

Synthesis of Benzo[4,5]imidazo[1,2-*a*]quinoxalines by **I₂-Mediated sp³ C–H Amination**

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1. General Information. ^1H and ^{13}C NMR spectra were recorded on a 400 MHz (100 MHz for ^{13}C NMR) spectrometer. Chemical shift values are reported in ppm (parts per million) with tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublets; dt, doublet of triplets. The coupling constants (J) are reported in Hertz (Hz). Melting points were determined on a micromelting point apparatus and are uncorrected. High-resolution mass spectra (HRMS) were obtained on a Q-TOF Mass Spectrometer equipped with an electrospray ion source (ESI), and operated in the positive mode. Flash column chromatography was performed over 200-300 mesh silica gel. Toluene used in the synthesis of products **2** was analytical reagent grade and used without any pretreatment.

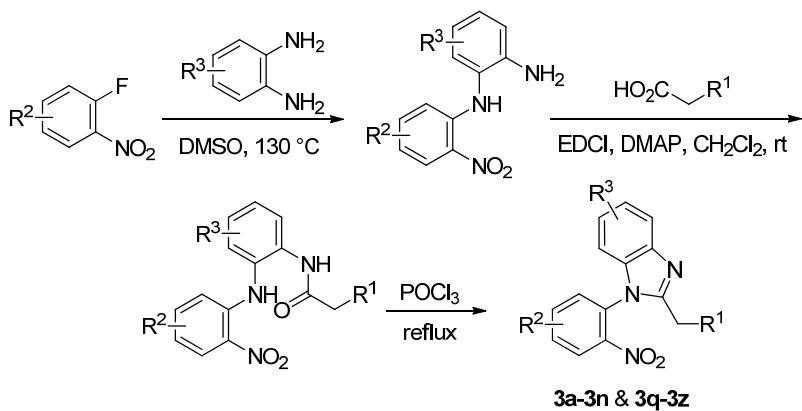
2. Preparation of Nitro Compounds **3.** The required nitro compounds **3** for the preparation of substrates **1** were synthesized as follows:

2.1. Method A. Using the synthesis of **3a** as an example, a reaction mixture of 1-fluoro-2-nitrobenzene (776 mg, 5.5 mmol) and 1,2-diaminobenzene (542 mg, 5 mmol) in DMSO (10 mL) was stirred at 130 °C for 8 h.¹ After cooling to room temperature, it was quenched with H₂O (10 mL) and extracted with EtOAc (3 × 20 mL). The combined organic layer was washed with brine (3 × 10 mL), dried over anhydrous Na₂SO₄, concentrated and purified through silica gel chromatography (EtOAc/petroleum ether (PE) 6:94) to give *N*¹-(2-nitrophenyl)benzene-1,2-diamine as a reddish brown solid (951 mg, 83% yield).

EDCI (1.2 g, 6 mmol) and DMAP (184 mg, 1.5 mmol) were added in sequence to a mixture of phenylacetic acid (409 mg, 3 mmol) and *N*¹-(2-nitrophenyl)benzene-1,2-diamine (757 mg, 3.3 mmol) in CH₂Cl₂ (10 mL). The

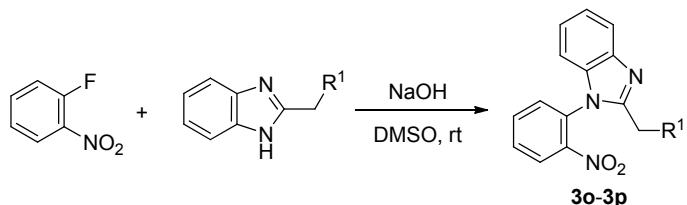
reaction mixture was stirred at room temperature for 5 h, then quenched with H₂O (10 mL), and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layer was dried over anhydrous Na₂SO₄, concentrated and purified through silica gel chromatography (EtOAc/PE 8:92) to give *N*-(2-((2-nitrophenyl)amino)phenyl)-2-phenylacetamide as a yellow solid (1.02 g, 98% yield).

A mixture of *N*-(2-((2-nitrophenyl)amino)phenyl)-2-phenylacetamide (696 mg, 2 mmol) in POCl₃ (5 mL) was refluxed for 1 h.² After cooling to 0 °C, the reaction was quenched and basified by sat. NaHCO₃, and then extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layer was dried over anhydrous Na₂SO₄, concentrated, and purified through silica gel chromatography (EtOAc/PE 12:88) to give nitro compound **3a** as a yellow solid (659 mg, 97% yield). Compounds **3b–3n** and **3q–3z** were prepared using this method.



2.2. Method B. Using the synthesis of **3o** as an example, a mixture of 1-fluoro-2-nitrobenzene (567 mg, 4 mmol) and 2-methyl-1*H*-benzo[*d*]imidazole (632 mg, 4.8 mmol) in DMSO (10 mL) was treated with NaOH (236 mg, 6 mmol). The reaction mixture was stirred at room temperature for 3 h and upon completion the reaction mixture was neutralized with 1 M HCl and extracted with EtOAc (3 × 20 mL). The combined organic layer was washed with brine (3 × 10 mL), dried over

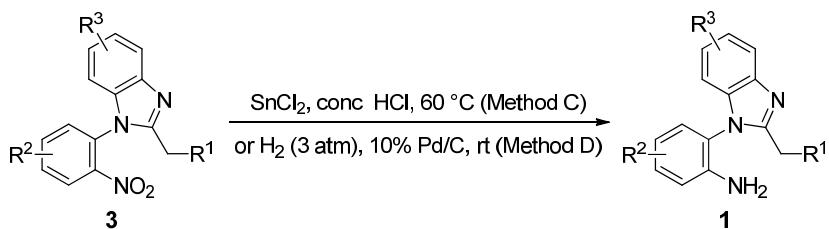
anhydrous Na_2SO_4 , concentrated, and purified through silica gel chromatography (EtOAc/PE 33:67) to give nitro compound **3o** as a yellow solid (1.0 g, 99% yield). Compound **3p** was synthesized similarly.



3. Preparation of Substrates 1.

3.1. Method C. The corresponding nitro compound **3** (2 mmol) was added to a stirred mixture of $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (1.4 g, 6 mmol) in conc. HCl (10 mL). Then the reaction mixture was heated at 60 °C until TLC indicated the completion of the reaction. After cooling to 0 °C, sat. NaOH was added slowly to the reaction mixture to adjust the pH to 9-10, and then it was extracted with EtOAc (3×20 mL). The combined organic layer was dried over anhydrous Na_2SO_4 , concentrated and purified through silica gel chromatography to afford substrates **1a**, **1c–1d**, **1h–1j**, **1l**, **1n–1q** and **1s–1y**.

3.2. Method D. A mixture of the corresponding nitro compound **3** (2 mmol) and 10% Pd/C (150 mg) in MeOH (50 mL) was hydrogenated under 3 atm of H_2 for 12 h. The catalyst was filtered off and the filtrate was concentrated and purified through silica gel chromatography to afford substrates **1b**, **1e–1g**, **1k**, **1m**, **1r**, and **1z**.



2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)aniline (1a). 5 h; eluent: EtOAc/PE 17:83; 479 mg, 80% yield; white solid, mp 157-158 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82

(d, $J = 8.0$ Hz, 1H), 7.30-7.26 (m, 2H, overlapped with the peak of chloroform), 7.21-7.14 (m, 4H), 7.04-7.00 (m, 3H), 6.92 (dd, $J = 8.0, 1.2$ Hz, 1H), 6.81-6.78 (m, 2H), 4.16-4.08 (m, 2H), 3.23 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.1, 143.6, 142.8, 136.2, 135.7, 130.5, 129.3, 128.8, 128.3, 126.6, 122.9, 122.5, 120.6, 119.5, 118.7, 116.4, 110.2, 34.4; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{20}\text{H}_{18}\text{N}_3$ 300.1495, found 300.1494.

2-(2-(4-Methylbenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1b). 12 h; eluent: EtOAc/PE 7:93; 595 mg, 95% yield; white solid, mp 168-169 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, $J = 8.0$ Hz, 1H), 7.30-7.24 (m, 2H, overlapped with the peak of chloroform), 7.19-7.15 (m, 1H), 7.00-6.91 (m, 6H), 6.81-6.77 (m, 2H), 4.11-4.01 (m, 2H), 3.28 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.5, 143.7, 142.9, 136.2, 135.7, 133.2, 130.5, 129.4, 129.1, 128.8, 122.8, 122.5, 120.7, 119.6, 118.7, 116.5, 110.3, 33.9, 21.1; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{21}\text{H}_{20}\text{N}_3$ 314.1652, found 314.1653.

2-(2-(4-Methoxybenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1c). 4.5 h; eluent: EtOAc/PE 28:72; 501 mg, 76% yield; white solid, mp 181-182 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 1H), 7.32-7.26 (m, 2H, overlapped with the peak of chloroform), 7.21-7.17 (m, 1H), 7.01 (d, $J = 8.0$ Hz, 1H), 6.96-6.93 (m, 3H), 6.83-6.80 (m, 2H), 6.70 (d, $J = 8.4$ Hz, 2H), 4.11-4.02 (m, 2H), 3.74 (s, 3H), 3.24 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.3, 154.5, 143.7, 142.9, 135.7, 130.5, 129.9, 129.4, 128.4, 122.9, 122.5, 120.7, 119.6, 118.8, 116.5, 113.8, 110.2, 55.3, 33.5; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{21}\text{H}_{20}\text{N}_3\text{O}$ 330.1601, found 330.1600.

2-(2-(4-Fluorobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1d). 4 h; eluent: EtOAc/PE 25:75; 584 mg, 92% yield; white solid, mp 173-174 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 7.65 (d, $J = 8.0$ Hz, 1H), 7.25-7.12 (m, 5H), 7.04 (t, $J = 9.2$ Hz,

2H), 6.95-6.89 (m, 3H), 6.66-6.62 (m, 1H), 5.00 (s, 2H), 4.09-3.93 (m, 2H); ^{13}C NMR (100 MHz, DMSO-*d*₆) δ 161.4 (d, $J_{\text{C}-\text{F}} = 240.5$ Hz), 154.3, 145.6, 143.2, 136.2, 133.4 (d, $J_{\text{C}-\text{F}} = 3.0$ Hz), 131.2 (d, $J_{\text{C}-\text{F}} = 8.1$ Hz), 130.6, 129.4, 122.7, 122.2, 119.4, 119.2, 116.7, 116.5, 115.3 (d, $J_{\text{C}-\text{F}} = 21.1$ Hz), 110.6, 33.0; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₇FN₃ 318.1401, found 318.1402.

2-(2-(4-Chlorobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1e). 12 h; eluent: EtOAc/PE 9:91; 641 mg, 96% yield; white solid, mp 170-171 °C; ^1H NMR (400 MHz, CDCl₃) δ 7.81 (d, $J = 8.0$ Hz, 1H), 7.32-7.26 (m, 2H), 7.22-7.18 (m, 1H), 7.13 (d, $J = 8.4$ Hz, 2H), 7.02 (d, $J = 8.0$ Hz, 1H), 6.97 (d, $J = 8.4$ Hz, 2H), 6.91 (dd, $J = 8.0, 1.6$ Hz, 1H), 6.84-6.79 (m, 2H), 4.13-4.03 (m, 2H), 3.32 (s, 2H); ^{13}C NMR (100 MHz, CDCl₃) δ 153.6, 143.6, 142.8, 135.6, 134.7, 132.5, 130.7, 130.2, 129.3, 128.5, 123.1, 122.7, 120.4, 119.6, 118.8, 116.5, 110.3, 33.8; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₇ClN₃ 334.1106, found 334.1108.

2-(2-(4-Bromobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1f). 12 h; eluent: EtOAc/PE 14:86; 743 mg, 98% yield; white solid, mp 157-158 °C; ^1H NMR (400 MHz, CDCl₃) δ 7.81 (d, $J = 8.0$ Hz, 1H), 7.32-7.27 (m, 4H), 7.21 (dt, $J = 8.0, 0.8$ Hz, 1H), 7.02 (d, $J = 8.0$ Hz, 1H), 6.93-6.91 (m, 3H), 6.84-6.79 (m, 2H), 4.12-4.02 (m, 2H), 3.31 (s, 2H); ^{13}C NMR (100 MHz, CDCl₃) δ 153.5, 143.5, 142.8, 135.6, 135.2, 131.4, 130.65, 135.57, 129.2, 123.0, 122.6, 120.6, 120.4, 119.6, 118.8, 116.4, 110.2, 33.8; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₇BrN₃ 378.0600, found 378.0603.

2-(2-(4-Iodobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1g). 12 h; eluent: EtOAc/PE 9:91; 808 mg, 95% yield; white solid, mp 163-164 °C; ^1H NMR (400 MHz, CDCl₃) δ 7.81 (d, $J = 8.0$ Hz, 1H), 7.49 (d, $J = 8.0$ Hz, 2H), 7.32-7.27 (m, 2H, overlapped with the peak of chloroform), 7.20 (t, $J = 7.6$ Hz, 1H), 7.02 (d, $J = 8.0$ Hz, 1H), 6.92 (d, $J =$

7.6 Hz, 1H), 6.84-6.79 (m, 4H), 4.10-4.00 (m, 2H), 3.31 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.5, 143.5, 142.8, 137.4, 136.0, 135.6, 130.9, 130.7, 129.3, 123.1, 122.7, 120.4, 119.6, 118.8, 116.5, 110.3, 92.2, 33.9; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{IN}_3$ 426.0462, found 426.0463.

2-(2-(4-(Trifluoromethyl)benzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1h). 2.5 h; eluent: EtOAc/PE 25:75; 441 mg, 60% yield; white solid, mp 143-144 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 1H), 7.43 (d, $J = 8.0$ Hz, 2H), 7.33-7.28 (m, 2H), 7.24-7.17 (m, 3H), 7.03 (d, $J = 8.0$ Hz, 1H), 6.91 (dd, $J = 8.0, 1.6$ Hz, 1H), 6.85-6.79 (m, 2H), 4.24-4.13 (m, 2H), 3.33 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.2, 143.5, 142.8, 140.3, 135.6, 130.8, 129.3, 129.2, 129.0 (q, $J_{\text{C}-\text{F}} = 32.2$ Hz), 125.3 (q, $J_{\text{C}-\text{F}} = 3.7$ Hz), 124.1 (q, $J_{\text{C}-\text{F}} = 270.5$ Hz), 123.2, 122.8, 120.3, 119.7, 118.9, 116.6, 110.3, 34.2; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{21}\text{H}_{17}\text{F}_3\text{N}_3$ 368.1369, found 368.1368.

2-(2-(3-Bromobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1i). 7 h; eluent: EtOAc/PE 25:75; 681 mg, 90% yield; white solid, mp 104-105 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.0$ Hz, 1H), 7.34-7.26 (m, 3H, overlapped with the peak of chloroform), 7.23-7.19 (m, 1H), 7.09 (s, 1H), 7.05-6.99 (m, 3H), 6.93 (dd, $J = 7.6, 1.2$ Hz, 1H), 6.85-6.81 (m, 2H), 4.14-4.06 (m, 2H), 3.28 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.5, 143.6, 142.9, 138.5, 135.8, 132.0, 130.9, 130.0, 129.9, 129.3, 127.7, 123.2, 122.8, 122.4, 120.4, 119.8, 118.9, 116.6, 110.4, 34.2; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{20}\text{H}_{17}\text{BrN}_3$ 378.0600, found 378.0597.

2-(2-(2-Bromobenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1j). 5 h; eluent: EtOAc/PE 17:83; 620 mg, 82% yield; white solid, mp 168-169 °C; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 7.63 (d, $J = 7.2$ Hz, 1H), 7.56 (d, $J = 7.6$ Hz, 1H), 7.32-7.31 (m, 2H), 7.25-7.16 (m, 4H), 7.02-6.93 (m, 3H), 6.66 (t, $J = 7.6$ Hz, 1H), 5.05 (s, 2H),

4.18-4.07 (m, 2H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 153.3, 145.7, 143.2, 137.0, 136.2, 132.8, 132.0, 130.6, 129.2, 129.1, 128.1, 124.5, 122.8, 122.2, 119.34, 119.27, 116.8, 116.6, 110.6, 34.2; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for C₂₀H₁₇BrN₃ 378.0600, found 378.0601.

2-(2-(2,5-Dimethylbenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1k). 12 h; eluent: EtOAc/CH₂Cl₂/PE 8:8:84; 635 mg, 97% yield; white solid, mp 139-140 °C; ^1H NMR (400 MHz, CDCl₃) δ 7.82 (d, J = 8.0 Hz, 1H), 7.30-7.25 (m, 2H), 7.19 (dt, J = 7.6, 1.2 Hz, 1H), 7.00 (d, J = 8.0 Hz, 1H), 6.92-6.89 (m, 2H), 6.87-6.85 (m, 1H), 6.81-6.77 (m, 2H), 6.69 (s, 1H), 4.09 (s, 2H), 3.24 (s, 2H), 2.14 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, CDCl₃) δ 154.1, 143.8, 142.8, 135.9, 135.2, 134.2, 133.5, 130.5, 130.4, 130.1, 129.3, 127.6, 122.8, 122.4, 120.8, 119.6, 118.8, 116.5, 110.1, 32.0, 20.9, 19.0; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for C₂₂H₂₂N₃ 328.1808, found 328.1810.

2-(2-(3,4-Dimethoxybenzyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1l). 4 h; eluent: EtOAc/PE 40:60; 647 mg, 90% yield; white solid, mp 55-56 °C; ^1H NMR (400 MHz, CDCl₃) δ 7.82 (d, J = 8.0 Hz, 1H), 7.32-7.27 (m, 2H, overlapped with the peak of chloroform), 7.19 (t, J = 7.6 Hz, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.96-6.94 (m, 1H), 6.84-6.81 (m, 2H), 6.66 (d, J = 8.4 Hz, 1H), 6.59 (dd, J = 8.0, 1.6 Hz, 1H), 6.51 (d, J = 1.6 Hz, 1H), 4.12-4.04 (m, 2H), 3.81 (s, 3H), 3.72 (s, 3H), 3.25 (s, 2H); ^{13}C NMR (100 MHz, CDCl₃) δ 154.4, 148.5, 147.6, 143.7, 142.8, 135.7, 130.5, 129.4, 128.6, 122.9, 122.5, 121.0, 120.7, 119.5, 118.7, 116.4, 112.0, 111.0, 110.2, 55.8, 55.7, 34.1; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for C₂₂H₂₂N₃O₂ 360.1707, found 360.1709.

2-(2-(Naphthalen-1-ylmethyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1m). 12 h; eluent: EtOAc/CH₂Cl₂/PE 6:47:47; 671 mg, 96% yield; white solid, mp 199-200 °C; ^1H NMR (400 MHz, DMSO- d_6) δ 8.07 (d, J = 5.6 Hz, 1H), 7.90 (d, J = 5.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 6.4 Hz, 1H), 7.48 (s, 2H), 7.35 (t, J = 7.6 Hz, 1H),

7.24-6.97 (m, 7H), 6.65 (t, J = 6.8 Hz, 1H), 5.09 (s, 2H), 4.56-4.38 (m, 2H); ^{13}C NMR (100 MHz, DMSO-*d*₆) δ 154.1, 145.7, 143.2, 136.3, 133.8, 133.3, 132.1, 130.6, 129.3, 128.8, 127.8, 127.6, 126.5, 126.0, 125.9, 124.7, 122.7, 122.1, 119.6, 119.2, 116.9, 116.7, 110.6, 31.6; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₄H₂₀N₃ 350.1652, found 350.1650.

2-(2-(Thiophen-2-ylmethyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1n). 5 h; eluent: EtOAc/PE 17:83; 446 mg, 73% yield; white solid, mp 134-135 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.83-7.81 (m, 1H), 7.31-7.26 (m, 2H), 7.20 (dt, J = 8.0, 0.8 Hz, 1H), 7.08-6.98 (m, 3H), 6.85-6.79 (m, 3H), 6.64-6.63 (m, 1H), 4.36-4.25 (m, 2H), 3.39 (s, 2H); ^{13}C NMR (100 MHz, CDCl₃) δ 153.2, 143.7, 142.8, 138.2, 135.6, 130.7, 129.2, 126.8, 126.2, 124.7, 123.1, 122.7, 120.4, 119.8, 118.8, 116.5, 110.4, 28.6; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₁₈H₁₆N₃S 306.1059, found 306.1061.

2-(2-Methyl-1*H*-benzo[*d*]imidazol-1-yl)aniline (1o). 5 h; eluent: EtOAc/PE 33:67; 397 mg, 89% yield; yellow oil; ¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, J = 8.0 Hz, 1H), 7.31-7.27 (m, 1H, overlapped with the peak of chloroform), 7.25-7.21 (m, 1H), 7.18-7.14 (m, 1H), 7.07 (dd, J = 7.6, 1.2 Hz, 1H), 7.01 (d, J = 7.6 Hz, 1H), 6.90-6.83 (m, 2H), 3.66 (s, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl₃) δ 152.5, 143.5, 142.8, 135.6, 130.5, 128.9, 122.6, 122.4, 120.7, 119.0, 118.7, 116.5, 110.1, 13.9; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₁₄H₁₄N₃ 224.1182, found 224.1181.

2-(2-Ethyl-1*H*-benzo[*d*]imidazol-1-yl)aniline (1p). 8 h; eluent: EtOAc/PE 25:75; 285 mg, 60% yield; white solid, mp 132-133 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.78 (d, J = 8.0 Hz, 1H), 7.32-7.23 (m, 2H, overlapped with the peak of chloroform), 7.17 (t, J = 8.0 Hz, 1H), 7.09 (dd, J = 7.6, 1.2 Hz, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.89-6.84 (m, 2H), 3.58 (s, 2H), 2.72 (q, J = 7.6 Hz, 2H), 1.33 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CDCl₃) δ 157.0, 143.5, 142.9, 135.5, 130.4, 129.0, 122.6, 122.4, 120.7,

119.2, 118.7, 116.4, 110.0, 21.0, 11.8; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₁₅H₁₆N₃ 238.1339, found 238.1338.

2-(2-(Cyclopropylmethyl)-1*H*-benzo[*d*]imidazol-1-yl)aniline (1q). 10 h; eluent: EtOAc/PE 25:75; 500 mg, 95% yield; white solid, mp 112-114 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.34-7.26 (m, 2H, overlapped with the peak of chloroform), 7.22-7.18 (m, 1H), 7.12 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.05-7.02 (m, 1H), 6.91-6.86 (m, 2H), 3.54 (s, 2H), 2.71-2.61 (m, 2H), 1.18-1.08 (m, 1H), 0.52-0.47 (m, 2H), 0.15-0.11 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 155.7, 143.5, 142.9, 135.6, 130.5, 129.2, 122.7, 122.4, 120.8, 119.4, 118.8, 116.4, 110.1, 32.6, 9.2, 4.9, 4.8; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₁₇H₁₈N₃ 264.1495, found 264.1496.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-6-methylaniline (1r). 12 h; eluent: EtOAc/PE 17:83; 613 mg, 98% yield; white solid, mp 166-167 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.30-7.26 (m, 1H, overlapped with the peak of chloroform), 7.20-7.13 (m, 5H), 7.00-6.99 (m, 3H), 6.84 (d, *J* = 7.6 Hz, 1H), 6.75 (t, *J* = 8.0 Hz, 1H), 4.15-4.06 (m, 2H), 3.04 (s, 2H), 2.16 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.3, 142.9, 142.1, 136.2, 135.8, 131.4, 129.0, 128.3, 126.9, 126.6, 123.9, 122.9, 122.5, 120.4, 119.6, 118.1, 110.3, 34.5, 17.6; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₂₀N₃ 314.1652, found 314.1651.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-5-methylaniline (1s). 3 h; eluent: EtOAc/PE 25:75; 464 mg, 74% yield; white solid, mp 131-132 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.29-7.24 (m, 1H, overlapped with the peak of chloroform), 7.20-7.13 (m, 4H), 7.07-7.05 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.62-6.60 (m, 2H), 4.15-4.06 (m, 2H), 3.17 (s, 2H), 2.35 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.4, 143.3, 142.9, 140.7, 136.4, 135.9, 129.0, 128.9, 128.4, 126.6, 122.8, 122.5, 119.8, 119.5, 118.2, 117.0, 110.3, 34.3, 21.5; HRMS

(ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₂₀N₃ 314.1652, found 314.1653.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-4-methylaniline (1t). 5 h; eluent: EtOAc/PE 25:75; 527 mg, 84% yield; white solid, mp 137-138 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.28-7.24 (m, 1H, overlapped with the peak of chloroform), 7.19-6.99 (m, 8H), 6.71 (d, *J* = 8.4 Hz, 1H), 6.64 (s, 1H), 4.17-4.04 (m, 2H), 3.13 (s, 2H), 2.19 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.2, 142.8, 141.1, 136.4, 135.8, 131.2, 129.6, 129.0, 128.3, 128.2, 126.6, 122.9, 122.5, 120.6, 119.5, 116.6, 110.3, 34.5, 20.2; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₂₀N₃ 314.1652, found 314.1653.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-3-methylaniline (1u). 4.5 h; eluent: EtOAc/PE 25:75; 338 mg, 54% yield; white solid, mp 159-160 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.82 (d, *J* = 8.0 Hz, 1H), 7.30-7.26 (m, 1H, overlapped with the peak of chloroform), 7.20-7.12 (m, 5H), 7.01-6.98 (m, 3H), 6.84 (d, *J* = 7.2 Hz, 1H), 6.75 (t, *J* = 7.6 Hz, 1H), 4.15-4.06 (m, 2H), 3.04 (s, 2H), 2.16 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.3, 142.8, 142.1, 136.2, 135.8, 131.4, 129.0, 128.3, 126.9, 126.6, 123.9, 122.9, 122.5, 120.4, 119.6, 118.1, 110.3, 34.5, 17.6; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₂₀N₃ 314.1652, found 314.1653.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-5-(trifluoromethyl)aniline (1v). 3 h; eluent: EtOAc/PE 25:75; 691 mg, 94% yield; white solid, mp 166-167 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.30 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.23-7.19 (m, 1H), 7.15-7.12 (m, 3H), 7.04-6.97 (m, 6H), 4.14-4.06 (m, 2H), 3.58 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 153.7, 144.1, 142.8, 135.9, 135.3, 132.7 (q, *J*_{C-F} = 32.3 Hz), 130.0, 128.8, 128.5, 126.9, 123.7 (q, *J*_{C-F} = 270.9 Hz), 123.3, 123.2 (q, *J*_{C-F} = 1.3 Hz), 122.9, 119.8, 115.0 (q, *J*_{C-F} = 3.8 Hz), 113.0 (q, *J*_{C-F} = 3.8 Hz), 110.0, 34.5; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₁₇F₃N₃ 368.1369, found 368.1372.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-5-chloroaniline (1w). 4.5 h; eluent: EtOAc/CH₂Cl₂/PE 17:17:66; 514 mg, 77% yield; white solid, mp 171-172 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.30-7.25 (m, 1H, overlapped with the peak of chloroform), 7.21-7.14 (m, 4H), 7.05-6.97 (m, 3H), 6.82-6.73 (m, 3H), 4.13-4.05 (m, 2H), 3.39 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 154.0, 144.7, 142.8, 136.10, 136.09, 135.6, 130.4, 128.8, 128.5, 126.8, 123.1, 122.8, 119.7, 119.0, 118.6, 116.0, 110.1, 34.4; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₇ClN₃ 334.1106, found 334.1109.

