Electronic Supplementary Information

A rapid construction of new boron heterocycles and evaluation for photophysical properties of iminoboronates

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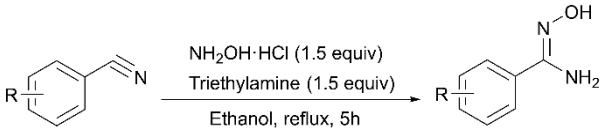
1. General Information.

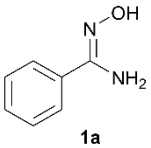
Commercial reagents were purchased from Meyer Reagent Co., Ltd., (Shanghai, China), Macklin Reagent Co., Ltd. (Shanghai, China), Chongqing Chuandong Chemical Co., Ltd. (Chongqing, China), etc., and used as received without further purification. ^{1}H, ^{13}C and ^{11}B NMR spectra were recorded at Bruker Avance - III spectrometer (600 MHz, 151 MHz and 193 MHz) using TMS as internal standard. Chemical shifts were reported in ppm and coupling constants (J) in Hz. The multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets(dd), multiplet (m), triplet (t). UV-Vis spectra and fluorescence spectra were recorded on Shimadzu UV2600 and RF-5301PC, respectively. High-resolution mass spectra were recorded on a JEOL AccuTOF-MS or Agilent Q-TOF6550. TLC plates were visualized by exposing UV light. Purification of crude compounds and separation of reaction mixtures were carried out by column chromatography using silica gel (200-300 meshes, Shanghai, China).

2. Synthesis and Characterization of Amidoximes (1a-1e)[1].



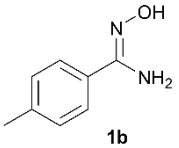
General procedure: To a round-bottom flask was charged with benzonitrile (19.4 mmol, 1.0 equiv), hydroxylamine hydrochloride (29.1 mmol, 1.5 equiv), triethylamine (29.1 mmol, 1.5 equiv) and ethanol (15 mL). The resulting mixture was warmed to 70 °C under reflux for 5 h. When the reaction was completed, reduced the temperature to 25 °C, then, the solvent was removed under reduced pressure and a saturated solution of NaCl (25 mL) was added. Subsequently, the aqueous phase was extracted with ethyl acetate (4 × 20 mL), and dried over anhydrous Na_2SO_4 and concentrated in vacuum with silica gel added. The residue was purified by column chromatography (petroleum ether/ethyl acetate 4:1) obtain the target product **1a**.

Characterization data:



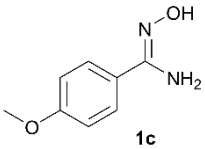
1a

Amidoxime (1a)[1]. White solid (2.20 g, 85% yield), PE/EA = 4:1, mp 67-69 °C. **^{1}H NMR** (600 MHz, DMSO-d_6): δ 9.63 (1 H, s), 7.69 – 7.67 (2 H, m), 7.38 – 7.36 (3 H, m), 5.80 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6): δ 151.29, 133.84, 129.33, 128.56, 125.85.



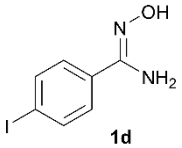
1b

Amidoxime (1b)[2]. White solid (2.20 g, 87% yield), PE/EA = 4:1, mp 124-127 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.52 (1 H, s), 7.56 (2 H, d, J 8.2), 7.17 (2 H, d, J 8.0), 5.73 (1 H, s), 2.31 (3 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 151.24, 138.71, 131.03, 129.10, 125.74, 21.28.



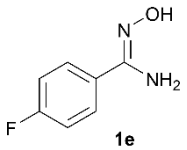
1c

Amidoxime (1c)[2]. White solid (2.20 g, 90% yield), PE/EA = 4:1, mp 107-110 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.44 (1 H, s), 7.61 (2 H, d, *J* 8.9), 6.92 (2 H, d, *J* 8.9), 5.71 (2 H, s), 3.77 (3 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 160.27, 151.05, 127.17, 126.24, 113.91, 55.61.



1d

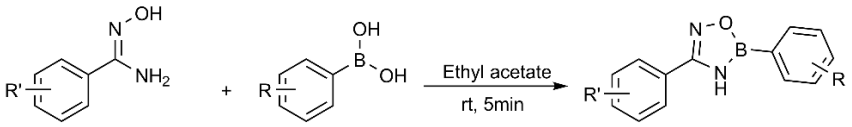
Amidoxime (1d)[3]. White solid (2.00 g, 87% yield), PE/EA = 4:1, mp 157-160 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.71 (1 H, s), 7.74 (2 H, d, *J* 8.3), 7.47 (2 H, d, *J* 8.1), 5.83 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 150.61, 137.36, 133.38, 127.90, 95.70.



1e

Amidoxime (1e)[3]**.** White solid (2.20 g, 85% yield), PE/EA = 4:1, mp 79-81 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.63 (1 H, s), 7.73 – 7.70 (2 H, m), 7.20 (2 H, t, *J* 8.9), 5.83 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 163.79, 162.16, 150.52, 130.31, 130.29, 128.02, 127.96, 115.49, 115.34.

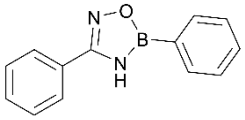
3. Synthesis and Characterization of the Oxadiazaborole Derivatives 3a–3k.



1 2 3

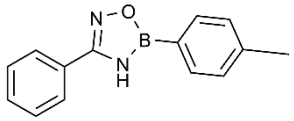
General procedure: Amidoxime **1** (1.1 mmol, 1.0 equiv), phenylboronic acid **2** (1.1 mmol, 1.0 equiv) derivatives and ethyl acetate (2 mL) were mixed together in round-bottom flask and stirred at room temperature for 5min. Reaction progress was monitored with TLC. When the reaction was completed, excess of petroleum ether (5 mL) was added to round bottom flask, the product immediately precipitated from the reaction system. After filtration and washing with a mixed solvent of ethyl acetate and petroleum ether (15:1), the pure product was obtained.

Characterization data:



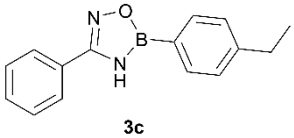
3a

3,5-diphenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3a)[4]. White solid (0.22 g, 92% yield); mp 158-160 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.46 (1 H, s), 8.00 (2 H, dd, *J* 6.5, 3.2), 7.96 (2 H, d, *J* 6.5), 7.59 (3 H, dd, *J* 7.0, 3.8), 7.55 (1 H, d, *J* 7.2), 7.52 (2 H, t, *J* 7.1). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.75, 134.38, 131.59, 131.24, 129.45, 128.73, 127.20, 126.78. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 32.07.



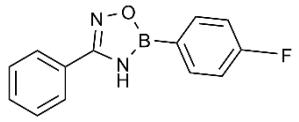
3b

3-phenyl-5-(p-tolyl)-4,5-dihydro-1,2,4,5-oxadiazaborole (3b)[4]. White solid (0.22 g, 85% yield); mp 143-146 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.36 (1 H, s), 7.98 – 7.95 (2 H, m), 7.83 (2 H, d, J 7.9), 7.58 – 7.53 (4 H, m), 7.32 (2 H, d, J 7.5), 2.37 (4 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.66, 141.31, 134.42, 131.22, 129.45, 129.41, 127.22, 126.74, 21.77. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.74.



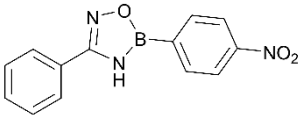
3c

5-(4-ethylphenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3c). White solid (0.23 g, 82% yield); mp 116-119 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.37 (1 H, s), 7.97 (2 H, dd, *J* 6.6, 2.9), 7.86 (2 H, d, *J* 7.8), 7.58 – 7.57 (3 H, m), 7.35 (2 H, d, *J* 7.8), 2.67 (2 H, q, *J* 7.6), 1.22 (4 H, t, *J* 7.6). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.67, 147.51, 134.51, 131.22, 129.44, 128.22, 127.23, 126.75, 28.83, 15.80. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 32.86. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{16}BN_2O$: 251.1350, found: 251.1344.



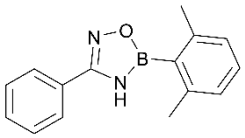
3d

5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3d). White solid (0.24 g, 90% yield); mp 192-194 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.46 (1 H, s), 8.03 – 8.00 (2 H, m), 7.99 – 7.97 (2 H, m), 7.60 – 7.58 (3 H, m), 7.36 (2 H, t, *J* 8.9). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 165.49, 163.84, 159.75, 136.91, 136.85, 131.27, 129.46, 127.12, 126.74, 115.99, 115.86. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.62. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{13}H_{11}BN_2OF$: 241.0943, found: 241.0939.



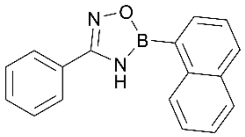
3e

5-(4-nitrophenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3e)[4]. White solid (0.27 g, 93% yield); mp 254-256 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.71 (1 H, s), 8.35 (2 H, d, *J* 8.5), 8.18 (2 H, d, *J* 8.5), 7.97 (2 H, dd, *J* 6.4, 2.9), 7.61 – 7.57 (3 H, m). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.96, 149.60, 135.57, 131.40, 129.49, 126.87, 126.75, 123.43. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 34.03.



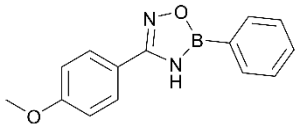
3f

5-(2,6-dimethylphenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3f). White solid (0.21 g, 80% yield); mp 148-151°C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.26 (1 H, s), 7.95 (3 H, dd, *J* 6.6, 3.0), 7.58 – 7.53 (4 H, m), 7.25 (2 H, t, *J* 7.6), 7.07 (3 H, d, *J* 7.6), 2.31 (9 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.34, 141.91, 131.25, 130.05, 129.48, 127.10, 126.89, 126.72, 22.89. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.97. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{16}BN_2O$: 251.1350, found: 251.1345.



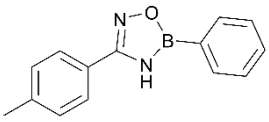
3g

5-(naphthalen-1-yl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3g). White solid (0.25 g, 84% yield); mp 134-136 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.58 (1 H, s), 8.66 (1 H, d, *J* 8.4), 8.23 (1 H, d, *J* 6.8), 8.12 (1 H, d, *J* 8.1), 8.06 (3 H, d, *J* 4.6), 8.01 (1 H, d, *J* 8.1), 7.67 (3 H, dd, *J* 13.0, 6.3), 7.60 (5 H, t, *J* 6.2). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.70, 136.00, 135.73, 133.44, 131.80, 131.32, 129.47, 129.08, 128.37, 127.34, 127.13, 126.97, 126.46, 125.81. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 34.99. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{17}H_{14}BN_2O$: 273.1193, found: 273.1196.



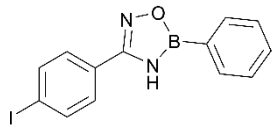
3h

3-(4-methoxyphenyl)-5-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3h)[5]**.** White solid (0.21 g, 92% yield); mp 176-179 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.33 (1 H, s), 7.94 (5 H, t, *J* 7.4), 7.55 (1 H, t, *J* 7.2), 7.51 (2 H, t, *J* 7.2), 7.13 (3 H, d, *J* 8.7), 3.85 (4 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 161.60, 159.41, 134.35, 131.52, 128.71, 128.34, 119.46, 114.85, 55.82. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.27.



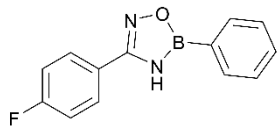
3i

5-phenyl-3-(p-tolyl)-4,5-dihydro-1,2,4,5-oxadiazaborole (3i)[5]**.** White solid (0.21 g, 90% yield); mp 151-154 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.37 (1 H, s), 7.94 (2 H, d, *J* 6.7), 7.87 (2 H, d, *J* 8.1), 7.55 (1 H, t, *J* 7.3), 7.51 (2 H, t, *J* 7.2), 7.38 (2 H, d, *J* 8.0), 2.39 (3 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.67, 141.05, 134.36, 131.55, 129.99, 128.72, 126.67, 124.38, 21.46. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.27.



3j

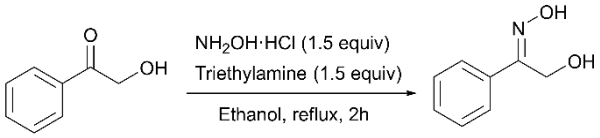
3-(4-iodophenyl)-5-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3j)[5]**.** White solid (0.16 g, 83% yield); mp 219-221 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.49 (1 H, s), 7.97 (2 H, d, *J* 8.4), 7.92 (2 H, d, *J* 6.7), 7.76 (2 H, d, *J* 7.9), 7.55 (1 H, t, *J* 7.3), 7.50 (2 H, t, *J* 7.1). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 159.22, 138.35, 134.36, 131.67, 128.76, 128.56, 126.63, 98.39. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.67.



3k

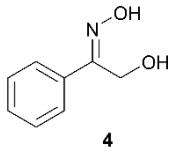
3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (3k). White solid (0.19 g, 82% yield); mp 192-195 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.48 (1 H, s), 8.04 (2 H, dd, *J* 8.7, 5.4), 7.94 (2 H, d, *J* 6.7), 7.56 (1 H, t, *J* 7.3), 7.52 (2 H, t, *J* 7.4), 7.44 (2 H, t, *J* 8.8). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 164.79, 163.15, 158.96, 134.35, 131.62, 129.24, 129.19, 128.74, 123.76, 123.74, 116.65, 116.50. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 33.47. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{13}H_{11}BN_2OF$: 241.0943, found: 249.0941.

4. Synthesis and Characterization of α-Hydroxyl Oxime 4[6].



General procedure: To a round-bottom flask was charged with 2-hydroxyacetophenone (14.7 mmol, 1.0 equiv), hydroxylamine hydrochloride (22.0 mmol, 1.5 equiv), triethylamine (22.0 mmol, 1.5 equiv) and ethanol (15 mL). The resulting mixture was warmed to 70 °C under reflux for 2 h. When the reaction was completed, reduced the temperature to 25 °C, then, the solvent was removed under reduced pressure and a saturated solution of NaCl (25 mL) was added. Subsequently, the aqueous phase was extracted with ethyl acetate (4 × 20 mL), and dried over anhydrous Na_2SO_4 and concentrated in vacuum with silica gel added. The residue was purified by column chromatography (petroleum ether/ethyl acetate 3:1) obtain the target product **4**.

Characterization data:



4

α-hydroxyl oxime 4. White solid (1.20 g ,55% yield); PE/EA = 3:1, mp 48-51 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.31 (1 H, s), 7.65 (2 H, dd, *J* 8.1, 1.5), 7.39 – 7.33 (3 H, m), 5.00 (1 H, t, *J* 5.8), 4.60 (2 H, d, *J* 5.8). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 157.35, 135.78, 128.81, 128.48, 127.23, 53.46.

5. References

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2. C.-C. Lin, T.-H. Hsieh, P.-Y. Liao, Z.-Y. Liao, C.-W. Chang, Y.-C. Shih, W.-H. Yeh and T.-C. Chien, *Org. Lett.*, 2014, **16**, 892-895.
3. M. Li, W. Li, C.-D. Lin, J.-H. Wang and L.-R. Wen, *The Journal of Organic Chemistry*, 2019, **84**, 6904-6915.
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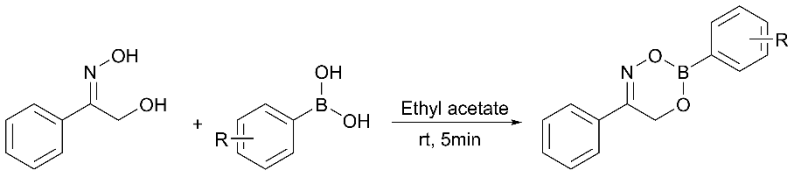
6. C. P. Park, A. Nagle, C. H. Yoon, C. Chen and K. W. Jung, *The Journal of Organic Chemistry*, 2009, **74**, 6231-6236.

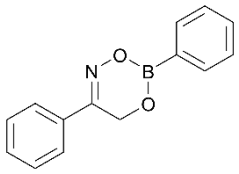
6. Synthesis and Characterization of Dioxazaborinine Derivatives 5a-5j.



4 2 5

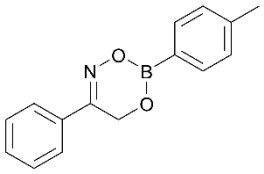
General procedure: α-hydroxyl oxime **4** (1.0 mmol, 1.0 equiv), phenylboronic acid **2** (1.0 mmol, 1.0 equiv) derivatives and ethyl acetate (2 mL) were mixed together in round-bottom flask and stirred at room temperature for 5min. Reaction progress was monitored with TLC. When the reaction was completed, excess of petroleum ether (5 mL) was added to round bottom flask, the product immediately precipitated from the reaction system. After filtration and washing with a mixed solvent of ethyl acetate and petroleum ether (15:1), the pure product was obtained.

Characterization data:



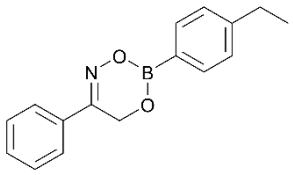
5a

2,5-diphenyl-6H-1,3,4,2-dioxazaborinine (5a). White solid (0.21 g, 91% yield); mp 130-133 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 (1 H, d, *J* 7.8), 7.68 (1 H, d, *J* 7.0), 7.50 (1 H, dd, *J* 15.9, 7.3), 7.45 (1 H, t, *J* 7.3), 7.41 (1 H, t, *J* 7.5), 4.94 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.82, 134.27, 131.88, 131.66, 131.14, 128.98, 127.90, 125.65, 57.40. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 24.13. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{13}BNO_2$: 238.1033, found: 238.1030.



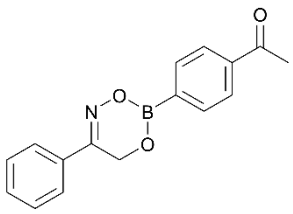
5b

5-phenyl-2-(p-tolyl)-6H-1,3,4,2-dioxazaborinine (5b). White solid (0.21 g, 85% yield); mp 154-156 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.84 (1 H, d, *J* 7.9), 7.67 (1 H, d, *J* 7.0), 7.48 (0 H, t, *J* 7.2), 7.44 (1 H, t, *J* 7.3), 7.23 (1 H, d, *J* 7.8), 4.91 (1 H, s), 2.38 (2 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.79, 142.14, 134.34, 131.74, 131.07, 128.95, 128.74, 125.63, 57.33, 21.83. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 24.77. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{15}BNO_2$: 252.1190, found: 252.1189.



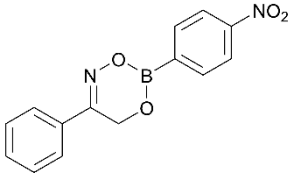
5c

2-(4-ethylphenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (5c). White solid (0.22 g, 83% yield); mp 107-110 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 7.72 (1 H, t, *J* 7.7), 7.54 – 7.51 (0 H, m), 7.49 (0 H, t, *J* 7.2), 7.26 (0 H, d, *J* 8.0), 5.00 (0 H, s), 2.64 (0 H, q, *J* 7.6), 1.19 (1 H, t, *J* 7.6). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 158.79, 147.48, 134.08, 132.47, 131.20, 129.27, 127.80, 126.15, 57.57, 28.82, 15.81. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.10. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{17}BNO_2$: 266.1346, found: 266.1343.



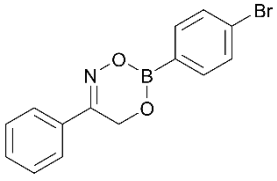
5d

1-(4-(5-phenyl-6H-1,3,4,2-dioxazaborinin-2-yl) phenyl) ethan-1-one (5d). White solid (0.24 g, 87% yield); mp 226-228 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.03 (1 H, d, *J* 8.2), 7.98 (1 H, d, *J* 8.2), 7.68 (1 H, d, *J* 7.1), 7.51 (1 H, t, *J* 7.3), 7.47 (1 H, t, *J* 7.3), 4.98 (1 H, s), 2.63 (2 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 198.39, 157.89, 139.51, 134.44, 131.42, 131.30, 129.02, 127.45, 125.67, 57.53, 26.79. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.34. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{15}BNO_3$: 280.1139, found: 280.1137.



5e

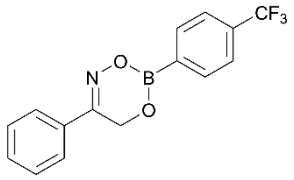
2-(4-nitrophenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (5e). White solid (0.25 g, 90% yield); mp 218-220 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 8.12 (1 H, d, *J* 8.6), 7.78 (1 H, d, *J* 8.6), 7.66 (1 H, dd, *J* 6.7, 2.9), 7.43 (1 H, s), 4.64 (1 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 158.21, 147.45, 135.70, 134.55, 133.14, 129.88, 129.04, 125.41, 122.32, 57.36. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.75. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{12}BN_2O_4$: 283.0884, found: 283.0876.



5f

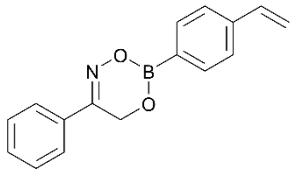
2-(4-bromophenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (5f). White solid (0.25 g, 90% yield); mp 164-166 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.79 (1 H, d, *J* 8.2), 7.67 (1 H, d, *J* 7.1), 7.55 (1 H,

d, *J* 8.2), 7.50 (0 H, t, *J* 7.3), 7.46 (1 H, t, *J* 7.3), 4.94 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.85, 135.79, 131.49, 131.23, 131.20, 129.00, 126.97, 125.65, 57.46. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 17.54. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{12}BNO_2Br$: 316.0139, found: 316.0139.



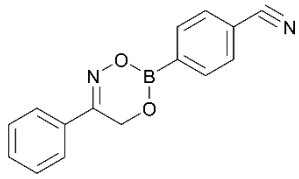
5g

5-phenyl-2-(4-(trifluoromethyl) phenyl)-6H-1,3,4,2-dioxazaborinine (5g). White solid (0.25 g, 84% yield); mp 164-167 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.04 (1 H, d, *J* 7.9), 7.67 (2 H, t, *J* 8.8), 7.51 (1 H, t, *J* 7.3), 7.47 (1 H, t, *J* 7.4), 4.98 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.91, 134.51, 131.37, 131.32, 129.03, 125.66, 124.54, 124.52, 57.55. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 11.36. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{12}BNO_2F_3$: 306.0907, found: 306.0905.



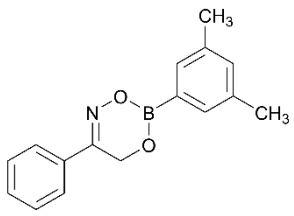
5h

5-phenyl-2-(4-vinylphenyl)-6H-1,3,4,2-dioxazaborinine (5h). White solid (0.21 g, 80% yield); mp 129-132 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (1 H, d, *J* 8.1), 7.67 (1 H, d, *J* 7.0), 7.49 (0 H, t, *J* 7.2), 7.45 (2 H, dd, *J* 7.8, 4.7), 6.75 (1 H, dd, *J* 17.6, 10.9), 5.83 (1 H, d, *J* 17.6), 5.31 (1 H, d, *J* 10.9), 4.94 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.82, 140.80, 136.84, 134.55, 131.67, 131.12, 128.97, 125.71, 125.64, 115.22, 57.39. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 21.10. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{15}BNO_2$: 264.1190, found: 264.1187.



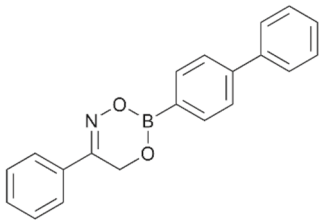
5i

4-(5-phenyl-6H-1,3,4,2-dioxazaborinin-2-yl) benzonitrile (5i). White solid (0.21 g, 82% yield); mp 169-171 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02 (1 H, d, *J* 8.2), 7.70 – 7.66 (2 H, m), 7.51 (0 H, t, *J* 7.3), 7.47 (1 H, t, *J* 7.4), 4.98 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.94, 134.57, 131.42, 131.34, 131.23, 129.06, 125.67, 118.76, 115.15, 57.63. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.23. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{12}BN_2O_2$: 263.0986, found: 263.0982.



5j

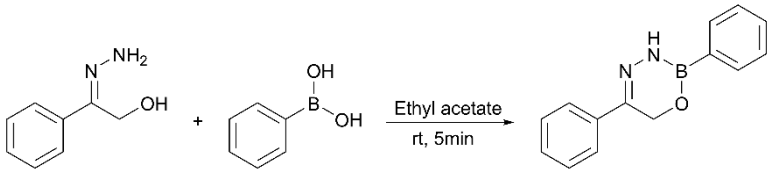
2-(3,5-dimethylphenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (5j). White solid (0.21 g, 81% yield); mp 80-82 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.67 (1 H, d, *J* 7.0), 7.56 (1 H, s), 7.48 (0 H, t, *J* 7.2), 7.44 (1 H, t, *J* 7.2), 7.14 (0 H, s), 4.92 (1 H, s), 2.34 (3 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.74, 137.24, 133.61, 131.99, 131.73, 131.07, 128.95, 125.64, 57.36, 21.27. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 25.06. **HRMS** (ESI): **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{16}BNO_2$: 266.1322, found: 266.1357.



5l

2-([1,1'-biphenyl]-4-yl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (5l). White solid (0.09 g, 60% yield); mp 208-210 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.01 (1 H, d, J 8.2), 7.69 (1 H, d, J 6.9), 7.66 – 7.63 (2 H, m), 7.52 – 7.48 (1 H, m), 7.46 (2 H, dd, J 14.8, 7.6), 7.36 (1 H, t, J 7.4), 4.97 (1 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 157.84, 144.45, 140.90, 134.76, 131.70, 131.08, 128.94, 128.78, 127.65, 127.22, 126.58, 125.65, 57.42. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.76. APCI-MS$[M+H]^+$ = 313.7.

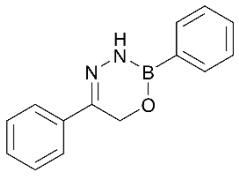
7. Synthesis and Characterization of Oxadiazaborinine Derivatives 7a-7j.



6 2 7

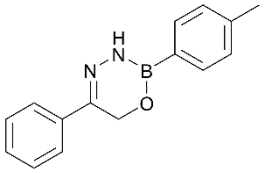
General procedure: α-hydroxyl hydrazone **6** (1.0 mmol, 1.0 equiv), phenylboronic acid **2** (1.0 mmol, 1.0 equiv) derivatives and ethyl acetate (2 mL) were mixed together in round-bottom flask and stirred at room temperature for 5min. Reaction progress was monitored with TLC. When the reaction was completed, excess of petroleum ether (5 mL) was added to round bottom flask, the product immediately precipitated from the reaction system. After filtration and washing with a mixed solvent of ethyl acetate and petroleum ether (15:1), the pure product was obtained.

Characterization data:



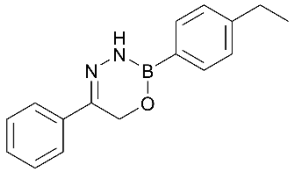
7a

2,5-diphenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7a). White solid (0.21 g, 90% yield); mp 185-188 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.75 (1 H, s), 7.82 (2 H, d, *J* 6.7), 7.70 (3 H, d, *J* 6.9), 7.48 – 7.37 (8 H, m), 5.04 (3 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 145.44, 135.35, 133.54, 131.19, 129.49, 128.99, 128.21, 125.22, 59.57. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.22. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{14}BN_2O$: 237.1193, found:237.1198.



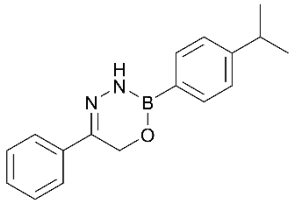
7b

5-phenyl-2-(p-tolyl)-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7b). White solid (0.21 g, 84% yield); mp 135-138 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.69 (1 H, s), 7.70 (4 H, dd, *J* 18.4, 7.4), 7.46 – 7.39 (3 H, m), 7.21 (2 H, d, *J* 7.6), 5.02 (2 H, s), 2.33 (1 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 150.04, 145.52, 140.16, 138.38, 134.18, 133.73, 133.65, 129.95, 64.24, 26.47. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.45. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{15}BN_2O$: 251.1360, found:251.1360.



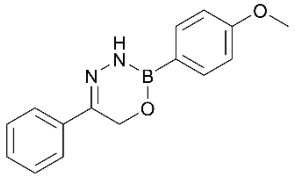
7c

2-(4-ethylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7c). White solid (0.22 g, 82% yield); mp 122-125 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) 9.69 (1 H, s), 7.74 (2 H, d, *J* 8.0), 7.69 (2 H, d, *J* 6.9), 7.45 – 7.38 (3 H, m), 7.23 (2 H, d, *J* 8.0), 5.02 (2 H, s), 2.62 (2 H, q, *J* 7.6), 1.19 (3 H, t, *J* 7.6). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 147.02, 145.30, 135.41, 133.70, 129.43, 128.98, 127.70, 125.20, 59.49, 28.78, 15.86. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.46. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{18}BN_2O$: 265.1506, found: 265.1504.



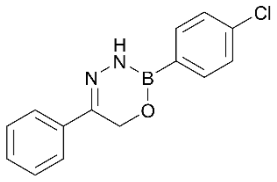
7d

2-(4-isopropylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7d). White solid (0.22 g, 81% yield); mp 119-121 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.63 (1 H, t, *J* 7.8), 7.54 (0 H, s), 7.41 – 7.34 (1 H, m), 7.26 (0 H, d, *J* 7.8), 5.02 (1 H, s), 2.96 – 2.88 (0 H, m), 1.26 (1 H, d, *J* 6.9). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 152.01, 145.76, 134.99, 132.89, 129.28, 128.62, 126.22, 124.95, 59.80, 34.29, 23.85. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.64. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{17}H_{20}BN_2O$: 279.1663, found: 279.1662.



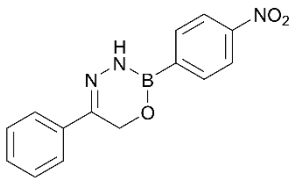
7e

2-(4-methoxyphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7e). White solid (0.22 g, 84% yield); mp 183-185 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.65 (1 H, s), 7.77 (2 H, d, *J* 8.5), 7.68 (2 H, d, *J* 7.2), 7.41 (3 H, dt, *J* 21.3, 7.0), 6.95 (2 H, d, *J* 8.5), 5.00 (2 H, s), 3.79 (3 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 166.68, 149.87, 140.21, 140.07, 134.13, 133.72, 129.92, 118.61, 64.19, 60.16. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.27. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{16}BN_2O_2$: 267.1299, found: 267.1300.



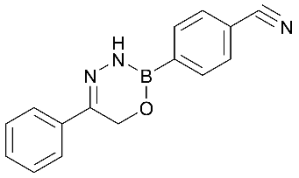
7f

2-(4-chlorophenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7f). White solid (0.24g, 88% yield); mp 179-181 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.80 (1 H, s), 7.82 (2 H, d, *J* 8.3), 7.69 (2 H, d, *J* 6.7), 7.47 (2 H, d, *J* 8.3), 7.45 – 7.39 (3 H, m), 5.04 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 145.62, 136.23, 135.36, 135.25, 129.56, 128.98, 128.34, 125.25, 59.67. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.93. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{13}BN_2OCl$: 271.0804, found: 271.0798.



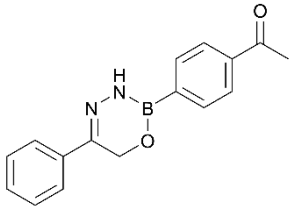
7g

2-(4-nitrophenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7g). Yellow solid (0.24 g, 86%); mp 191-194 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.97 (1 H, s), 8.23 (2 H, d, *J* 8.6), 8.06 (2 H, d, *J* 8.6), 7.71 (2 H, d, *J* 6.4), 7.49 – 7.34 (3 H, m), 5.09 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 149.51, 146.08, 135.08, 134.71, 129.73, 129.00, 125.34, 122.87, 59.90. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 27.68. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{14}H_{13}BN_3O_3$: 282.1044, found: 282.1040.



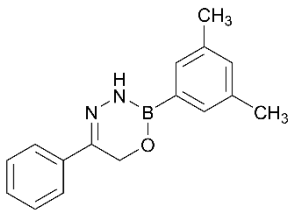
7h

4-(5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinin-2-yl) benzonitrile (7h). White solid (0.22 g, 83%); mp 161-163 °C, **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.97 (1 H, s), 8.23 (2 H, d, *J* 8.6), 8.06 (2 H, d, *J* 8.6), 7.71 (2 H, d, *J* 6.4), 7.49 – 7.34 (3 H, m), 5.09 (2 H, s). **^{13}C NMR** (151 MHz, DMSO-d_6) δ 146.00, 135.11, 134.06, 131.81, 129.70, 129.00, 125.32, 119.31, 113.49, 59.85. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.17. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{15}H_{13}BN_3O$: 262.1146 , found: 262.1141.



7i

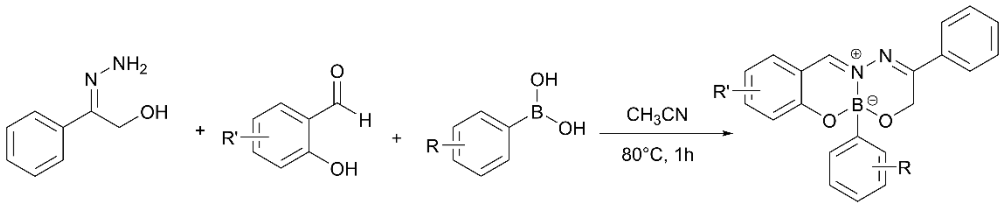
1-(4-(5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinin-2-yl) phenyl) ethan-1-one (7i). White solid (0.24 g, 85%); mp 205-207 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 14.61 (1 H, s), 12.69 (4 H, s), 12.44 (2 H, d, *J* 6.7), 12.20 – 12.12 (3 H, m), 9.80 (2 H, s), 7.34 (3 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 203.35, 150.55, 143.55, 139.97, 138.48, 134.37, 133.75, 132.47, 130.04, 64.48, 32.03. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.57. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{16}BN_2O_2$: 279.1299, found: 279.1303.



7j

2-(3,5-dimethylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (7j). White solid (0.21 g, 80%); mp 69-71 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.63 (1 H, dd, *J* 8.1, 1.5), 7.56 (0 H, s), 7.42 – 7.35 (2 H, m), 7.32 (1 H, s), 7.10 (0 H, s), 5.02 (1 H, s), 2.33 (3 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 145.71, 137.38, 134.98, 132.70, 130.47, 129.29, 128.62, 124.96, 59.83, 21.33. **^{11}B NMR** (193 MHz, DMSO-d_6) δ 28.54. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{16}H_{18}BN_2O$: 265.1506, found: 265.1500.

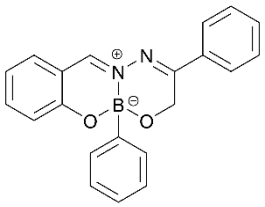
8. Synthesis and Characterization of Iminoboronate 9a-9g.



6 **8** **2** **9**

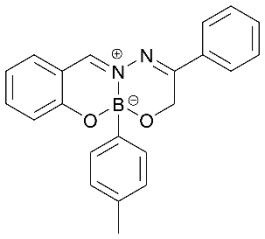
General procedure: α-hydroxyl hydrazine **6** (1.0 mmol, 1.0 equiv), salicylaldehyde **8** (1.0 mmol, 1.0equiv), phenylboronic acid **2** (1.2 mmol, 1.2 equiv) derivatives and acetonitrile (2 mL) were mixed together in round-bottom flask and stirred and stirred at 80 °C for 1 h. Reaction progress was monitored with TLC. As soon as the reaction was complete, it was cooled to room temperature. After filtration and washing with methanol, the pure product was obtained.

Characterization data:



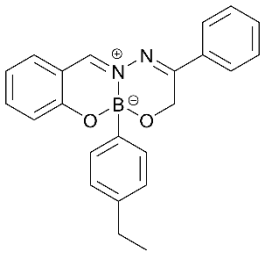
9a

Iminoboronate 9a. light green solid (0.21 g, 61% yield); mp 249-251 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ8.53 (1 H, s), 7.76 (2 H, d, *J* 7.3), 7.48 (1 H, t, *J* 7.4), 7.44 – 7.39 (5 H, m), 7.36 (1 H, dd, *J* 7.8, 1.6), 7.23 (2 H, t, *J* 7.1), 7.19 (1 H, t, *J* 7.2), 6.97 (1 H, d, *J* 8.4), 6.85 (1 H, t, *J* 7.5), 5.16 (1 H, d, *J* 19.2), 4.85 (1 H, d, *J* 19.2). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.87, 160.31, 156.17, 138.05, 132.87, 132.01, 131.81, 130.84, 128.82, 127.65, 127.43, 126.46, 120.02, 119.63, 116.14, 63.89. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 4.40. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{21}H_{18}BN_2O_2$: 341.1455, found: 341.1450.



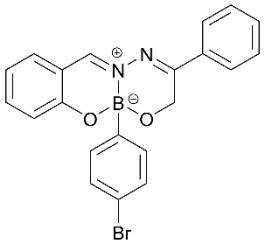
9b

Iminoboronate 9b. light green solid (0.20 g, 57% yield); mp 265-267 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (1 H, s), 7.76 (2 H, d, *J* 7.2), 7.48 (1 H, t, *J* 7.4), 7.44 – 7.39 (3 H, m), 7.36 (1 H, dd, *J* 7.8, 1.6), 7.32 (2 H, d, *J* 7.8), 7.05 (2 H, d, *J* 7.6), 6.96 (1 H, d, *J* 8.4), 6.84 (1 H, t, *J* 7.5), 5.16 (1 H, d, *J* 19.2), 4.85 (1 H, d, *J* 19.2), 2.25 (4 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.82, 160.35, 156.10, 137.98, 136.89, 132.91, 131.97, 131.78, 130.90, 128.80, 128.46, 126.45, 120.05, 119.57, 116.16, 63.90, 21.29. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 4.44. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{22}H_{20}BN_2O_2$: 355.1612, found: 355.1614.



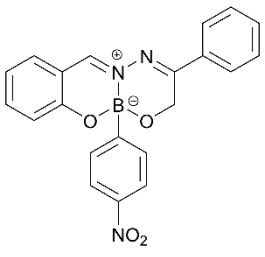
9c

Iminoboronate 9c. light green solid (0.20 g, 55% yield); mp 234-236 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (1 H, s), 7.76 (2 H, d, *J* 7.3), 7.48 (1 H, t, *J* 7.4), 7.44 – 7.39 (3 H, m), 7.35 (3 H, dd, *J* 14.1, 4.8), 7.07 (2 H, d, *J* 8.0), 6.96 (1 H, d, *J* 8.4), 6.84 (1 H, t, *J* 7.5), 5.16 (1 H, d, *J* 19.2), 4.86 (1 H, d, *J* 19.2), 2.56 (2 H, q, *J* 7.6), 1.17 (3 H, t, *J* 7.6). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.80, 160.38, 156.07, 143.14, 137.96, 132.93, 131.96, 131.78, 130.88, 128.80, 127.21, 126.46, 120.05, 119.54, 116.16, 63.90, 28.65, 15.30. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 4.52. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{23}H_{22}BN_2O_2$: 369.1768, found: 369.1771.



9d

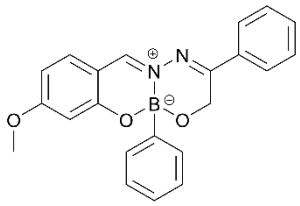
Iminoboronate 9d. light green solid (0.25 g, 60% yield); mp 263-265 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (1 H, s), 7.74 (2 H, d, *J* 7.4), 7.48 (1 H, t, *J* 7.4), 7.44 (1 H, t, *J* 7.8), 7.40 (2 H, t, *J* 7.7), 7.37 (1 H, d, *J* 6.3), 7.33 (2 H, d, *J* 8.2), 7.26 (2 H, d, *J* 8.1), 6.95 (1 H, d, *J* 8.4), 6.86 (1 H, t, *J* 7.5), 5.14 (1 H, d, *J* 19.3), 4.78 (1 H, d, *J* 19.2). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.92, 160.09, 156.26, 138.27, 132.67, 132.16, 131.86, 130.75, 128.88, 126.43, 121.78, 119.95, 119.87, 116.01, 63.78. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 4.18. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{21}H_{17}BN_2O_2Br$: 419.0561, found: 419.0566.



9e

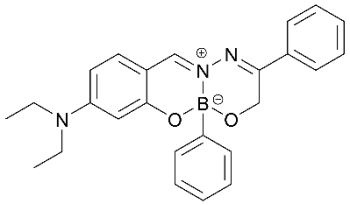
Iminoboronate 9e. light green solid (0.22 g, 58% yield); mp 235-238 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.61 (1 H, s), 8.05 (2 H, d, *J* 8.7), 7.76 (2 H, d, *J* 7.2), 7.56 (2 H, d, *J* 8.6), 7.49 (2 H, dt, *J* 8.7, 4.6), 7.43 (3 H, t, *J* 7.5), 6.98 (1 H, d, *J* 8.4), 6.92 (1 H, t, *J* 7.5), 5.18 (1 H, d, *J* 19.3), 4.77 (1 H, d, *J* 19.4). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 169.96, 159.81, 156.58, 147.73, 138.61, 132.41, 132.38, 132.02, 131.66, 128.96, 126.44, 122.58, 120.23, 119.88, 115.87, 63.62. **^{11}B NMR** (193 MHz,

$CDCl_3$) δ 3.66. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{21}H_{17}BN_3O_4$: 386.1306, found: 386.1308.



9f

Iminoboronate 9f. light green solid (0.21 g, 57% yield); mp 257-259 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.40 (1 H, s), 7.71 (2 H, d, *J* 7.3), 7.44 (1 H, t, *J* 7.4), 7.41 (1 H, d, *J* 6.7), 7.37 (2 H, t, *J* 7.6), 7.22 (3 H, dd, *J* 14.2, 6.2), 7.17 (1 H, t, *J* 7.2), 6.44 – 6.39 (2 H, m), 5.10 (1 H, d, *J* 19.0), 4.79 (1 H, d, *J* 19.0), 3.77 (3 H, s). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.27, 167.77, 162.95, 154.98, 133.20, 133.06, 131.59, 130.88, 128.74, 127.64, 127.35, 126.26, 109.97, 109.68, 102.48, 63.79, 55.68. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 4.11. **HRMS** (ESI): m/z $[M + H]^+$ calculated for $C_{22}H_{20}BN_2O_3$: 371.1561, found: 371.1565.



9g

Iminoboronate 9g. light green solid (0.25 g, 62% yield); mp 251-253 °C, **^{1}H NMR** (600 MHz, $CDCl_3$) δ8.23 (1 H, s), 7.71 (2 H, d, *J* 7.2), 7.45 (2 H, d, *J* 6.7), 7.41 (1 H, t, *J* 7.3), 7.36 (2 H, t, *J* 7.4), 7.22 (2 H, t, *J* 7.2), 7.16 (1 H, t, *J* 7.3), 7.12 (1 H, d, *J* 9.0), 6.21 (1 H, d, *J* 6.8), 6.12 (1 H, s), 5.07 (1 H, d, *J* 18.7), 4.76 (1 H, d, *J* 18.7), 3.39 (2 H, dq, *J* 14.3, 7.1), 3.31 (2 H, dq, *J* 14.4, 7.1), 1.16 (6 H, t, *J* 7.1). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 164.63, 162.19, 155.45, 153.38, 133.87, 133.54, 131.08, 130.89, 128.61, 127.48, 126.95, 125.99, 106.47, 105.72, 99.37, 63.53, 44.99, 12.68. **^{11}B NMR** (193 MHz, $CDCl_3$) δ 3.68. HRMS (ESI): m/z $[M + H]^+$ calculated for $C_{25}H_{27}BN_3O_2$: 412.2190, found: 412.2193.

9. NMR Spectra

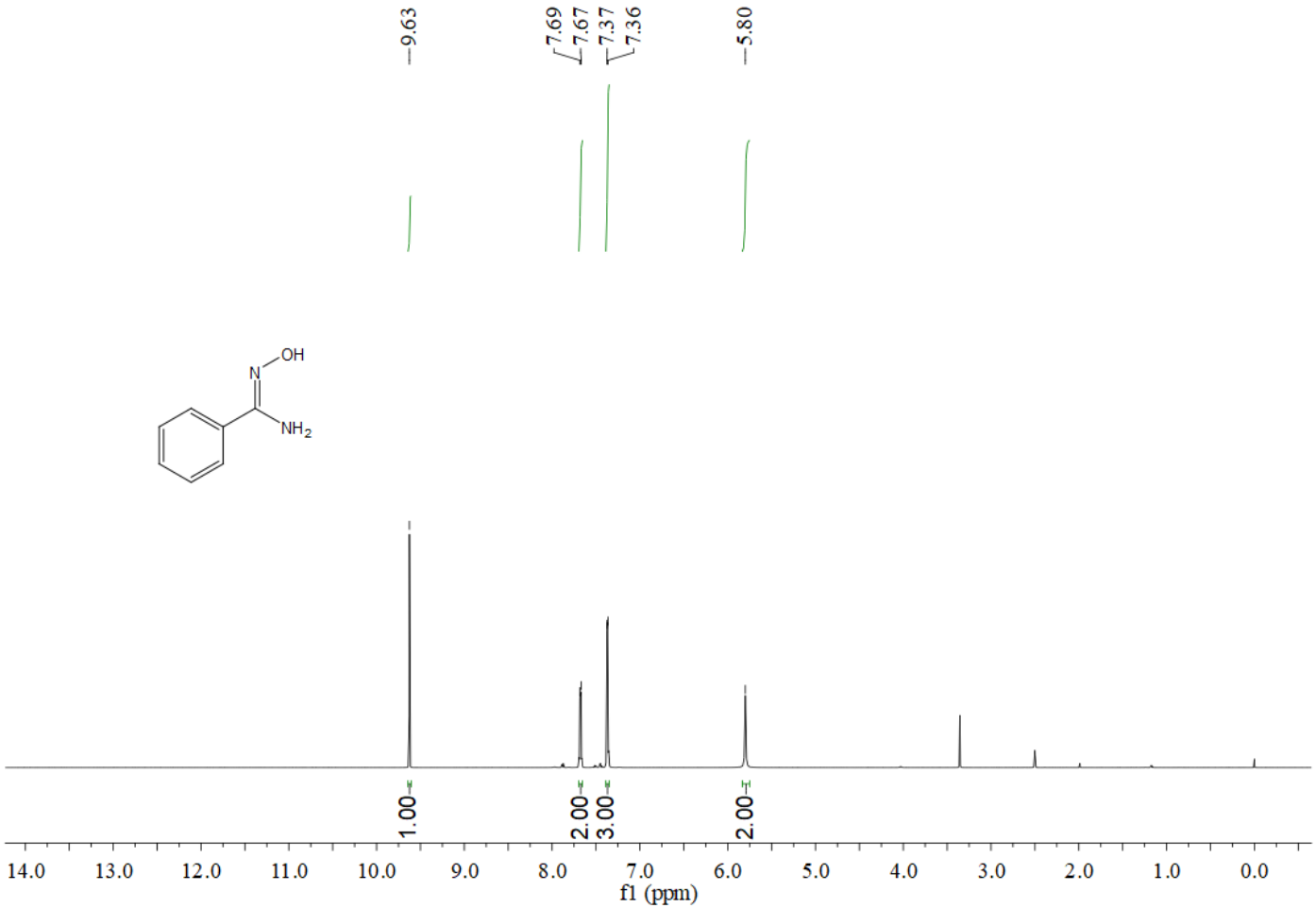


Fig. S1 ^{1}H NMR for compound **1a** (600 MHz, DMSO-d_6)

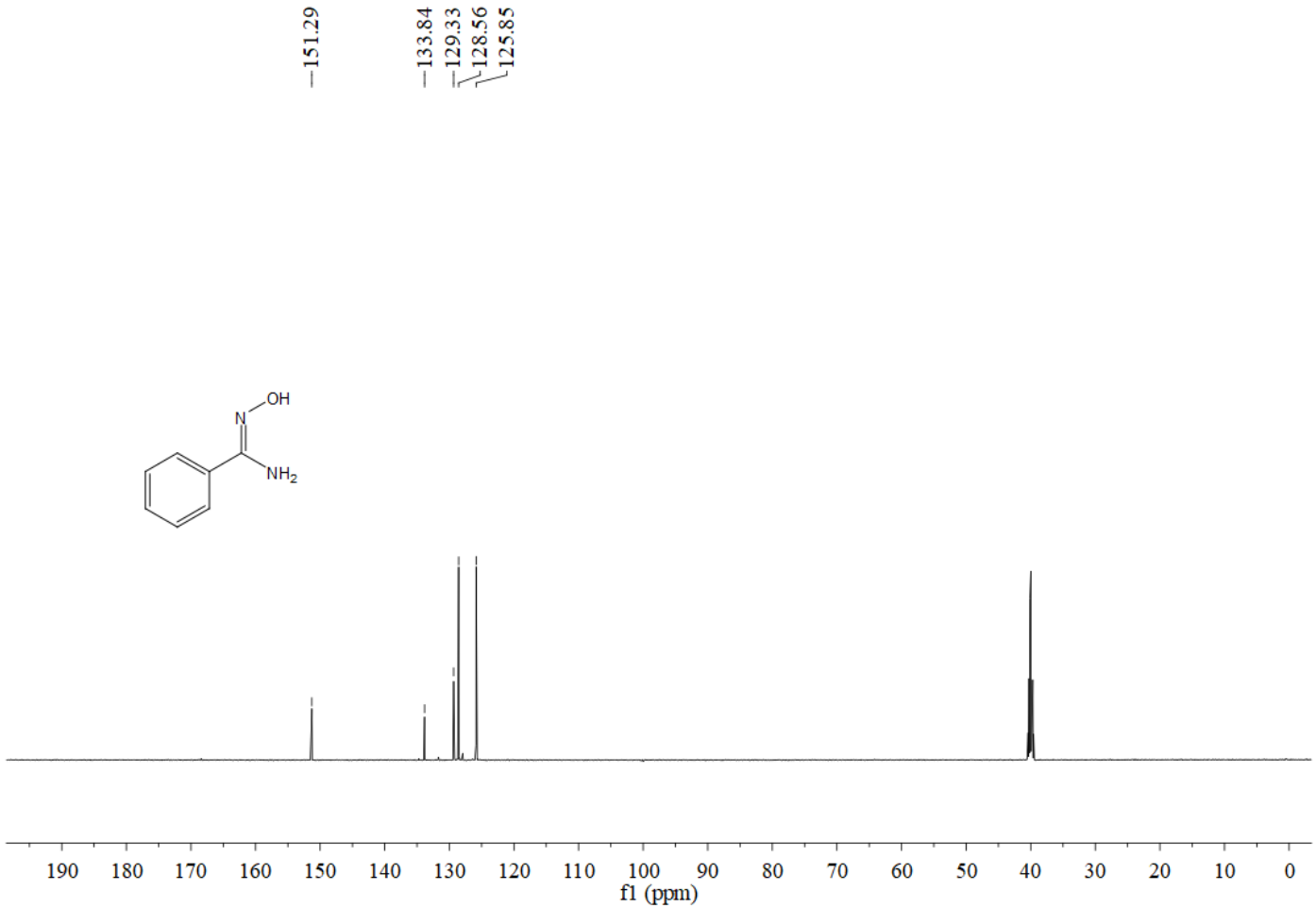


Fig. S2 ^{13}C NMR for compound **1a** (151 MHz, DMSO-d_6)

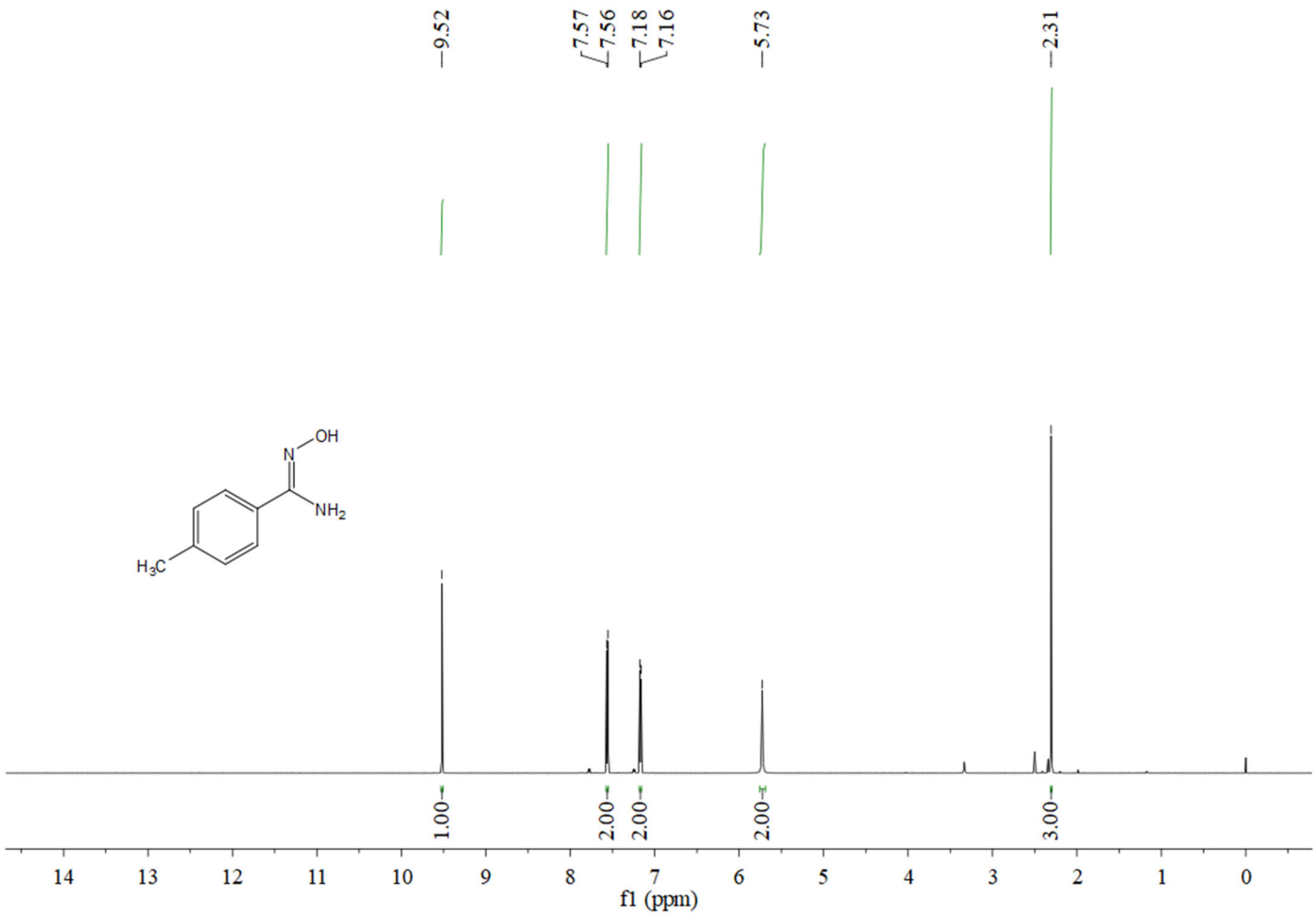


Fig. S3 ^{1}H NMR for compound **1b** (600 MHz, DMSO-d_6)

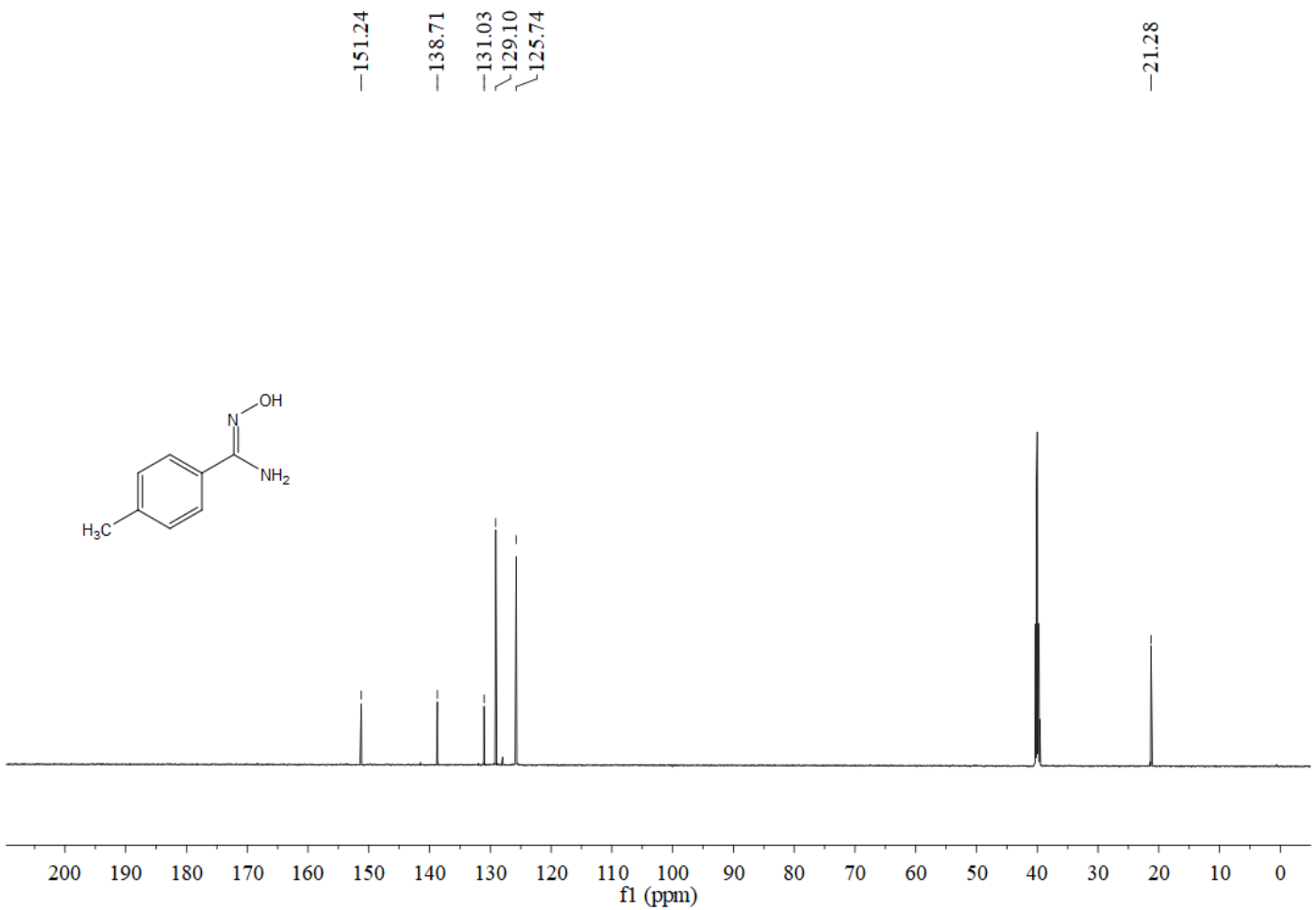


Fig. S4 ^{13}C NMR for compound **1b** (151 MHz, DMSO-d_6)

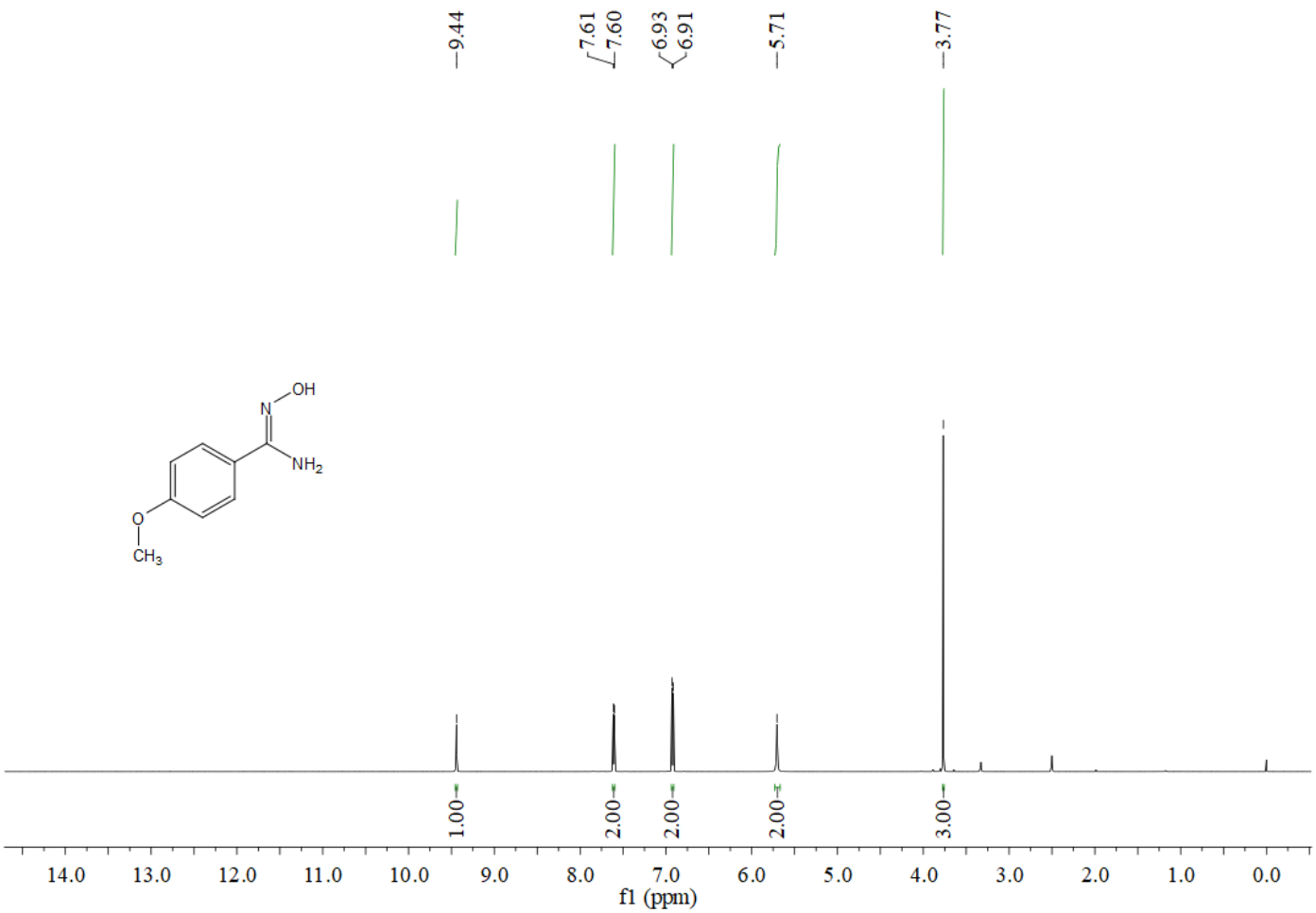


Fig. S5 ^{1}H NMR for compound **1c** (600 MHz, DMSO-d_6)

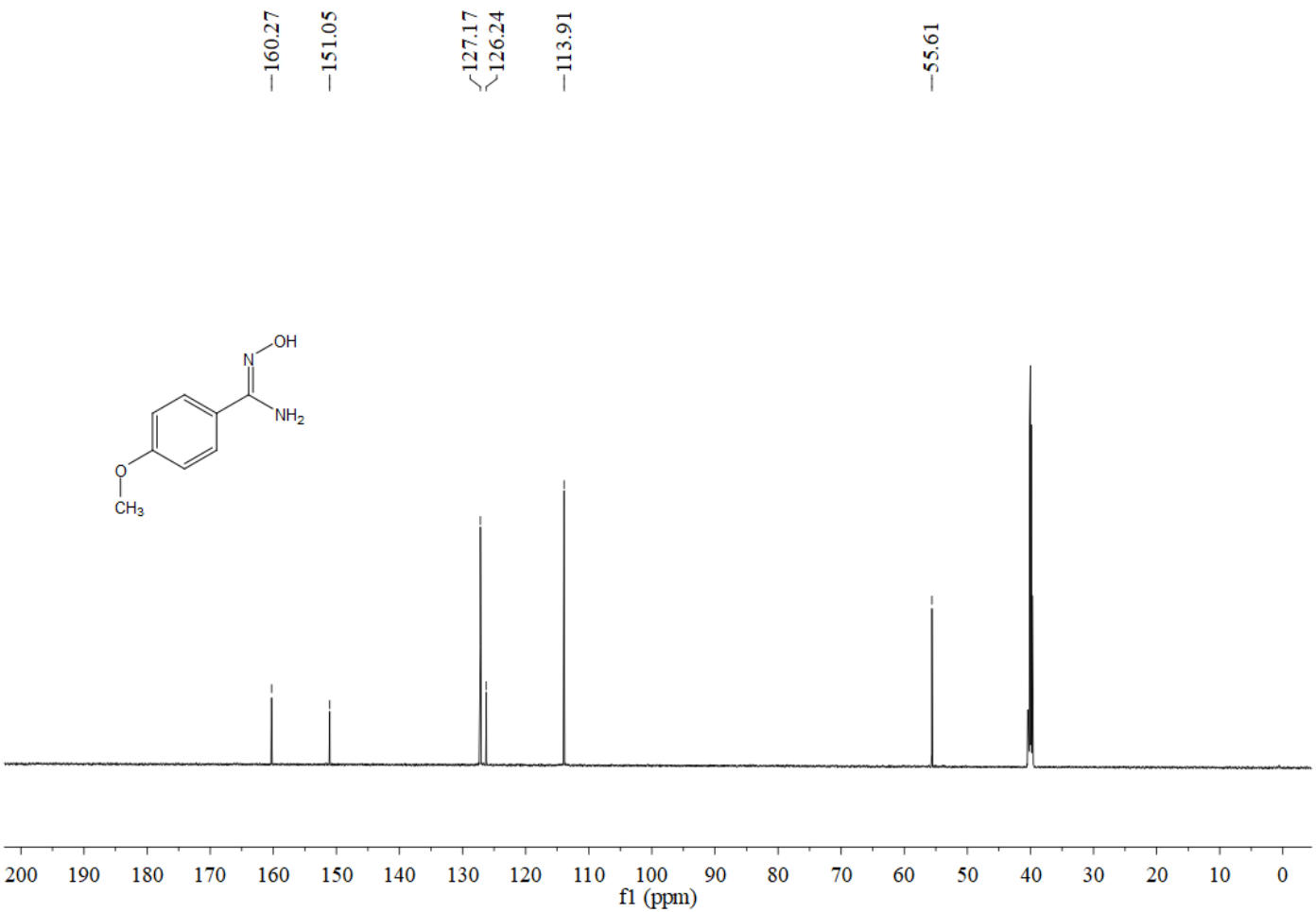


Fig. S6 ^{13}C NMR for compound **1c** (151 MHz, DMSO-d_6)

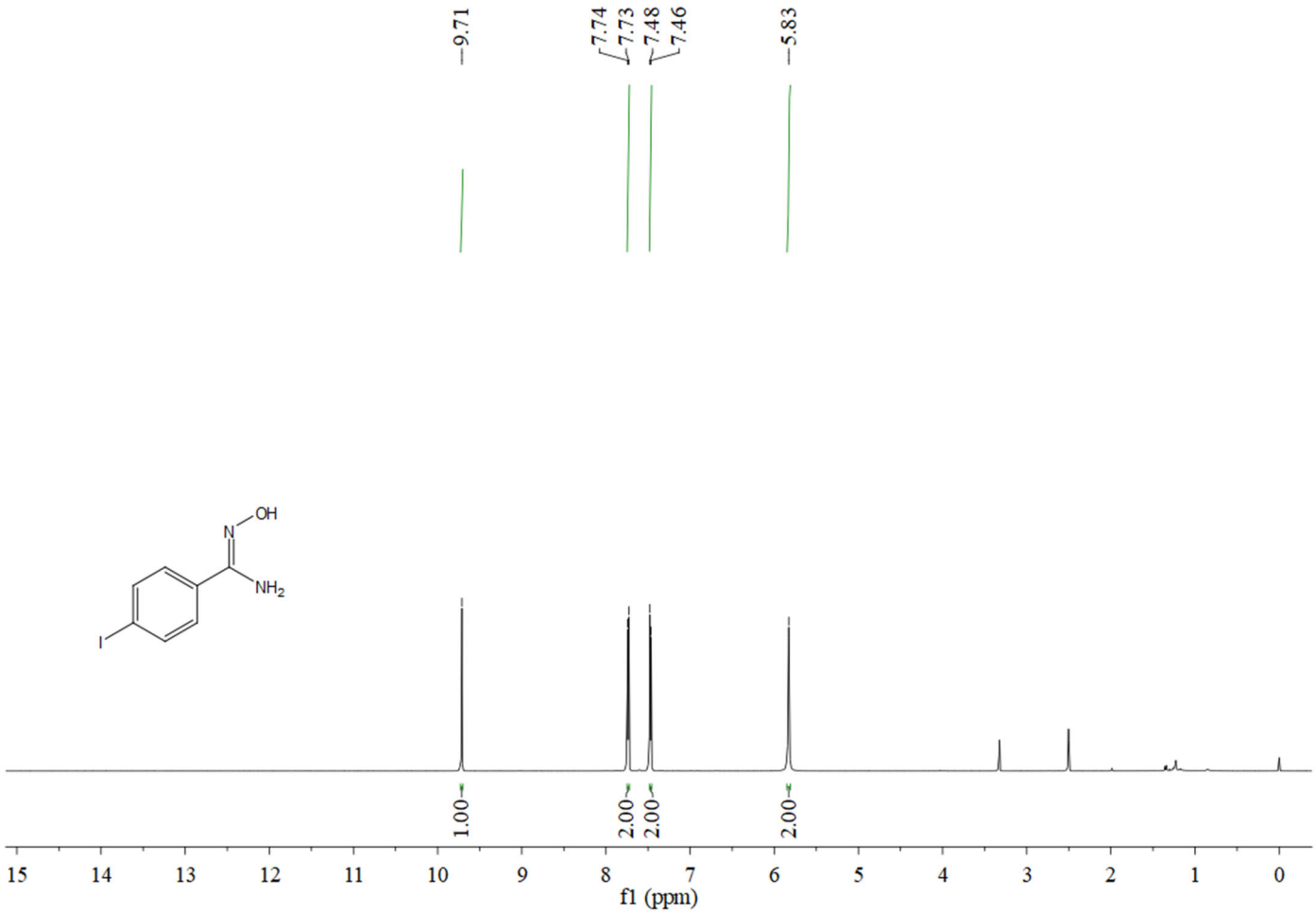


Fig. S7 ^{1}H NMR for compound **1d** (600 MHz, DMSO-d_6)

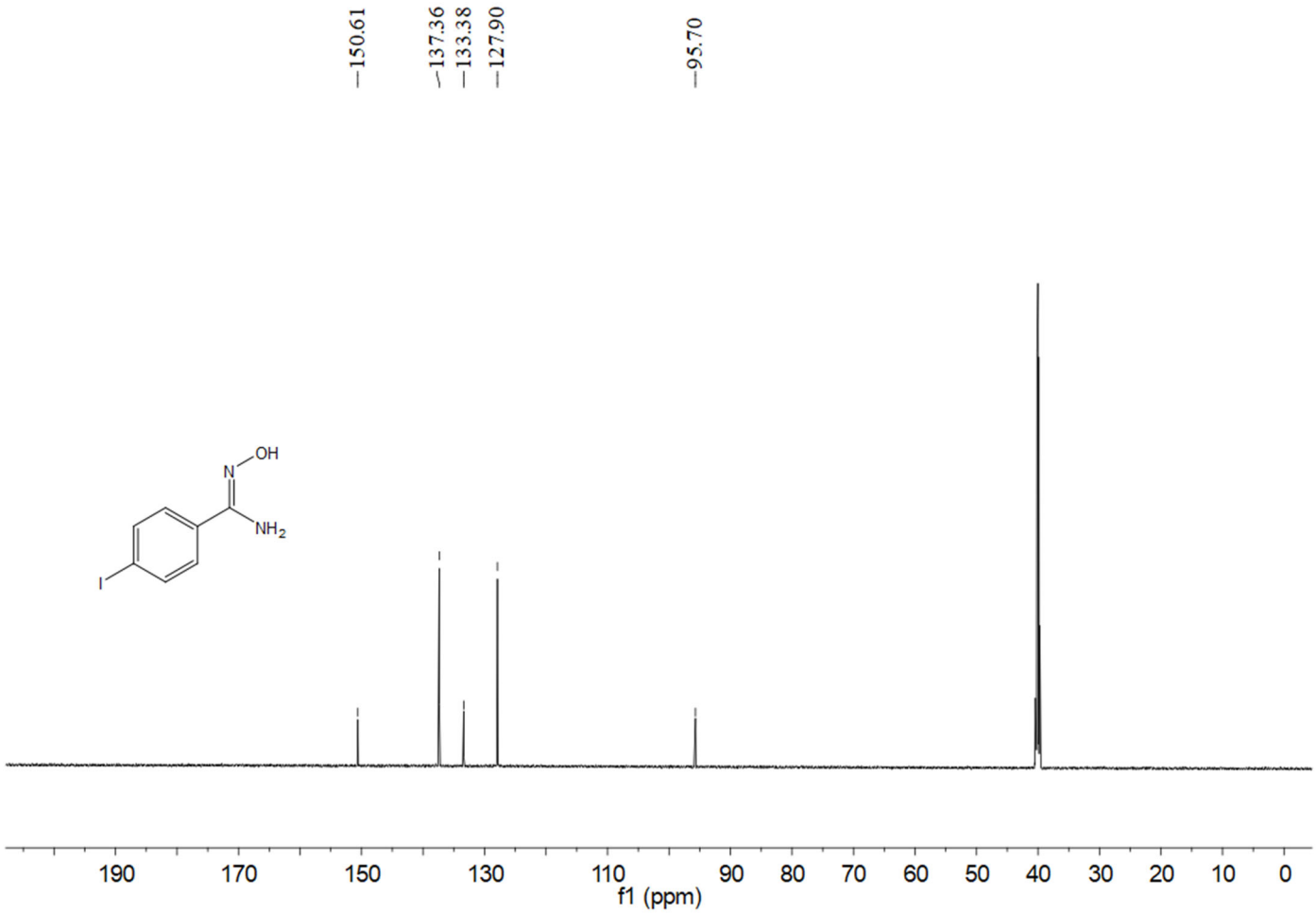


Fig. S8 ^{13}C NMR for compound **1d** (151 MHz, DMSO-d_6)

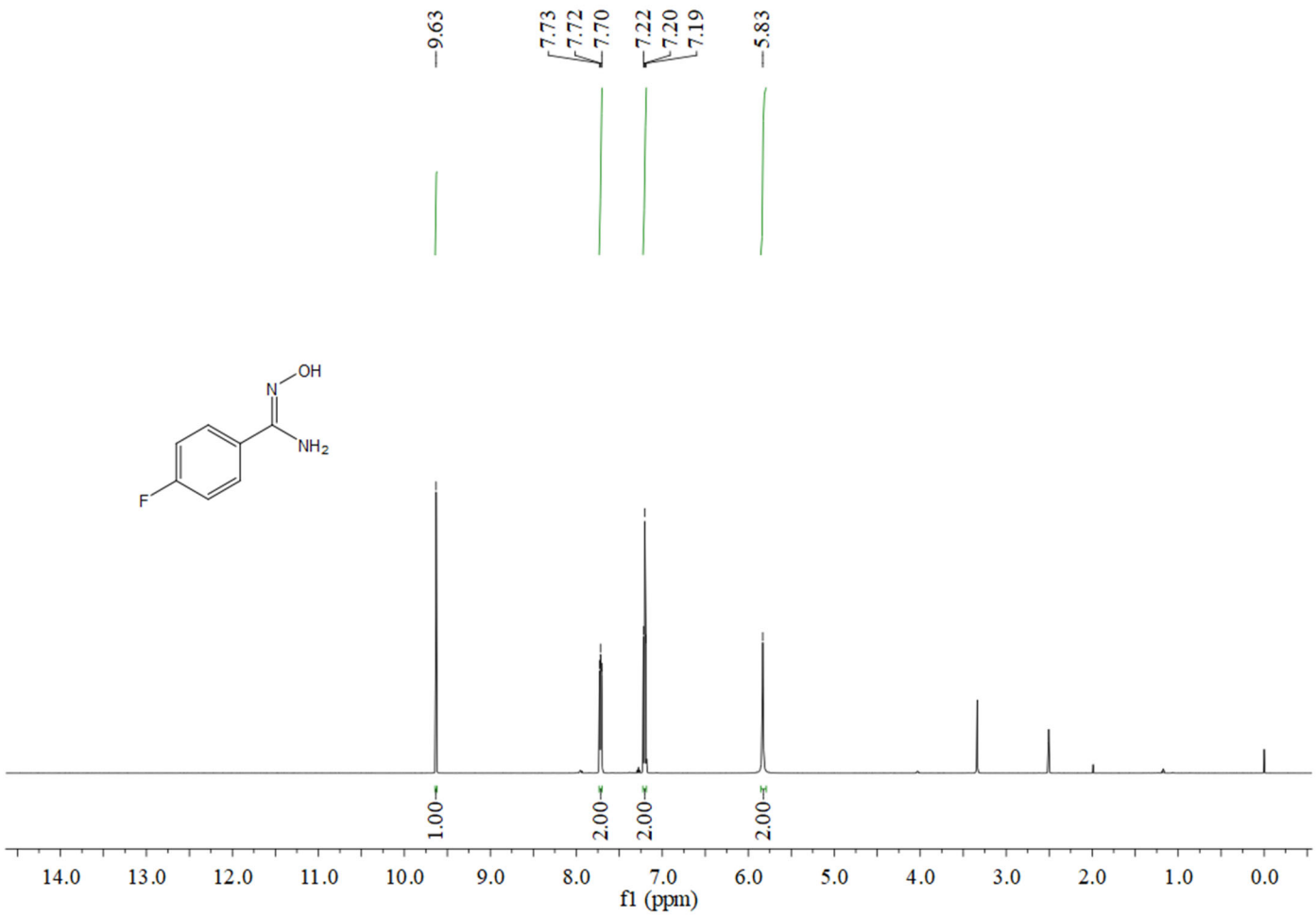


Fig. S9 ^{1}H NMR for compound **1e** (600 MHz, DMSO-d_6)

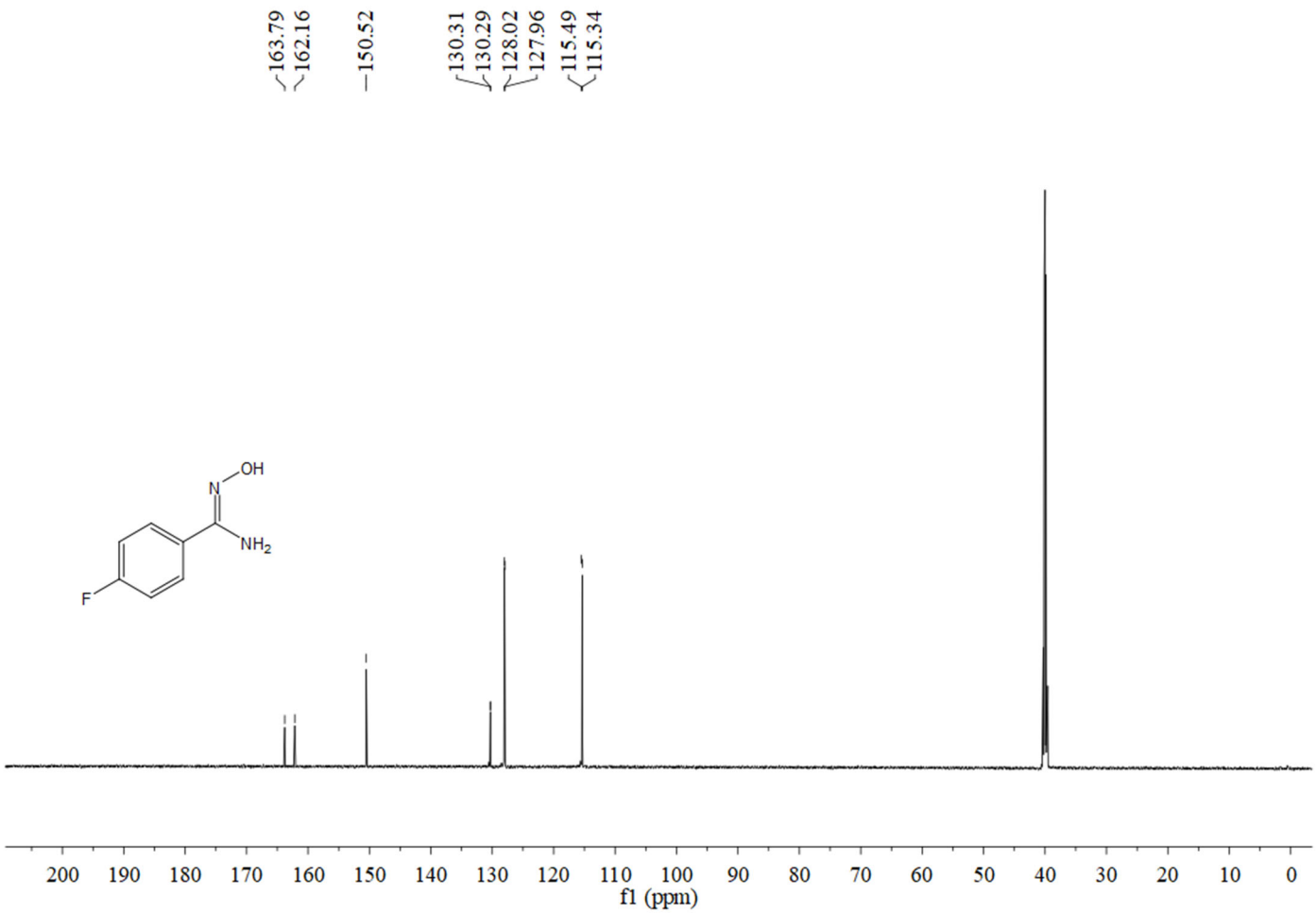


Fig. S10 ^{13}C NMR for compound **1e** (151 MHz, DMSO-d_6)