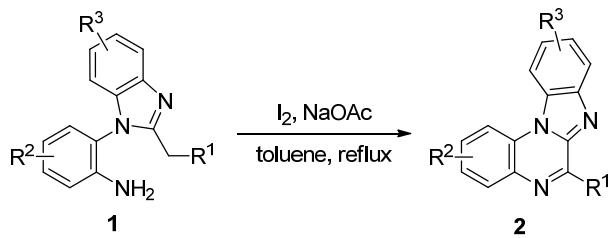
2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-4-chloroaniline (1x). 6.5 h; eluent: EtOAc/PE 25:75; 361 mg, 54% yield; white solid, mp 142-143 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.29-7.14 (m, 6H, overlapped with the peak of chloroform), 7.03-6.97 (m, 3H), 6.84 (d, *J* = 2.4 Hz, 1H), 6.72 (d, *J* = 8.8 Hz, 1H), 4.16-4.05 (m, 2H), 3.32 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 153.9, 142.8, 142.5, 136.0, 135.5, 130.6, 129.2, 128.9, 128.5, 126.8, 123.2, 122.8, 122.6, 121.2, 119.7, 117.3, 110.1, 34.5; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₇ClN₃ 334.1106, found 334.1107.

2-(2-Benzyl-1*H*-benzo[*d*]imidazol-1-yl)-4-chloro-5-methylaniline (1y). 6 h; eluent: EtOAc/PE 17:83; 487 mg, 70% yield; white solid, mp 162-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.31 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.24-7.17 (m, 4H), 7.10-7.07 (m, 2H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.88 (s, 1H), 6.70 (s, 1H), 4.19-4.08 (m, 2H), 3.26 (s, 2H), 2.40 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.1, 142.8, 142.3, 138.6, 136.1, 135.6, 129.3, 128.9, 128.5, 126.8, 123.1, 123.0, 122.7, 119.7, 119.1, 118.2, 110.1, 34.4, 20.1; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₁₉ClN₃ 348.1262, found 348.1264.

2-(2-Benzyl-5,6-dimethyl-1*H*-benzo[*d*]imidazol-1-yl)aniline (1z). 12 h; eluent:

EtOAc/PE 80:20; 622 mg, 95% yield; white solid, mp 152-153 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.58 (s, 1H), 7.29-7.25 (m, 1H, overlapped with the peak of chloroform), 7.15-7.12 (m, 3H), 7.01-7.00 (m, 2H), 6.89 (dd, J = 8.0 Hz, 1.6 Hz, 1H), 6.80-6.77 (m, 3H), 4.13-4.04 (m, 2H), 3.22 (s, 2H), 2.37 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.2, 143.7, 141.3, 136.5, 134.2, 132.0, 131.3, 130.4, 129.3, 128.8, 128.3, 126.5, 120.9, 119.6, 118.6, 116.4, 110.4, 34.3, 20.3, 20.2; HRMS (ESI-TOF) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{22}\text{H}_{22}\text{N}_3$ 328.1808, found 328.1809.

4. General Procedure for the Synthesis of Products 2. A solution of the substrate **1** (0.5 mmol) in toluene (10 mL) was treated sequentially with I₂ (279 mg, 1.1 mmol) and NaOAc (206 mg, 2.5 mmol), and then heated at reflux until TLC indicated the disappearance of the substrate. After cooling to room temperature, the reaction was quenched with sat. Na₂SO₃ (5 mL) followed by the addition of conc. ammonia solution (2 mL), and extracted with CH₂Cl₂ (3 × 20 mL). The combined organic layer was dried over anhydrous Na₂SO₄, concentrated and purified through silica gel chromatography to yield the product **2**.



6-Phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2a).³ eluent: EtOAc/PE 5:95; 145 mg, 98% yield (0.5 mmol, 1.5 h); 1.44 g, 97% (5 mmol, 2 h); yellow solid, mp 202-204 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.73-8.71 (m, 2H), 8.45 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.40-8.37 (m, 1H), 8.20 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.17-8.15 (m, 1H), 7.71-7.67 (m, 1H), 7.64-7.54 (m, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 151.9, 144.2,

140.7, 136.3, 135.6, 131.1, 130.7, 130.2, 130.0, 129.3, 129.1, 128.4, 125.5, 125.3, 124.6, 122.3, 114.4, 114.2; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₀H₁₄N₃ 296.1182, found 296.1180.

6-(*p*-Tolyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2b). 1 h; eluent: EtOAc/PE 5:95; 145 mg, 94% yield; yellow solid, mp 171-173 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.62 (d, J = 8.0 Hz, 2H), 8.40-8.30 (m, 2H), 8.15-8.11 (m, 2H), 7.63-7.59 (m, 1H), 7.56-7.48 (m, 3H), 7.40 (d, J = 8.0 Hz, 2H), 2.47 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 152.0, 144.2, 141.0, 140.8, 135.7, 133.5, 131.0, 130.2, 129.9, 129.3, 129.2, 128.9, 125.5, 125.3, 124.6, 122.3, 114.4, 114.2, 21.7; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₁₆N₃ 310.1339, found 310.1340.

6-(4-Methoxyphenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2c). 1 h; eluent: EtOAc/CH₂Cl₂/PE 5:5:90; 157 mg, 96% yield; yellow solid, mp 201-203 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.33 (d, J = 8.8 Hz, 2H), 8.58-8.56 (m, 2H), 8.33-8.31 (m, 2H), 7.71-7.56 (m, 4H), 7.23 (d, J = 8.8 Hz, 2H), 3.74 (s, 3H); ¹³C NMR (100 MHz, C₅D₅N) δ 162.1, 150.2, 144.3, 140.7, 135.7, 132.4, 130.6, 130.2, 129.2, 129.1, 128.9, 125.6, 125.5, 124.6, 121.9, 115.02, 114.98, 113.8, 55.1; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₁₆N₃O 326.1288, found 326.1291.

6-(4-Fluorophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2d). 1.5 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 146 mg, 93% yield; yellow solid, mp 209-210 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.29-9.24 (m, 2H), 8.58-8.55 (m, 2H), 8.33-8.30 (m, 2H), 7.75-7.60 (m, 4H), 7.44-7.38 (m, 2H); ¹³C NMR (100 MHz, C₅D₅N) δ 164.5 (d, J_{C-F} = 248.6 Hz), 144.2, 140.4, 135.3, 132.93, 132.87, 132.8, 130.8, 130.1, 129.4, 129.2, 125.6 (d, J_{C-F} = 6.7 Hz), 124.8, 121.9, 115.1 (d, J_{C-F} = 29.5 Hz), 115.0; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₀H₁₃FN₃ 314.1088, found 314.1089.

6-(4-Chlorophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2e). 1 h; eluent:

EtOAc/PE 2:98; 157 mg, 95% yield; yellow solid, mp 208-209 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.20 (d, *J* = 8.4 Hz, 2H), 8.60 (d, *J* = 7.6 Hz, 2H), 8.33 (d, *J* = 8.0 Hz, 2H), 7.78-7.60 (m, 6H); ¹³C NMR (100 MHz, C₅D₅N) δ 144.2, 140.4, 136.6, 135.1, 132.1, 130.9, 130.1, 129.7, 129.3, 128.4, 125.7, 125.6, 124.8, 121.9, 115.1, 115.0; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₃ClN₃ 330.0793, found 330.0791.

6-(4-Bromophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2f).⁴ 1 h; eluent: EtOAc/PE 2:98; 178 mg, 95% yield; yellow solid, mp 233-234 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.12 (d, *J* = 8.4 Hz, 2H), 8.60-8.58 (m, 2H), 8.32 (d, *J* = 8.0 Hz, 2H), 7.84 (d, *J* = 8.8 Hz, 2H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.70-7.59 (m, 3H); ¹³C NMR (100 MHz, C₅D₅N) δ 149.4, 144.2, 140.3, 135.5, 132.3, 131.4, 130.9, 130.1, 129.7, 129.3, 125.7, 125.6, 125.4, 124.9, 121.9, 115.1, 115.0; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₃BrN₃ 374.0287, found 374.0289.

6-(4-Iodophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2g). 2 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 202 mg, 96% yield; yellow solid, mp 238-239 °C; ¹H NMR (400 MHz, C₅D₅N) δ 8.95-8.93 (m, 2H), 8.60-8.57 (m, 2H), 8.31-8.29 (m, 2H), 8.06-8.03 (m, 2H), 7.76-7.71 (m, 1H), 7.68-7.57 (m, 3H); ¹³C NMR (100 MHz, C₅D₅N) δ 149.7, 144.2, 140.3, 137.5, 136.0, 135.4, 132.2, 130.9, 130.1, 129.7, 129.3, 125.7, 125.6, 124.8, 121.9, 115.1, 115.0, 98.7; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₀H₁₃IN₃ 422.0149, found 422.0150.

6-(4-(Trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2h). 5 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 171 mg, 94% yield; yellow solid, mp 189-190 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.26 (d, *J* = 8.0 Hz, 2H), 8.58 (d, *J* = 7.6 Hz, 2H), 8.31 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.70-7.64 (m, 2H), 7.63-7.61 (m, 1H, overlapped with the peak of pyridine); ¹³C NMR (100 MHz, C₅D₅N) δ 149.1, 144.2, 140.3, 140.0, 135.2, 131.4 (q, *J*_{C-F} = 31.9 Hz), 131.1, 131.0,

130.1, 130.0, 129.4, 125.7, 125.0 (q, $J_{C-F} = 3.8$ Hz), 124.9, 124.7 (q, $J_{C-F} = 270.7$ Hz), 121.9, 115.1, 115.0; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₁₃F₃N₃ 364.1056, found 364.1053.

6-(3-Bromophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2i). 5 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 176 mg, 94% yield; yellow solid, mp 149-150 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.44 (d, $J = 1.6$ Hz, 1H), 9.22 (dd, $J = 8.0, 0.8$ Hz, 1H), 8.60-8.56 (m, 2H), 8.33-8.28 (m, 2H), 7.79-7.72 (m, 2H), 7.67-7.60 (m, 3H, overlapped with the peak of pyridine), 7.50 (t, $J = 8.0$ Hz, 1H); ¹³C NMR (100 MHz, C₅D₅N) δ 149.2, 144.6, 140.7, 139.0, 135.6, 133.9, 133.4, 131.4, 130.5, 130.2, 129.8, 129.7, 126.13, 126.06, 125.3, 122.8, 122.4, 115.5, 115.4; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₀H₁₃BrN₃ 374.0287, found 374.0284.

6-(2-Bromophenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2j). 1.5 h; eluent: EtOAc/CH₂Cl₂/PE 6:12:82; 178 mg, 95% yield; yellow solid, mp 210-211 °C; ¹H NMR (400 MHz, C₅D₅N) δ 8.60 (t, $J = 7.2$ Hz, 2H), 8.33 (dd, $J = 8.0, 1.2$ Hz, 1H), 8.21-8.19 (m, 1H), 8.08 (dd, $J = 8.0, 1.2$ Hz, 1H), 7.83 (d, $J = 8.0$ Hz, 1H), 7.79-7.75 (m, 1H), 7.65-7.57 (m, 3H), 7.52 (dt, $J = 7.6, 0.8$ Hz, 1H), 7.36 (dt, $J = 8.0, 1.6$ Hz, 1H); ¹³C NMR (100 MHz, C₅D₅N) δ 154.1, 144.7, 140.8, 138.3, 135.5, 133.2, 131.9, 131.1, 131.0, 130.6, 130.1, 129.7, 127.5, 125.7, 125.6, 124.8, 122.9, 122.0, 115.4, 115.1; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₀H₁₃BrN₃ 374.0287, found 374.0289.

6-(2,5-Dimethylphenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2k). 2 h; eluent: EtOAc/CH₂Cl₂/PE 4:4:92; 156 mg, 96% yield; white solid, mp 183-184 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.56 (d, $J = 8.4$ Hz, 1H), 8.47-8.44 (m, 1H), 8.24 (dd, $J = 8.4, 1.6$ Hz, 1H), 8.17-8.14 (m, 1H), 7.79-7.75 (m, 1H), 7.64-7.58 (m, 3H), 7.50 (s, 1H), 7.30-7.24 (m, 2H, overlapped with the peak of chloroform), 2.41 (s, 3H), 2.33 (s, 3H);

¹³C NMR (100 MHz, CDCl₃) δ 155.9, 144.5, 141.1, 135.9, 135.6, 135.4, 133.8, 131.1, 130.9, 130.7, 130.4, 130.0, 129.5, 129.4, 125.7, 125.4, 124.8, 122.6, 114.6, 114.3, 21.1, 19.8; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₂H₁₈N₃ 324.1495, found 324.1496.

6-(3,4-Dimethoxyphenyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2l). 2 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 171 mg, 96% yield; yellow solid, mp 163-164 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.21 (dd, *J* = 8.8, 2.0 Hz, 1H), 8.93 (d, *J* = 1.6 Hz, 1H), 8.61 (d, *J* = 7.6 Hz, 2H), 8.35 (d, *J* = 8.4 Hz, 2H), 7.73-7.63 (m, 3H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.18-7.17 (m, 1H, overlapped with the peak of pyridine), 3.97 (s, 3H), 3.82 (s, 3H); ¹³C NMR (100 MHz, C₅D₅N) δ 152.3, 150.1, 149.3, 144.3, 140.8, 135.6, 130.6, 130.2, 129.4, 129.2, 128.9, 125.6, 125.5, 125.0, 124.7, 122.0, 115.1, 115.0, 113.8, 111.2, 55.8, 55.6; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₂H₁₈N₃O₂ 356.1394, found 356.1395.

6-(Naphthalen-1-yl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2m). 2.5 h; eluent: EtOAc/CH₂Cl₂/PE 8:8:84; 167 mg, 97% yield; yellow solid, mp 210-211 °C; ¹H NMR (400 MHz, C₅D₅N) δ 8.70-8.65 (m, 2H, overlapped with the peak of pyridine), 8.47-8.41 (m, 2H), 8.34 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.01-7.98 (m, 1H), 7.83-7.79 (m, 1H), 7.71-7.58 (m, 4H), 7.52-7.48 (m, 2H); ¹³C NMR (100 MHz, C₅D₅N) δ 154.2, 144.6, 141.8, 135.7, 134.4, 134.2, 132.2, 131.0, 130.7, 130.1, 129.8, 129.6, 129.3, 128.6, 126.7, 126.4, 126.2, 125.7, 125.5, 125.3, 124.8, 122.0, 115.4, 115.1; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₄H₁₆N₃ 346.1339, found 346.1337.

6-(Thiophen-2-yl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2n). 7 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 138 mg, 91% yield; yellow solid, mp 195-196 °C; ¹H NMR (400 MHz, C₅D₅N) δ 9.47 (dd, *J* = 3.6, 0.8 Hz, 1H), 8.53 (t, *J* = 7.6 Hz, 2H),

8.35-8.33 (m, 1H), 8.22 (dd, J = 8.0, 1.2 Hz, 1H), 7.82 (dd, J = 5.2, 0.8 Hz, 1H), 7.67-7.60 (m, 3H), 7.54-7.51 (m, 1H, overlapped with the peak of pyridine), 7.35-7.33 (m, 1H); ^{13}C NMR (100 MHz, $\text{C}_5\text{D}_5\text{N}$) δ 145.9, 144.3, 141.4, 139.3, 135.4, 133.9, 131.5, 130.3, 130.2, 129.00, 128.98, 128.7, 125.7, 125.6, 124.8, 121.9, 115.1, 115.0; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{18}\text{H}_{12}\text{N}_3\text{S}$ 302.0746, found 302.0749.

Benzo[4,5]imidazo[1,2-*a*]quinoxaline (2o).³ 8 h; eluent: EtOAc/PE 17:83; 103 mg, 94% yield; yellow solid, mp 153-154 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.12 (s, 1H), 8.20 (d, J = 8.4 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 7.2 Hz, 1H), 7.62 (t, J = 8.4 Hz, 1H), 7.52-7.45 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 146.1, 144.3, 141.1, 135.6, 131.1, 129.9, 129.8, 129.6, 125.6, 124.8, 122.0, 114.8, 114.2; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{14}\text{H}_{10}\text{N}_3$ 220.0869, found 220.0868.

6-Methylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2p).³ 10 h; eluent: EtOAc/PE 18:82; 52 mg, 44% yield; yellow solid, mp 150-151 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.45 (d, J = 8.0 Hz, 1H), 8.40-8.38 (m, 1H), 8.15-8.13 (m, 1H), 8.10 (dd, J = 8.0, 1.2 Hz, 1H), 7.73-7.69 (m, 1H), 7.64-7.56 (m, 3H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.6, 143.9, 141.4, 135.3, 130.5, 130.2, 129.4, 128.7, 125.6, 125.5, 124.7, 122.0, 114.6, 114.3, 21.8; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{N}_3$ 234.1026, found 234.1022.

6-Cyclopropylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2q). 8 h; eluent: EtOAc/PE 5:95; 31 mg, 24% yield; yellow solid, mp 149-150 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.45-8.39 (m, 2H), 8.17-8.15 (m, 1H), 8.01 (dd, J = 8.0, 1.6 Hz, 1H), 7.67-7.57 (m, 3H), 7.55-7.51 (m, 1H), 3.28-3.22 (m, 1H), 1.52-1.48 (m, 2H), 1.30-1.25 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 158.6, 144.1, 141.7, 135.7, 130.6, 130.0, 128.9, 127.9, 125.4, 125.3, 124.5, 121.9, 114.5, 114.3, 13.5, 11.1; HRMS (ESI-TOF) m/z : [M + H] $^+$

calcd for C₁₇H₁₄N₃ 260.1182, found 260.1184.

4-Methyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2r). 1.5 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 153 mg, 99% yield; yellow solid, mp 170-171 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.84-8.82 (m, 2H), 8.31 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.62-7.46 (m, 6H), 7.34 (d, *J* = 7.2 Hz, 1H), 2.84 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 149.5, 144.2, 140.6, 139.7, 136.7, 133.9, 130.5, 130.2, 130.1, 129.2, 128.6, 128.4, 126.6, 125.2, 124.3, 122.1, 114.4, 112.1, 18.5; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₁₆N₃ 310.1339, found 310.1338.

3-Methyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2s). 2 h; eluent: EtOAc/CH₂Cl₂/PE 5:5:90; 152 mg, 98% yield; yellow solid, mp 195-196 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.71-8.69 (m, 2H), 8.38-8.31 (m, 2H), 8.18-8.13 (m, 1H), 7.99 (d, *J* = 1.2 Hz, 1H), 7.64-7.54 (m, 5H), 7.48 (dd, *J* = 8.4, 1.6 Hz, 1H), 2.53 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 151.9, 144.2, 140.7, 136.4, 135.58, 135.57, 130.9, 130.6, 130.3, 130.1, 129.9, 128.5, 127.1, 125.3, 124.5, 122.2, 114.2, 114.1, 21.1; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₁₆N₃ 310.1339, found 310.1340.

2-Methyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2t). 1.5 h; eluent: EtOAc/PE 17:83; 152 mg, 98% yield; yellow solid, mp 191-192 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70-8.68 (m, 2H), 8.31 (d, *J* = 7.6 Hz, 1H), 8.14-8.10 (m, 2H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.63-7.50 (m, 5H), 7.30 (d, *J* = 8.4 Hz, 1H), 2.57 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 150.7, 144.2, 140.8, 139.9, 136.4, 133.6, 130.6, 130.5, 130.0, 129.9, 129.1, 128.5, 126.8, 125.2, 124.4, 122.1, 114.4, 114.3, 22.3; HRMS (ESI-TOF) *m/z*: [M + H]⁺ calcd for C₂₁H₁₆N₃ 310.1339, found 310.1342.

1-Methyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2u). 1.5 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:94; 152 mg, 98% yield; yellow solid, mp 171-172 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.84 (d, *J* = 6.8 Hz, 2H), 8.36 (d, *J* = 7.6 Hz, 1H), 8.27 (d,

$J = 8.0$ Hz, 1H), 8.16 (d, $J = 7.2$ Hz, 1H), 7.63-7.50 (m, 6H), 7.38 (d, $J = 7.2$ Hz, 1H), 2.86 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 149.5, 144.3, 140.6, 139.7, 136.7, 133.9, 130.5, 130.3, 130.1, 129.3, 128.6, 128.4, 126.6, 125.3, 124.4, 122.1, 114.4, 112.2, 18.5; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{N}_3$ 310.1339, found 310.1338.

6-Phenyl-3-(trifluoromethyl)benzo[4,5]imidazo[1,2-*a*]quinoxaline (2v). 1.5 h; eluent: EtOAc/PE 3:97; 173 mg, 95% yield; yellow solid, mp 162-163 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.65-8.63 (m, 2H), 8.27 (d, $J = 1.2$ Hz, 1H), 8.15 (d, $J = 8.8$ Hz, 1H), 7.98 (d, $J = 8.0$ Hz, 1H), 7.90-7.88 (m, 1H), 7.70 (dd, $J = 8.8, 2.0$ Hz, 1H), 7.53-7.47 (m, 3H), 7.40-7.33 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.4, 143.9, 140.0, 135.4, 134.8, 131.1, 130.9 (q, $J_{\text{C}-\text{F}} = 0.9$ Hz), 130.0, 129.5, 128.4, 128.2 (q, $J_{\text{C}-\text{F}} = 3.9$ Hz), 127.3 (q, $J_{\text{C}-\text{F}} = 33.3$ Hz), 125.6, 125.1, 125.0 (q, $J_{\text{C}-\text{F}} = 3.5$ Hz), 123.7, (q, $J_{\text{C}-\text{F}} = 270.5$ Hz), 122.3, 114.7, 113.6; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{21}\text{H}_{13}\text{F}_3\text{N}_3$ 364.1056, found 364.1054.

3-Chloro-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2w). 2 h; eluent: EtOAc/ CH_2Cl_2 /PE 4:8:88; 162 mg, 98% yield; yellow solid, mp 200-201 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.68-8.66 (m, 2H), 8.13-8.01 (m, 4H), 7.57-7.55 (m, 3H), 7.48-7.41 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.4, 143.9, 140.1, 136.1, 135.7, 131.0, 130.6, 130.11, 130.06, 129.6, 128.8, 128.4, 127.5, 125.5, 124.9, 122.3, 115.1, 113.7; HRMS (ESI-TOF) m/z : [M + H] $^+$ calcd for $\text{C}_{20}\text{H}_{13}\text{ClN}_3$ 330.0793, found 330.0795.

2-Chloro-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2x). 1 h; eluent: EtOAc/ CH_2Cl_2 /PE 5:5:90; 161 mg, 98% yield; yellow solid, mp 214-215 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.75-8.73 (m, 2H), 8.48 (d, $J = 2.0$ Hz, 1H), 8.39-8.36 (m, 1H), 8.20-8.15 (m, 2H), 7.66-7.56 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 152.0, 144.3, 140.4, 135.9, 134.8, 134.1, 132.0, 130.9, 130.0, 129.9, 129.7, 128.5, 126.0,

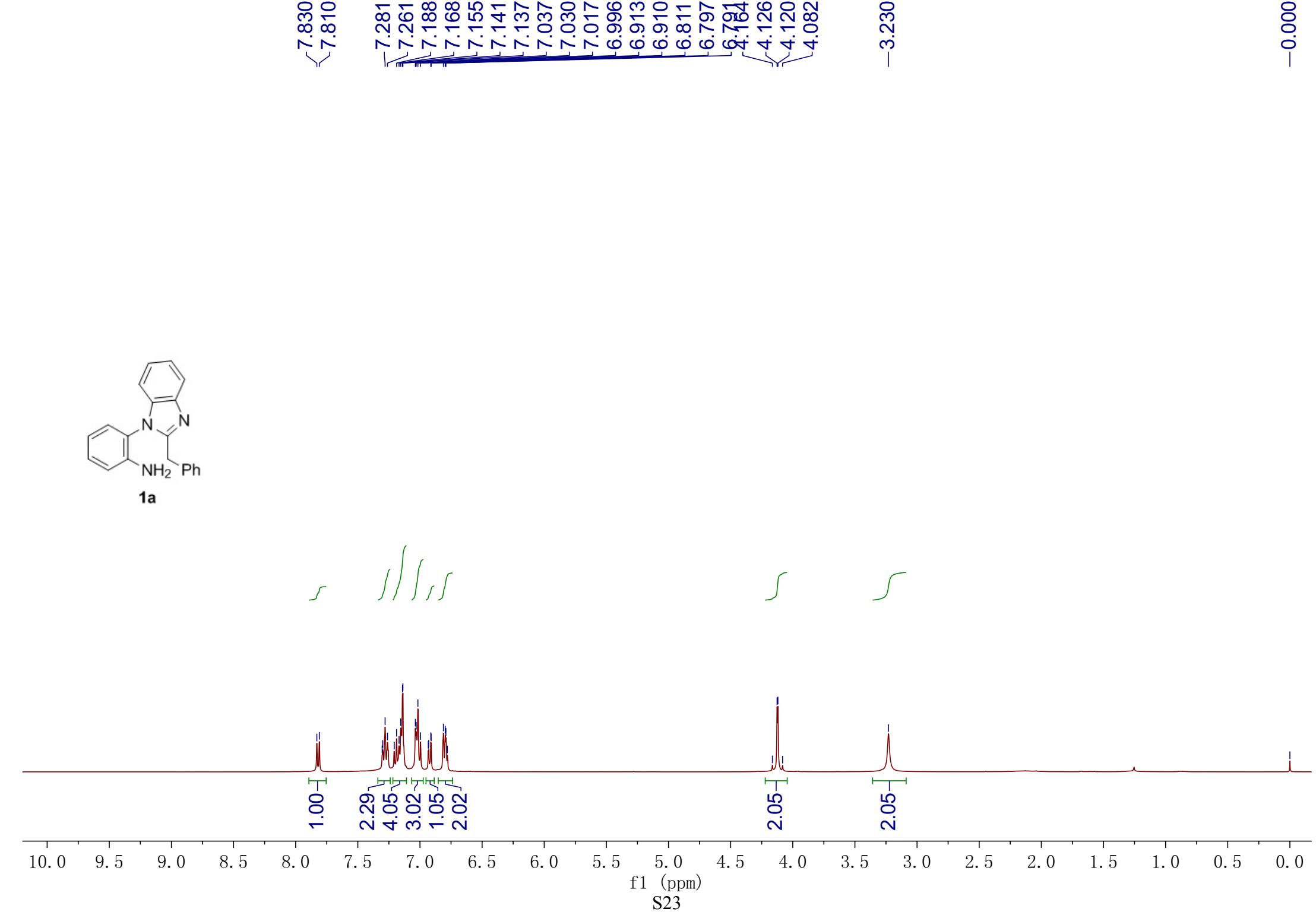
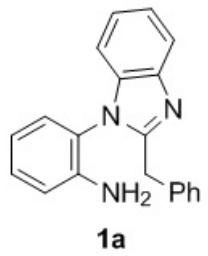
125.7, 125.1, 122.5, 114.5, 114.0; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₀H₁₃ClN₃ 330.0793, found 330.0794.