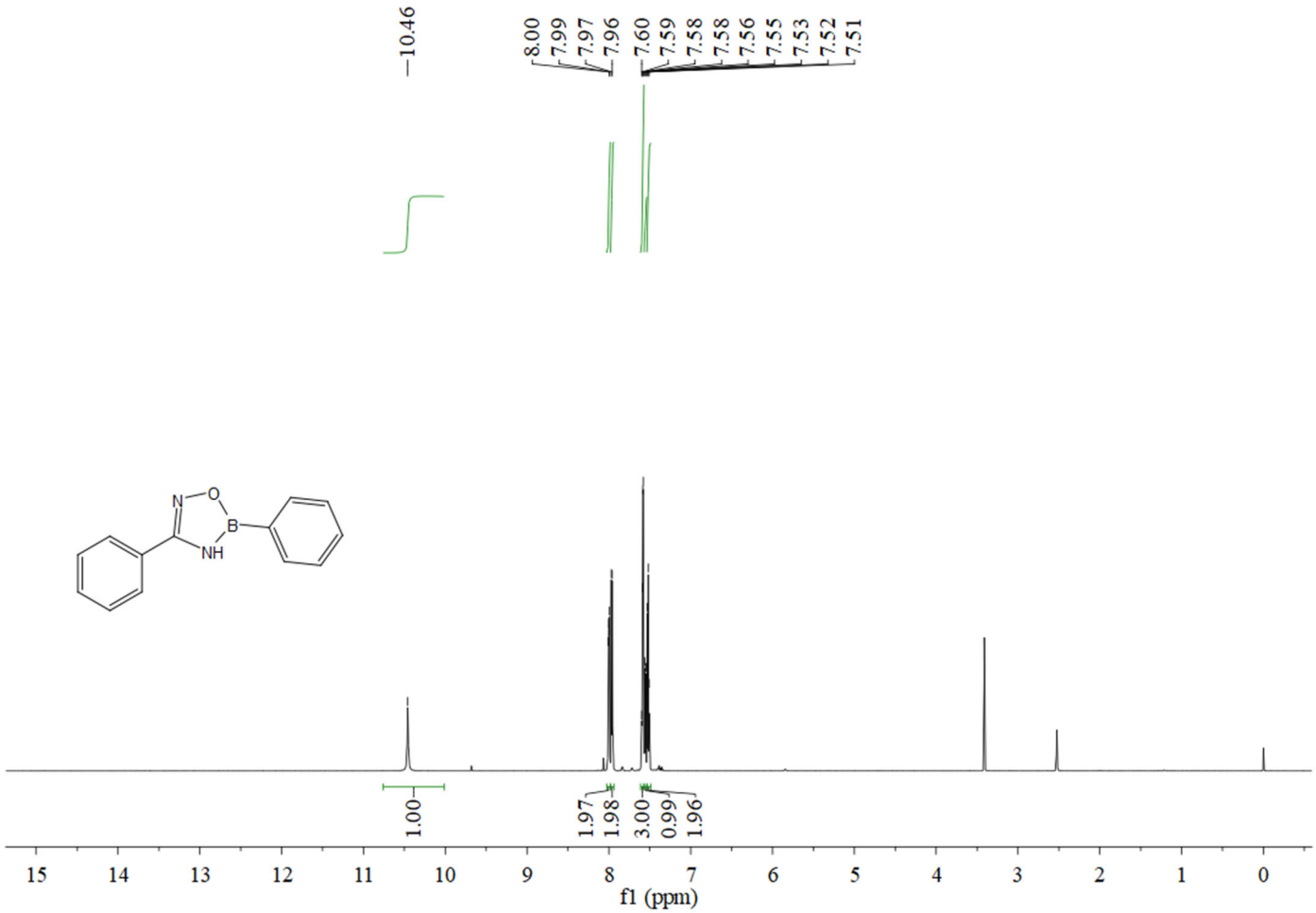


Fig. S11 ^{1}H NMR for compound **3a** (600 MHz, DMSO-d_6)

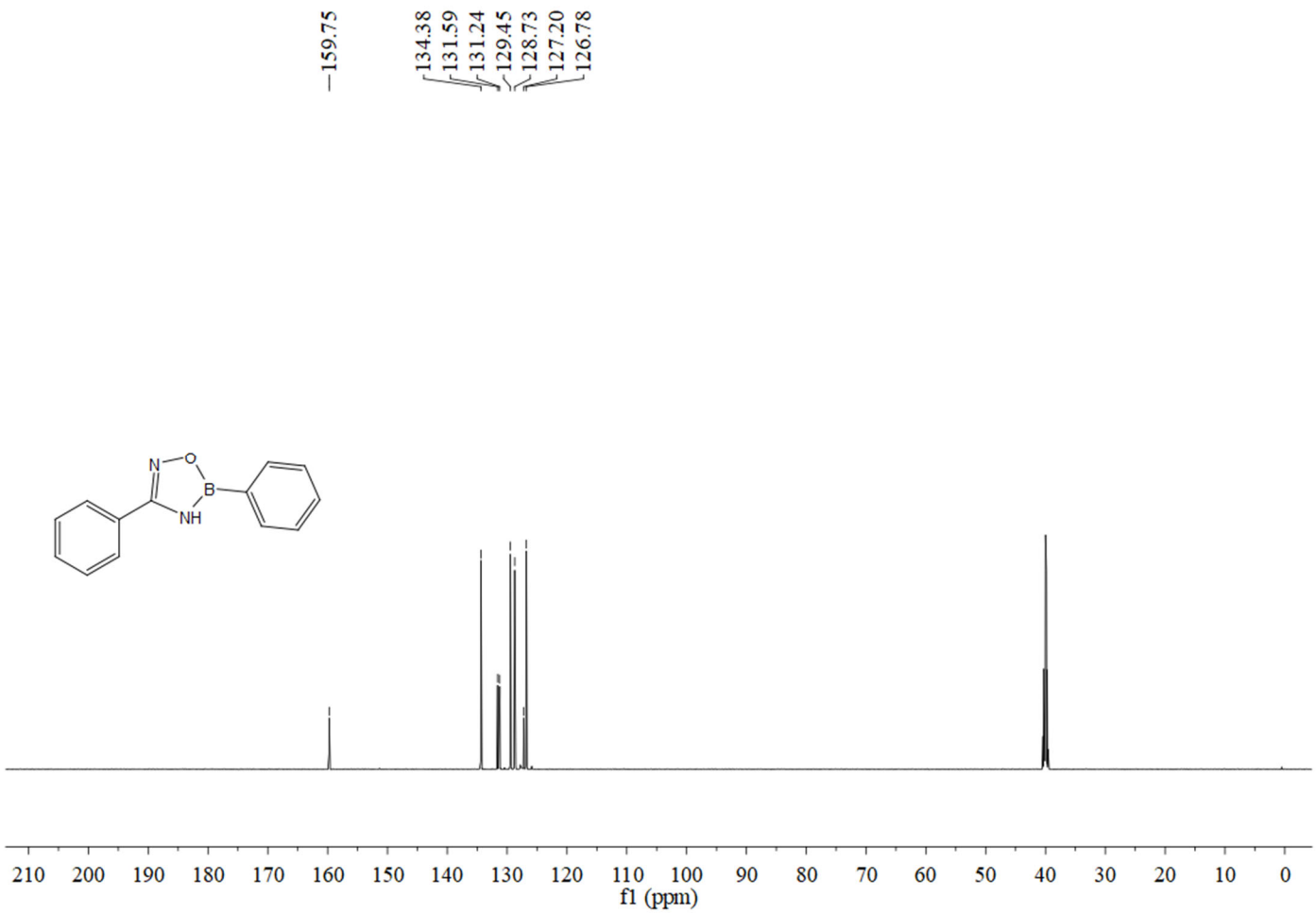


Fig. S12 ^{13}C NMR for compound **3a** (151 MHz, DMSO-d_6)

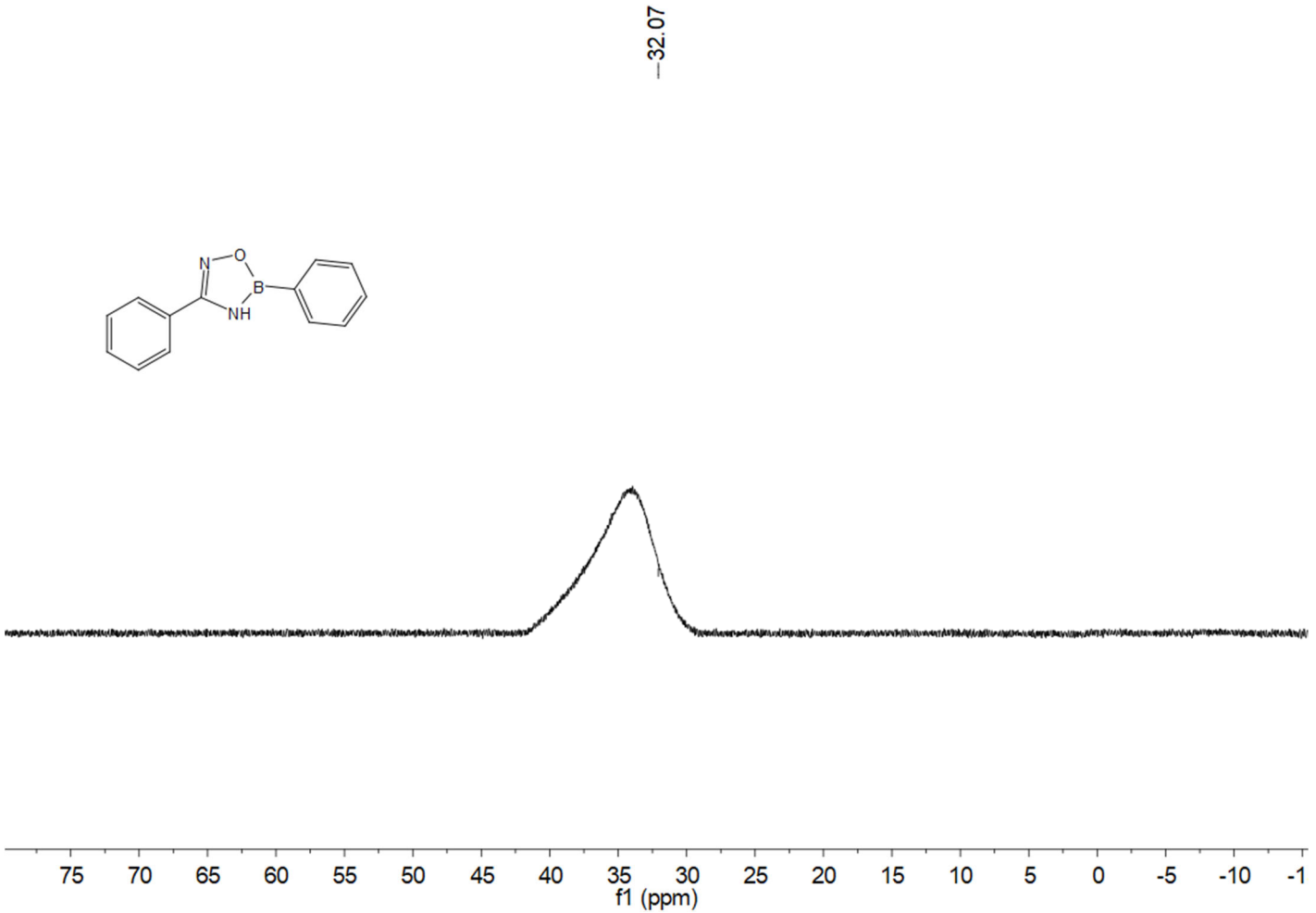


Fig. S13 ^{11}B NMR for compound **3a** (193 MHz, DMSO-d_6)

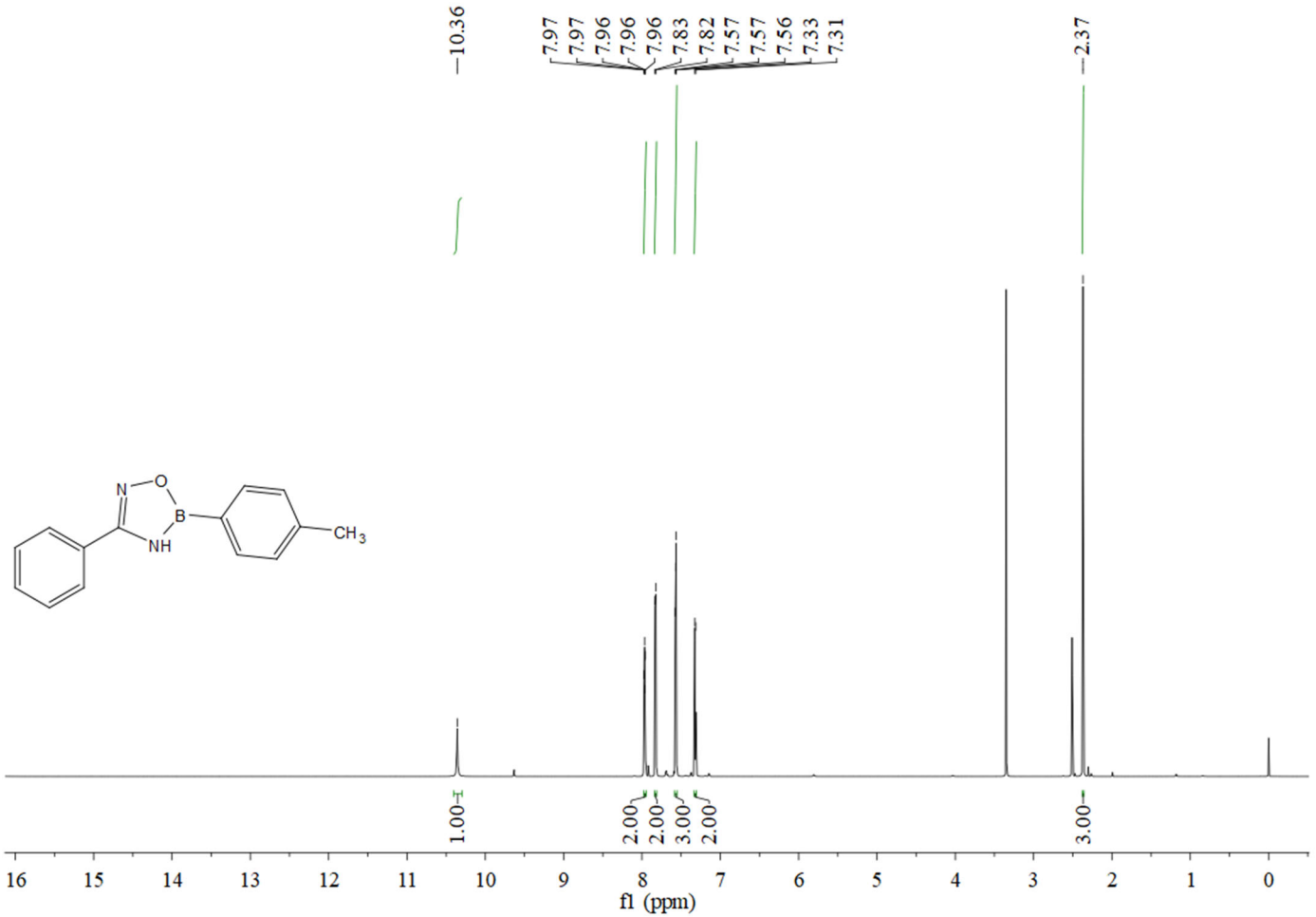


Fig. S14 ^{1}H NMR for compound **3b** (600 MHz, DMSO-d_6)

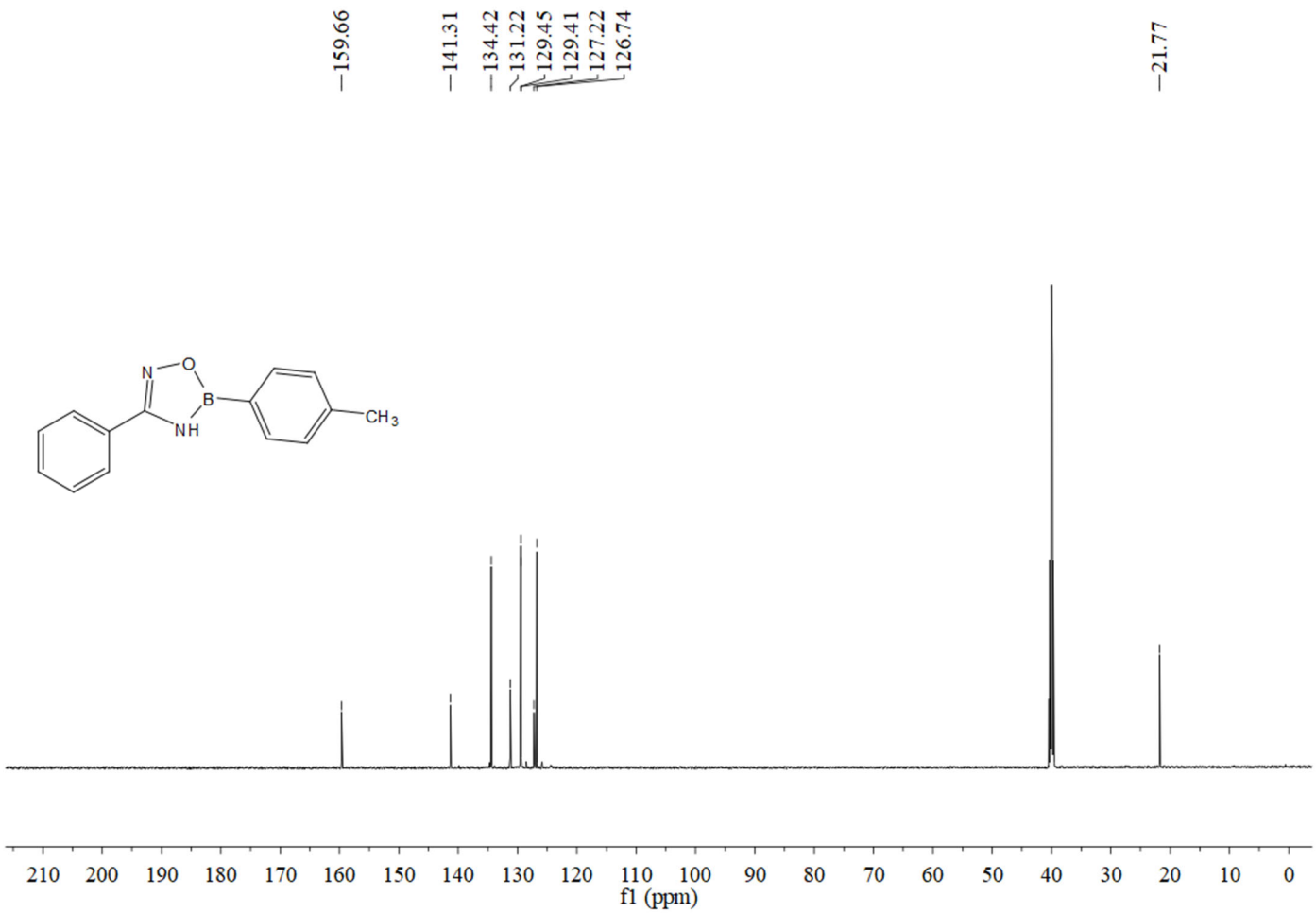


Fig. S15 ^{13}C NMR for compound **3b** (151 MHz, DMSO-d_6)

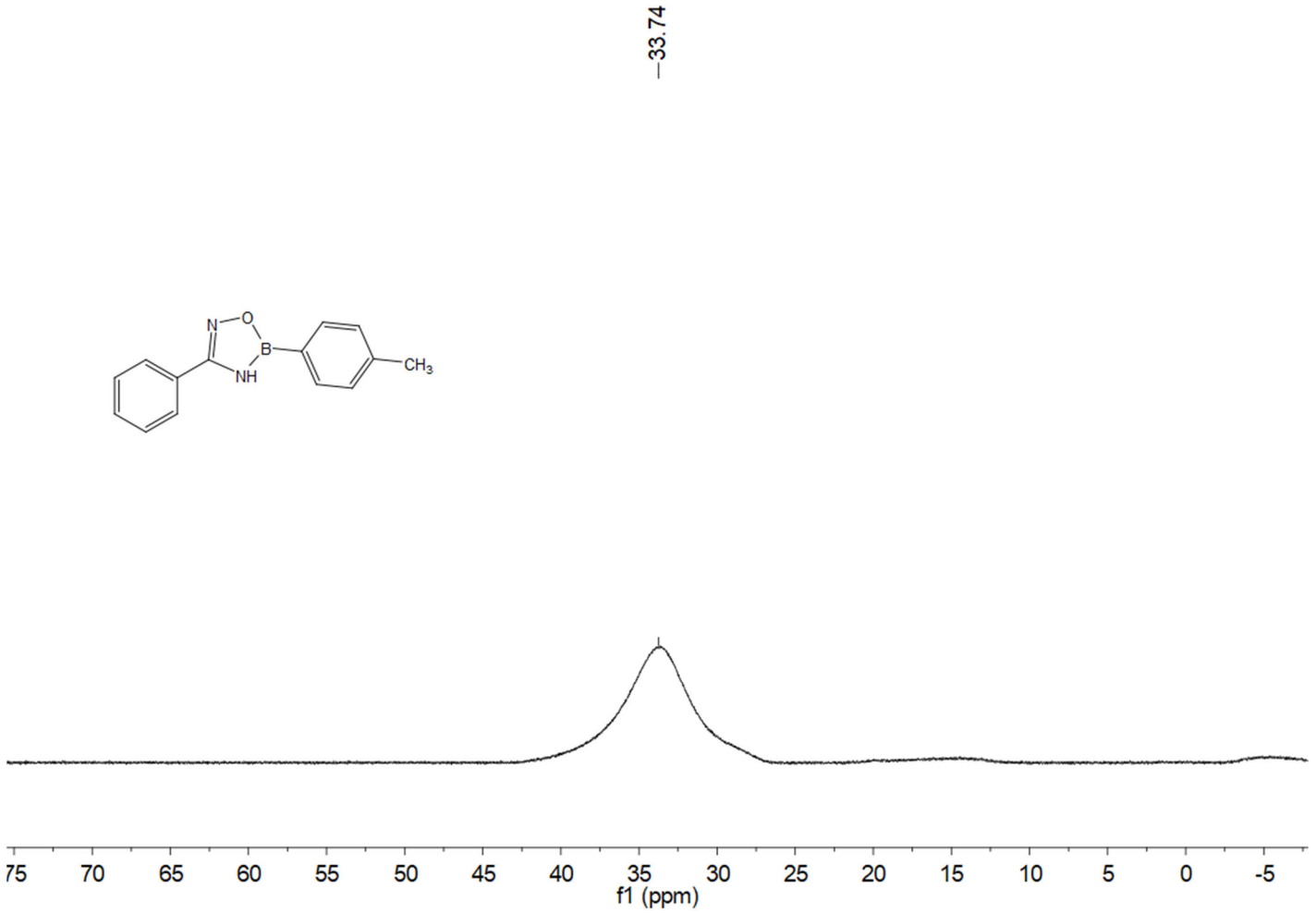


Fig. S16 ^{11}B NMR for compound **3b** (193 MHz, DMSO-d_6)

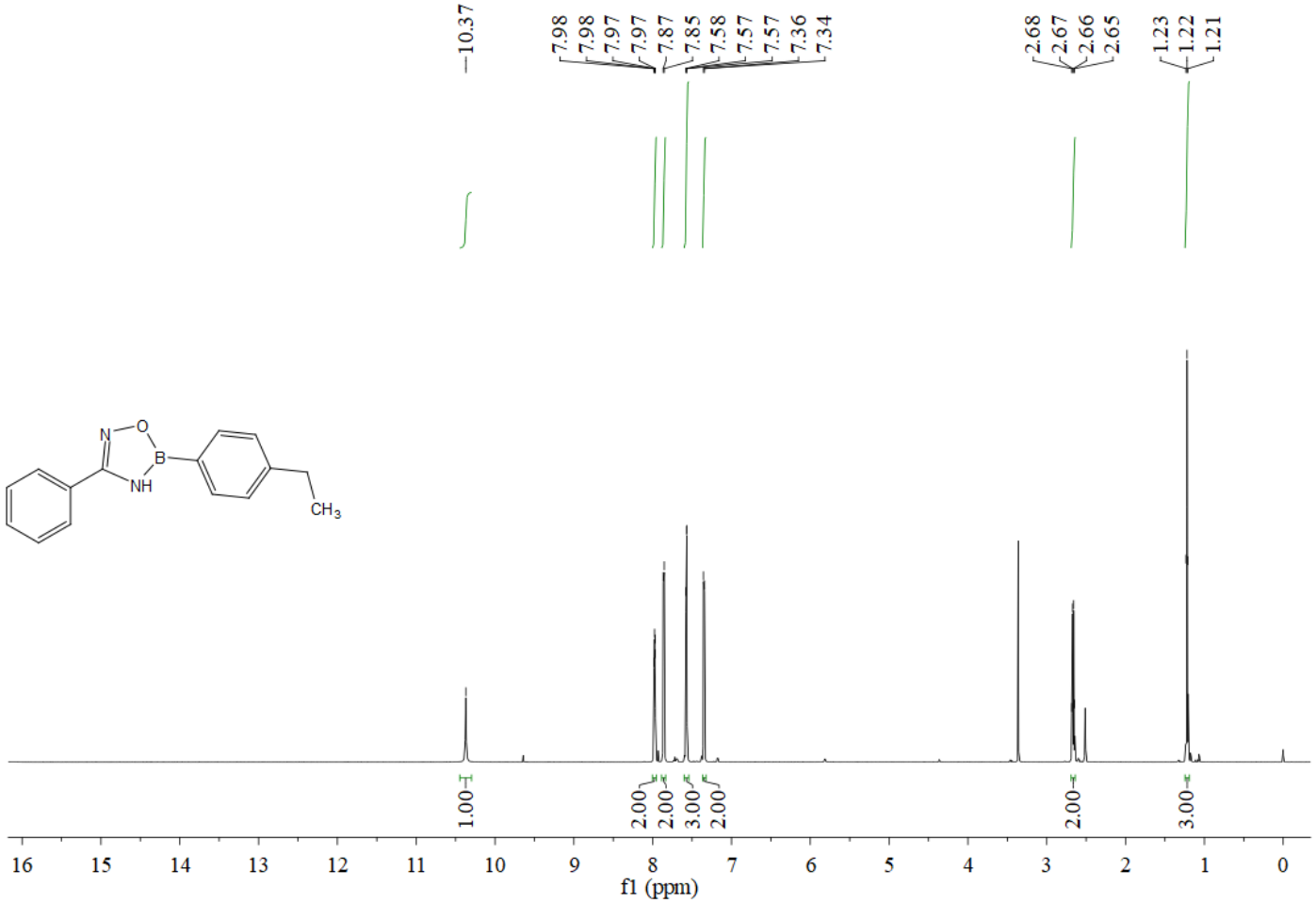


Fig. S17 ^{1}H NMR for compound **3c** (600 MHz, DMSO-d_6)

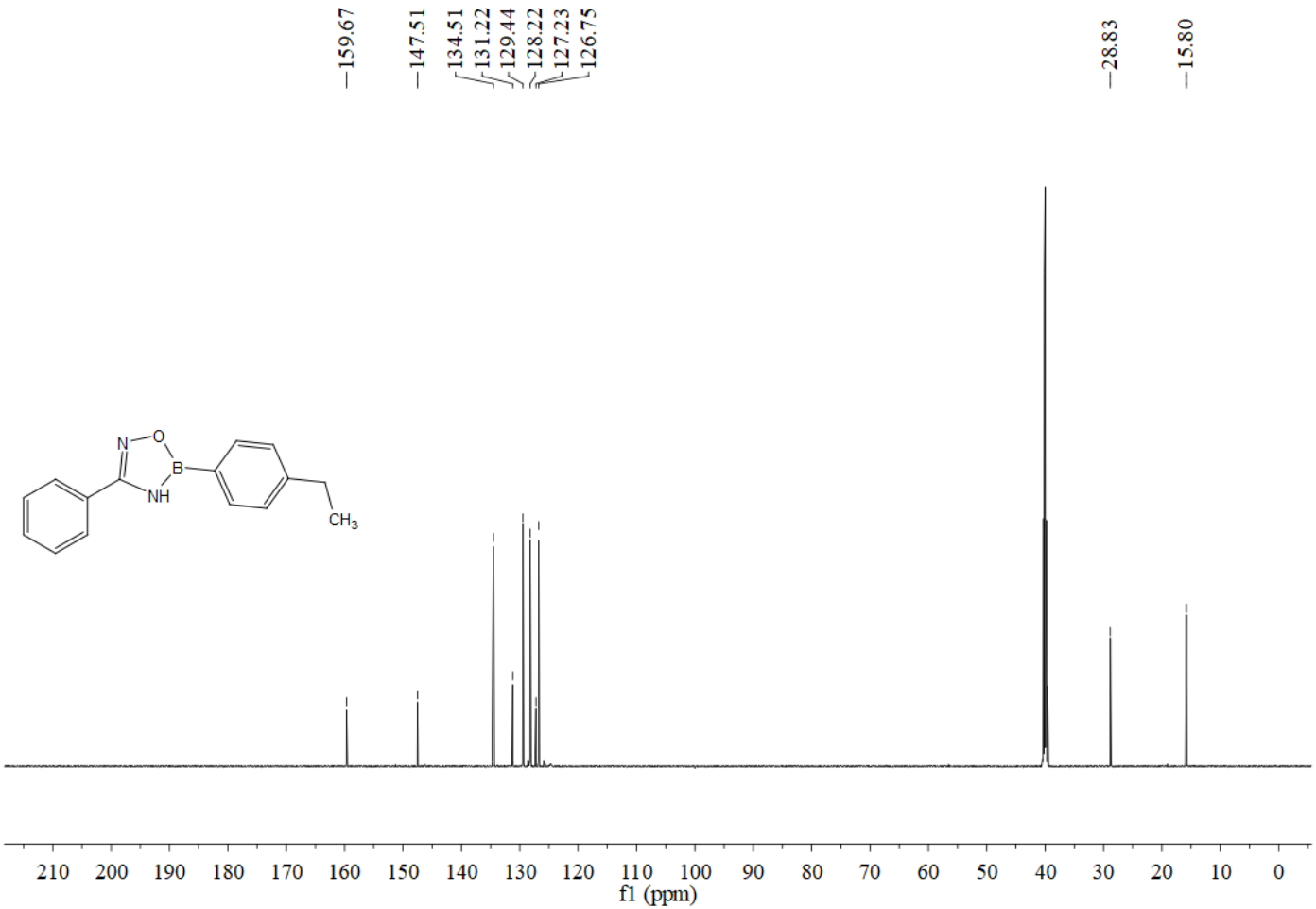


Fig. S18 ^{13}C NMR for compound **3c** (151 MHz, DMSO-d_6)

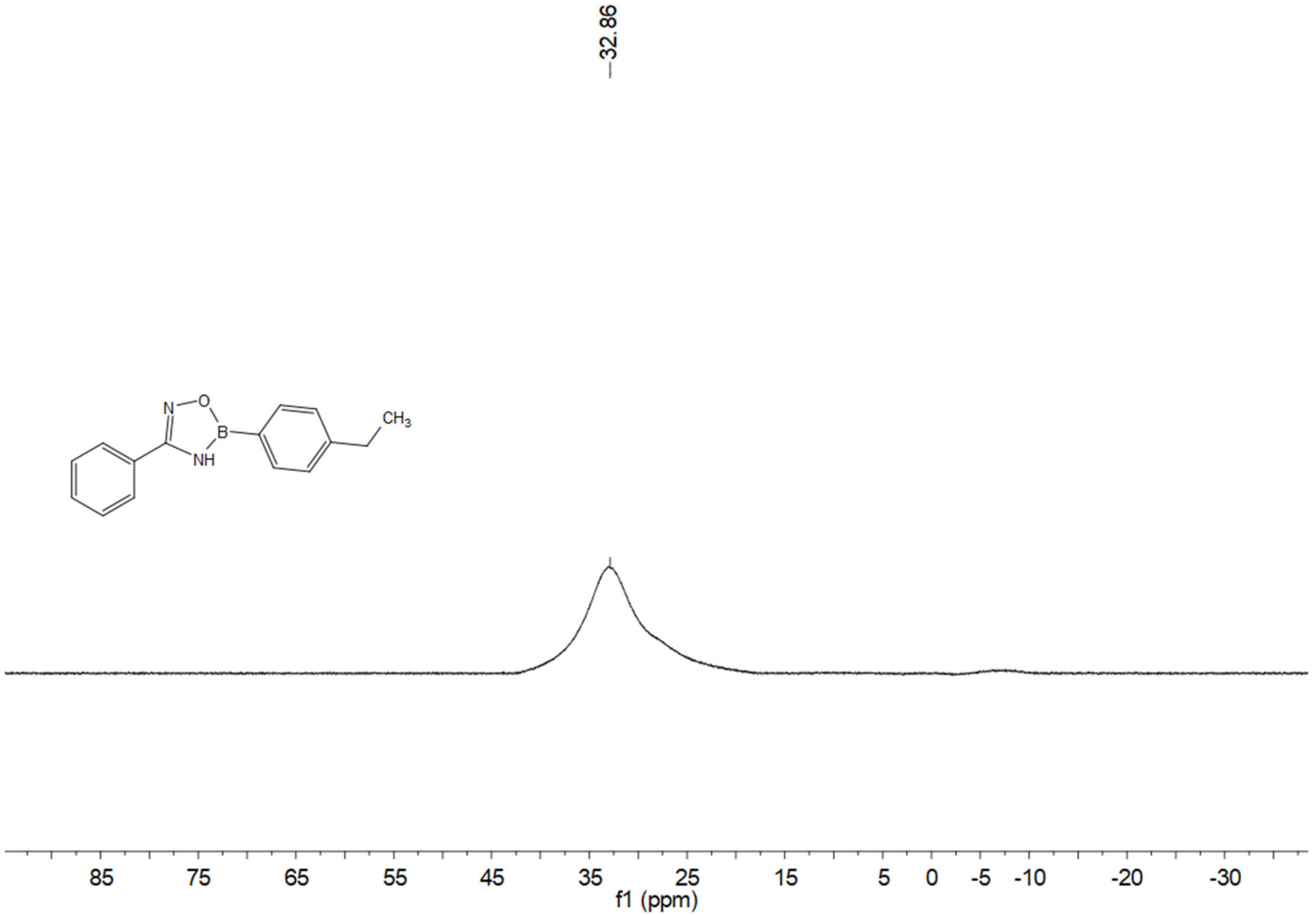


Fig. S19 ^{11}B NMR for compound **3c** (193 MHz, DMSO-d_6)

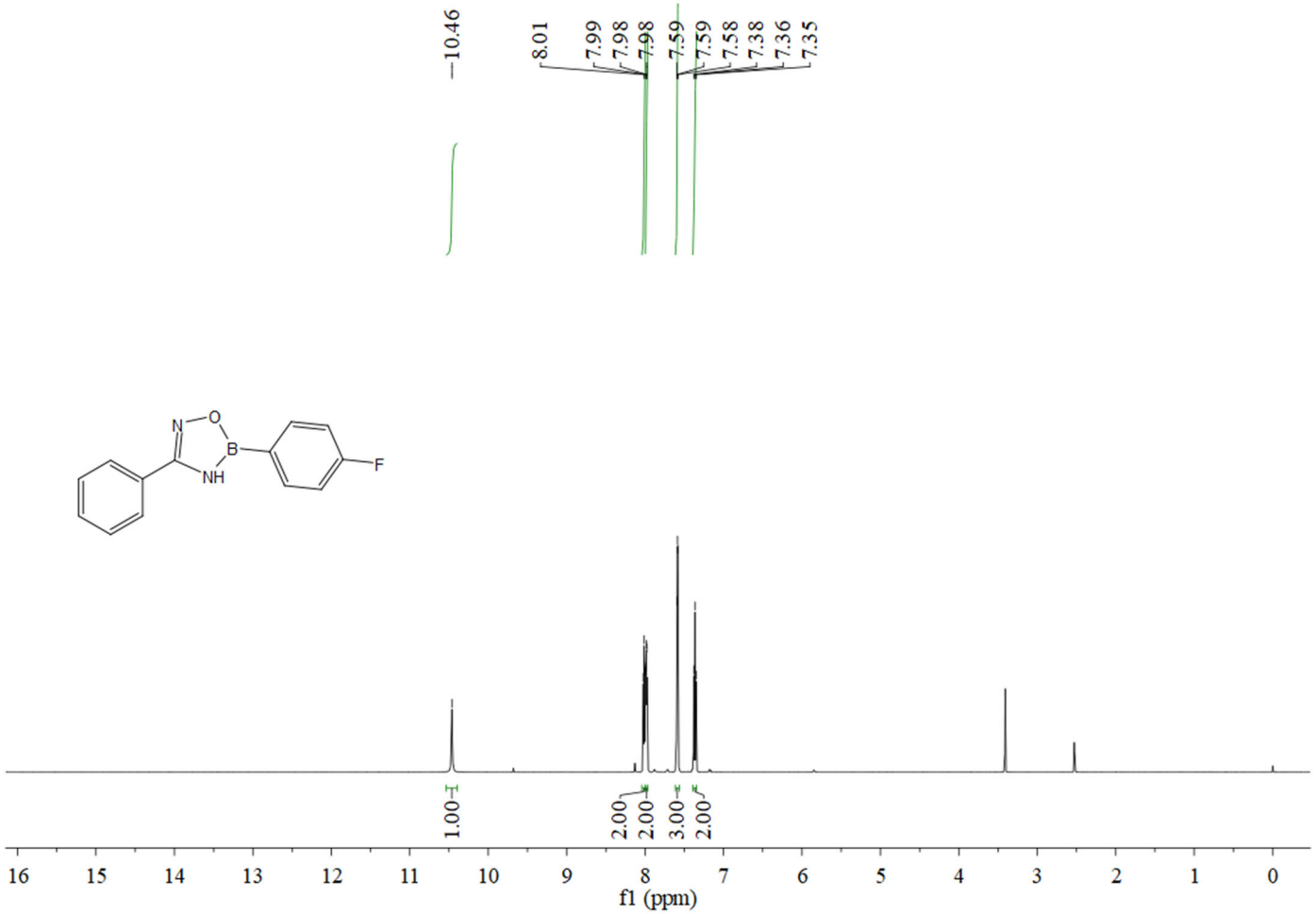


Fig. S20 ^{1}H NMR for compound **3d** (600 MHz, DMSO-d_6)

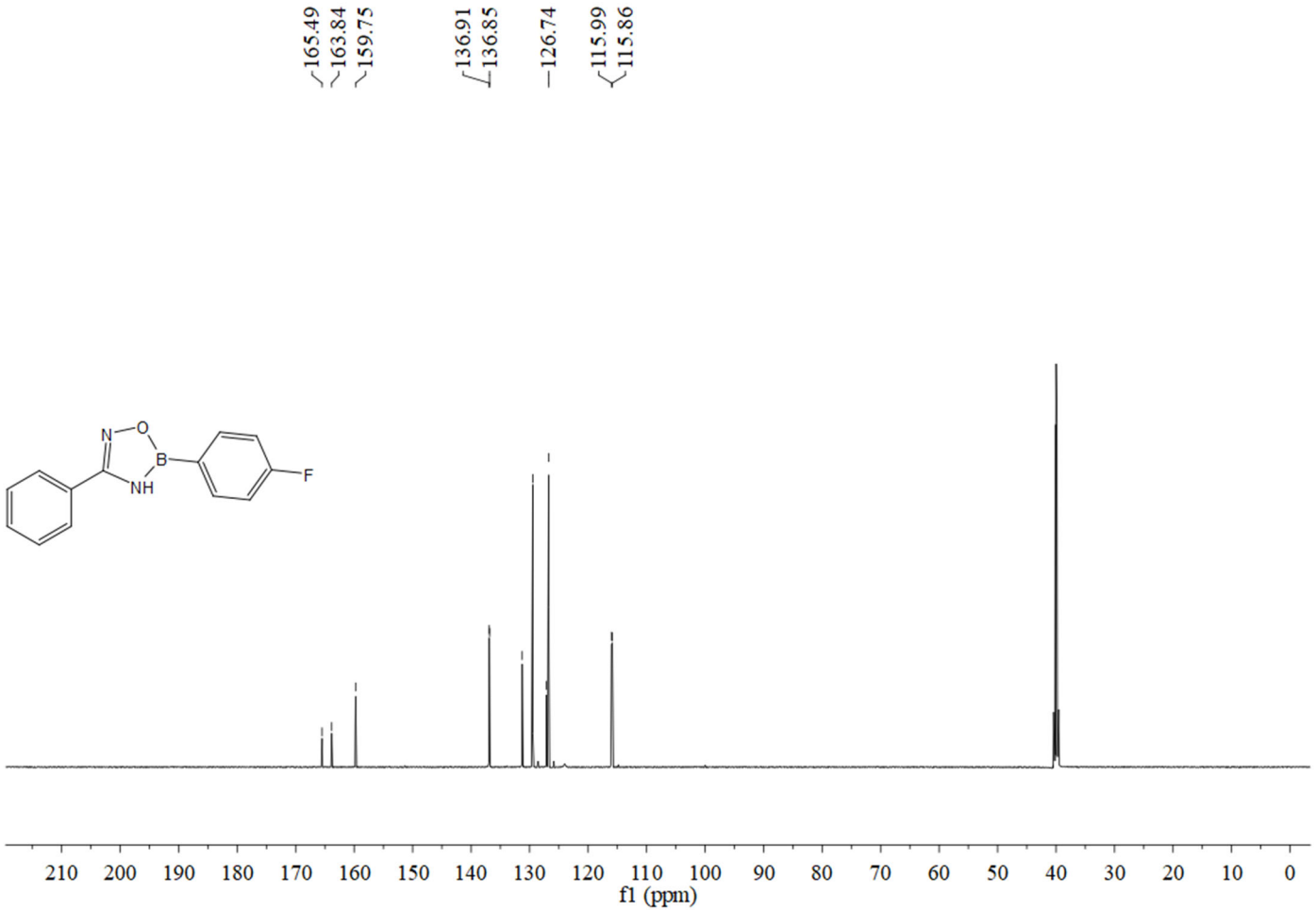


Fig. S21 ^{13}C NMR for compound **3d** (151 MHz, DMSO-d_6)

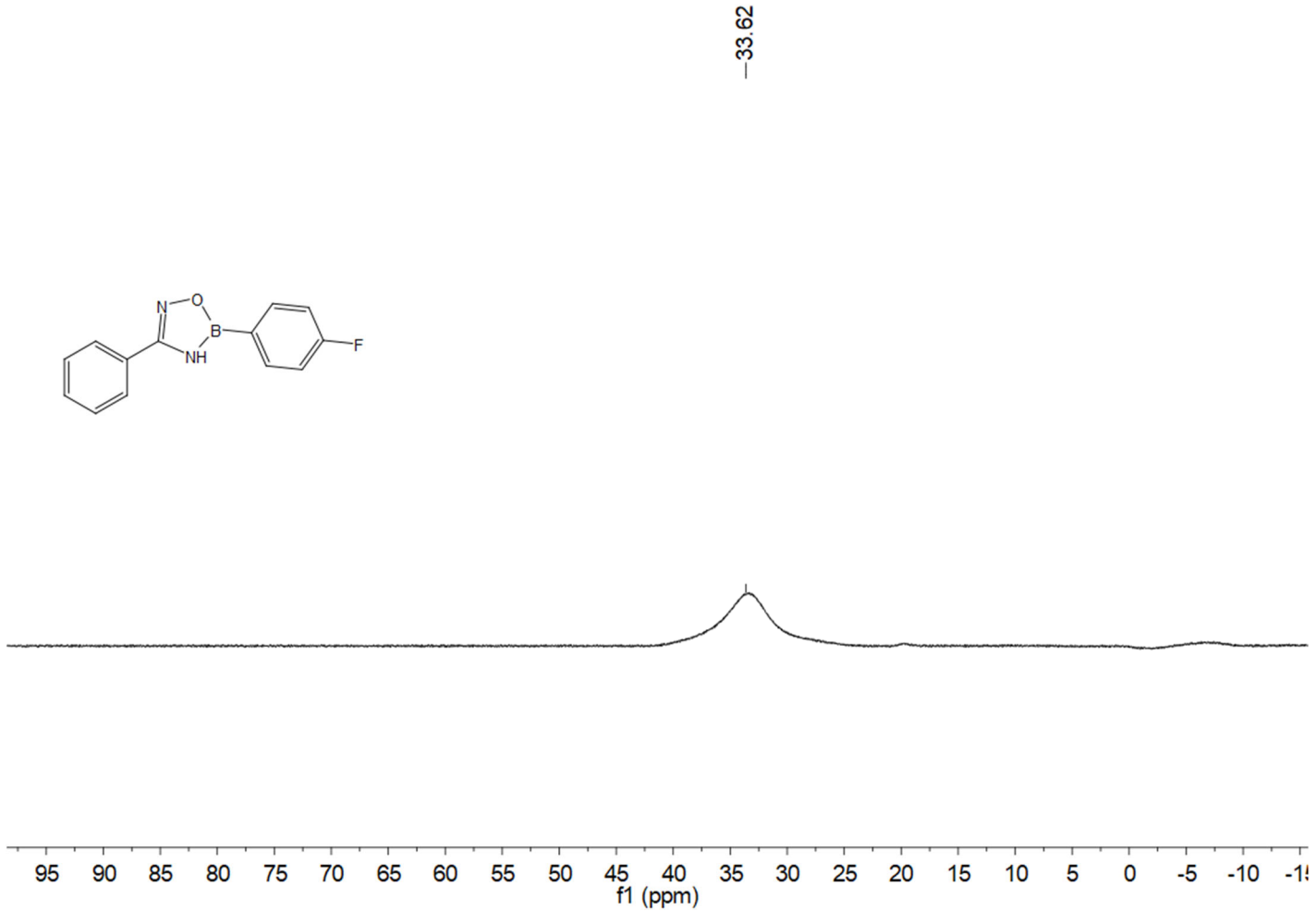


Fig. S22 ^{11}B NMR for compound **3d** (193 MHz, DMSO-d_6)

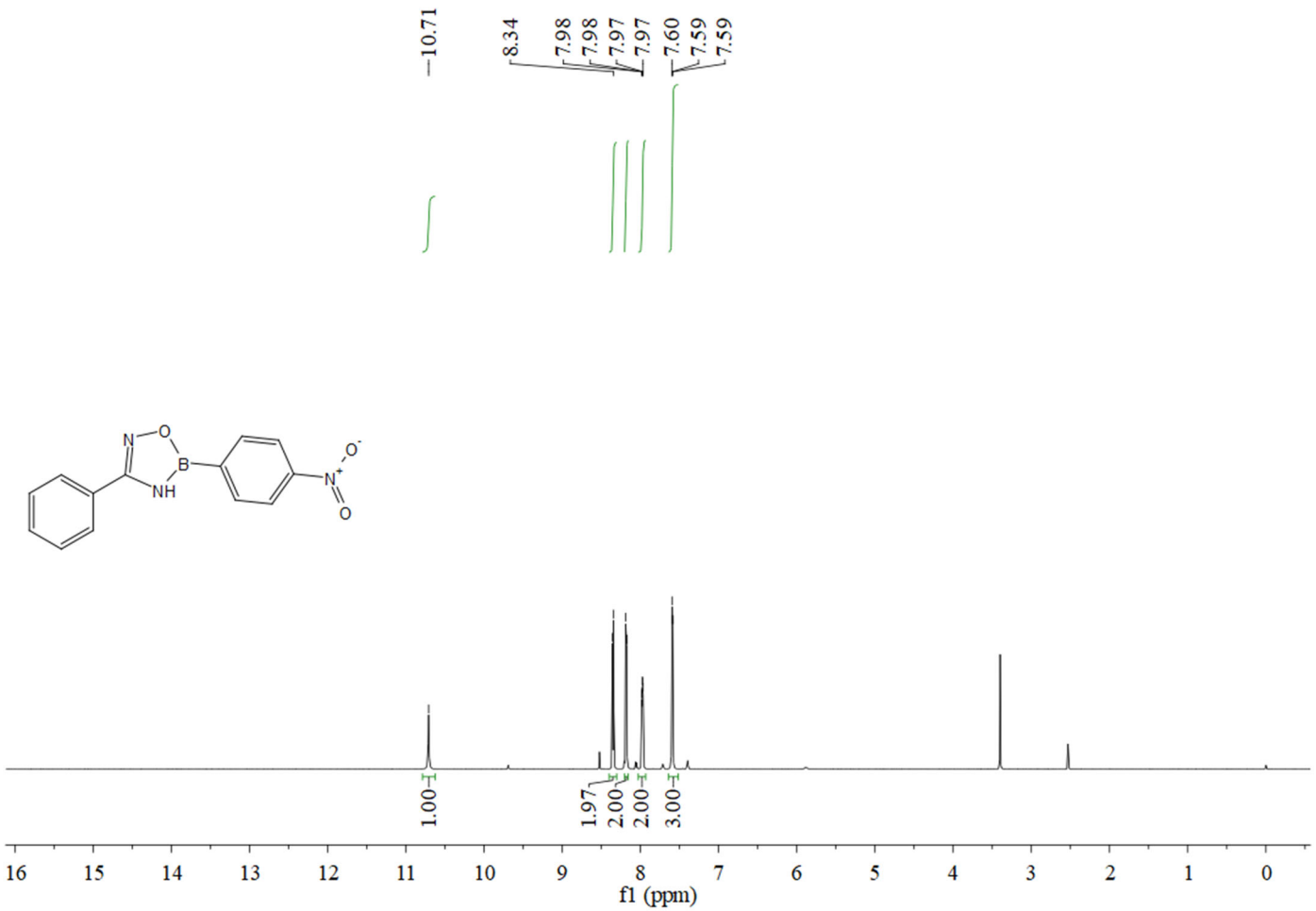


Fig. S23 ^{1}H NMR for compound **3e** (600 MHz, DMSO-d_6)

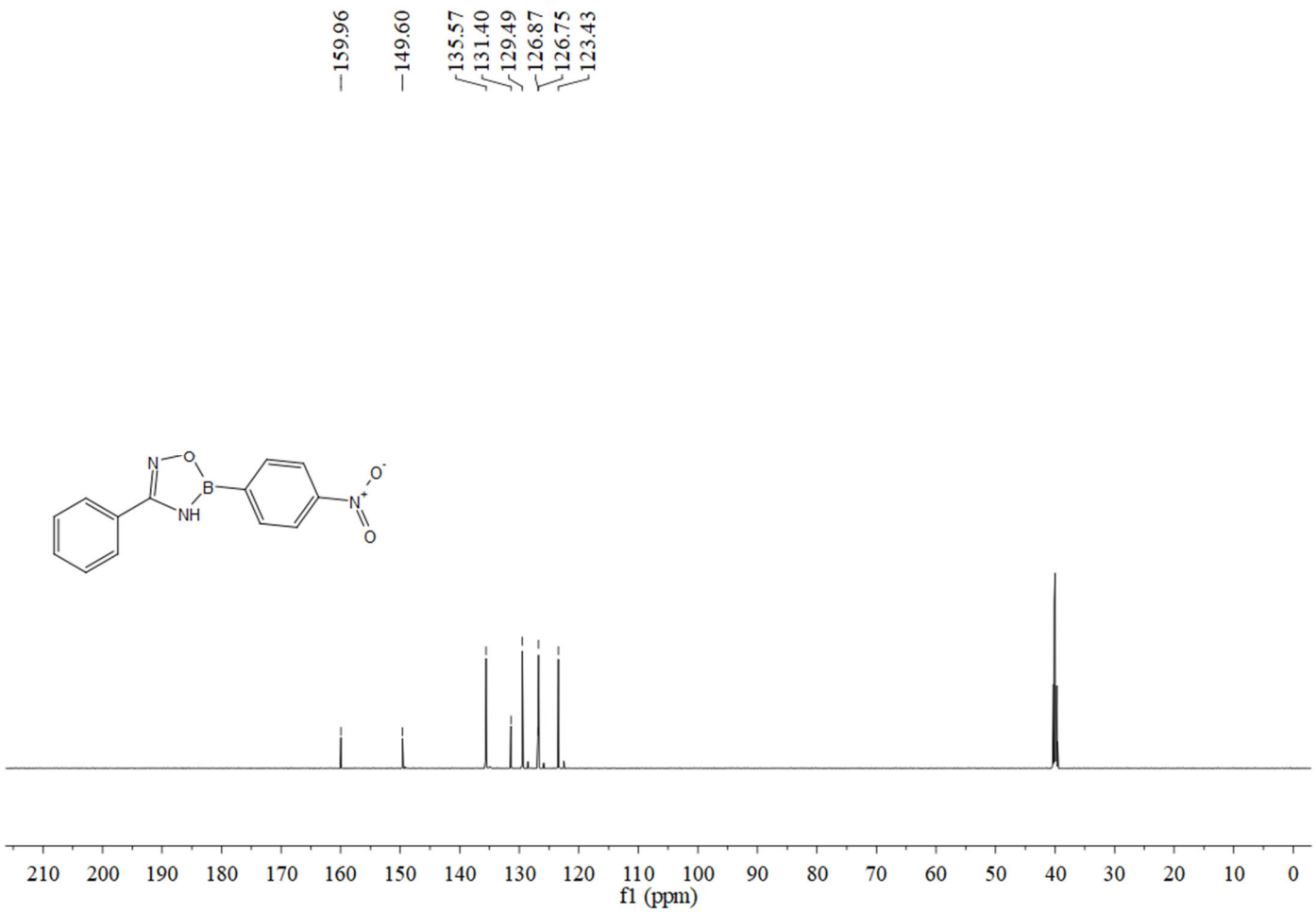


Fig. S24 ^{13}C NMR for compound **3e** (151 MHz, DMSO-d_6)

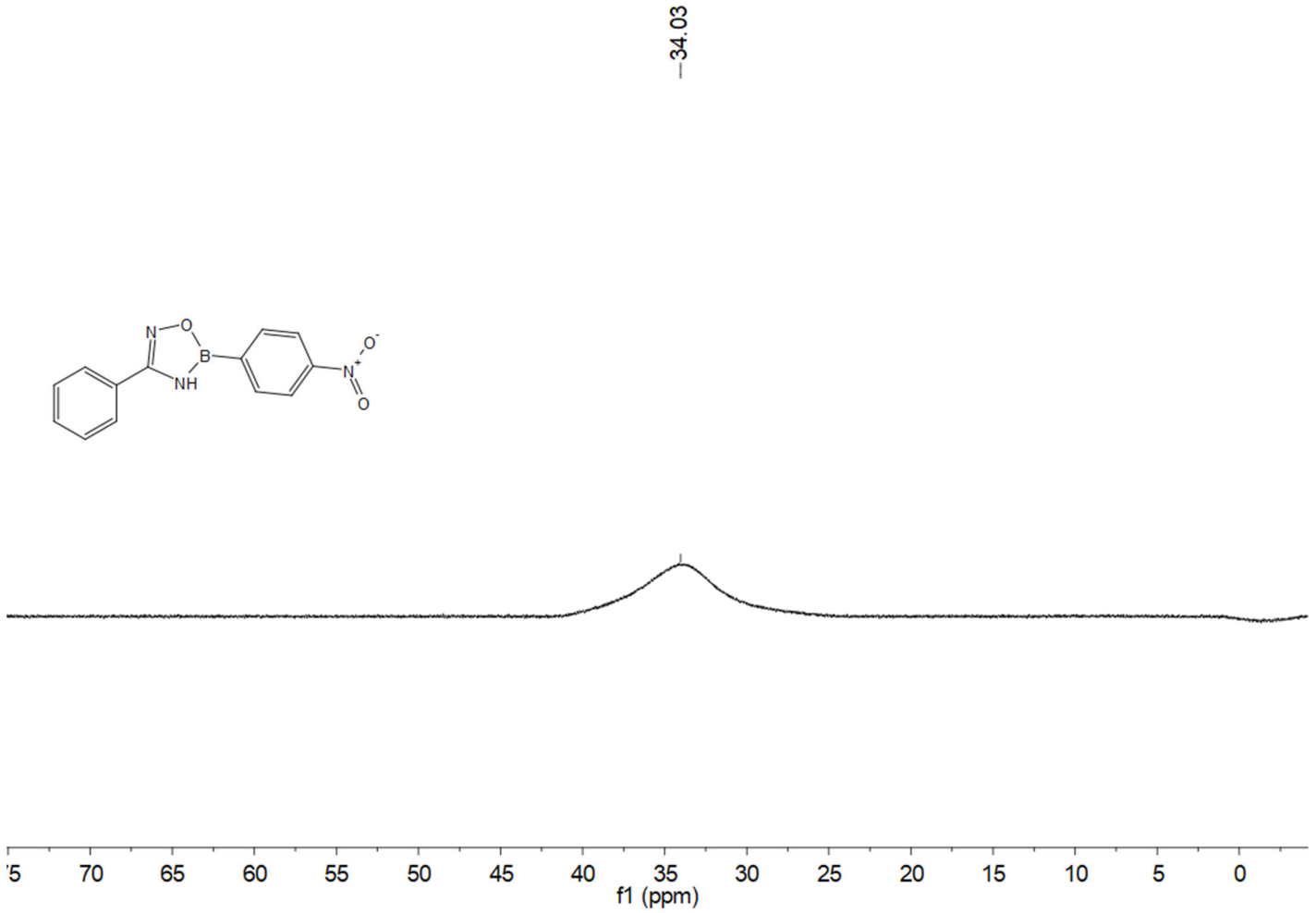


Fig. S25 ^{11}B NMR for compound **3e** (193 MHz, DMSO-d_6)

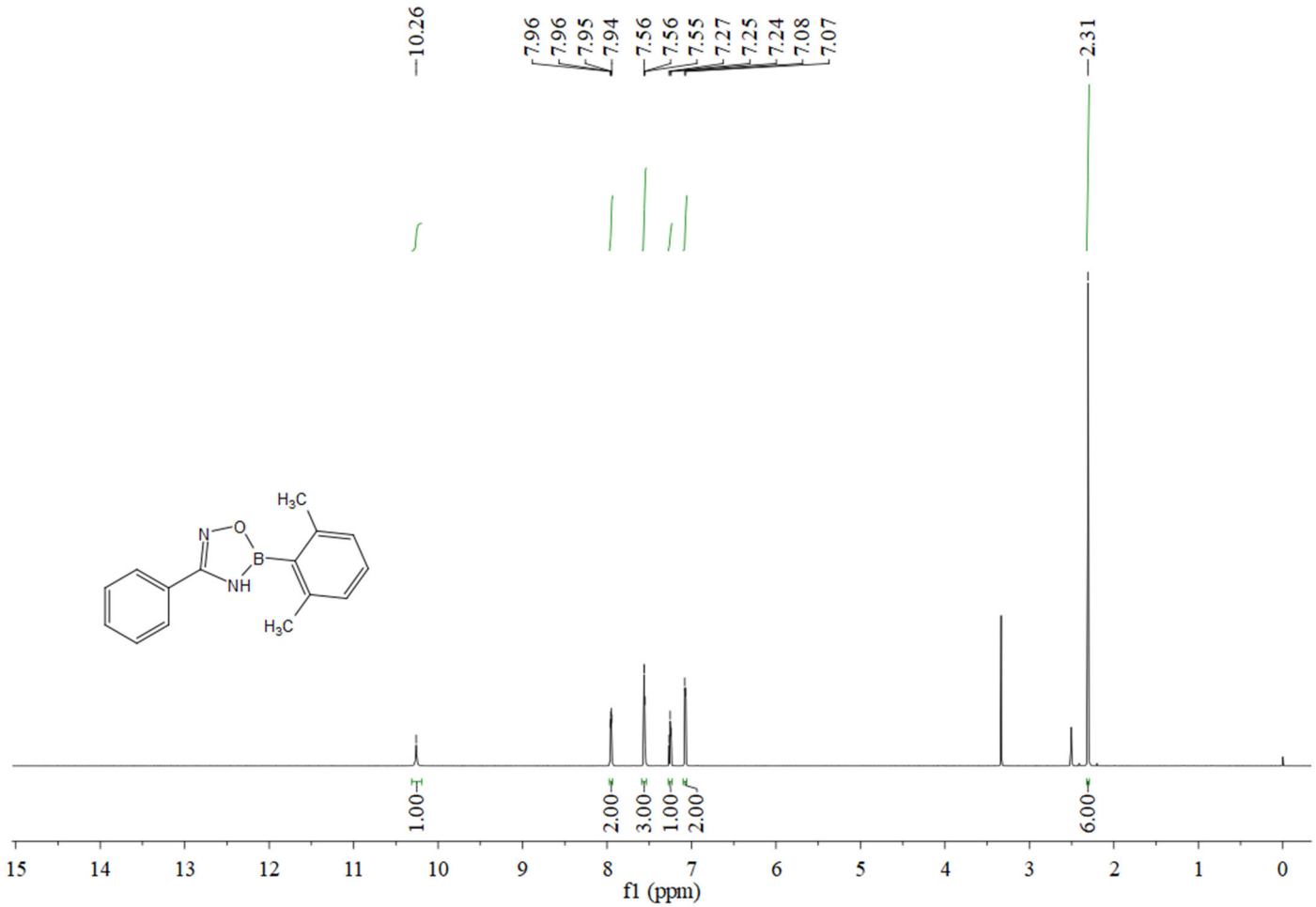


Fig. S26 ^{1}H NMR for compound **3f** (600 MHz, DMSO-d_6)

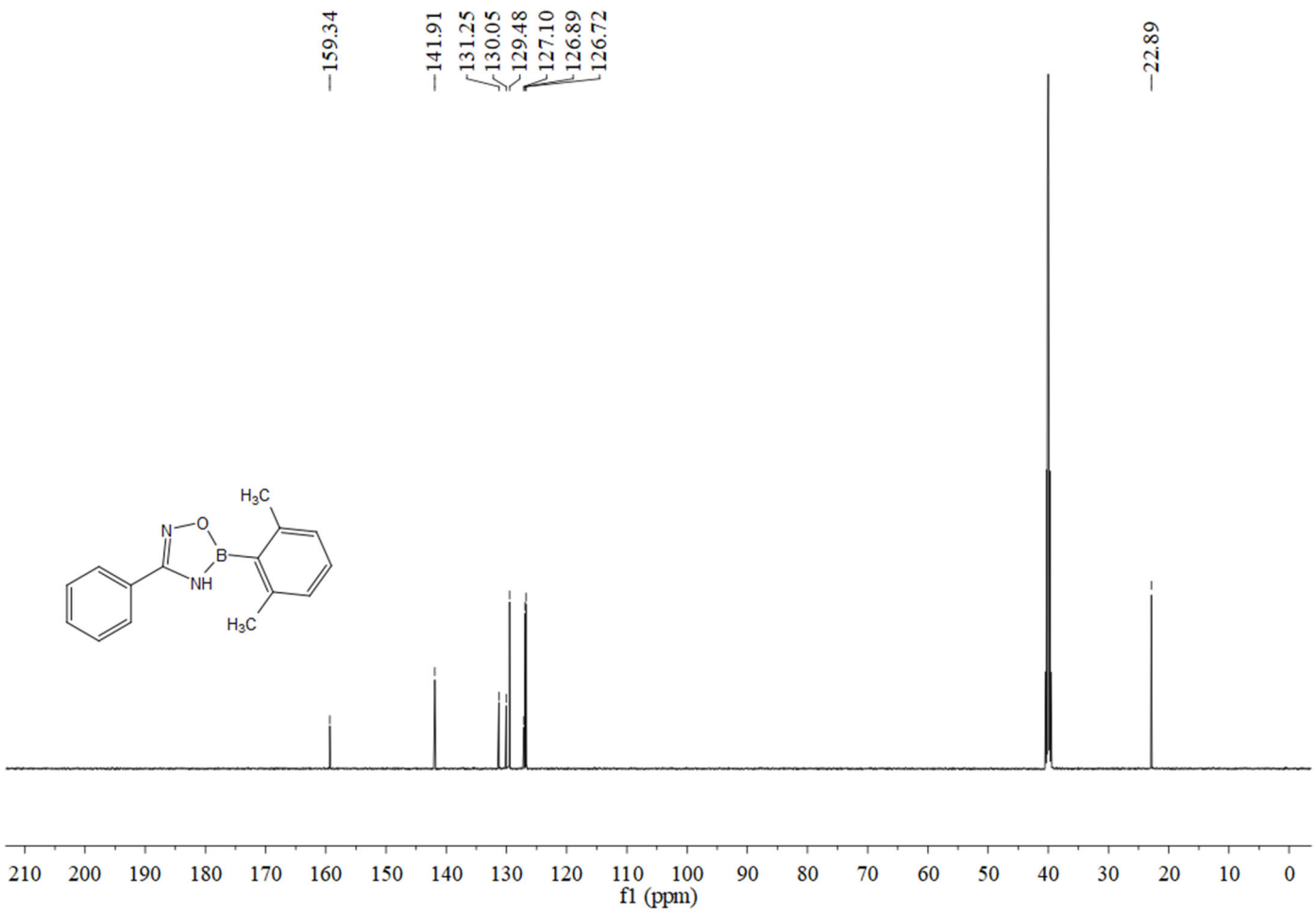


Fig. S27 ^{13}C NMR for compound **3f** (151 MHz, DMSO-d_6)

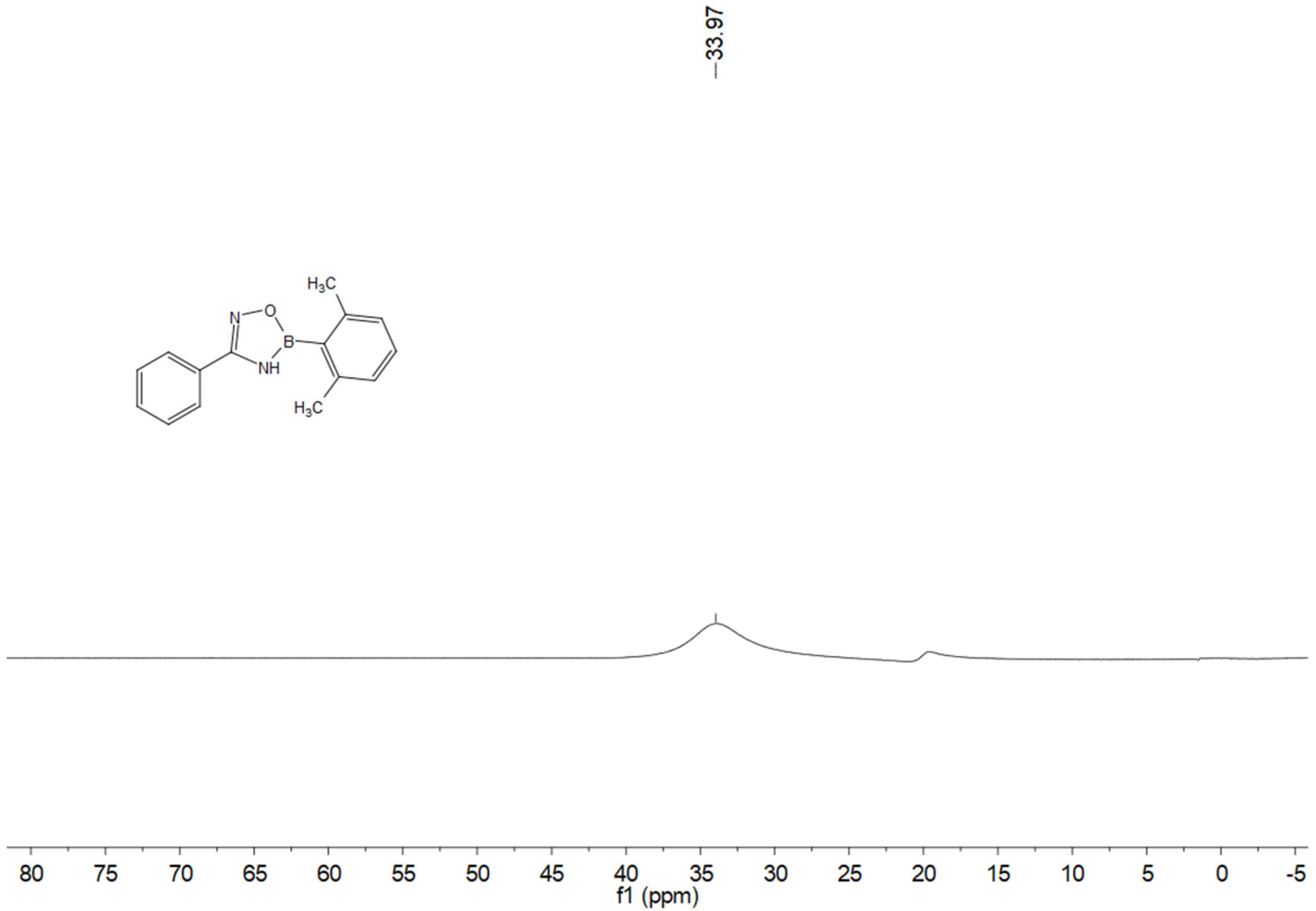


Fig. S28 ^{11}B NMR for compound **3f** (193 MHz, DMSO-d_6)

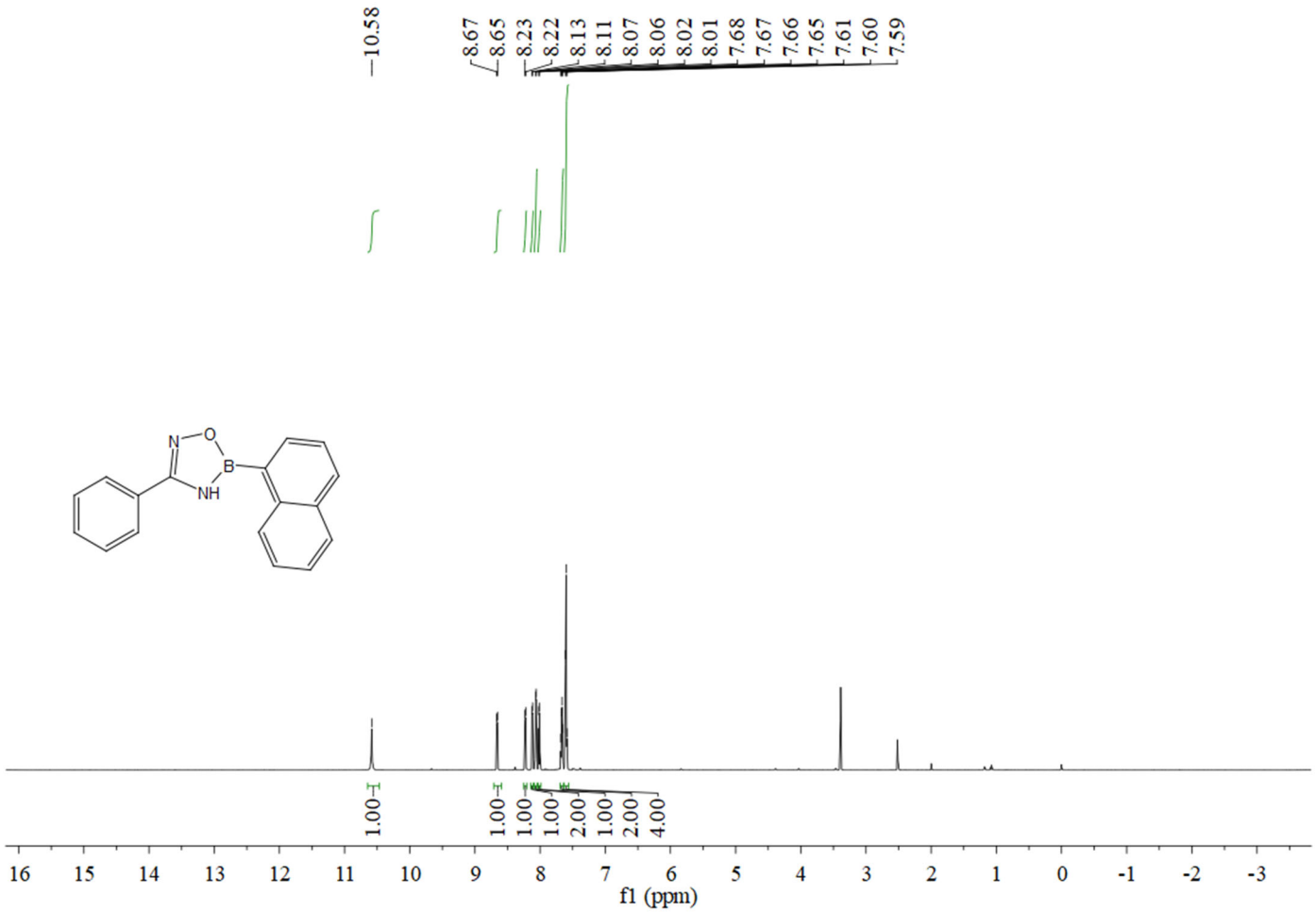


Fig. S29 ^{1}H NMR for compound **3g** (600 MHz, DMSO-d_6)

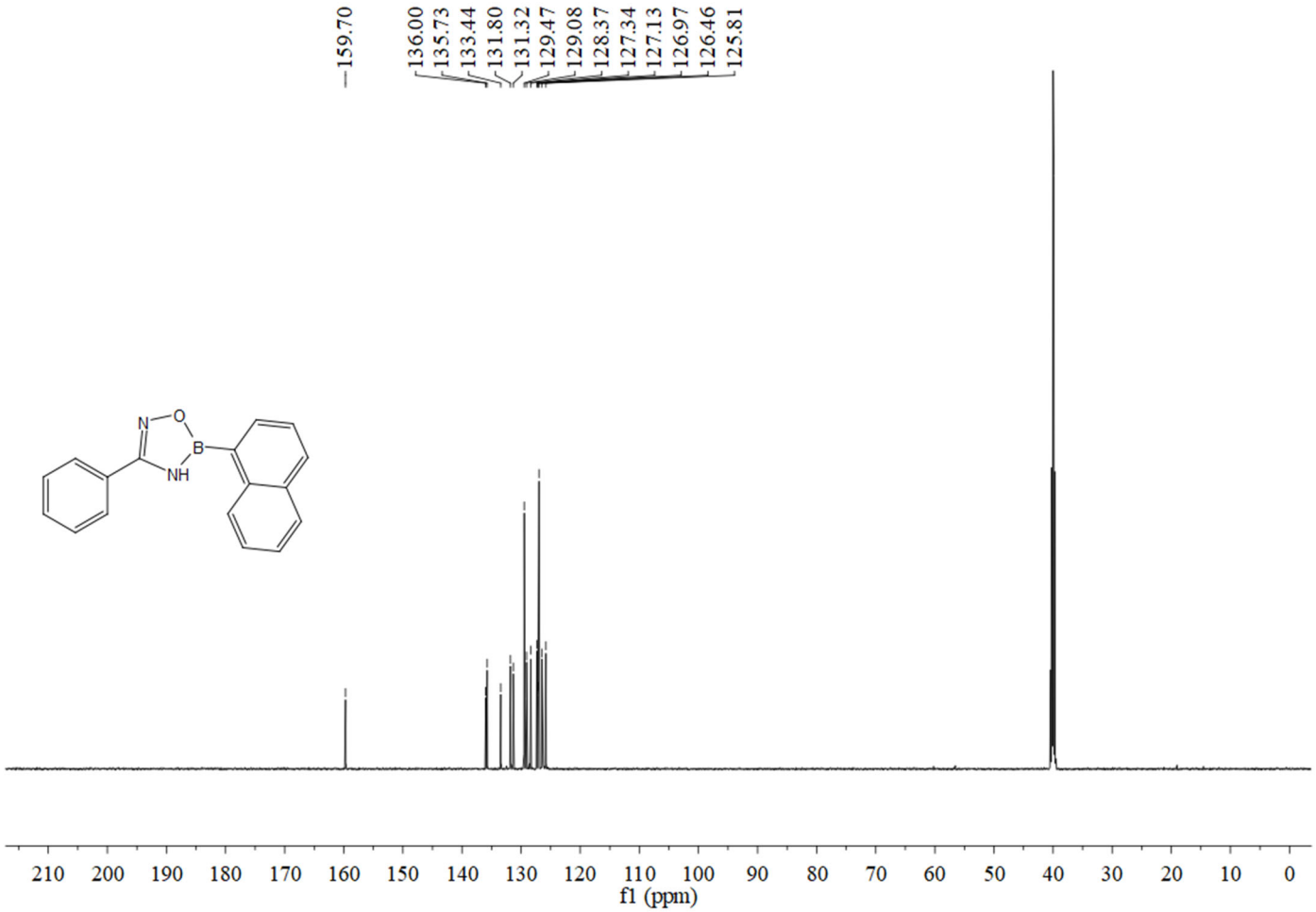


Fig. S30 ^{13}C NMR for compound **3g** (151 MHz, DMSO-d_6)

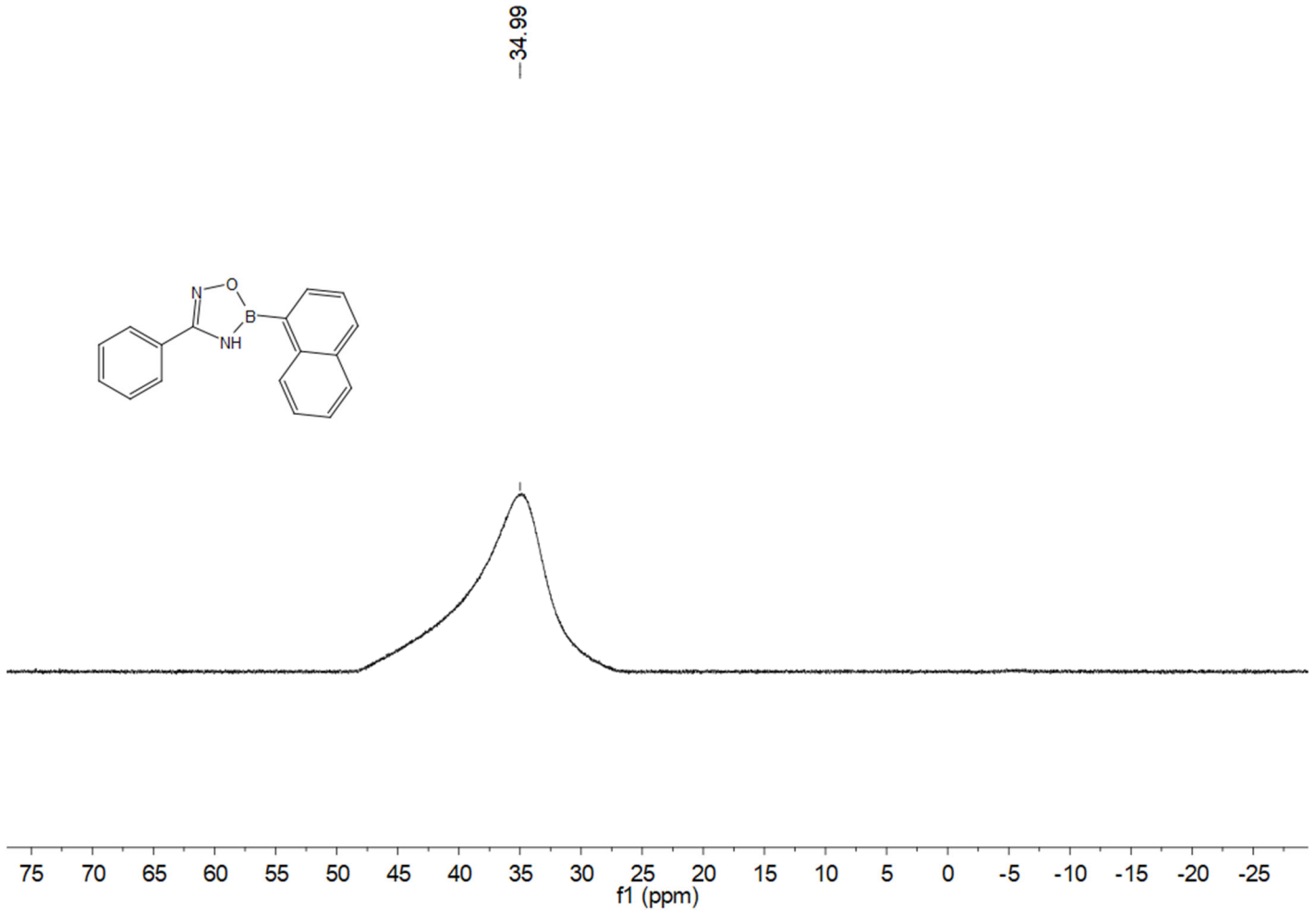


Fig. S31 ^{11}B NMR for compound **3g** (193 MHz, DMSO-d_6)

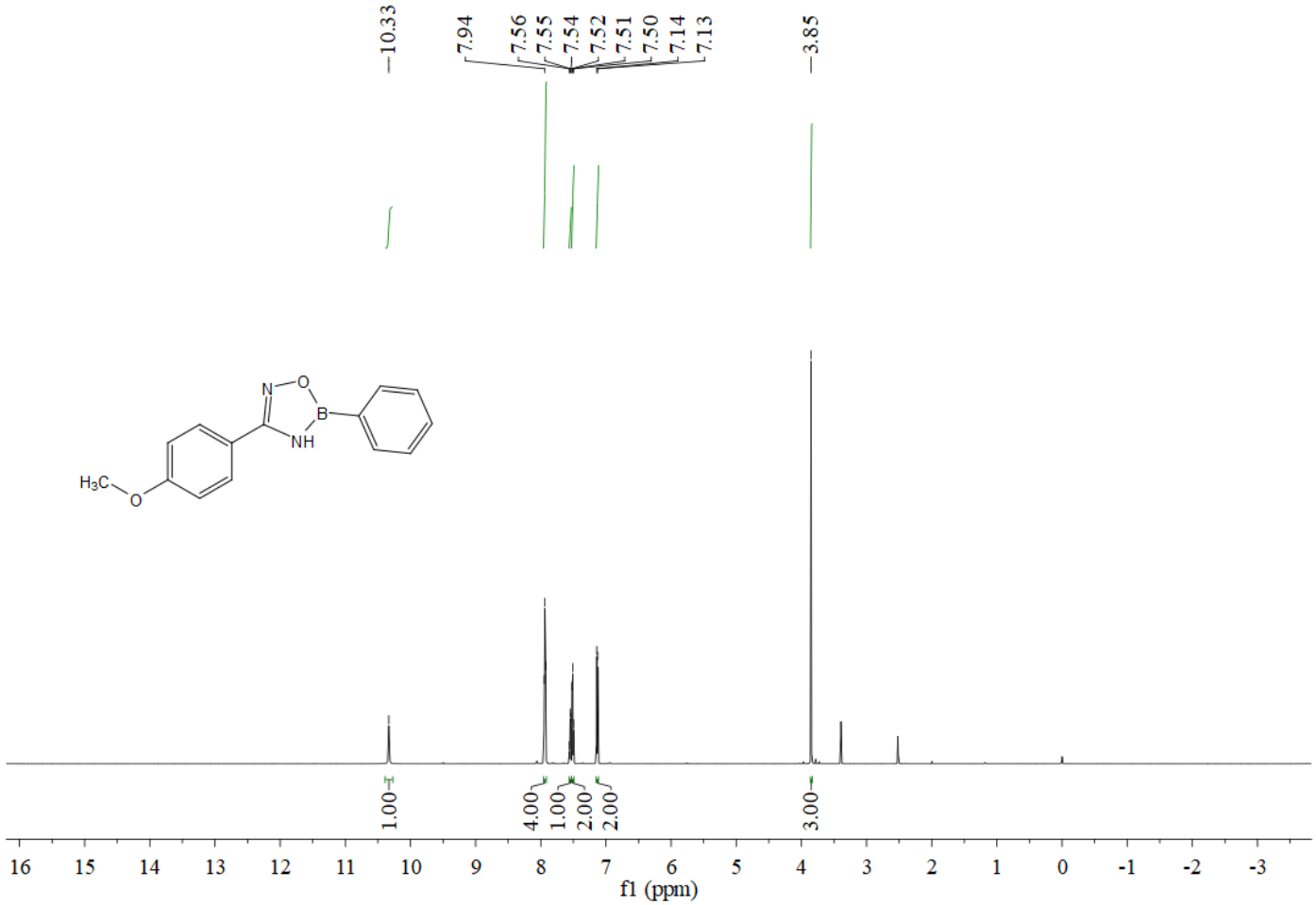


Fig. S32 ^{1}H NMR for compound **3h** (600 MHz, DMSO-d_6)

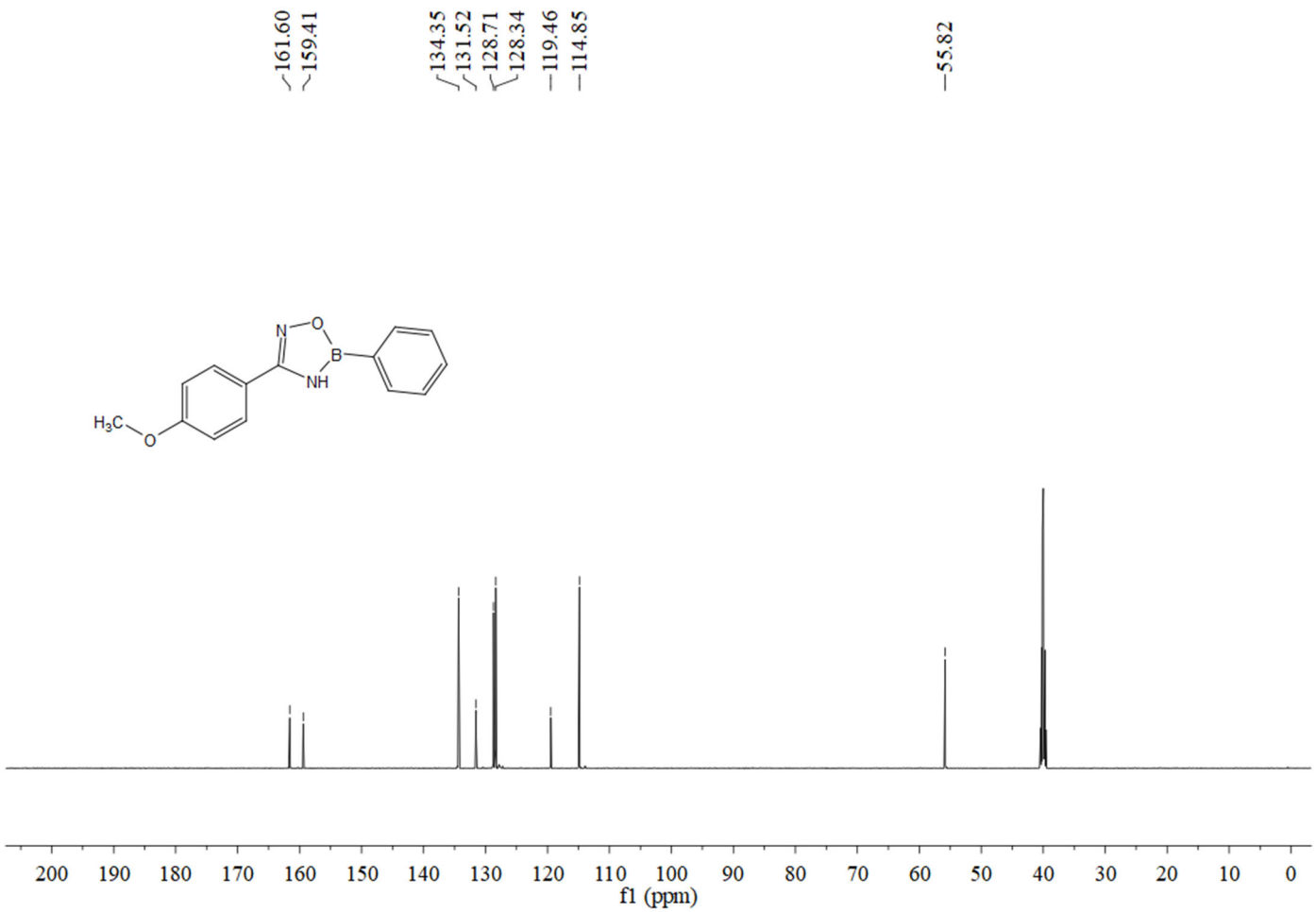


Fig. S33 ^{13}C NMR for compound **3h** (151 MHz, DMSO-d_6)

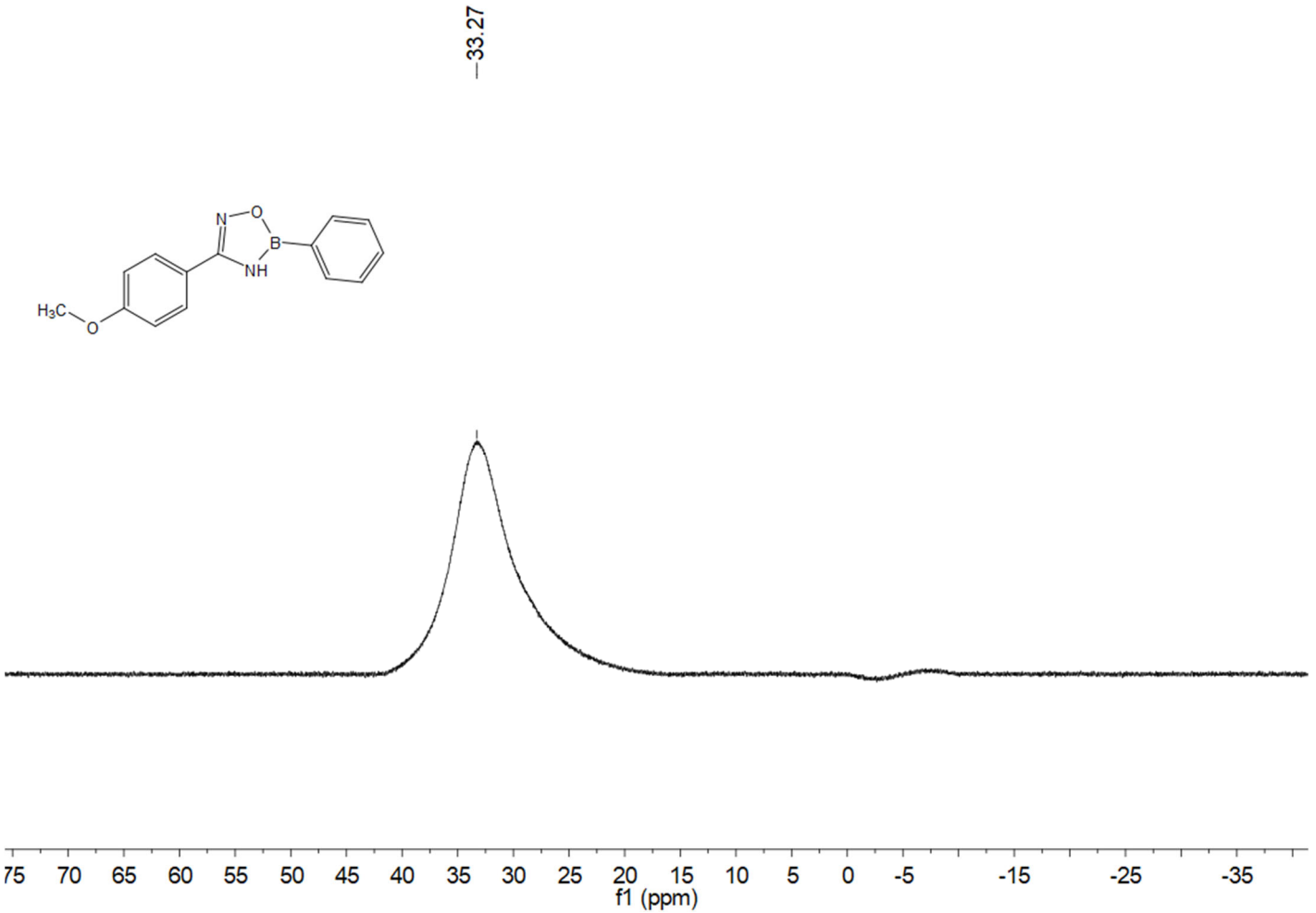


Fig. S34 ^{11}B NMR for compound **3h** (193 MHz, DMSO-d_6)

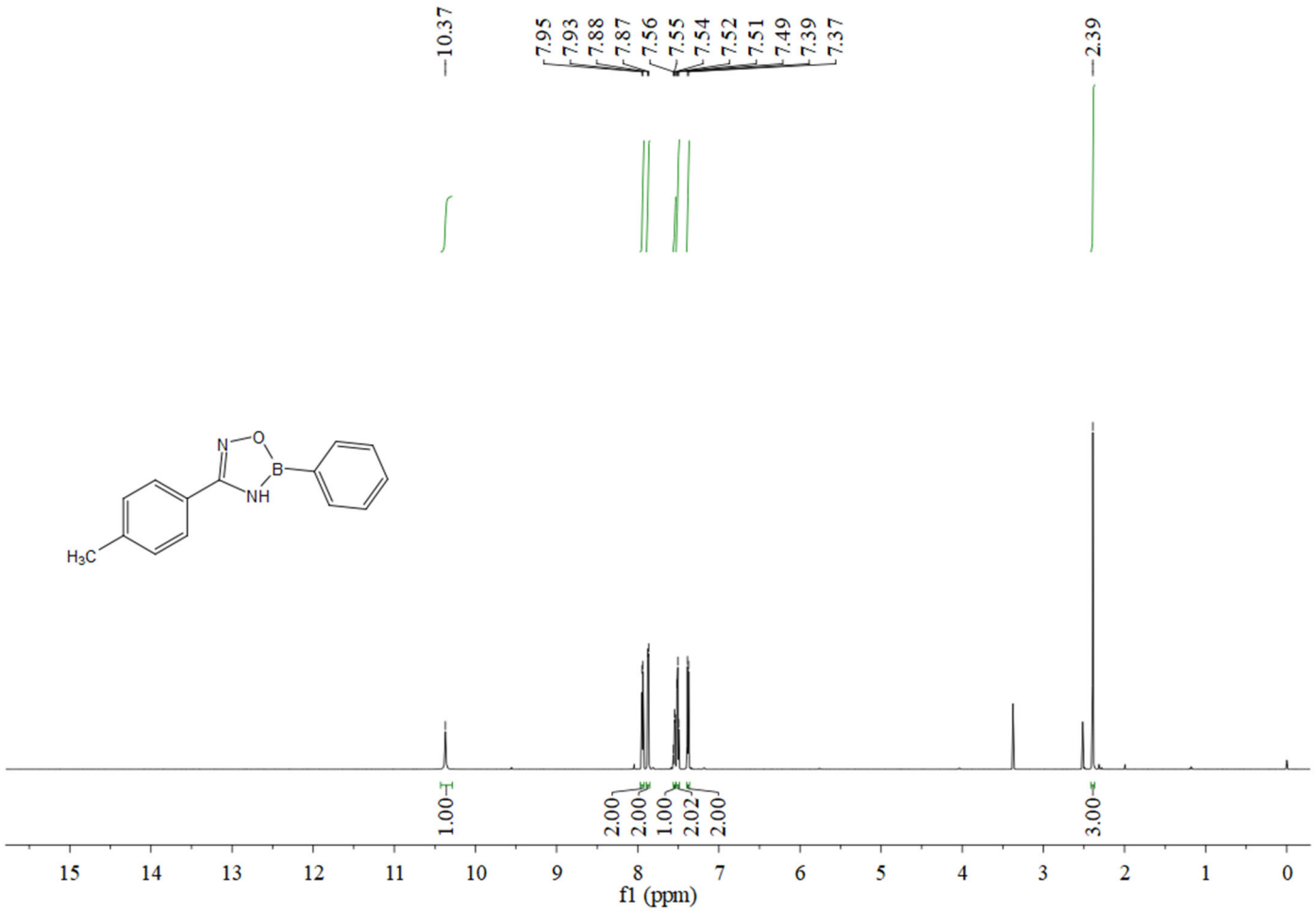


Fig. S35 ^{1}H NMR for compound **3i** (600 MHz, DMSO-d_6)

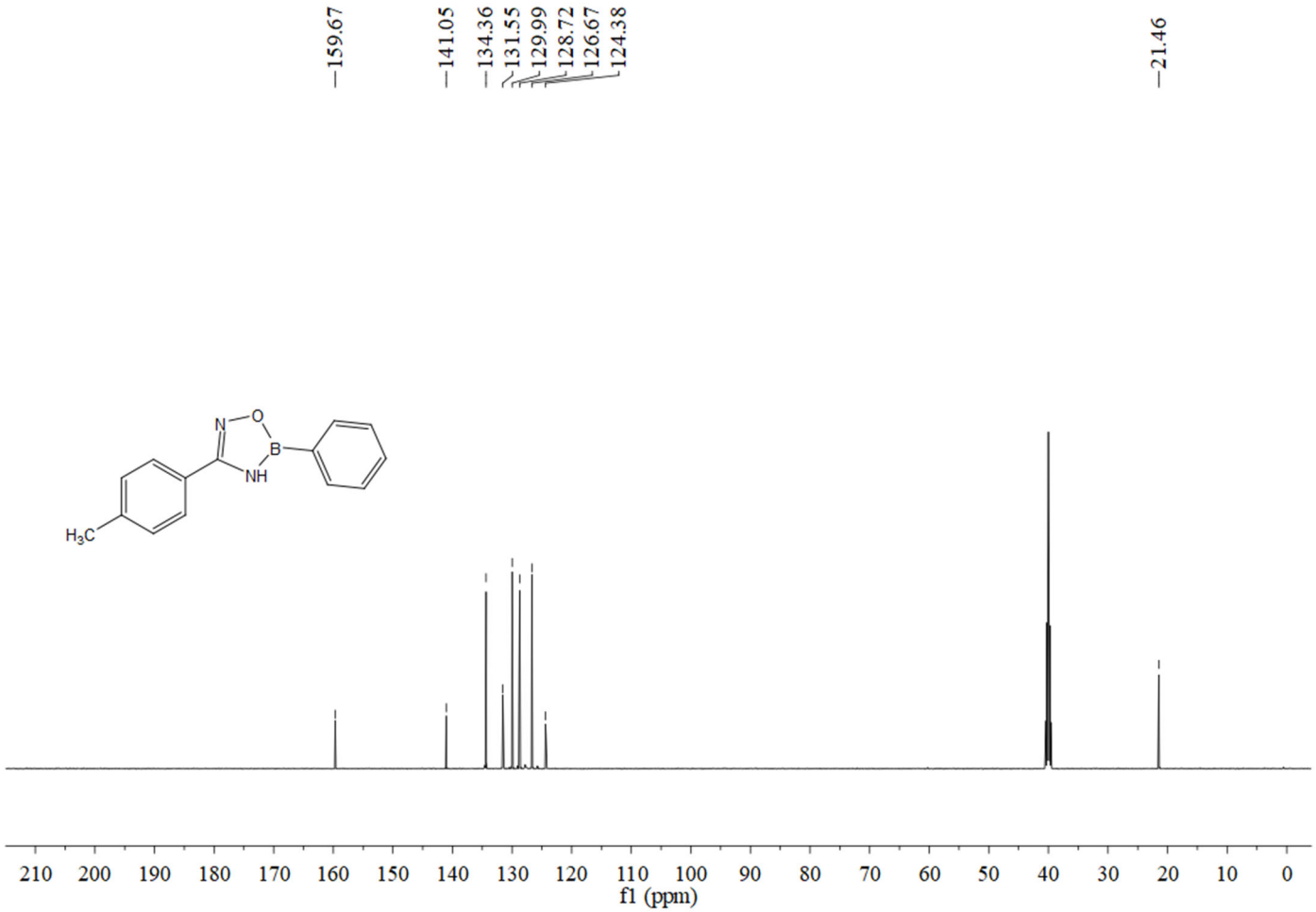


Fig. S36 ^{13}C NMR for compound **3i** (151 MHz, DMSO-d_6)

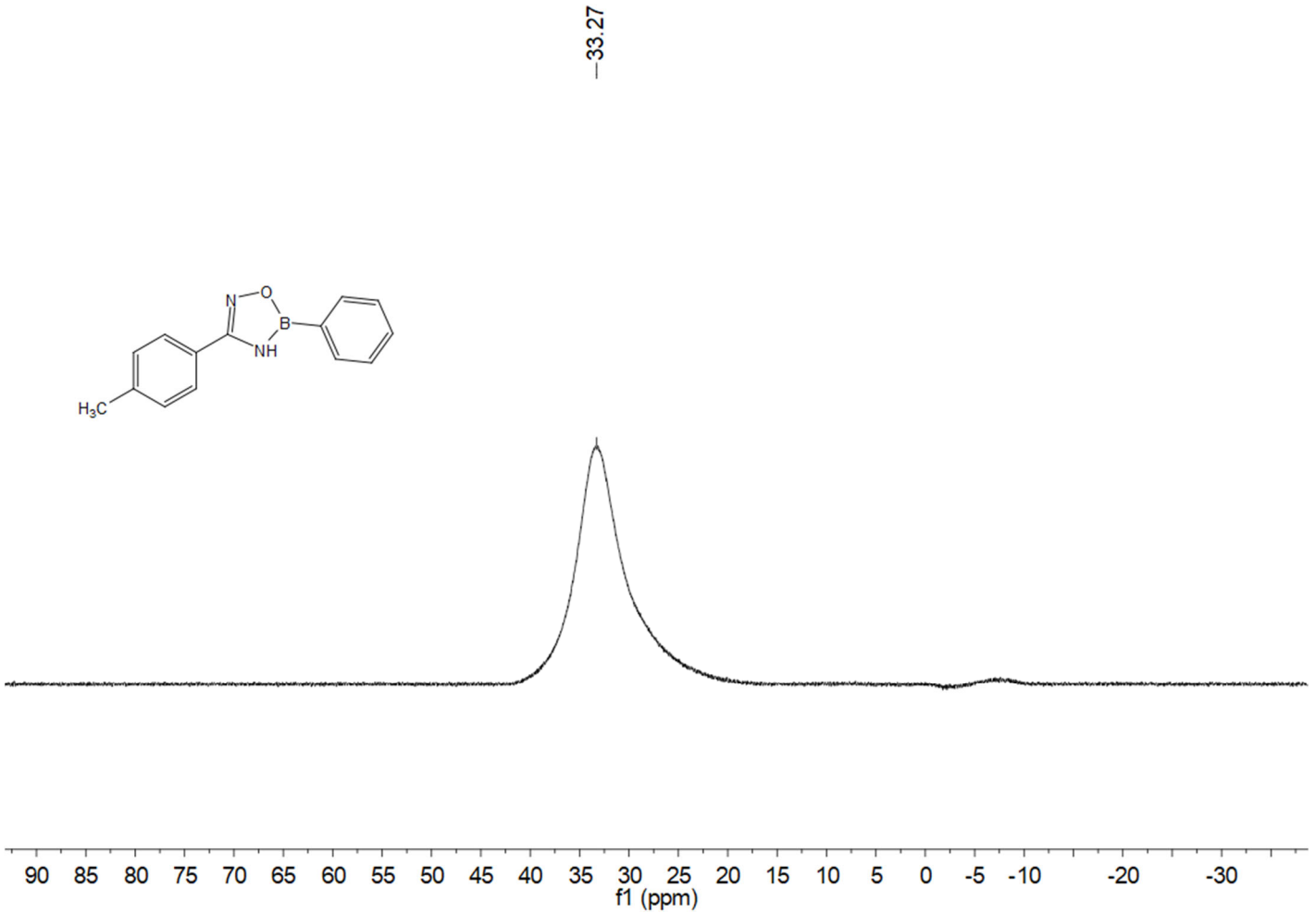


Fig. S37 ^{11}B NMR for compound **3i** (193 MHz, DMSO-d_6)

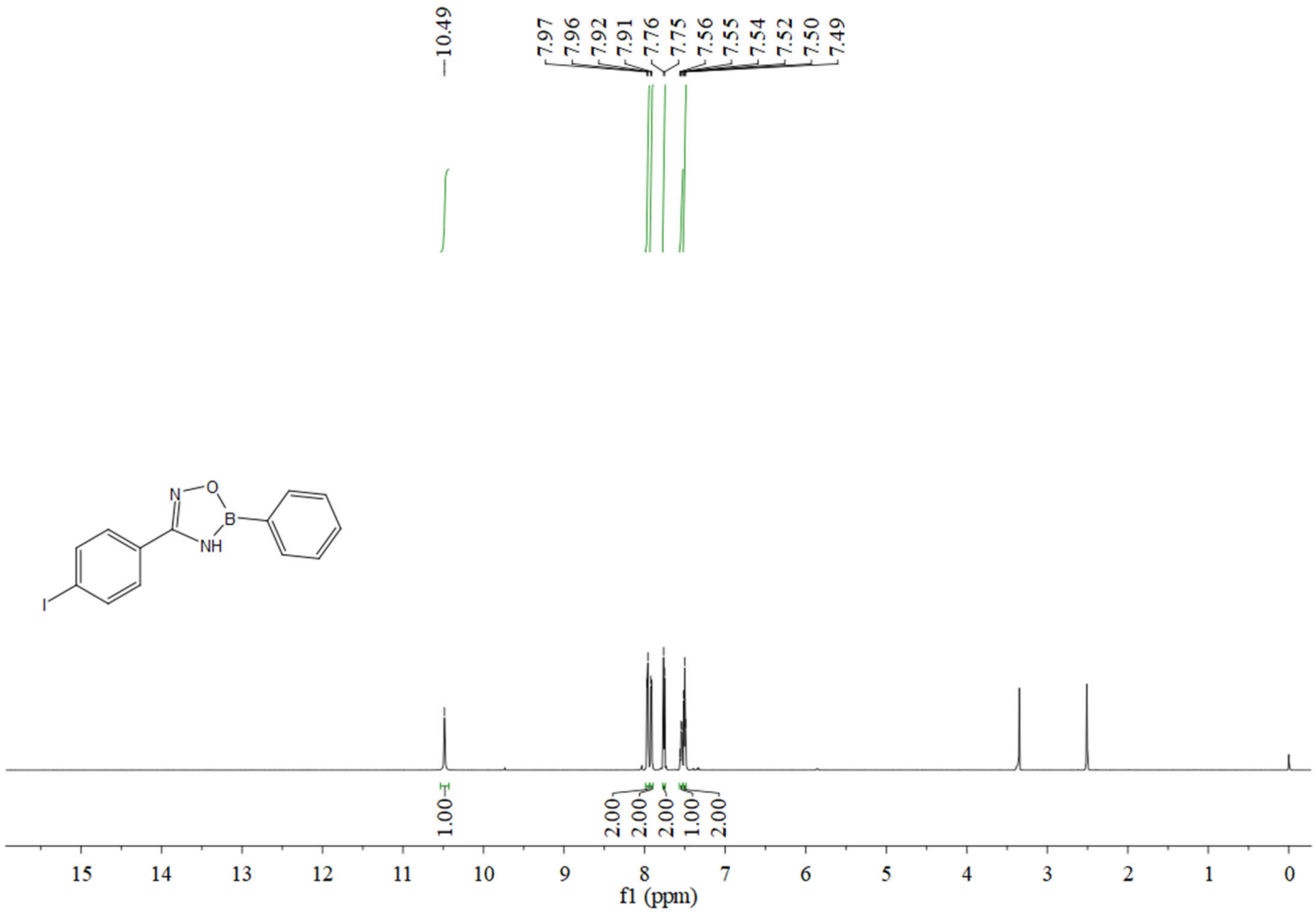


Fig. S38 ^{1}H NMR for compound **3j** (600 MHz, DMSO-d_6)

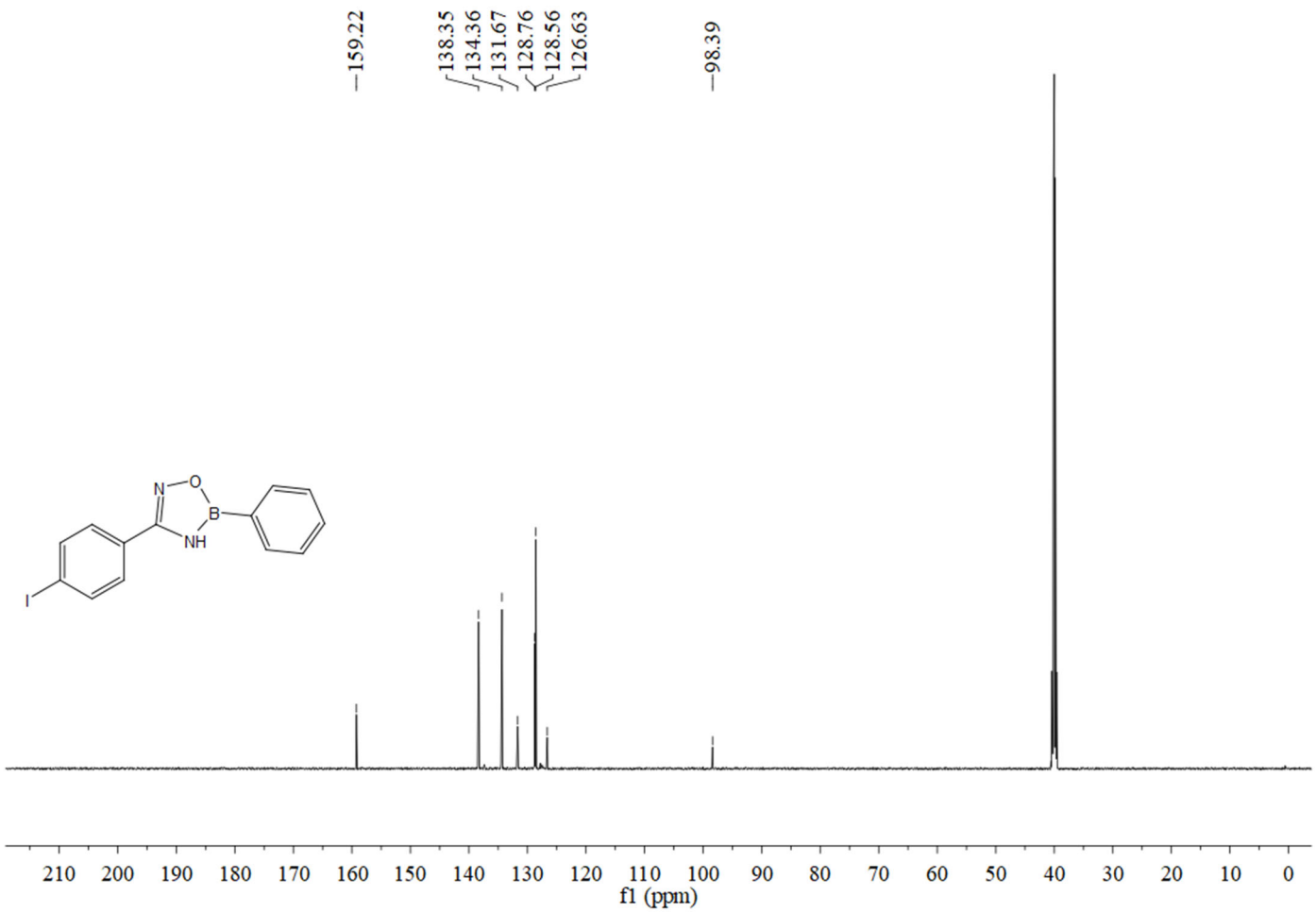


Fig. S39 ^{13}C NMR for compound **3j** (151 MHz, DMSO-d_6)

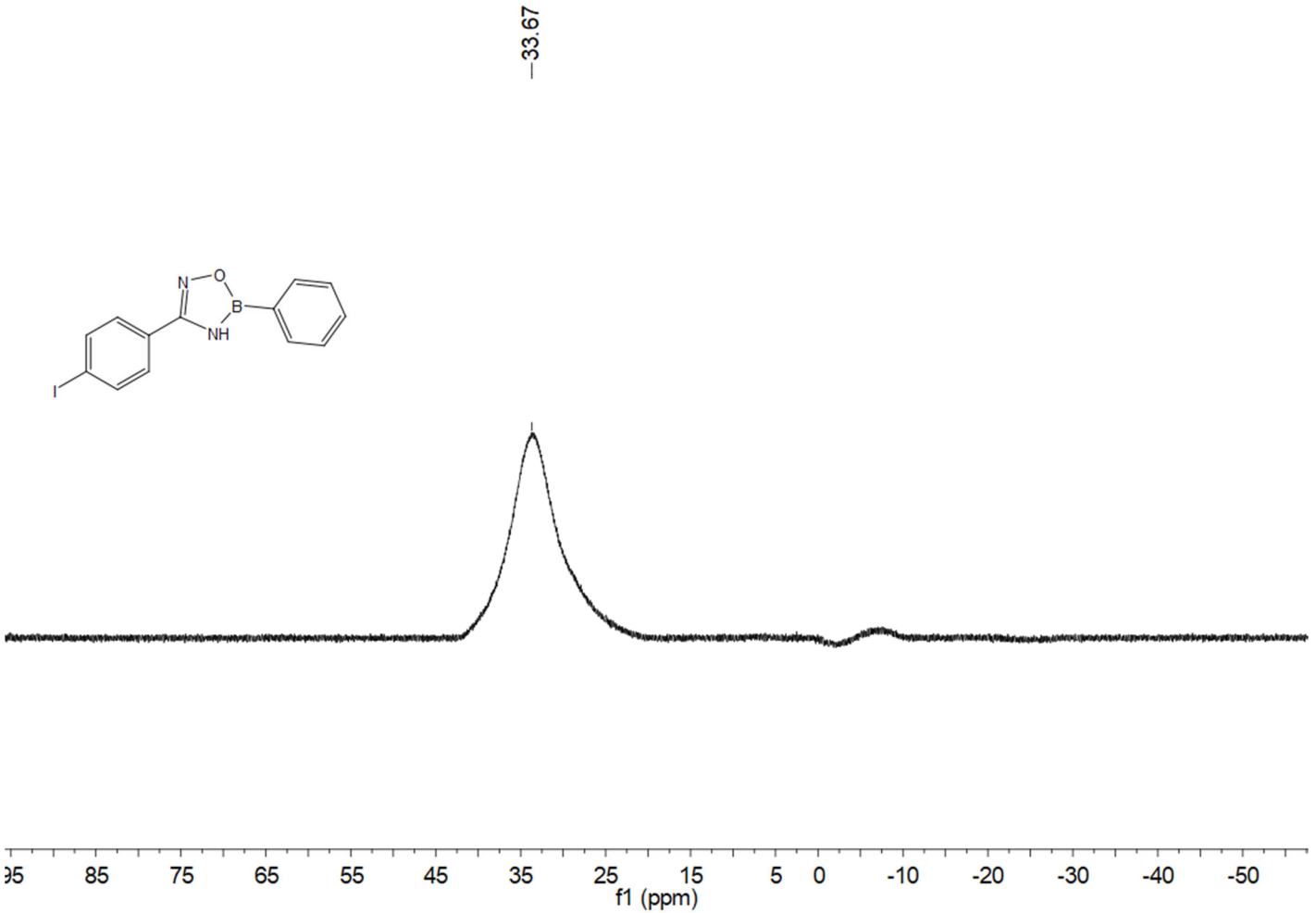


Fig. S40 ^{11}B NMR for compound **3j** (193 MHz, DMSO-d_6)

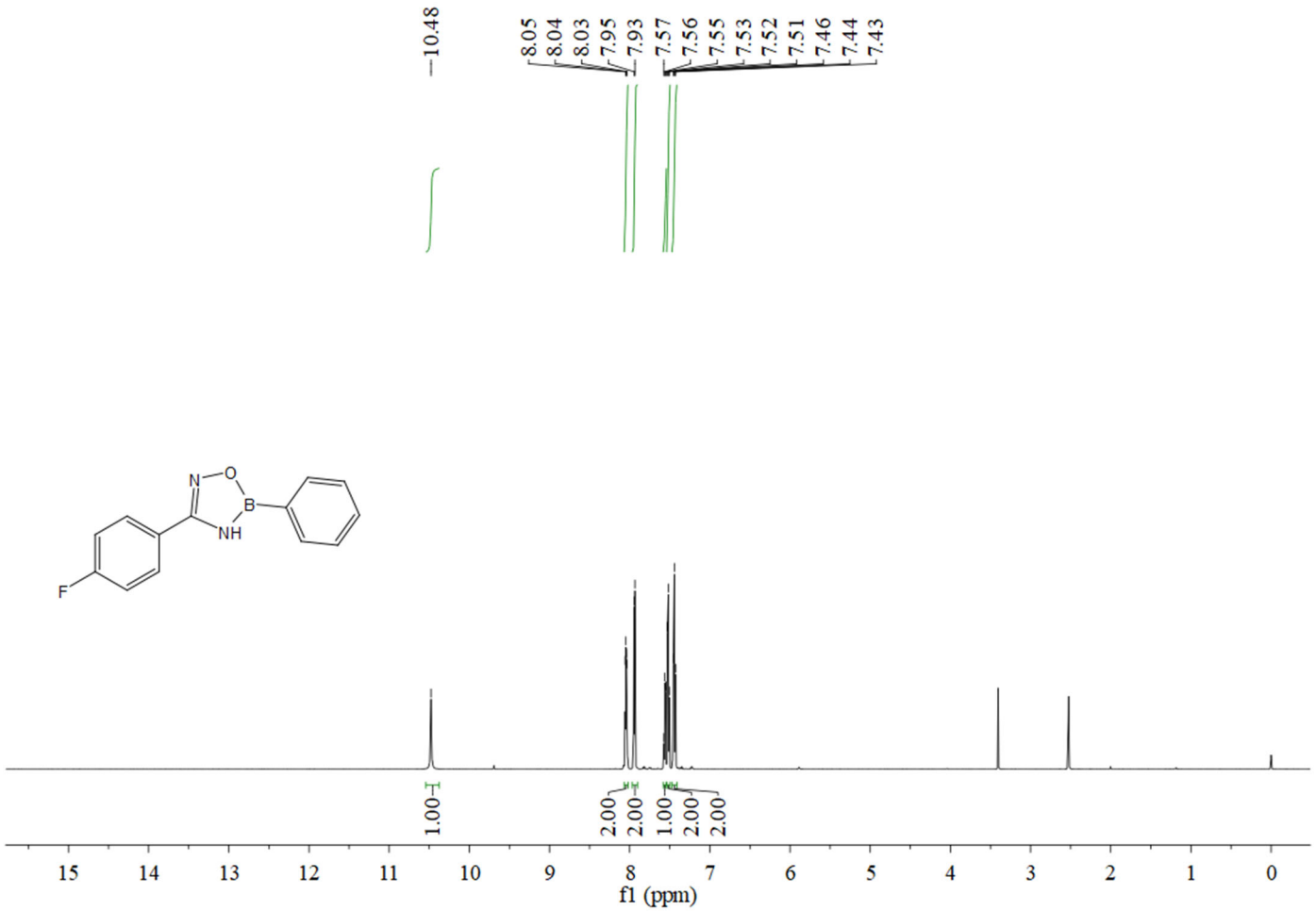


Fig. S41 ^{1}H NMR for compound **3k** (600 MHz, DMSO-d_6)

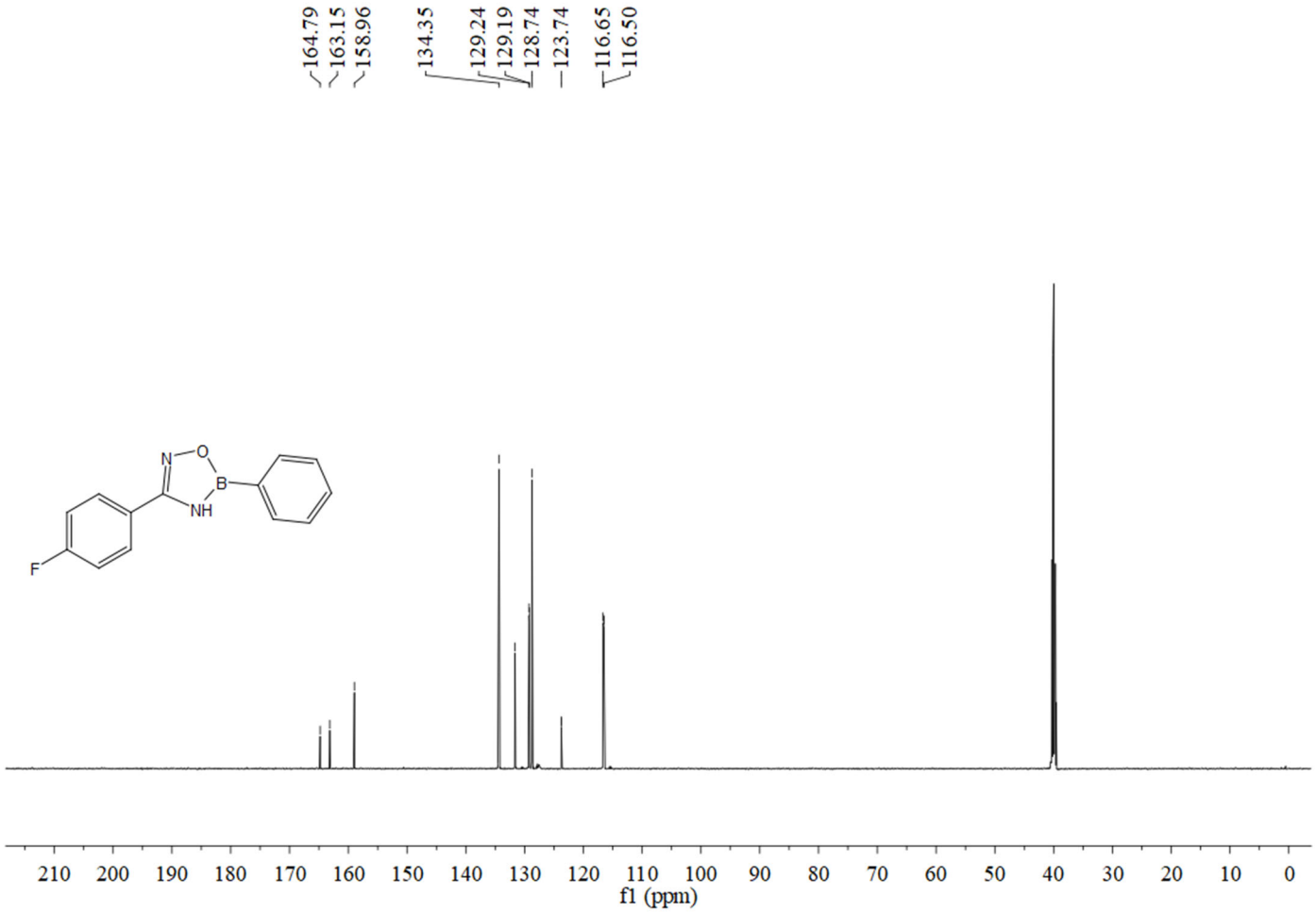


Fig. S42 ^{13}C NMR for compound **3k** (151 MHz, DMSO-d_6)

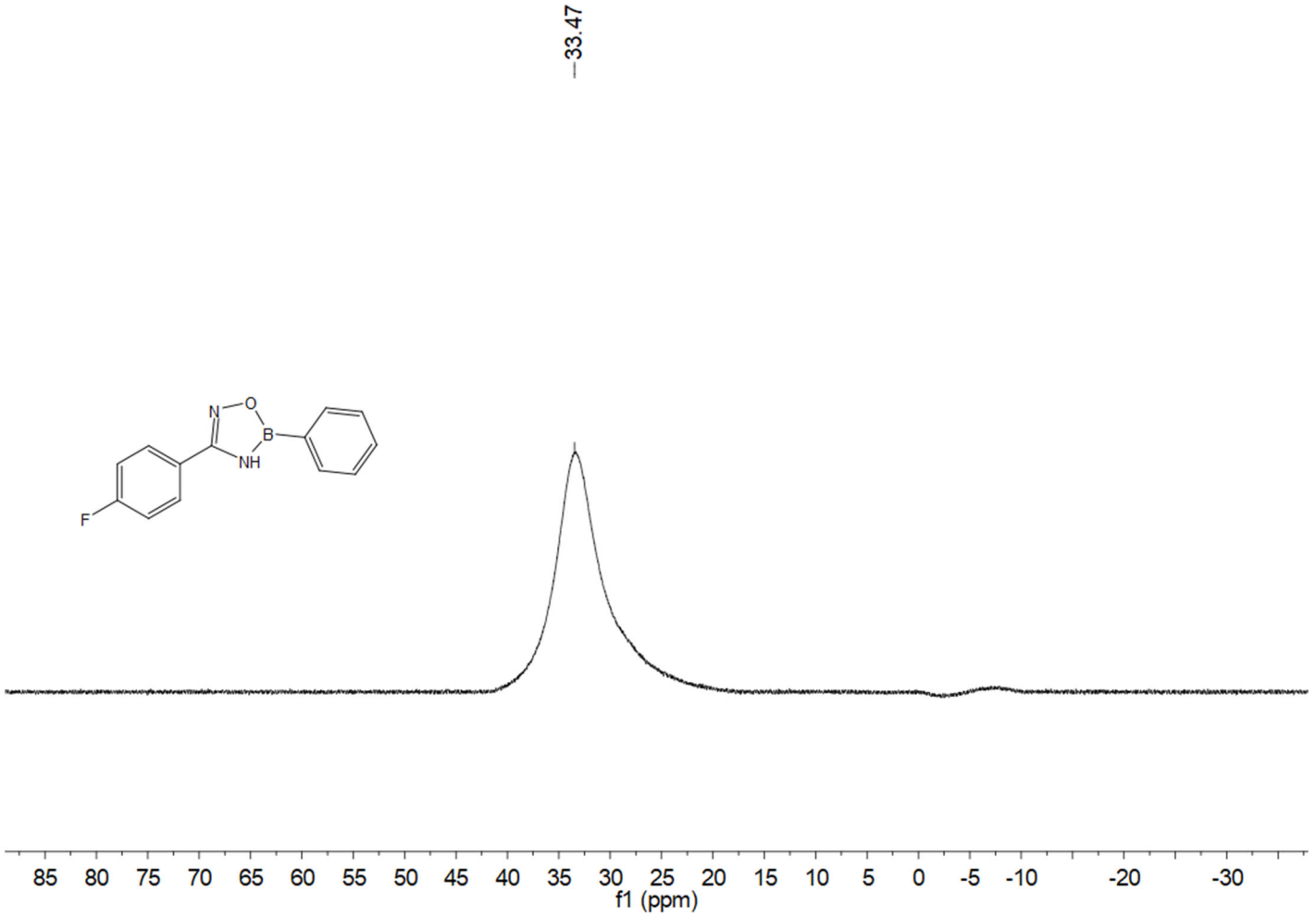


Fig. S43 ^{11}B NMR for compound **3k** (193 MHz, DMSO-d_6)

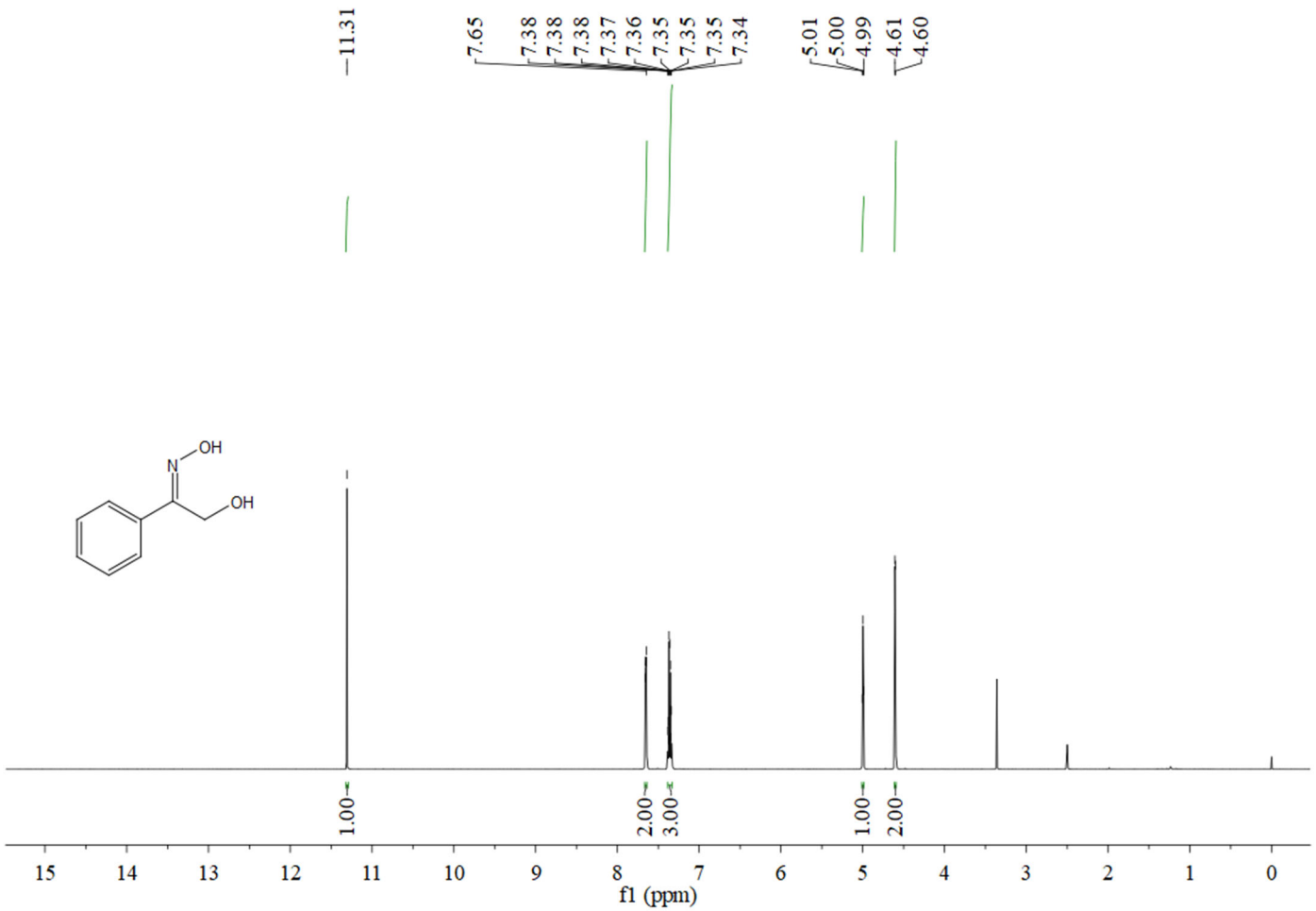


Fig. S44 ^{1}H NMR for compound **4a** (600 MHz, DMSO-d_6)

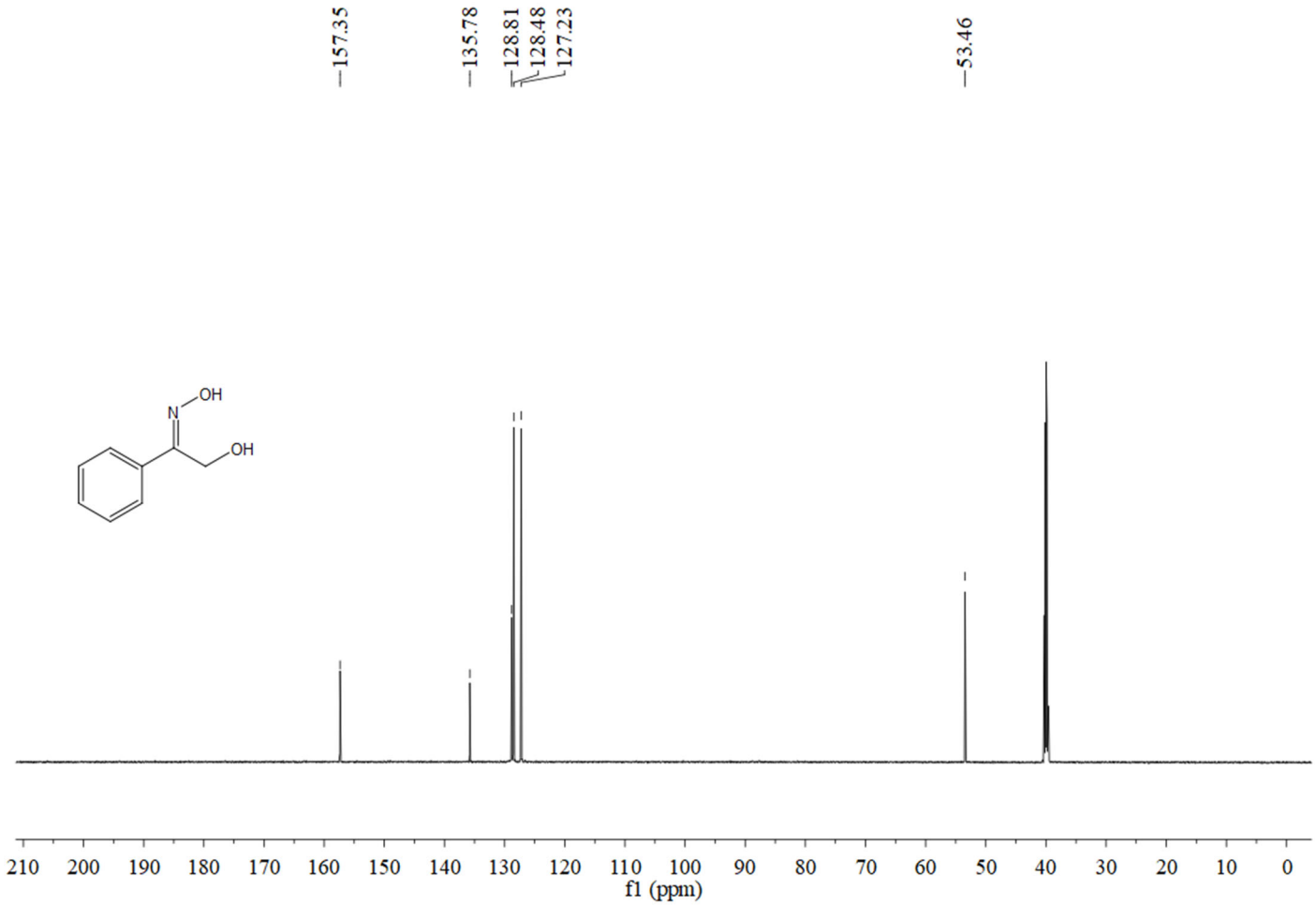


Fig. S45 ^{13}C NMR for compound **4a** (151 MHz, DMSO-d_6)

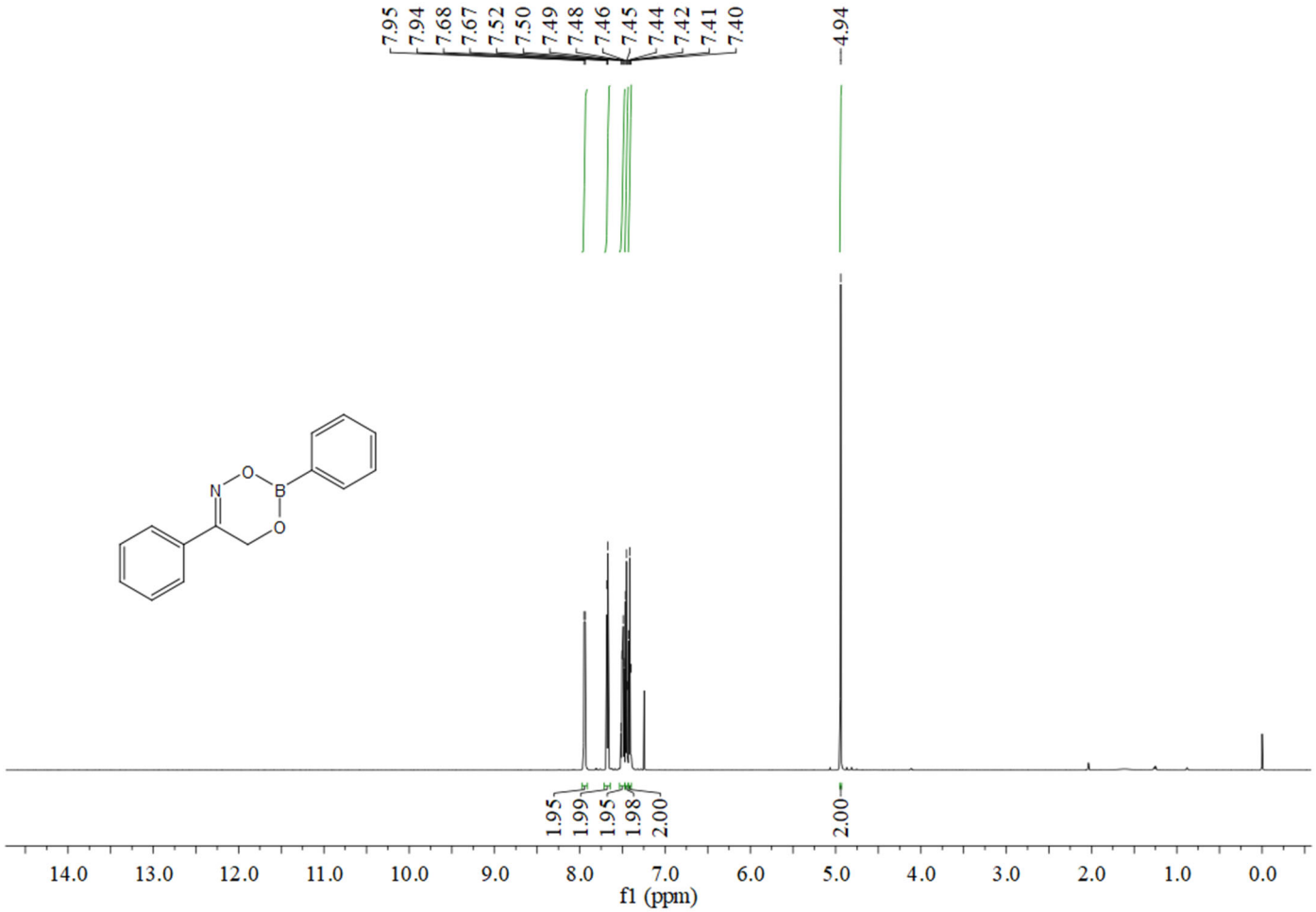


Fig. S46 ^{1}H NMR for compound **5a** (600 MHz, $CDCl_3$)

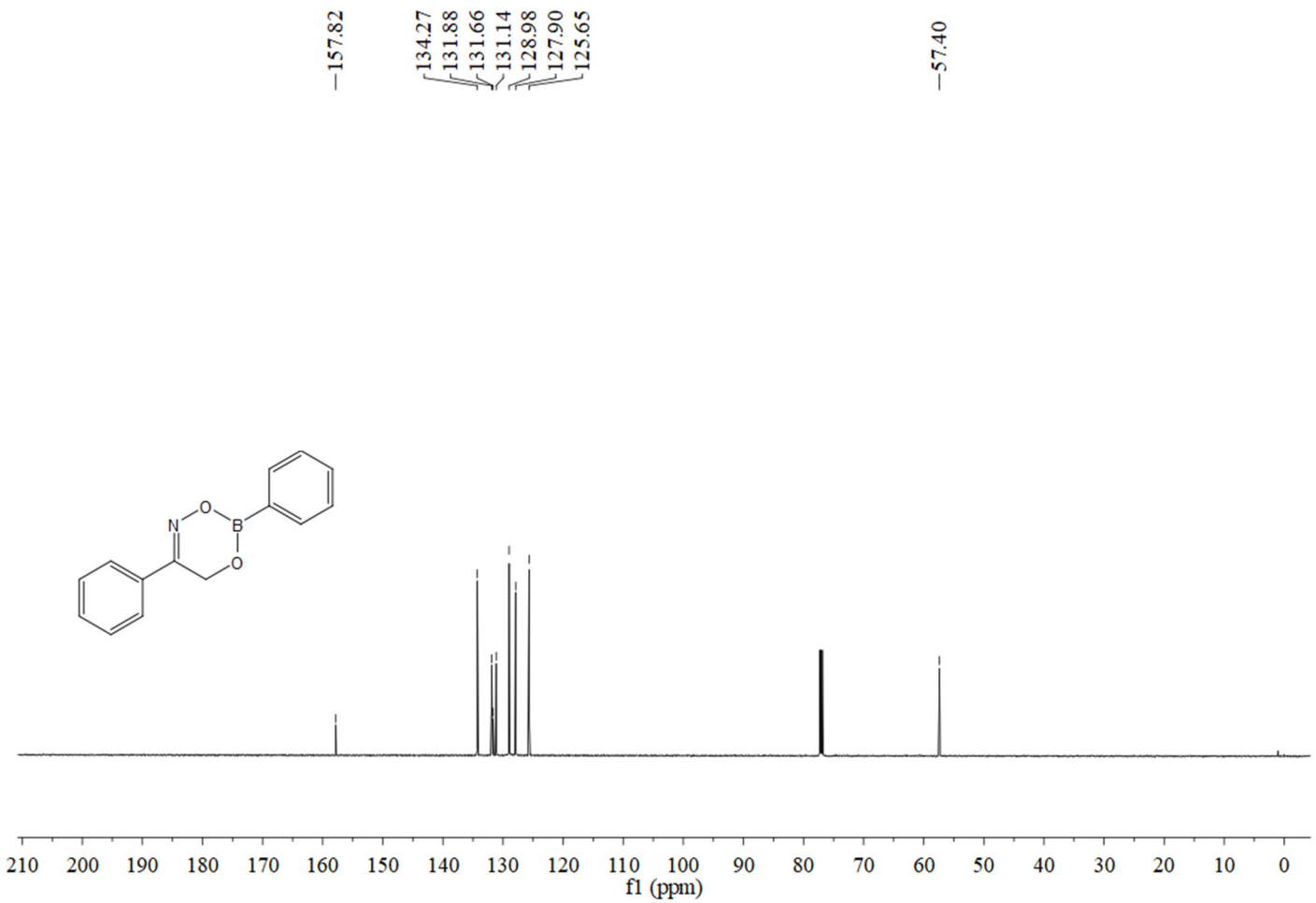


Fig. S47 ^{13}C NMR for compound **5a** (151 MHz, $CDCl_3$)

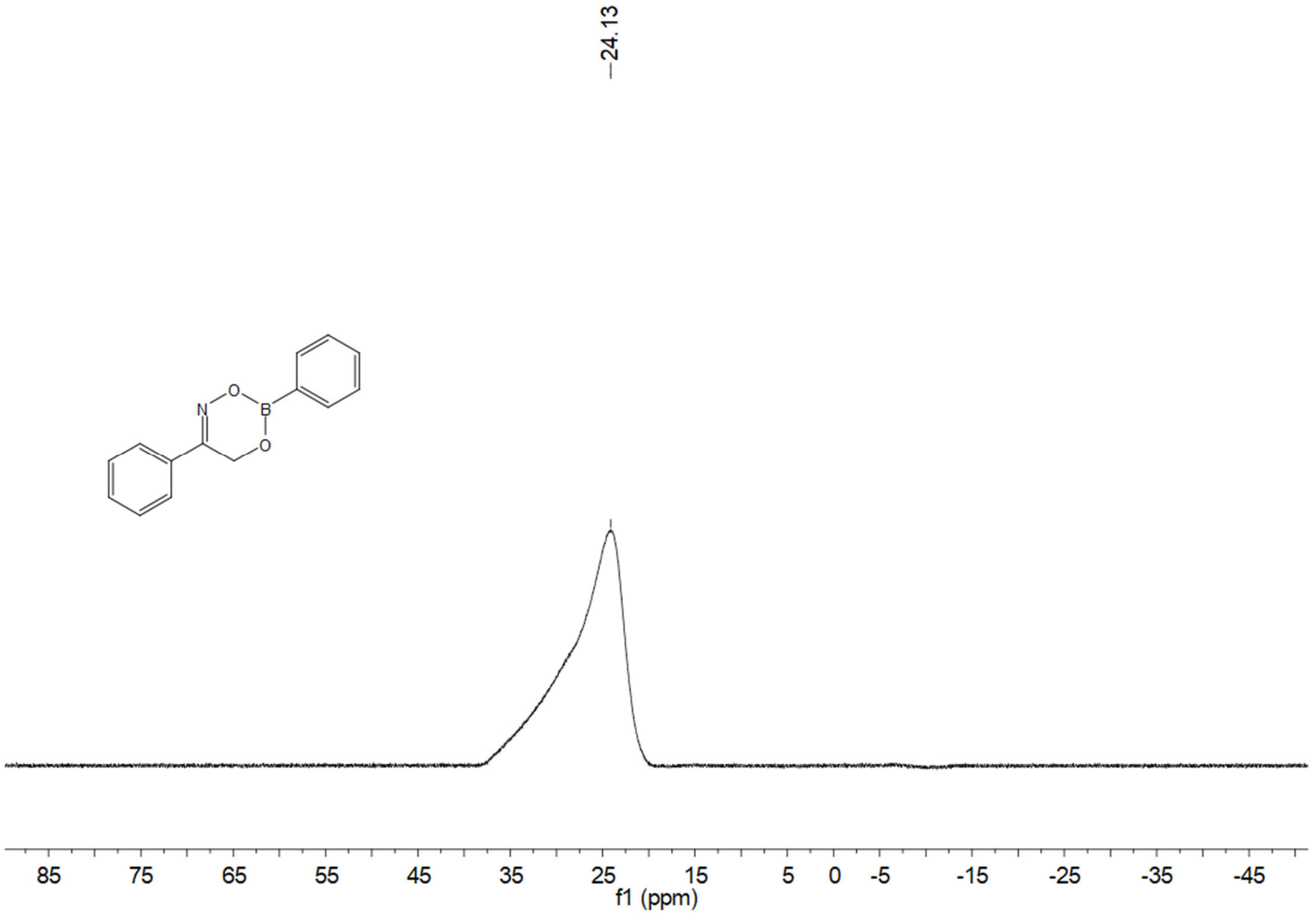


Fig. S48 ^{11}B NMR for compound **5a** (193 MHz, DMSO-d_6)

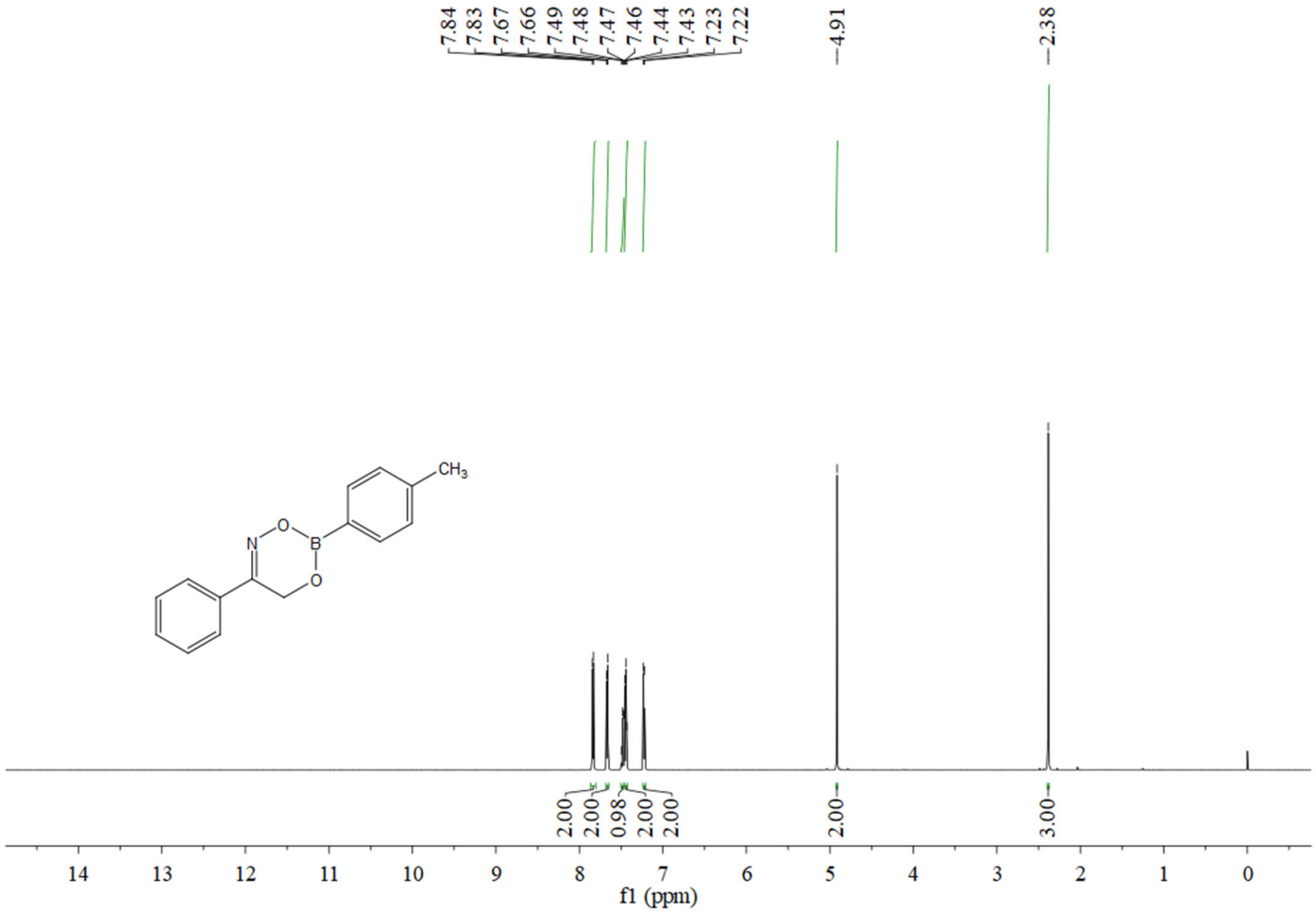


Fig. S49 ^{1}H NMR for compound **5b** (600 MHz, $CDCl_3$)

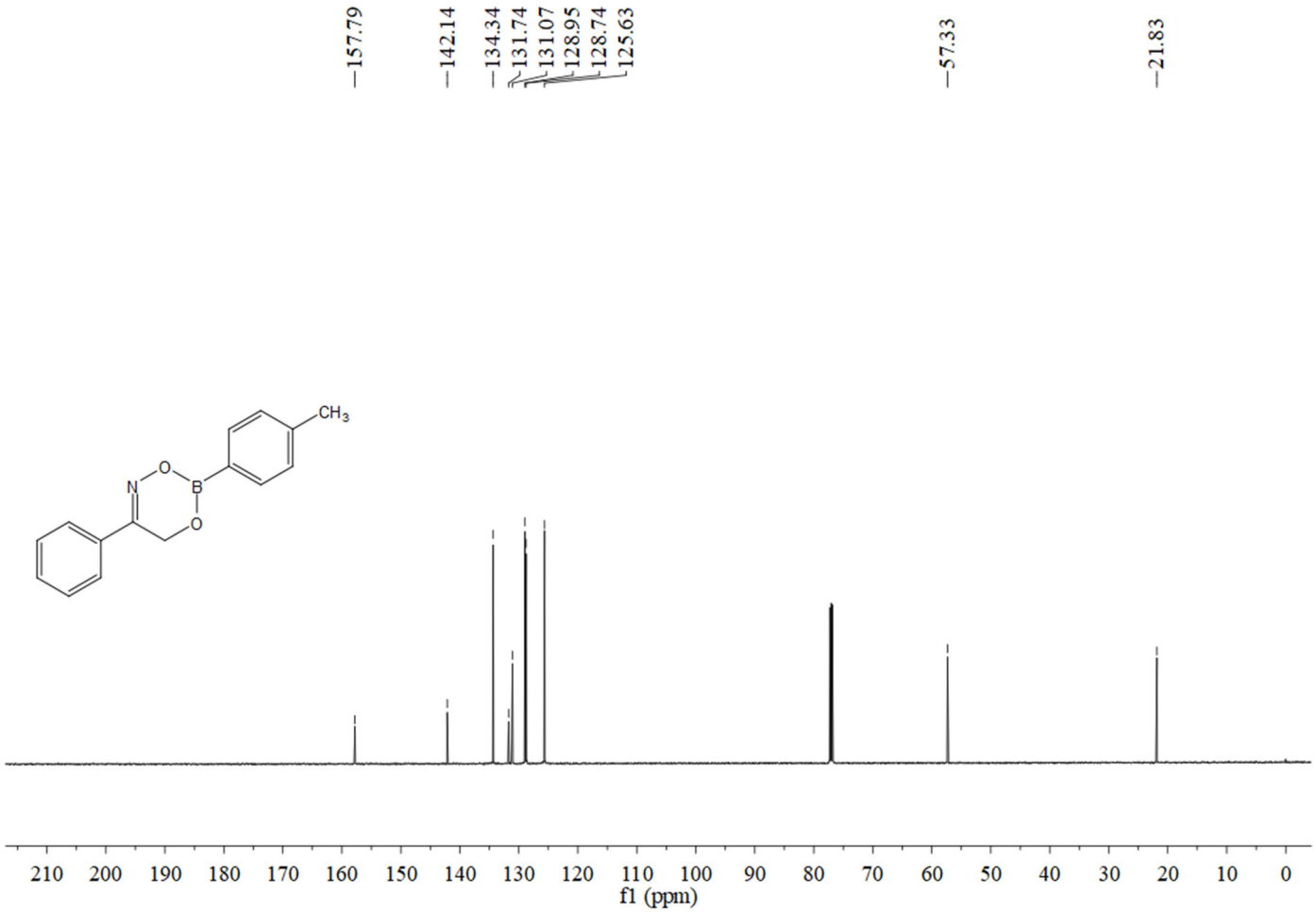


Fig. S50 ^{13}C NMR for compound **5b** (151 MHz, $CDCl_3$)

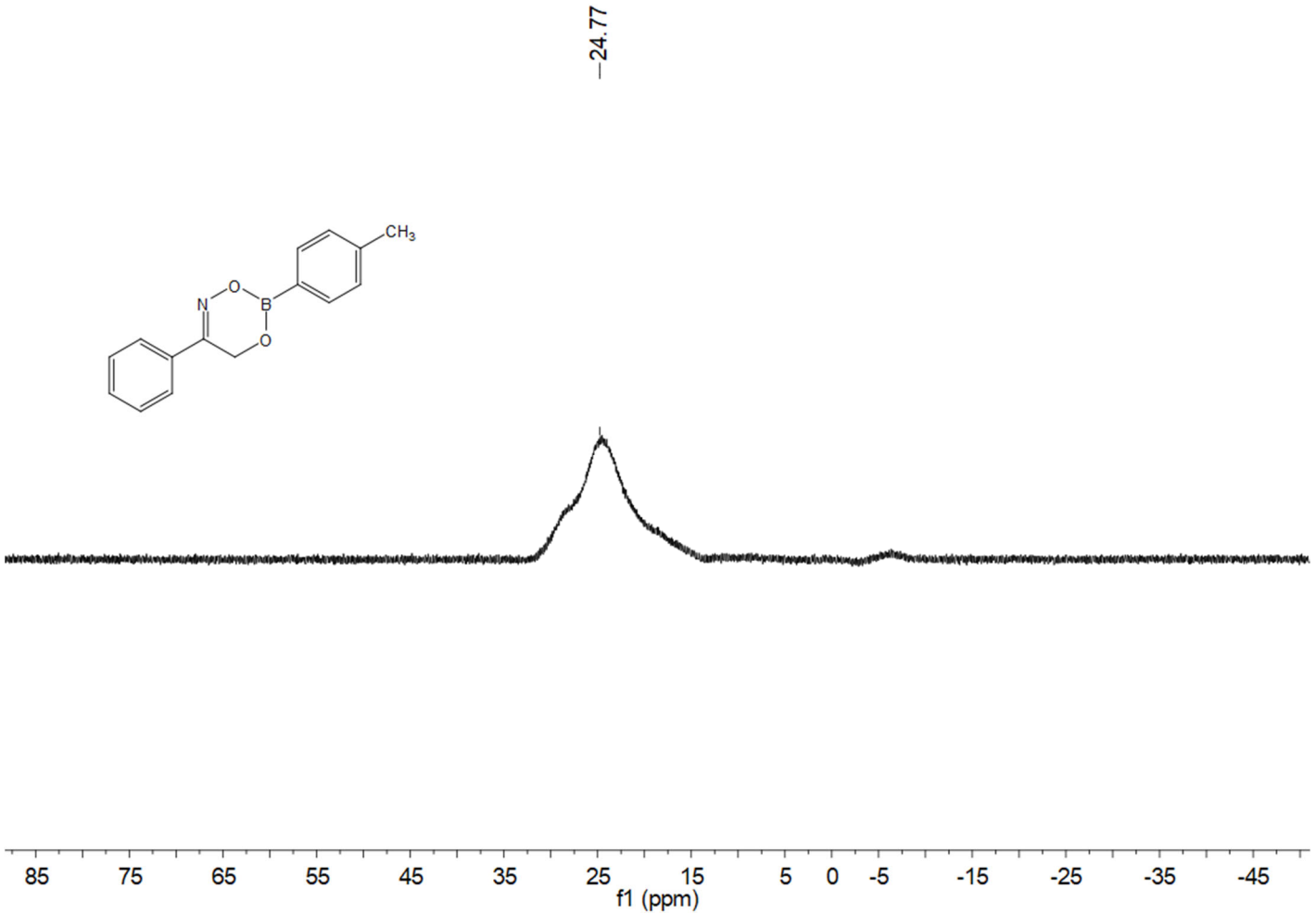


Fig. S51 ^{11}B NMR for compound **5b** (193 MHz, DMSO-d_6)

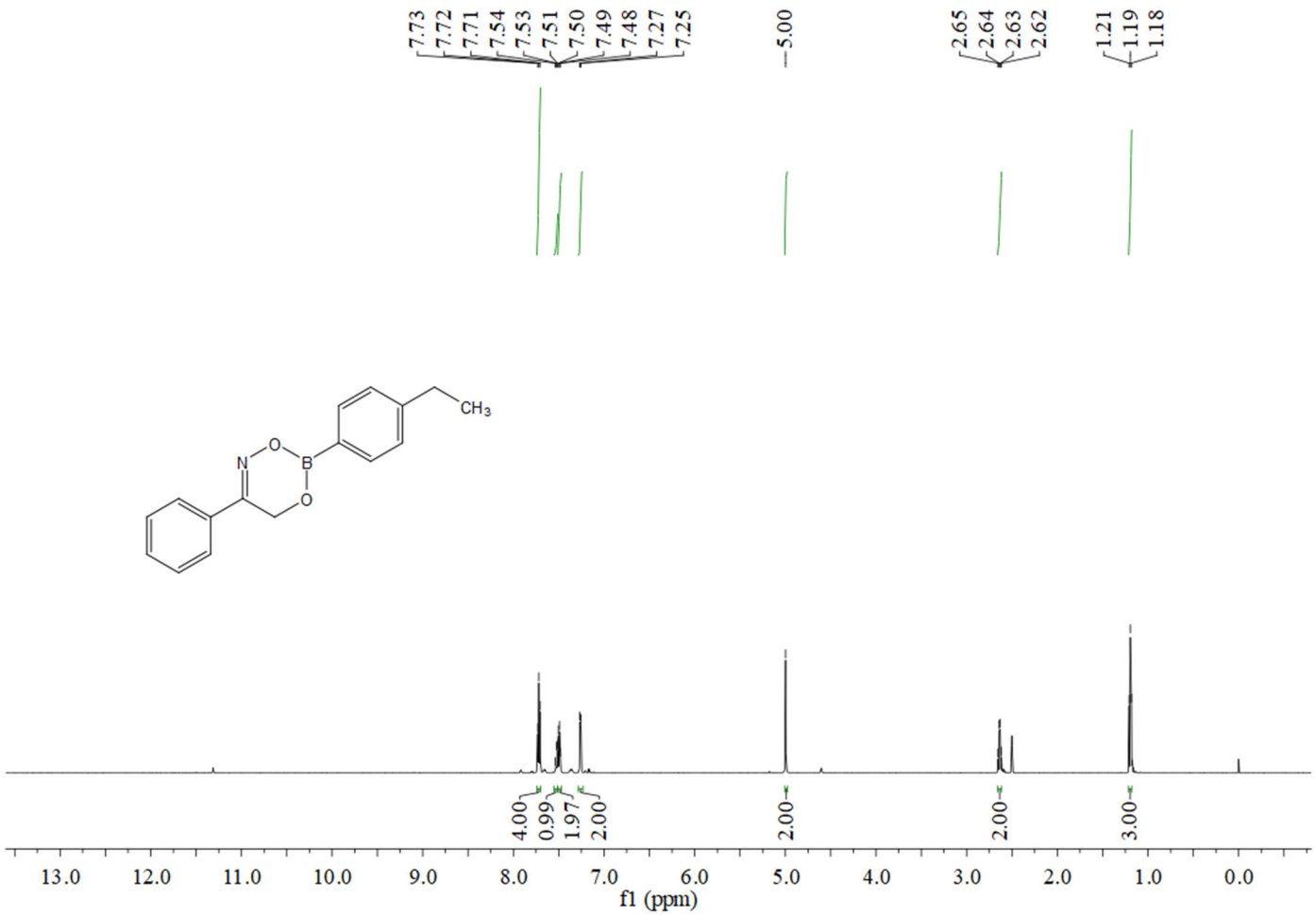


Fig. S52 ^{1}H NMR for compound **5c** (600 MHz, DMSO-d_6)

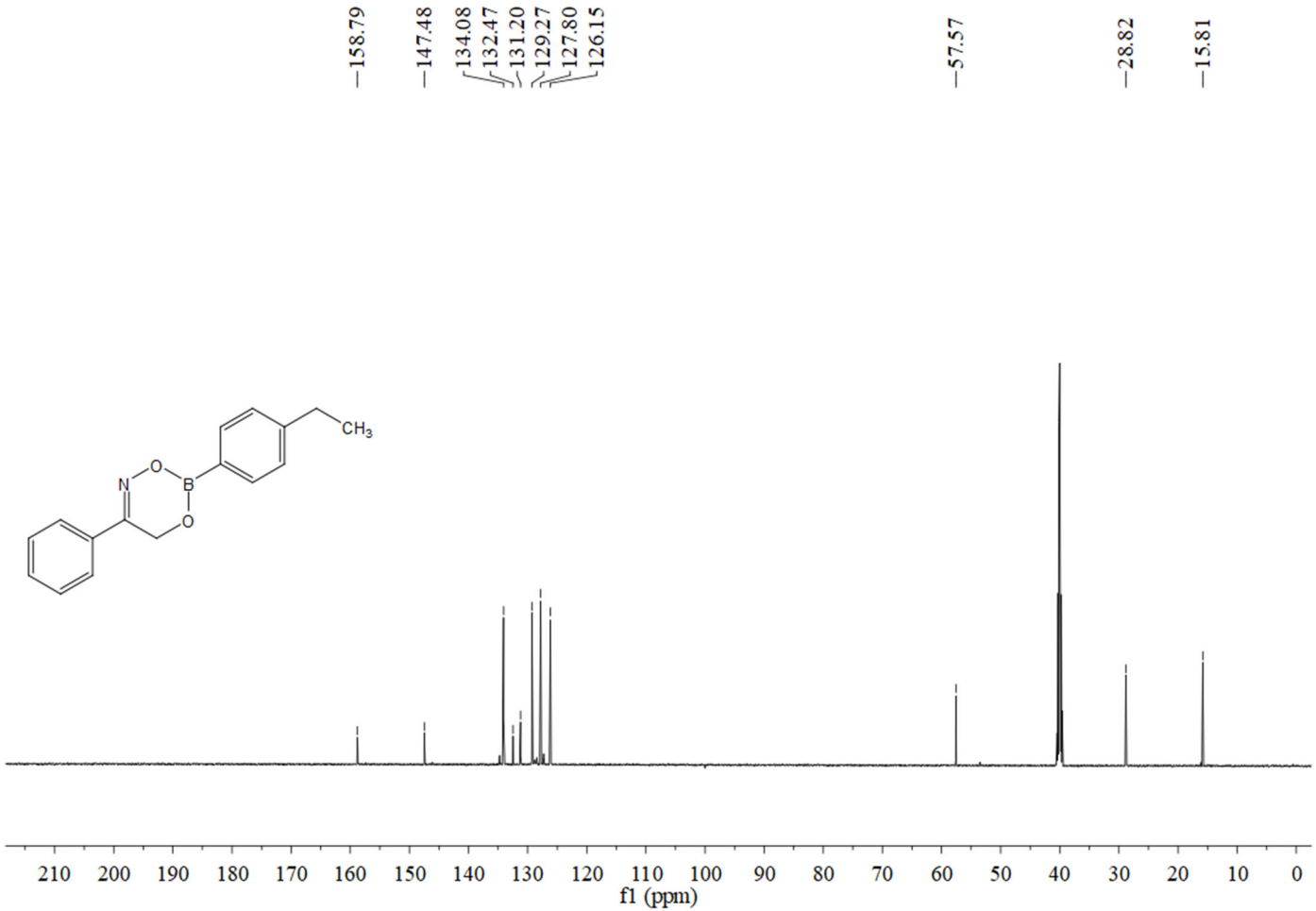


Fig. S53 ^{13}C NMR for compound **5c** (151 MHz, DMSO-d_6)

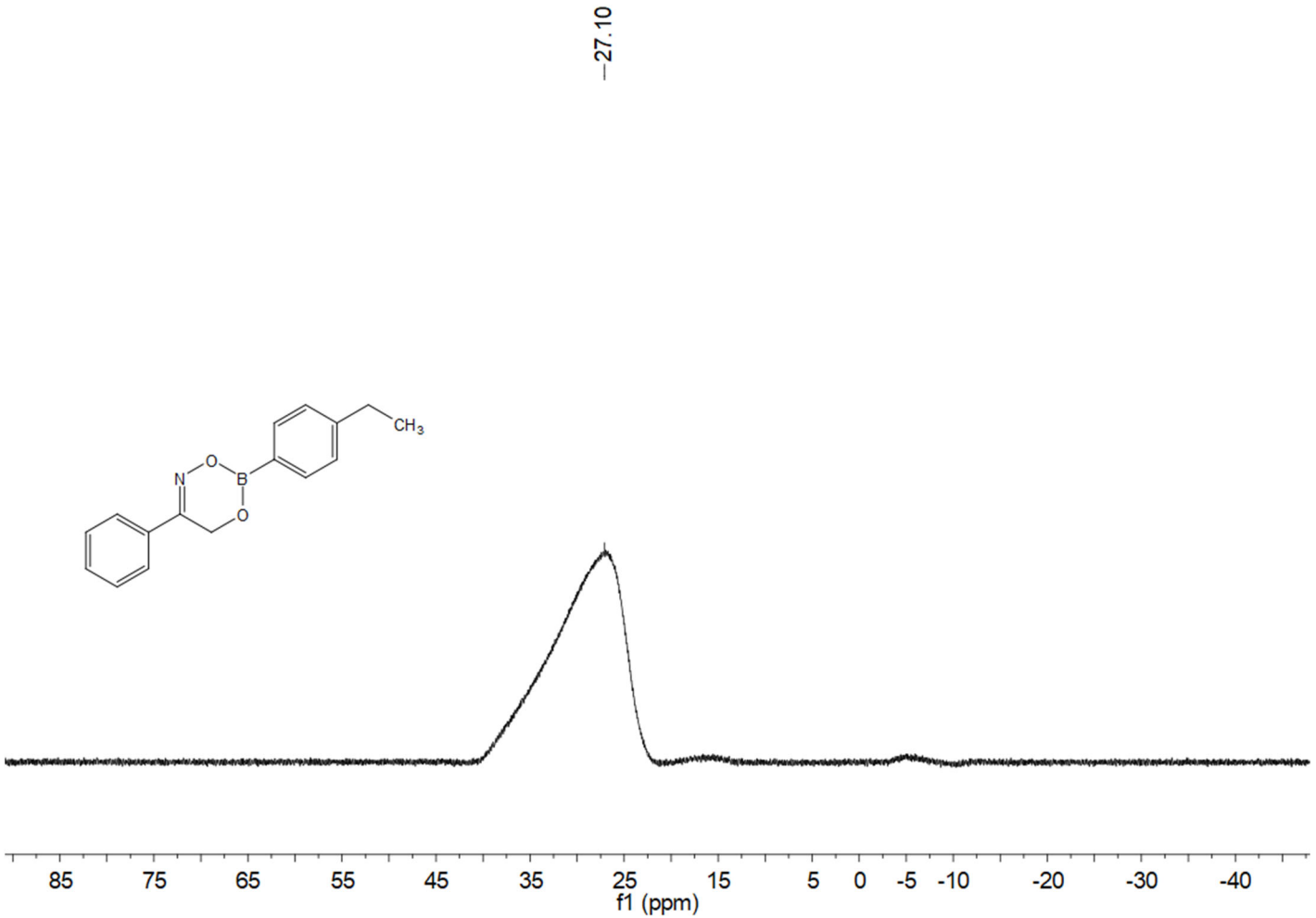


Fig. S54 ^{11}B NMR for compound **5c** (193 MHz, DMSO-d_6)