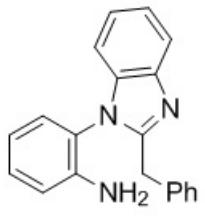
2-Chloro-3-methyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2y). 3.5 h; eluent: CH₂Cl₂/PE 20:80; 169 mg, 98% yield; yellow solid, mp 201-202 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.69-8.66 (m, 2H), 8.25 (s, 1H), 8.19-8.15 (m, 1H), 8.10-8.06 (m, 1H), 7.91 (s, 1H), 7.61-7.49 (m, 5H), 2.43 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 151.6, 144.1, 140.2, 136.0, 135.1, 134.1, 133.6, 132.1, 130.8, 129.9, 129.7, 128.4, 127.6, 125.4, 124.8, 122.2, 114.5, 113.8, 19.8; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₁H₁₅ClN₃ 344.0949, found 344.0948.

9,10-Dimethyl-6-phenylbenzo[4,5]imidazo[1,2-*a*]quinoxaline (2z). 2 h; eluent: EtOAc/CH₂Cl₂/PE 3:3:92; 153 mg, 95% yield; yellow solid, mp 190-191 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (d, J = 7.2 Hz, 2H), 8.23 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.0 Hz, 1H), 7.90 (s, 1H), 7.75 (s, 1H), 7.62-7.56 (m, 4H), 7.46 (t, J = 7.6 Hz, 1H), 2.40 (s, 3H), 2.34 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 151.5, 142.9, 140.0, 136.4, 135.4, 134.8, 134.3, 130.7, 130.5, 130.0, 129.2, 128.7, 128.5, 128.4, 125.1, 121.6, 114.3, 113.8, 21.1, 20.5; HRMS (ESI-TOF) m/z : [M + H]⁺ calcd for C₂₂H₁₈N₃ 324.1495, found 324.1497.

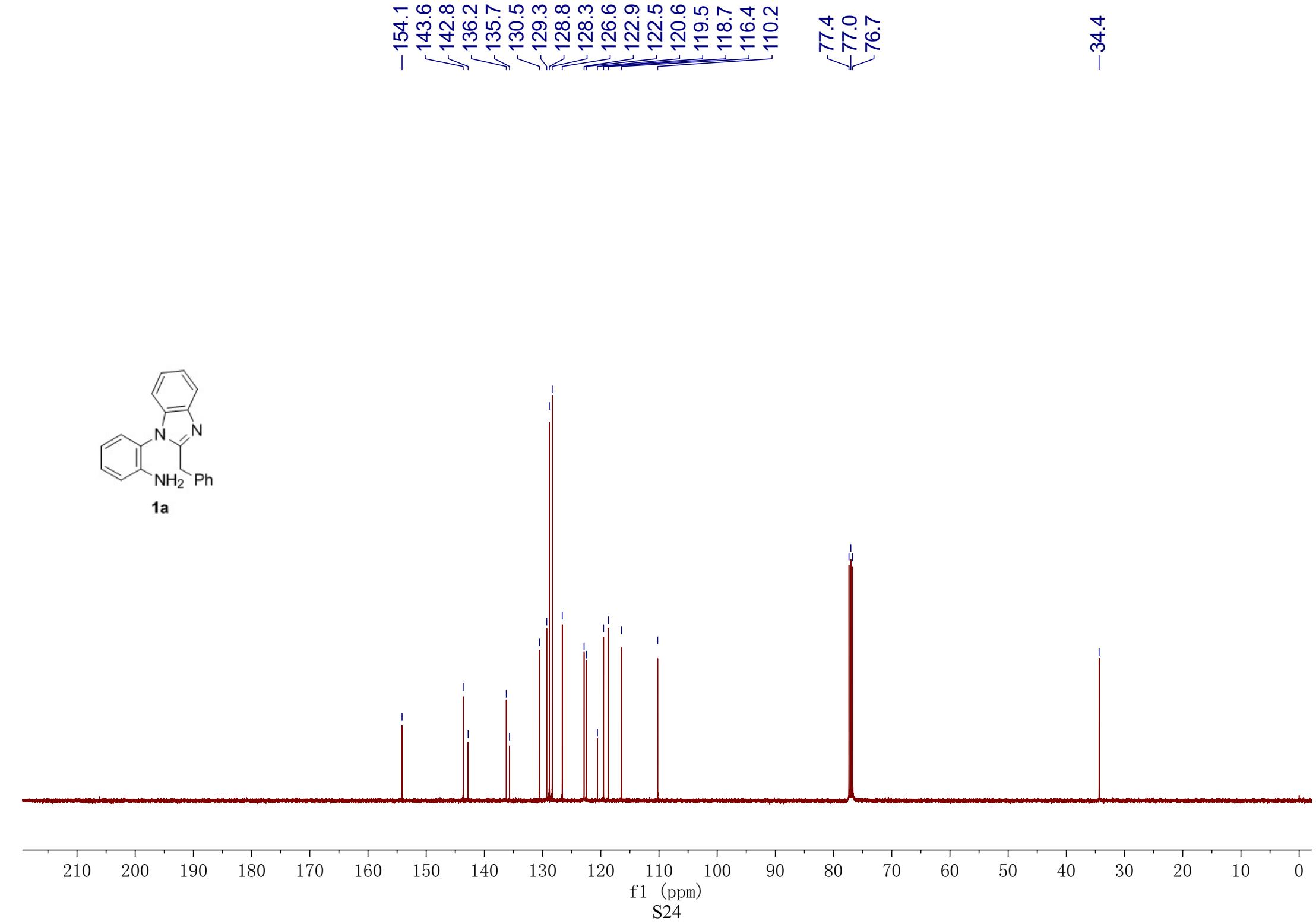
5. References

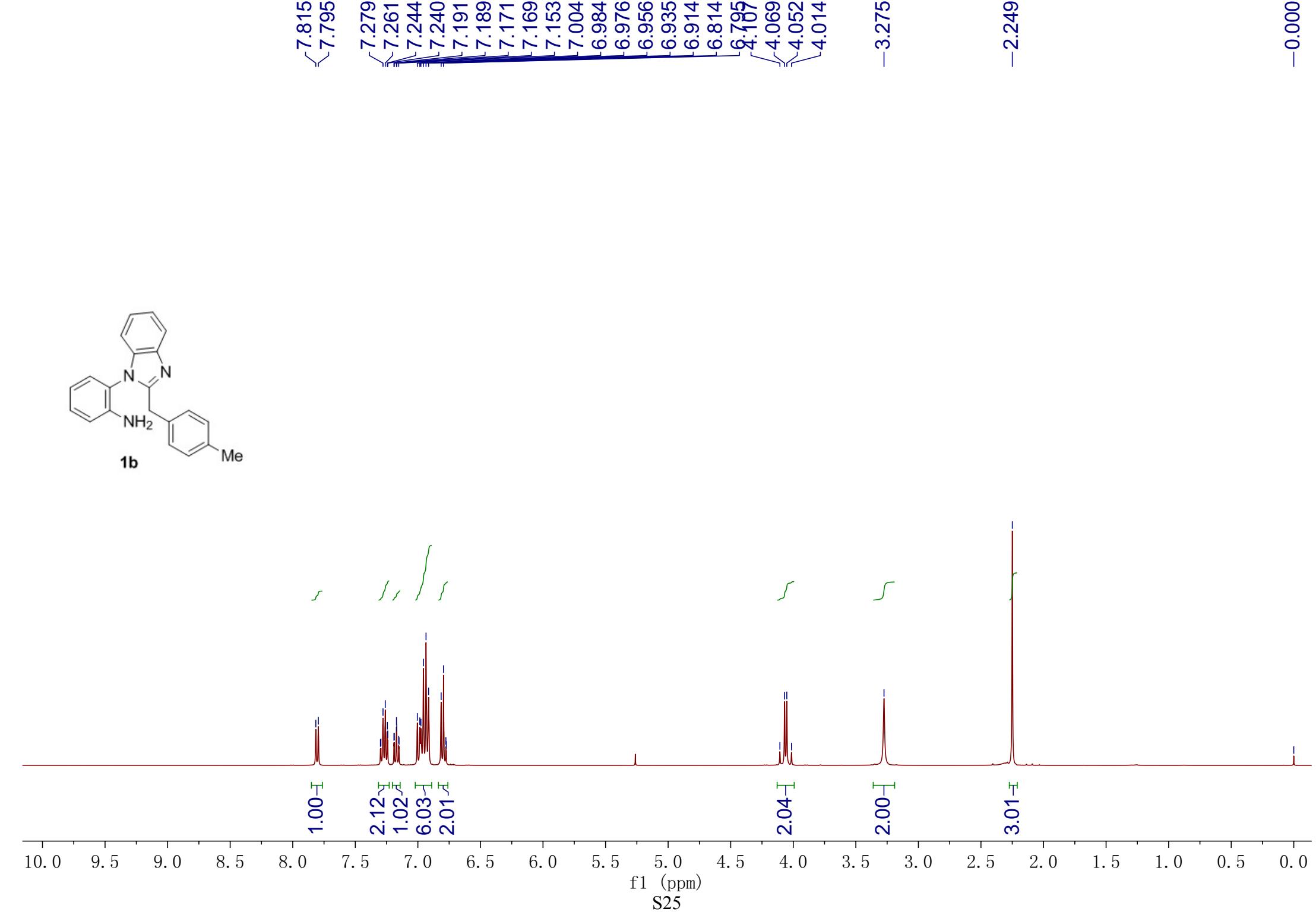
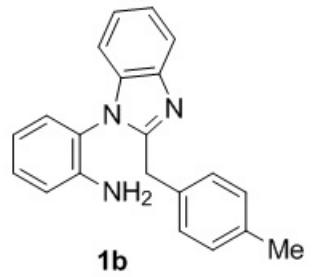
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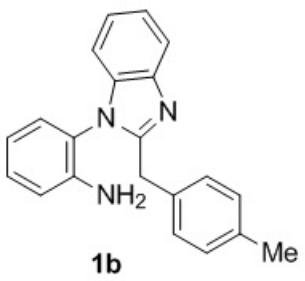




1a





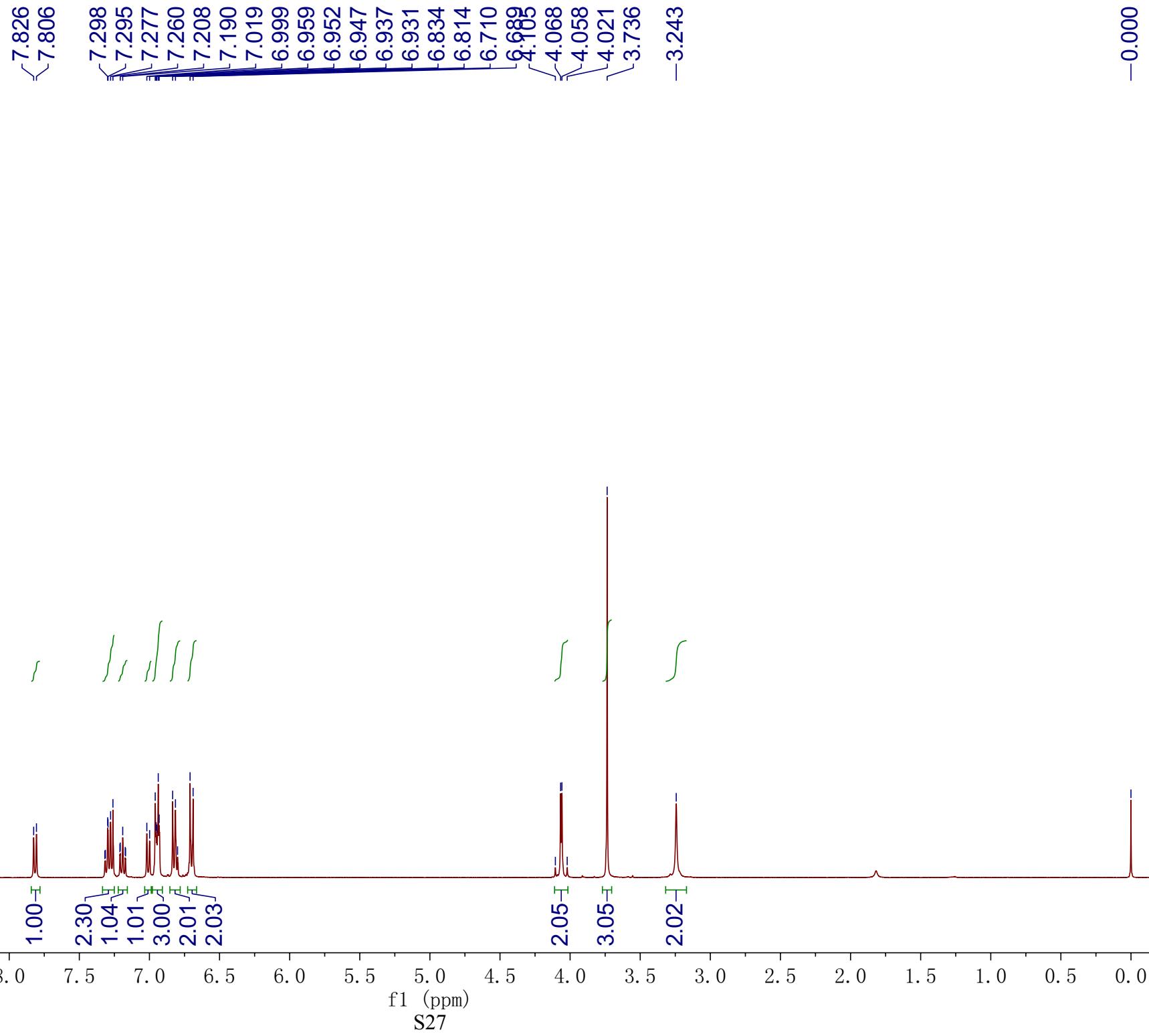
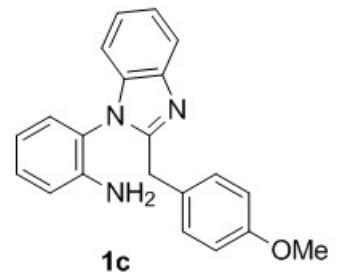


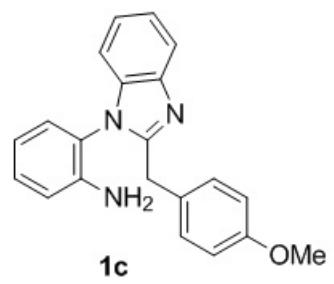
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S26

-33.9

-21.1





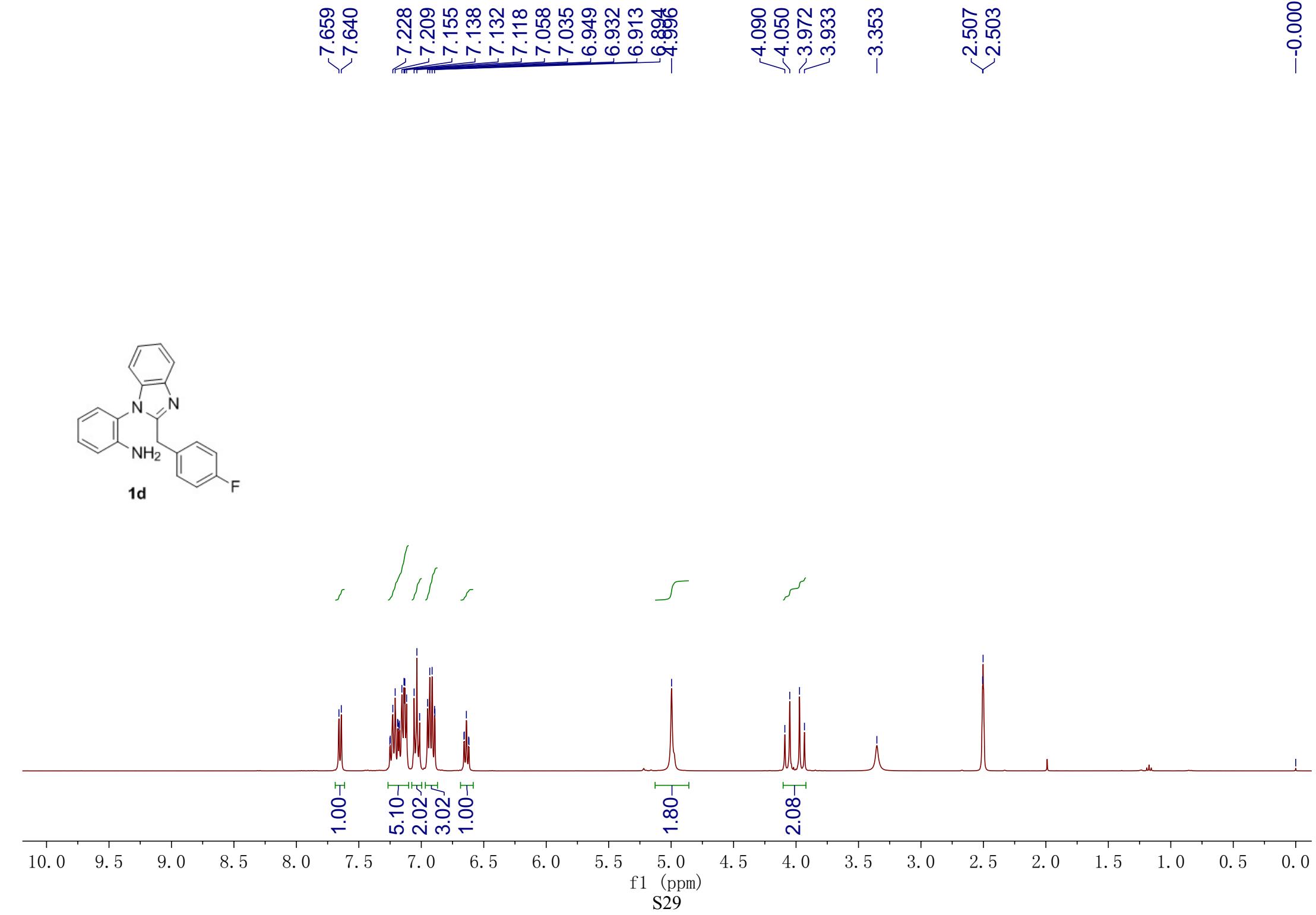
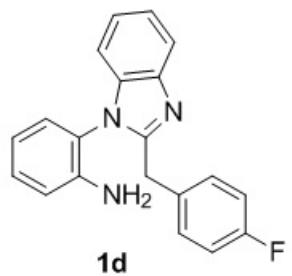
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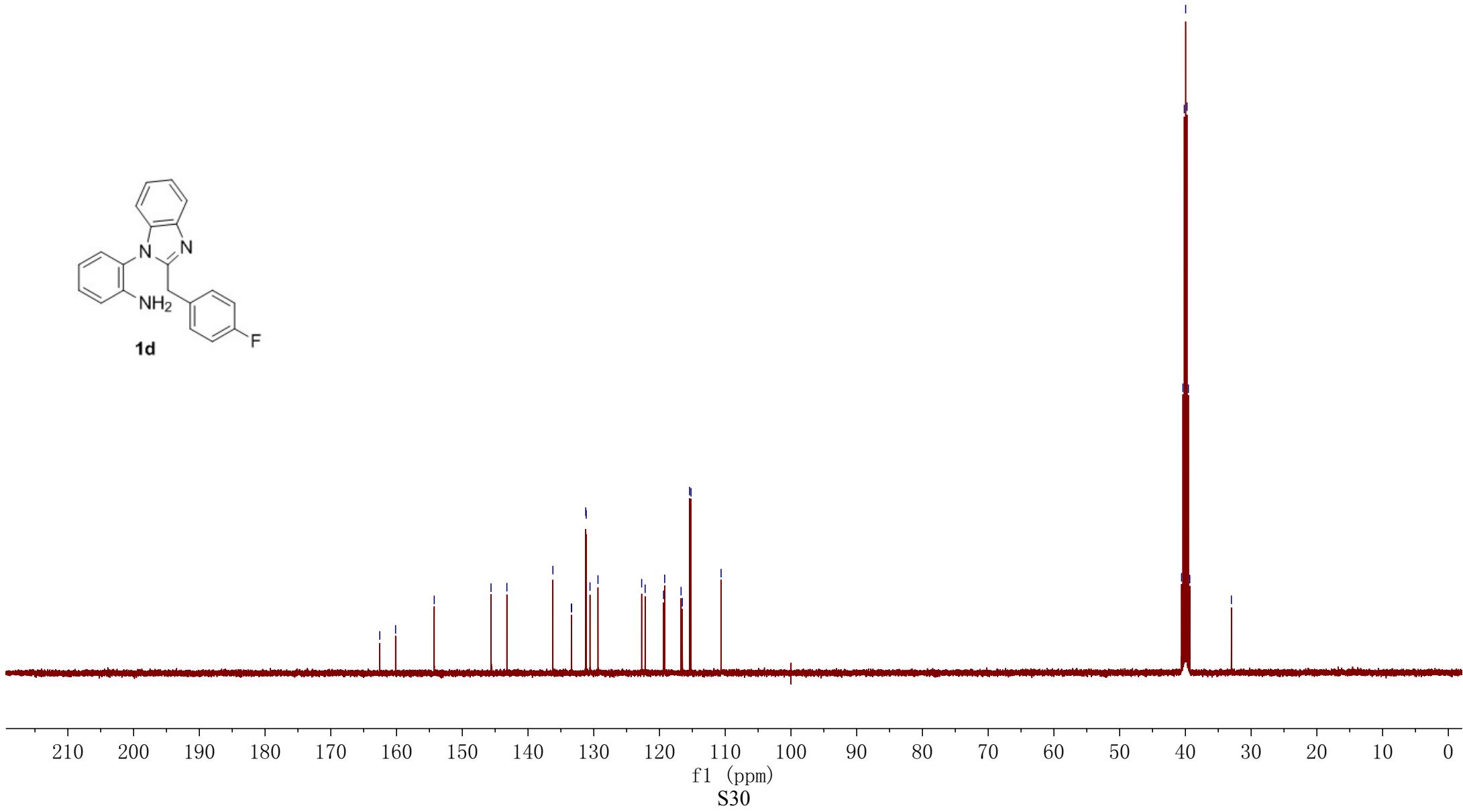
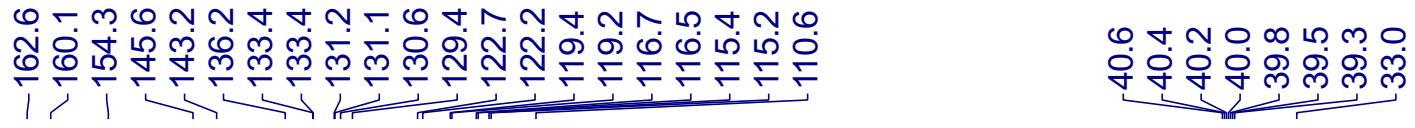
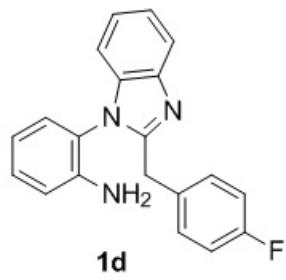
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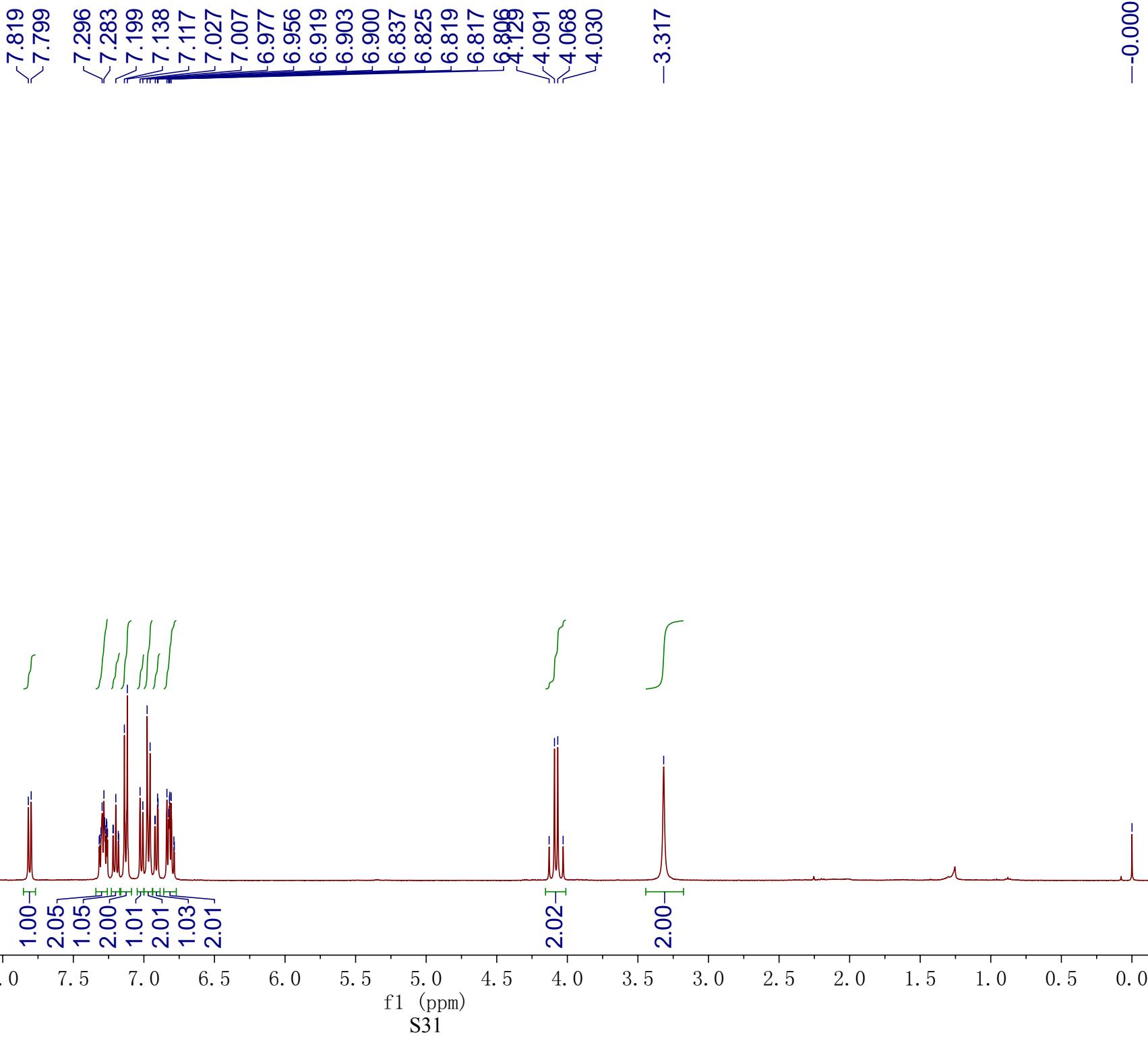
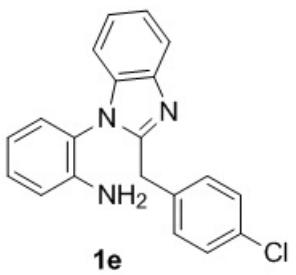
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77.1
76.7