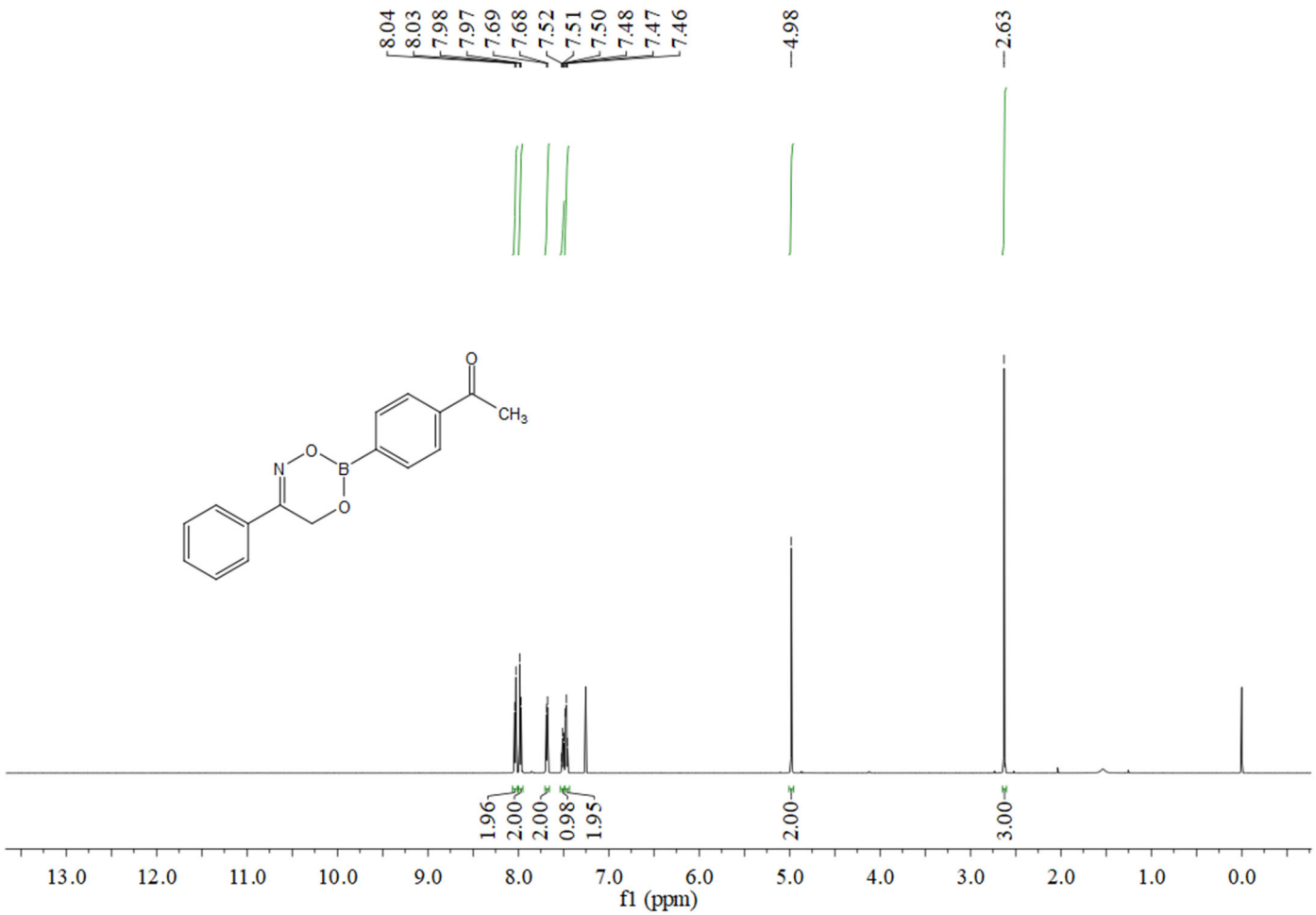


Fig. S55 ^{1}H NMR for compound **5d** (600 MHz, $CDCl_3$)

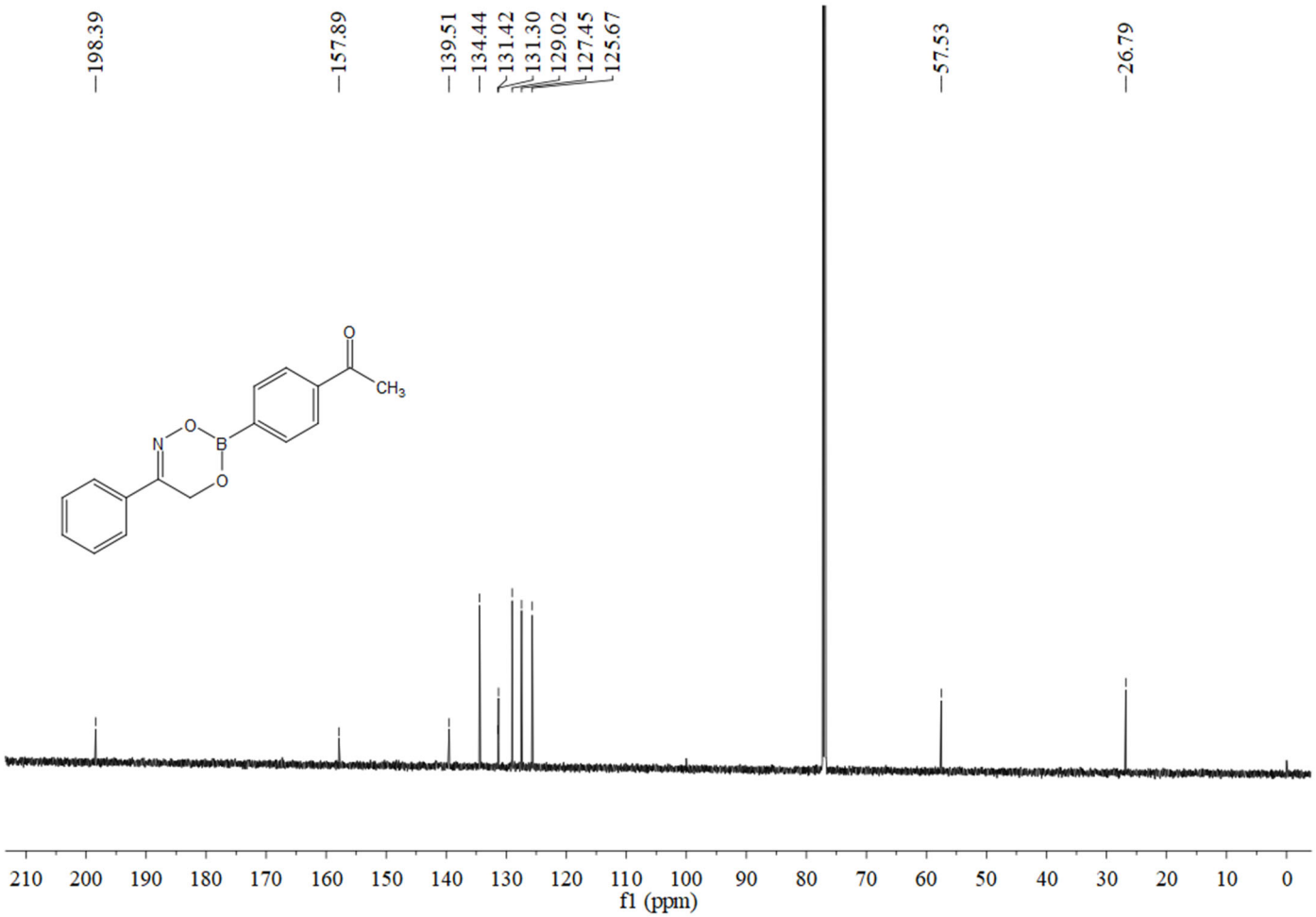


Fig. S56 ^{13}C NMR for compound **5d** (151 MHz, $CDCl_3$)

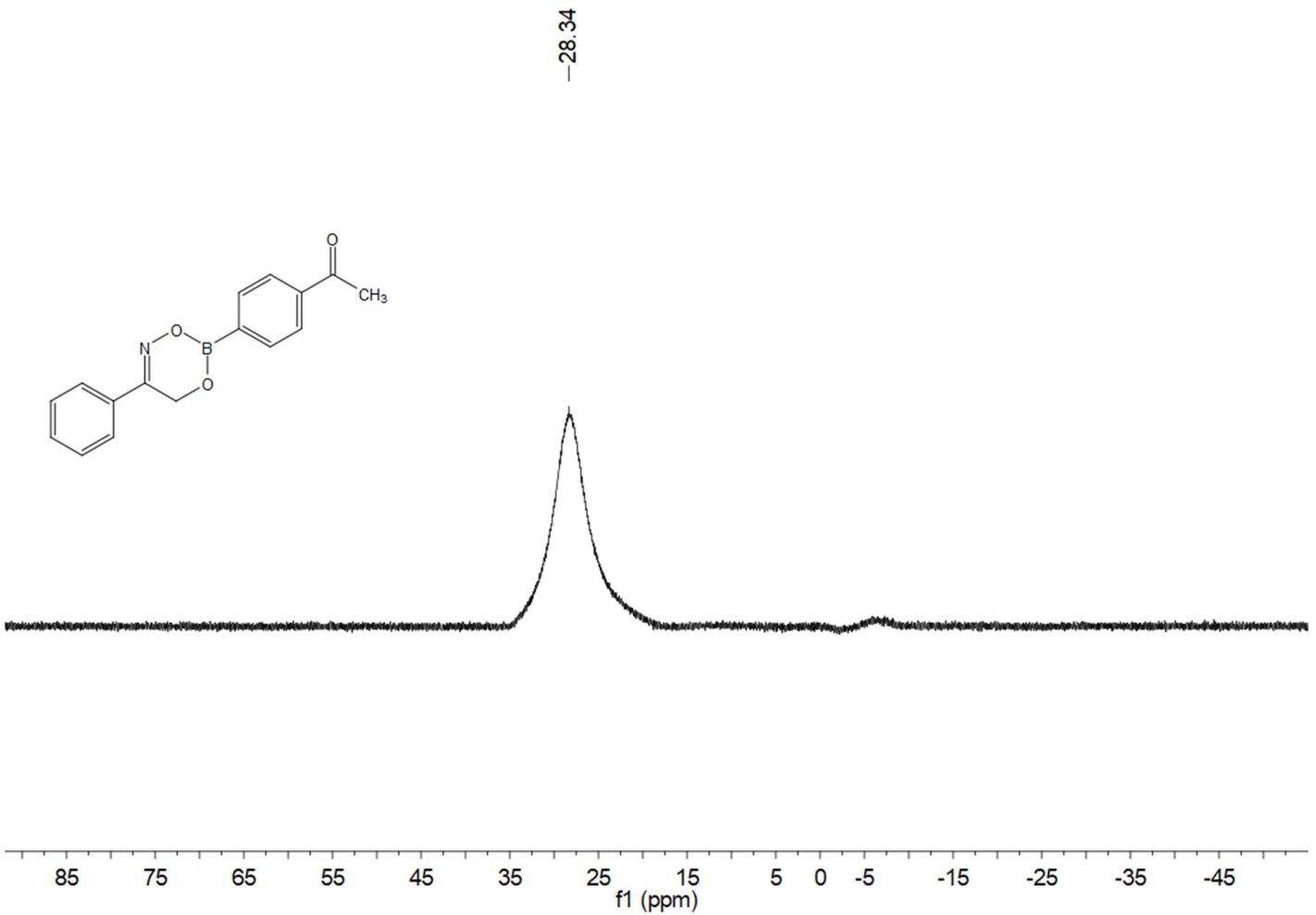


Fig. S57 ^{11}B NMR for compound **5d** (193 MHz, DMSO-d_6)

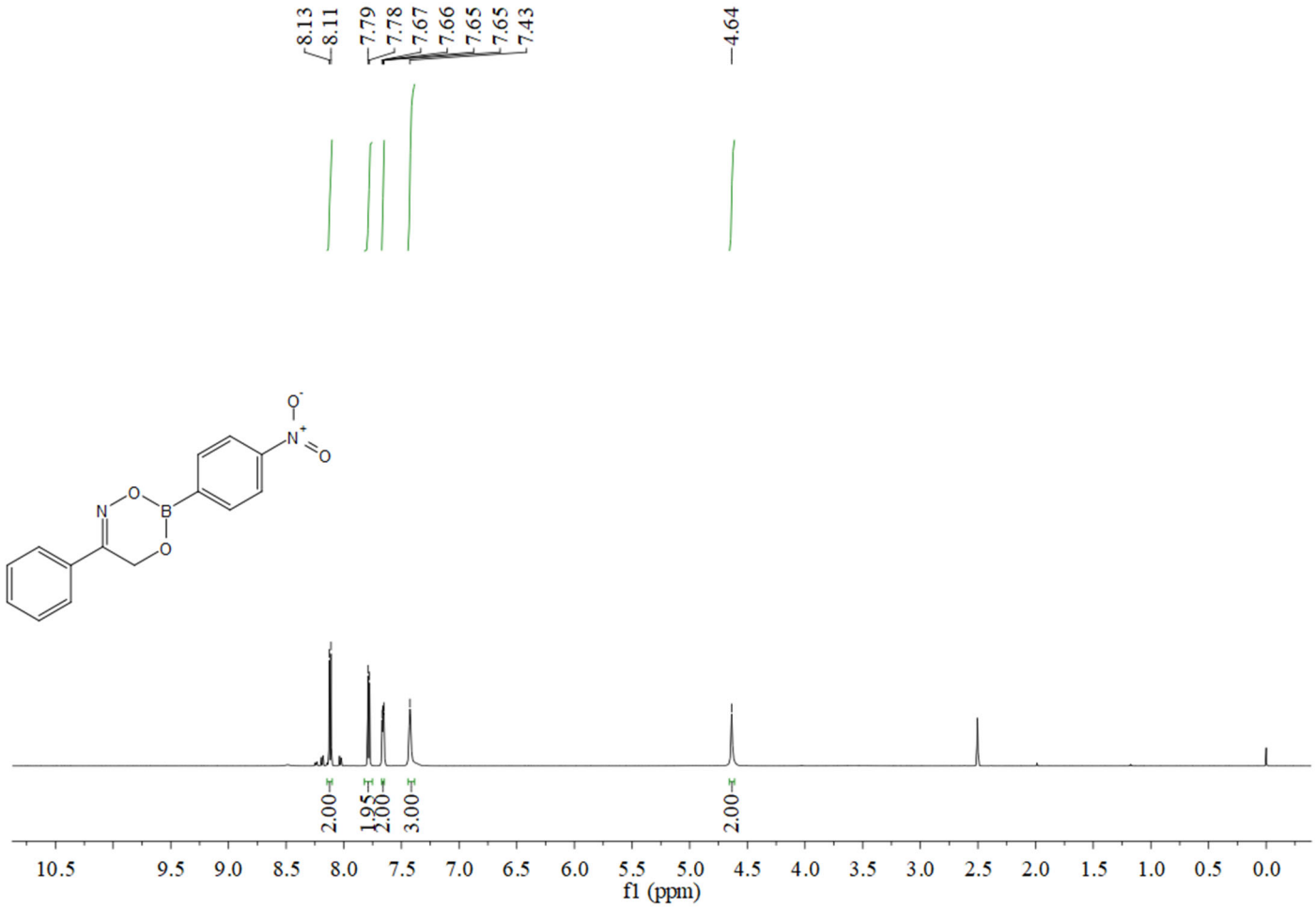


Fig. S58 ^{1}H NMR for compound **5e** (600 MHz, DMSO-d_6)

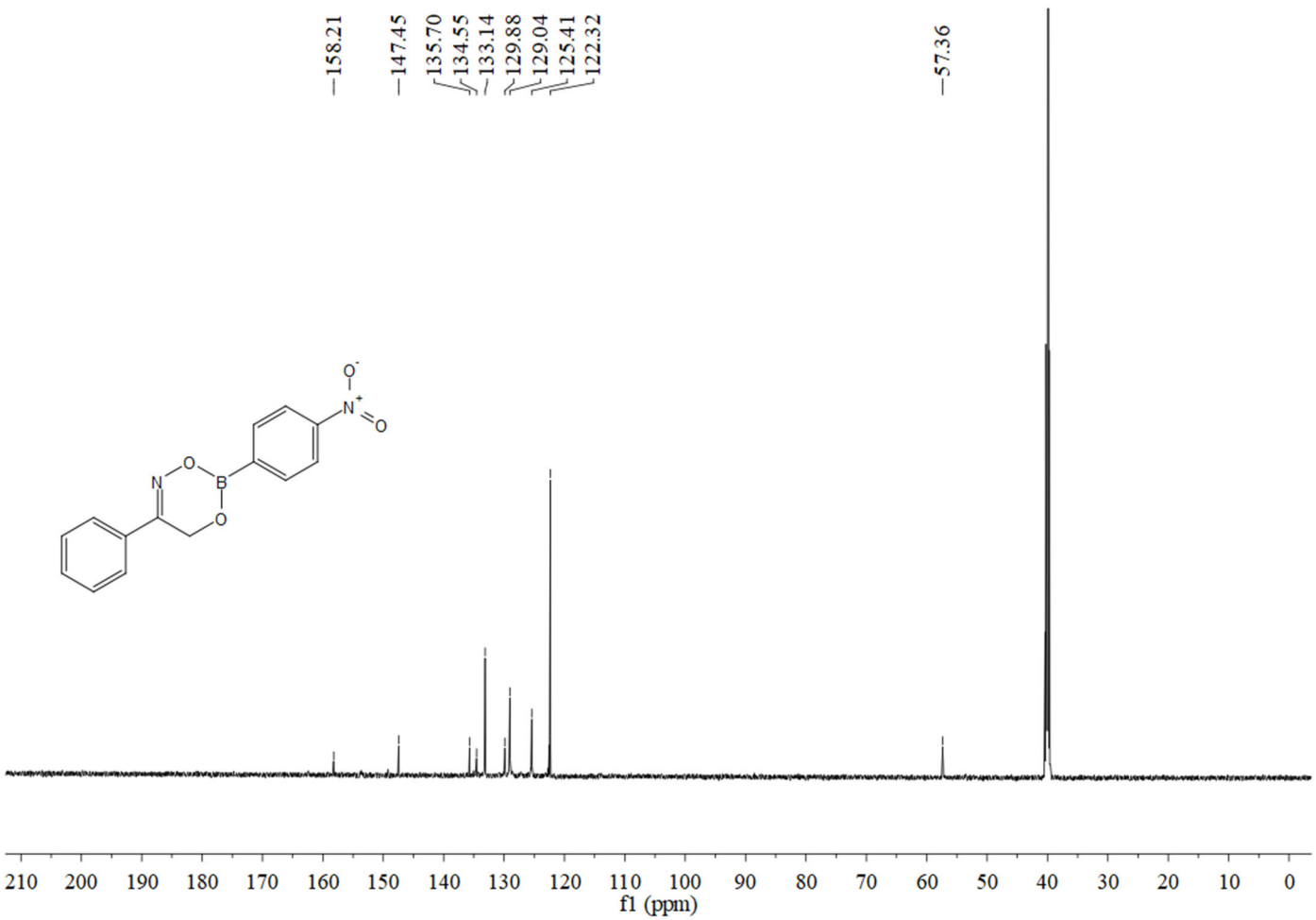


Fig. S59 ^{13}C NMR for compound **5e** (151 MHz, DMSO-d_6)

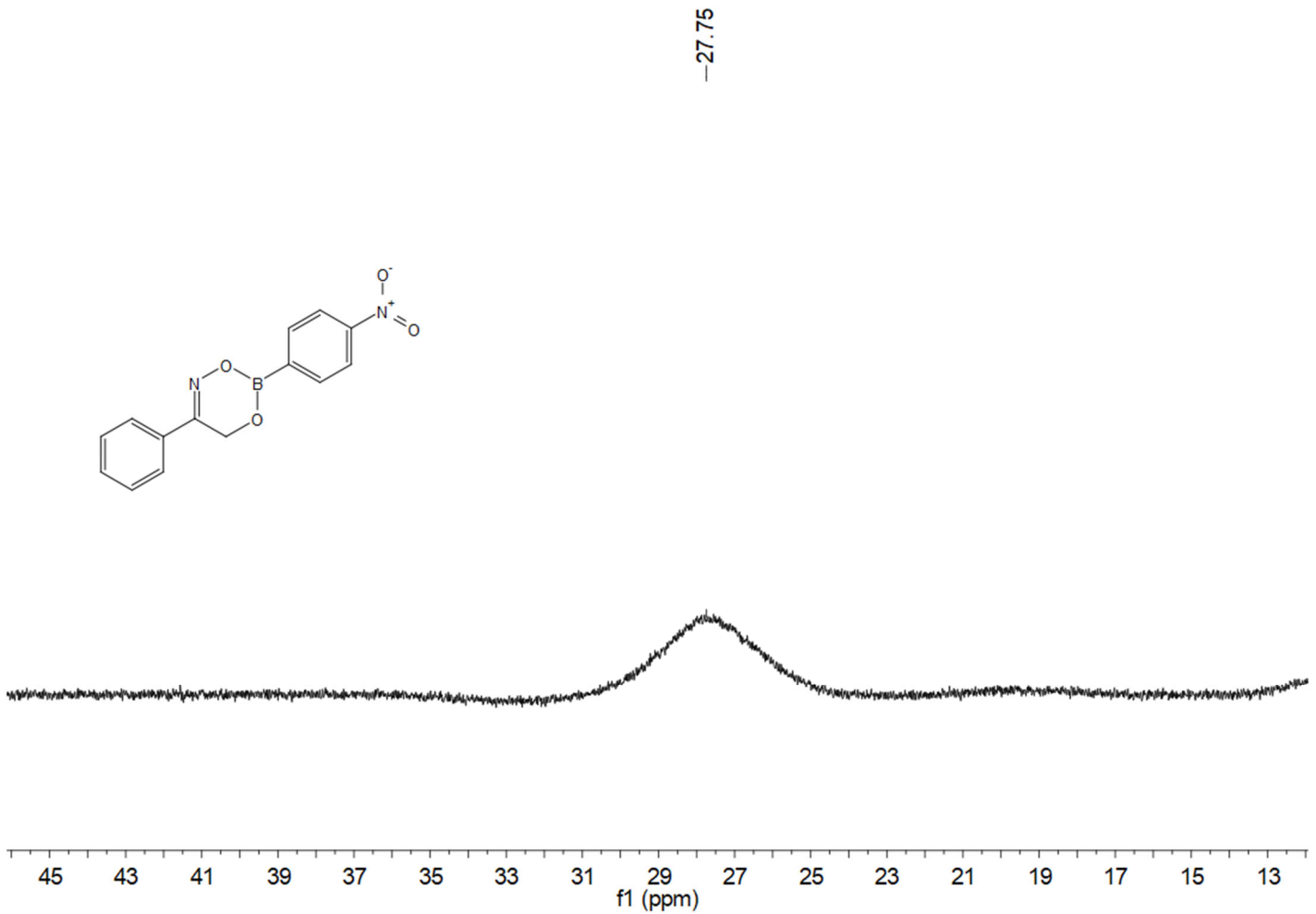


Fig. S60 ^{11}B NMR for compound **5e** (193 MHz, DMSO-d_6)

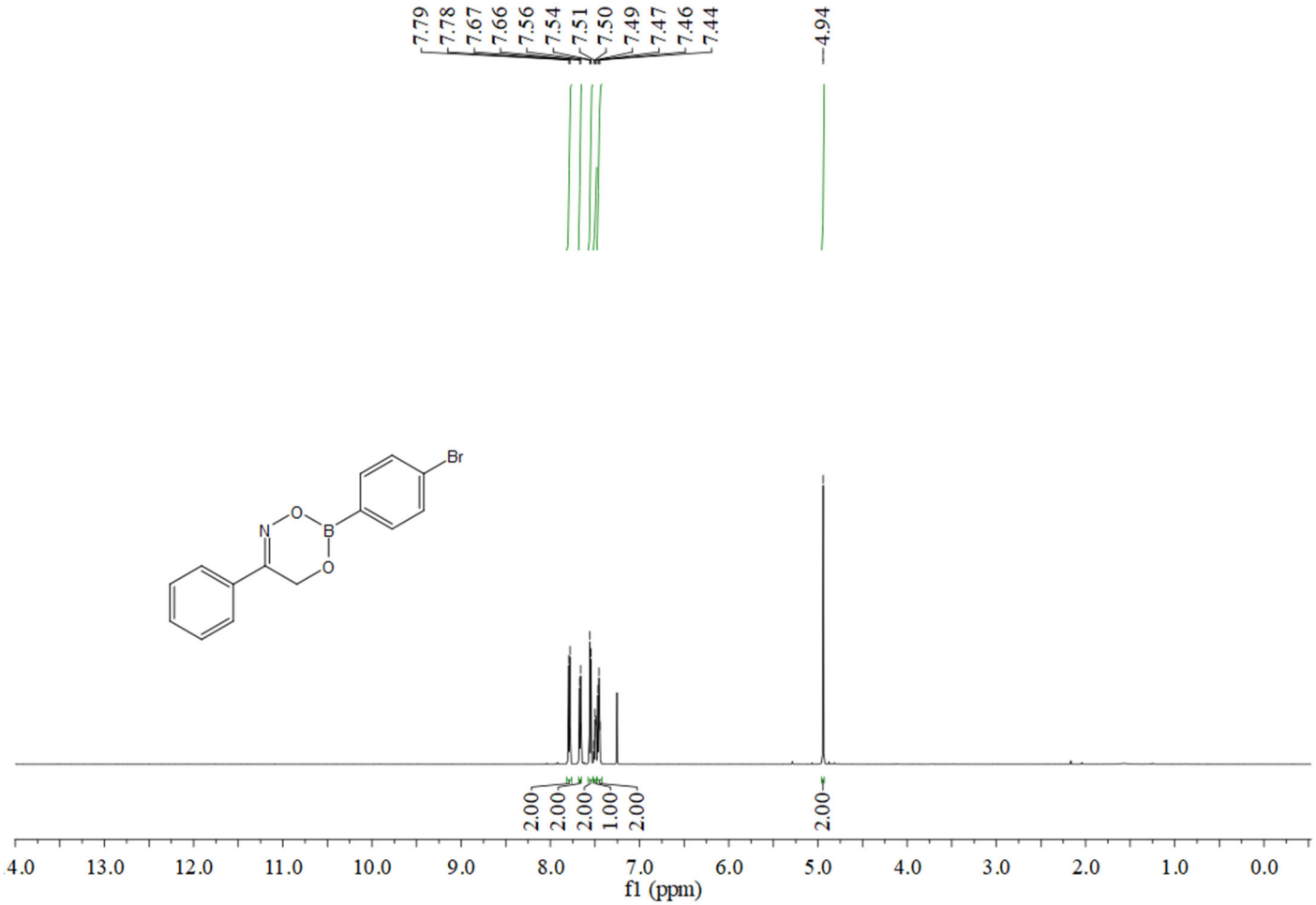


Fig. S61 ^{1}H NMR for compound **5f** (600 MHz, $CDCl_3$)

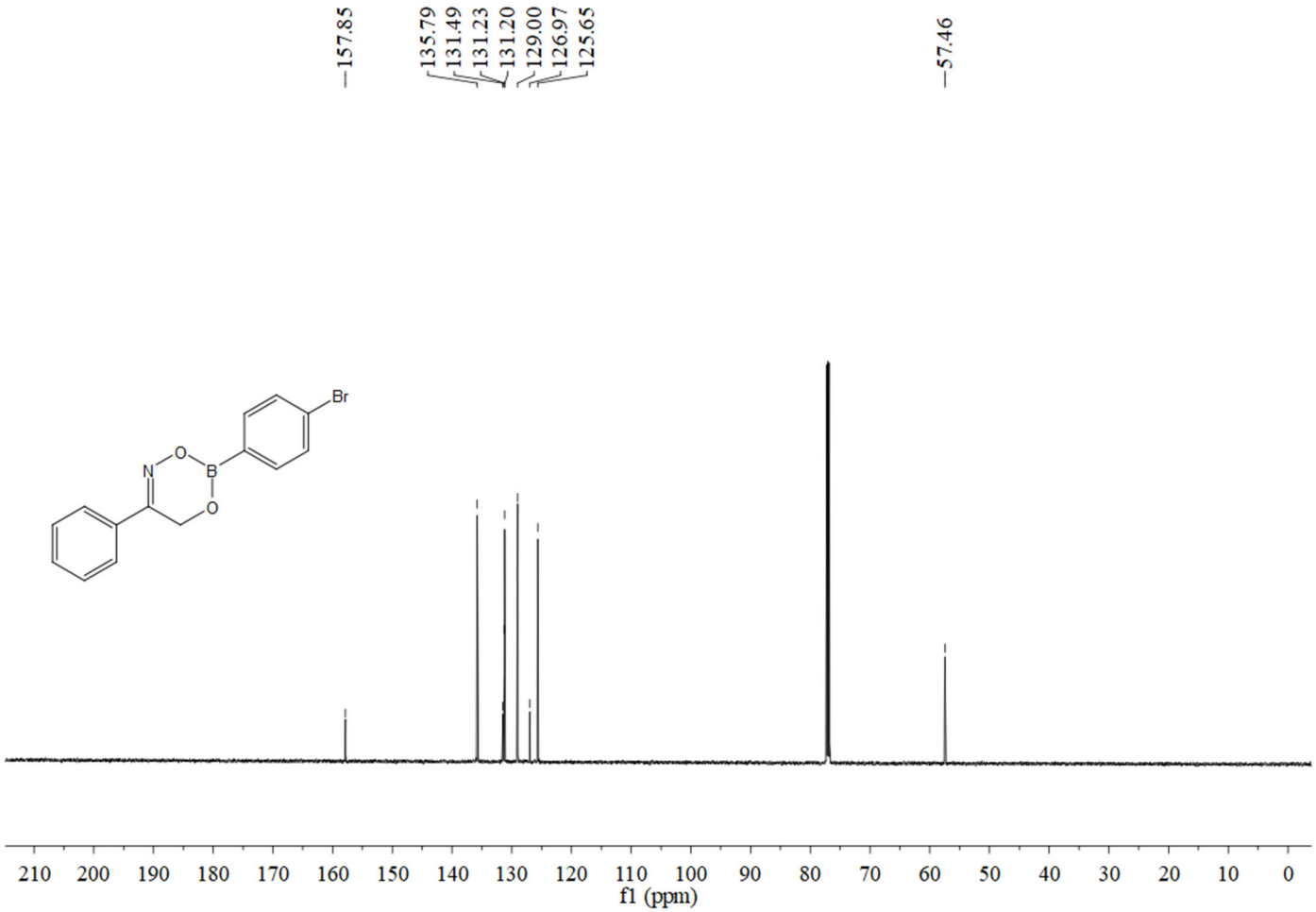


Fig. S62 ^{13}C NMR for compound **5f** (151 MHz, $CDCl_3$)

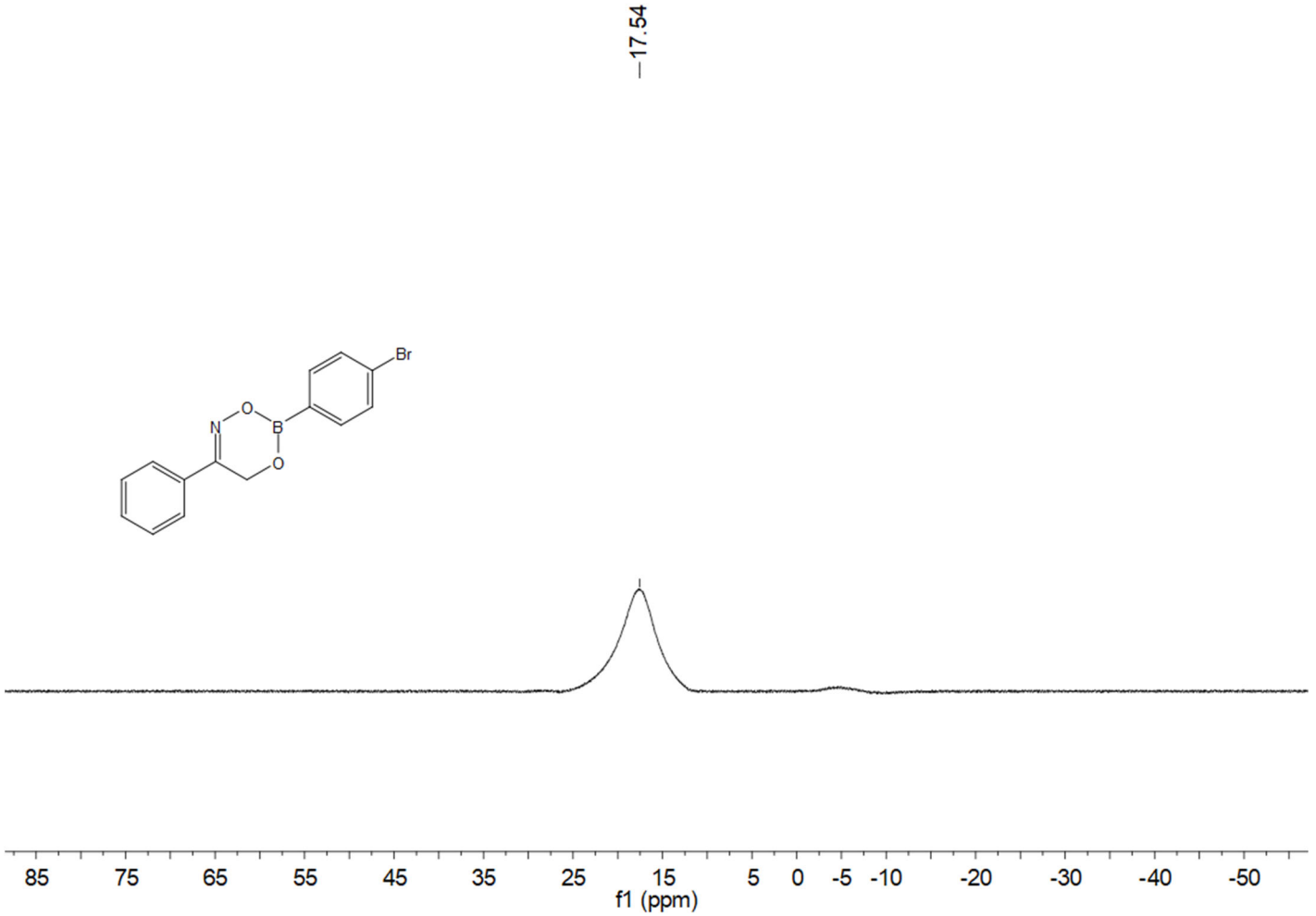


Fig. S63 ^{11}B NMR for compound **5f** (193 MHz, DMSO-d_6)

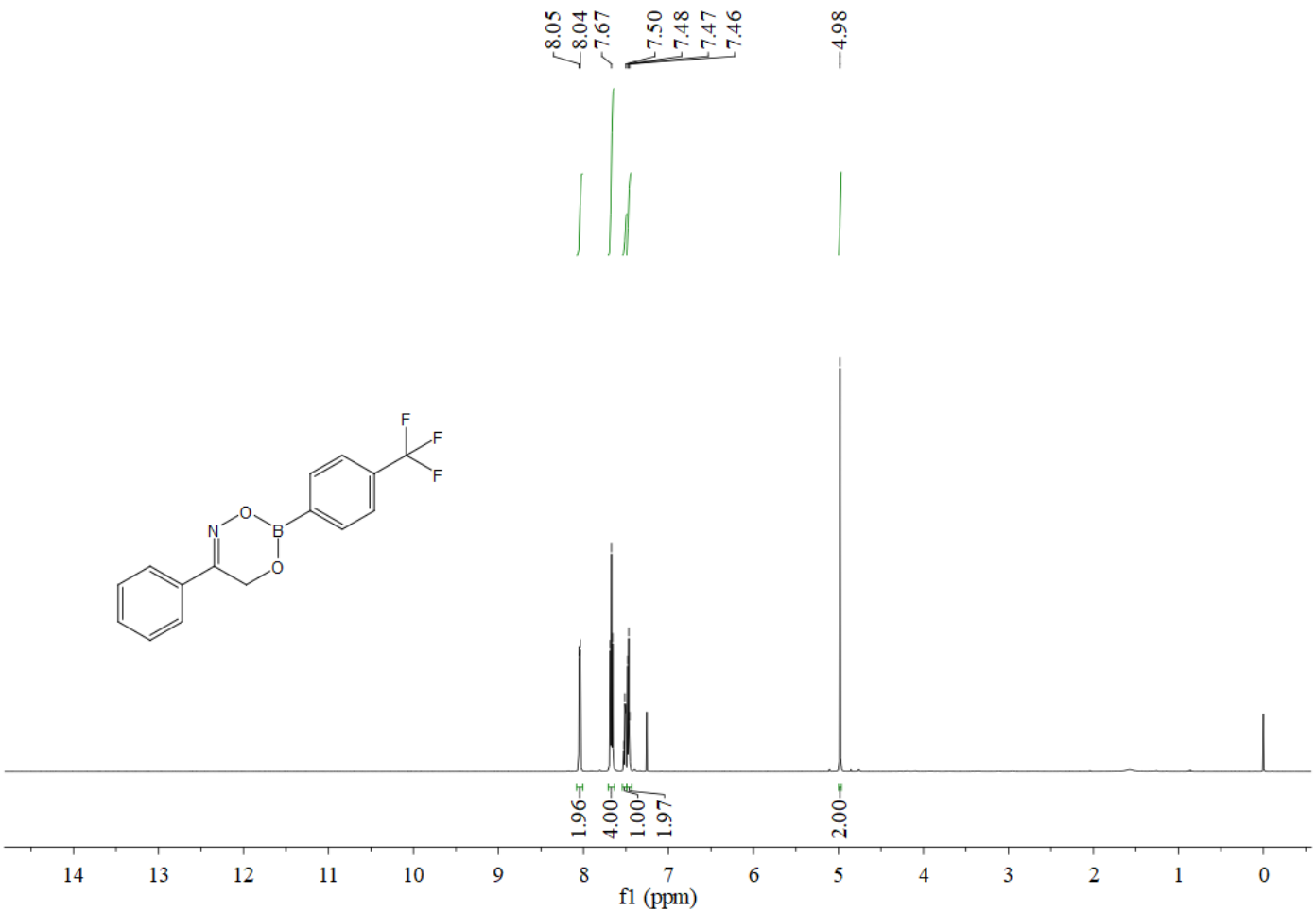


Fig. S64 ^{1}H NMR for compound **5g** (600 MHz, $CDCl_3$)

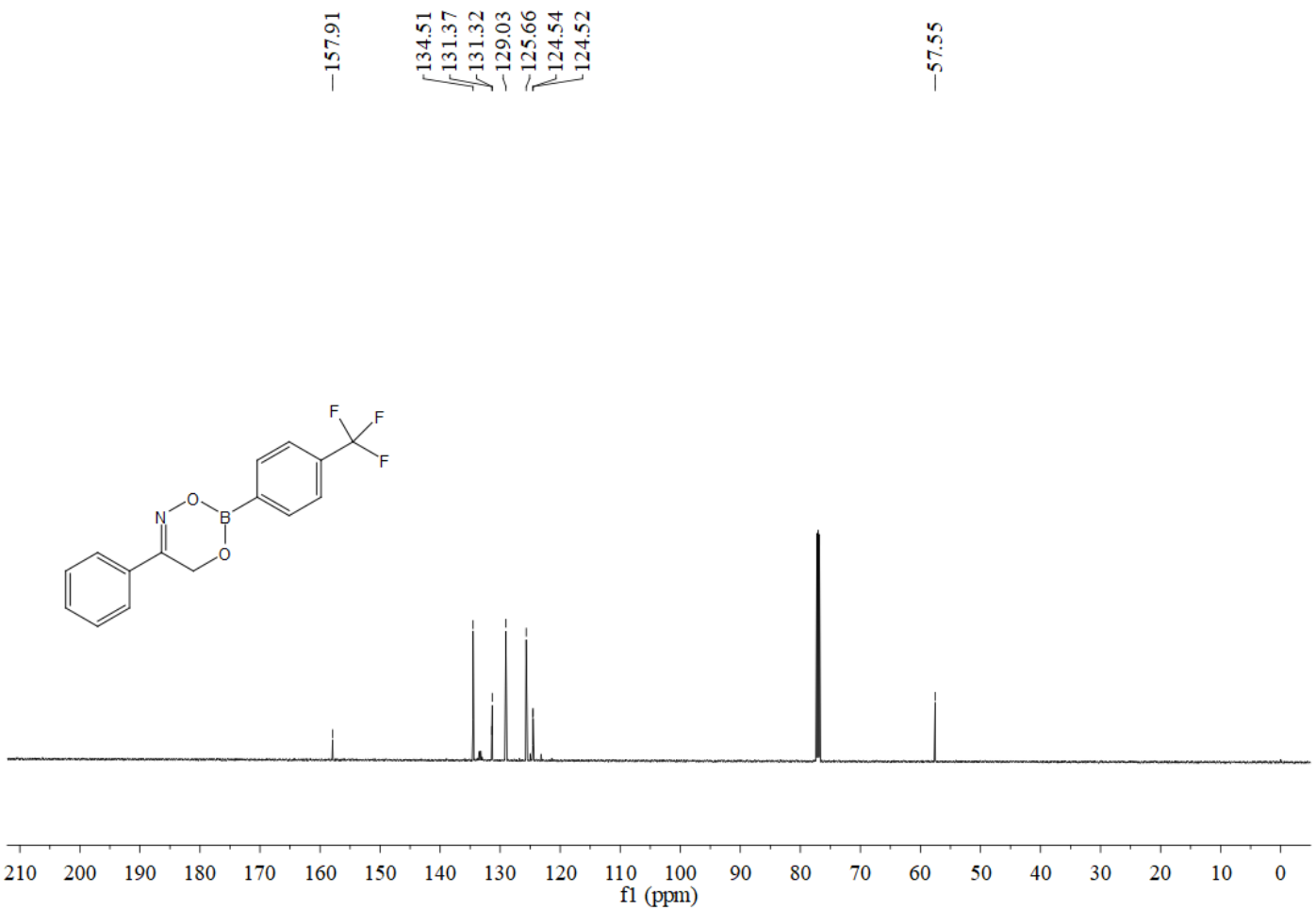


Fig. S65 ^{13}C NMR for compound **5g** (151 MHz, $CDCl_3$)

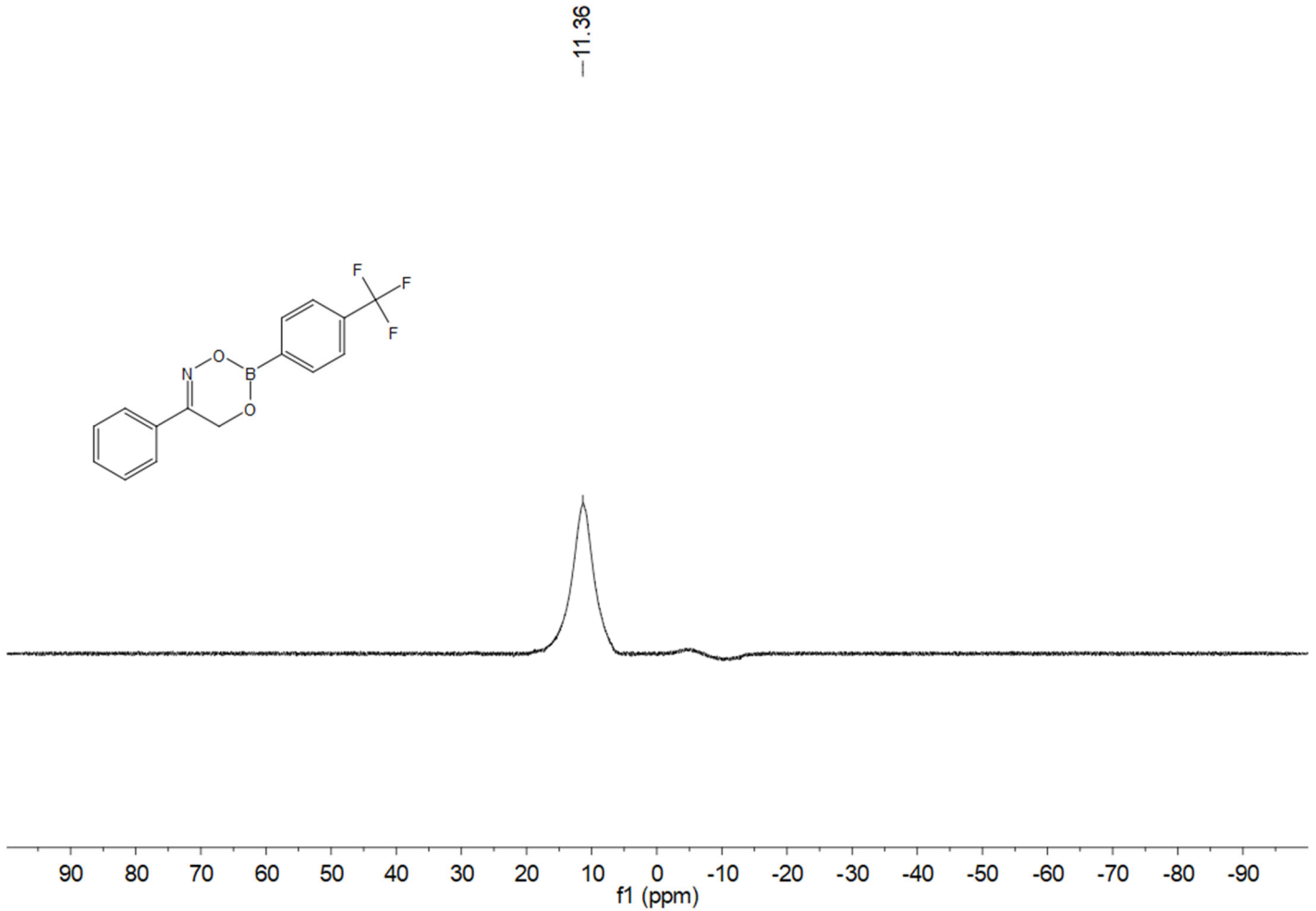


Fig. S66 ^{11}B NMR for compound **5g** (193 MHz, DMSO-d_6)

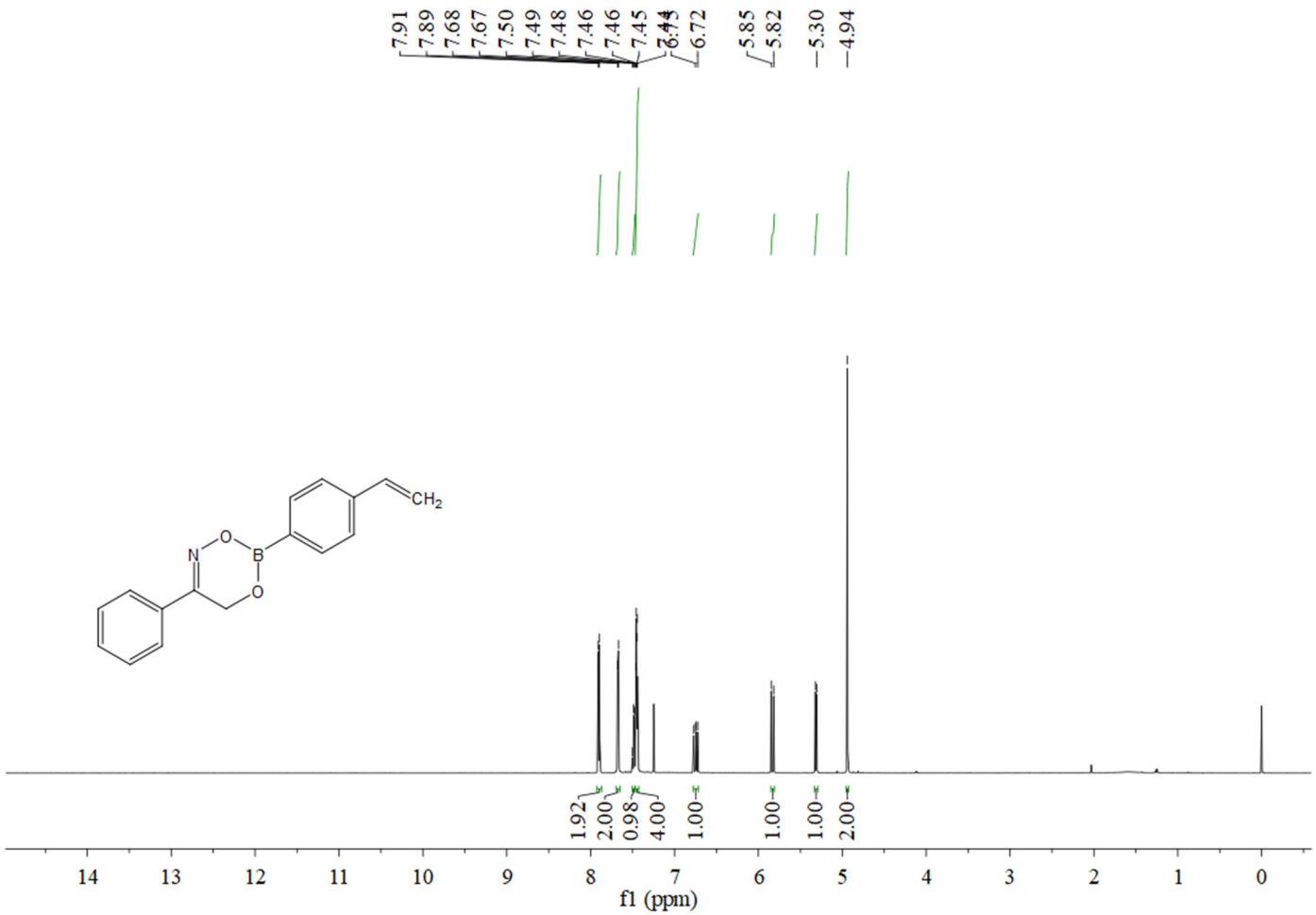


Fig. S67 ^{1}H NMR for compound **5h** (600 MHz, $CDCl_3$)

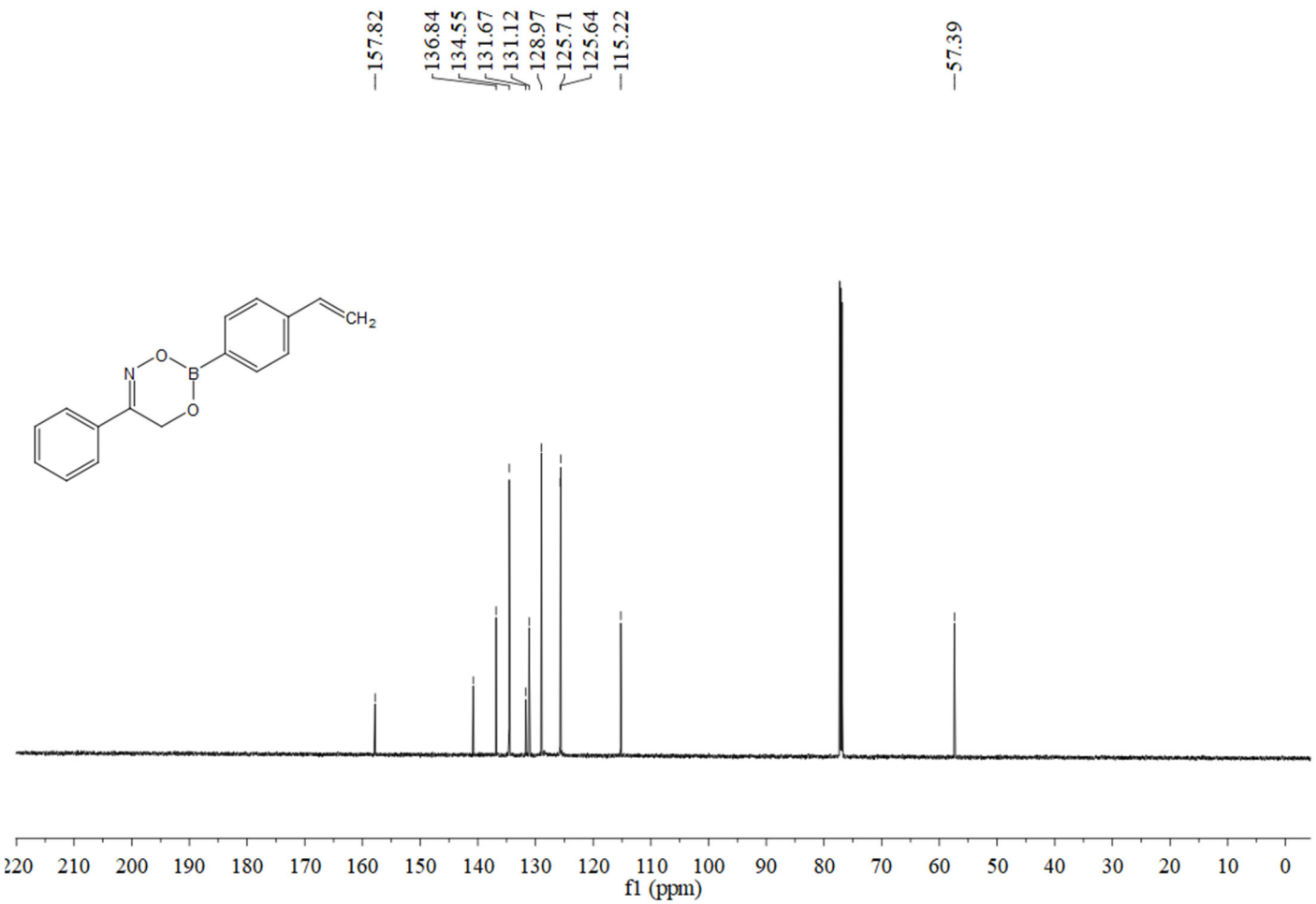


Fig. S68 ^{13}C NMR for compound **5h** (151 MHz, $CDCl_3$)

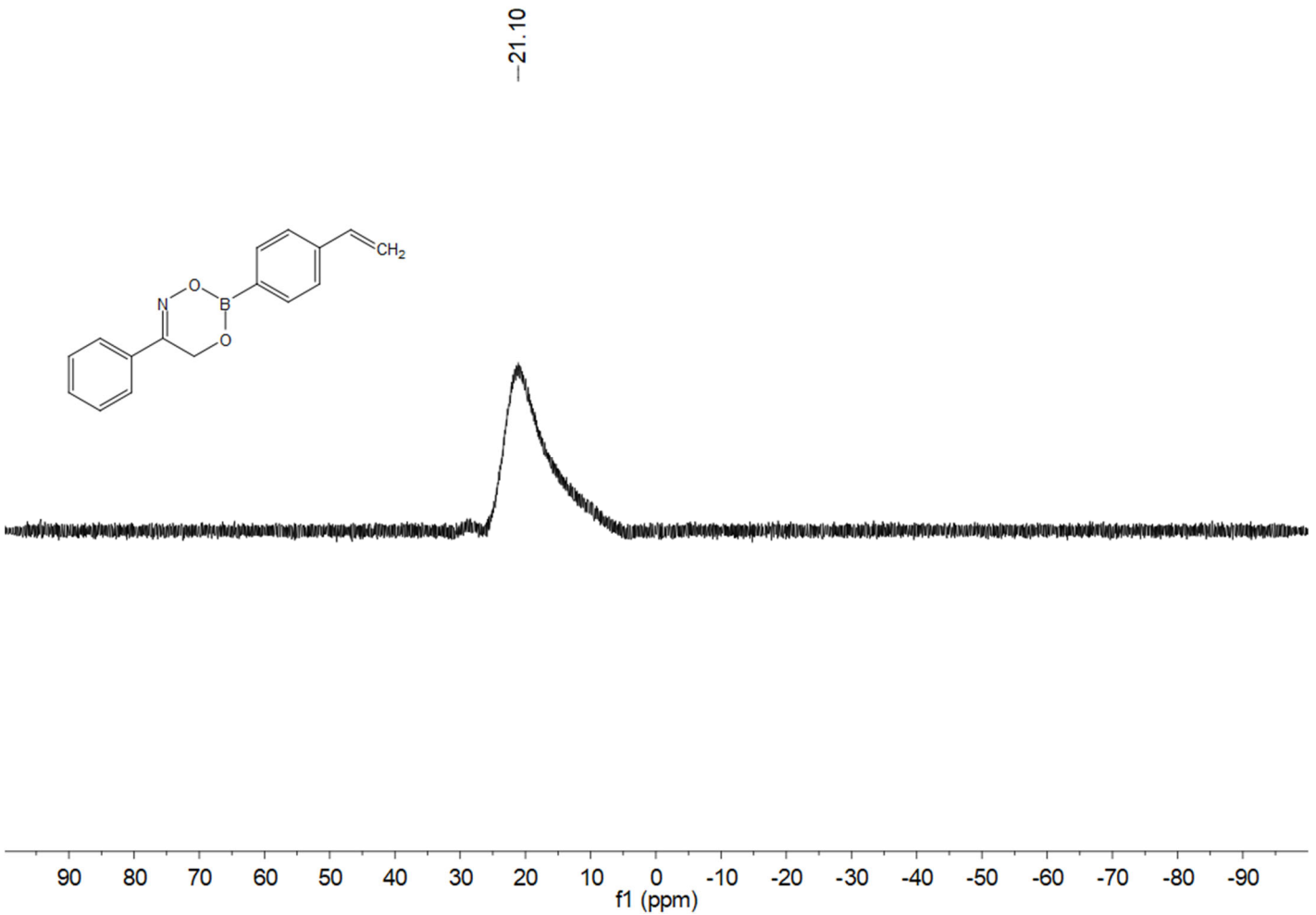


Fig. S69 ^{11}B NMR for compound **5h** (193 MHz, DMSO-d_6)

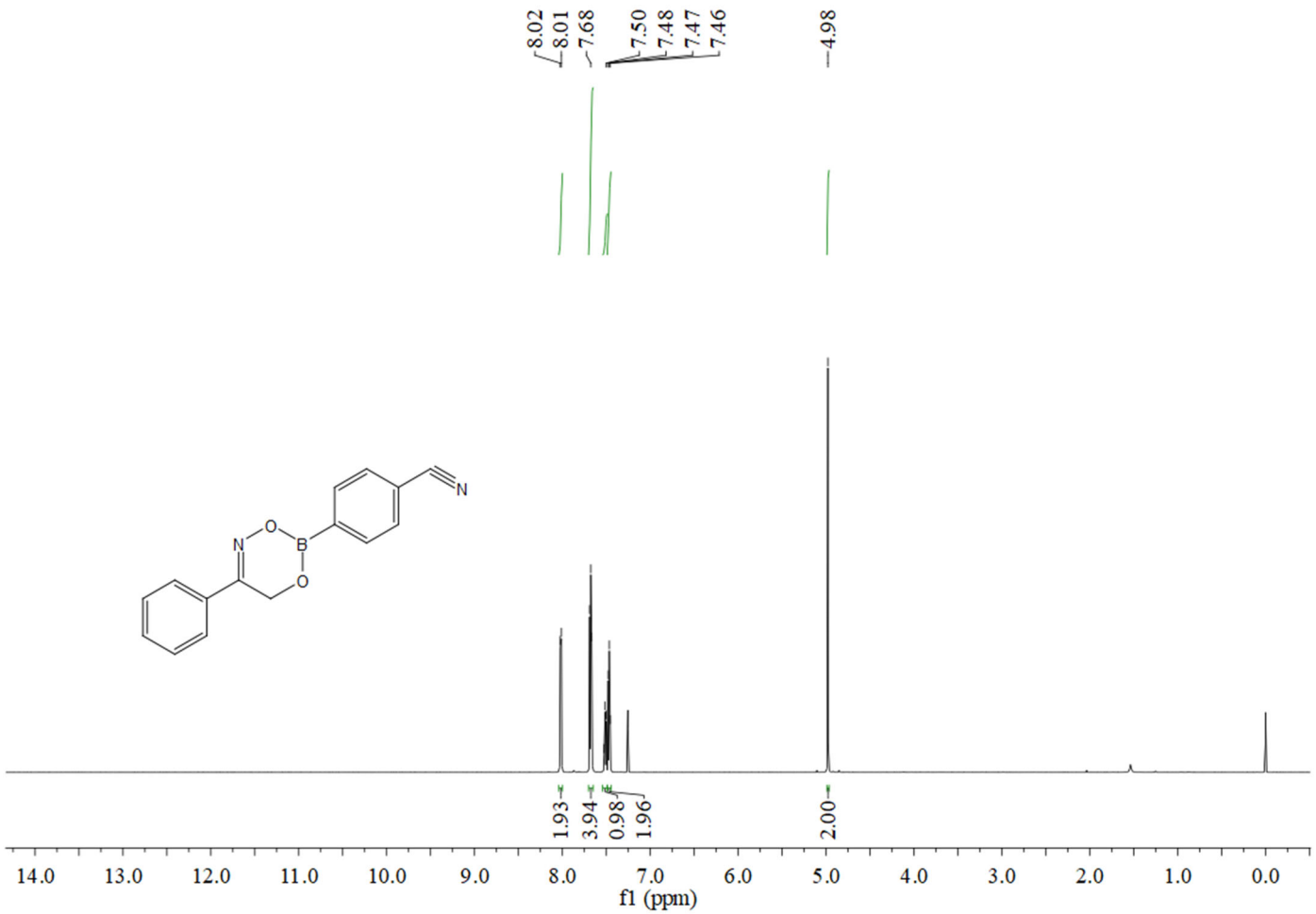


Fig. S70 ^{1}H NMR for compound **5i** (600 MHz, $CDCl_3$)

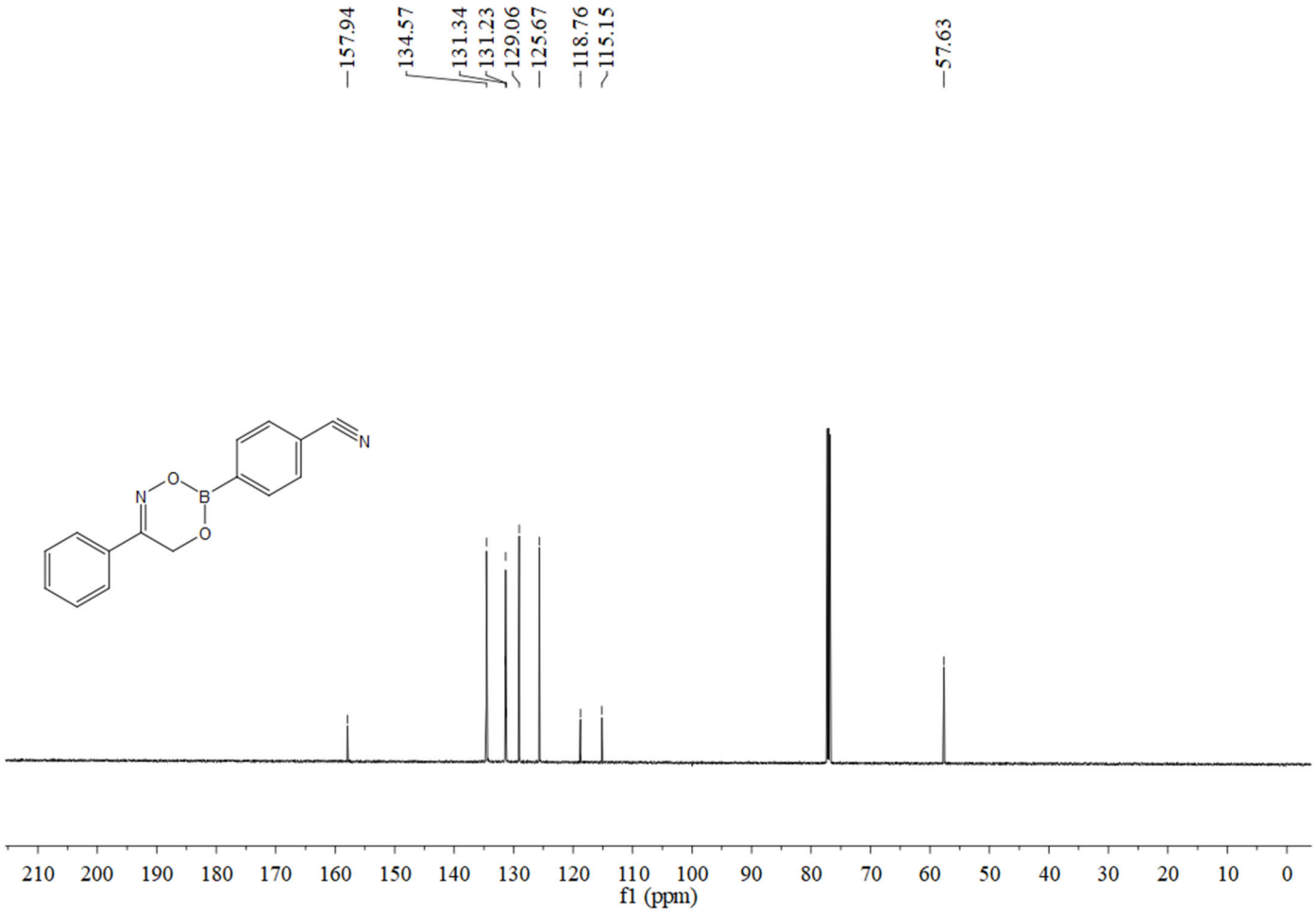


Fig. S71 ^{13}C NMR for compound **5i** (151 MHz, $CDCl_3$)

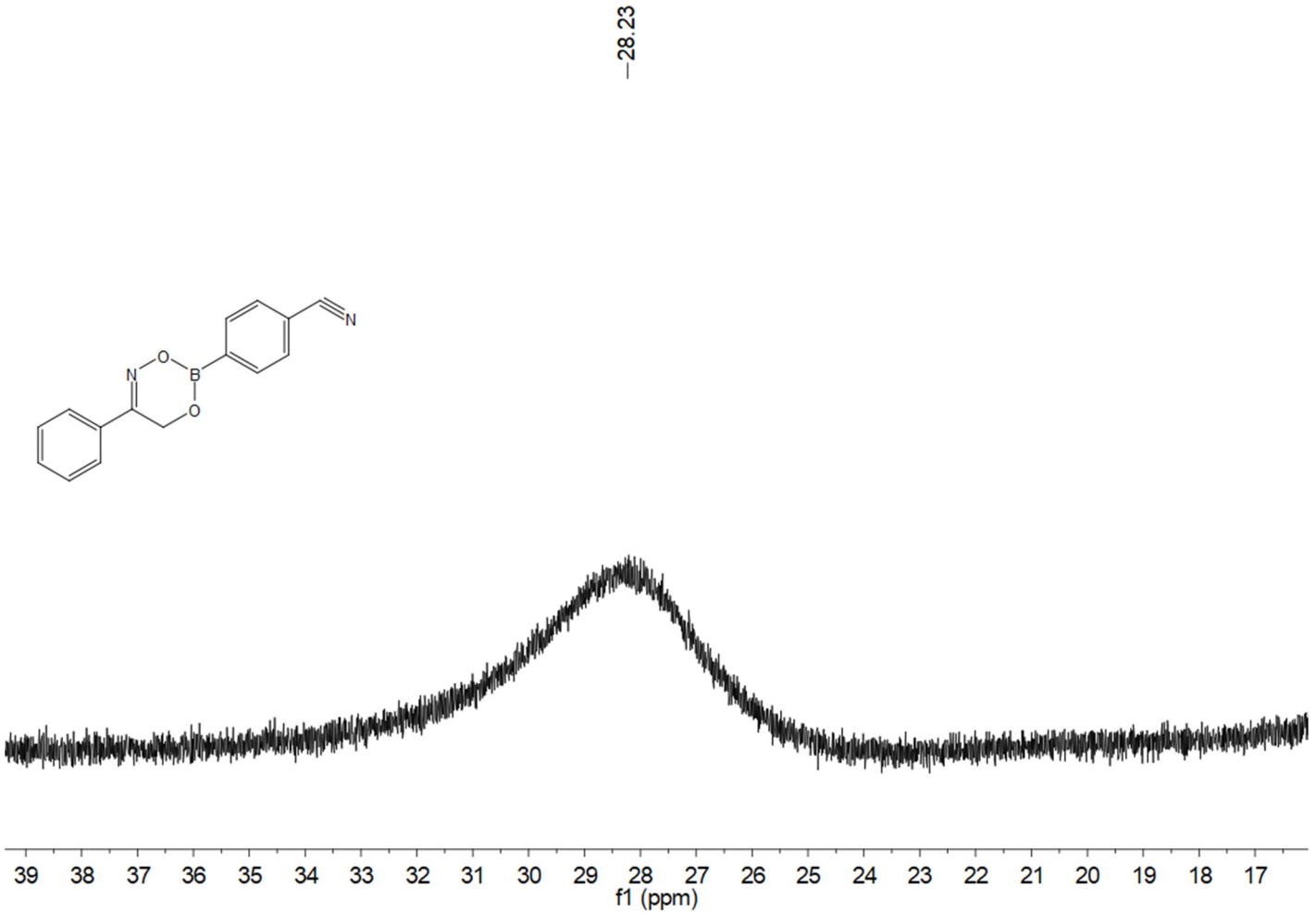


Fig. S72 ^{11}B NMR for compound **5i** (193 MHz, DMSO-d_6)

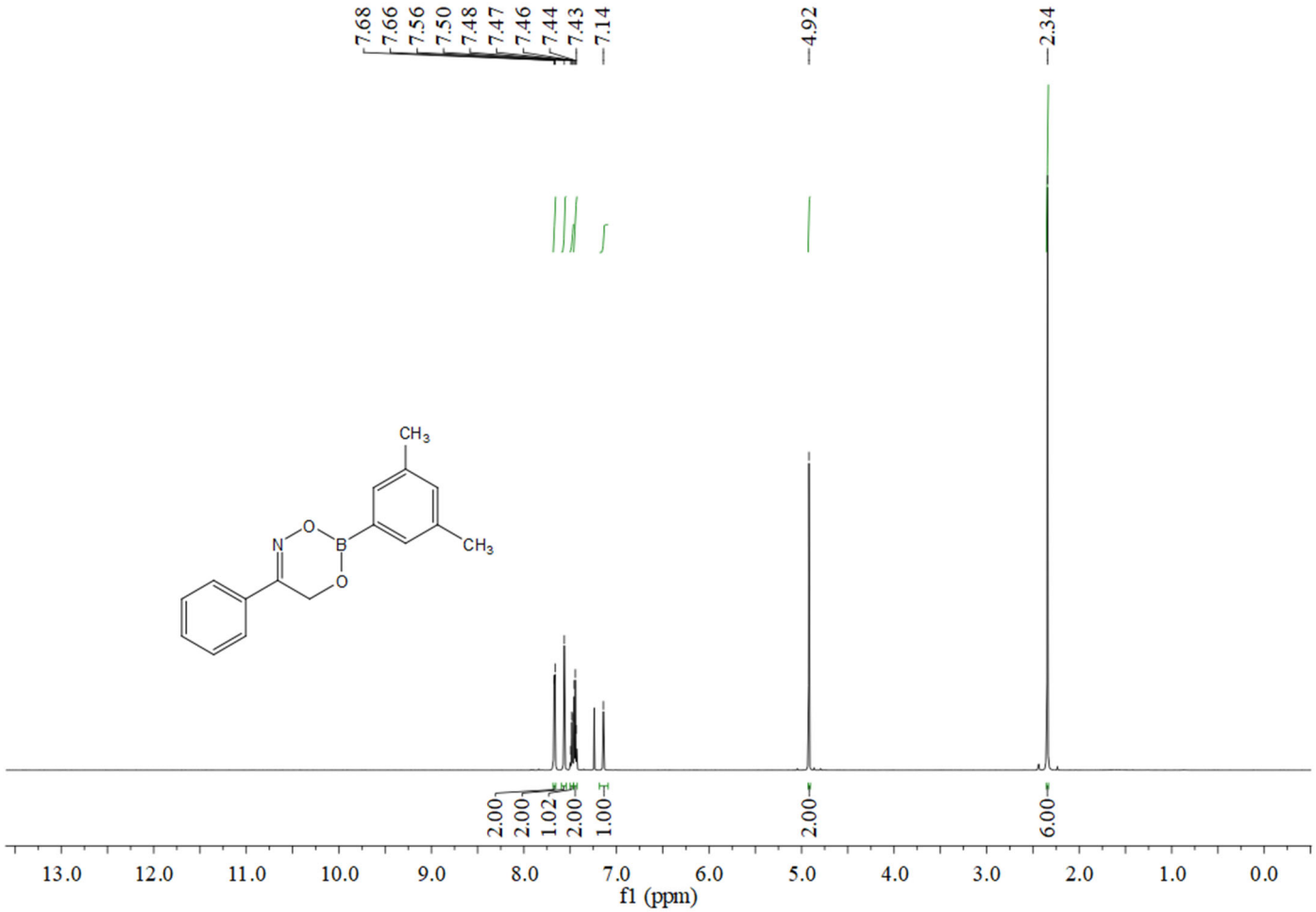


Fig. S73 ^{1}H NMR for compound **5j** (600 MHz, $CDCl_3$)

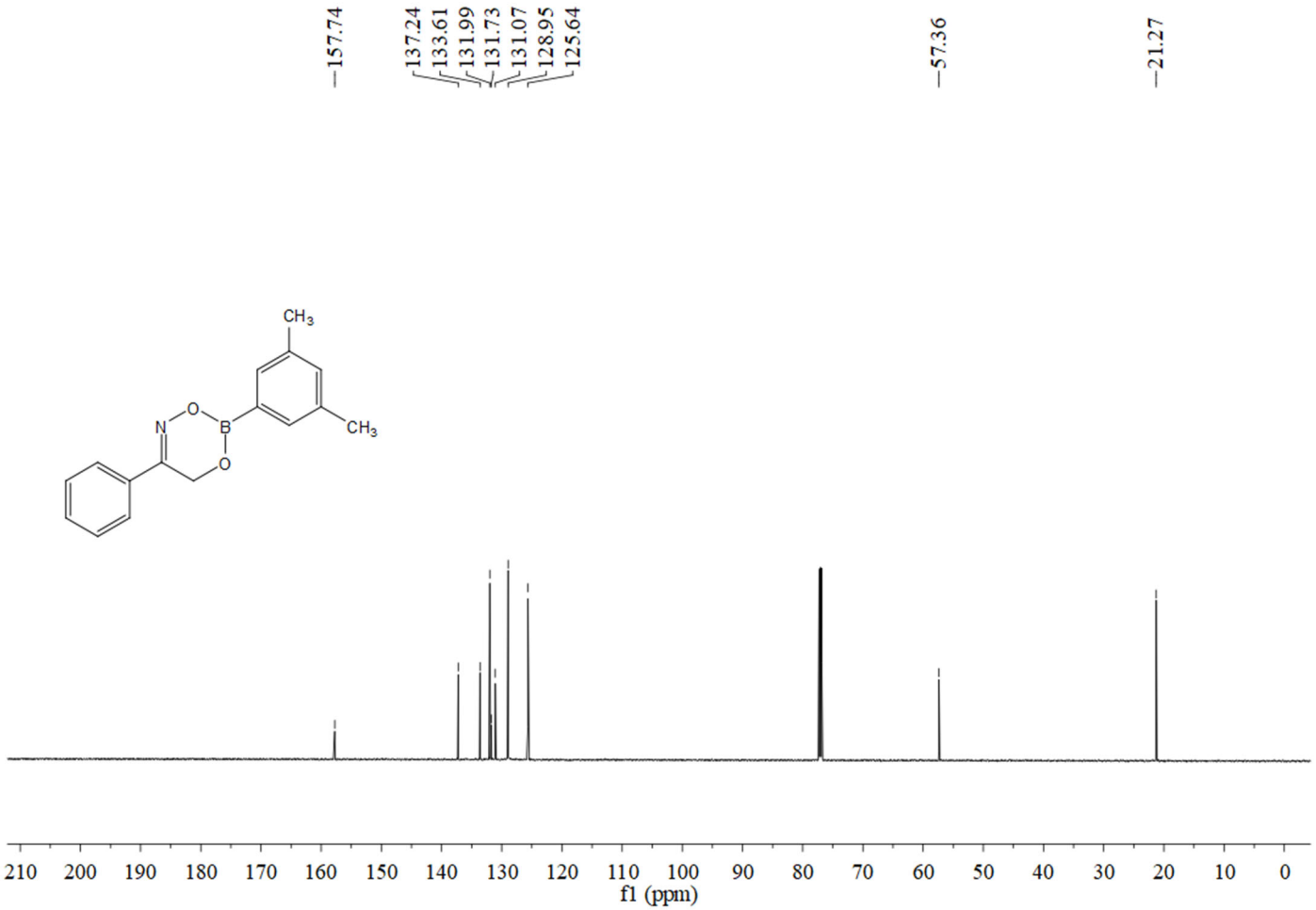


Fig. S74 ^{13}C NMR for compound **5j** (151 MHz, $CDCl_3$)

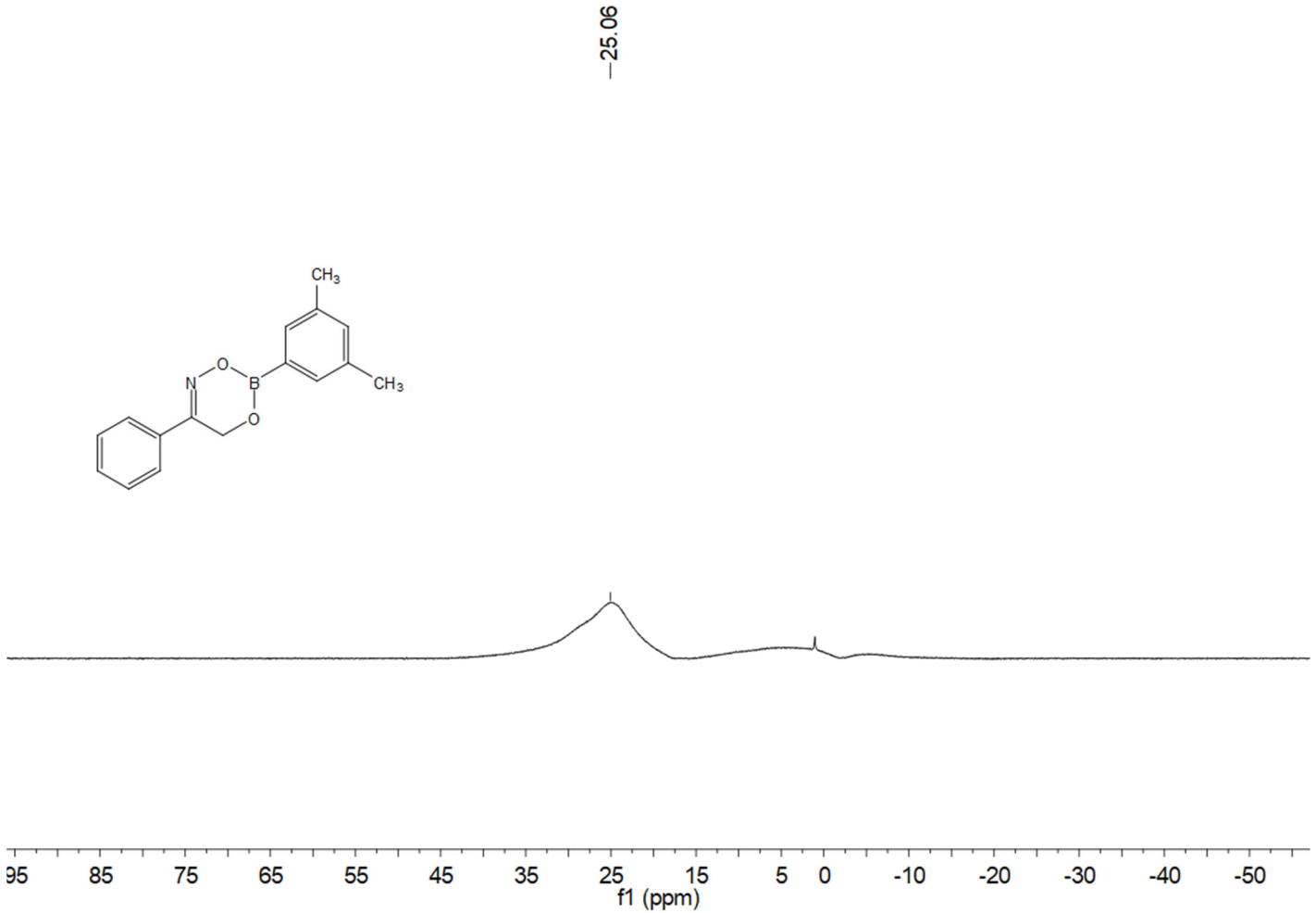


Fig. S75 ^{11}B NMR for compound **5j** (193 MHz, DMSO-d_6)

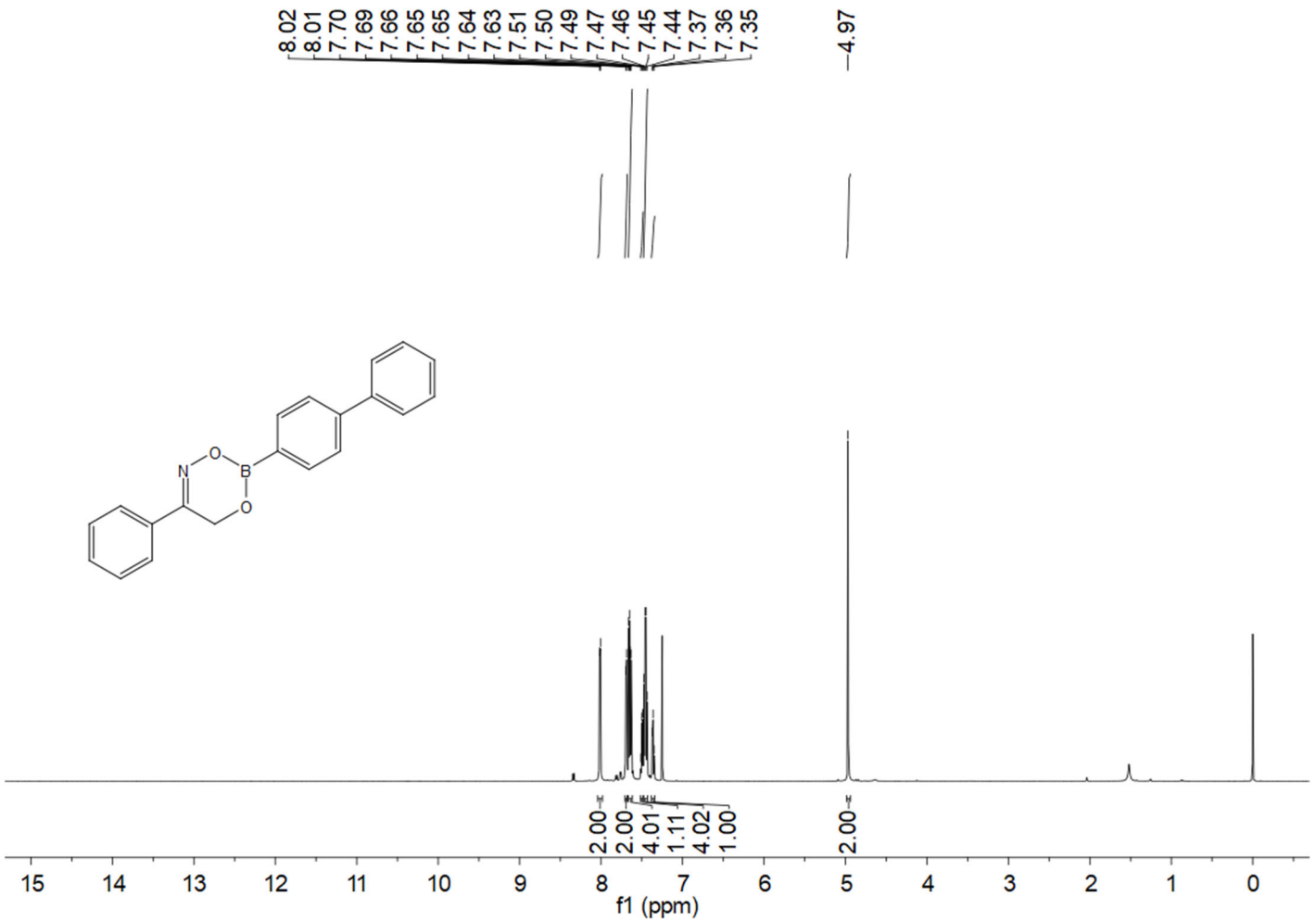


Fig. S76 ^{1}H NMR for compound **5l** (600 MHz, $CDCl_3$)

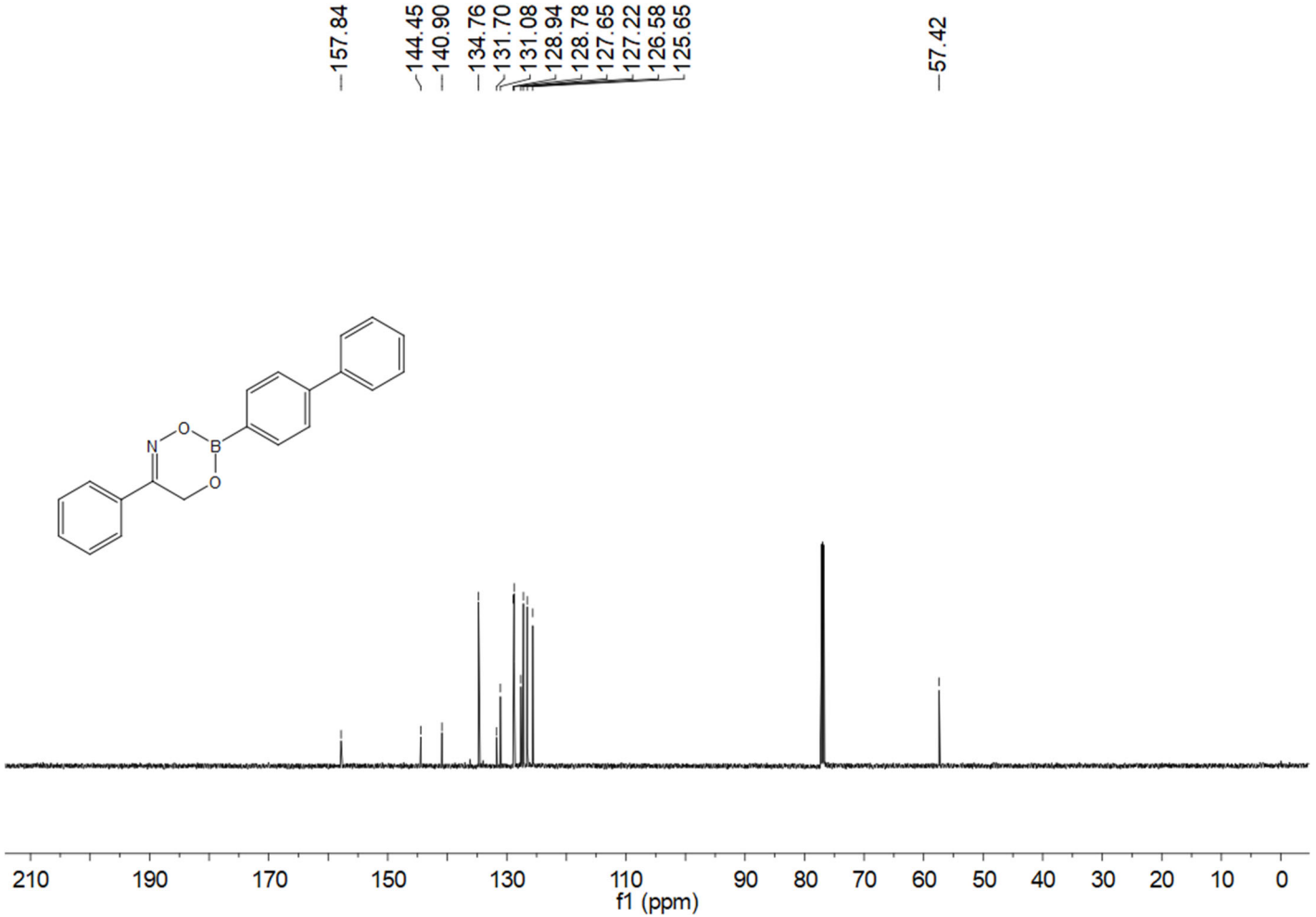


Fig. S77 ^{13}C NMR for compound **5l** (151 MHz, $CDCl_3$)

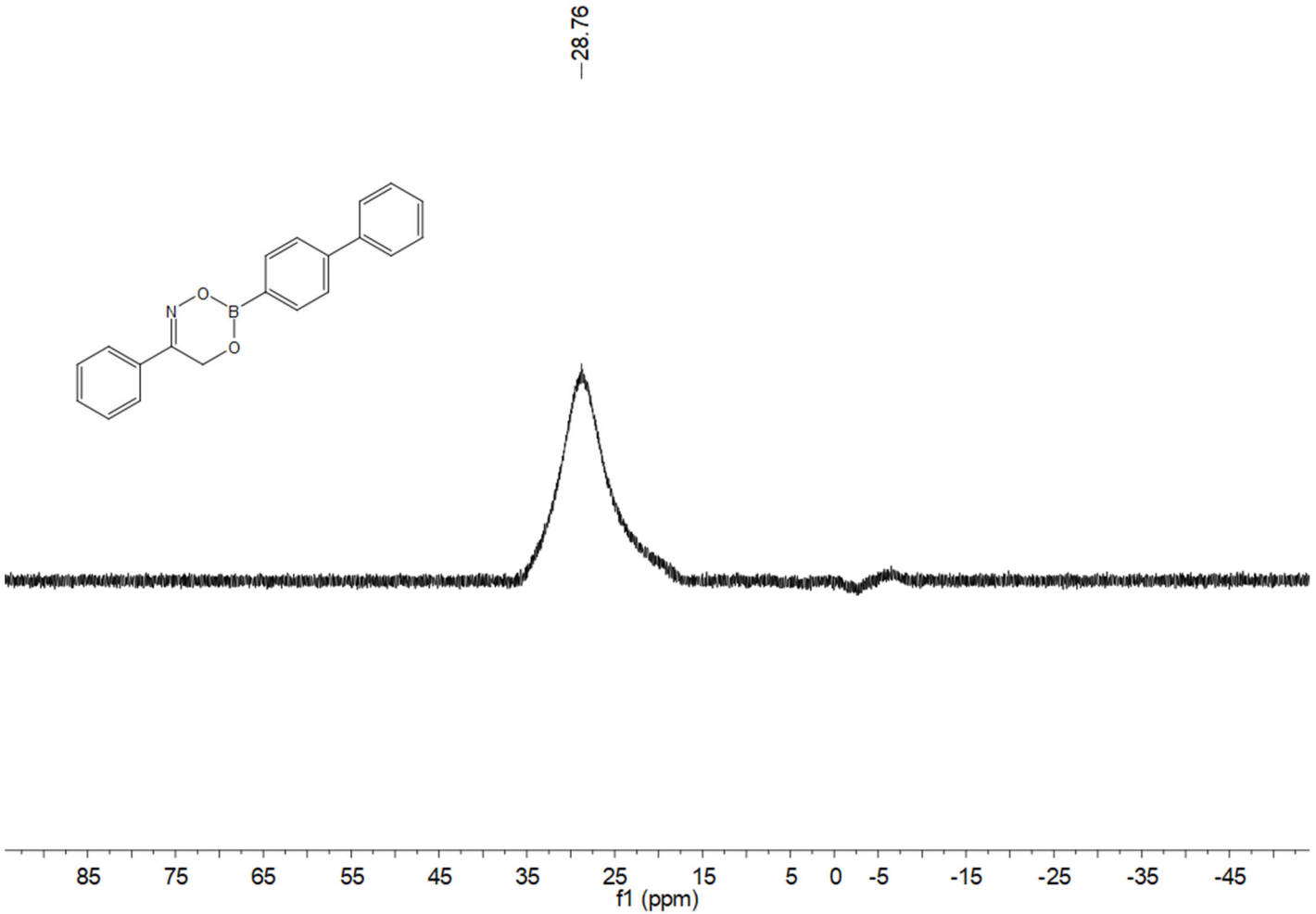


Fig. S78 ^{11}B NMR for compound **5l** (193 MHz, DMSO-d_6)

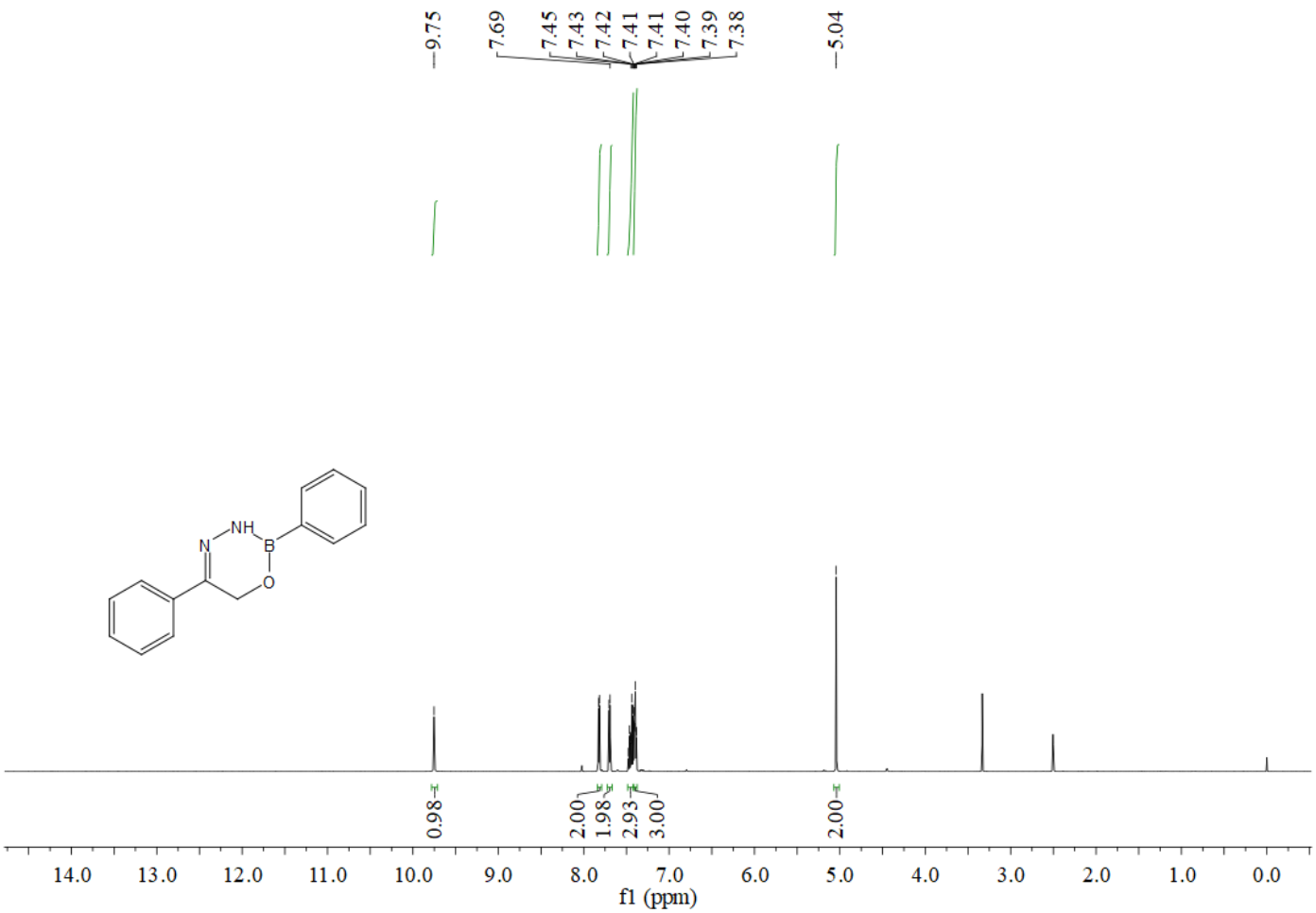


Fig. S79 ^{1}H NMR for compound **7a** (600 MHz, DMSO-d_6)

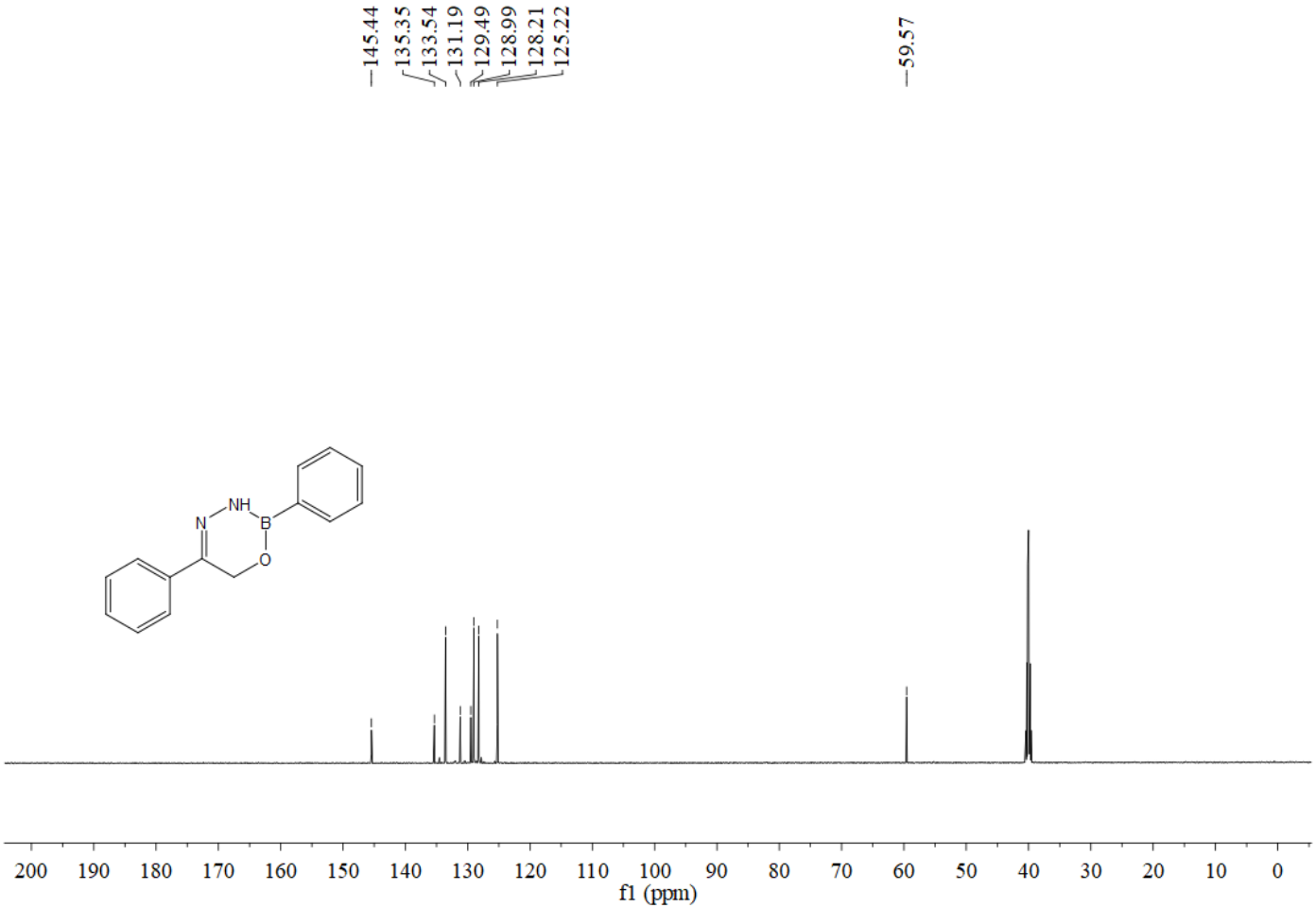


Fig. S80 ^{13}C NMR for compound **7a** (151 MHz, DMSO-d_6)

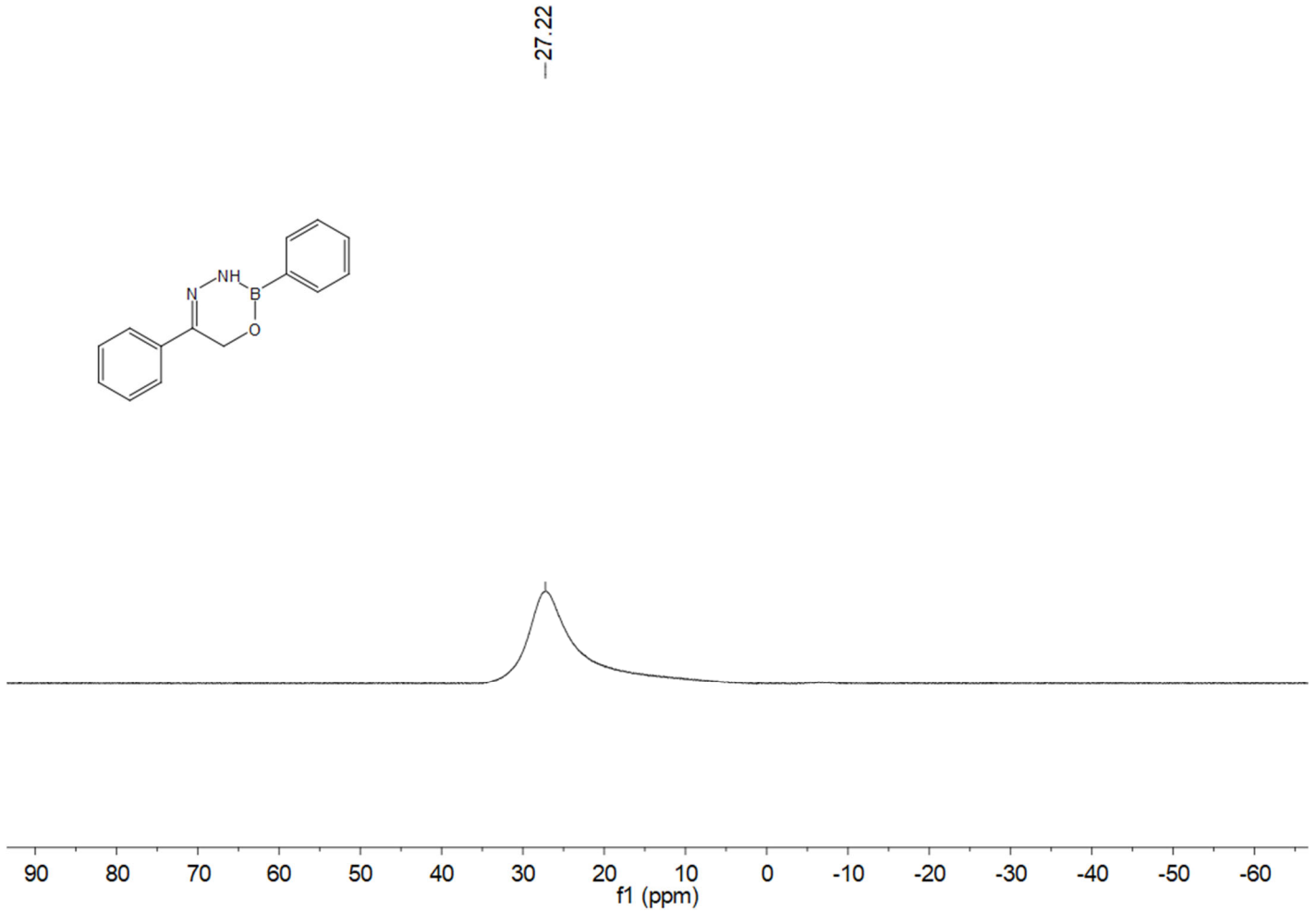


Fig. S81 ^{11}B NMR for compound **7a** (193 MHz, DMSO-d_6)

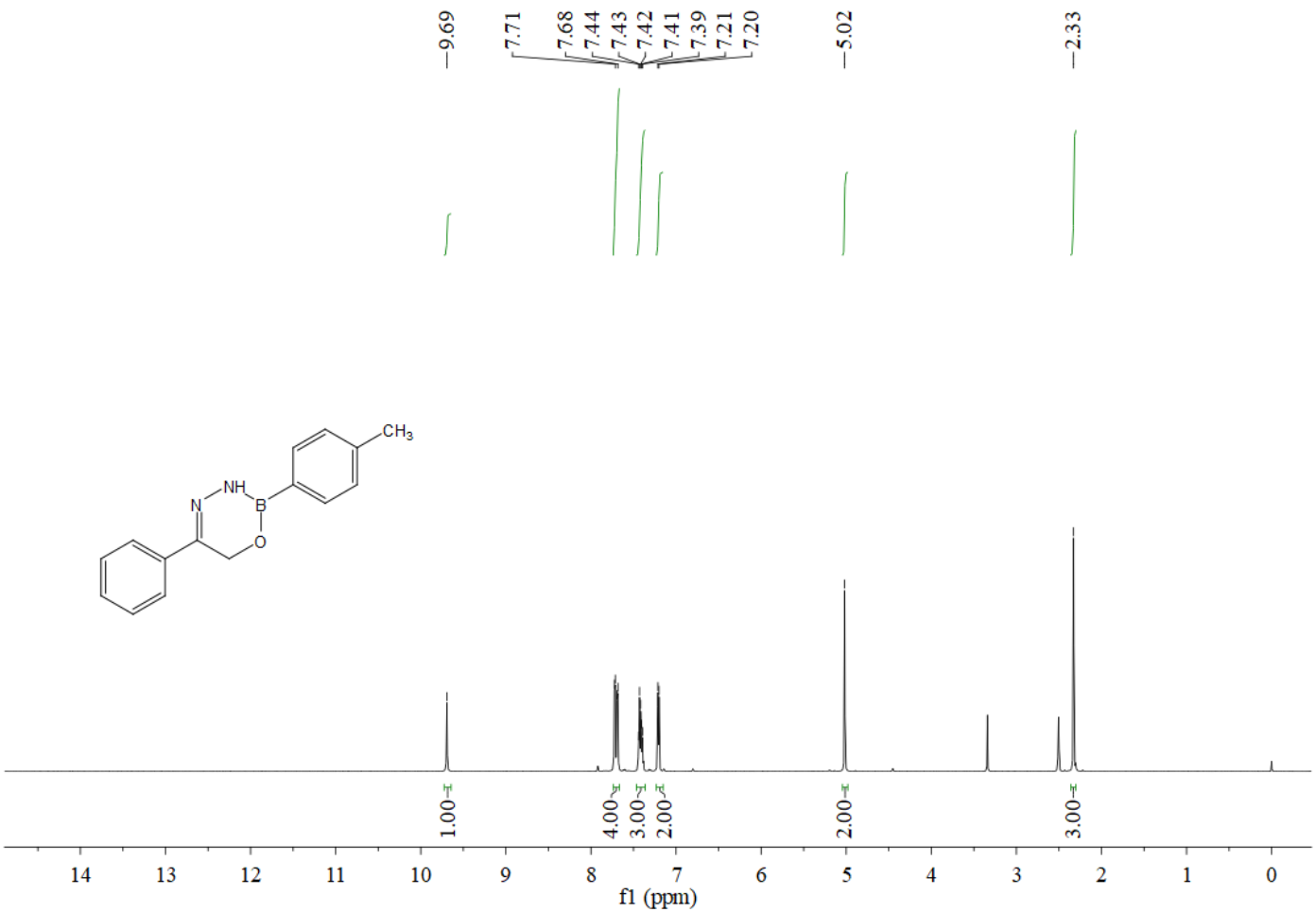


Fig. S82 ^{1}H NMR for compound **7b** (600 MHz, DMSO-d_6)

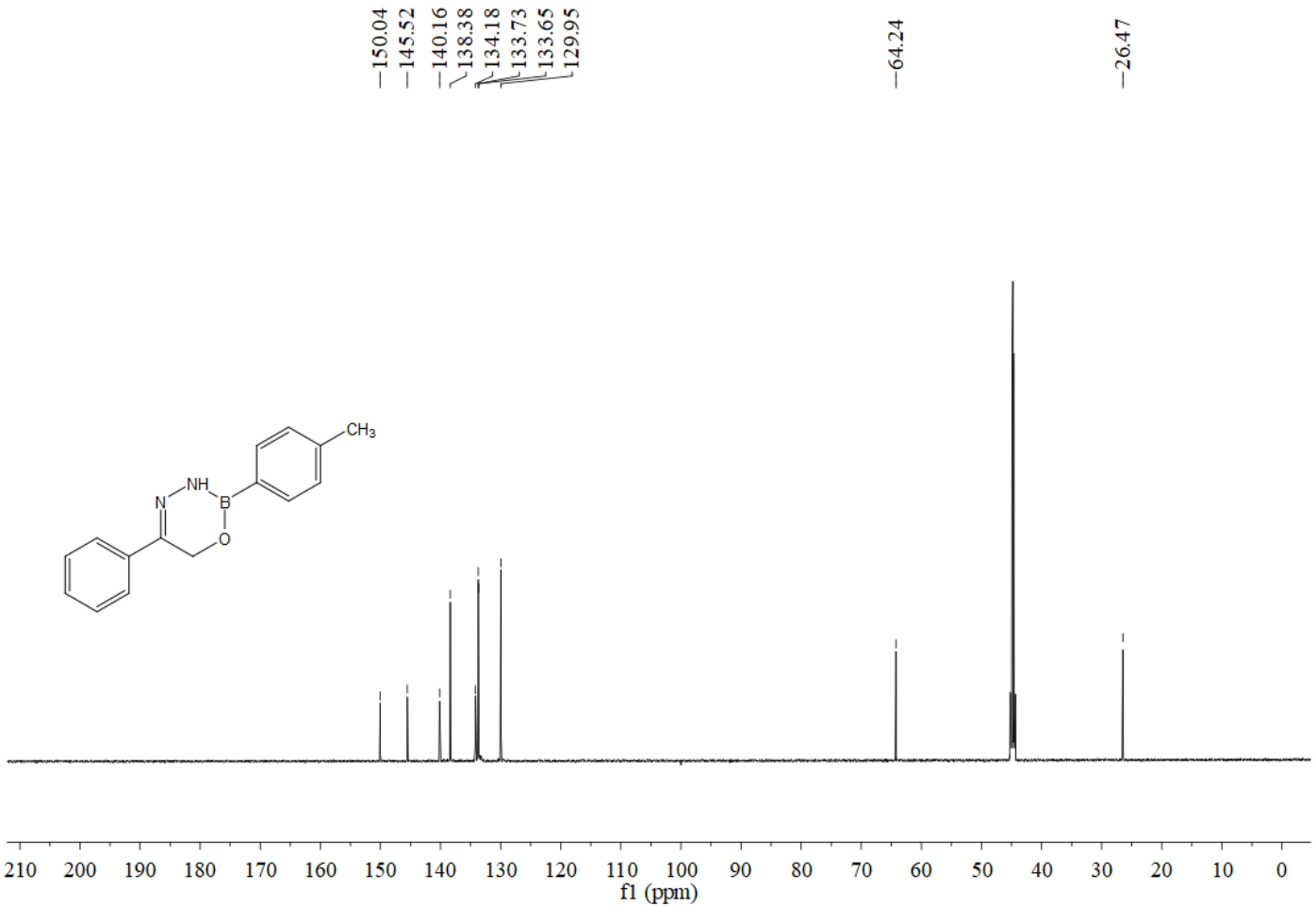


Fig. S83 ^{13}C NMR for compound **7b** (151 MHz, DMSO-d_6)

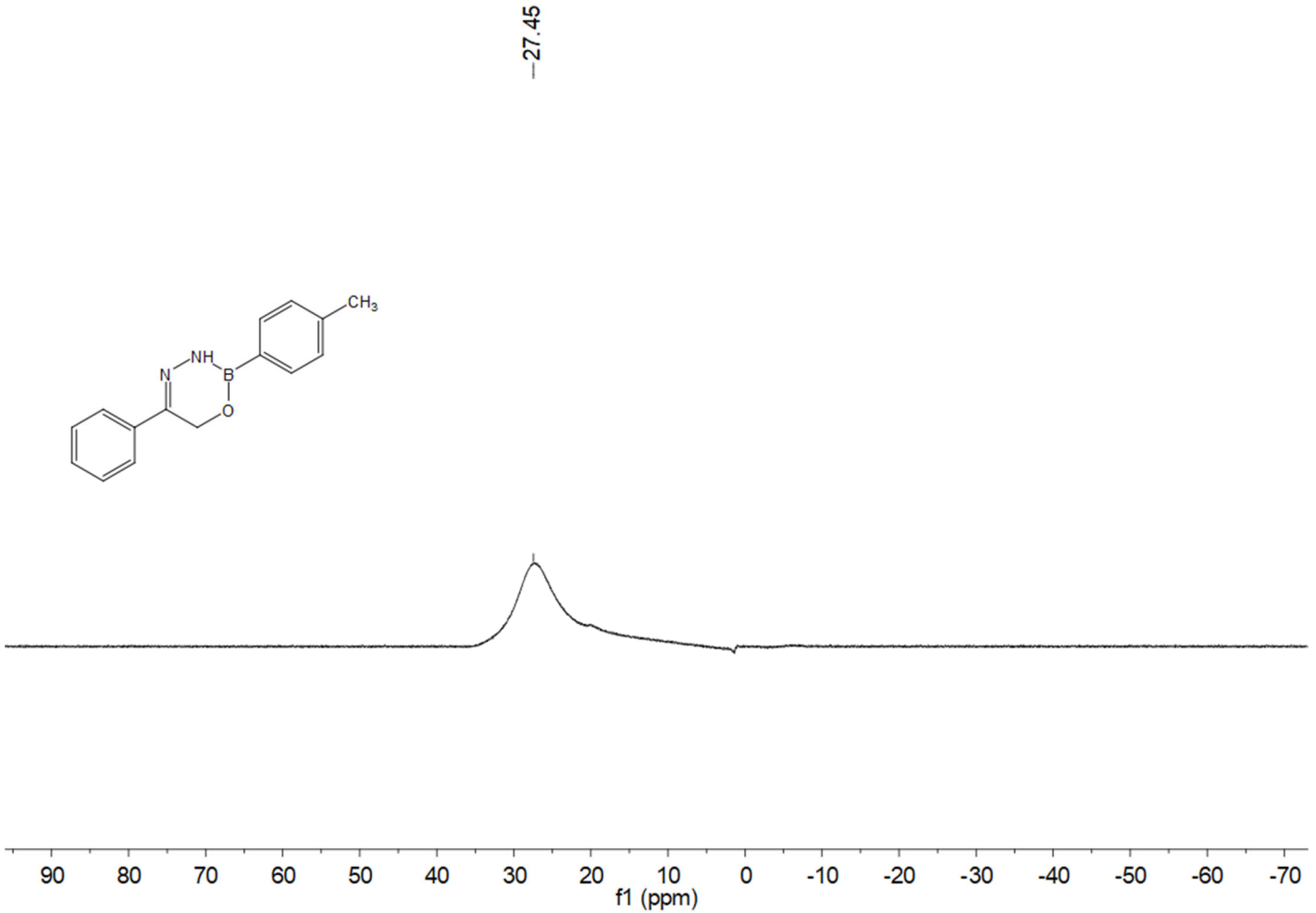


Fig. S84 ^{11}B NMR for compound **7b** (193 MHz, DMSO-d_6)

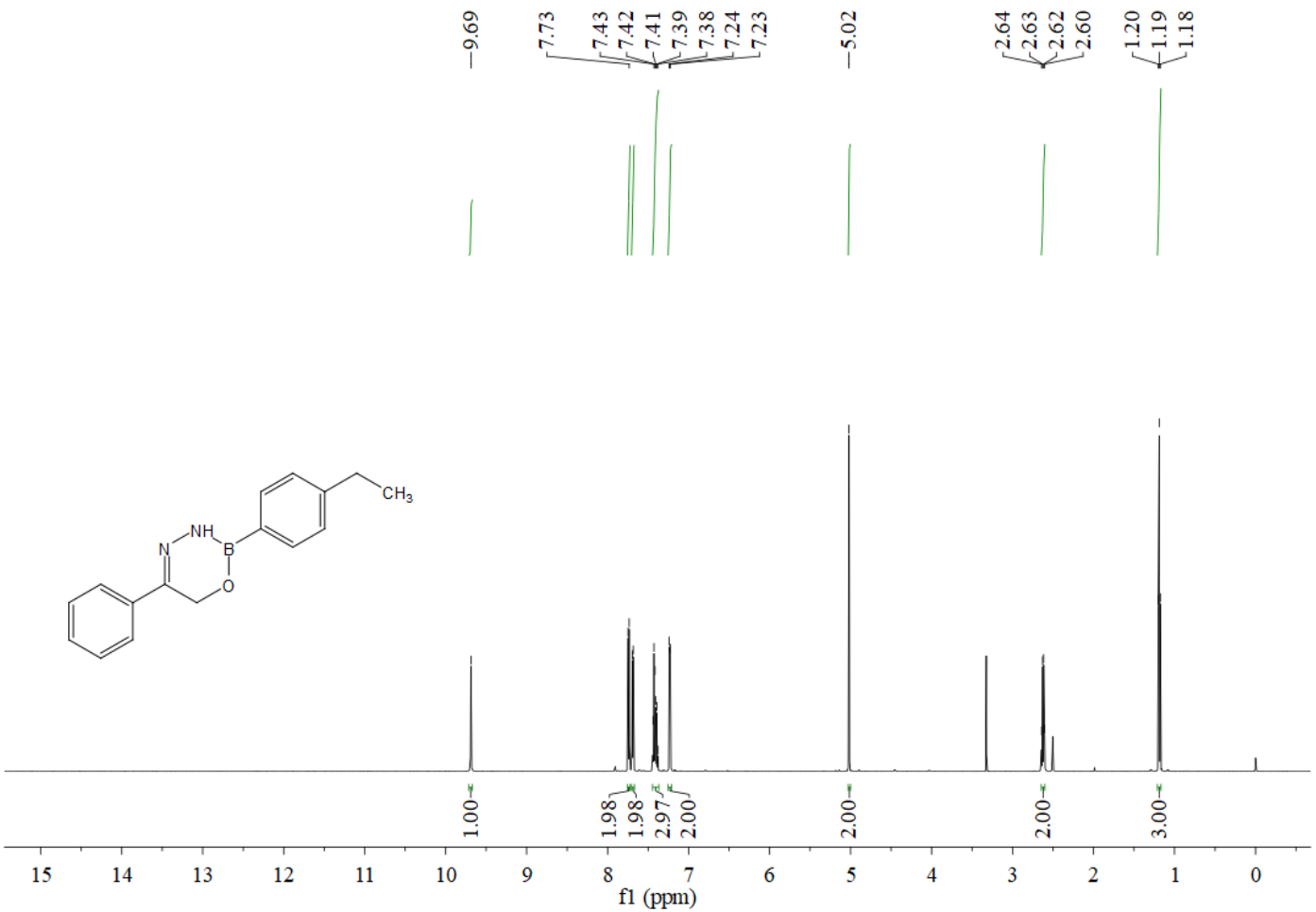


Fig. S85 ^{1}H NMR for compound **7c** (600 MHz, DMSO-d_6)

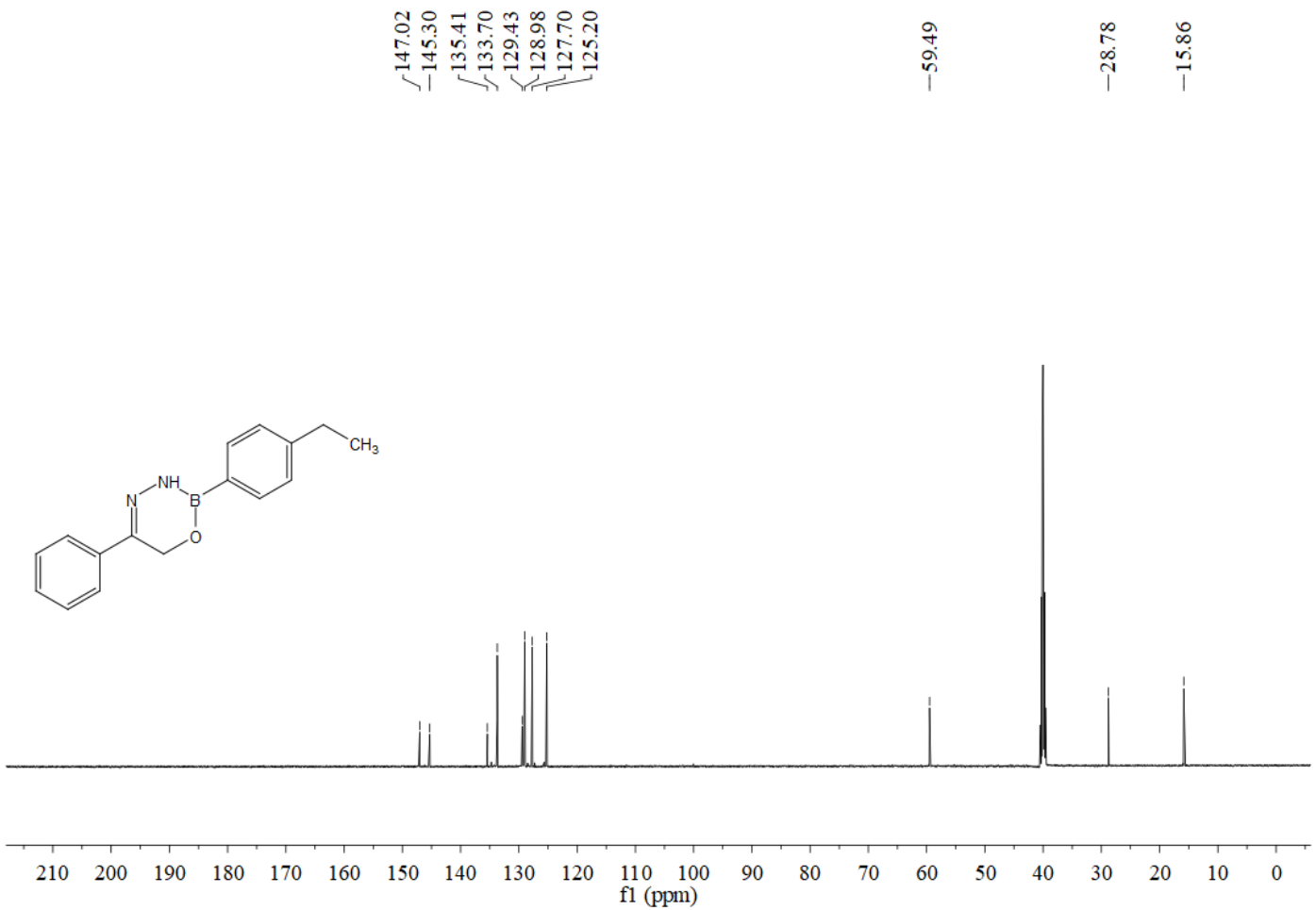


Fig. S86 ^{13}C NMR for compound **7c** (151 MHz, DMSO-d_6)

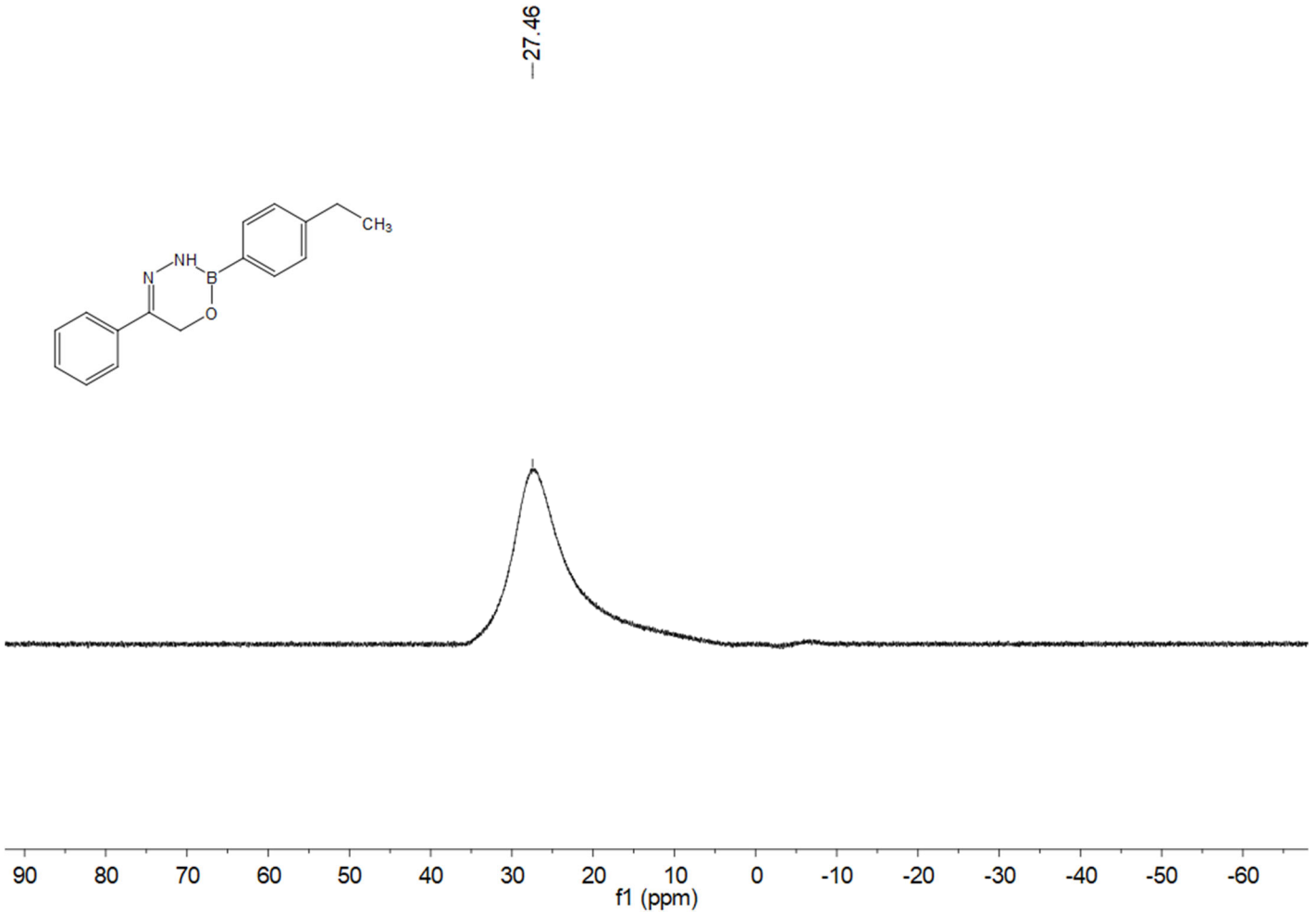


Fig. S87 ^{11}B NMR for compound **7c** (193 MHz, DMSO-d_6)

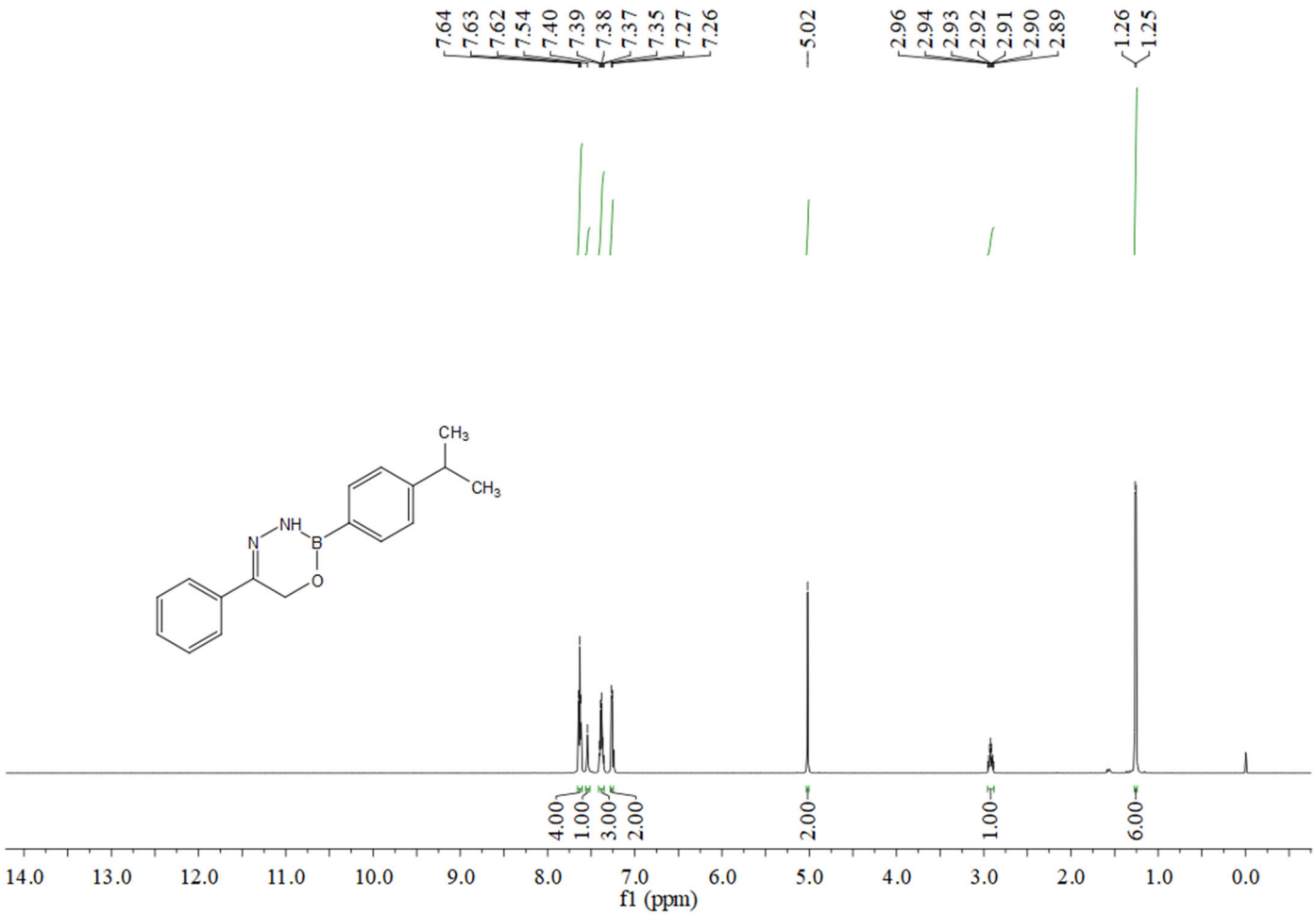


Fig. S88 ^{1}H NMR for compound **7d** (600 MHz, $CDCl_3$)

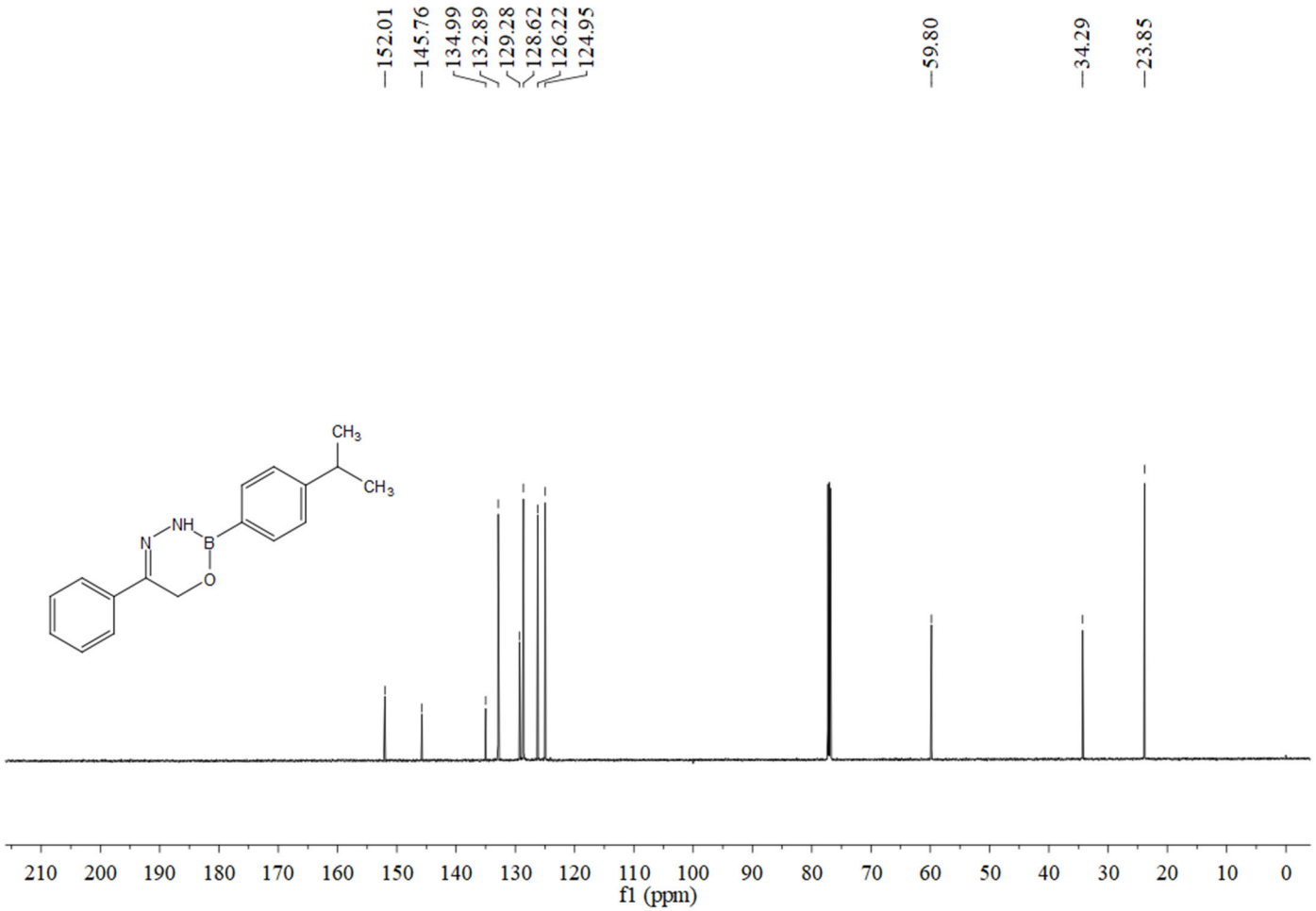


Fig. S89 ^{13}C NMR for compound **7d** (151 MHz, $CDCl_3$)

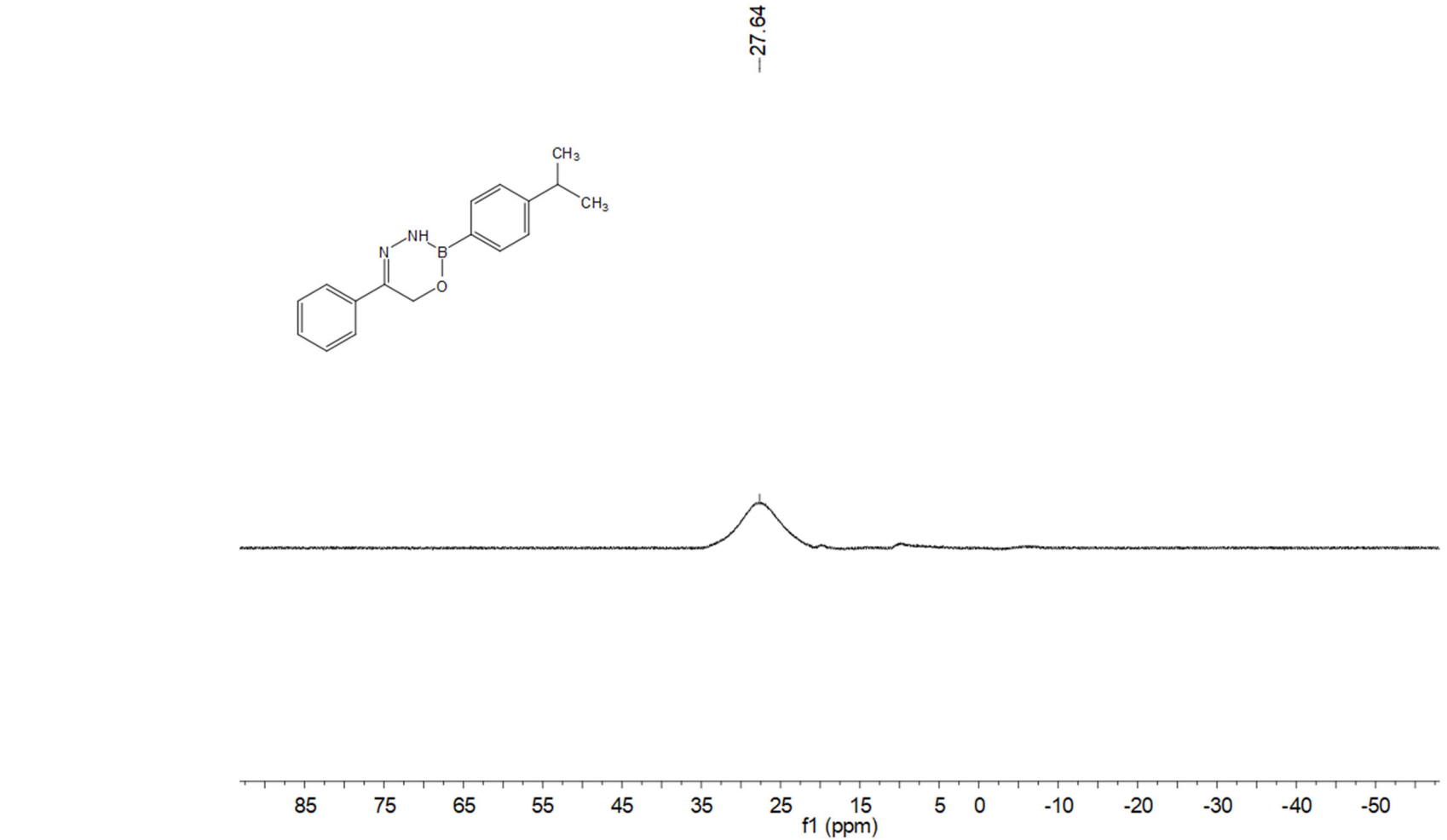


Fig. S90 ^{11}B NMR for compound **7d** (193 MHz, DMSO-d_6)

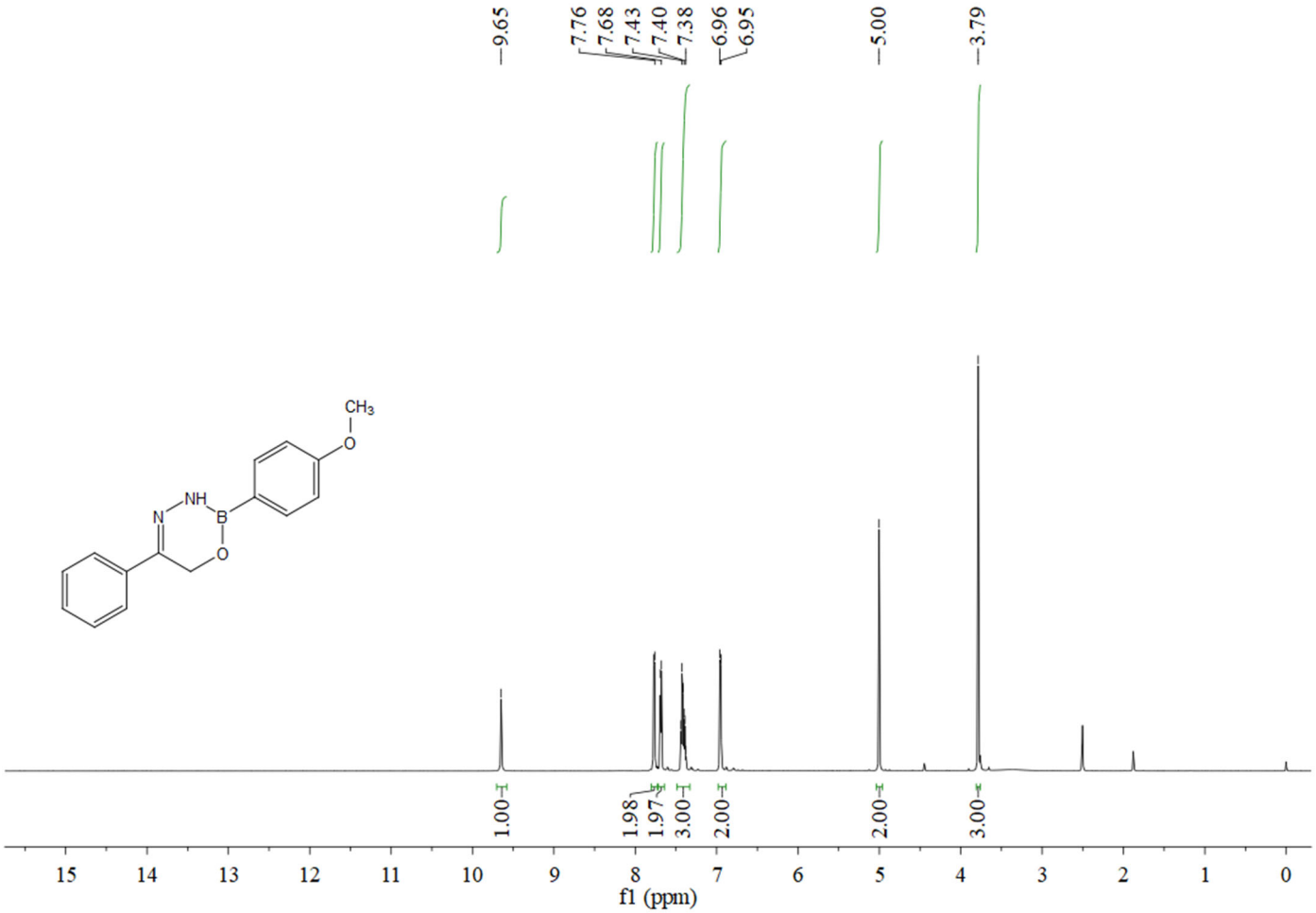


Fig. S91 ^{1}H NMR for compound **7e** (600 MHz, DMSO-d_6)

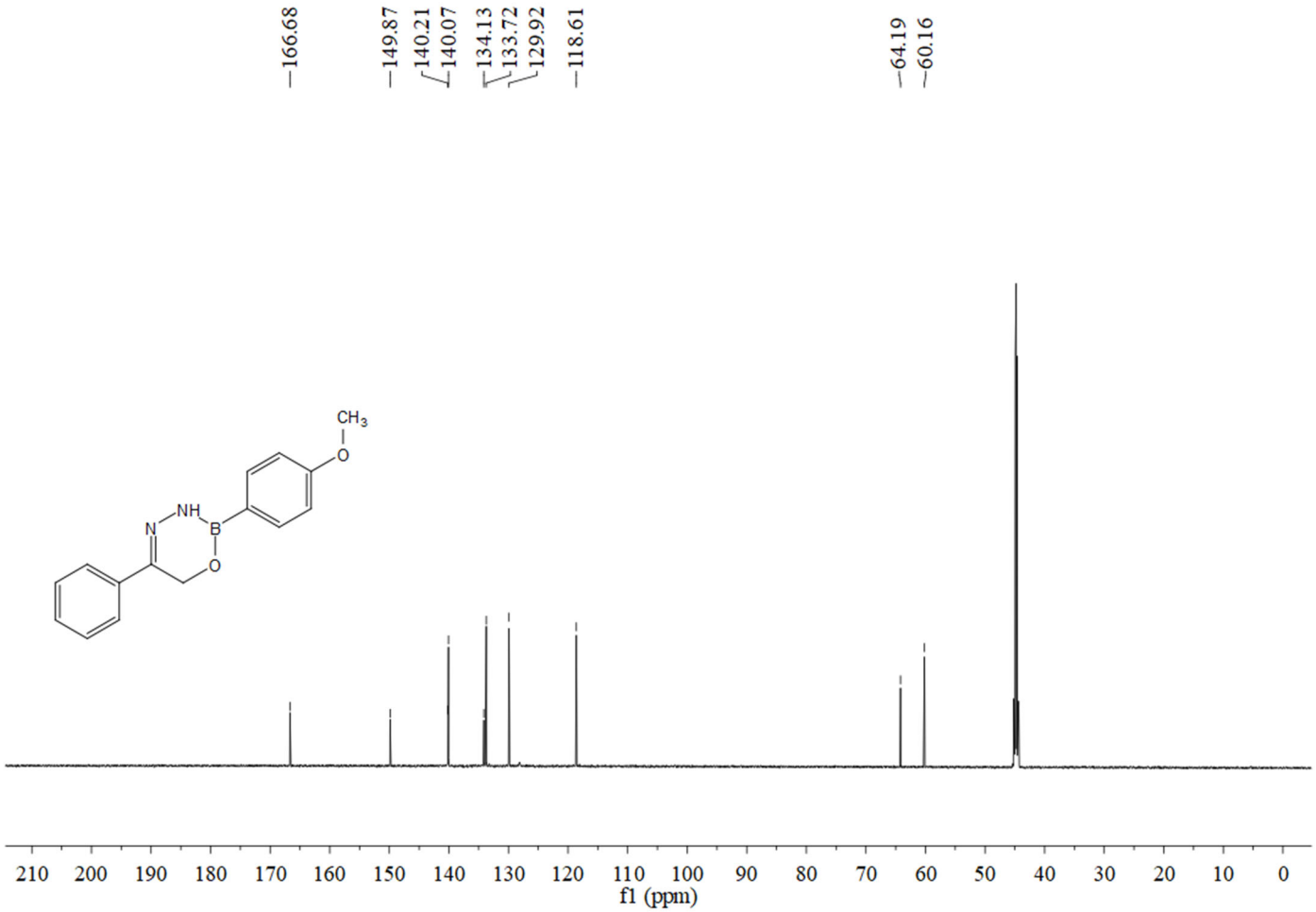


Fig. S92 ^{13}C NMR for compound **7e** (151 MHz, DMSO-d_6)

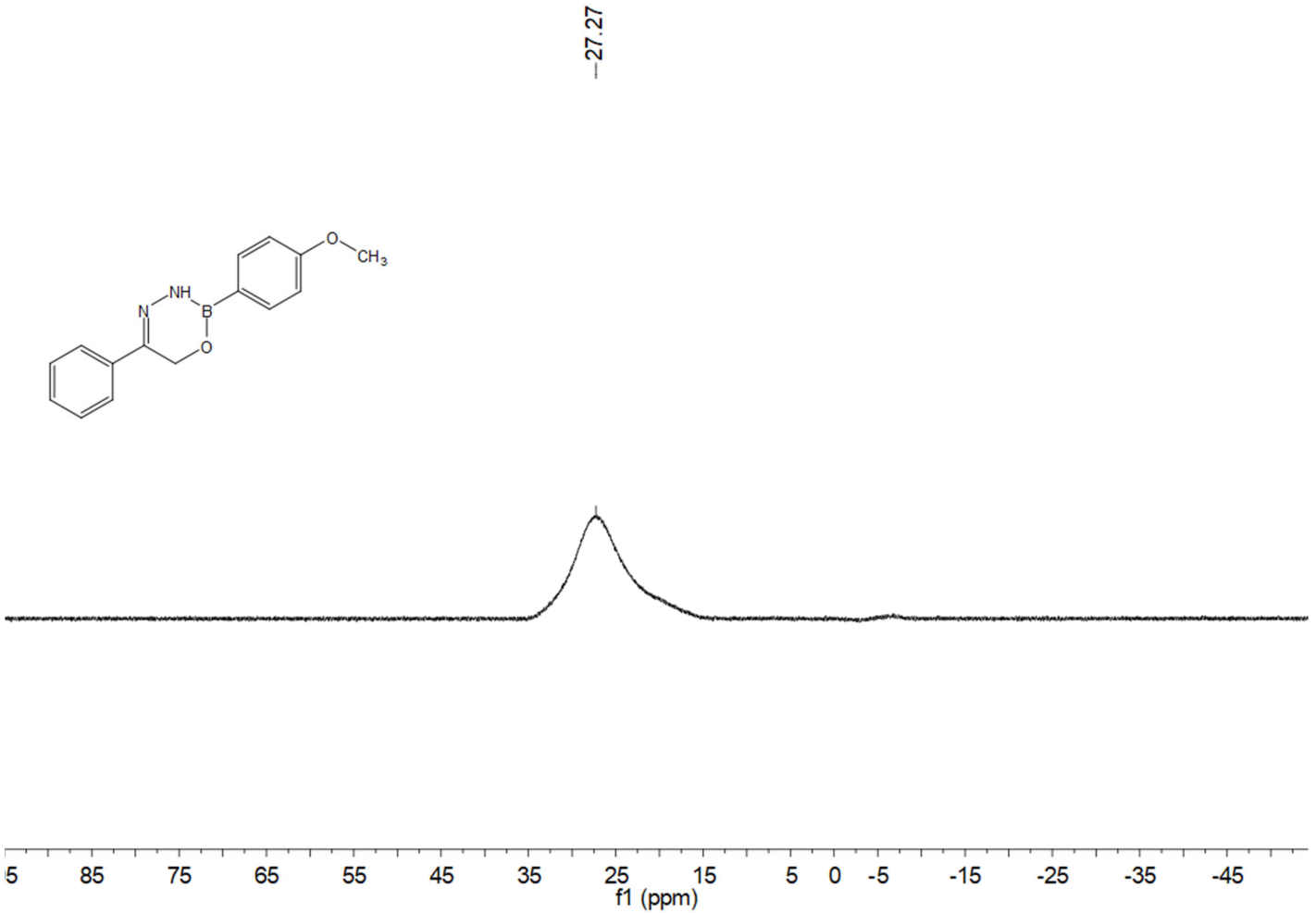


Fig. S93 ^{11}B NMR for compound **7e** (193 MHz, DMSO-d_6)

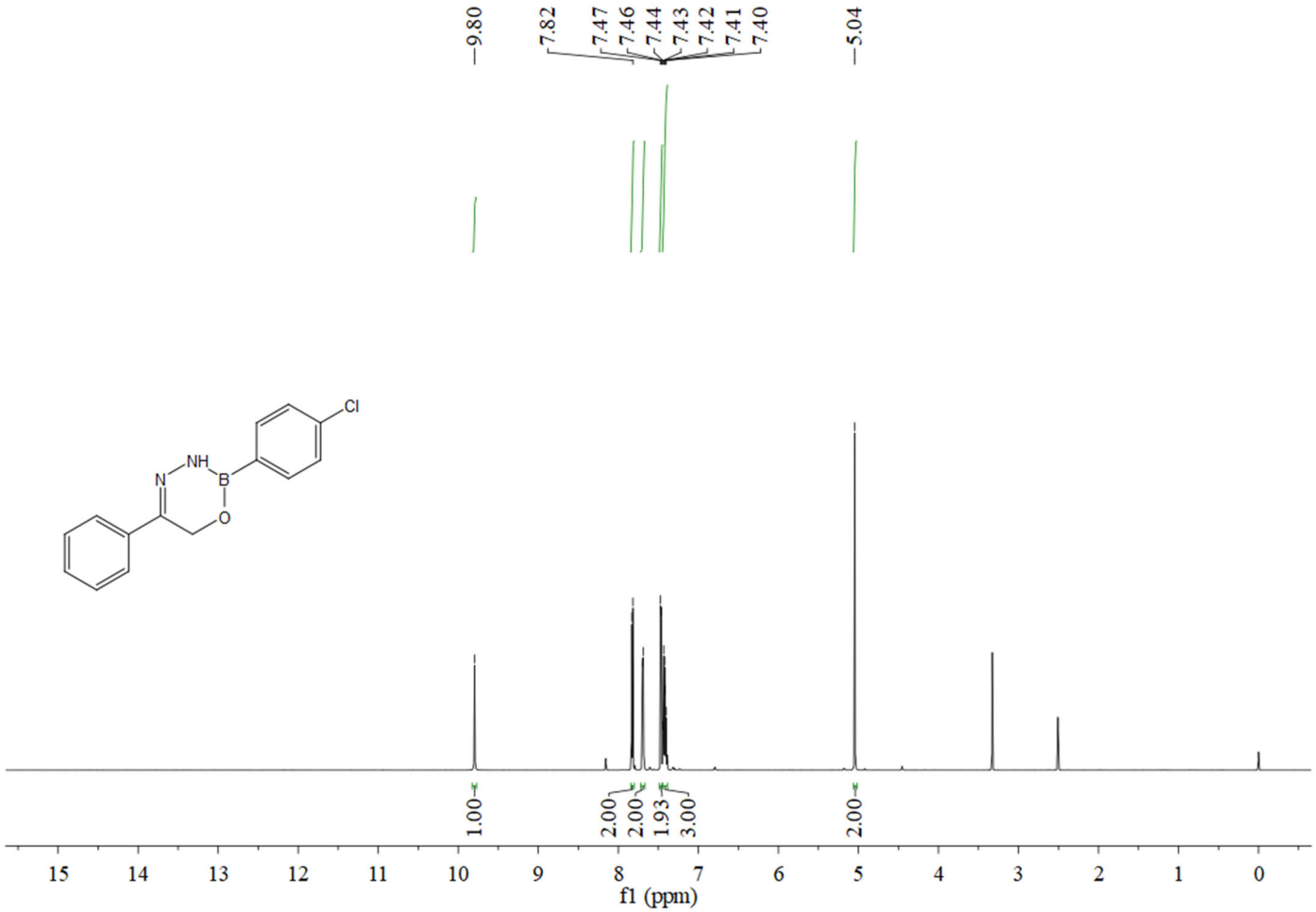


Fig. S94 ^{1}H NMR for compound **7f** (600 MHz, DMSO-d_6)

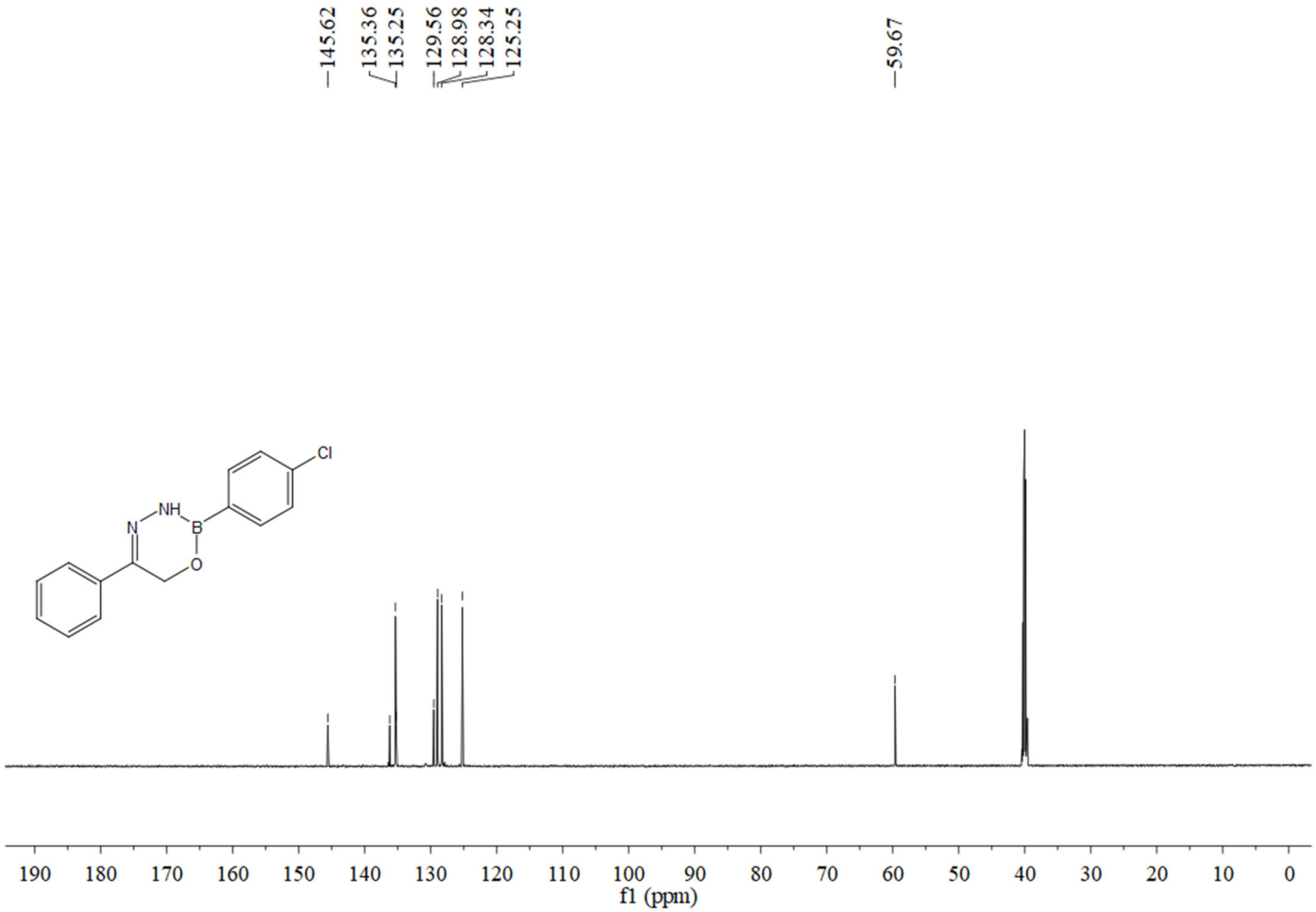


Fig. S95 ^{13}C NMR for compound **7f** (151 MHz, DMSO-d_6)

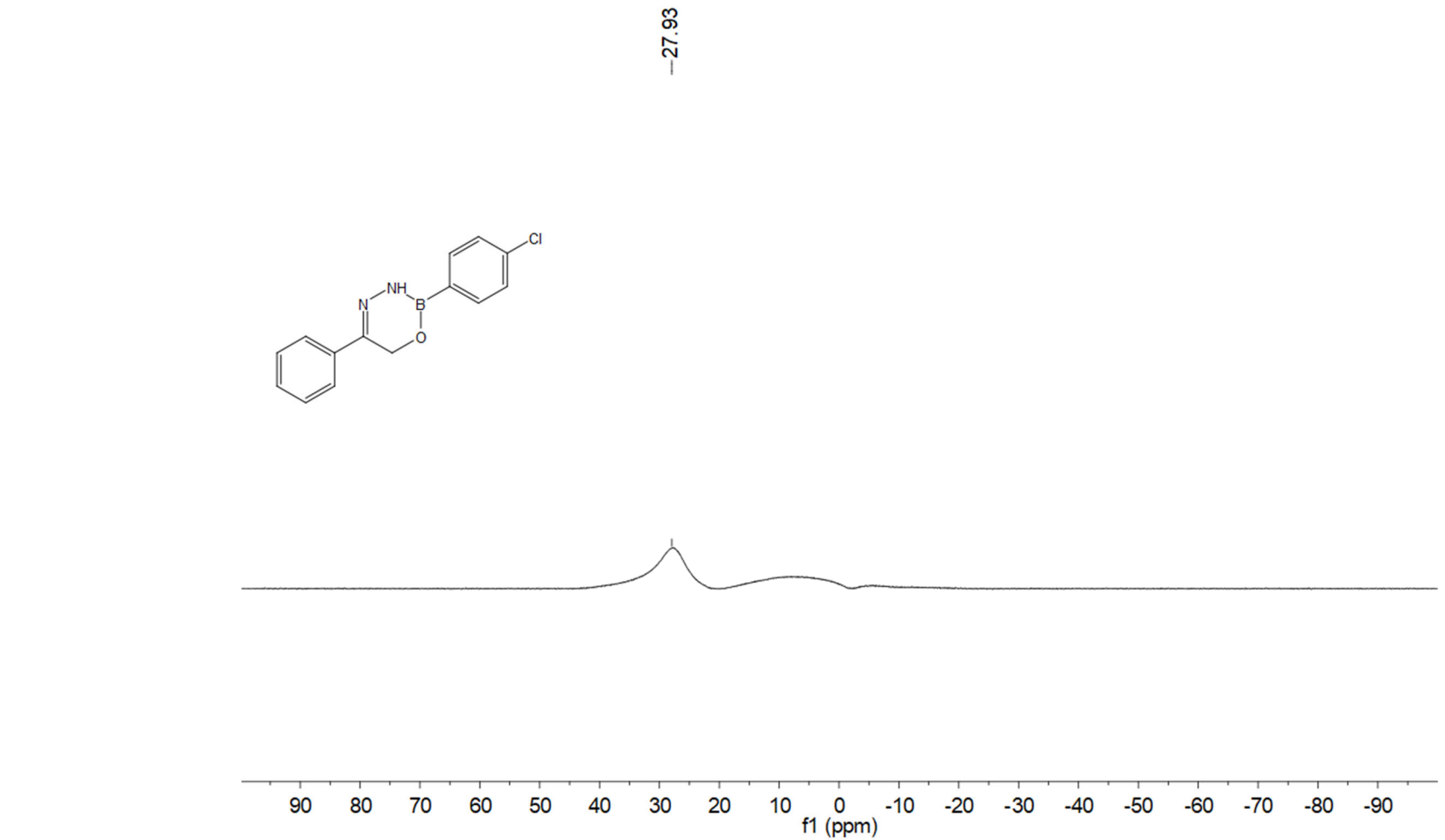


Fig. S96 ^{11}B NMR for compound **7f** (193 MHz, DMSO-d_6)

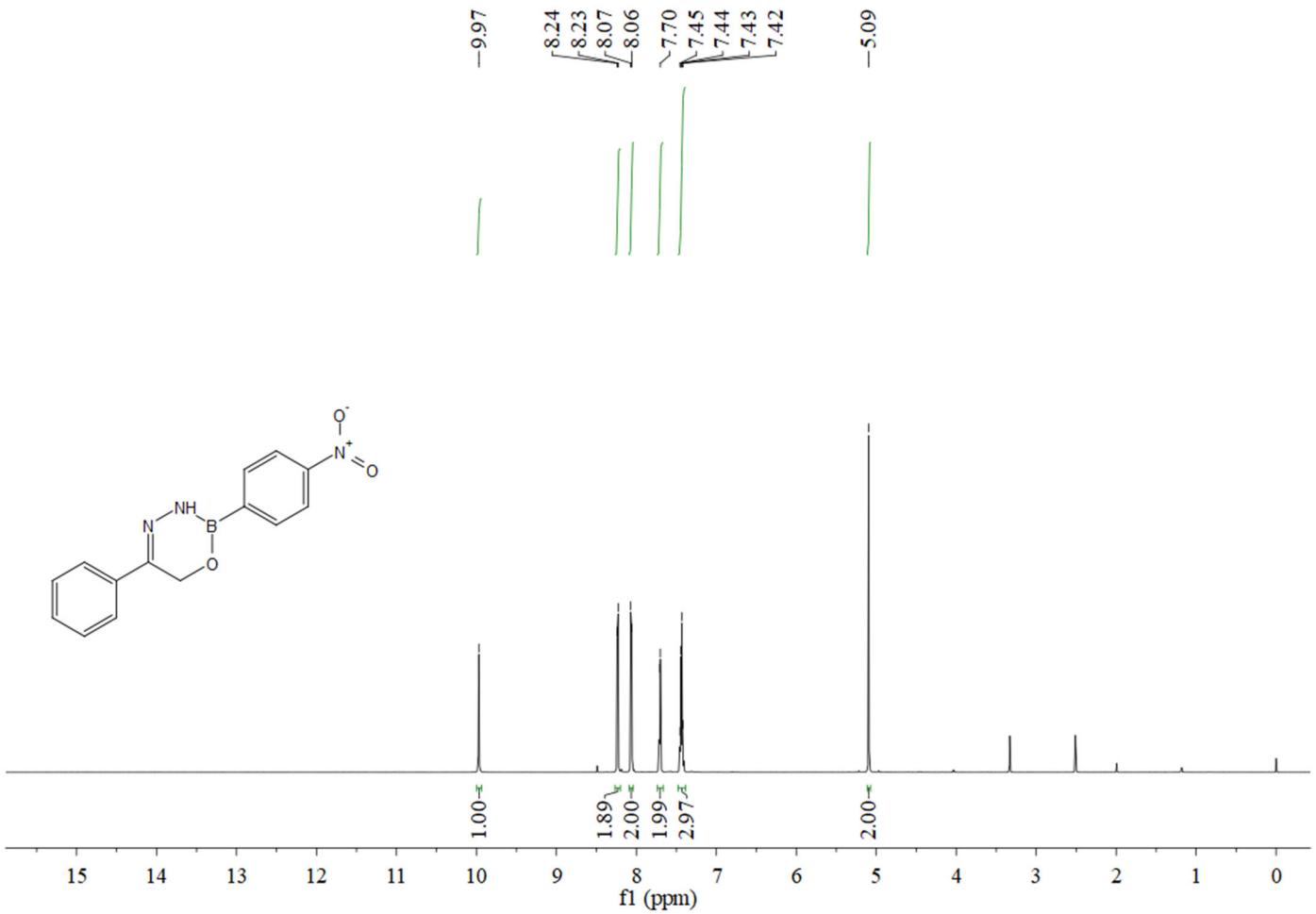


Fig. S97 ^{1}H NMR for compound **7g** (600 MHz, DMSO-d_6)