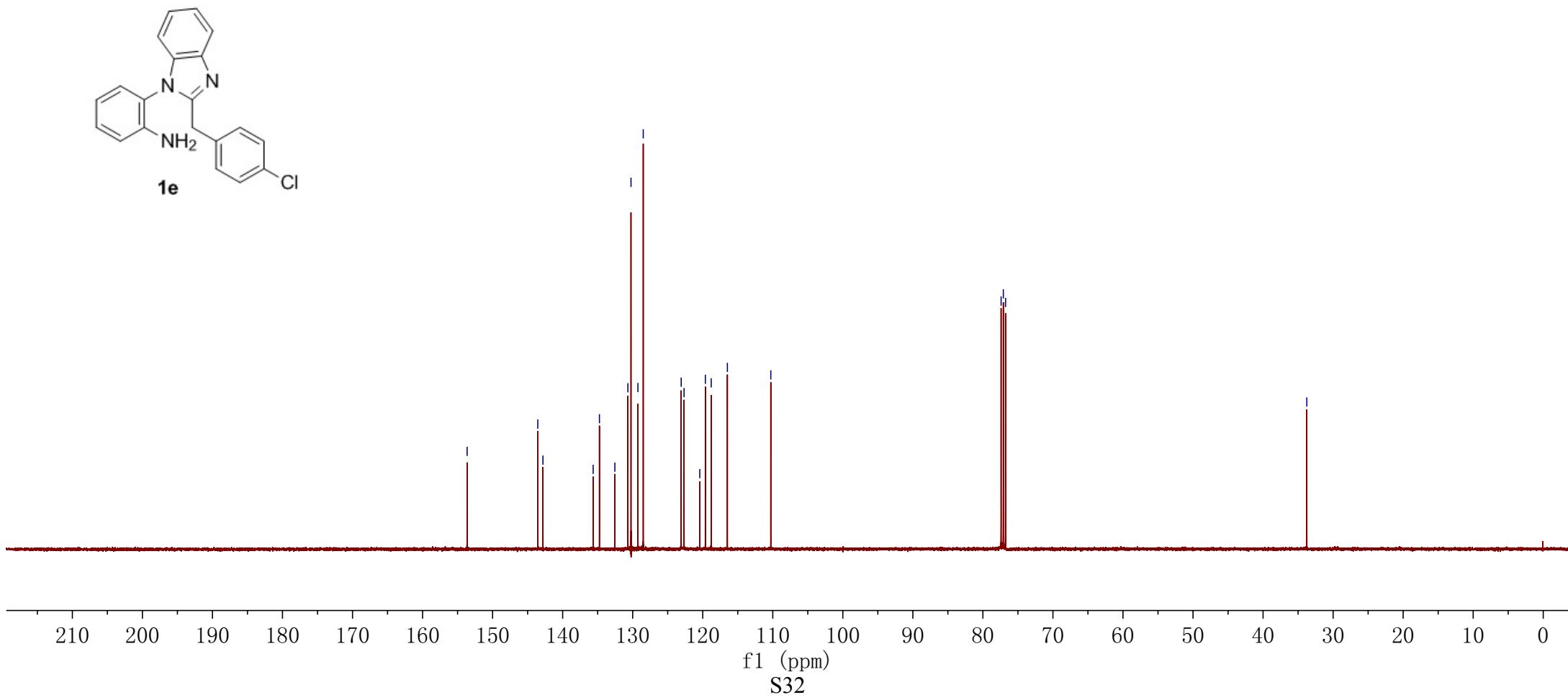
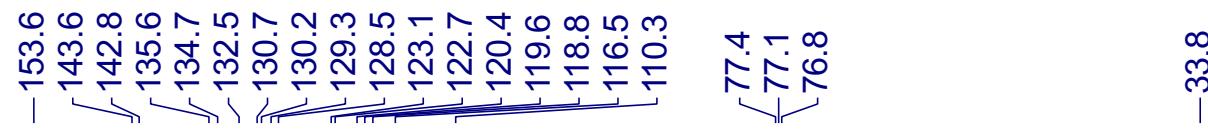
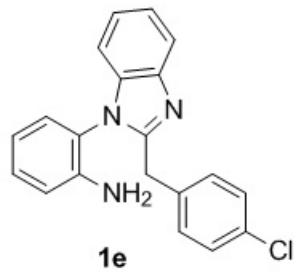
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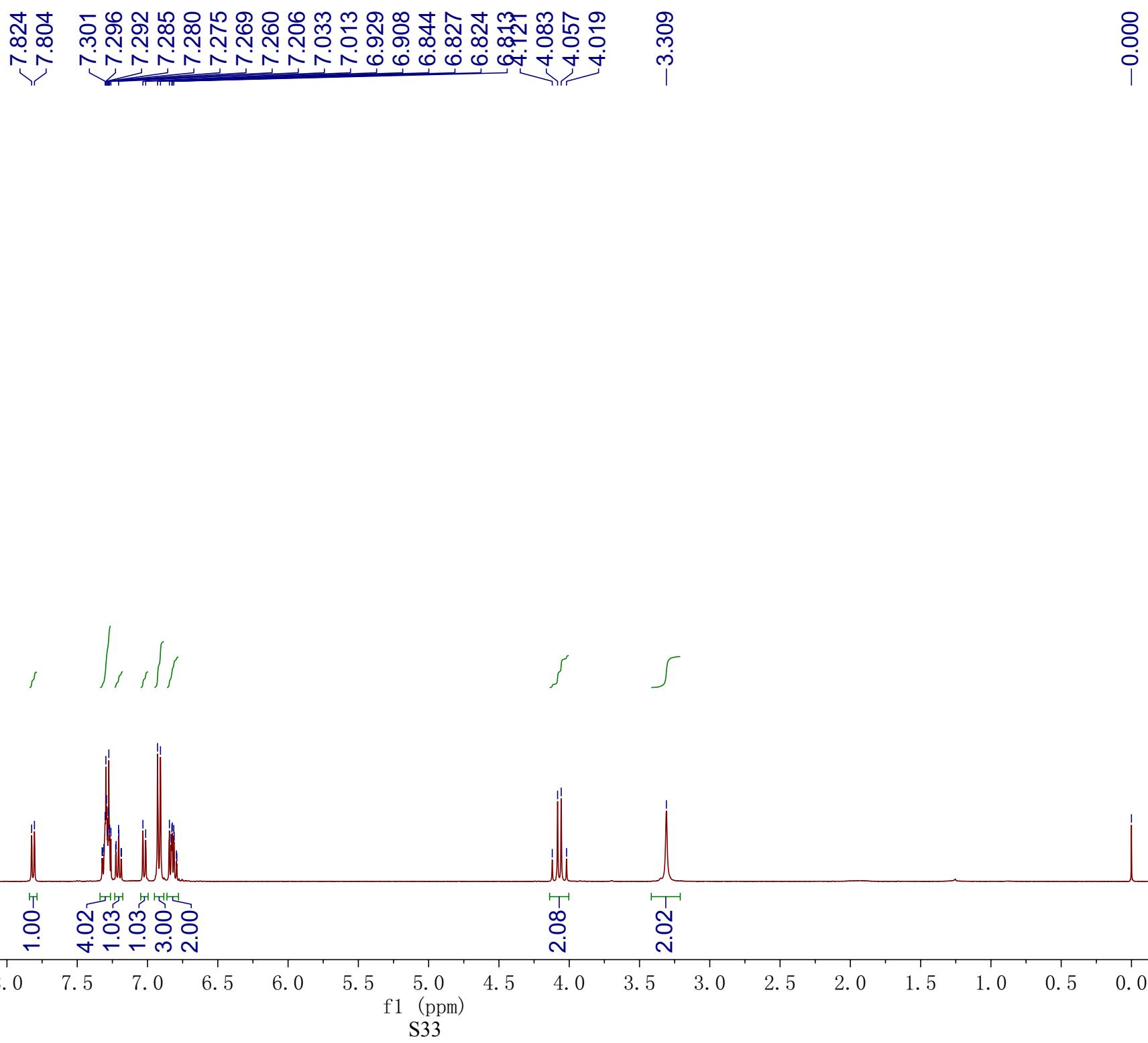
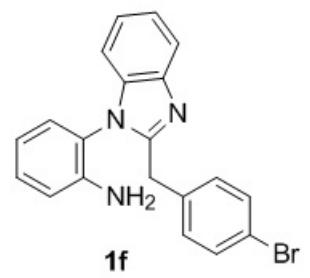
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S28

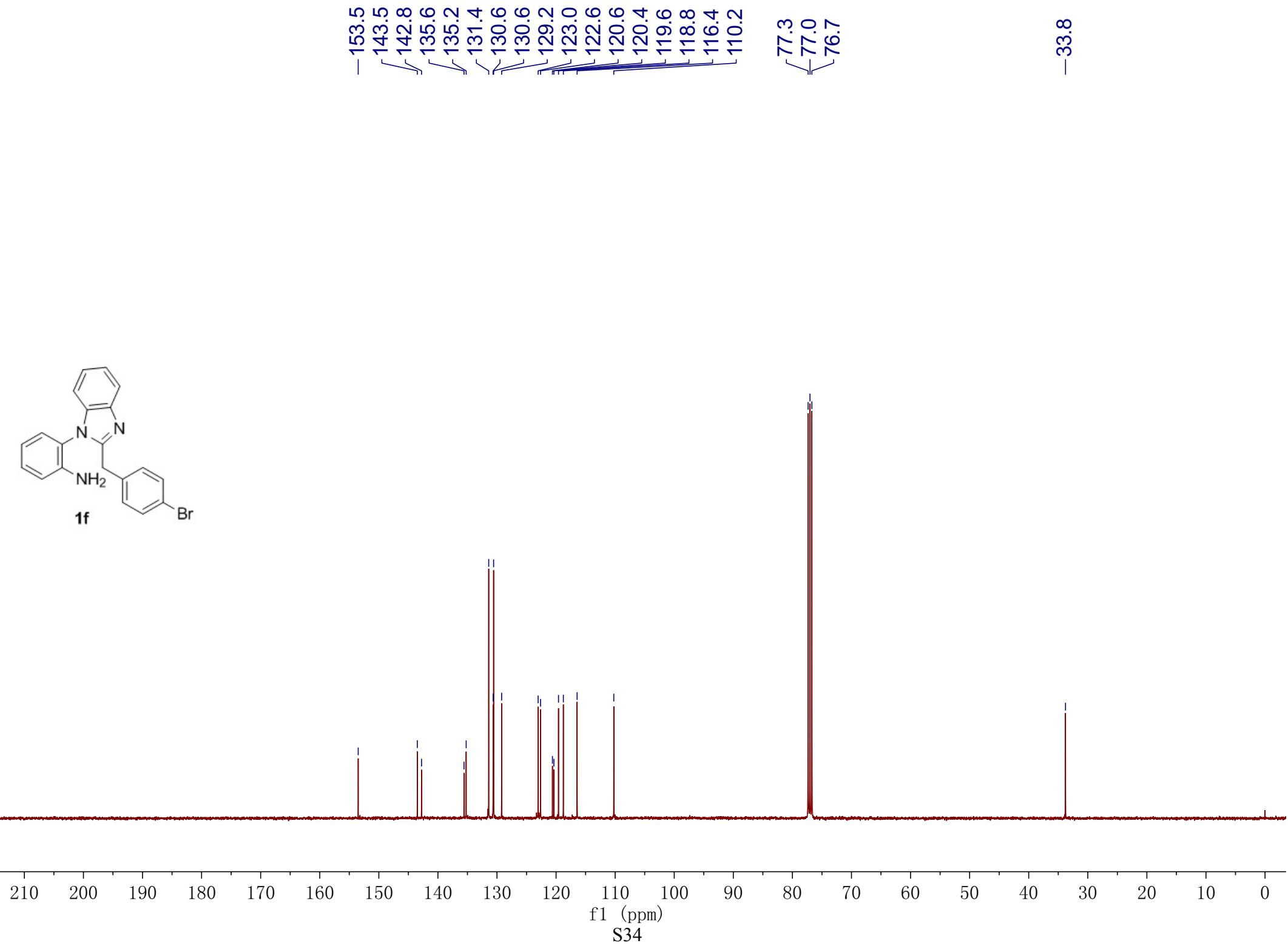
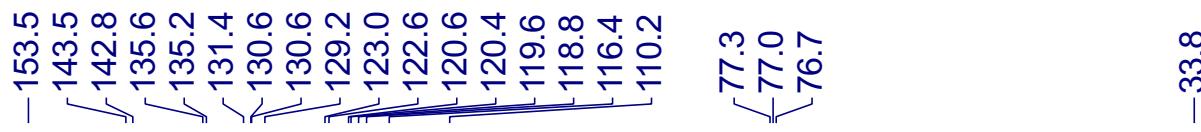
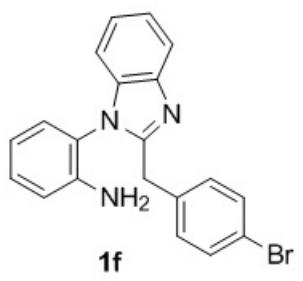


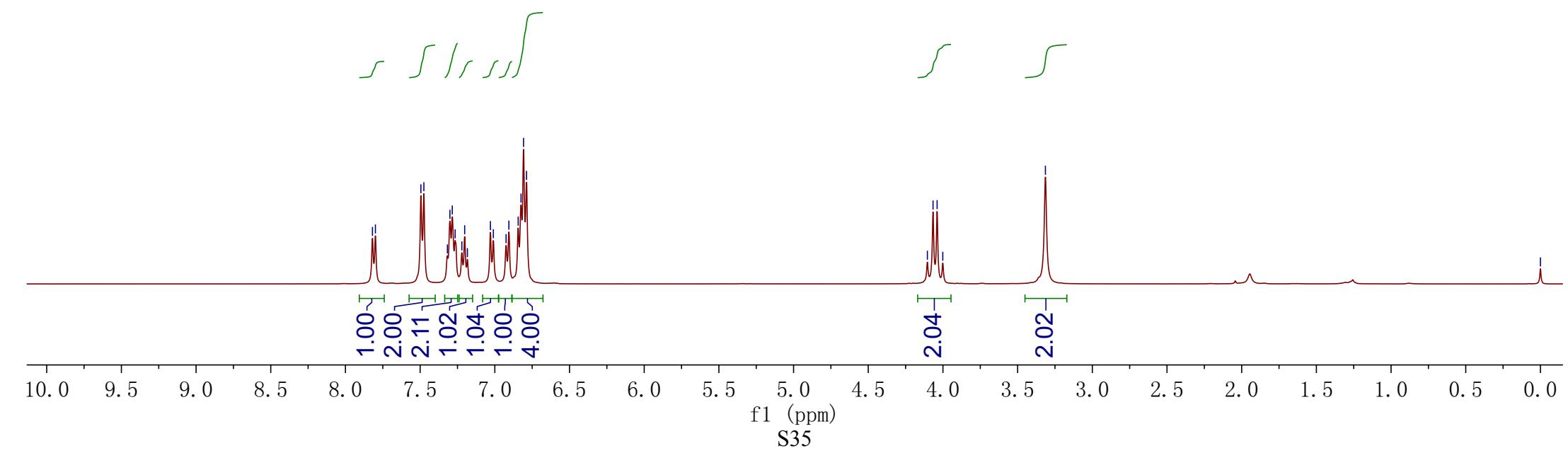
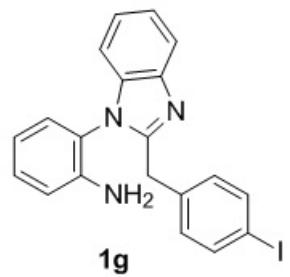
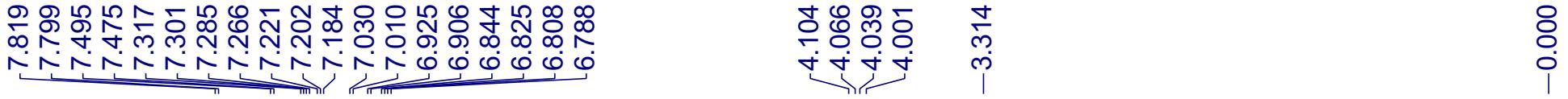


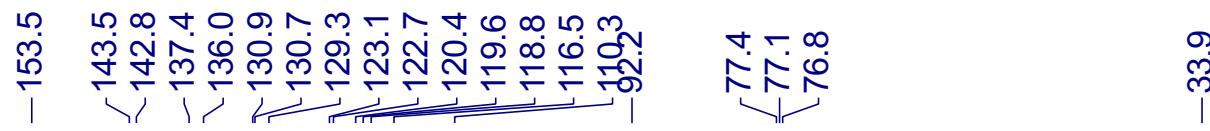
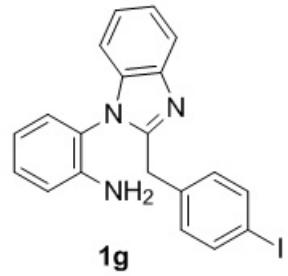




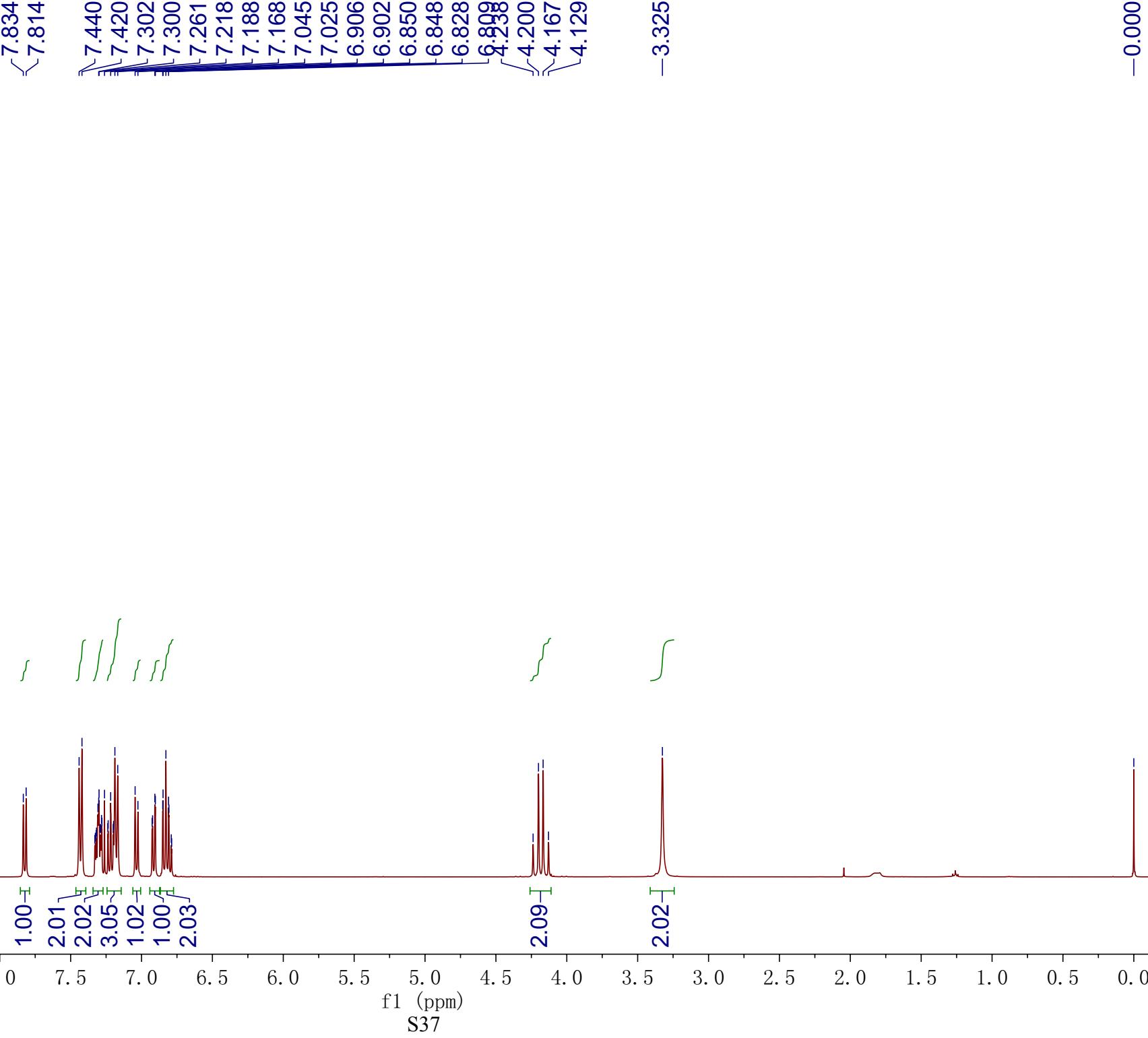
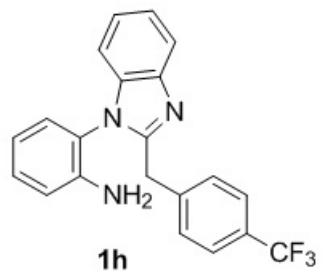


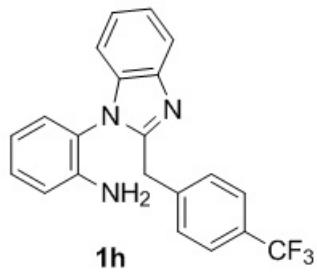






210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



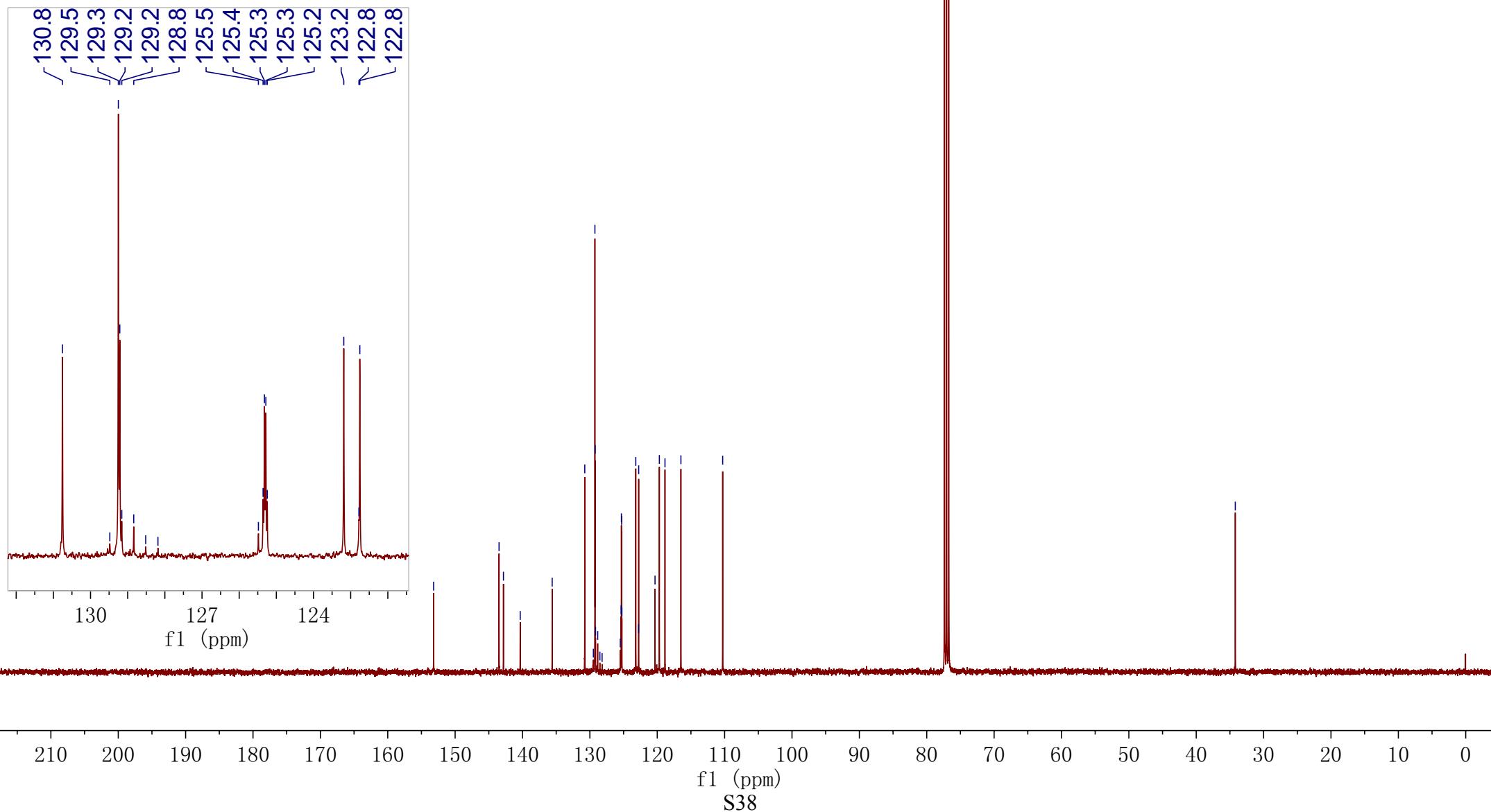


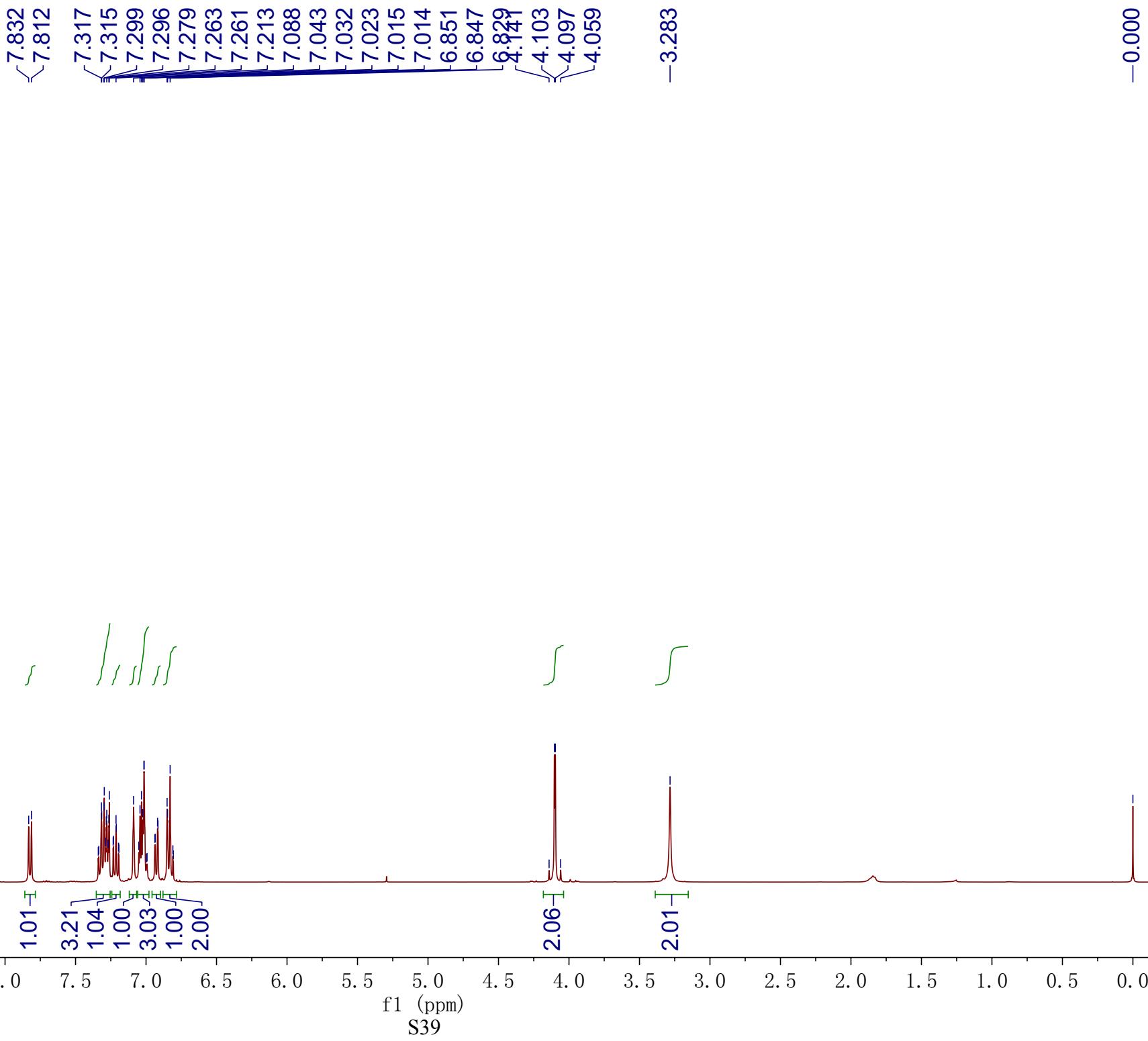
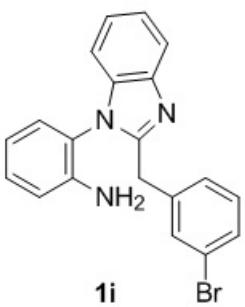
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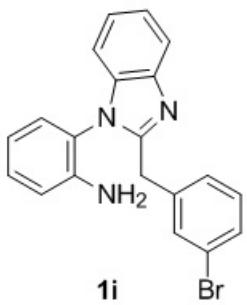
143.5
142.8
135.6
130.8
129.3
129.2
128.8
125.5
125.4
125.3
125.3
125.2
123.2
122.8
122.8

-34.2

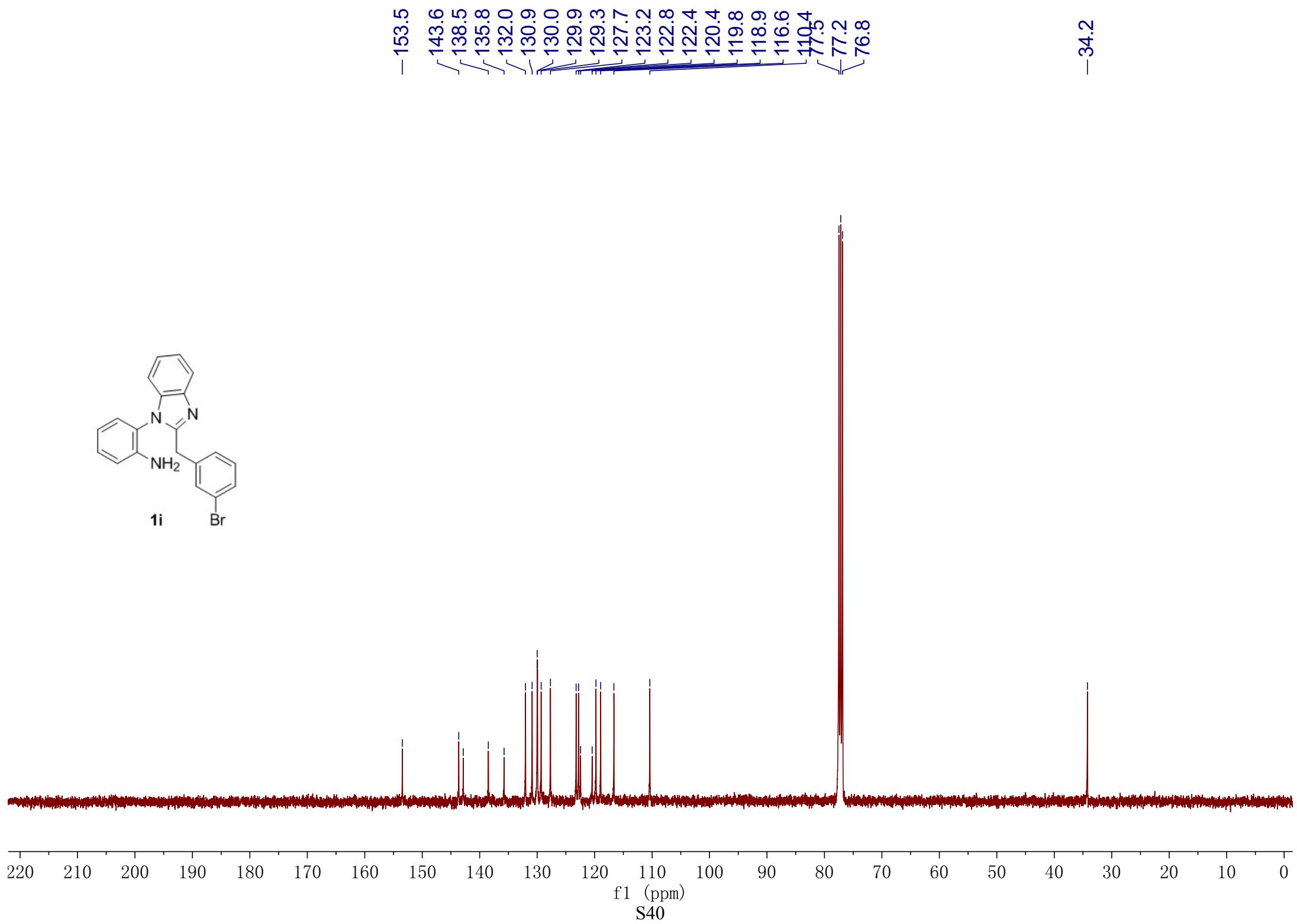
77.1
76.7





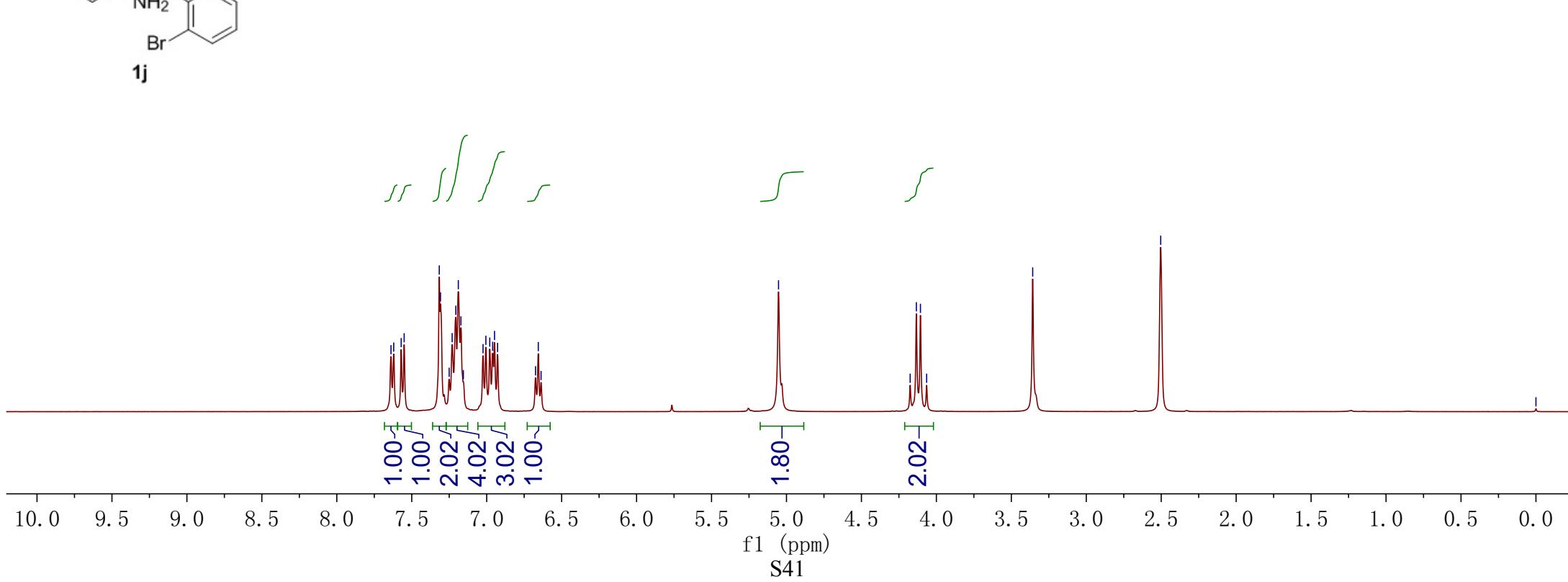


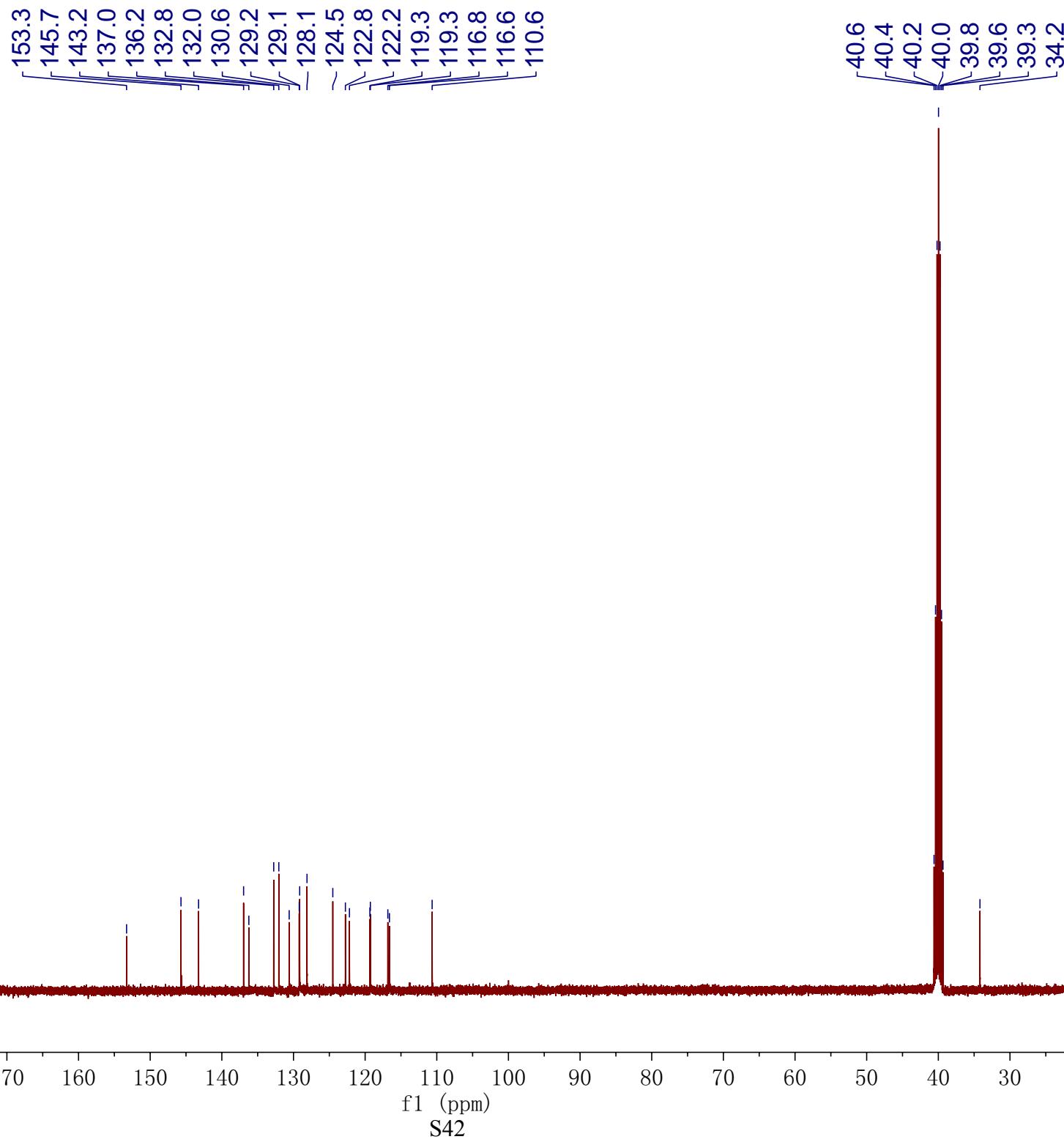
1i

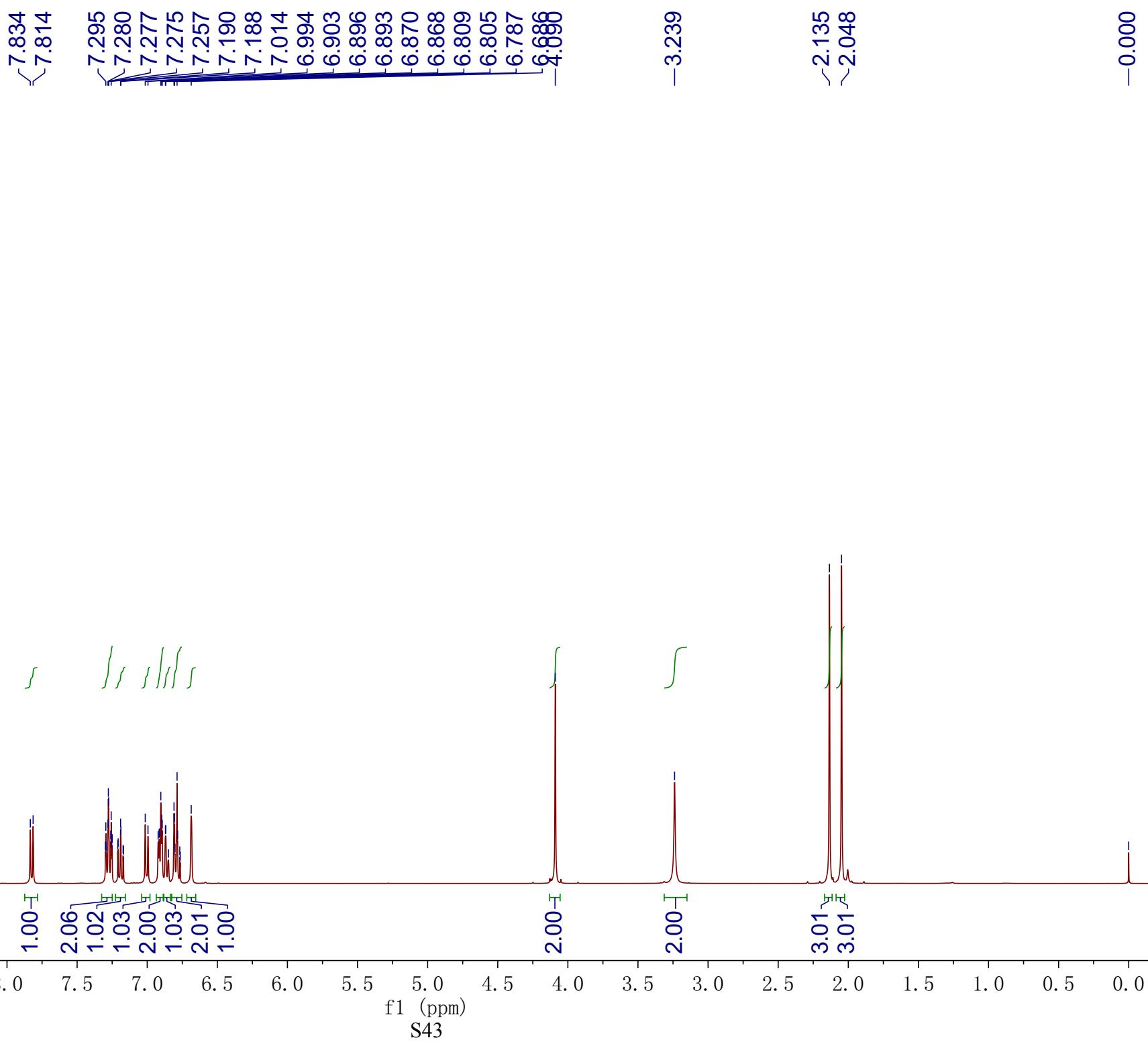
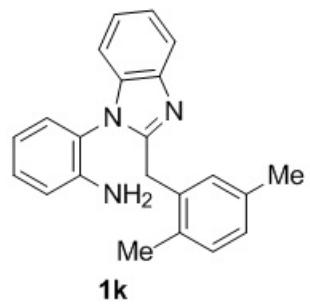


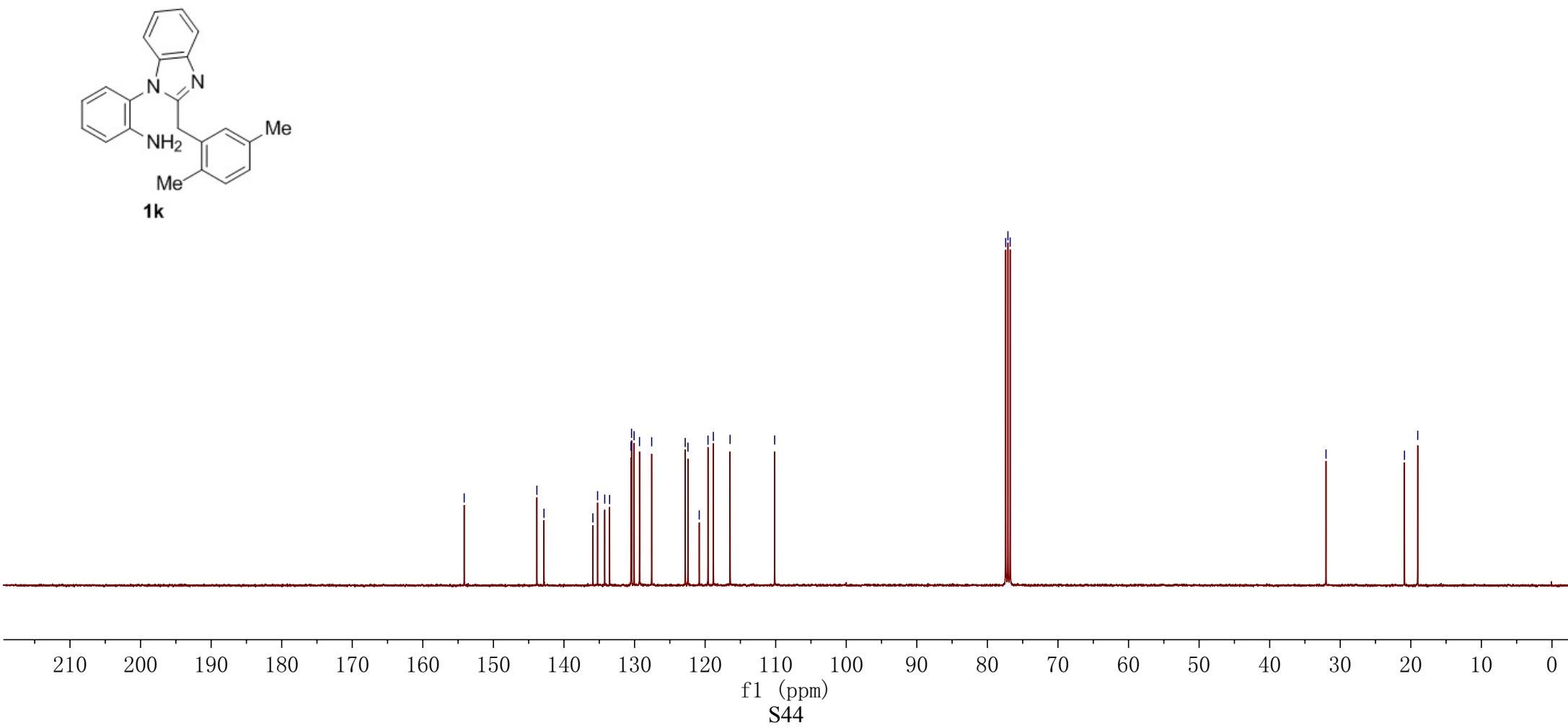
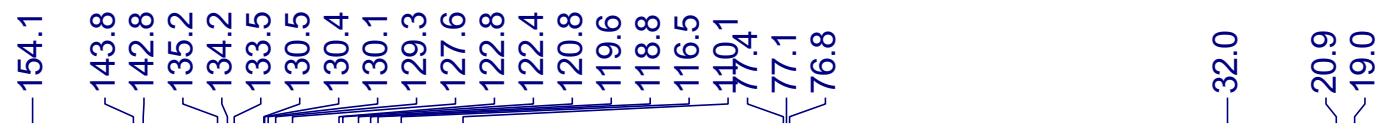
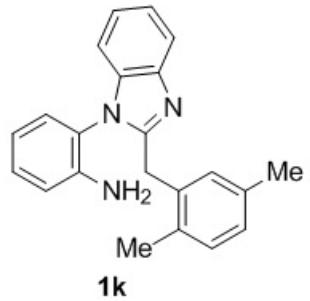
-34.2

-153.5





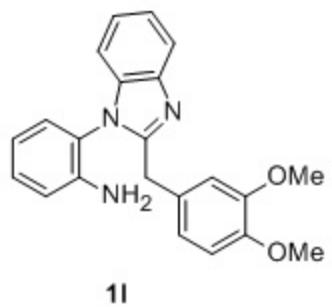




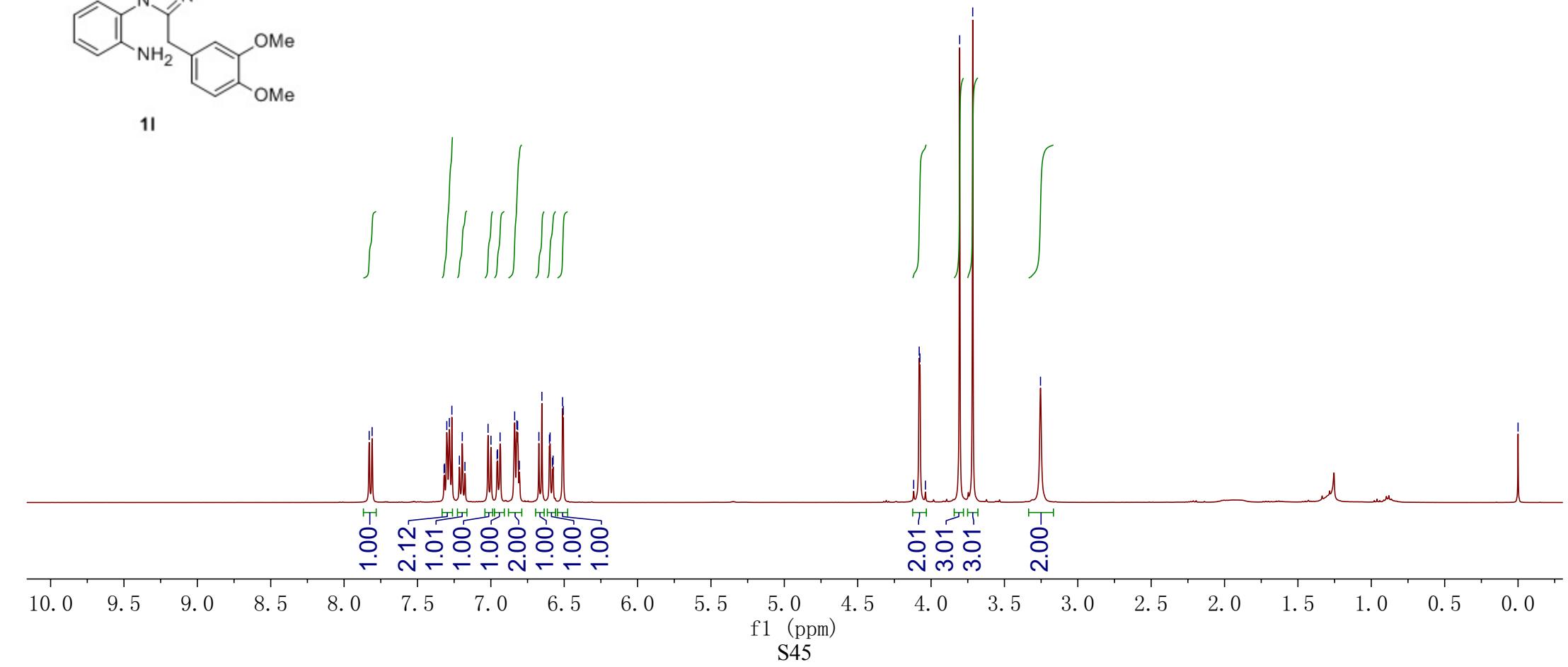
-0.000

7.829
7.809

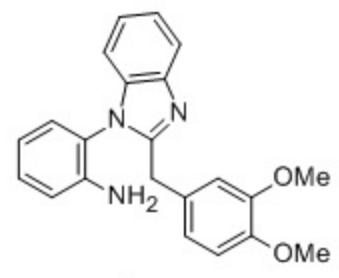
7.300
7.283
7.265
7.195
7.019
6.999
6.937
6.838
6.823
6.817
6.673
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6.600
6.596
6.511
6.507
4.081
4.076
4.038
3.805
3.716
3.254