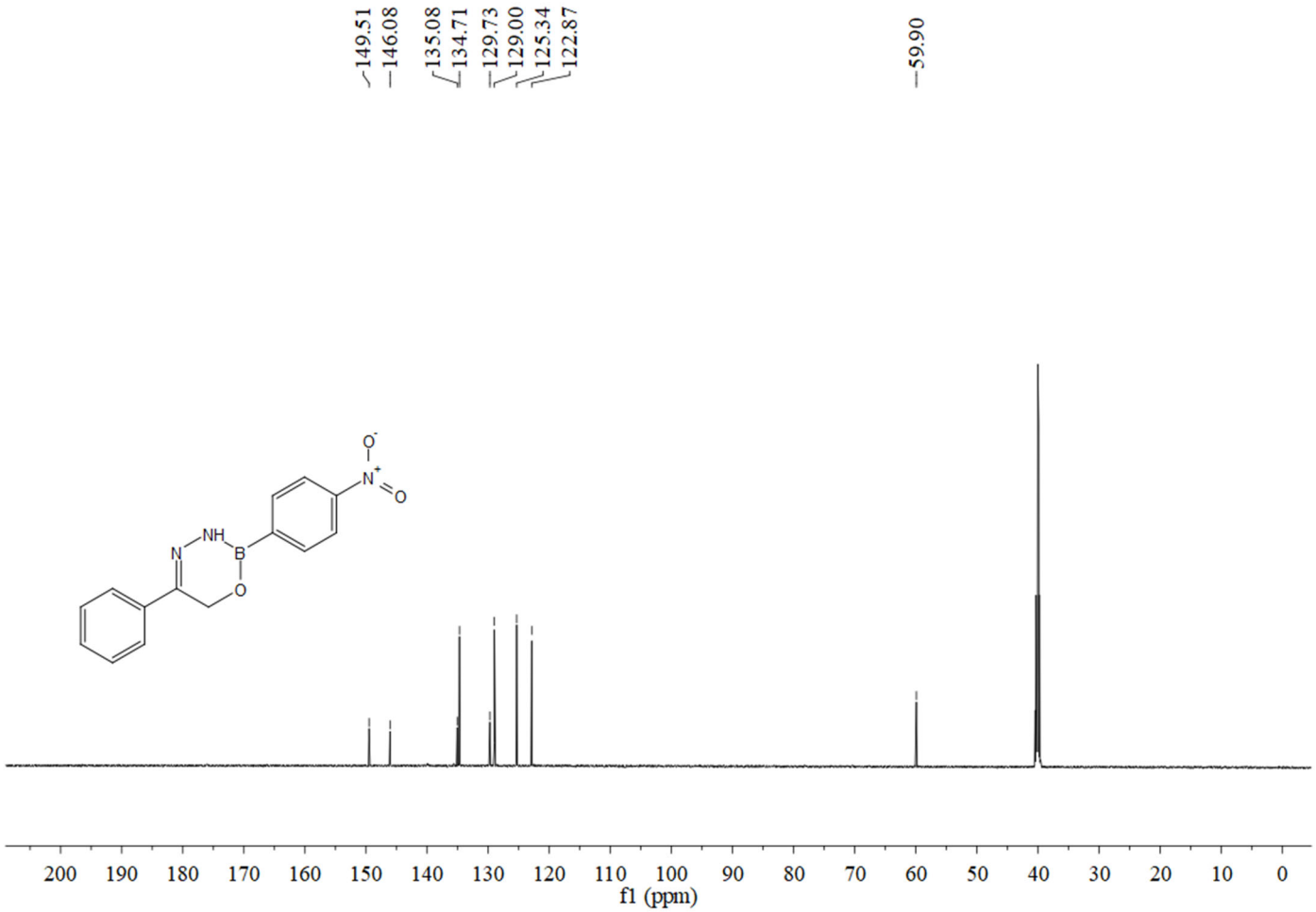


Fig. S98 ^{13}C NMR for compound **7g** (151 MHz, DMSO-d_6)

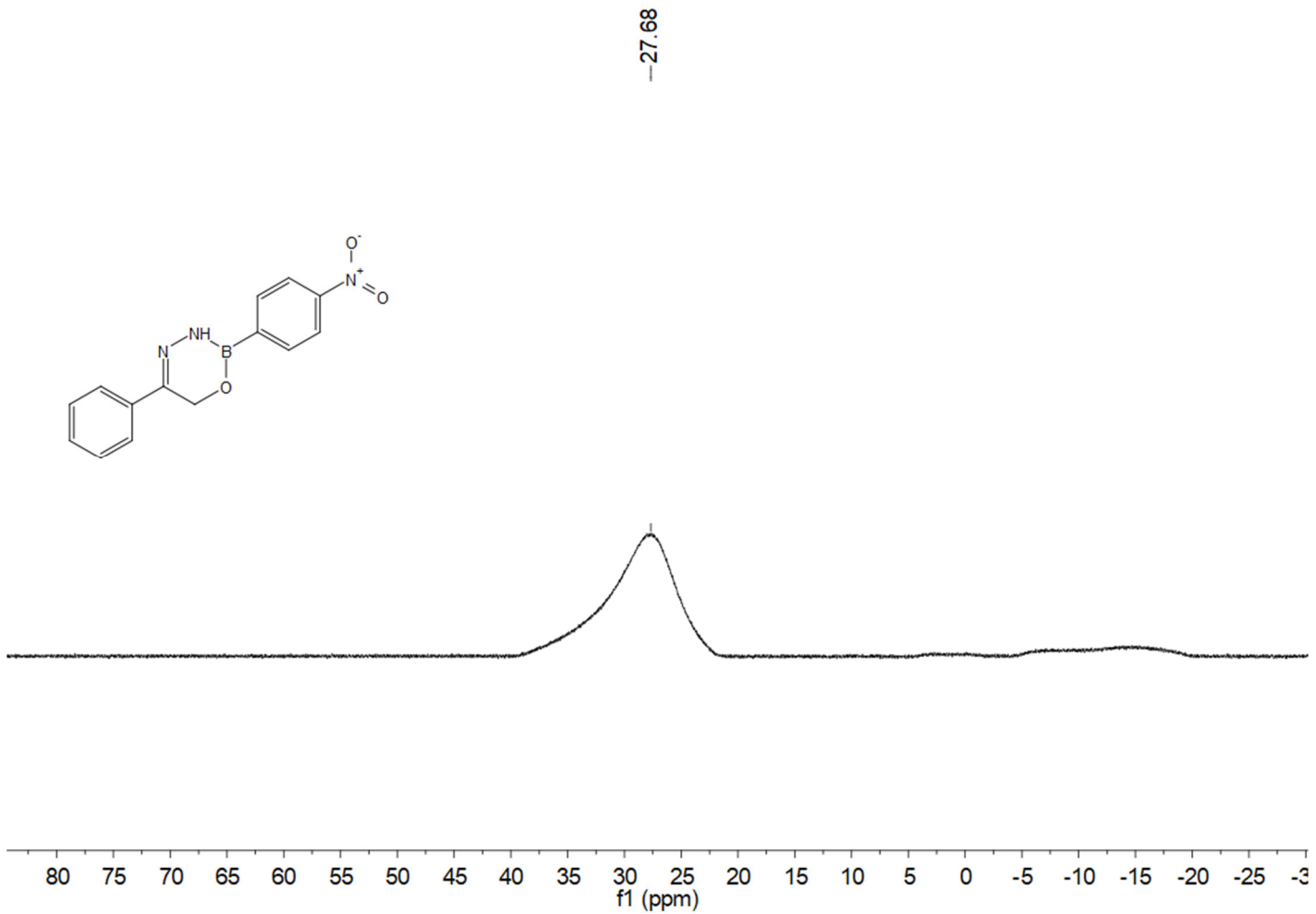


Fig. S99 ^{11}B NMR for compound **7g** (193 MHz, DMSO-d_6)

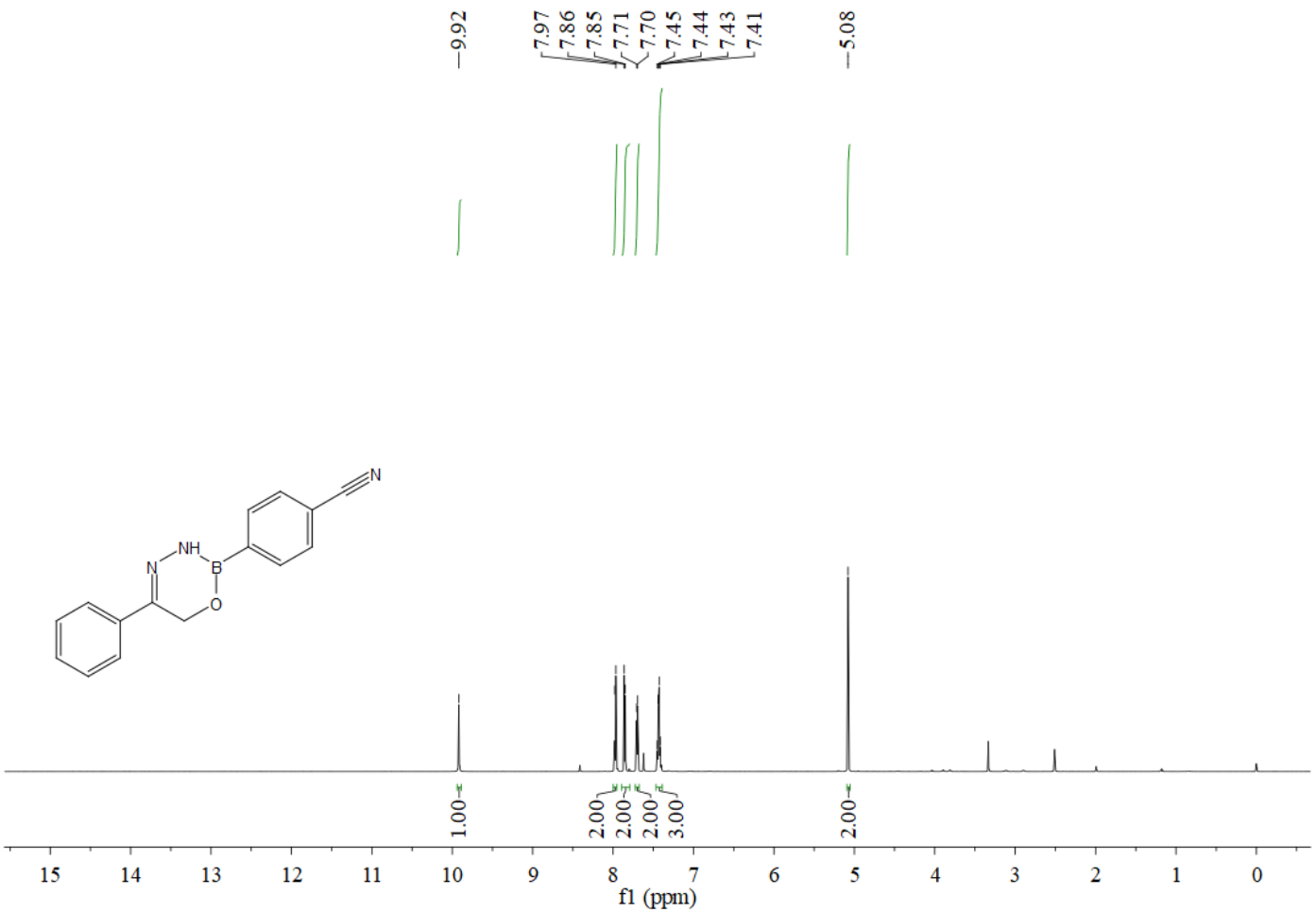


Fig. S100 ^{1}H NMR for compound **7h** (600 MHz, $CDCl_3$)

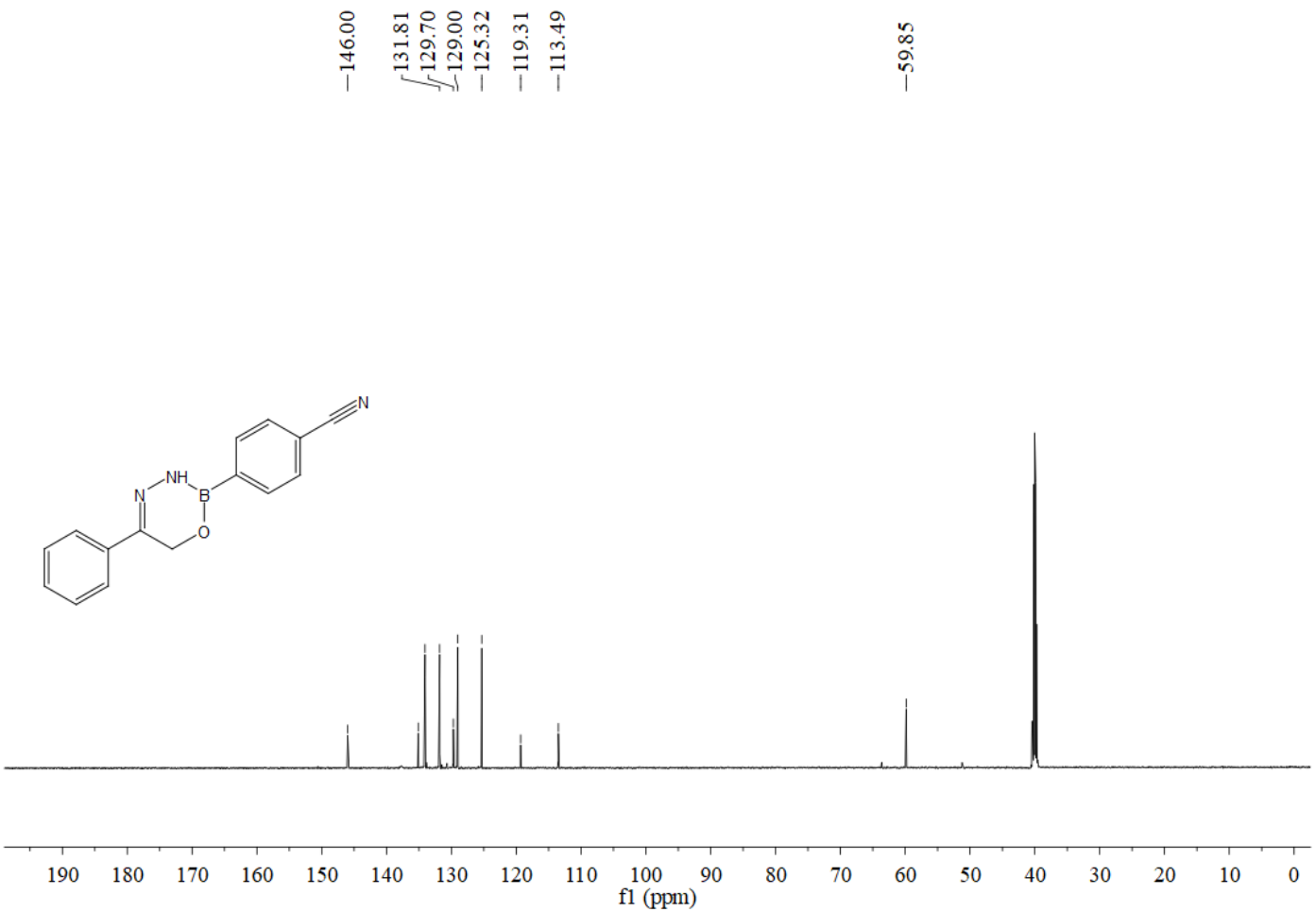


Fig. S101 ^{13}C NMR for compound **7h** (151 MHz, $CDCl_3$)

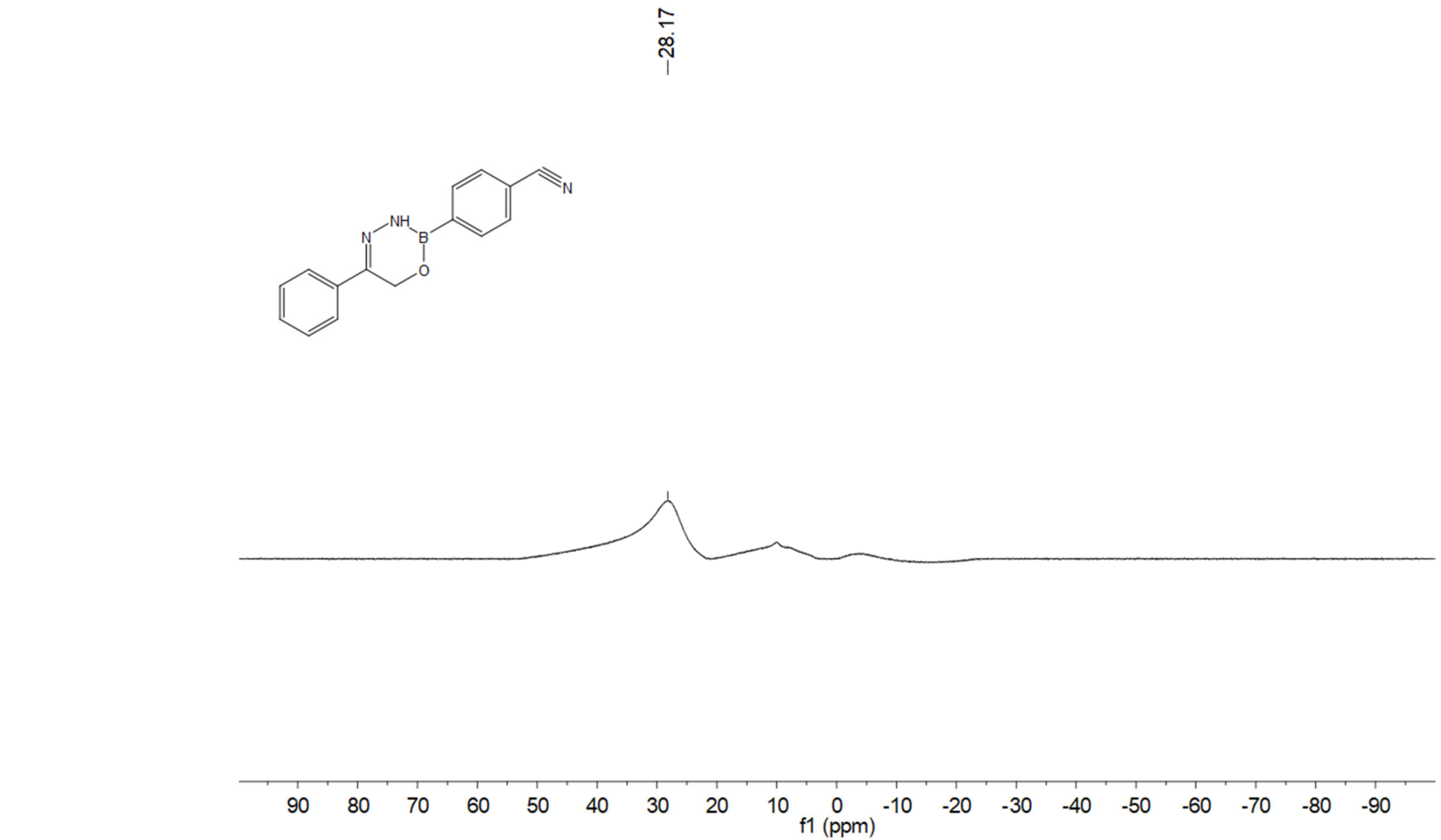


Fig. S102 ^{11}B NMR for compound **7h** (193 MHz, DMSO-d_6)

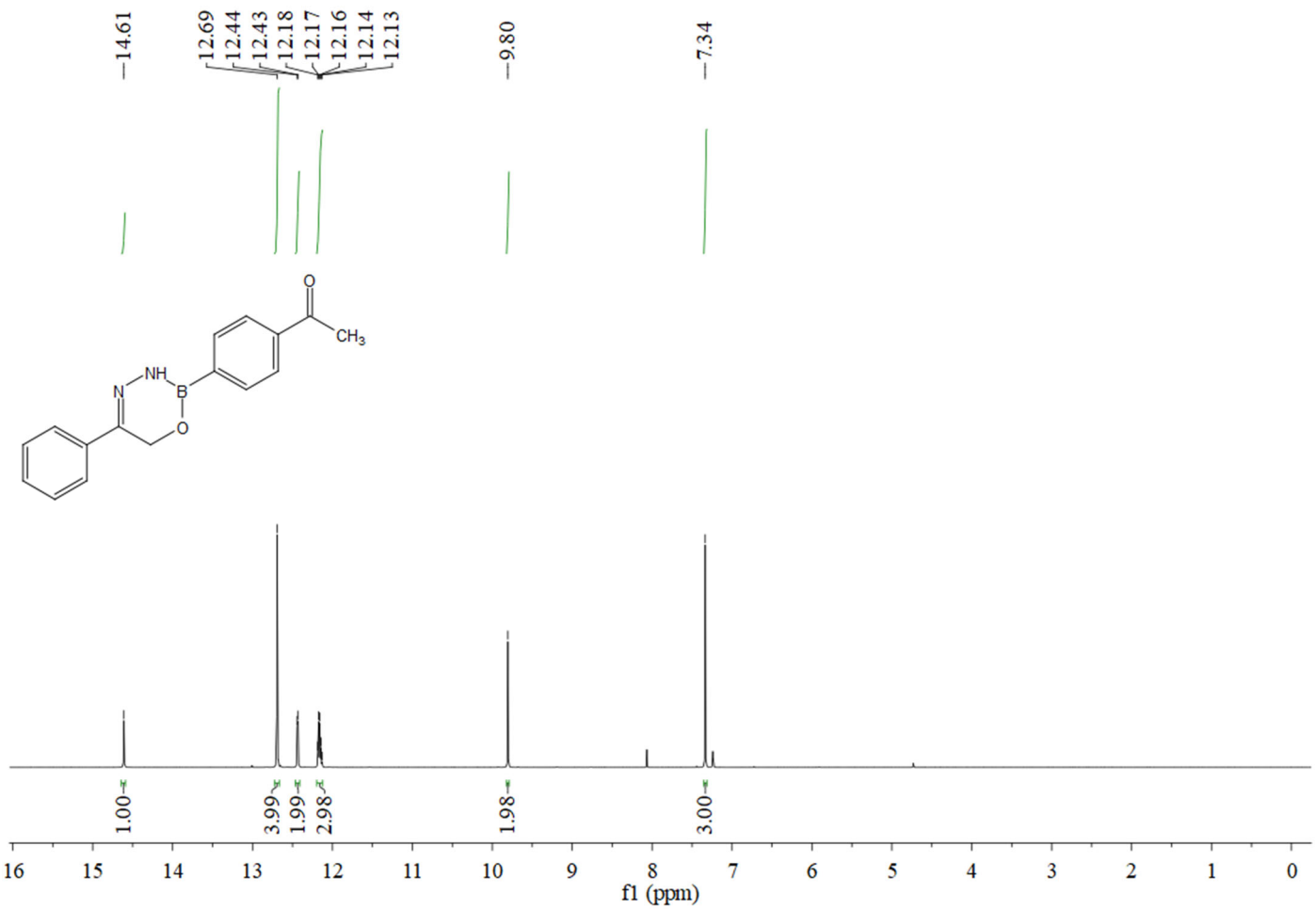


Fig. S103 ^{1}H NMR for compound **7i** (600 MHz, $CDCl_3$)

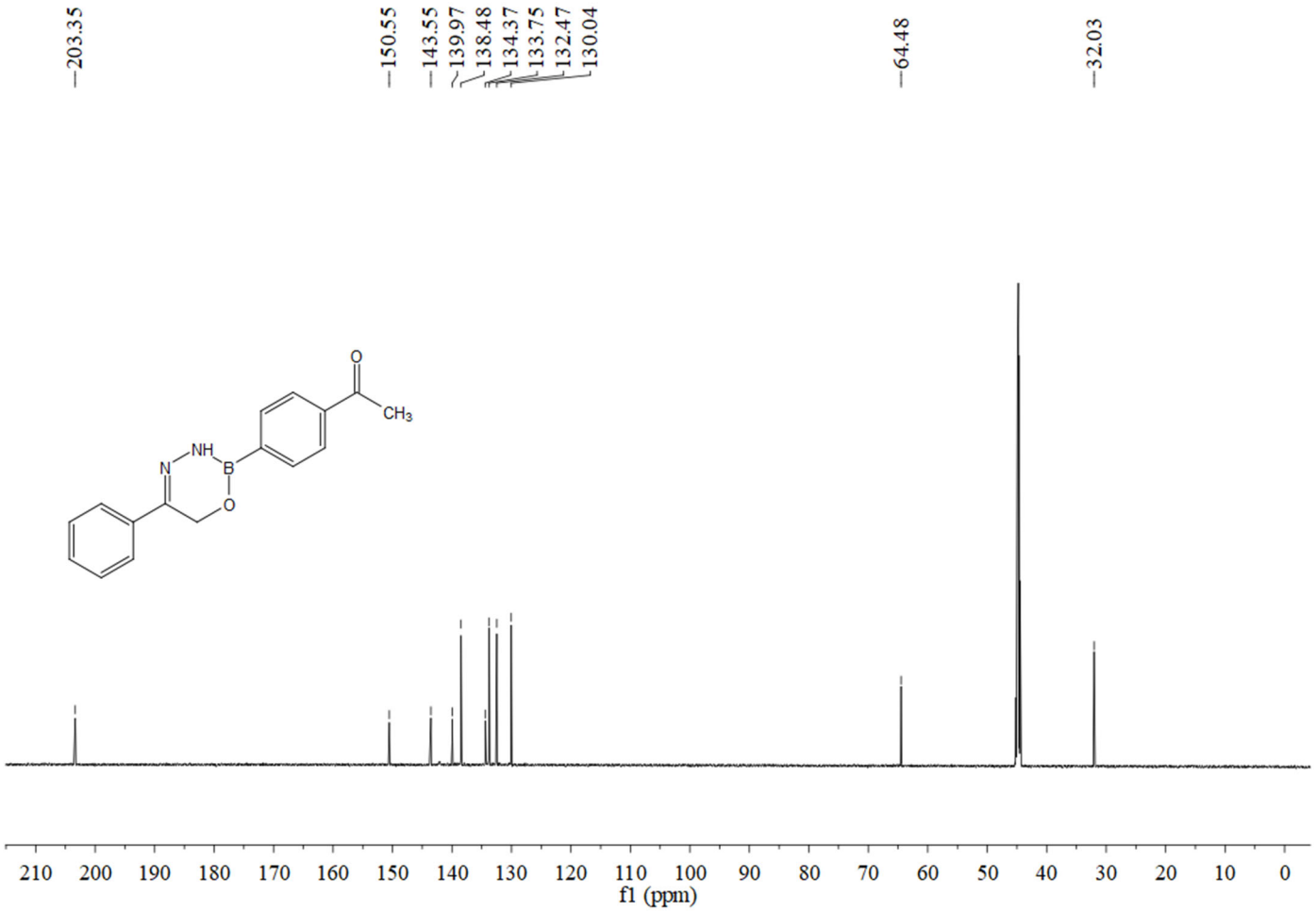


Fig. S104 ^{13}C NMR for compound **7i** (151 MHz, $CDCl_3$)

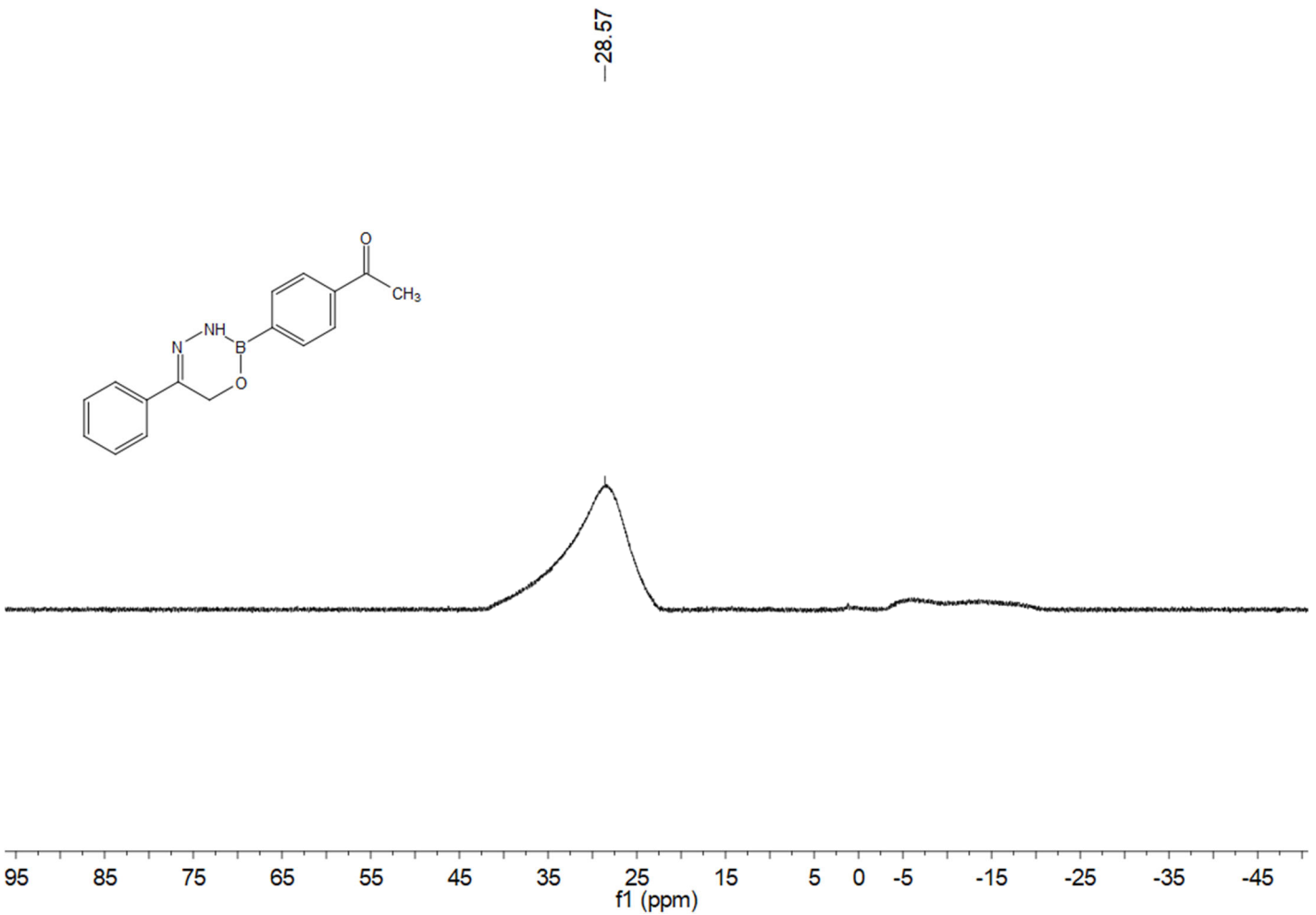


Fig. S105 ^{11}B NMR for compound **7i** (193 MHz, DMSO-d_6)

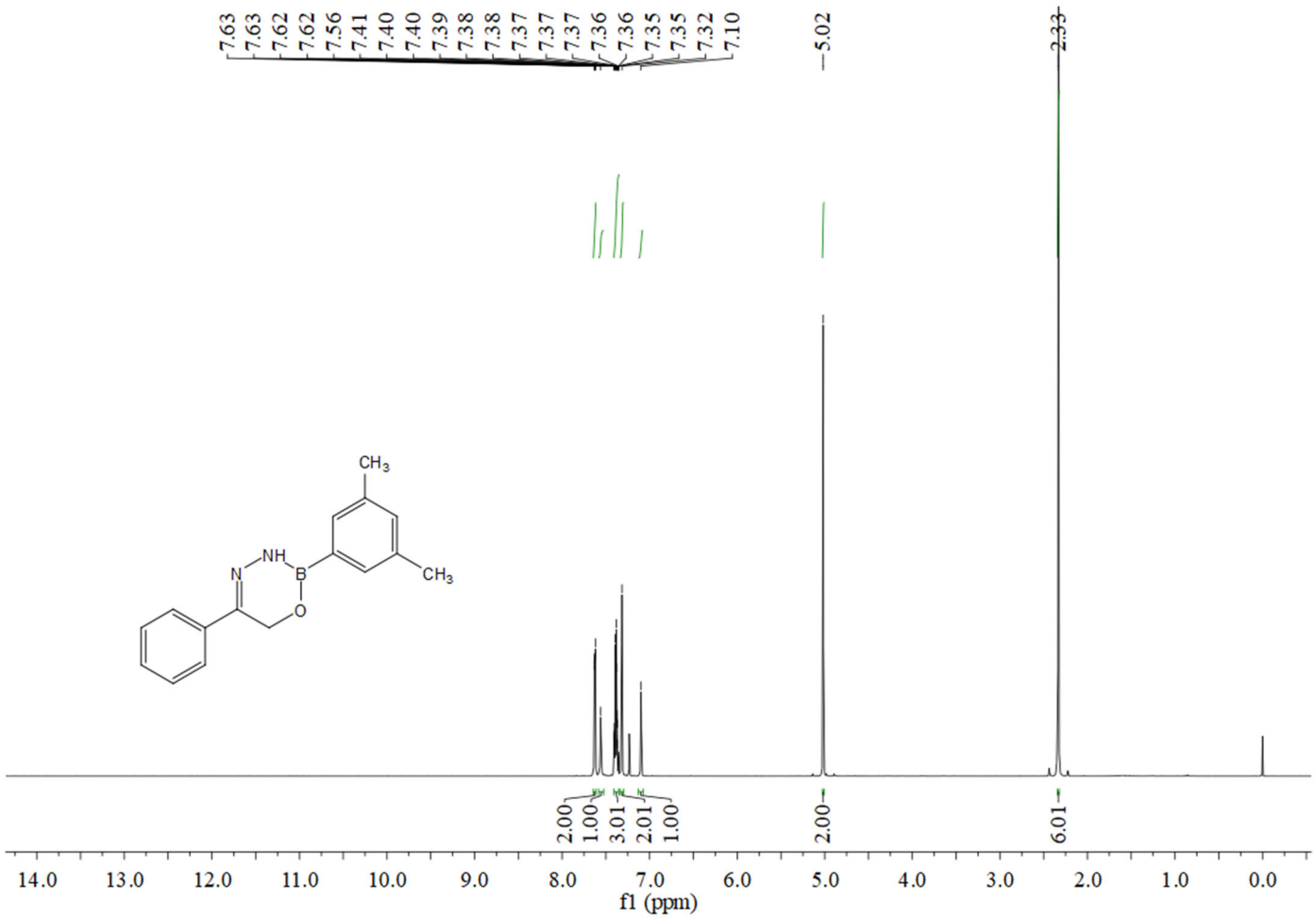


Fig. S106 ^{1}H NMR for compound **7j** (600 MHz, $CDCl_3$)

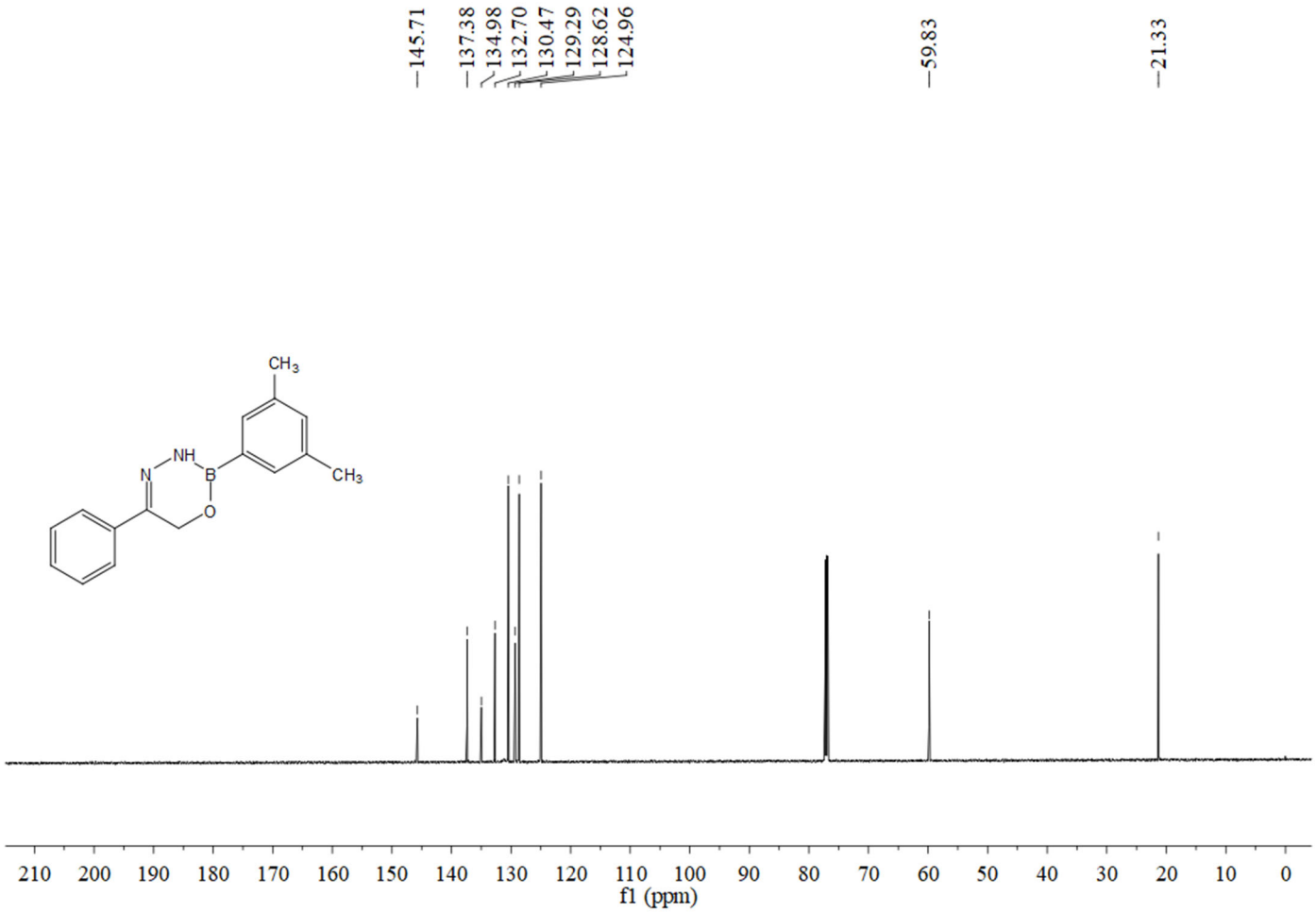


Fig. S107 ^{13}C NMR for compound **7j** (151 MHz, $CDCl_3$)

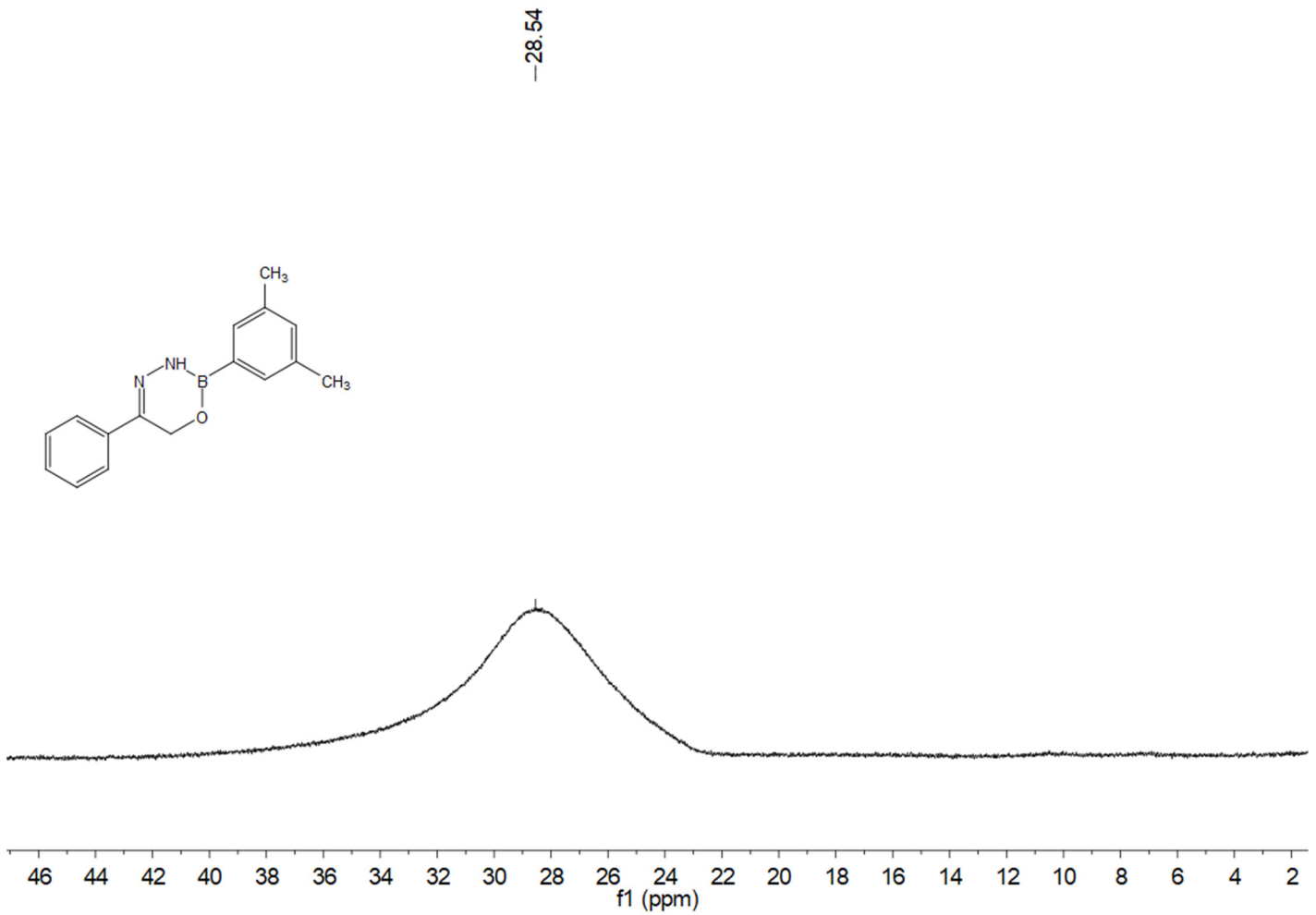


Fig. S108 ^{11}B NMR for compound **7j** (193 MHz, DMSO-d_6)

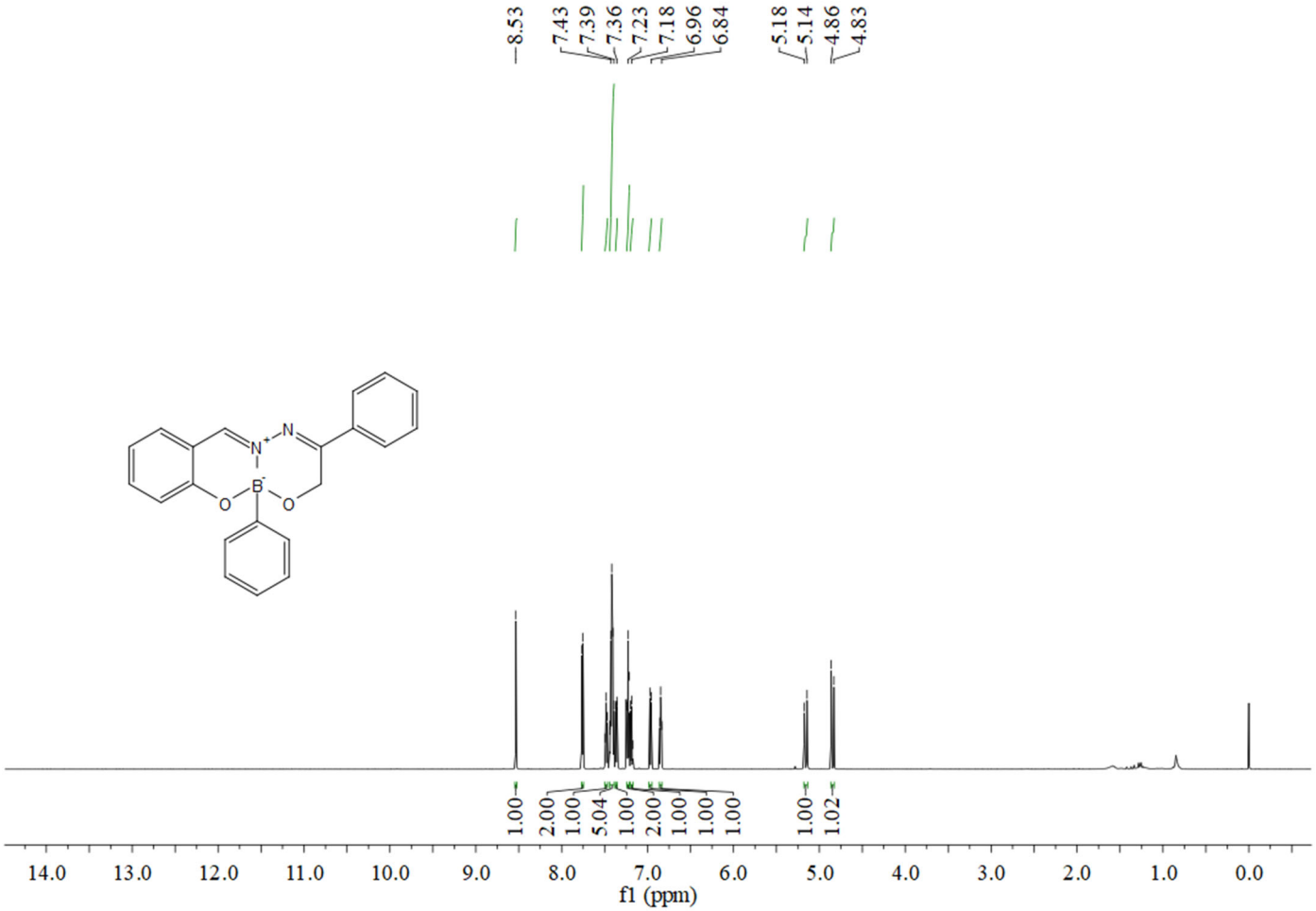


Fig. S109 ^{1}H NMR for compound **9a** (600 MHz, $CDCl_3$)

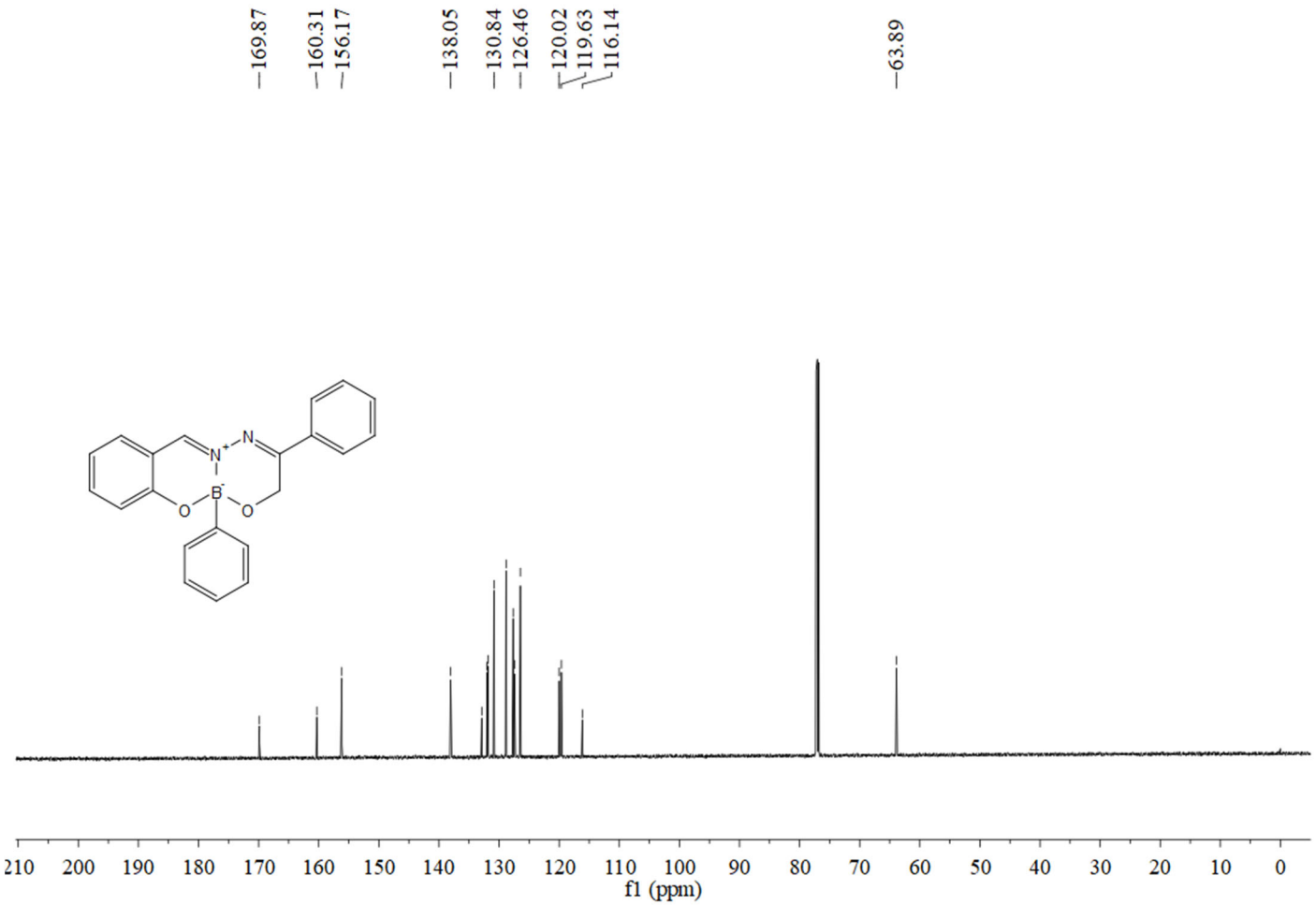


Fig. S110 ^{13}C NMR for compound **9a** (151 MHz, $CDCl_3$)

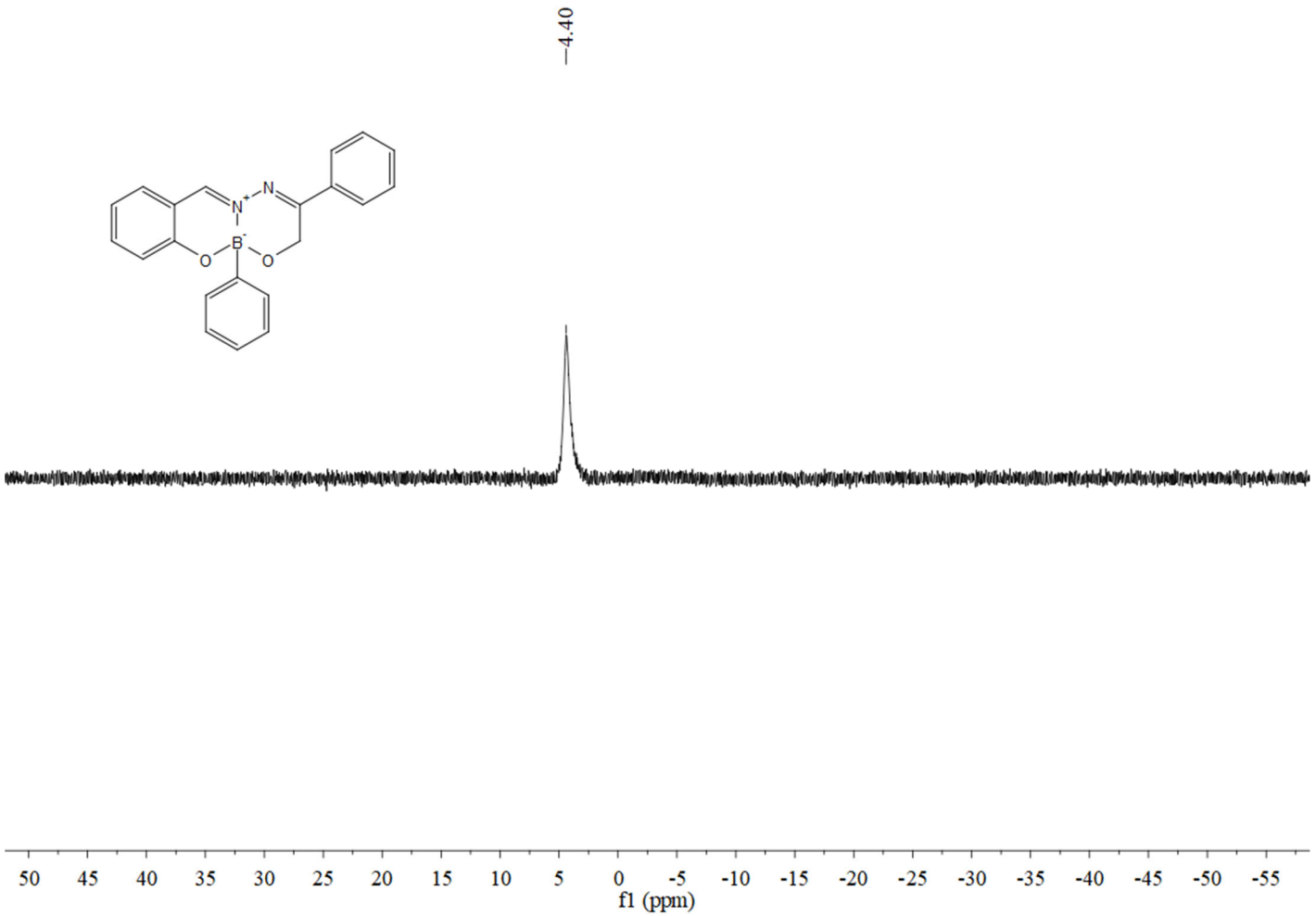


Fig. S111 ^{11}B NMR for compound **9a** (193 MHz, $CDCl_3$)

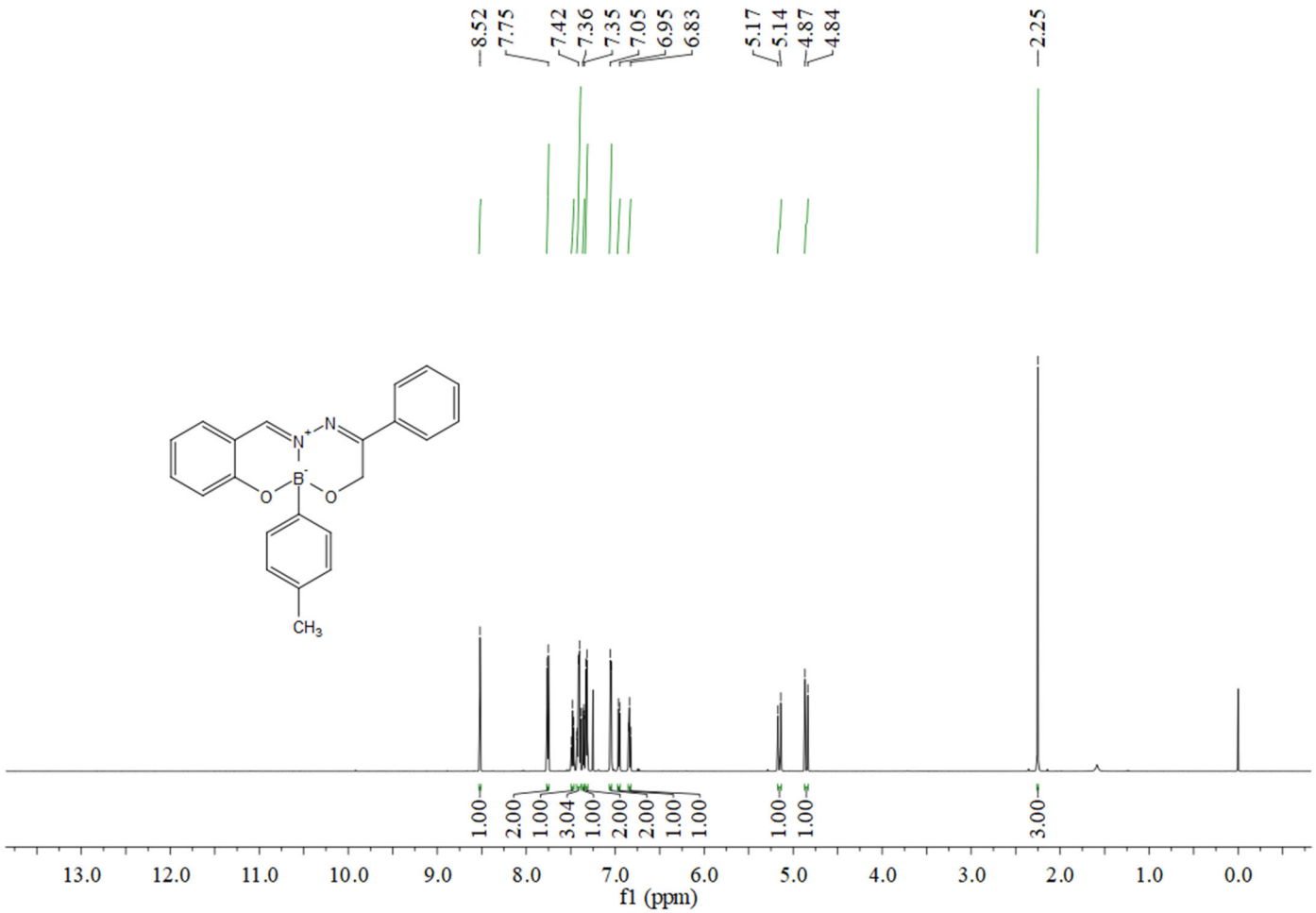


Fig. S112 ^{1}H NMR for compound **9b** (600 MHz, $CDCl_3$)

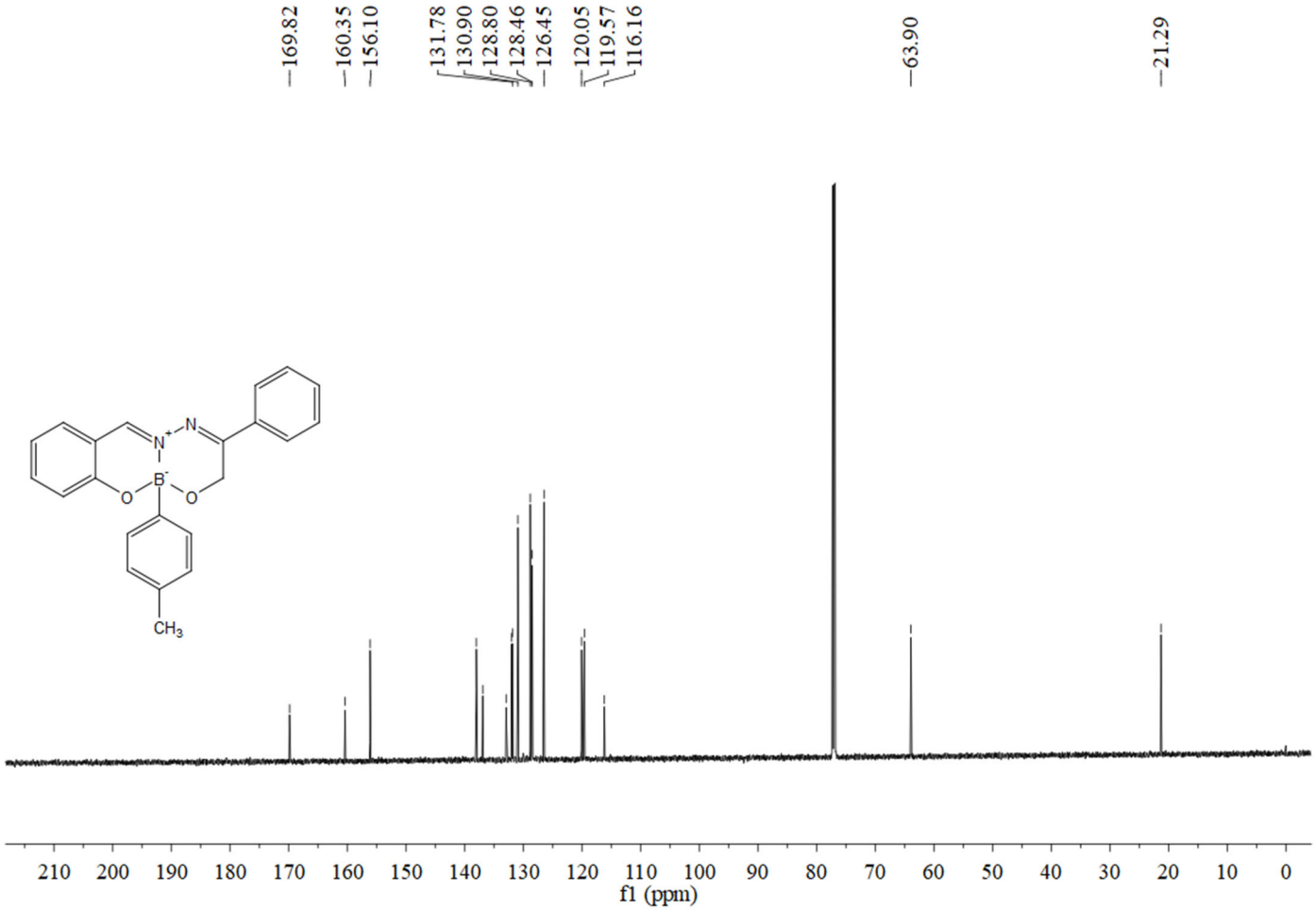


Fig. S113 ^{13}C NMR for compound **9b** (151 MHz, $CDCl_3$)

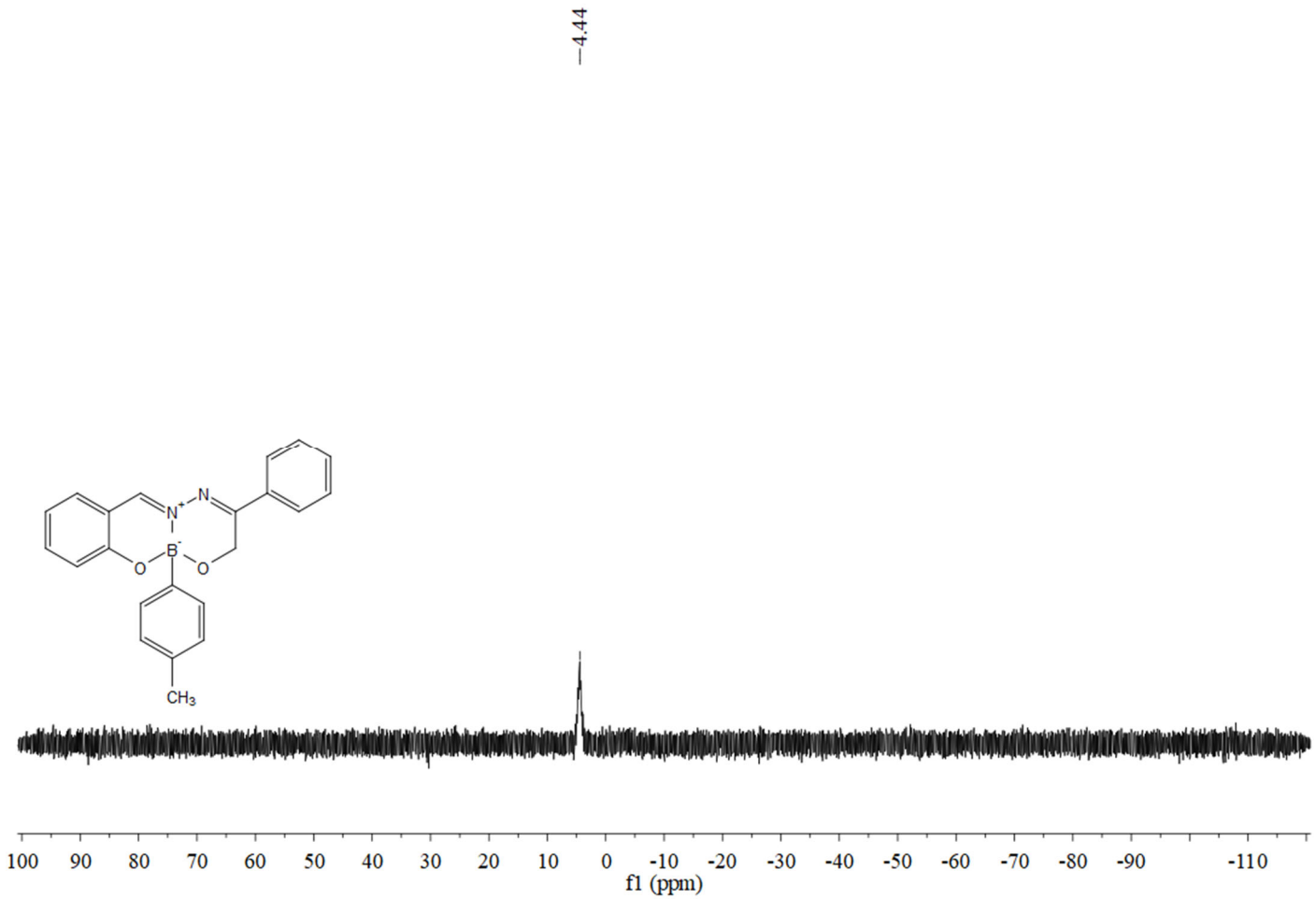


Fig. S114 ^{11}B NMR for compound **9b** (193 MHz, $CDCl_3$)

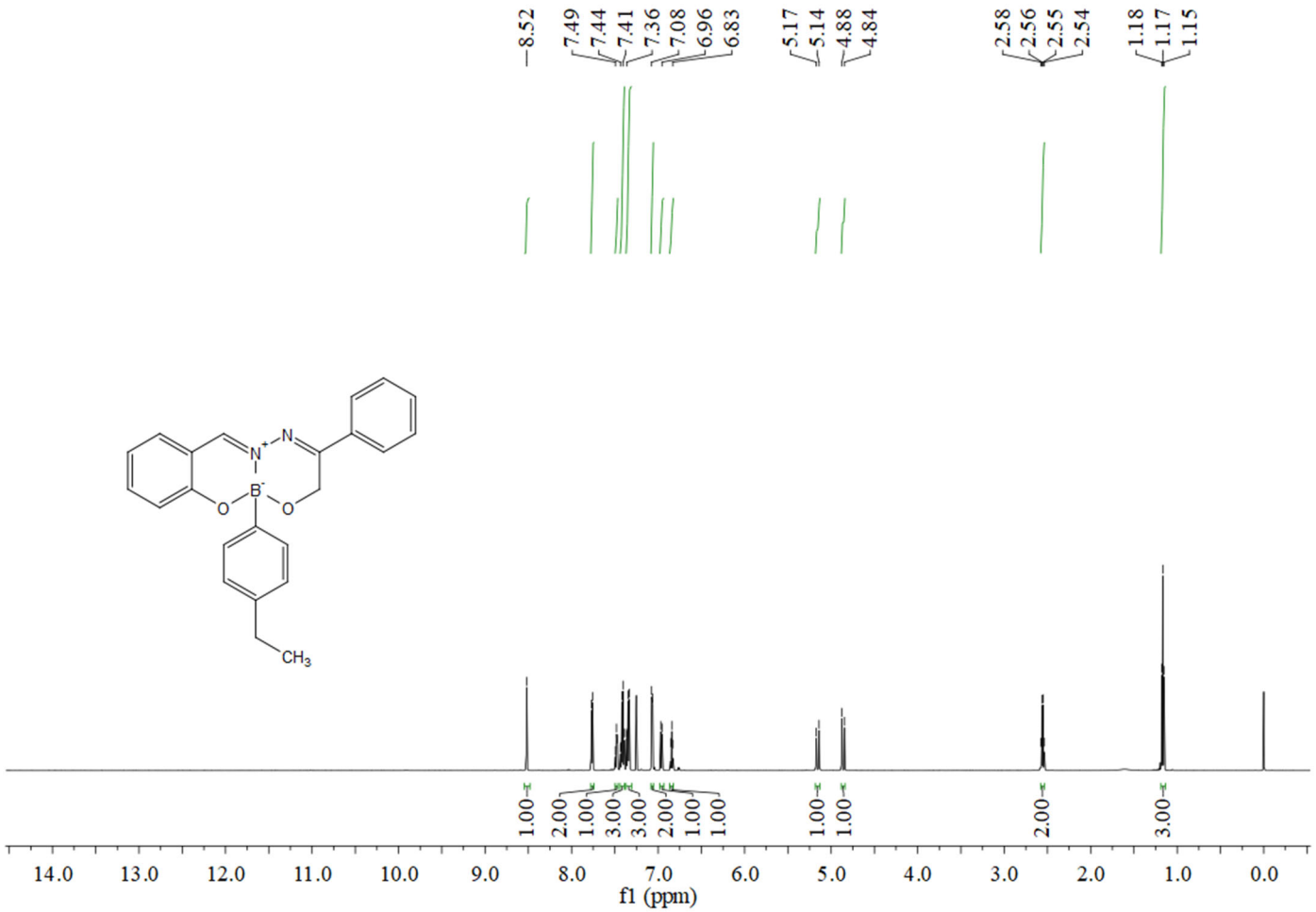


Fig. S115 ^{1}H NMR for compound **9c** (600 MHz, $CDCl_3$)

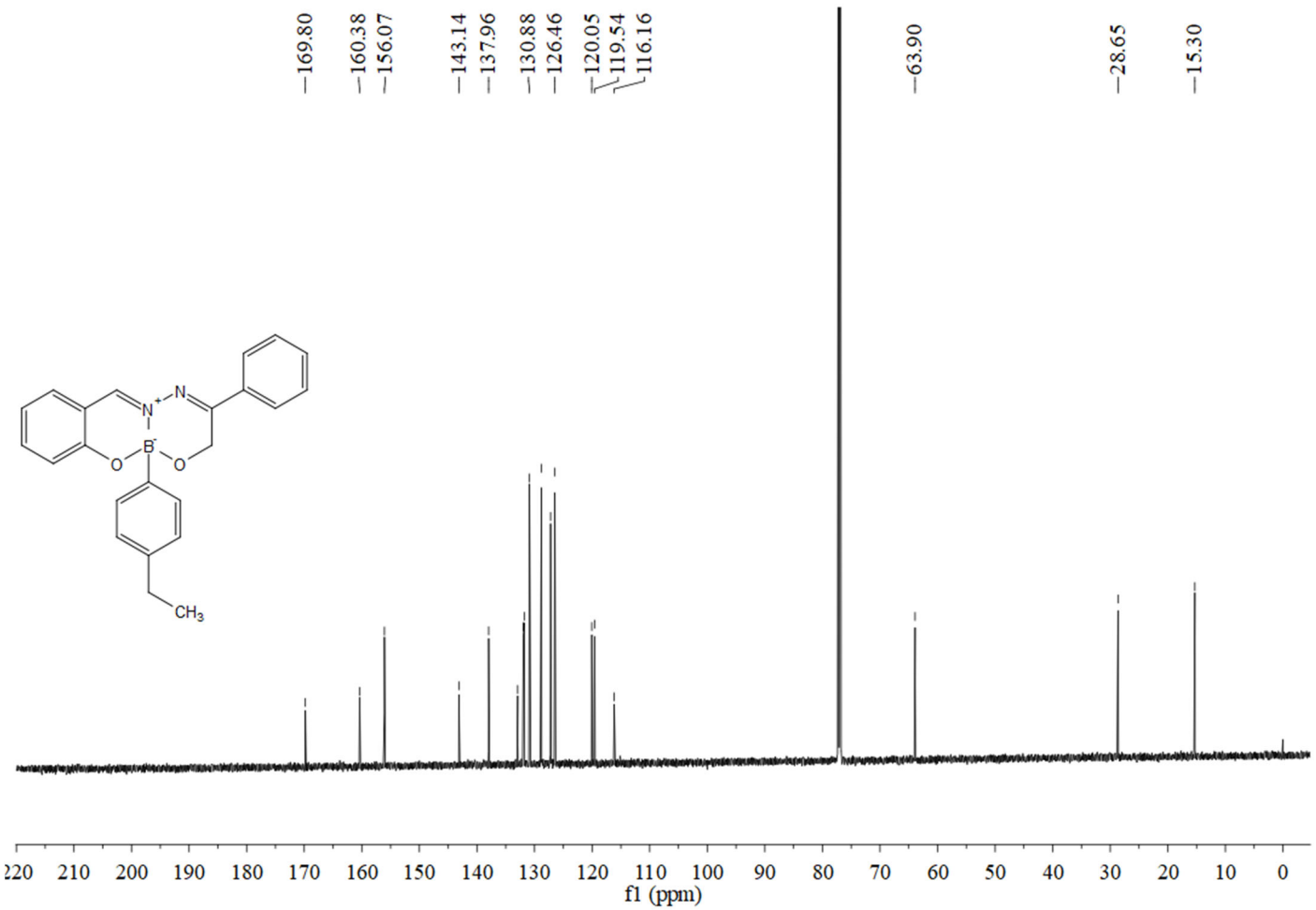


Fig. S116 ^{13}C NMR for compound **9c** (151 MHz, $CDCl_3$)

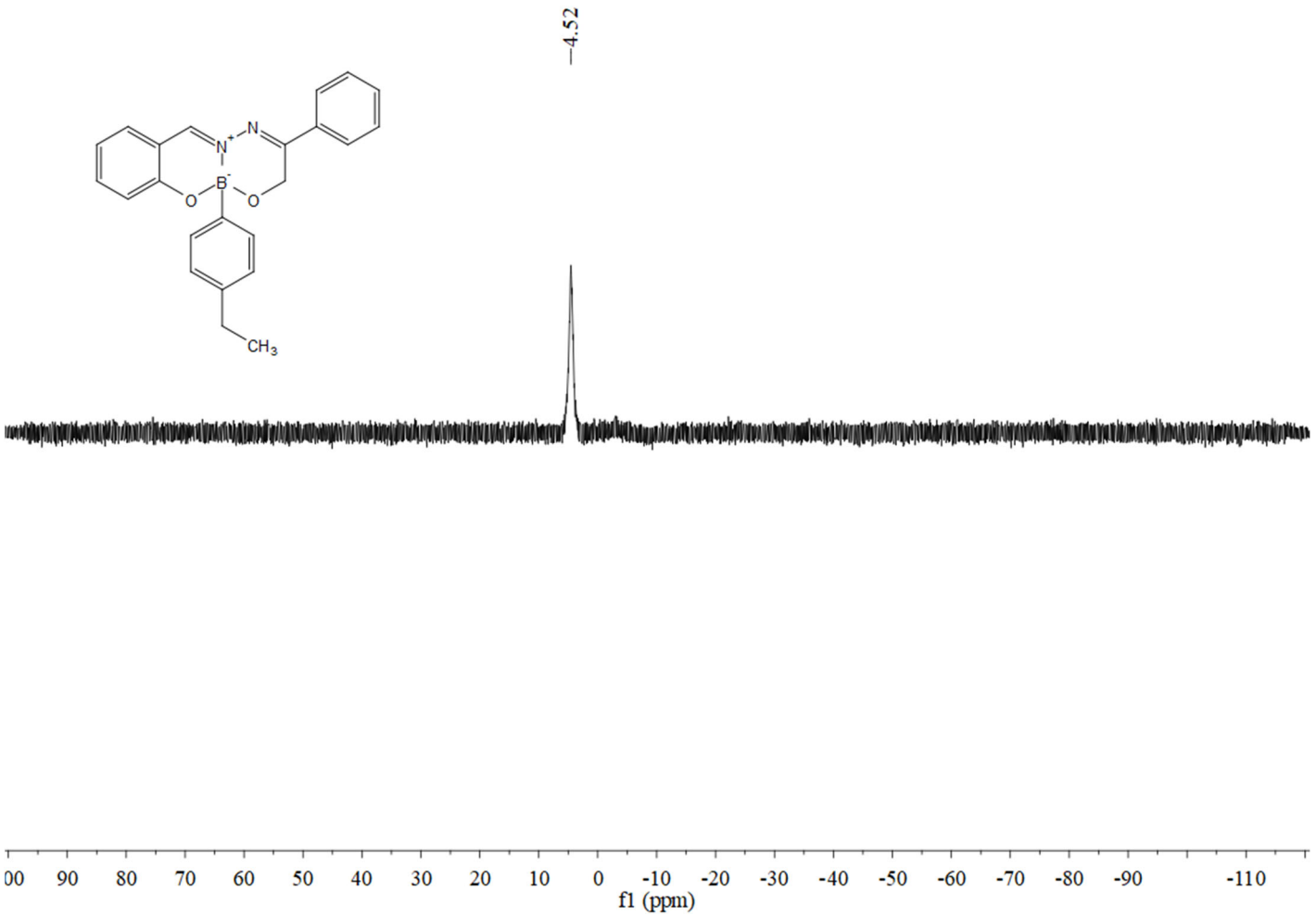


Fig. S117 ^{11}B NMR for compound **9c** (193 MHz, $CDCl_3$)

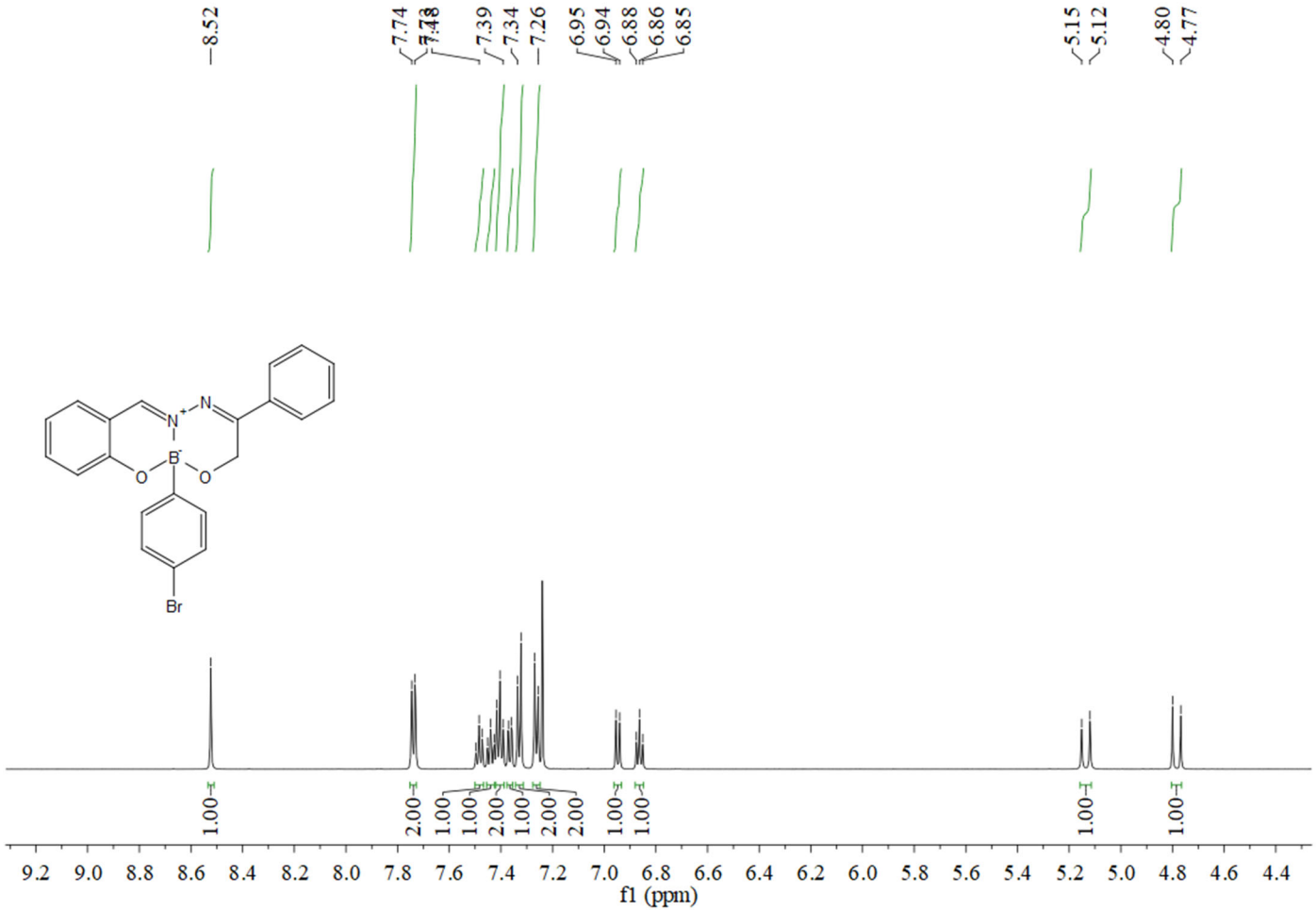


Fig. S118 ^{1}H NMR for compound **9d** (600 MHz, $CDCl_3$)

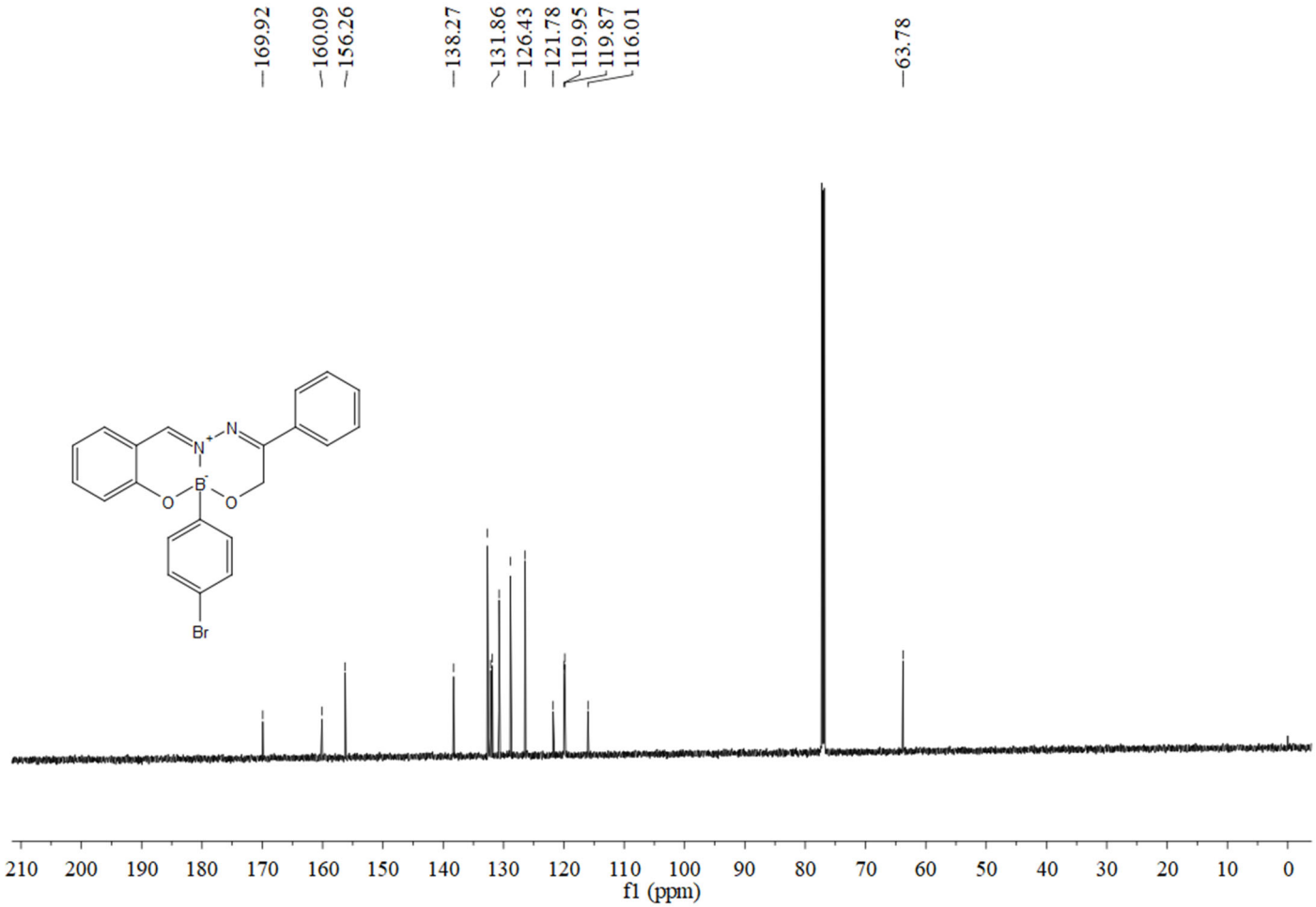


Fig. S119 ^{13}C NMR for compound **9d** (151 MHz, $CDCl_3$)

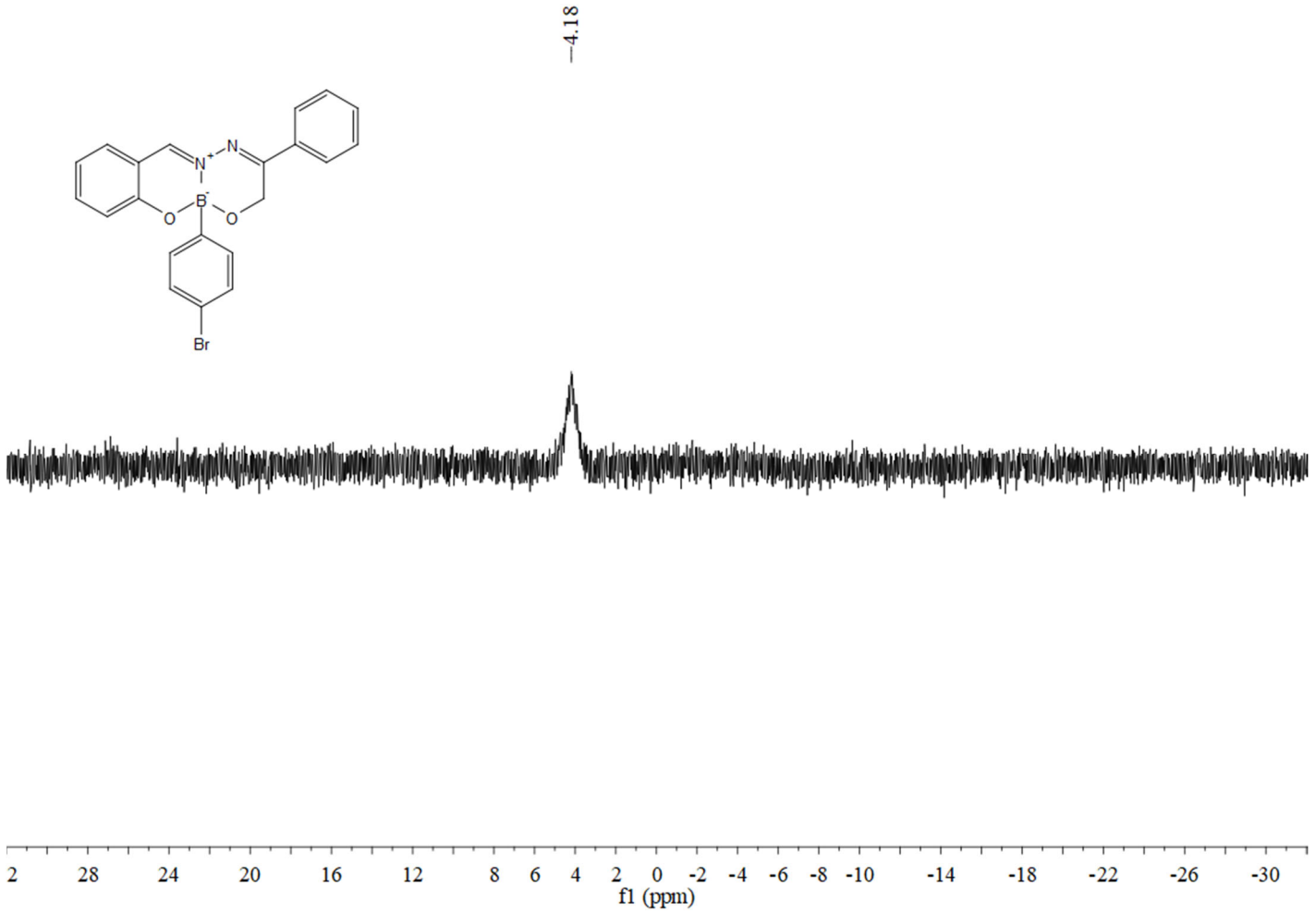


Fig. S120 ^{11}B NMR for compound **9d** (193 MHz, $CDCl_3$)

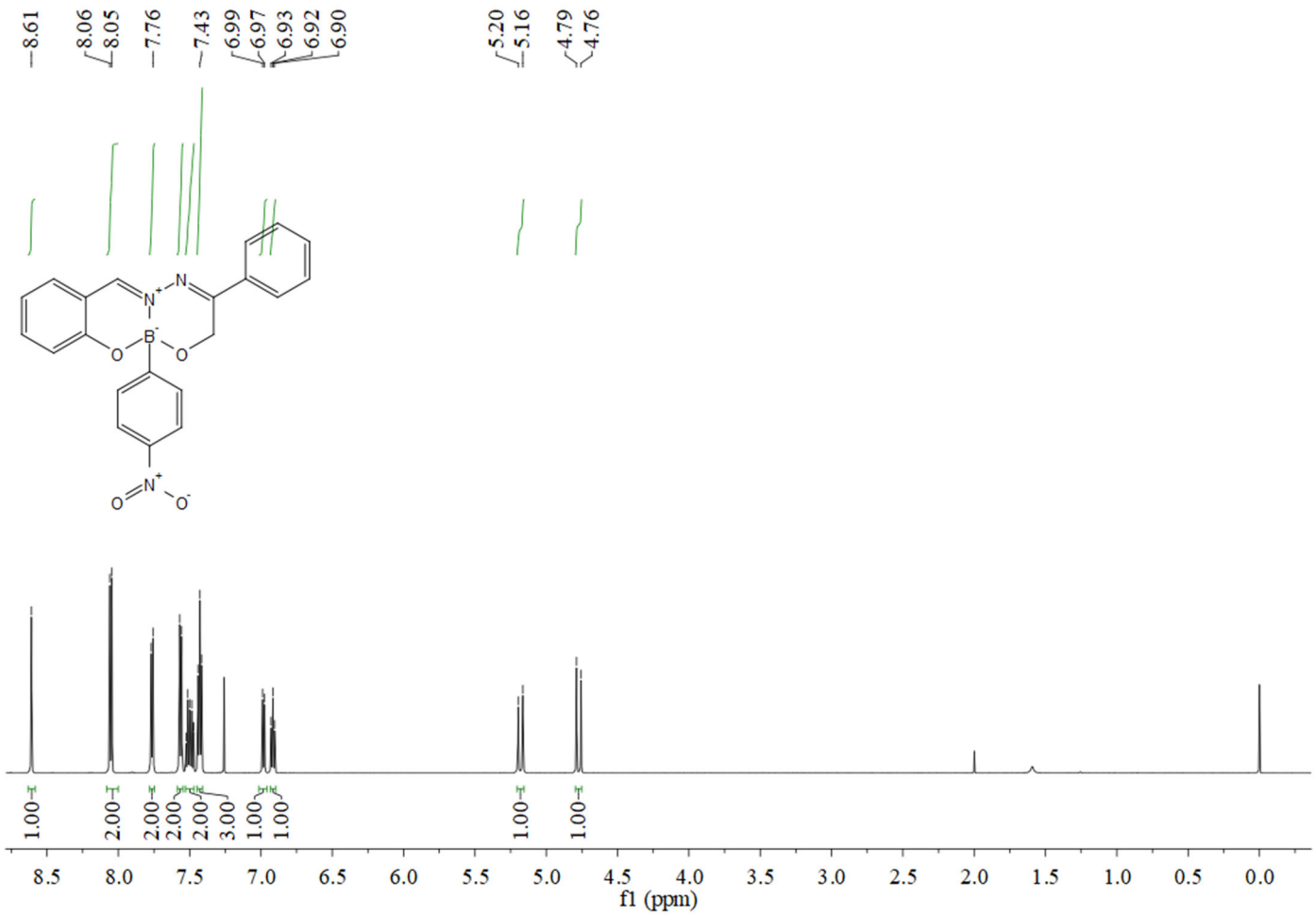


Fig. S121 ^{1}H NMR for compound **9e** (600 MHz, $CDCl_3$)

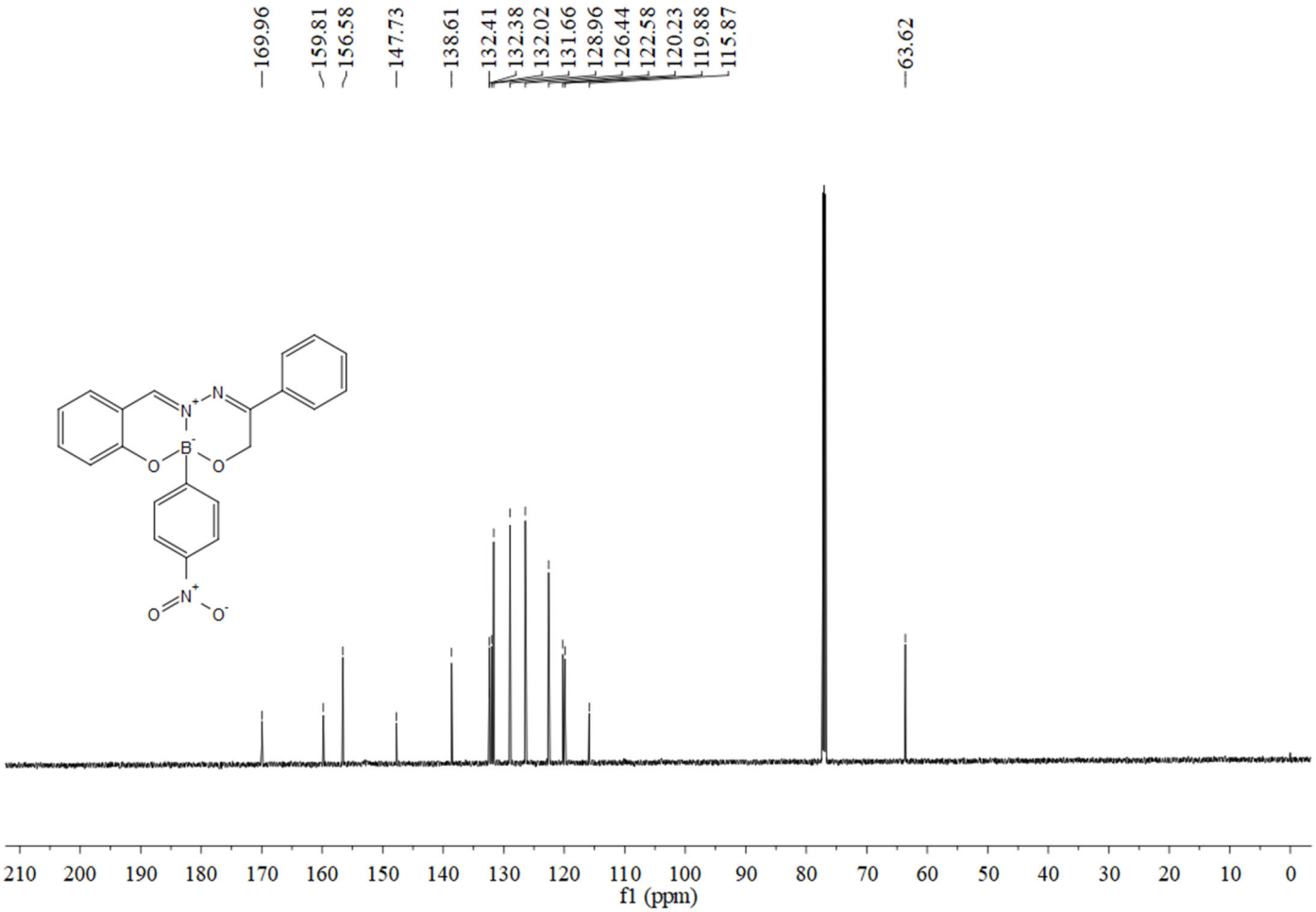


Fig. S122 ^{13}C NMR for compound **9e** (151 MHz, $CDCl_3$)

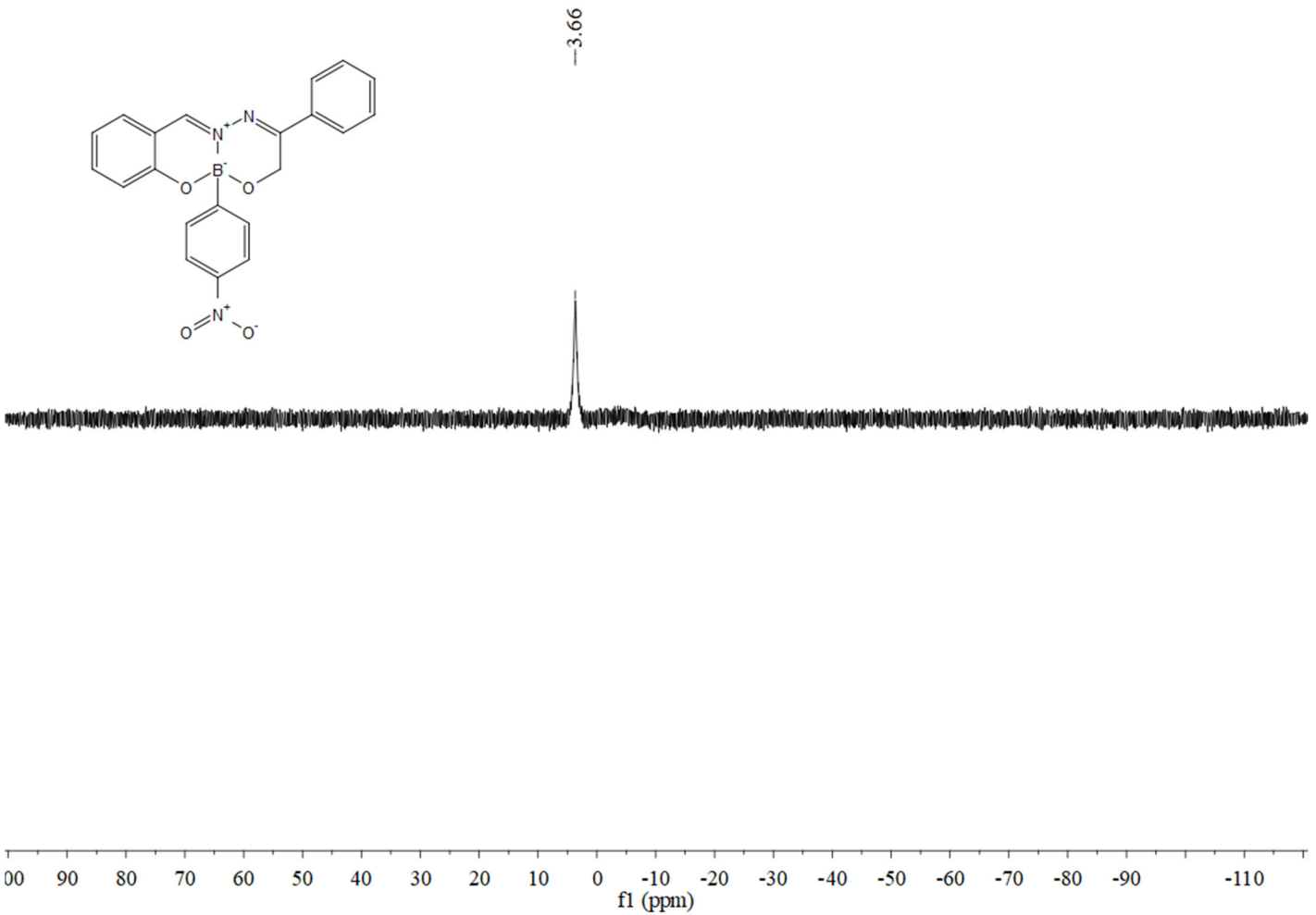


Fig. S123 ^{11}B NMR for compound **9e** (193 MHz, $CDCl_3$)

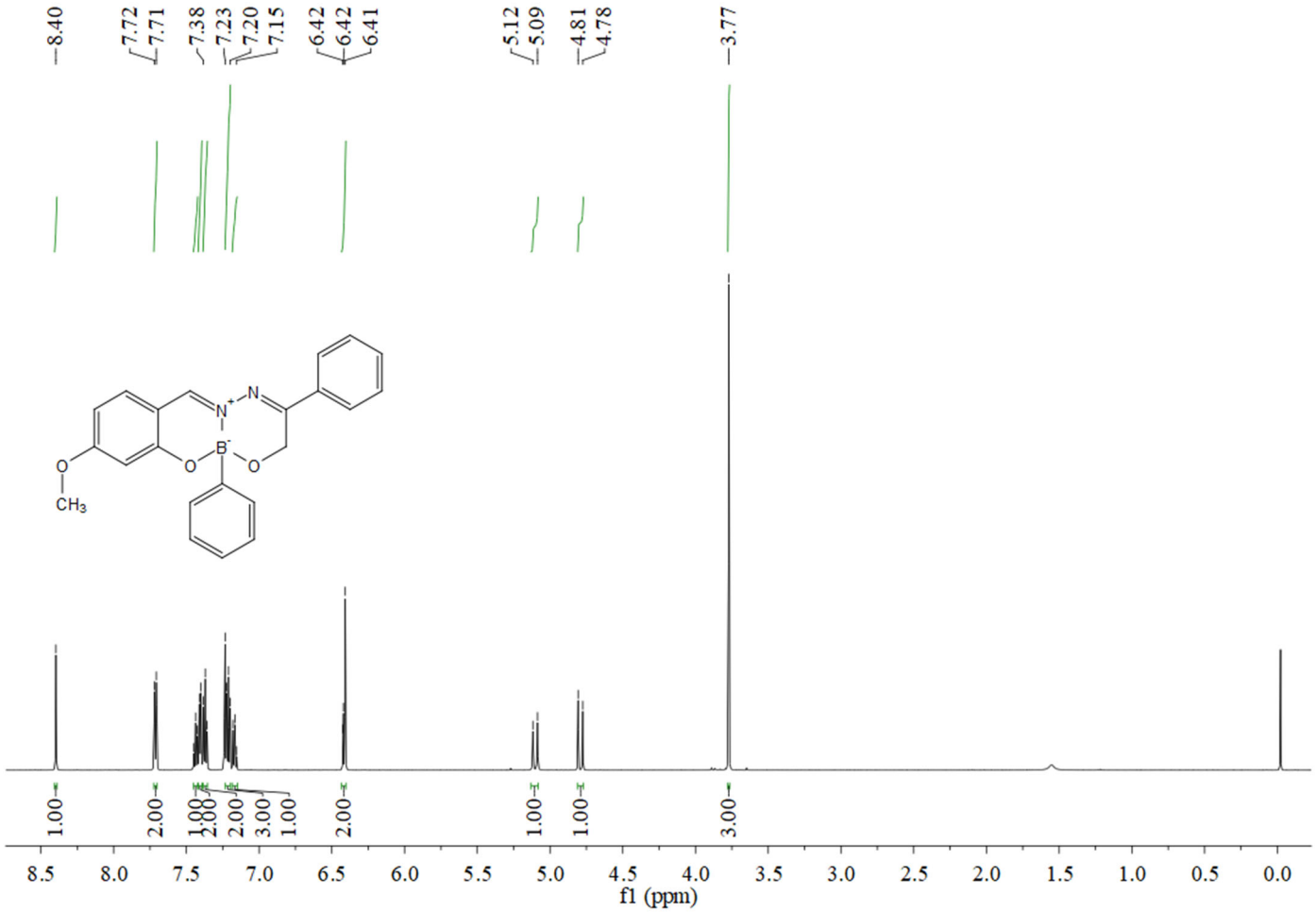


Fig. S124 ^{1}H NMR for compound **9f** (600 MHz, $CDCl_3$)

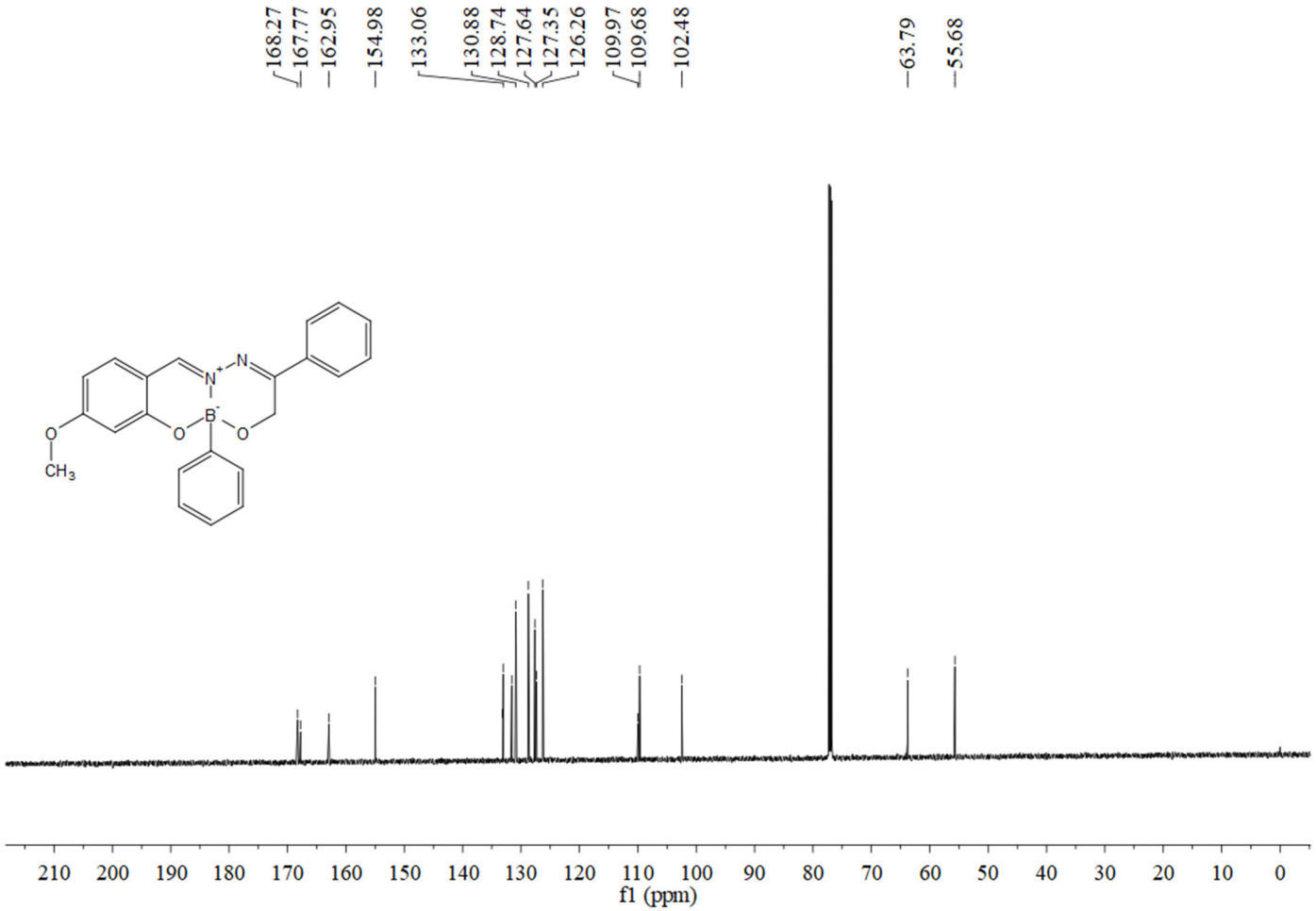


Fig. S125 ^{13}C NMR for compound **9f** (151 MHz, $CDCl_3$)

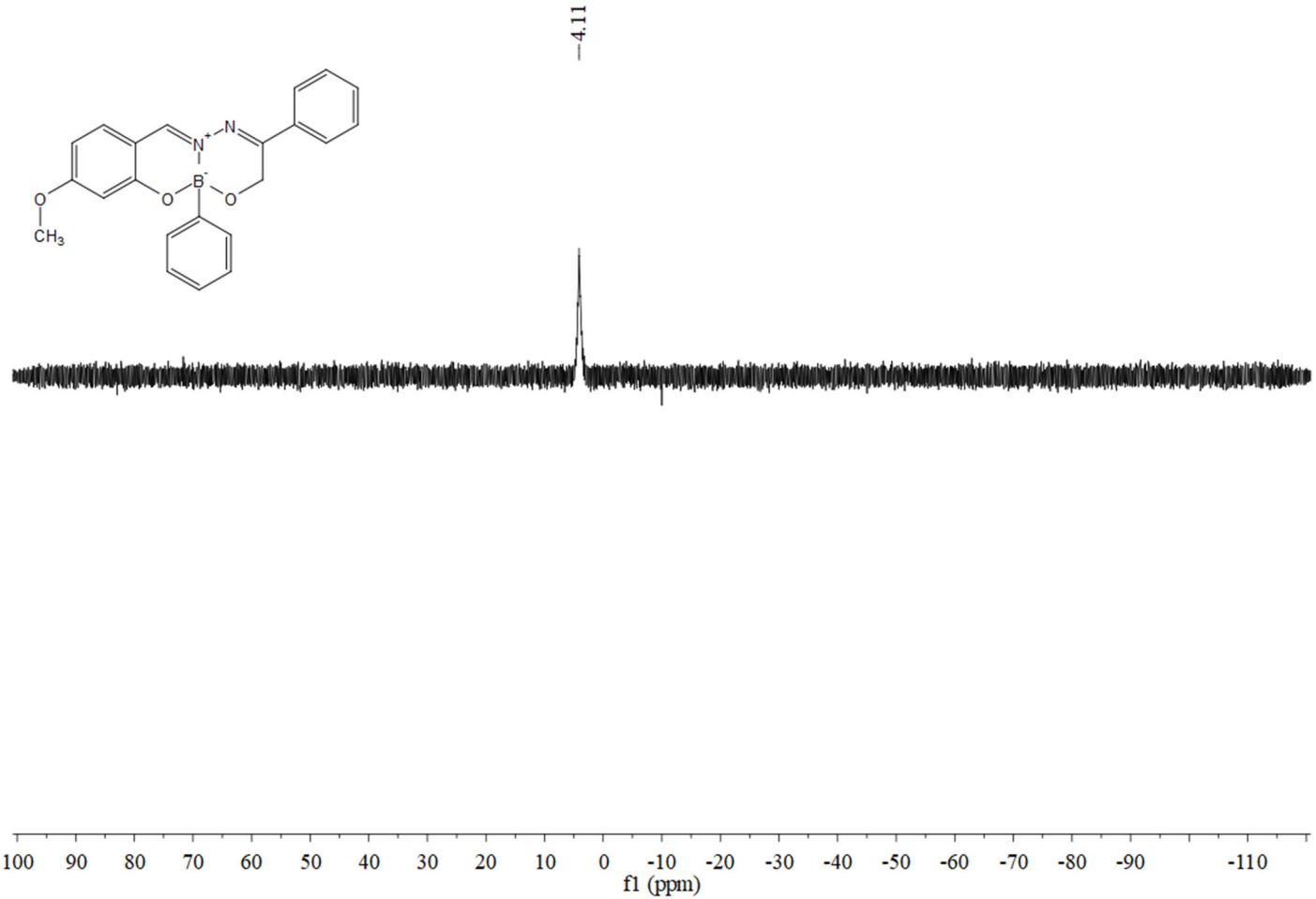


Fig. S126 ^{11}B NMR for compound **9f** (193 MHz, $CDCl_3$)

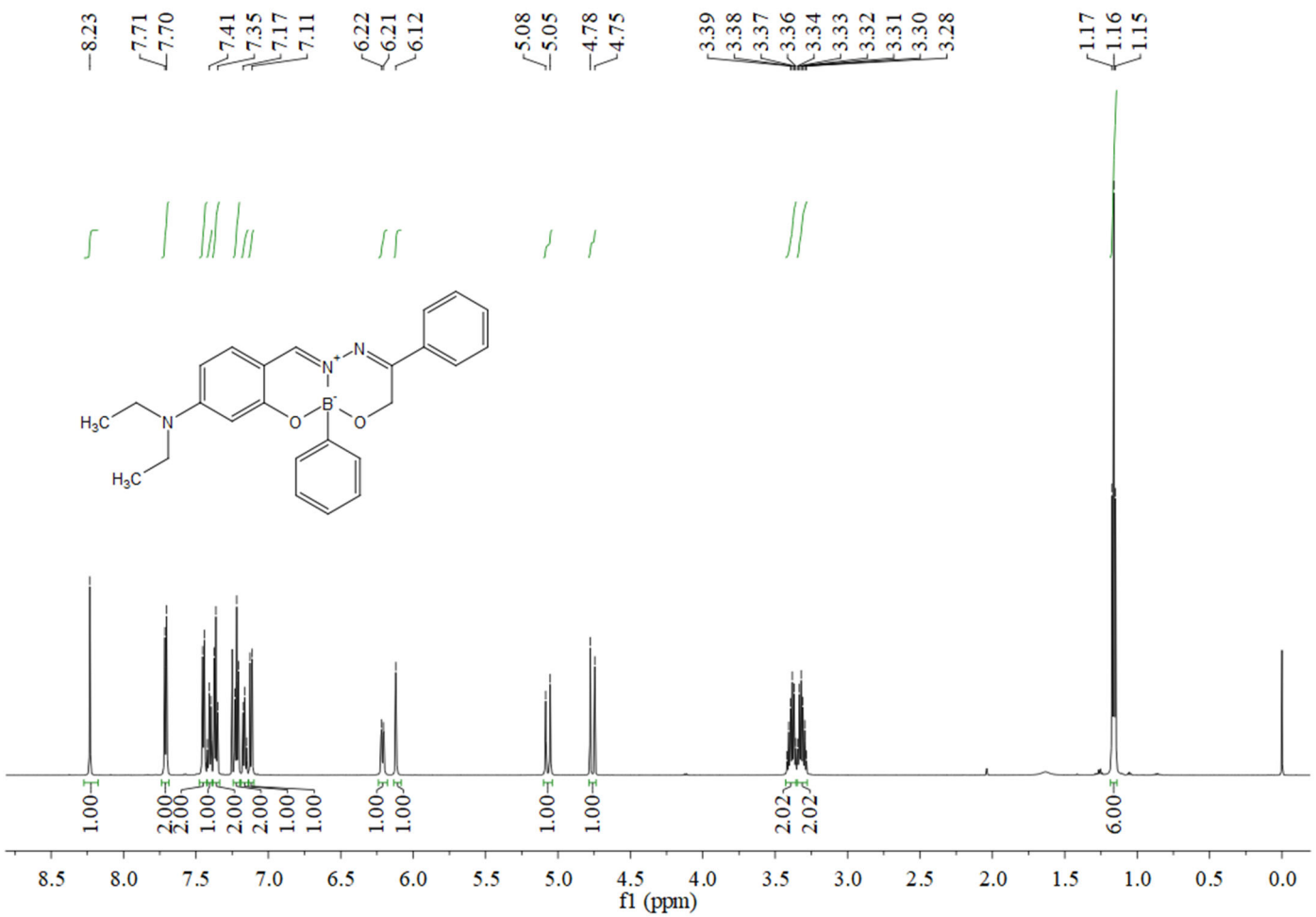


Fig. S127 ^{1}H NMR for compound **9g** (600 MHz, $CDCl_3$)

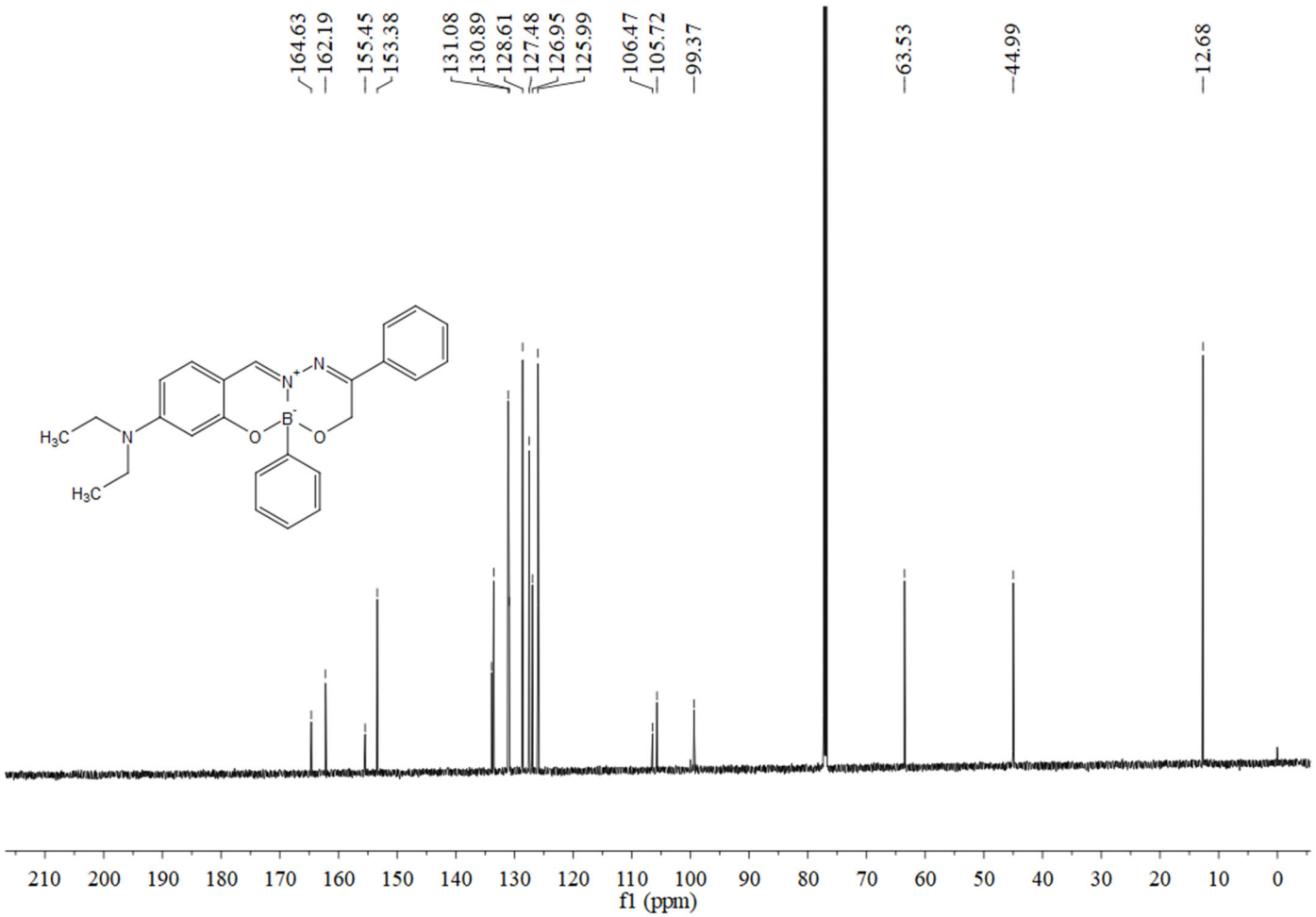


Fig. S128 ^{13}C NMR for compound **9g** (151 MHz, $CDCl_3$)

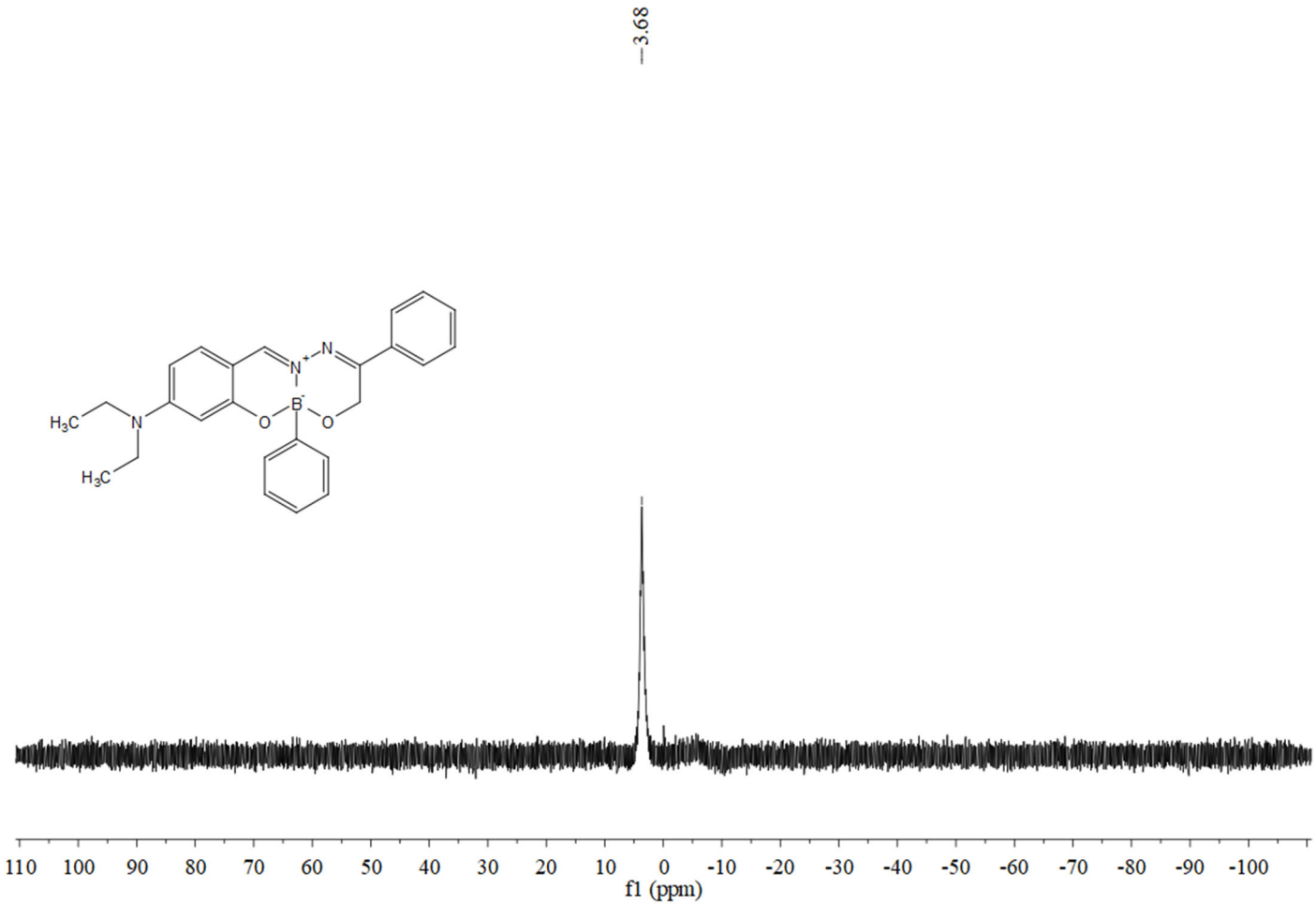


Fig. S129 ^{11}B NMR for compound **9g** (193 MHz, $CDCl_3$)

10. High-resolution mass spectra of new compounds

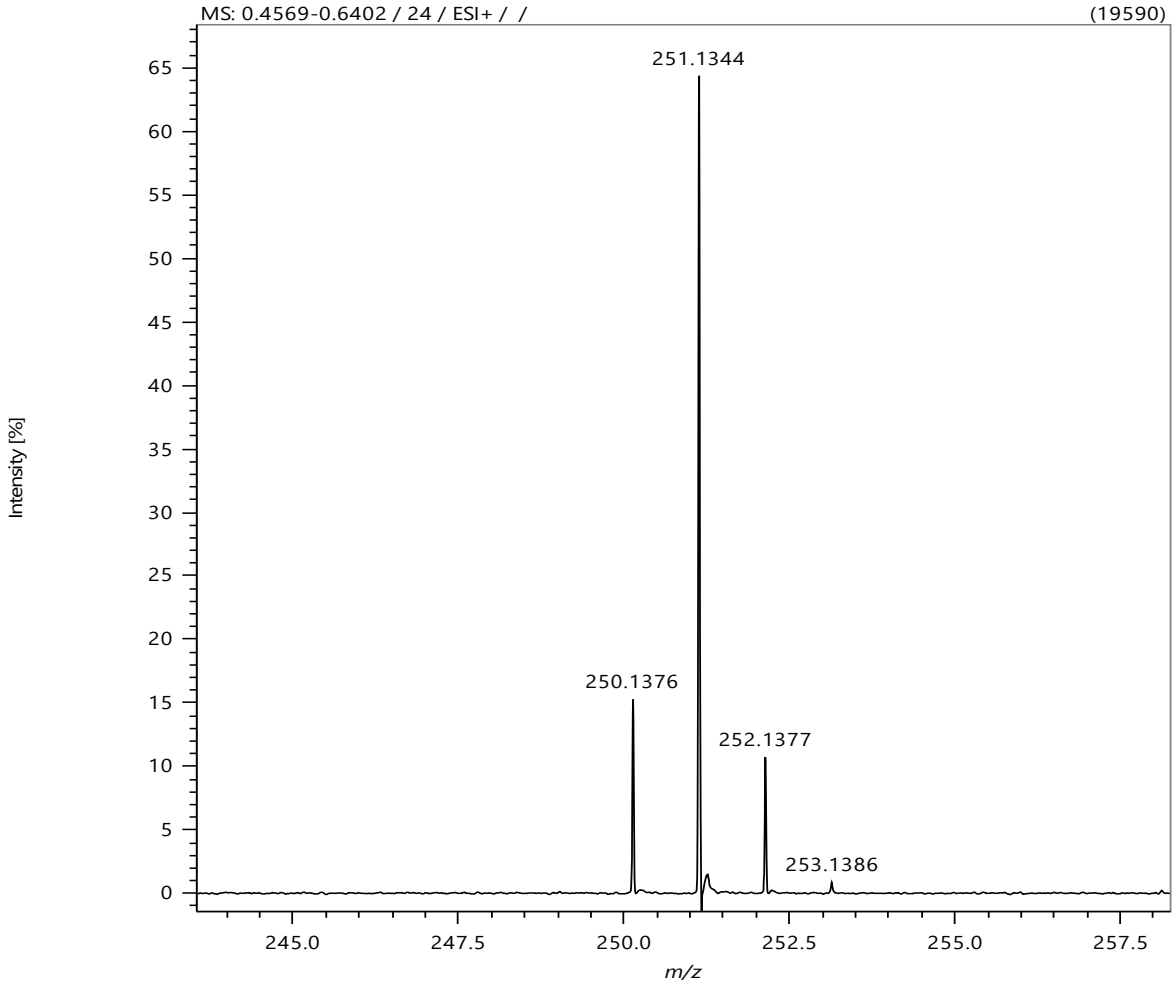


Fig. S130 5-(4-ethylphenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (**3c**).

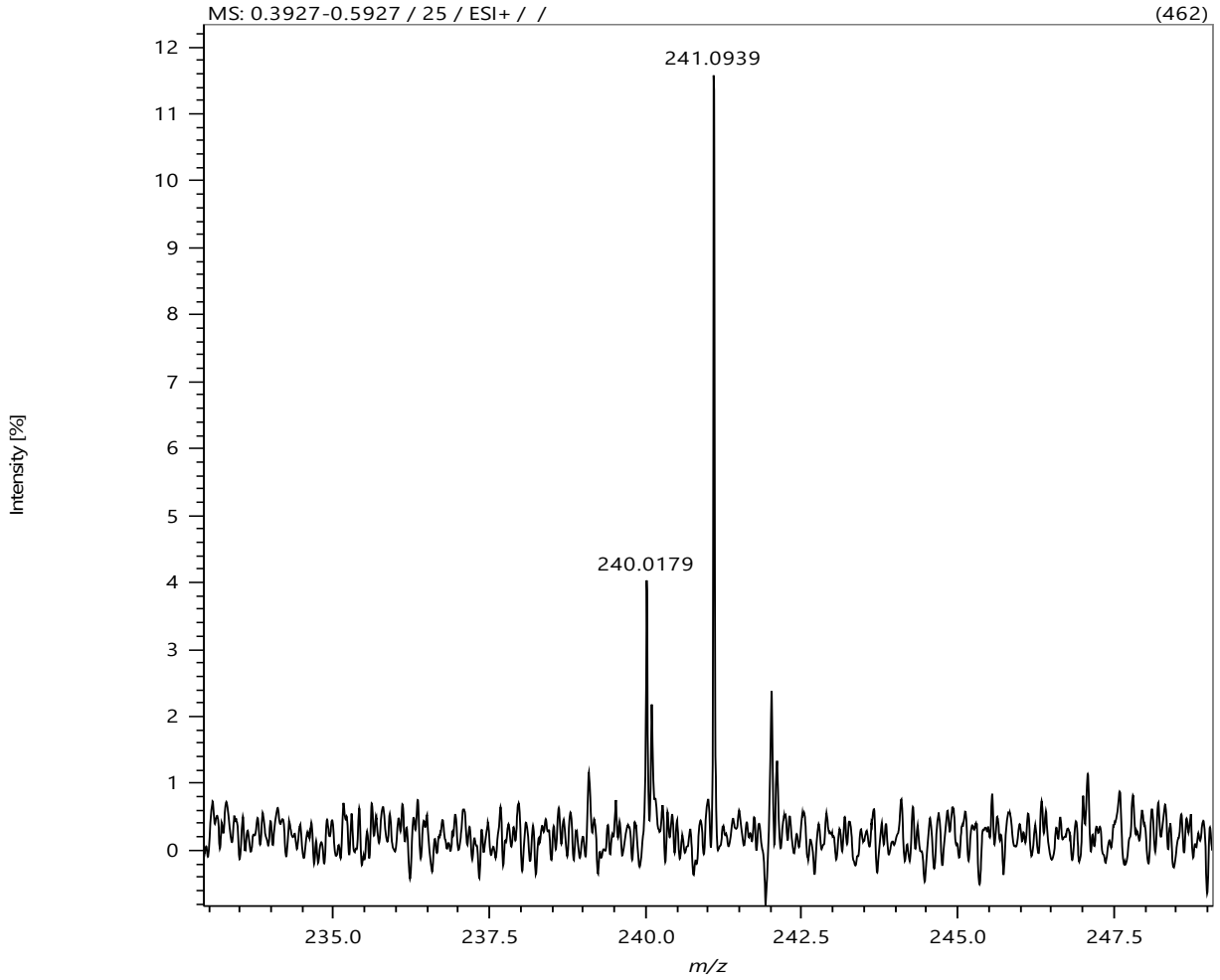


Fig. S131 5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (**3d**).

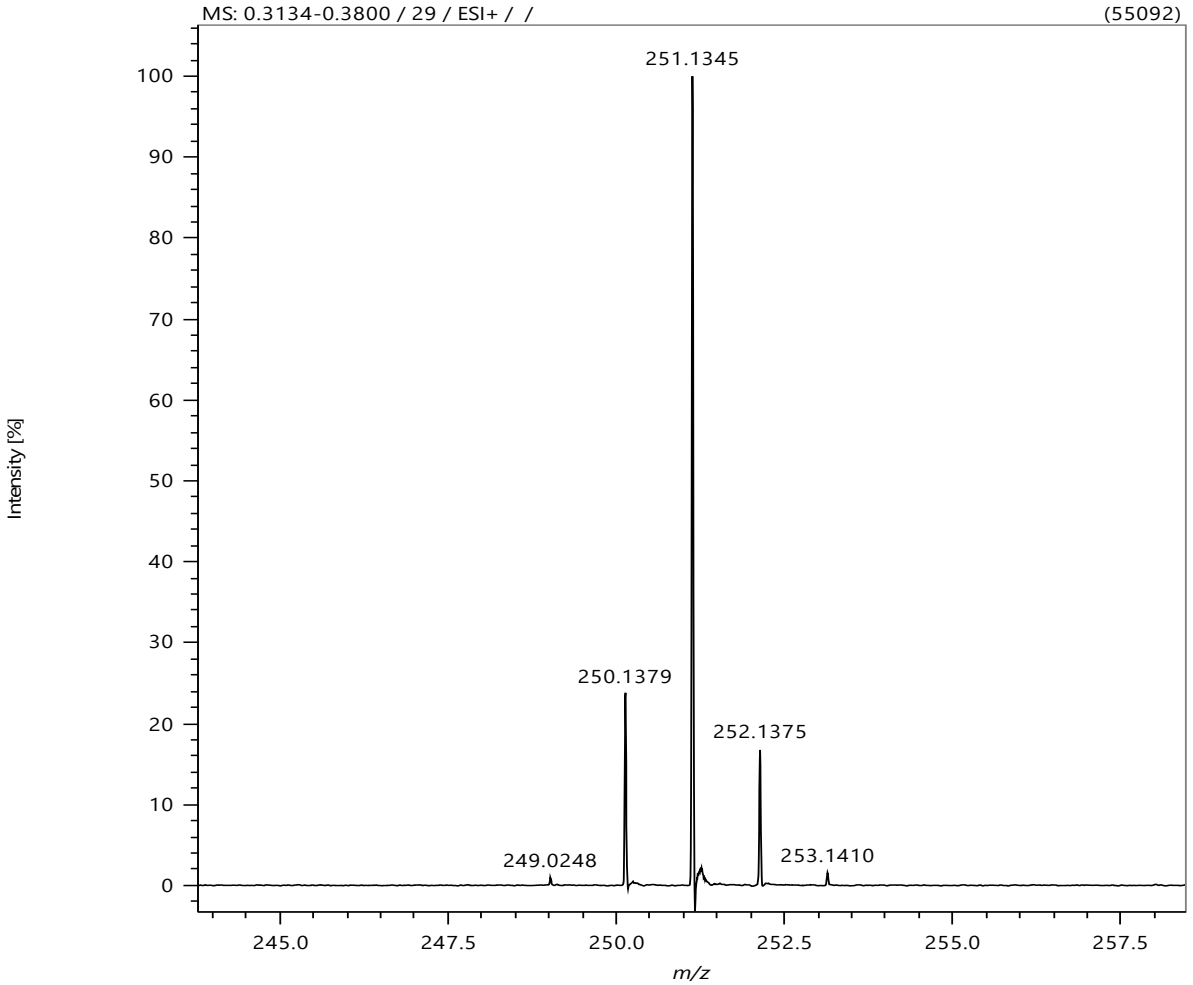


Fig. S132 5-(2,6-dimethylphenyl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (**3f**).

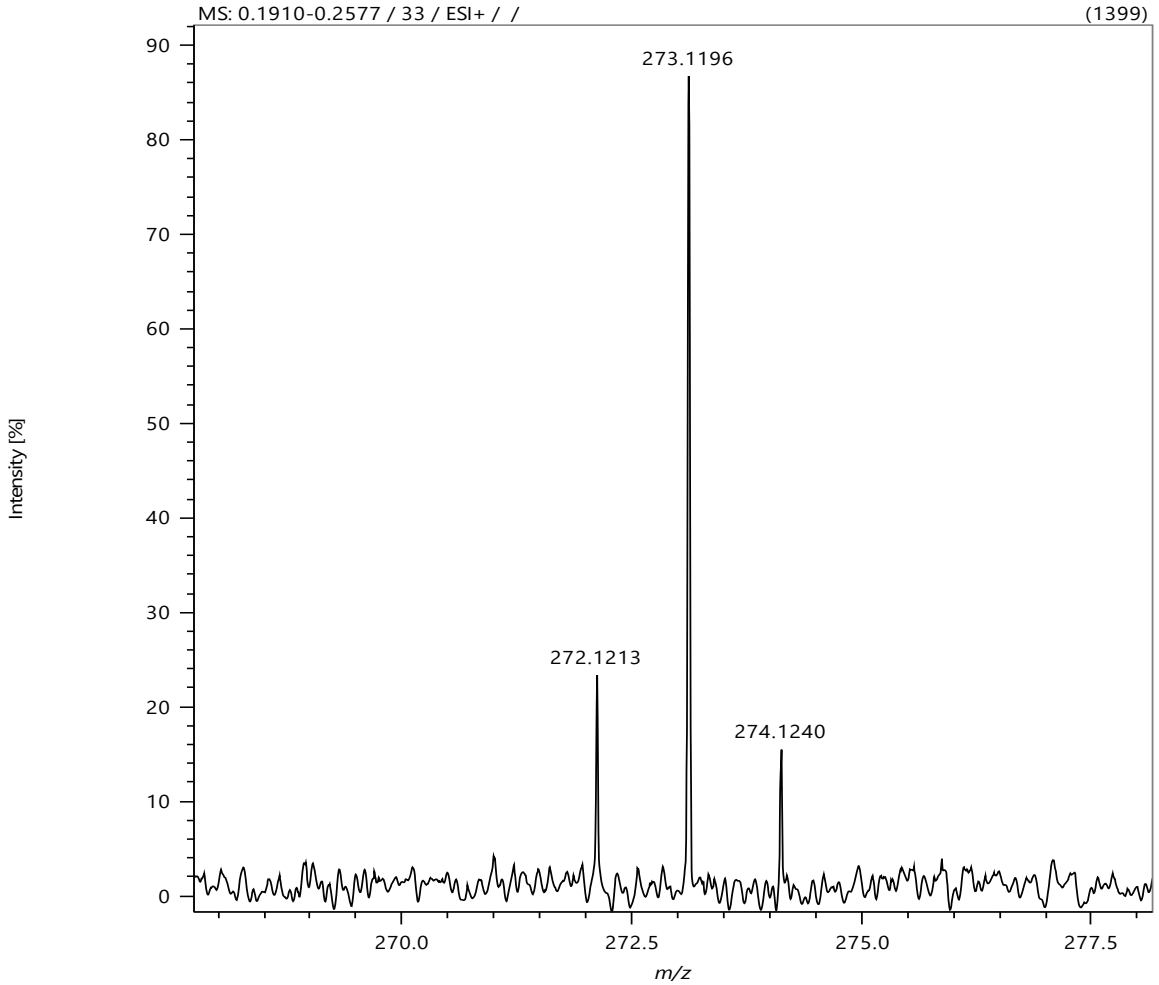


Fig. S133 5-(naphthalen-1-yl)-3-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (**3g**).

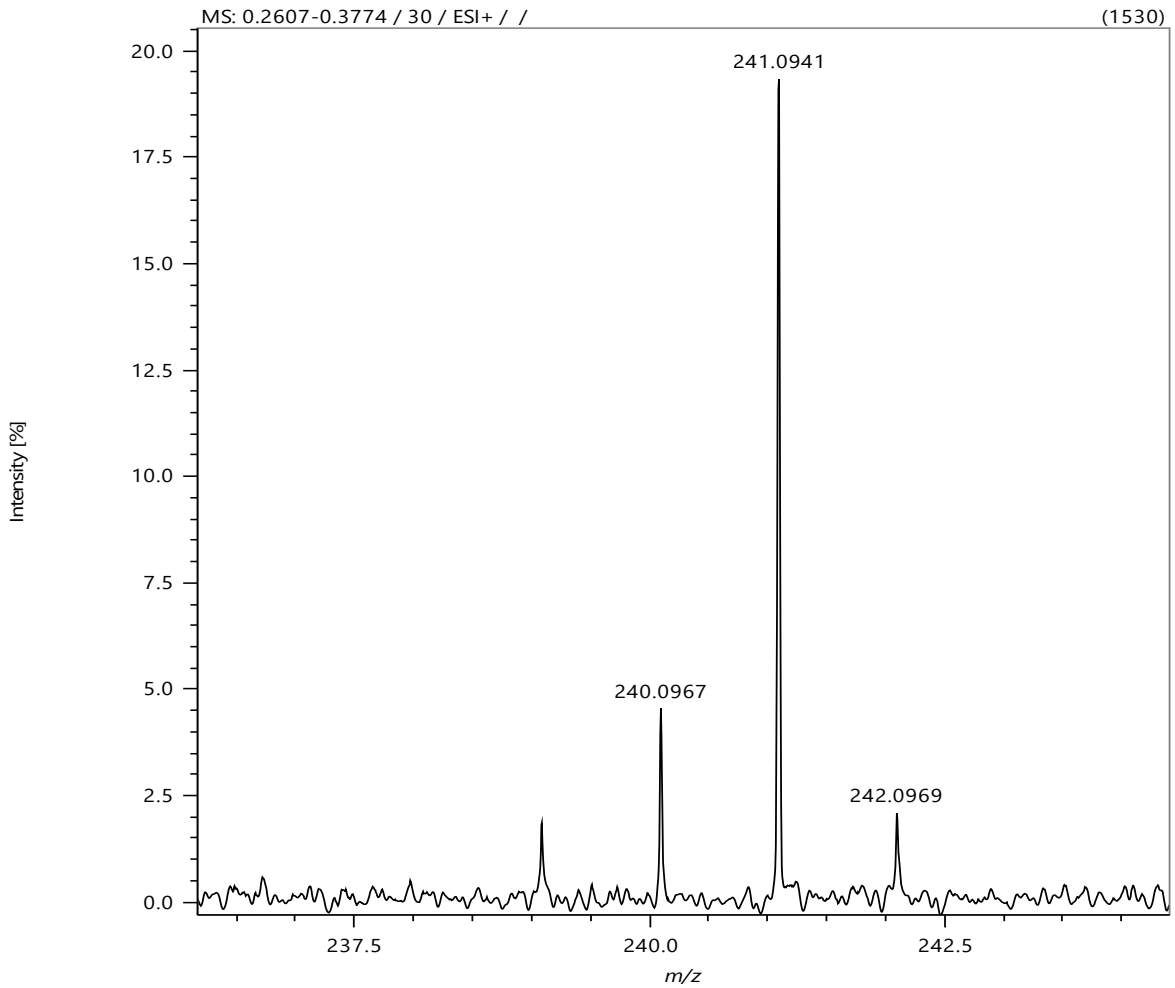


Fig. S134 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1,2,4,5-oxadiazaborole (**3k**).

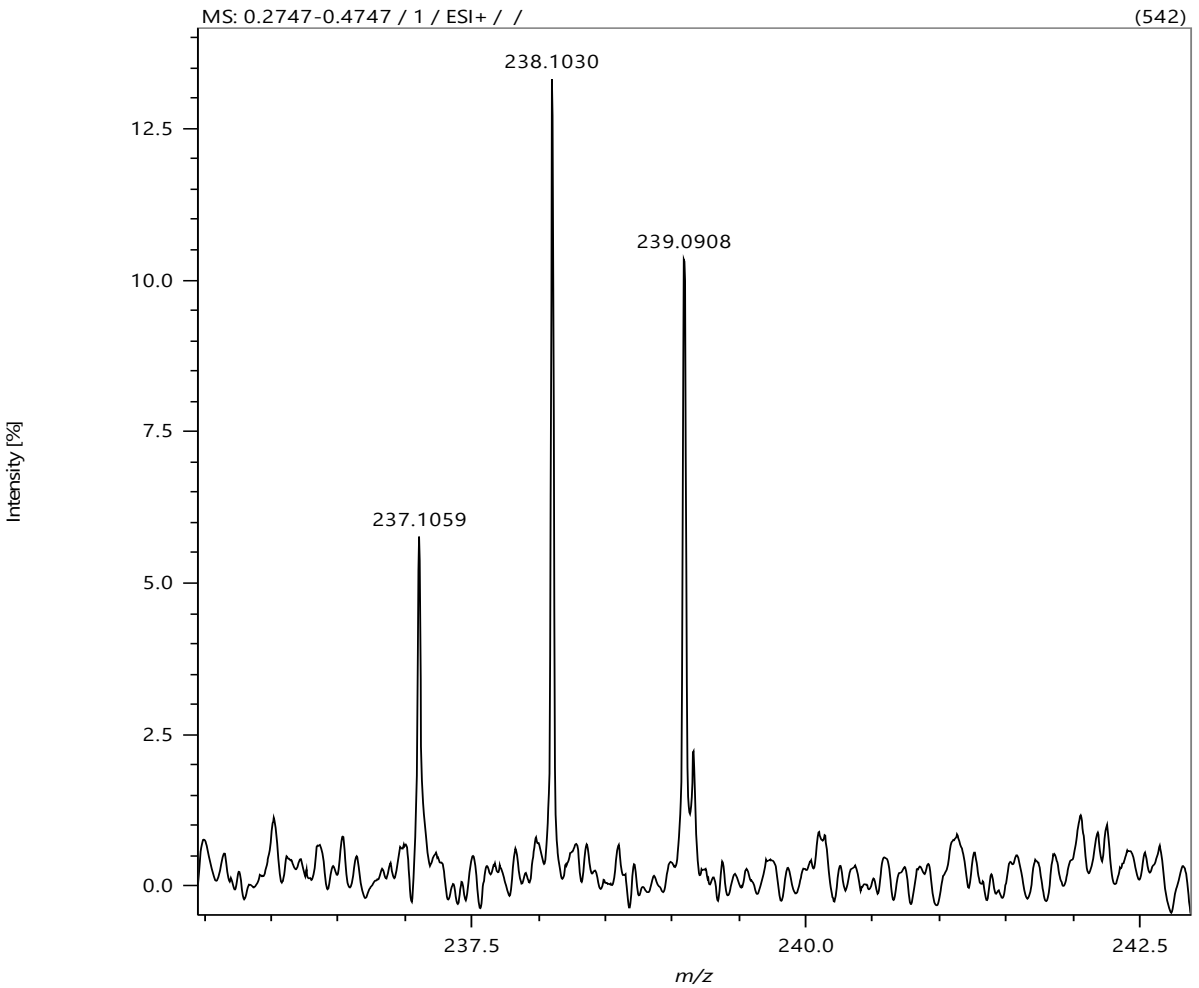


Fig. S135 2,5-diphenyl-6H-1,3,4,2-dioxazaborinine (**5a**).

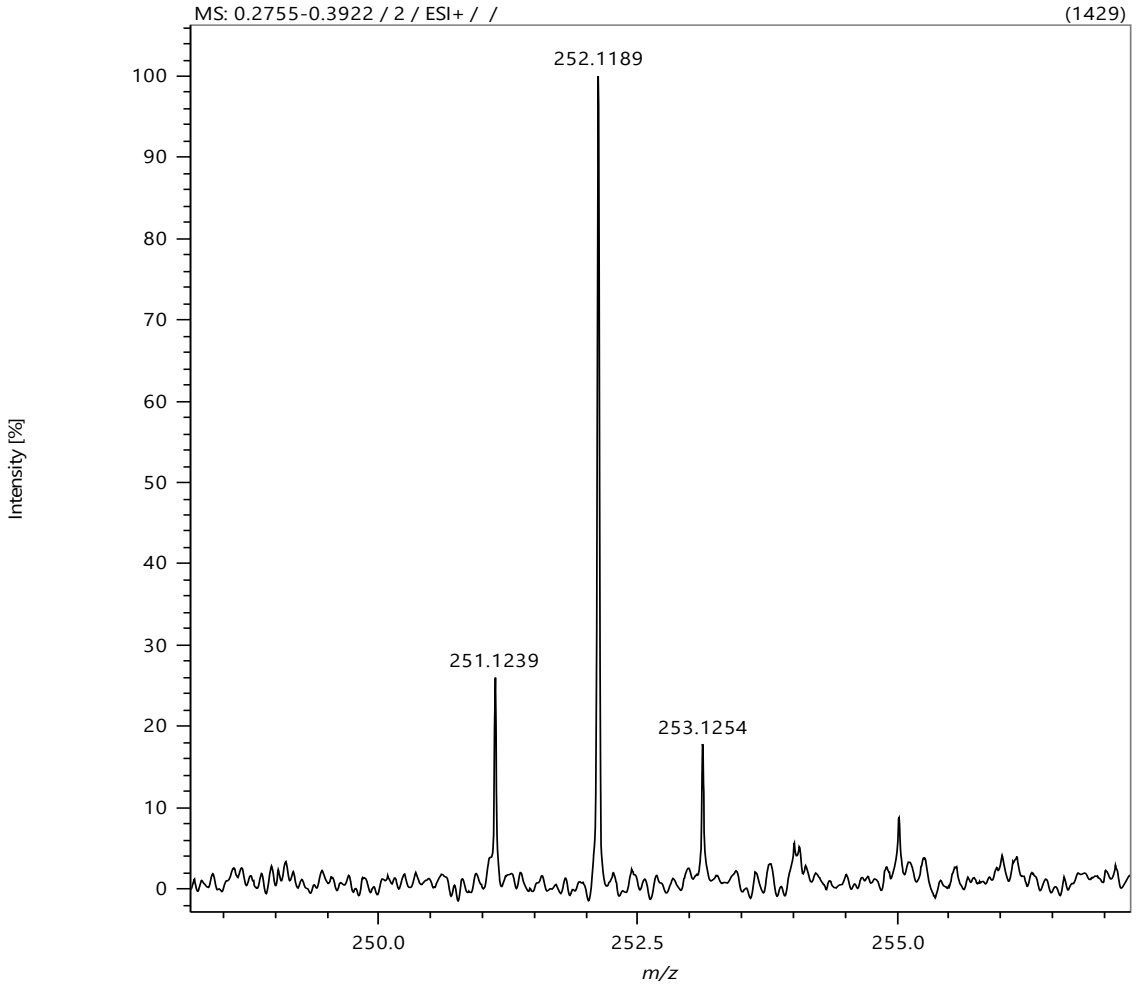


Fig. S136 5-phenyl-2-(p-tolyl)-6H-1,3,4,2-dioxazaborinine (**5b**).

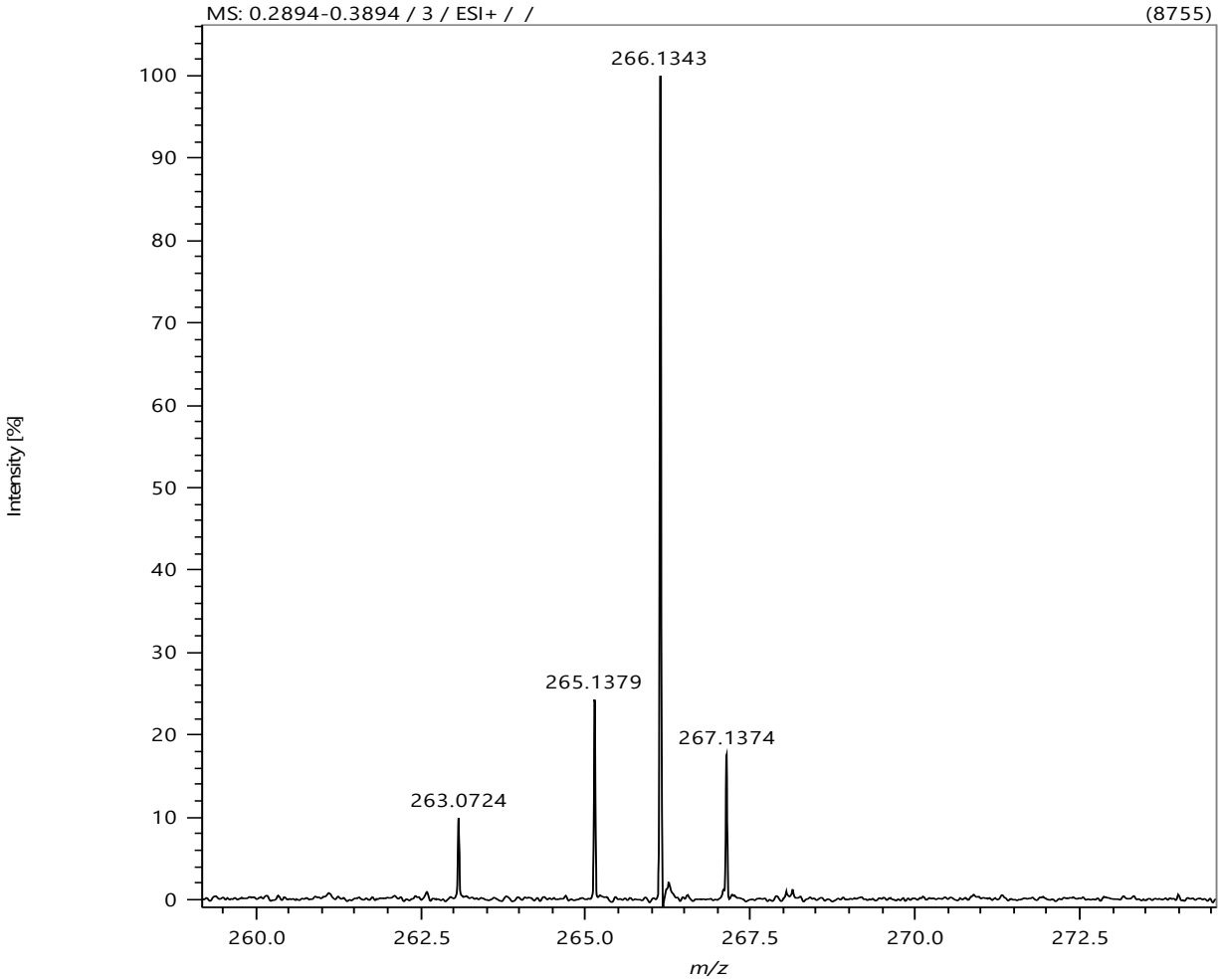


Fig. S137 2-(4-ethylphenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (**5c**).

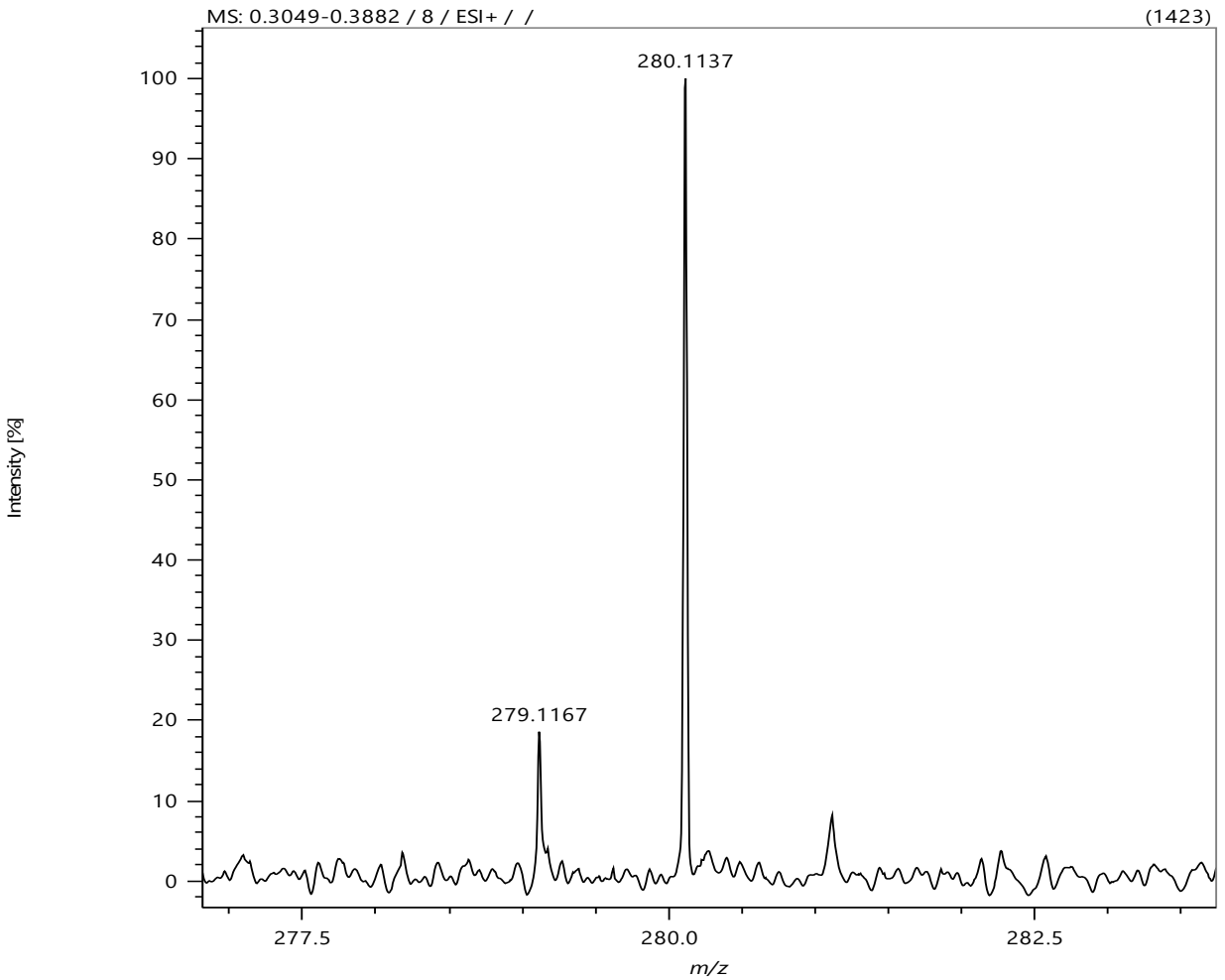


Fig. S138 1-(4-(5-phenyl-6H-1,3,4,2-dioxazaborinin-2-yl)phenyl)ethan-1-one (**5d**).

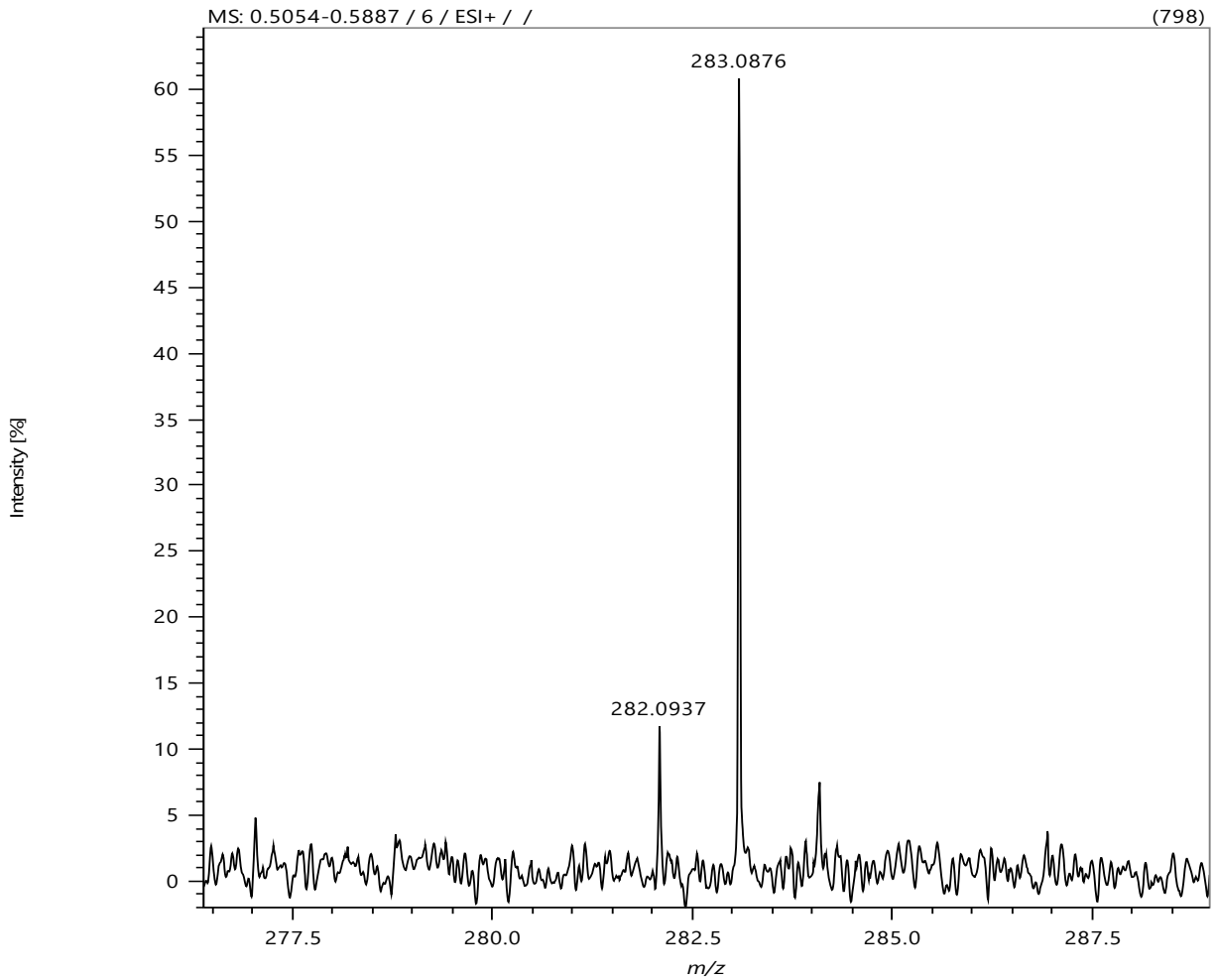


Fig. S139 2-(4-nitrophenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (**5e**).

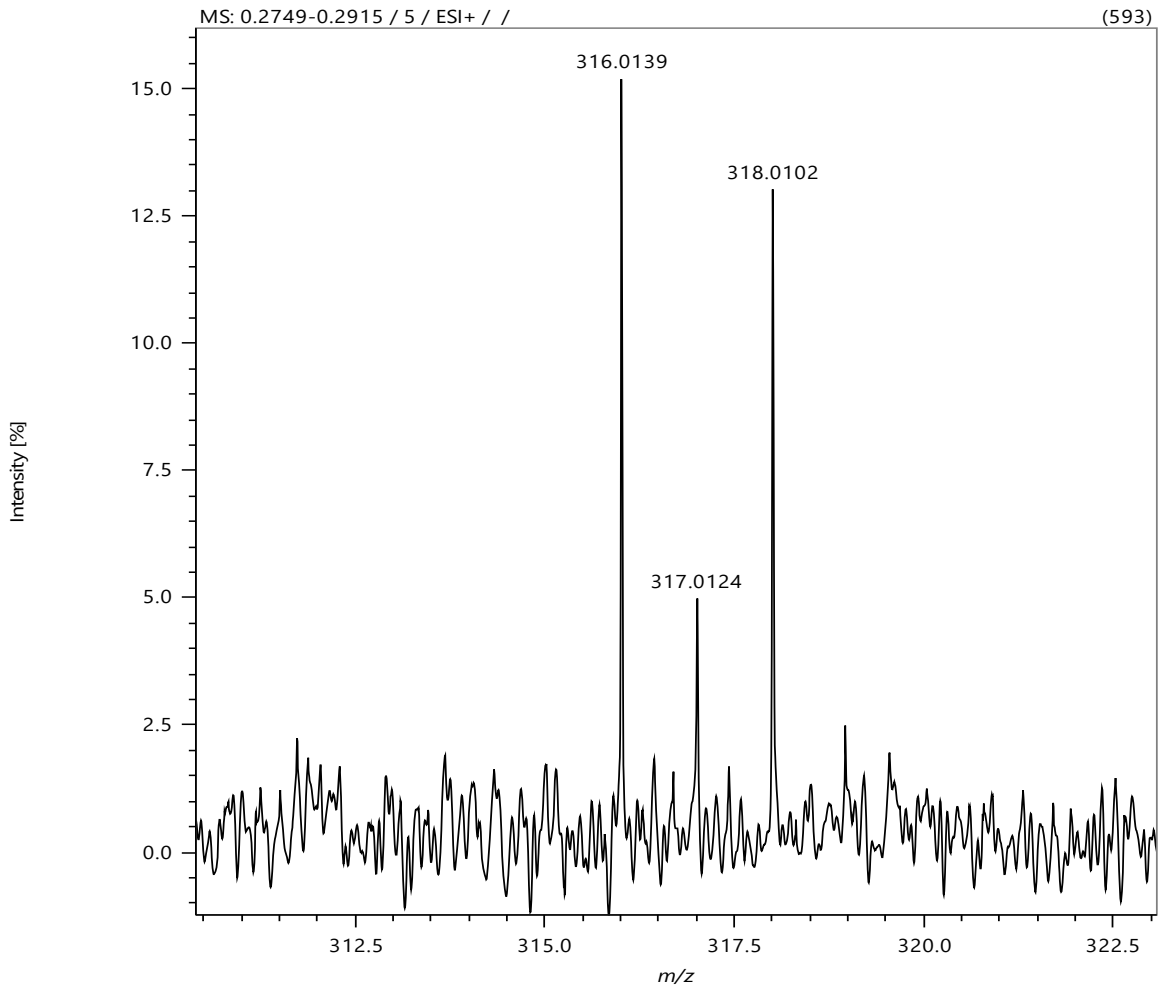


Fig. S140 2-(4-bromophenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (**5f**).