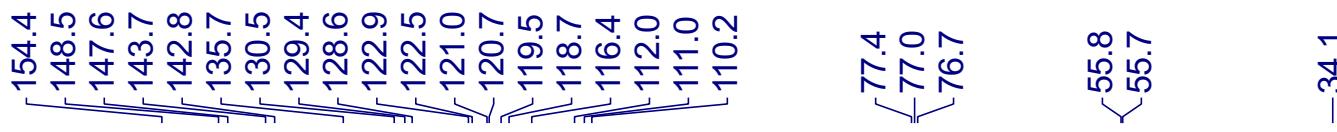
11



f1 (ppm)
S45

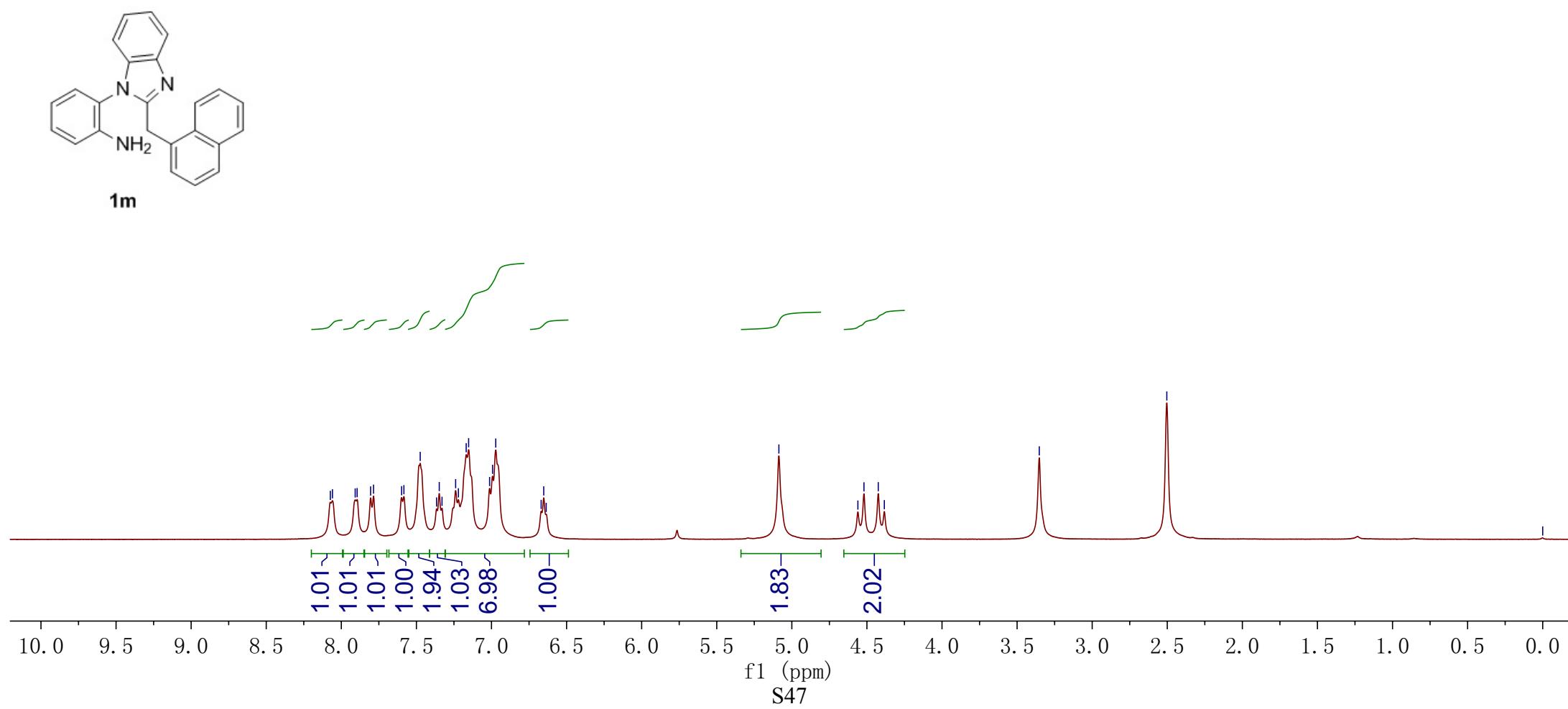
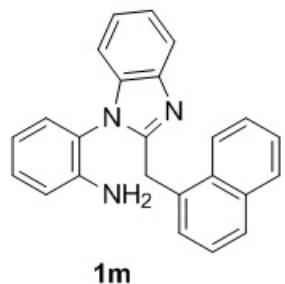


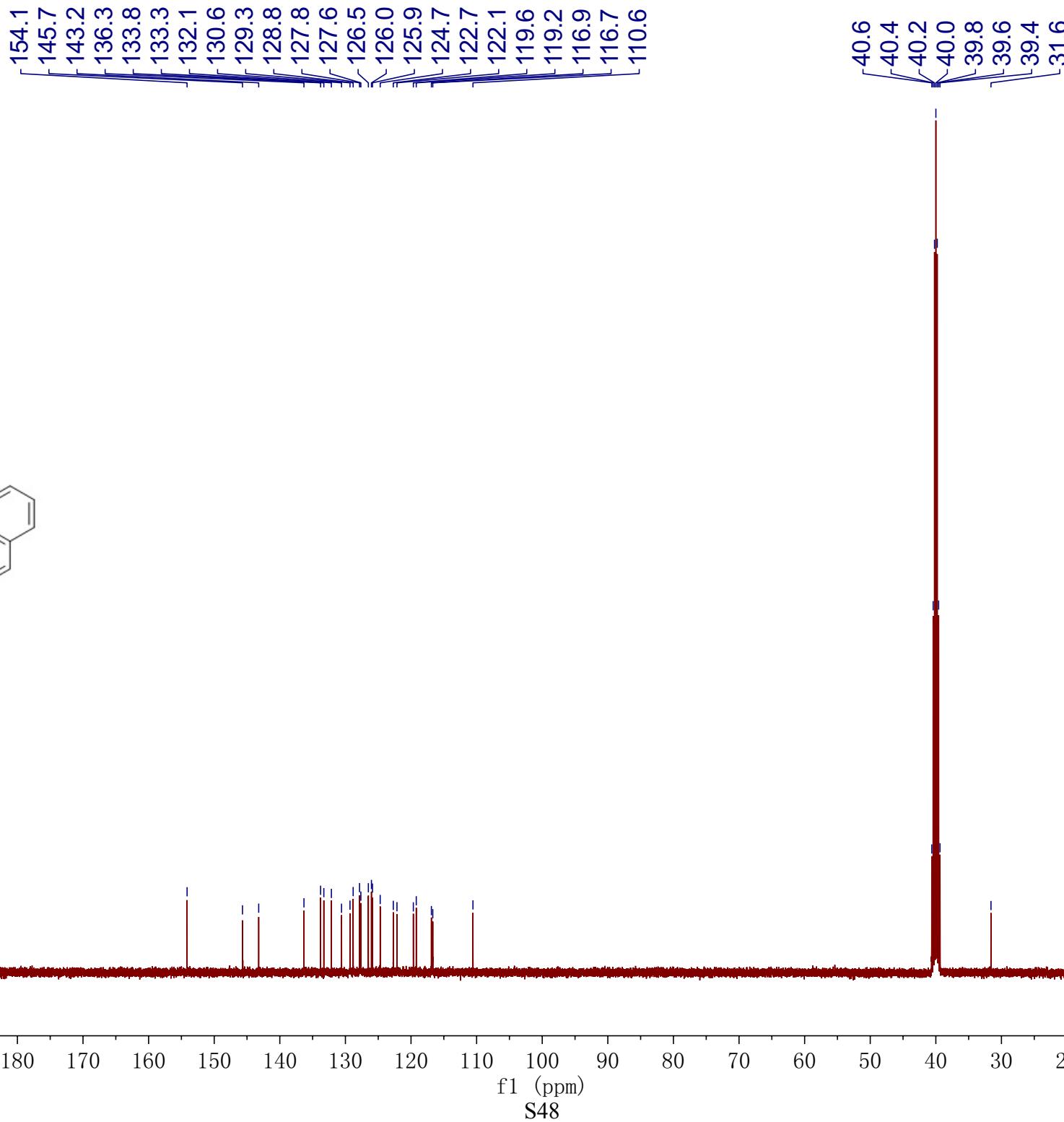
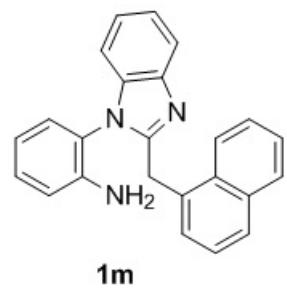
11



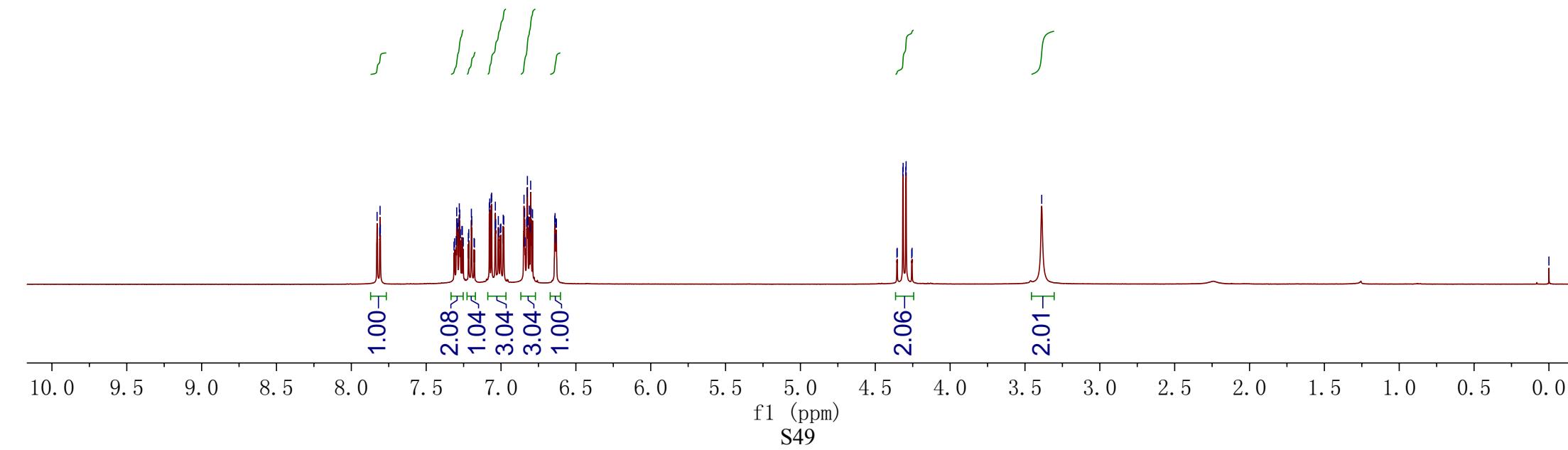
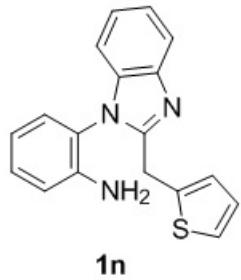
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

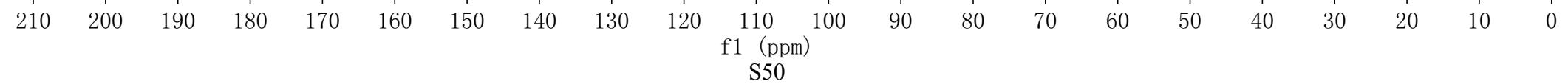
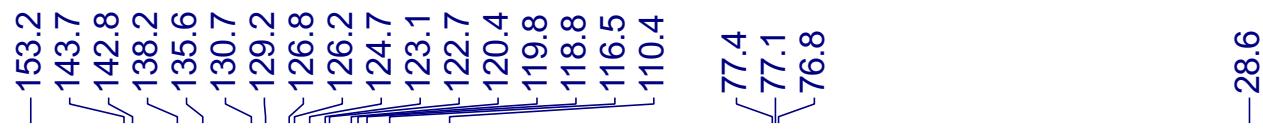
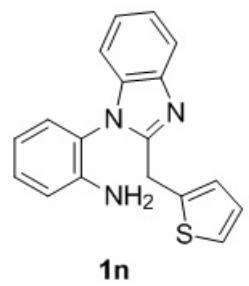
f1 (ppm)
S46

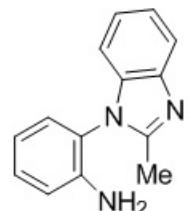




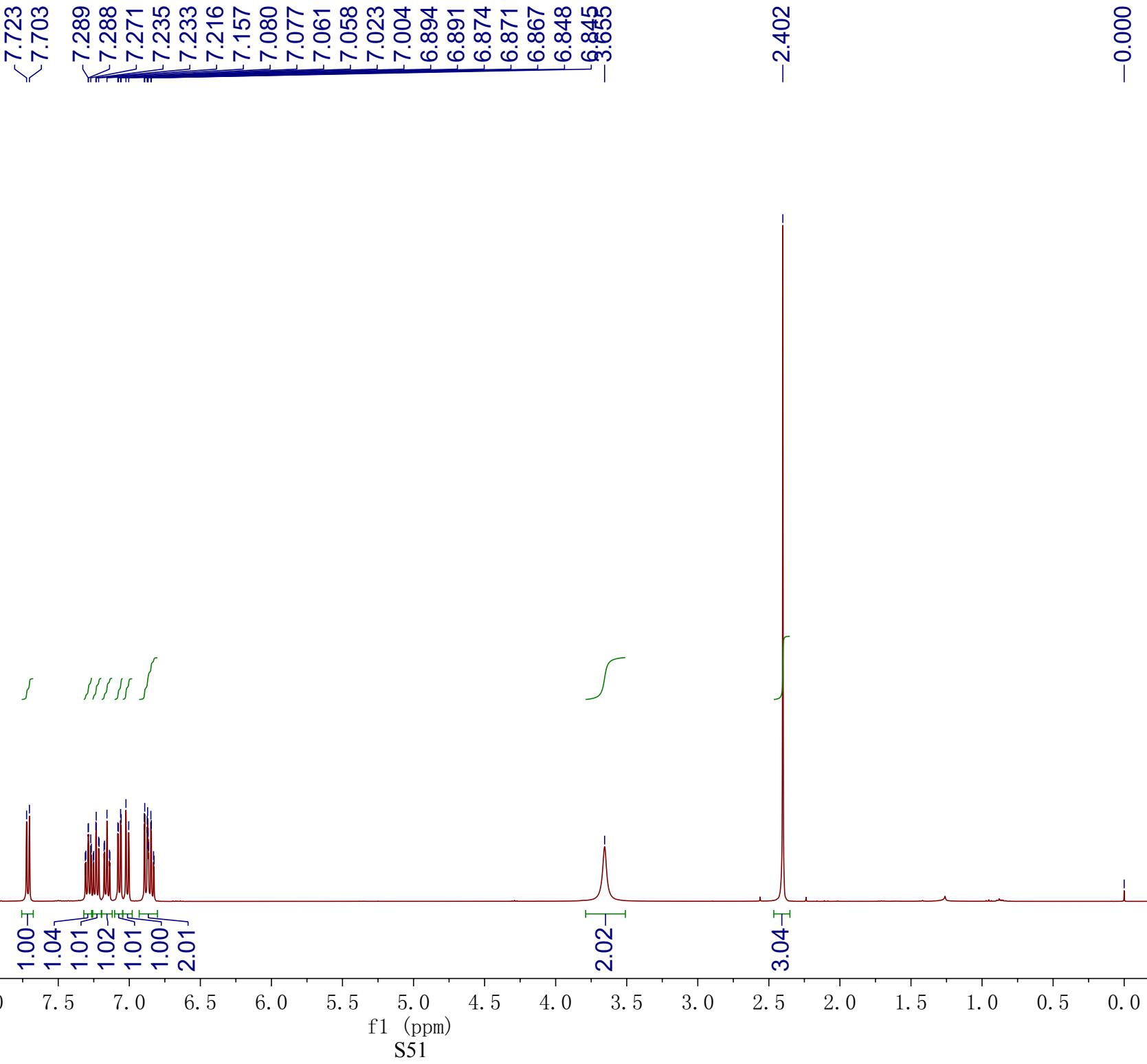
7.828	7.810	7.808	7.806	7.299	7.296	7.294	7.292	7.290	7.281	7.279	7.277	7.276	7.272	7.261	7.258	7.252	7.218	7.216	7.198	7.196	7.078	7.075	7.065	7.062	7.040	7.038	7.036	7.005	7.001	6.985	6.982	6.847	6.842	6.839	6.828	6.826	6.824	6.804	6.798	6.789	6.641	6.639	6.636	6.633	6.630	4.316	4.314	4.296	4.294	3.388
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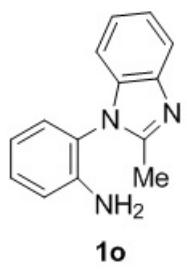
1o



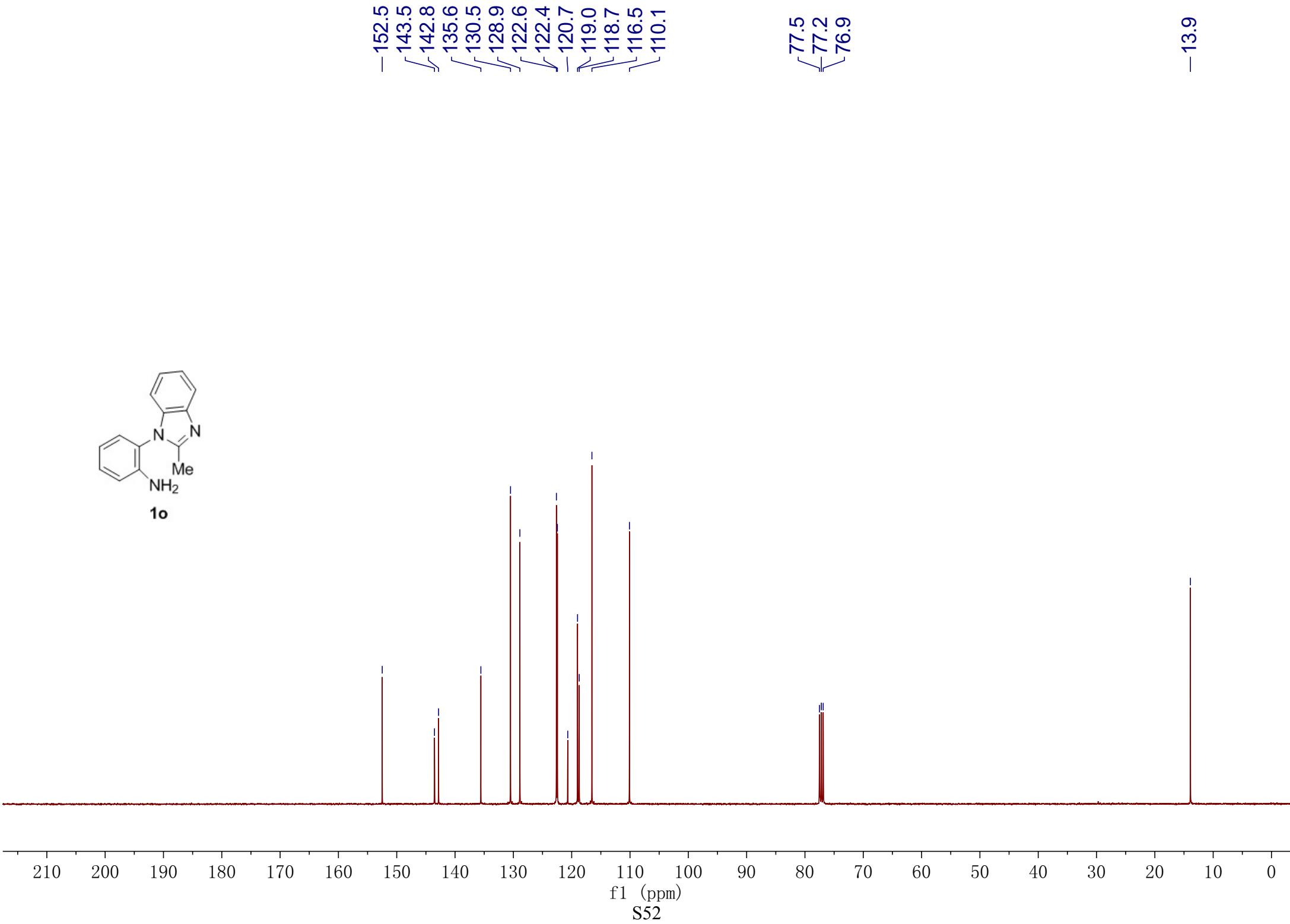
- 13.9

77.5
77.2
76.9

152.5
143.5
142.8
135.6
130.5
128.9
122.6
122.4
120.7
119.0
118.7
116.5
110.1

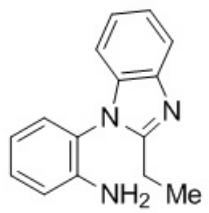


1o

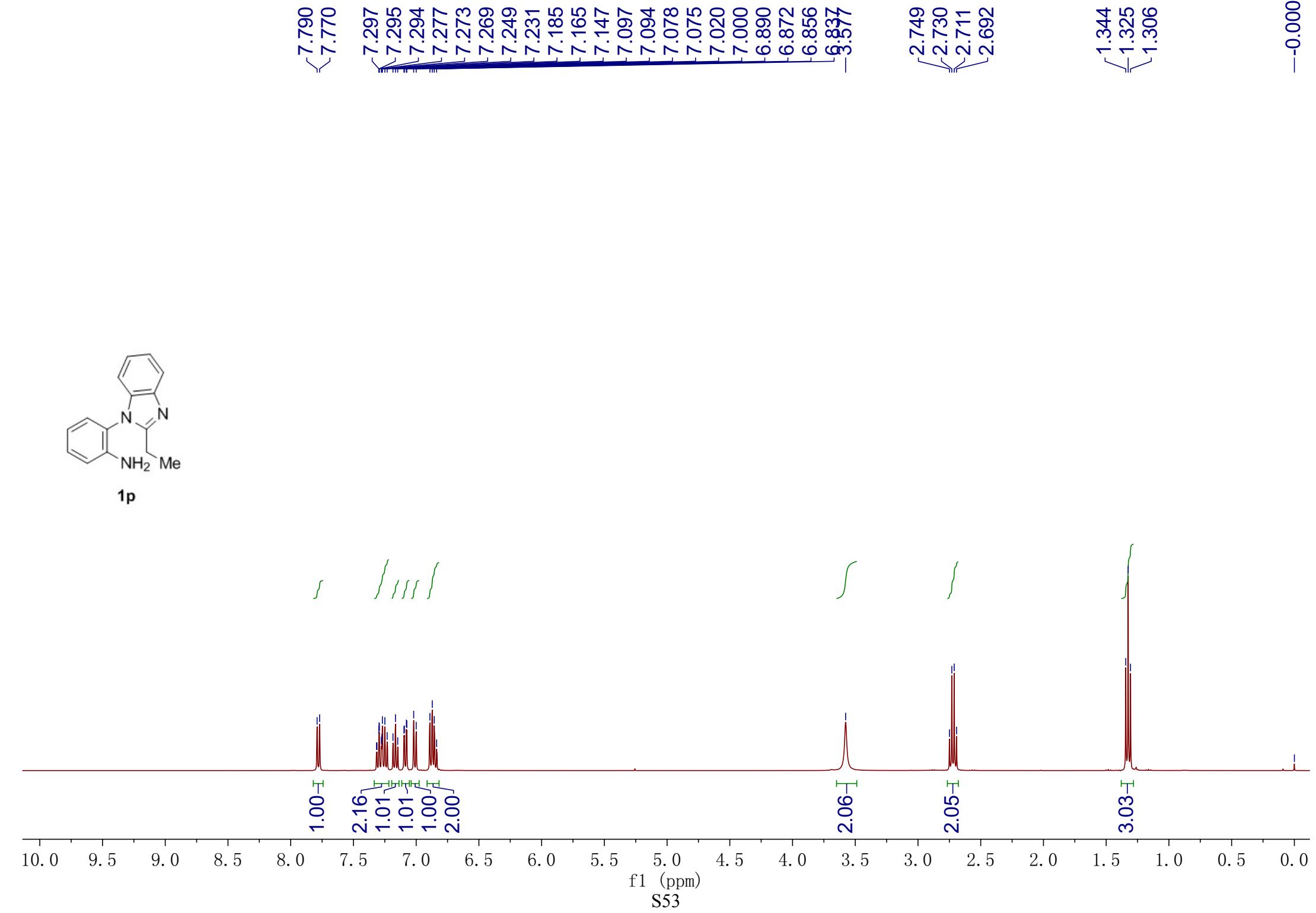


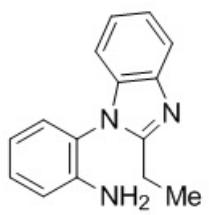
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S52