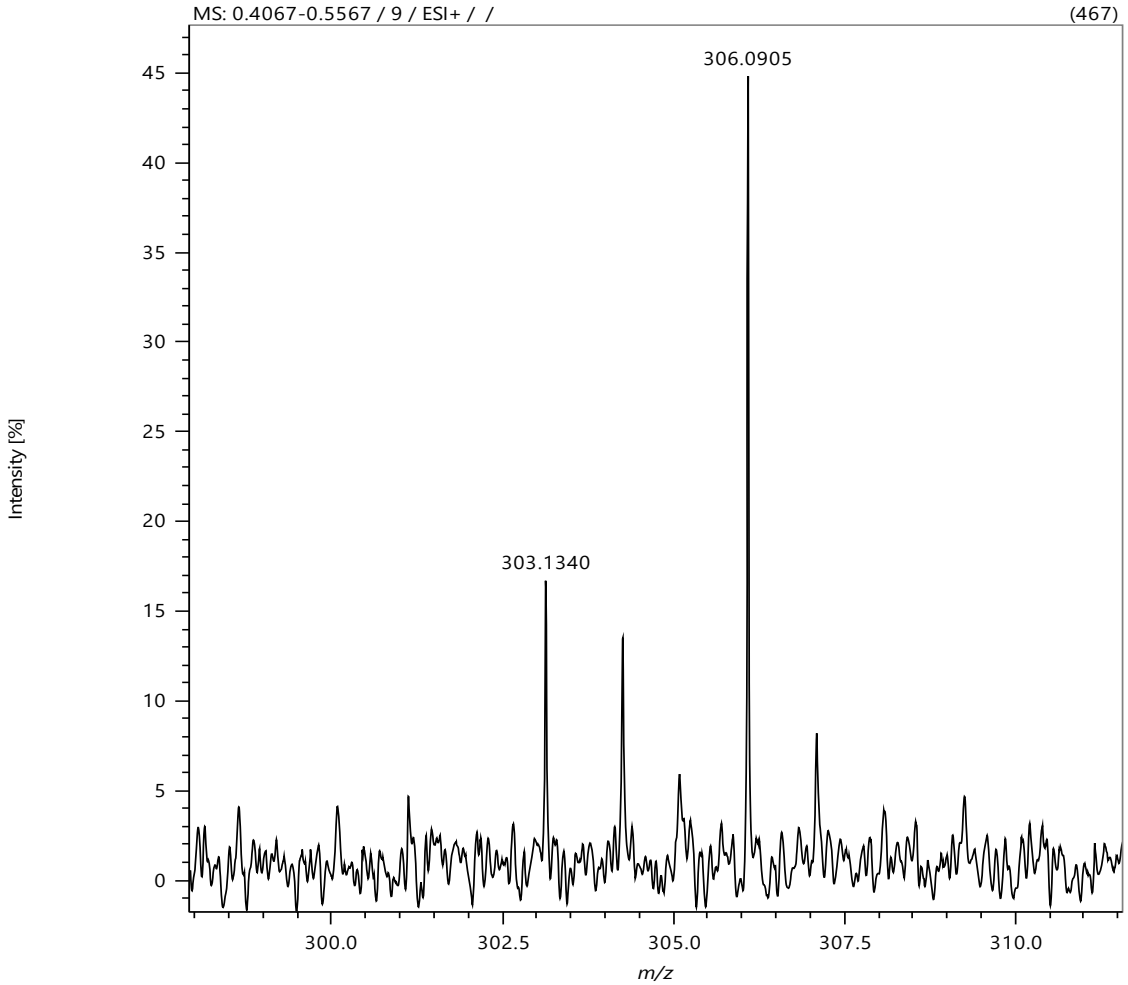


Fig. S141 5-phenyl-2-(4-(trifluoromethyl) phenyl)-6H-1,3,4,2-dioxazaborinine (**5g**).

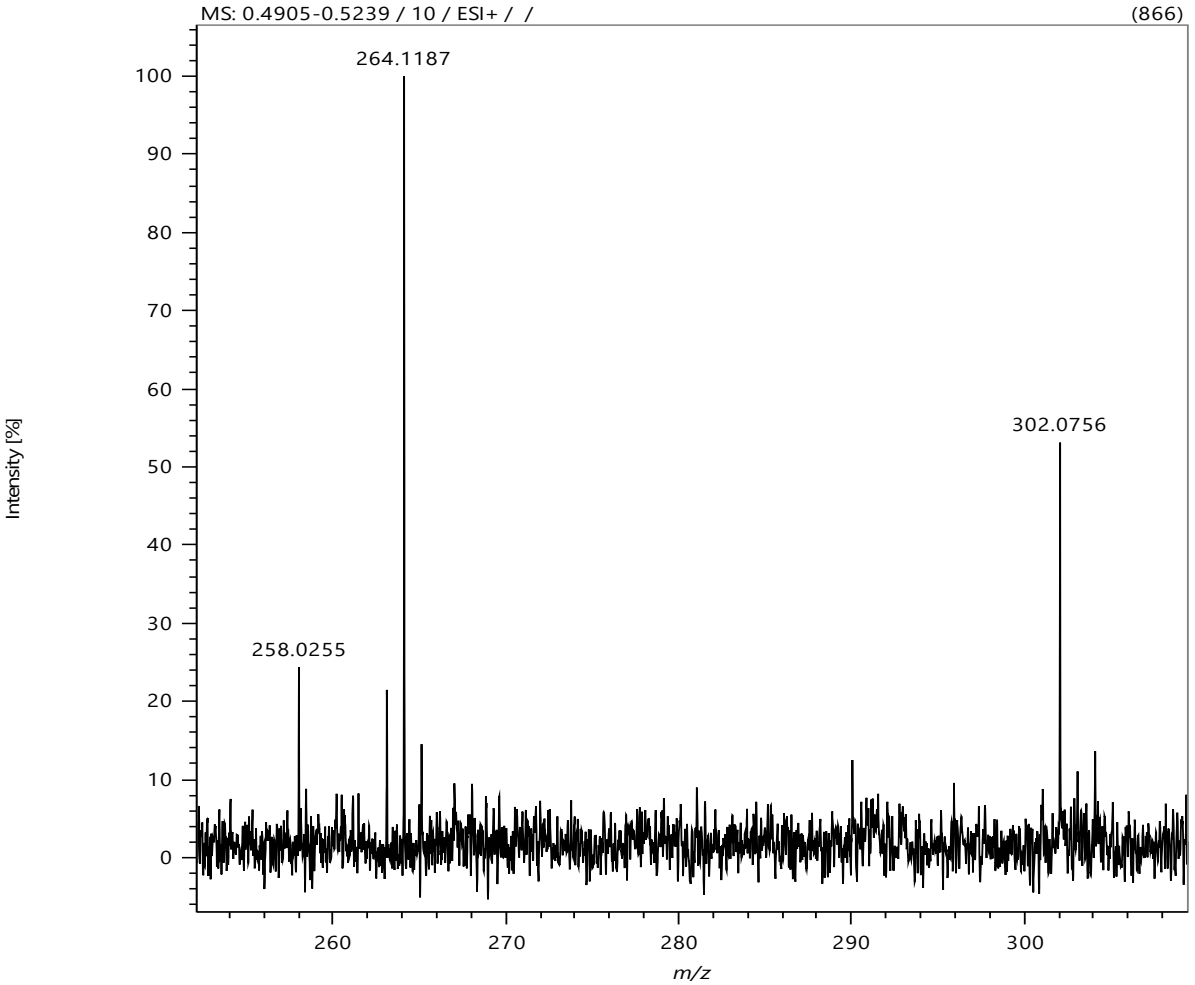


Fig. S142 5-phenyl-2-(4-vinylphenyl)-6H-1,3,4,2-dioxazaborinine (**5h**).

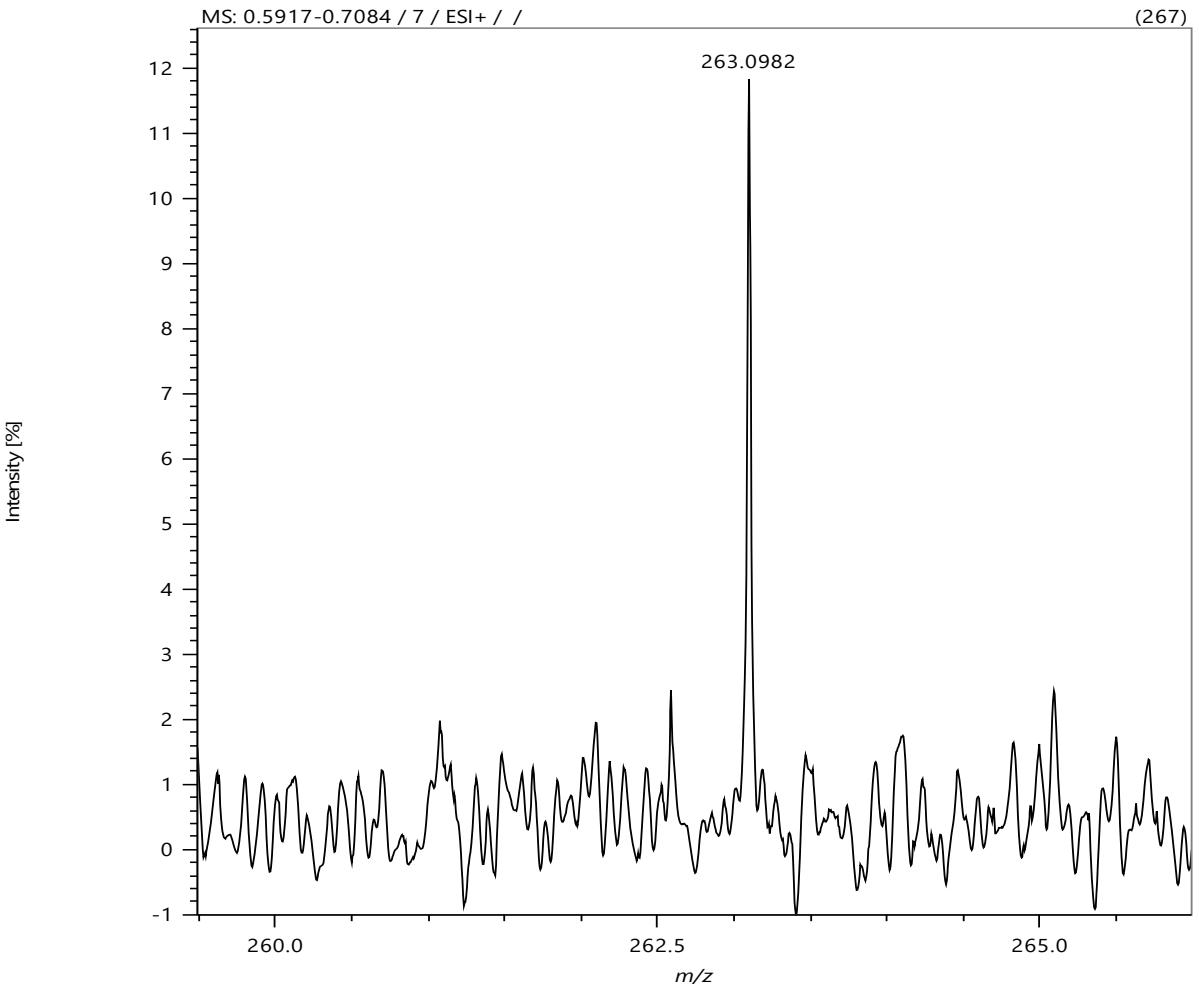


Fig. S143 4-(5-phenyl-6H-1,3,4,2-dioxazaborinin-2-yl) benzonitrile (**5i**).

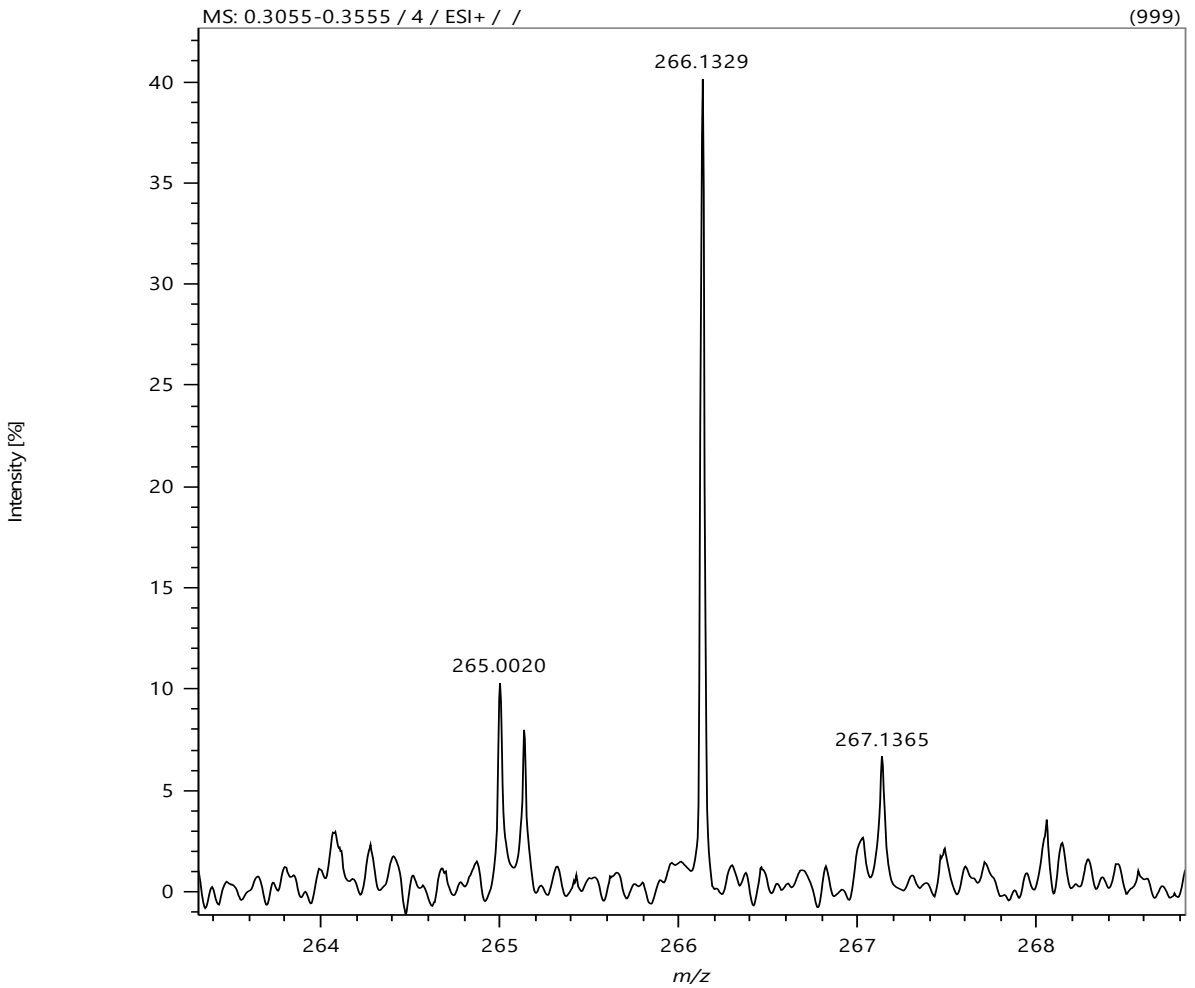


Fig. S144 2-(3,5-dimethylphenyl)-5-phenyl-6H-1,3,4,2-dioxazaborinine (**5j**).

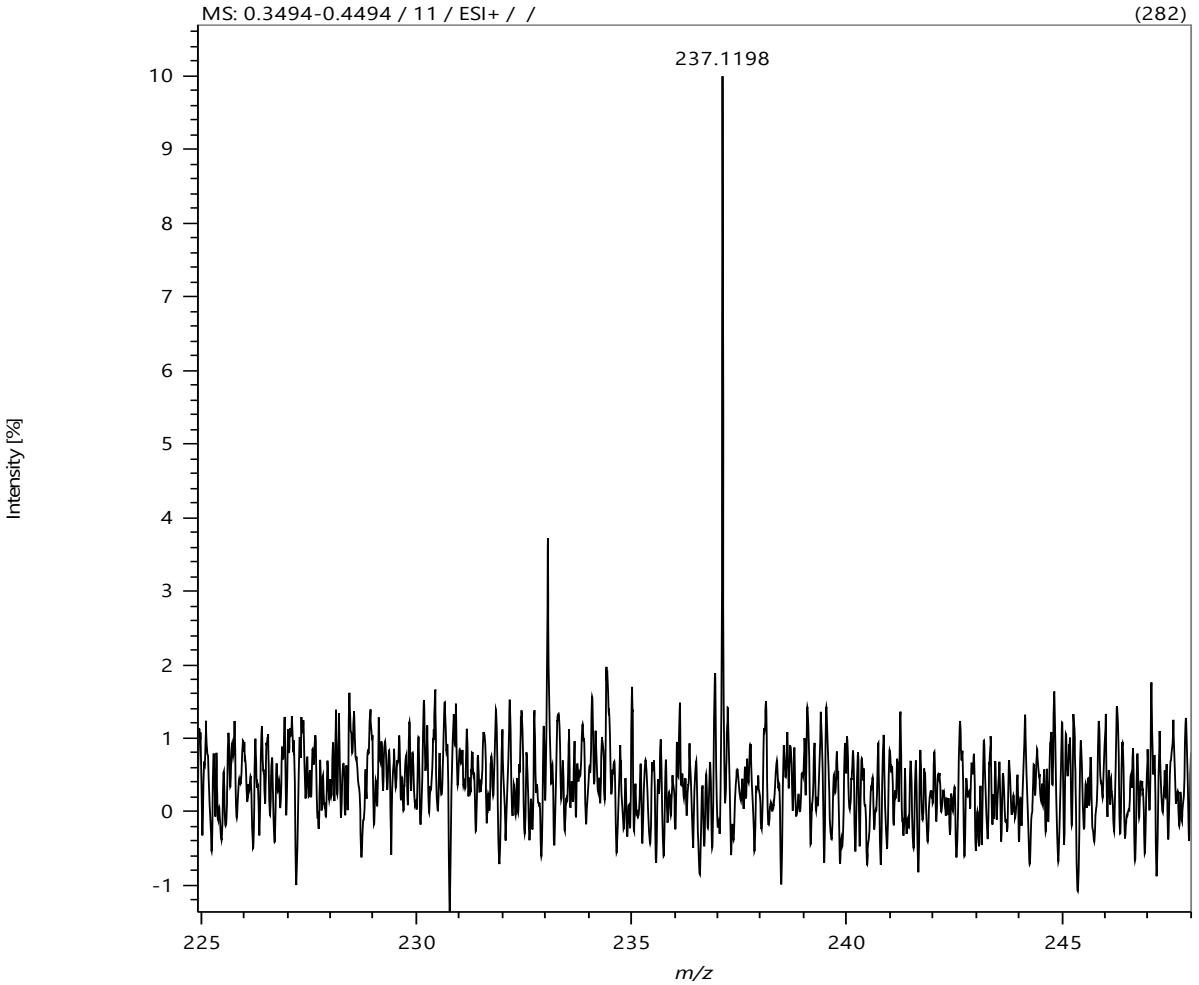


Fig. S145 2,5-diphenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7a**).

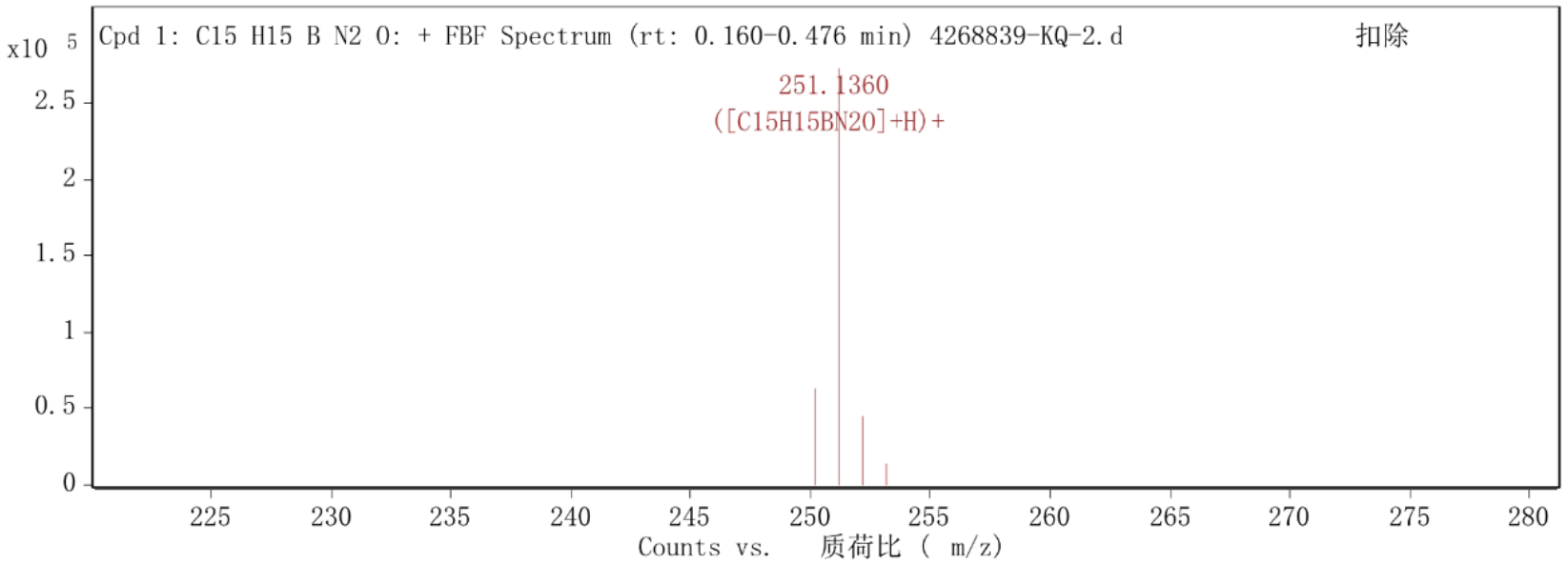


Fig. S146 5-phenyl-2-(p-tolyl)-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7b**).

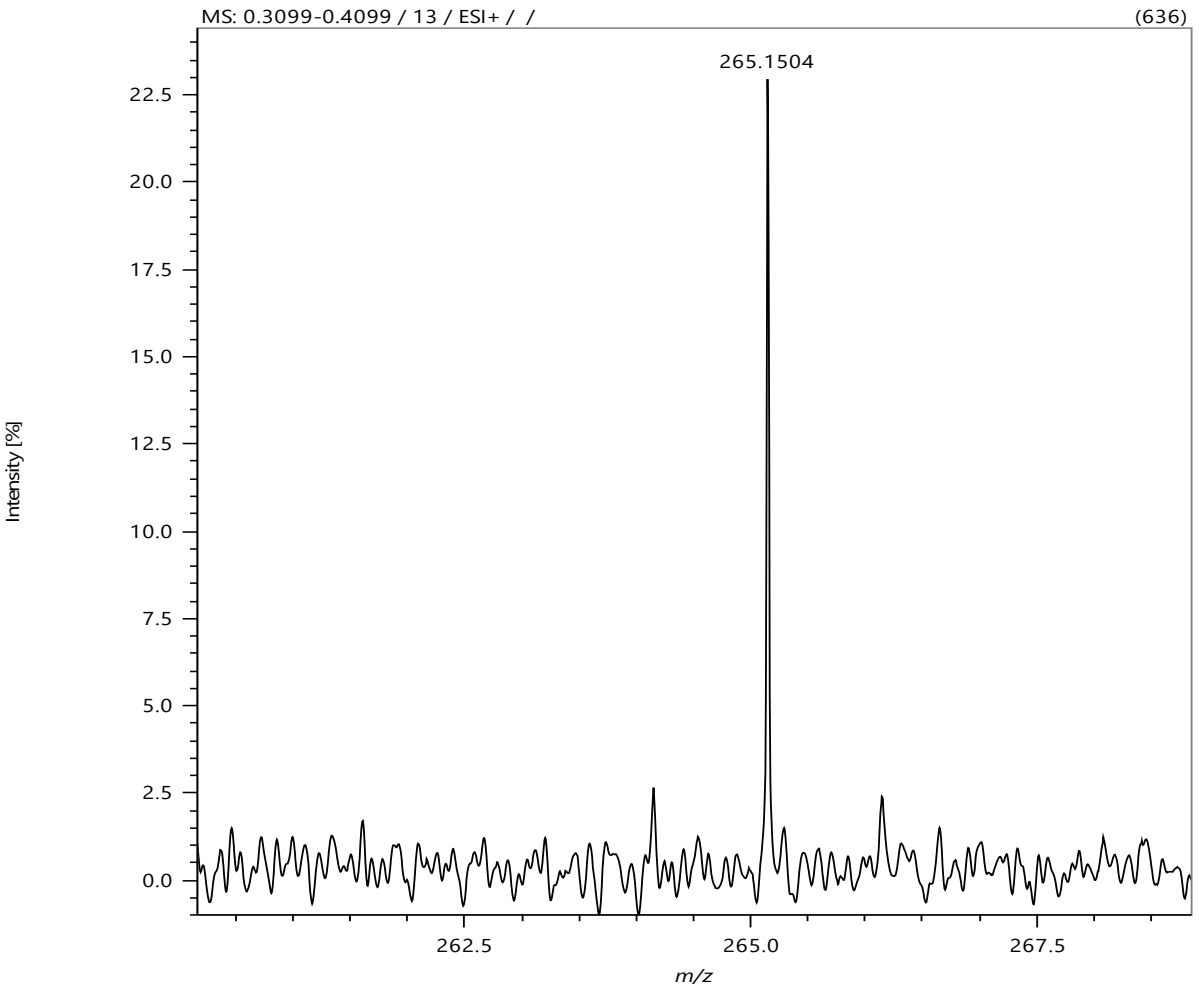


Fig. S147 2-(4-ethylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7c**).

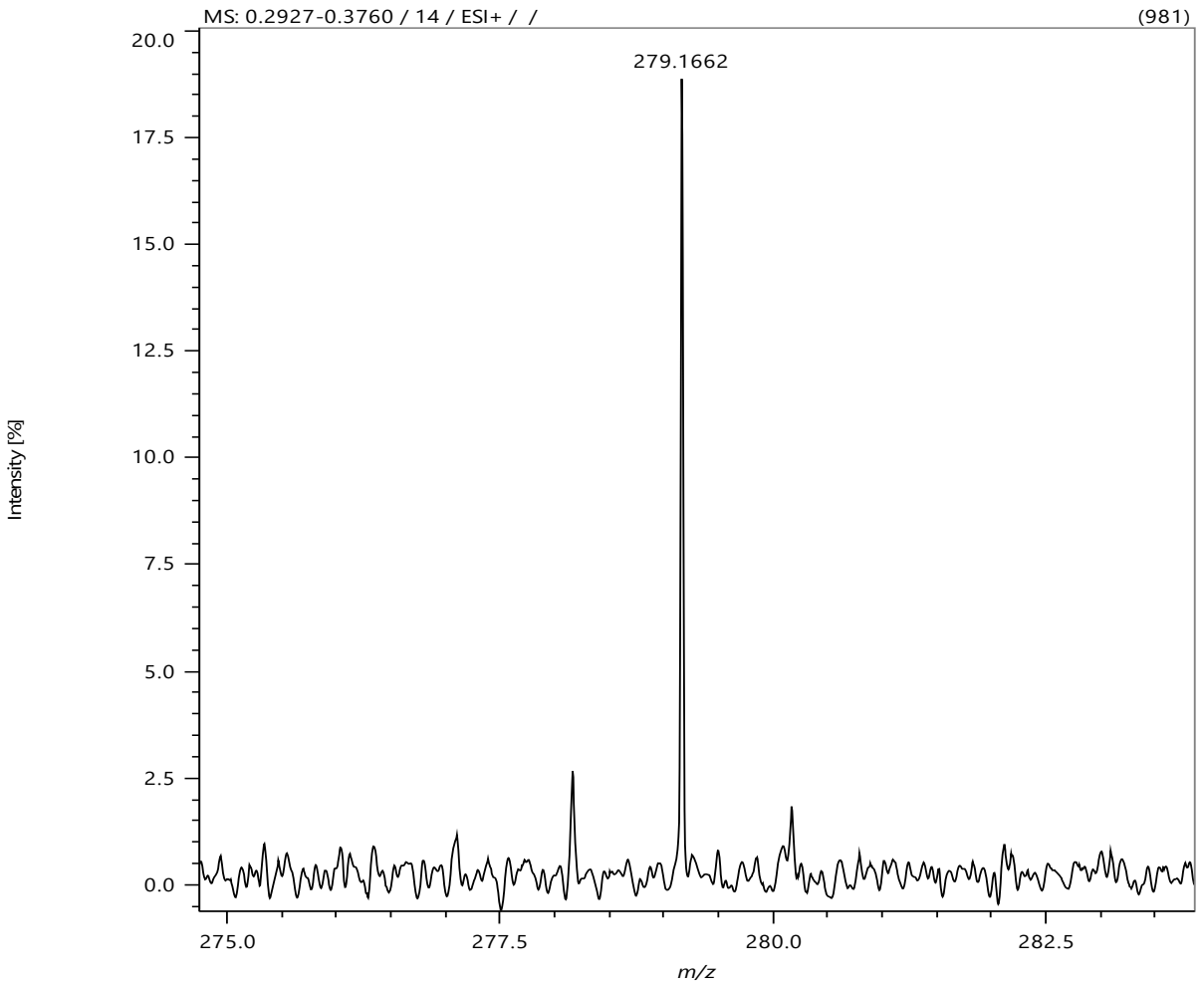


Fig. S148 2-(4-isopropylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7d**).

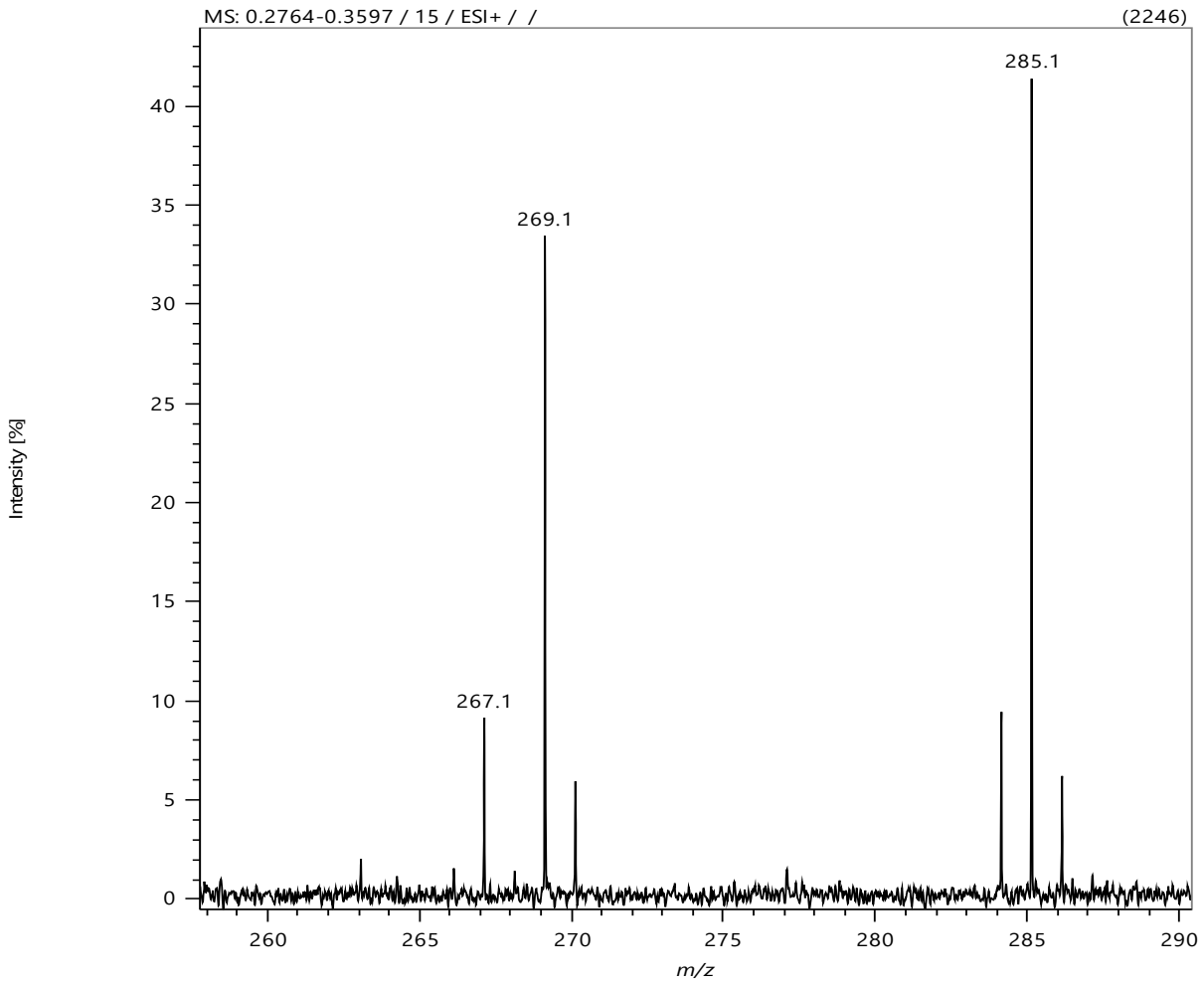


Fig. S149 2-(4-methoxyphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7e**).

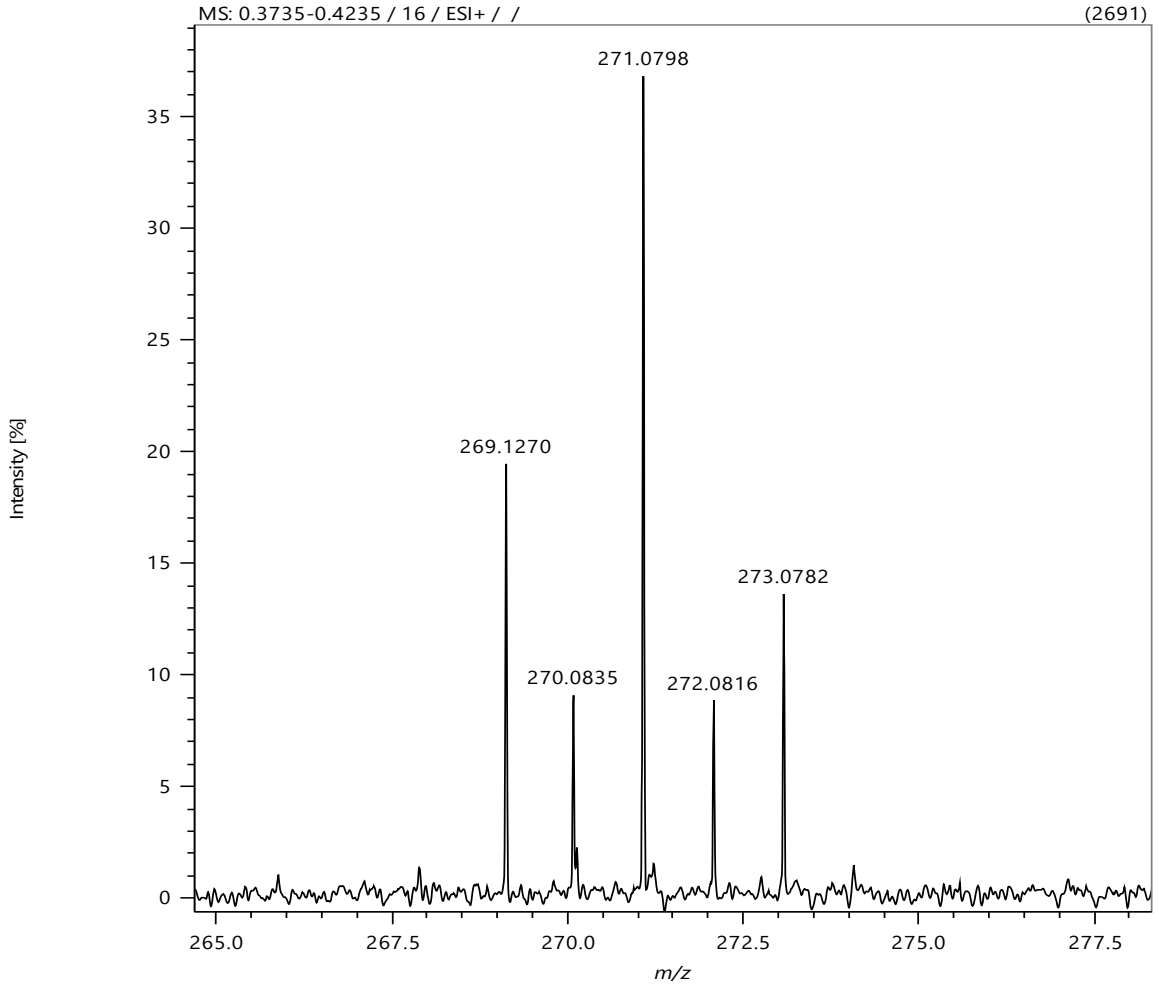


Fig. S150 2-(4-chlorophenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7f**).

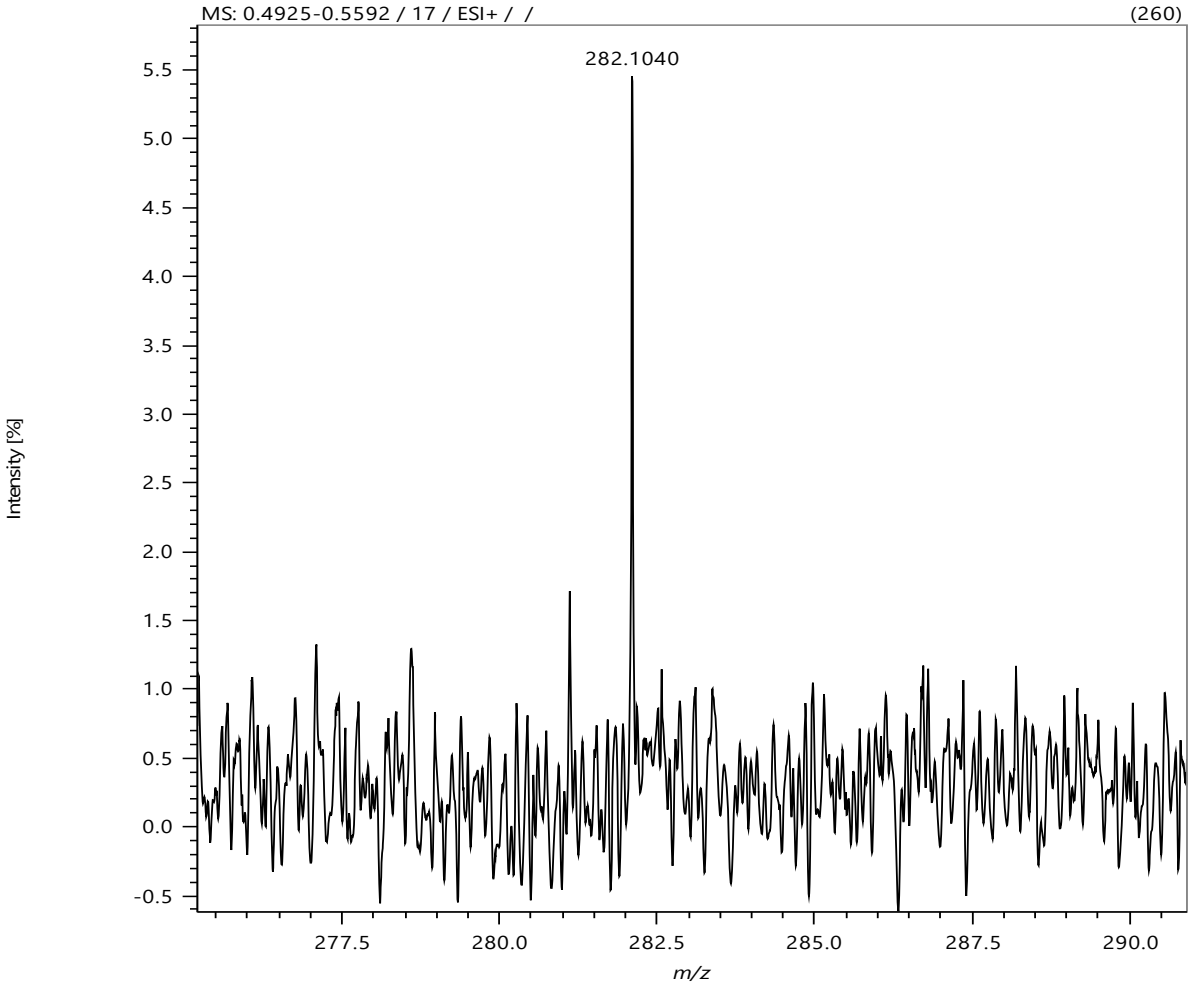


Fig. S151 2-(4-nitrophenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7g**).

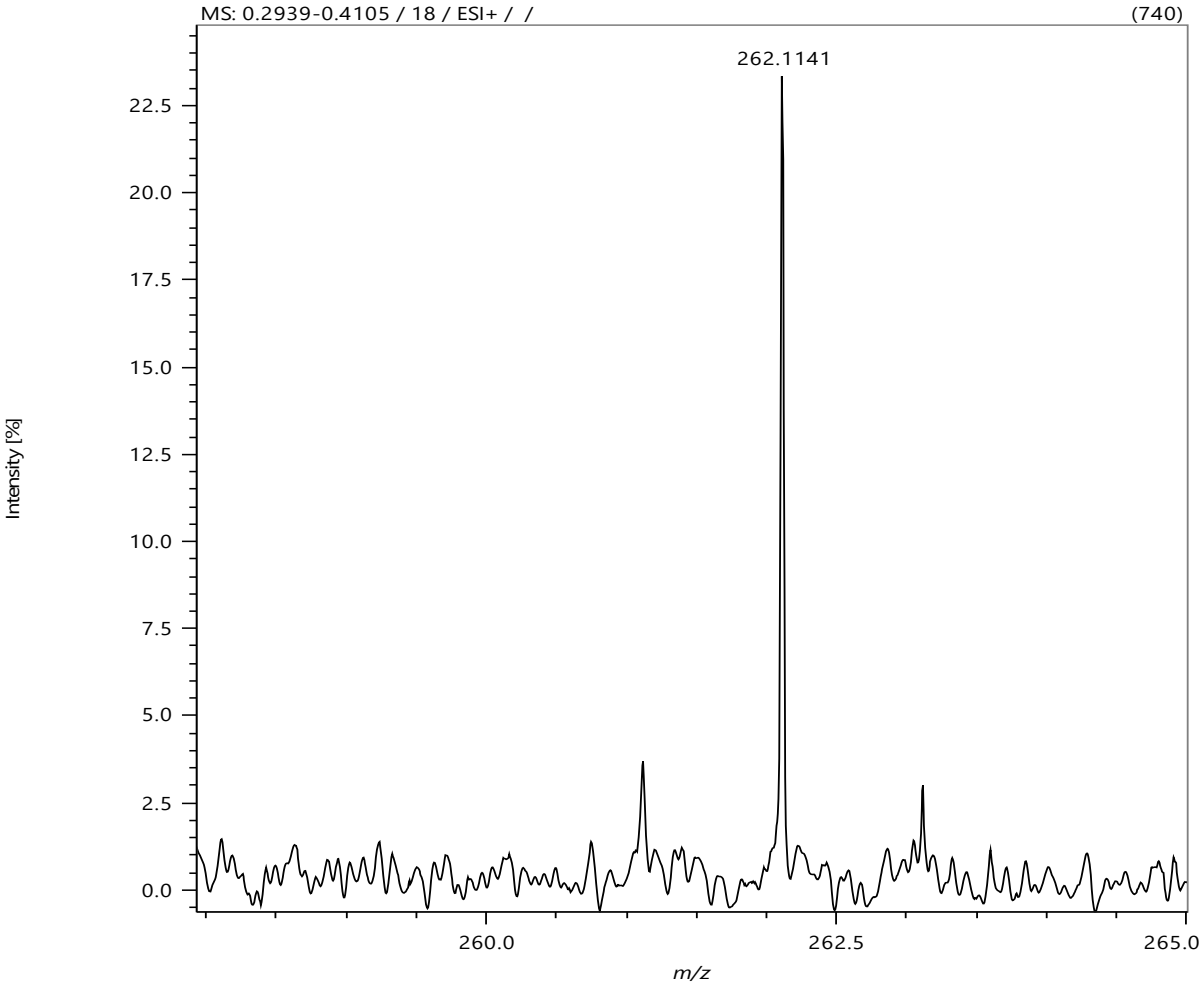


Fig. S152 4-(5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinin-2-yl) benzonitrile (**7h**).

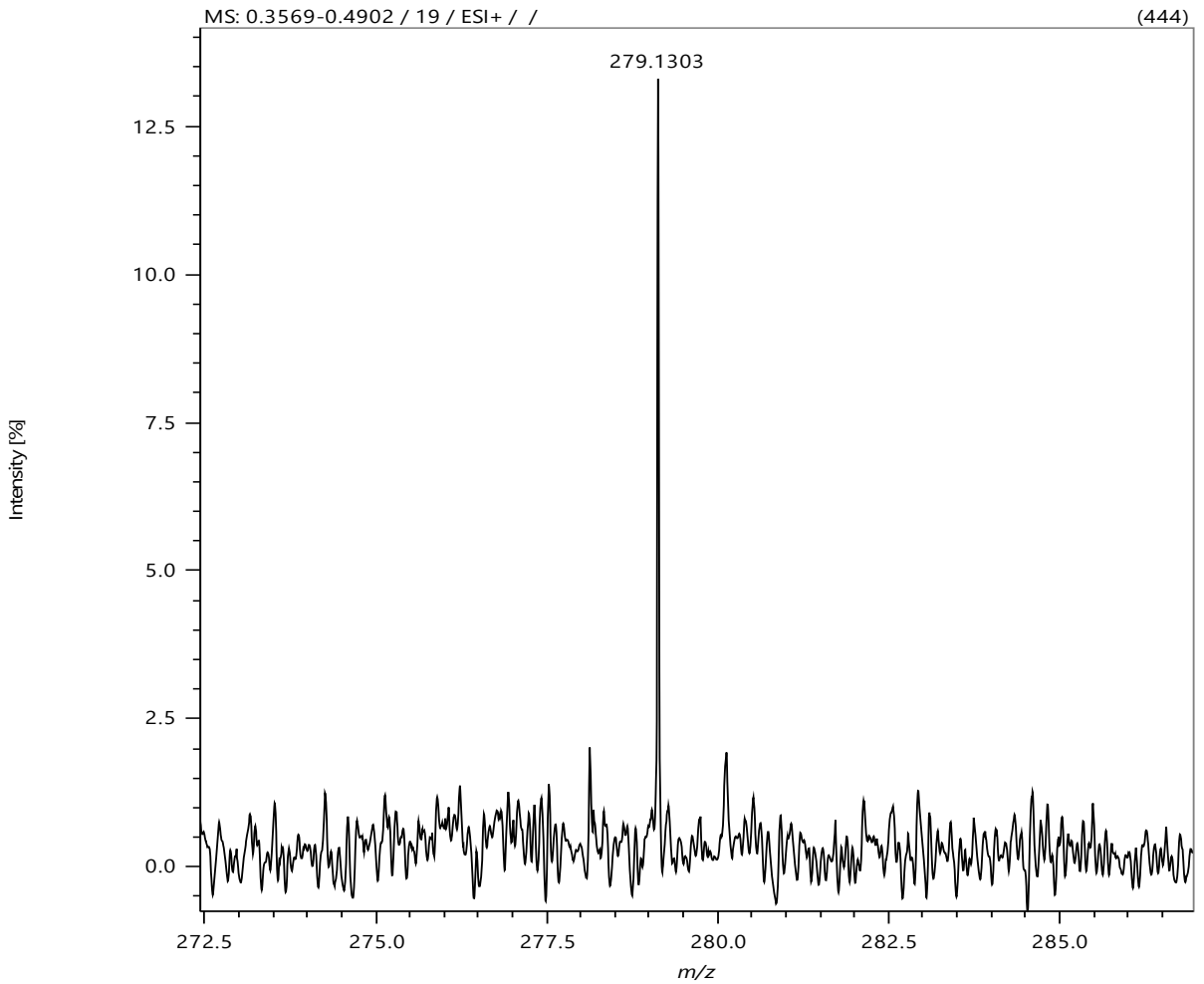


Fig. S153 1-(4-(5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinin-2-yl) phenyl) ethan-1-one (**7i**).

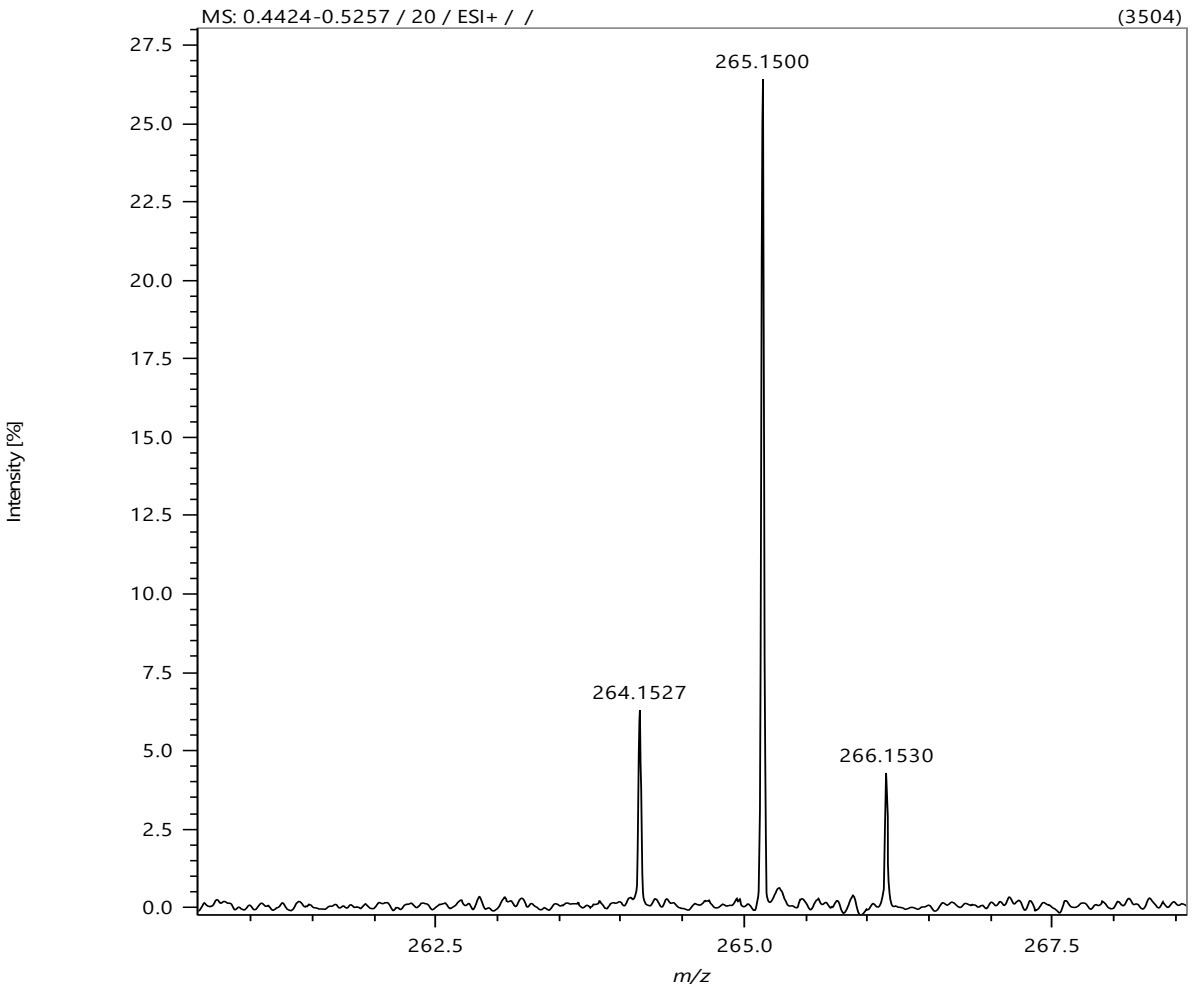


Fig. S154 2-(3,5-dimethylphenyl)-5-phenyl-3,6-dihydro-2H-1,3,4,2-oxadiazaborinine (**7j**).

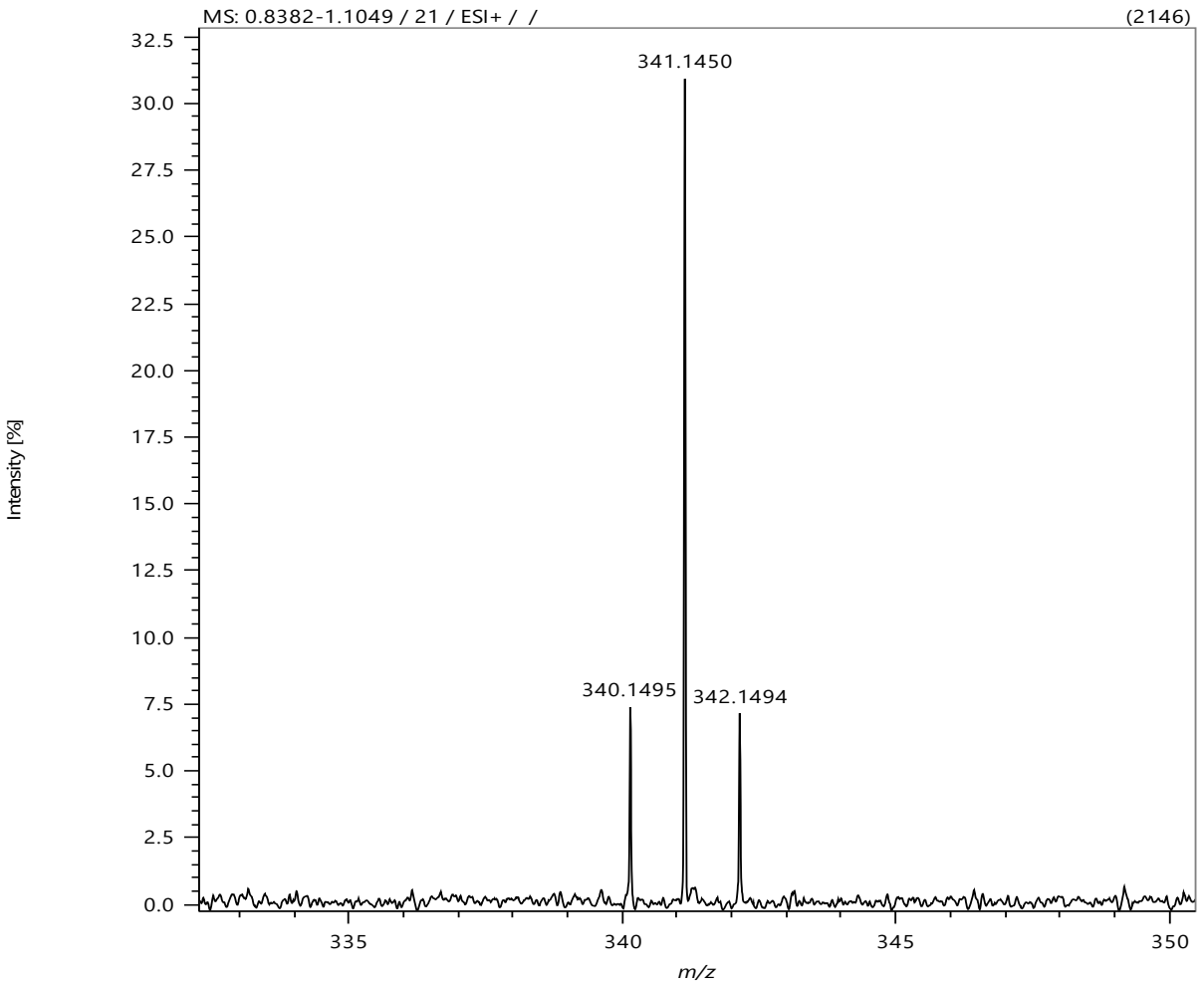


Fig. S155 Iminoboronates (**9a**).

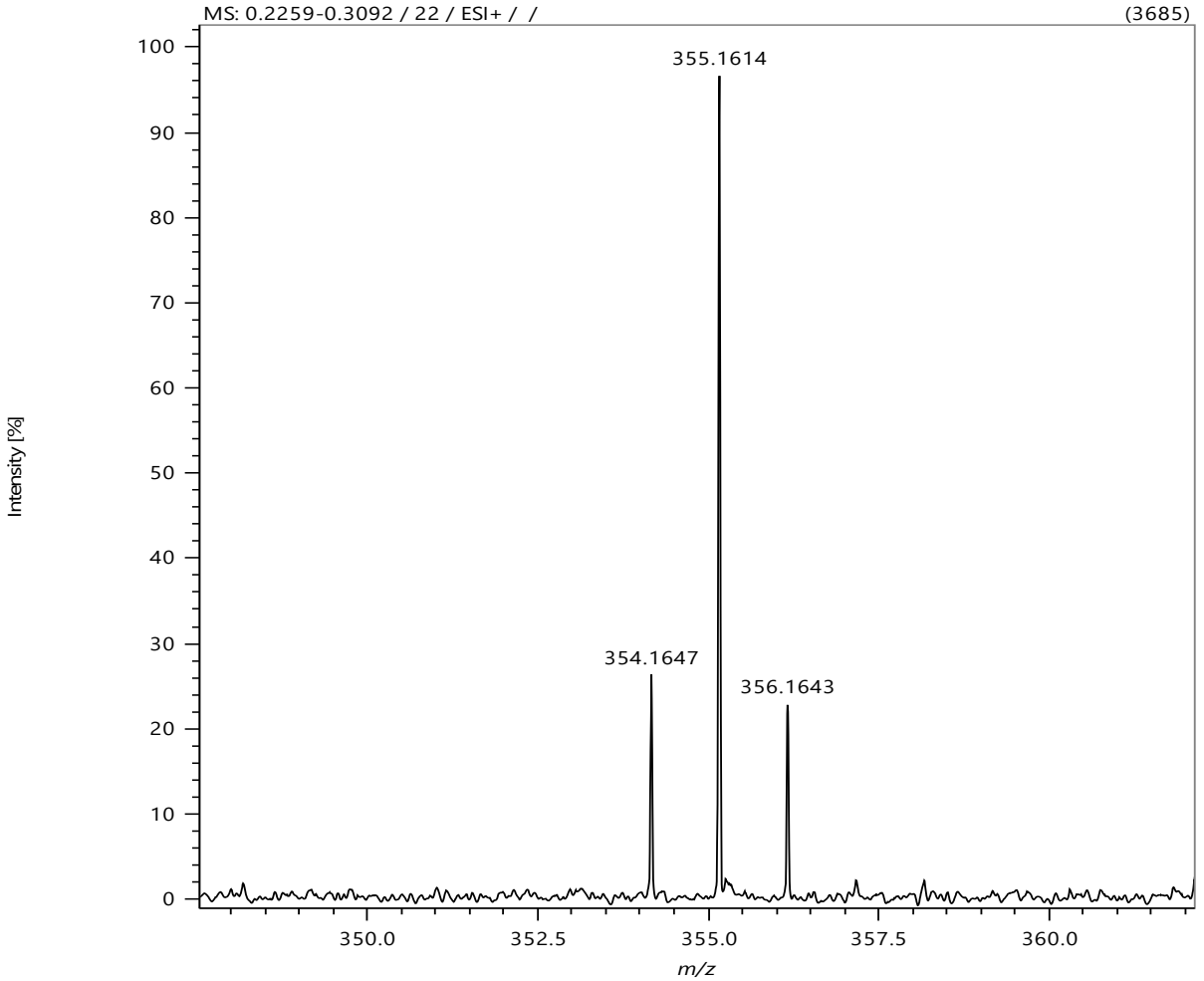


Fig. S156 Iminoboronates (**9b**).

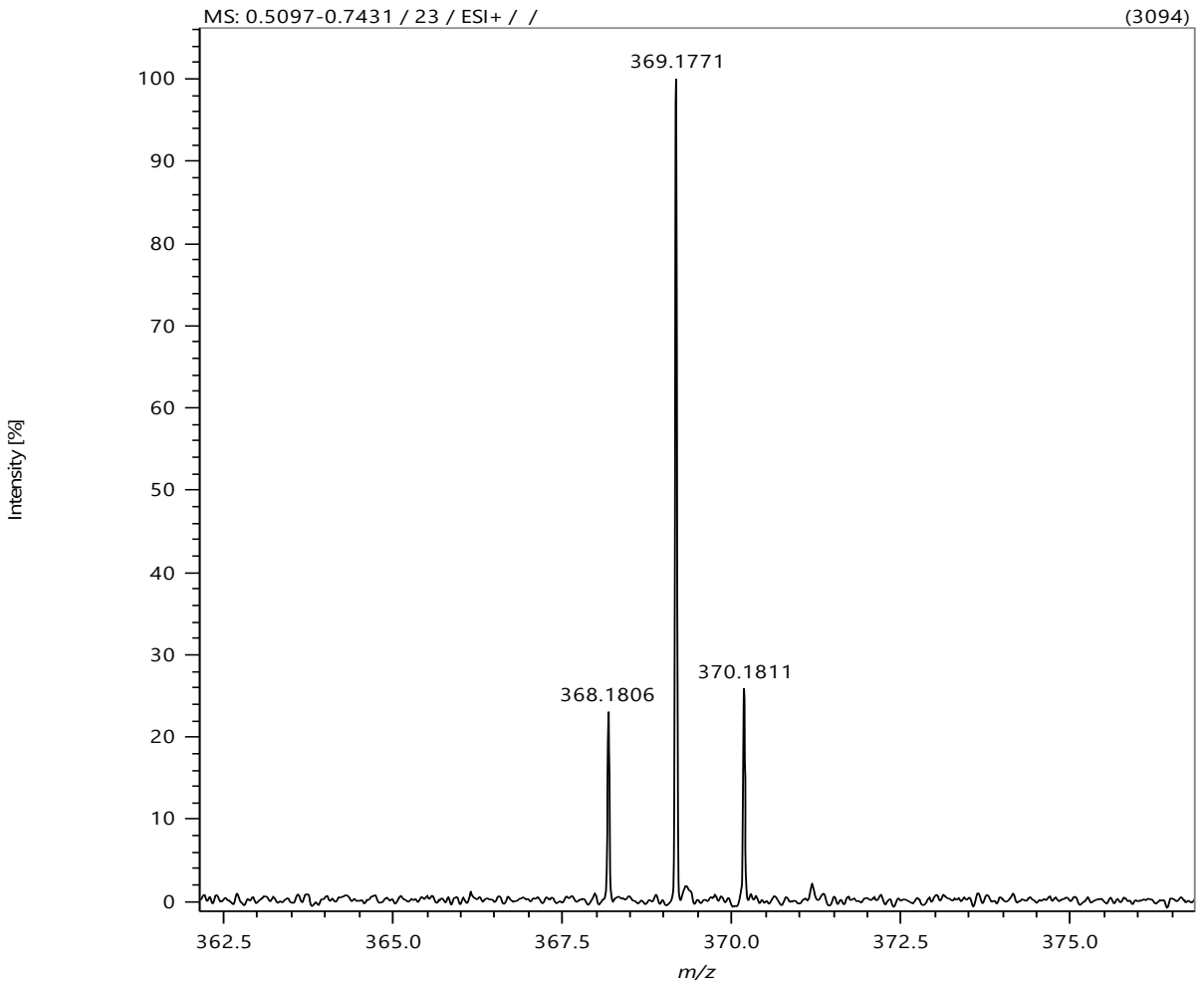


Fig. S157 Iminoboronates (**9c**).

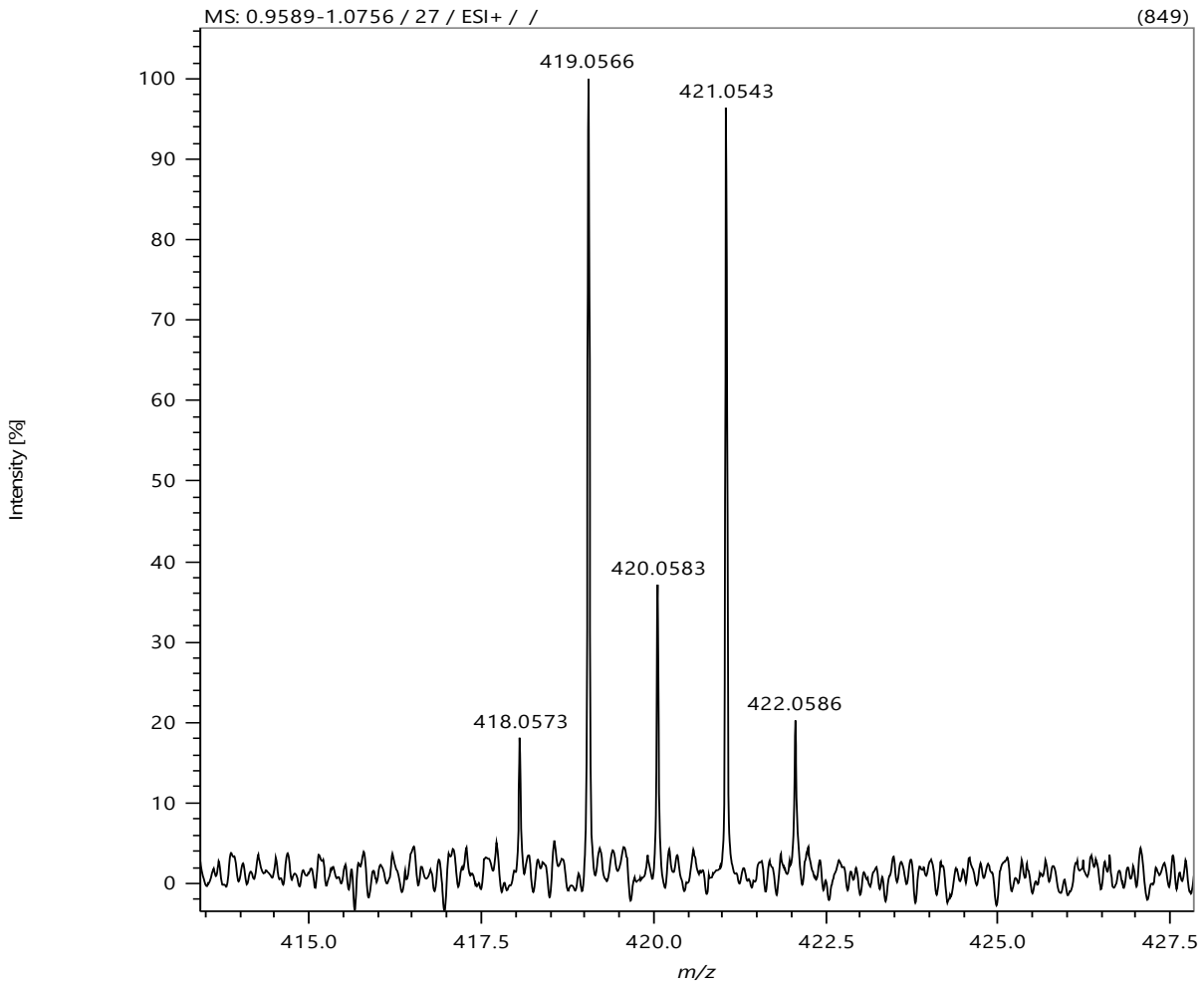


Fig. S158 Iminoboronates (**9d**).

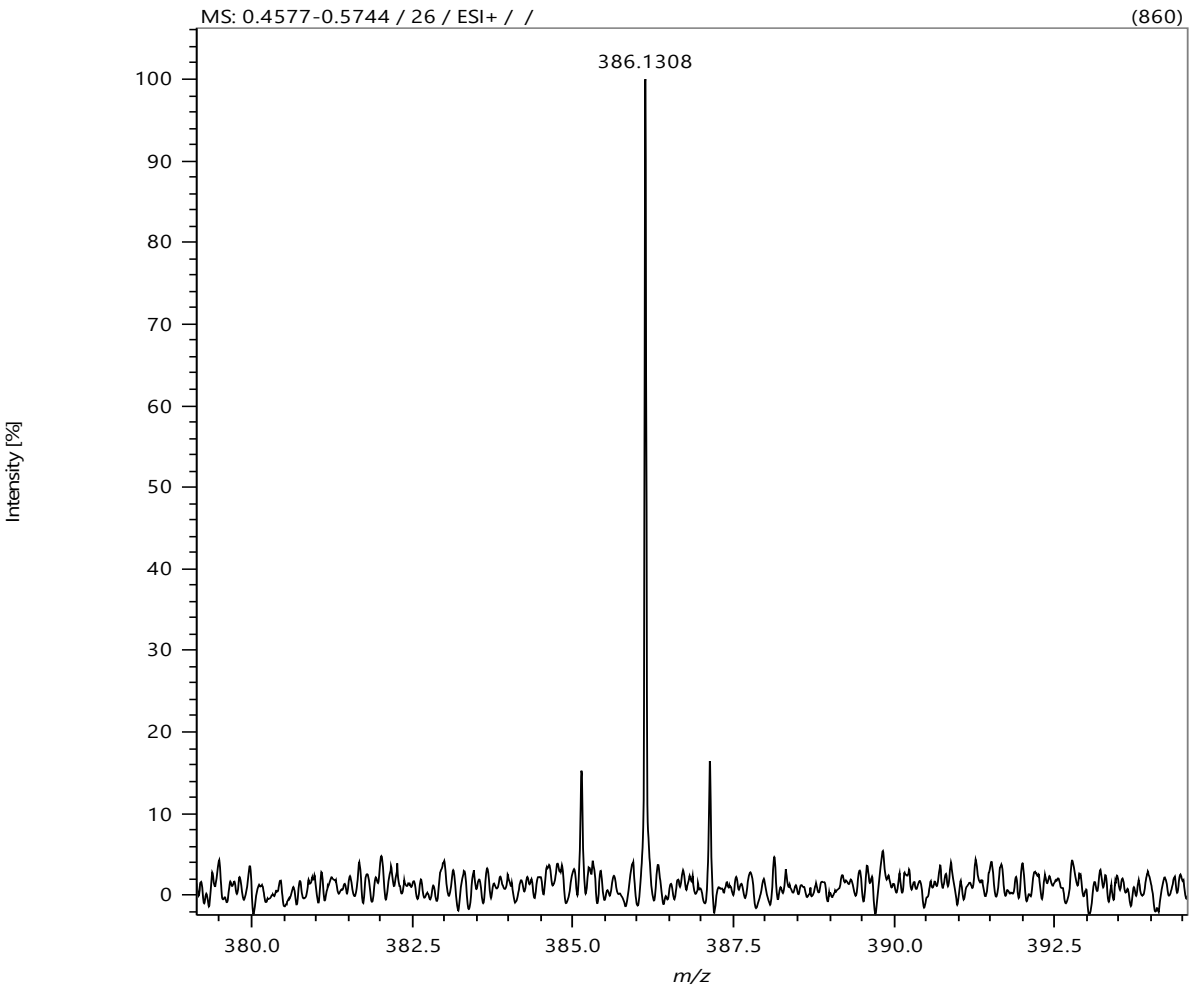


Fig. S159 Iminoboronates (**9e**).

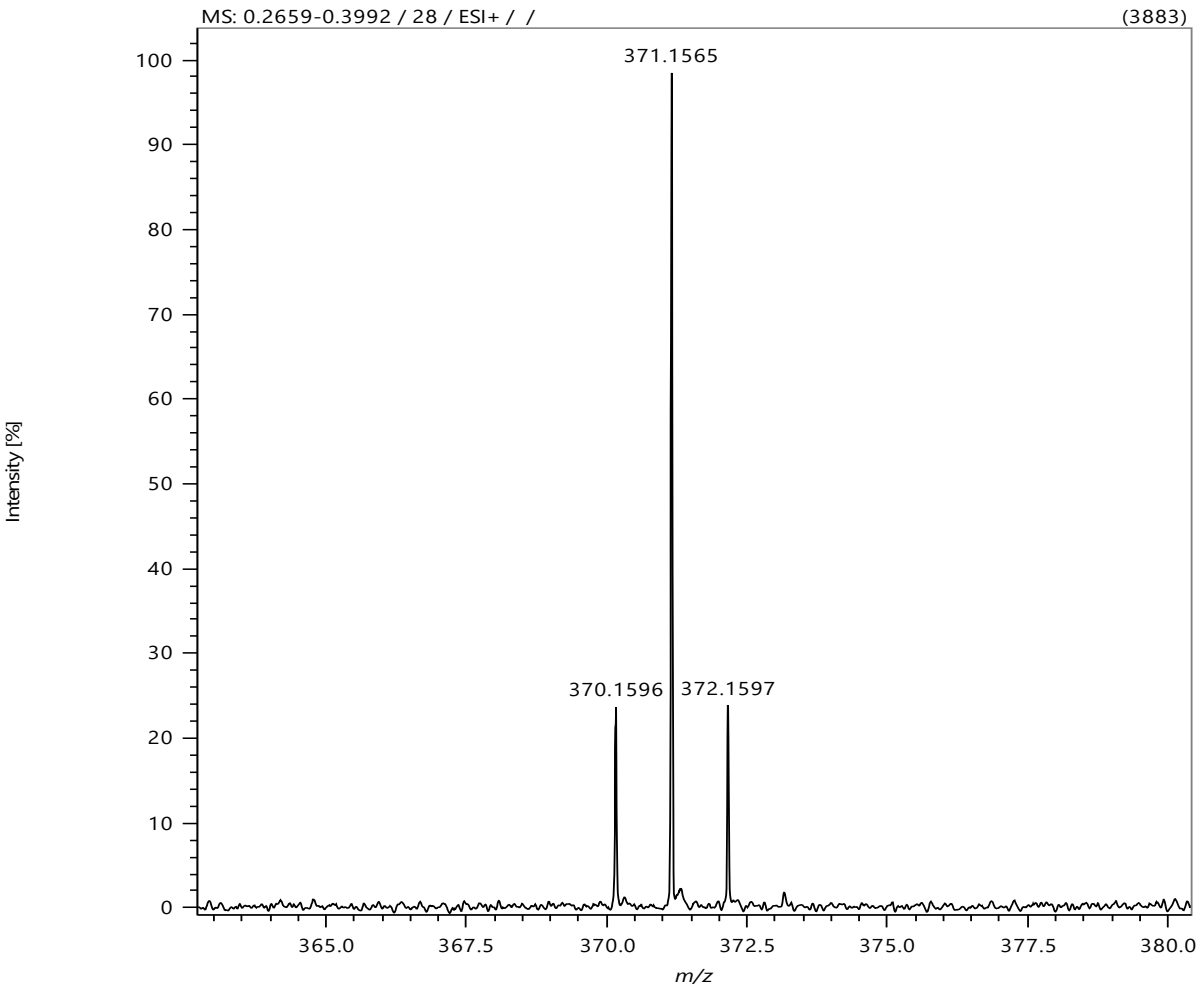


Fig. S160 Iminoboronates (**9f**).

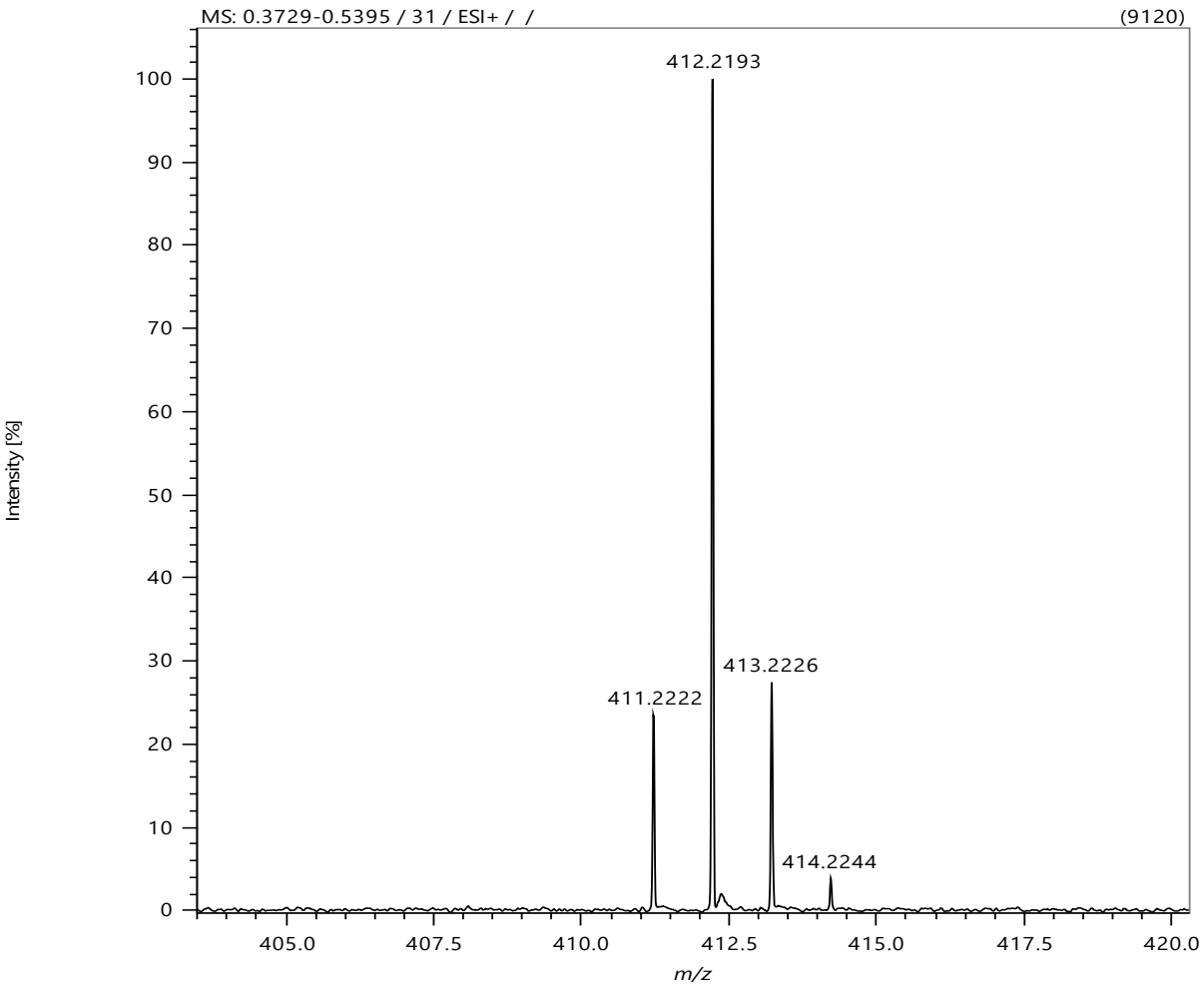


Fig. S161 Iminoboronates (**9g**).

11. Photophysical properties of 9a-9g.

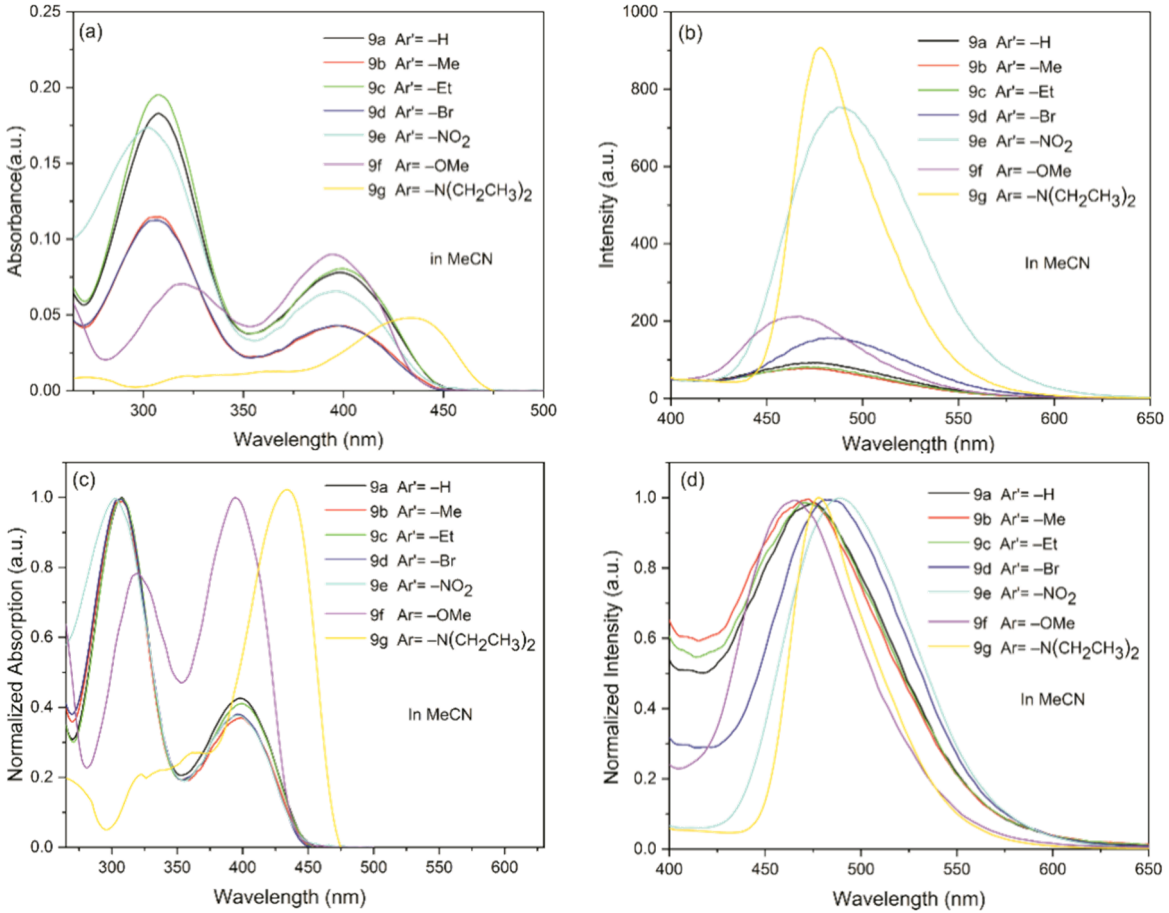


Fig. S162 (a) Absorption spectra of 9a-9e (1×10^{-5} M), 9f (4×10^{-6} M) and 9g (1×10^{-6} M) in acetonitrile; (b) Fluorescence spectra of 9a-9e (1×10^{-5} M), 9f (4×10^{-6} M) and 9g (1×10^{-6} M) in acetonitrile (λ_{ex} = 295 nm); (c) and (d) Normalized absorption and emission spectra of 9a-9g, respectively.

Table S163. Photophysical Data of **9a-9g** in Acetonitrile[a]

Entry	Compound	λ_{abs} (nm)	ε_{max} ($M^{-1}cm^{-1}$)	λ_{fl} (nm)	Stokes shift (nm)	Φ_{fl}[b,c]
1	9a	306, 396	18300 7800	474	78	0.01
2	9b	310, 395	11600 4300	470	75	0.02
3	9c	308, 399	19600 8100	471	72	0.01
4	9d	304, 394	11300 4300	481	87	0.04
5	9e	302, 395	17400 6600	487	92	0.09
6	9f	319, 393	18000 22500	467	74	0.02
7	9g	425	47000	478	53	0.26

[a] Absorption and fluorescence spectra of 9a-9e (1×10^{-5} M), 9f (4×10^{-6} M) and 9g (1×10^{-6} M) in acetonitrile (λ_{ex} = 348 nm) at room temperature.

[b] Fluorescence quantum yields (Φ_F) were measured in acetonitrile at room temperature (9a-9e (1×10^{-5} M), 9f (4×10^{-6} M) and 9g (1×10^{-6} M)) and the reference standard is 1×10^{-6} M Rhodamine B (λ_{ex} = 348 nm, quantum yield = 0.7 in methanol).

[c] The Φ_F values of the compounds were calculated according to the following equation:

$$\Phi_F(\mathrm{s}) = \Phi_F(\mathrm{ref}) \times \frac{F(\mathrm{s})}{F(\mathrm{ref})} \times \frac{\mathrm{Ab(ref)}}{\mathrm{Ab(s)}} \times \frac{n(\mathrm{ref})^2}{n(\mathrm{s})^2}$$

where F is the area under the emission spectra with excitation at 348 nm, Ab is the absorbance at 348 nm (no more than 0.05), n is the index of the refractive index of the solvent (MeCN: 1.34 MeOH: 1.32), and the symbols s and ref in brackets represent the sample and reference, respectively.