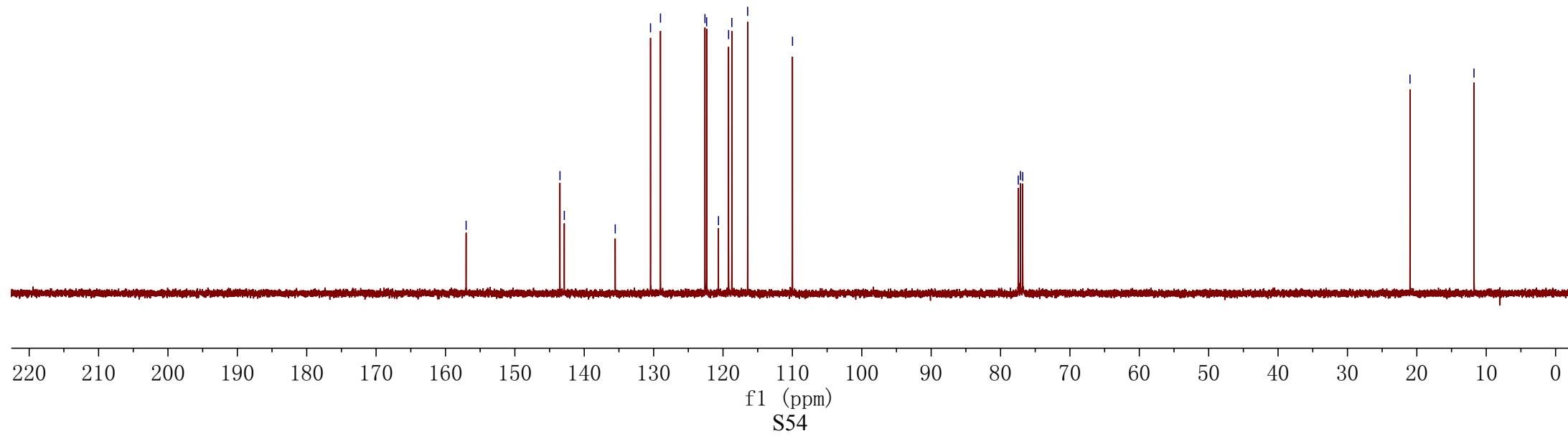
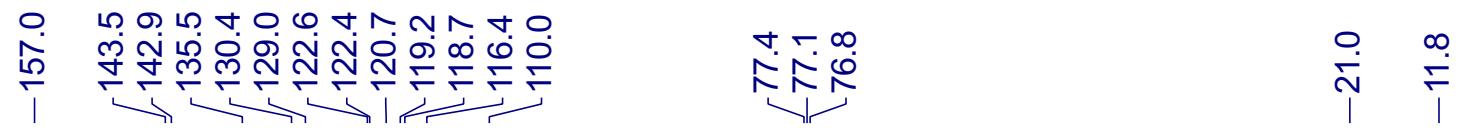


1p

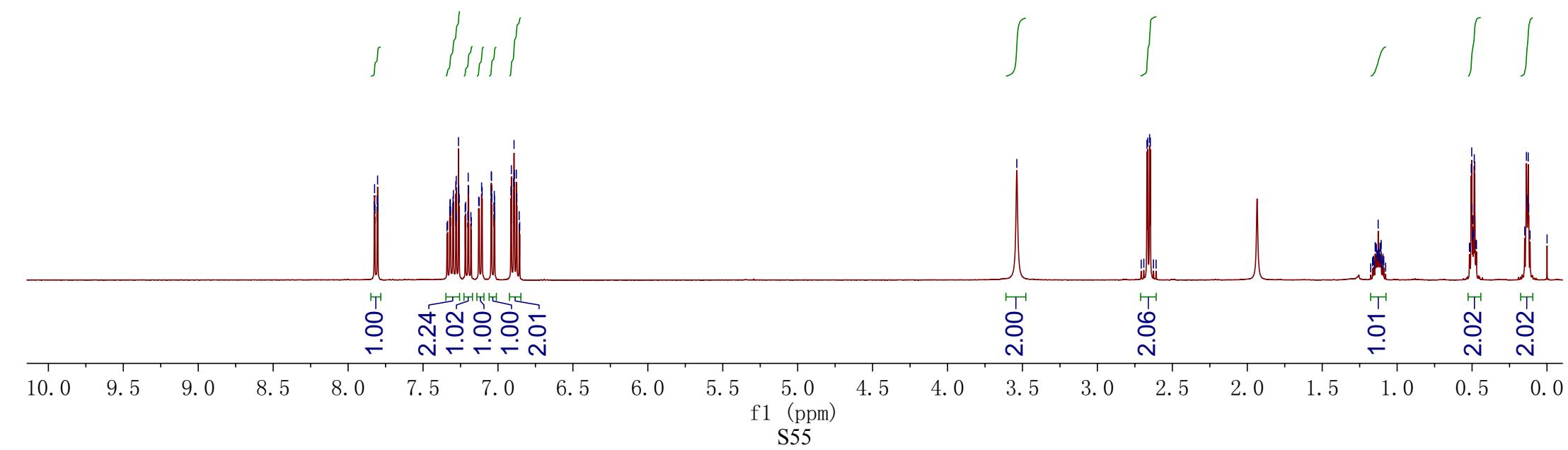
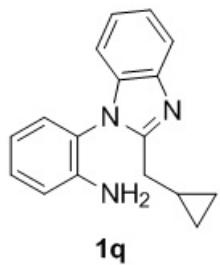


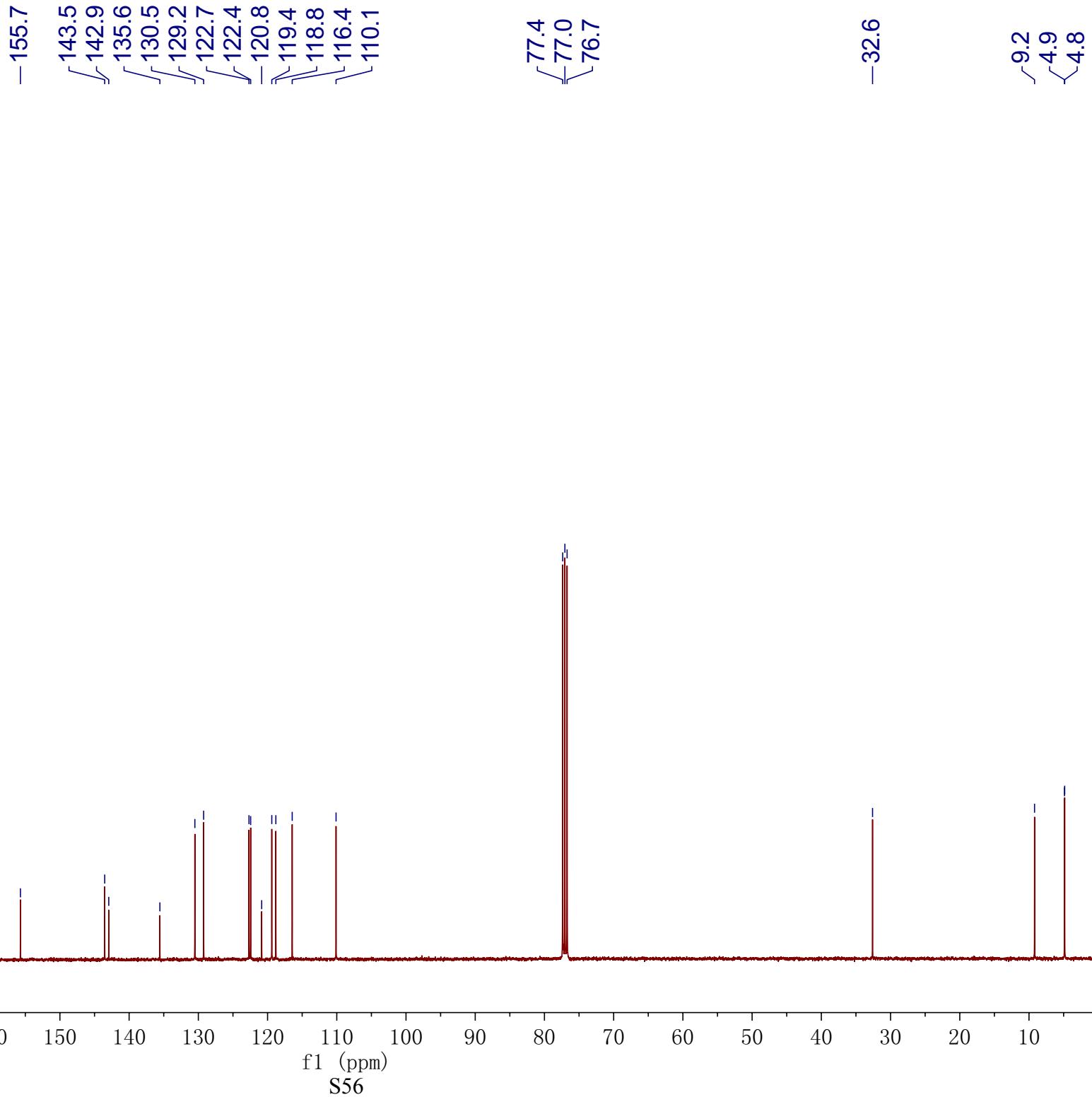
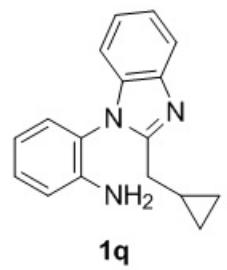


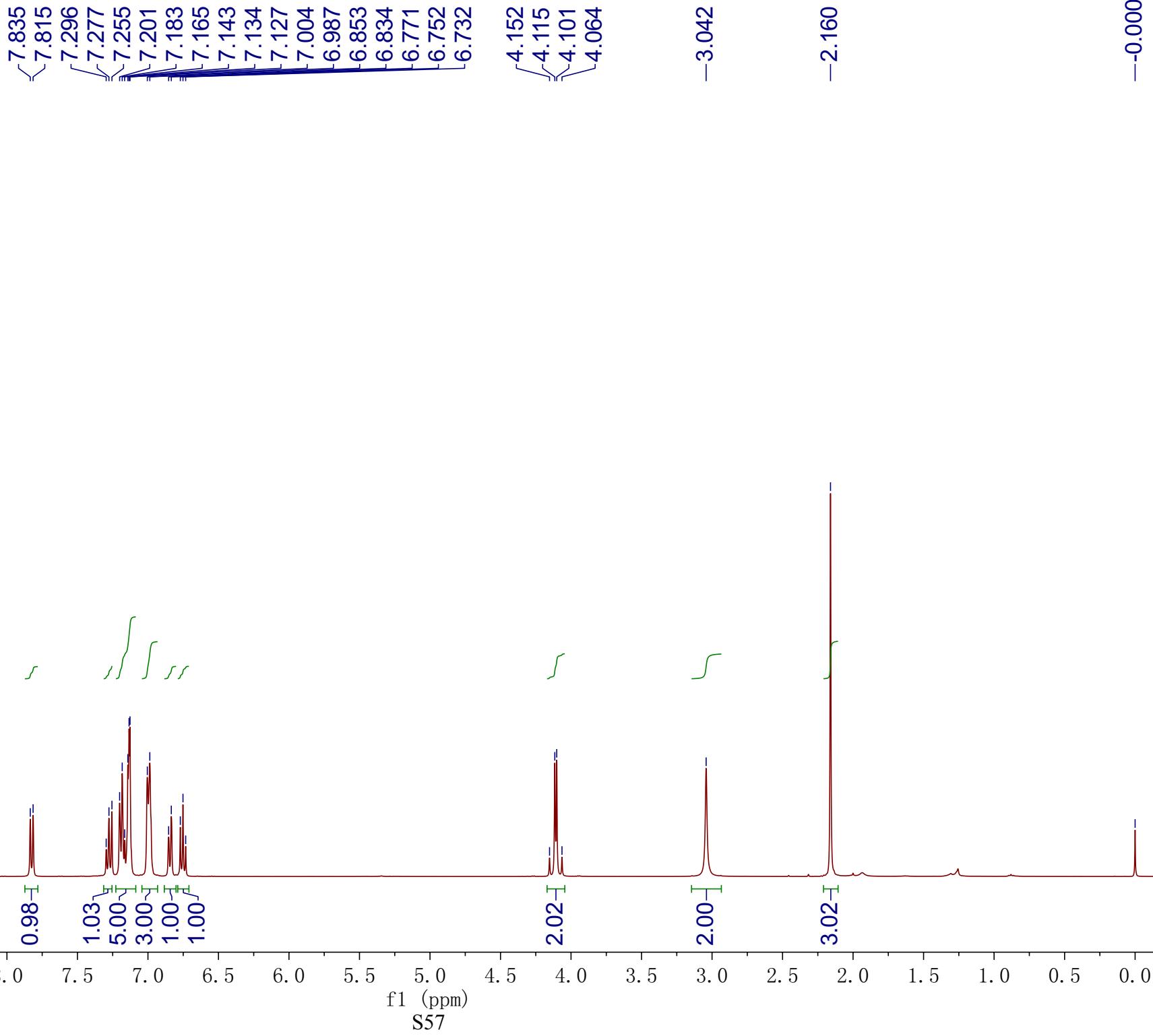
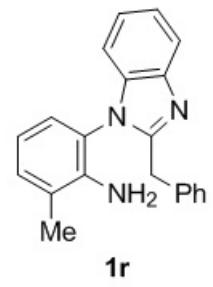
1p

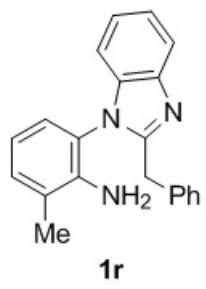


7.825	
7.823	
7.821	
7.805	
7.803	
7.801	
7.322	7.320
7.318	7.316
7.316	7.301
7.299	7.297
7.278	7.281
7.263	7.261
7.258	7.255
7.219	7.216
7.199	7.196
7.129	7.125
7.109	7.106
7.046	7.044
7.043	7.041
7.026	7.024
7.024	7.023
7.021	7.013
6.911	6.896
6.893	6.890
6.877	6.874
3.538	2.699
2.664	2.652
2.652	2.647
2.647	0.505
0.502	0.485
0.500	0.482
0.137	0.134
0.125	0.122
0.122	



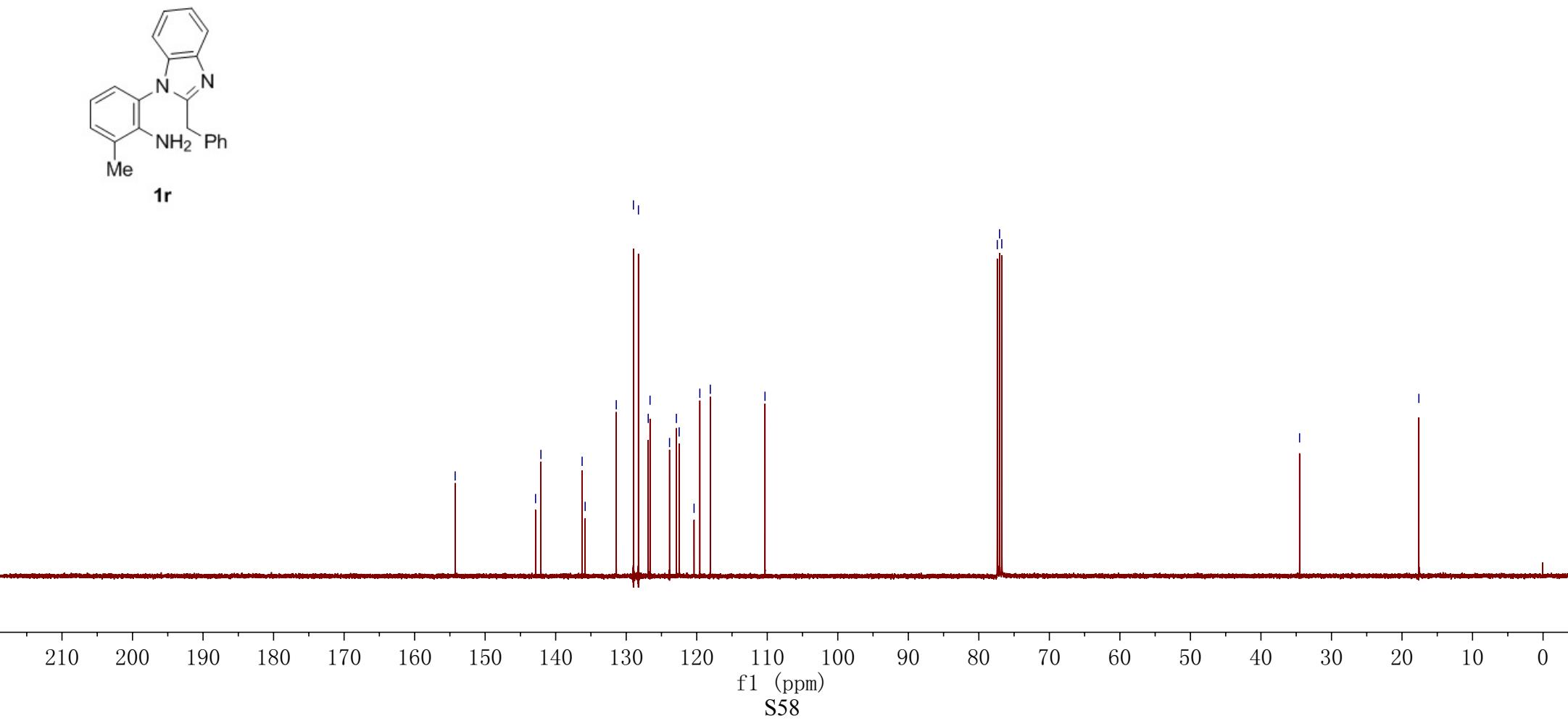


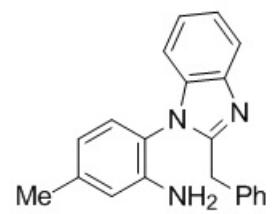




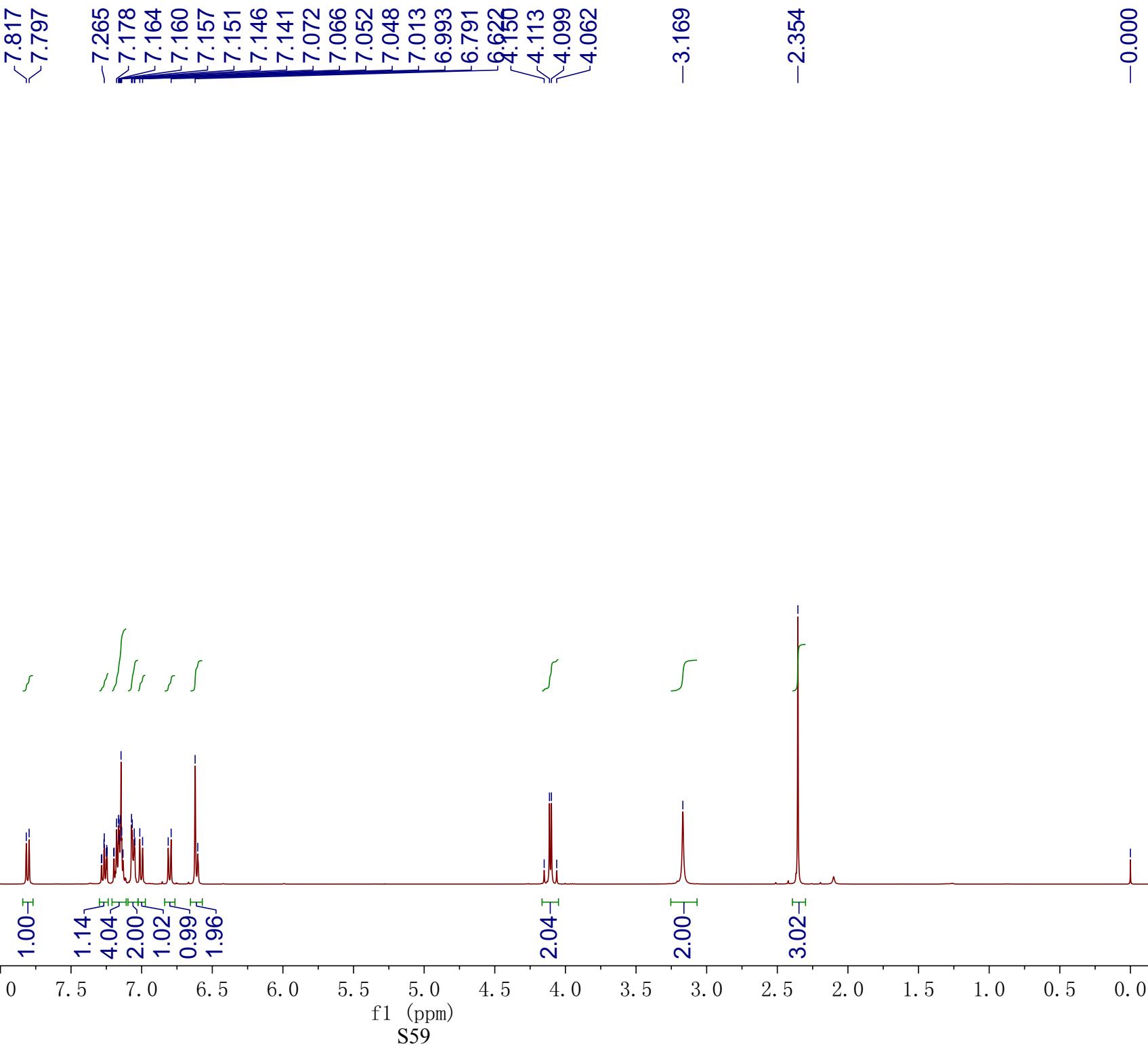
—154.3
—142.9
—142.1
—136.2
—135.8
—131.4
—129.0
—128.3
—126.9
—126.6
—123.9
—122.9
—122.5
—120.4
—119.6
—118.1
—110.3

—34.5
—17.6





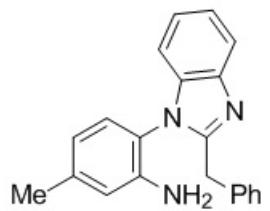
1s



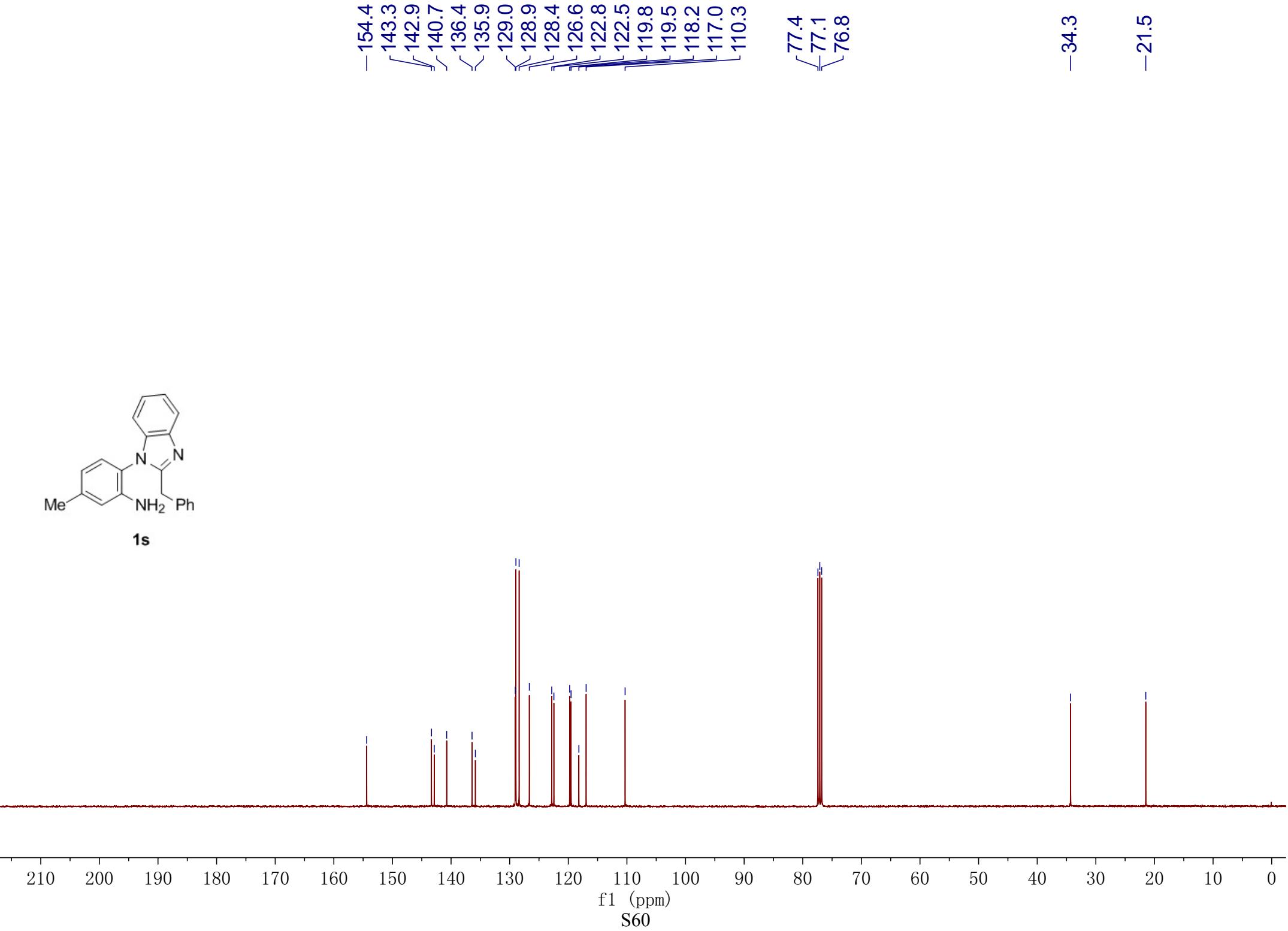
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

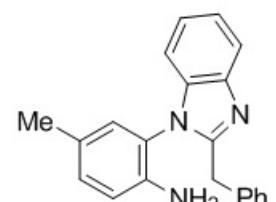
f1 (ppm)
S59

-0.000

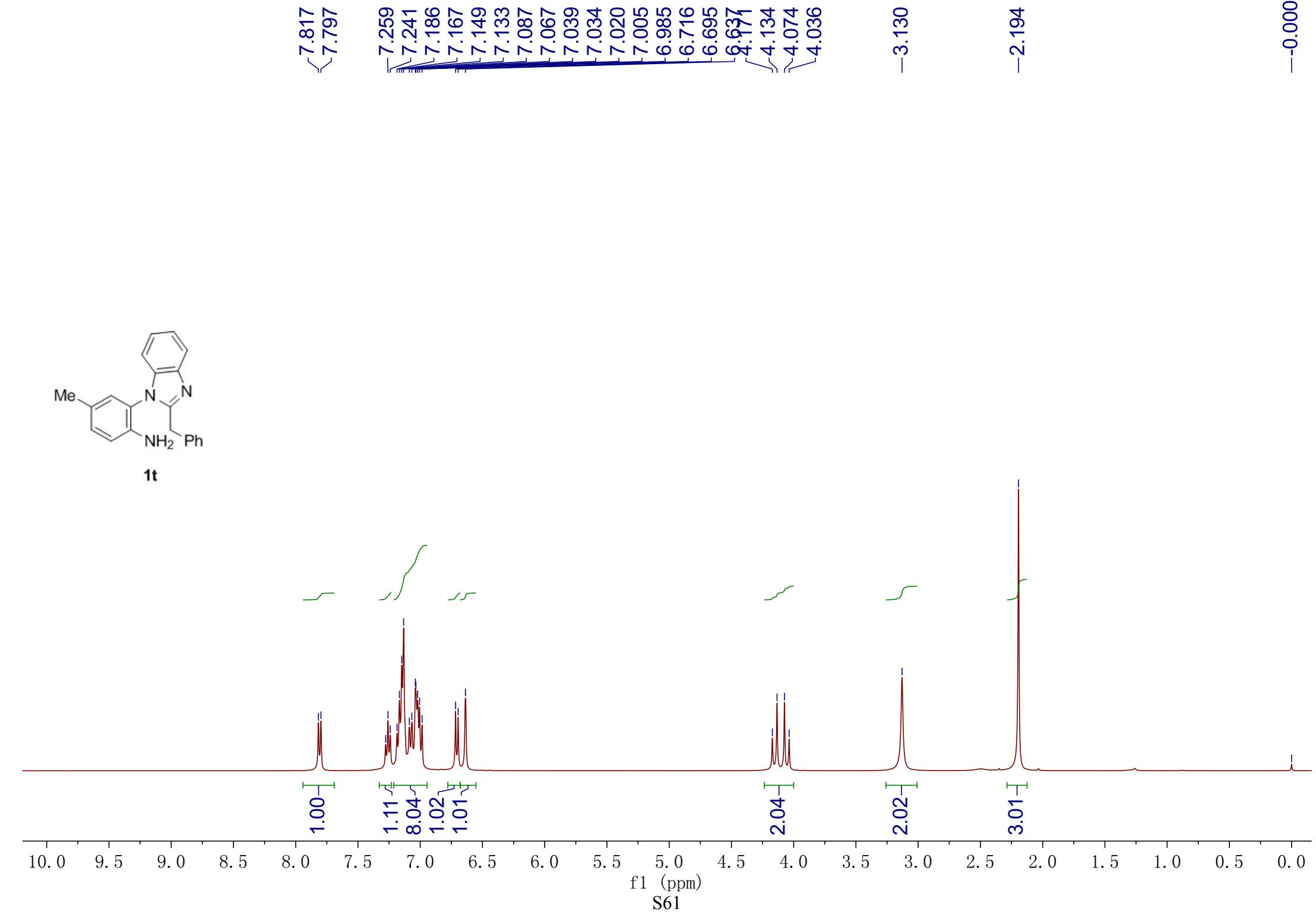


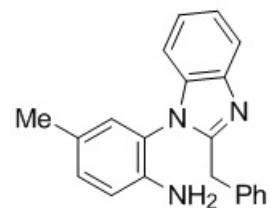
1s





1t



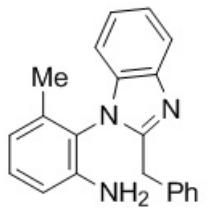


1t

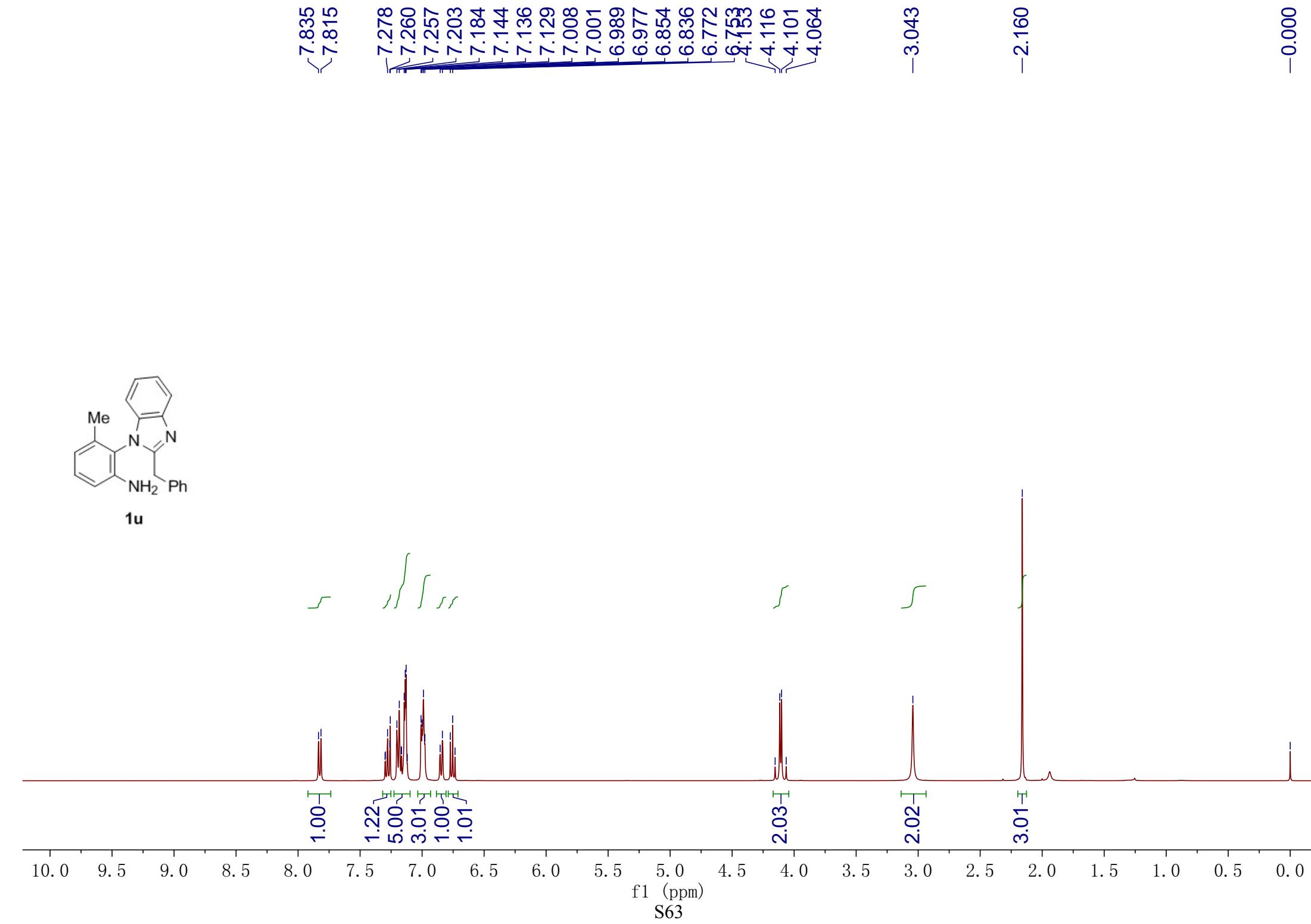
— 154.2 142.8 141.1 136.4 135.8 131.2 129.6 129.0 128.3 128.2 126.6 122.9 122.5 120.6 119.5 116.6 110.3
— 77.5 77.2 76.8
— 34.5
— 20.2

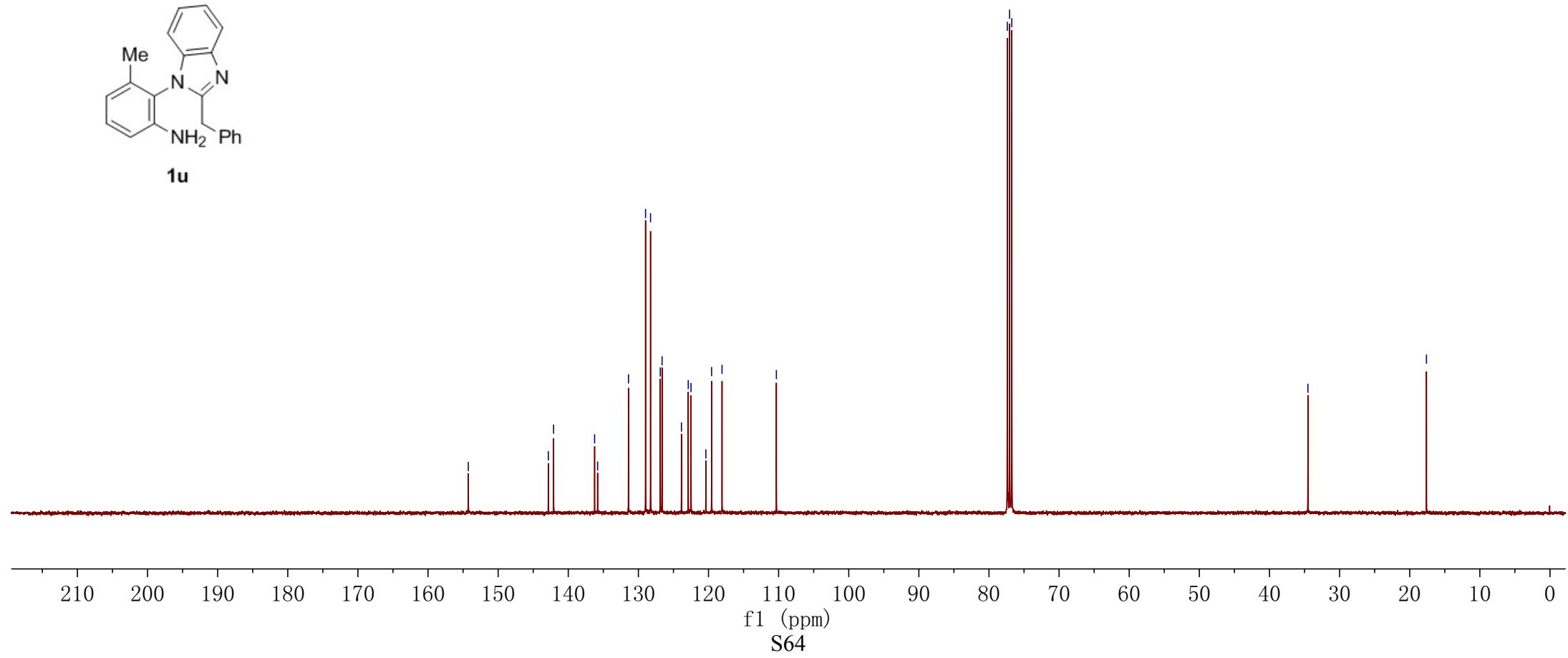
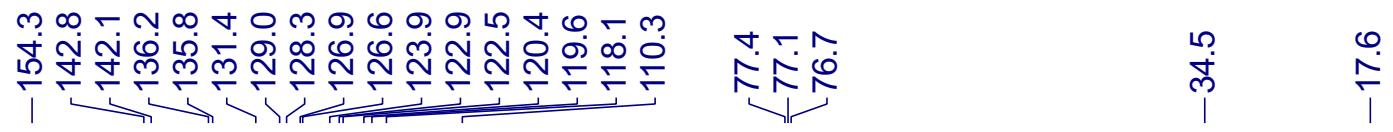
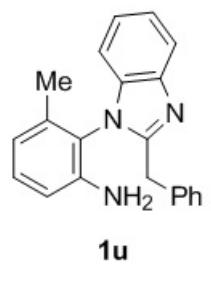
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

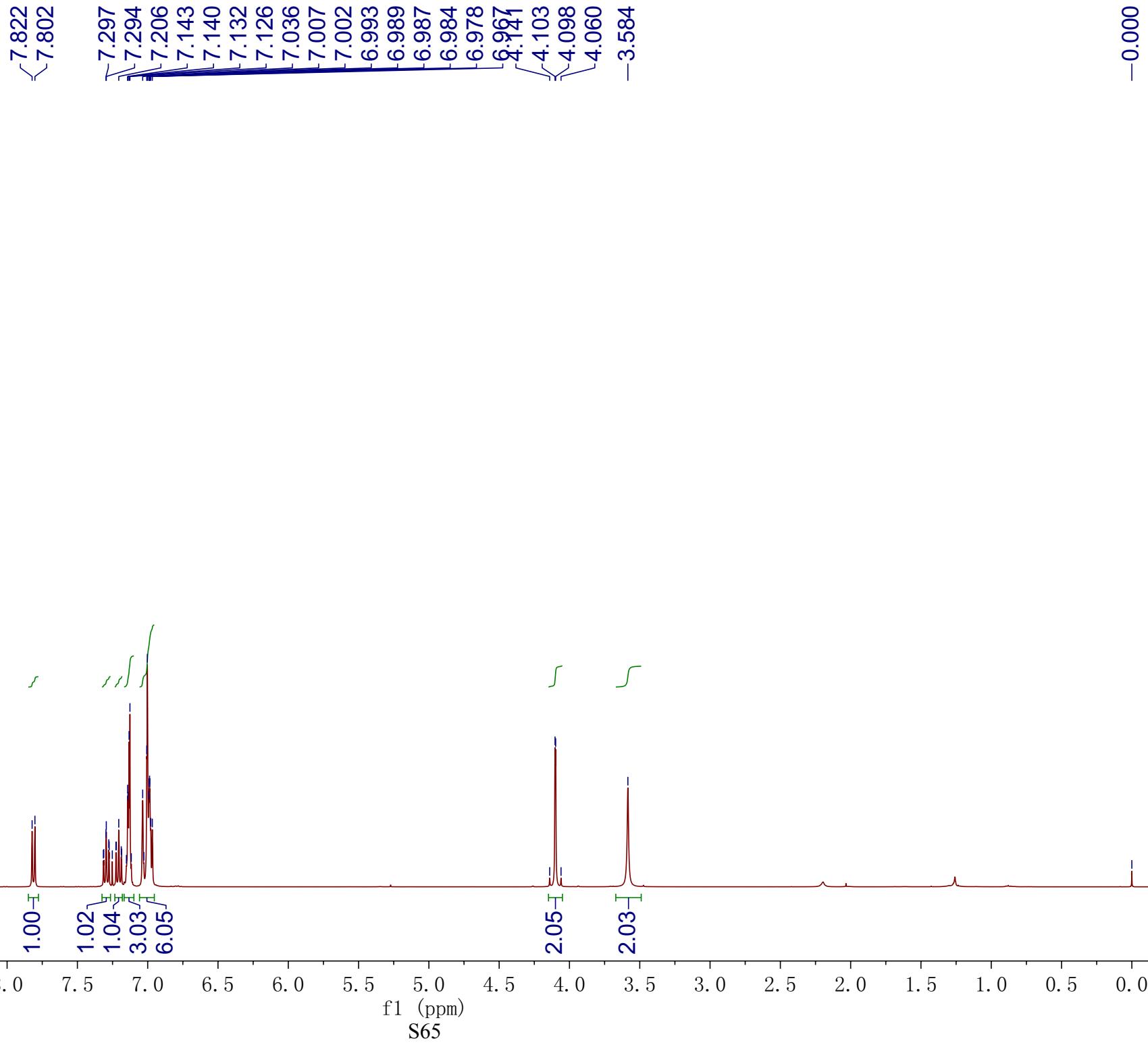
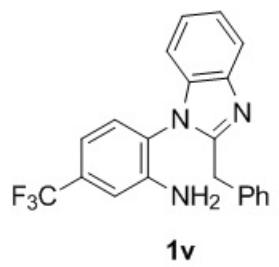
f1 (ppm)
S62

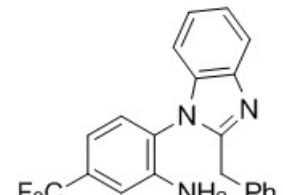


1u

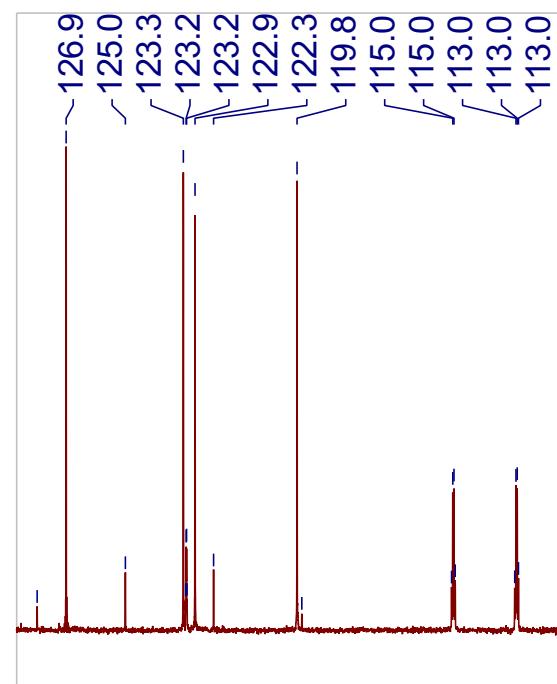
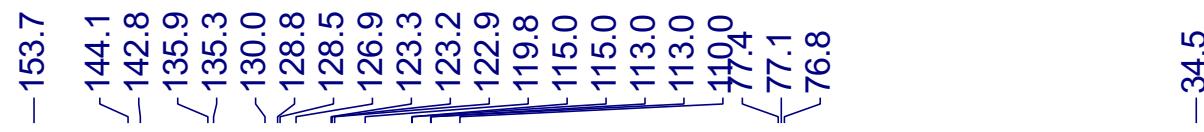








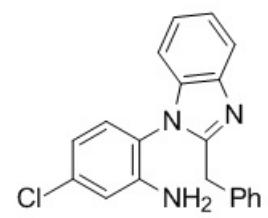
1v



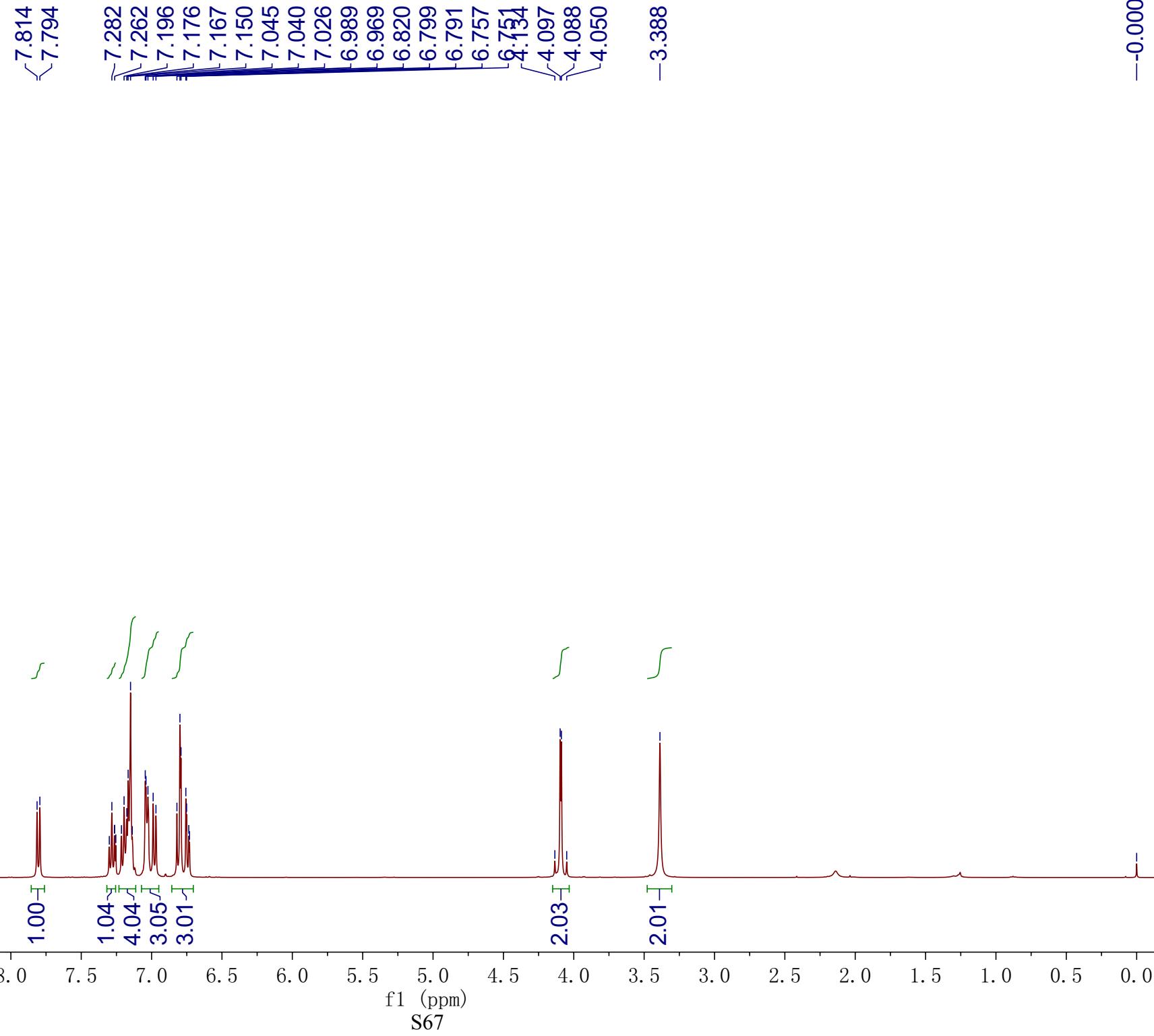
126
122
118
114
f1 (ppm)

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S66

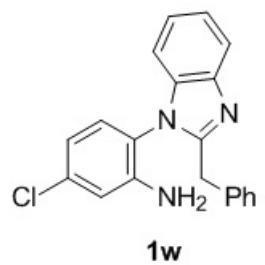


1w



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)
S67



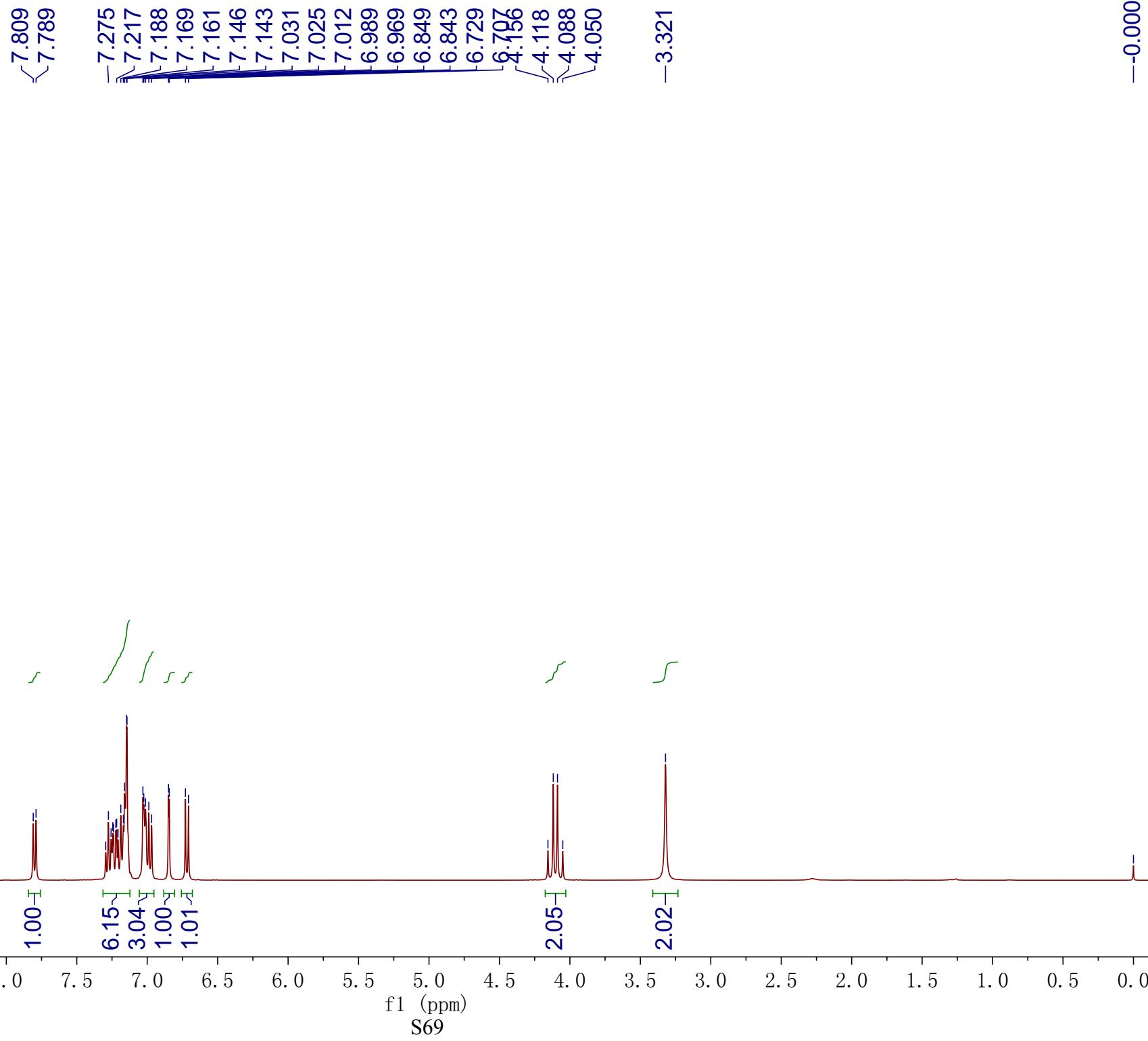
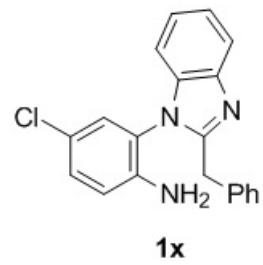
154.0
144.7
142.8
136.1
136.1
135.6
130.4
128.8
128.5
126.8
123.1
122.8
119.7
119.0
118.6
116.0
110.1

77.4
77.1
76.8

-34.4

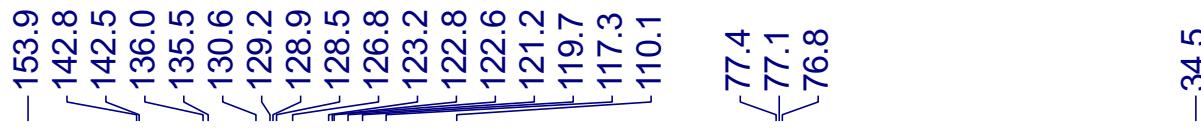
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S68



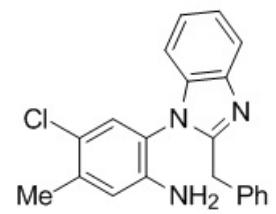


1x

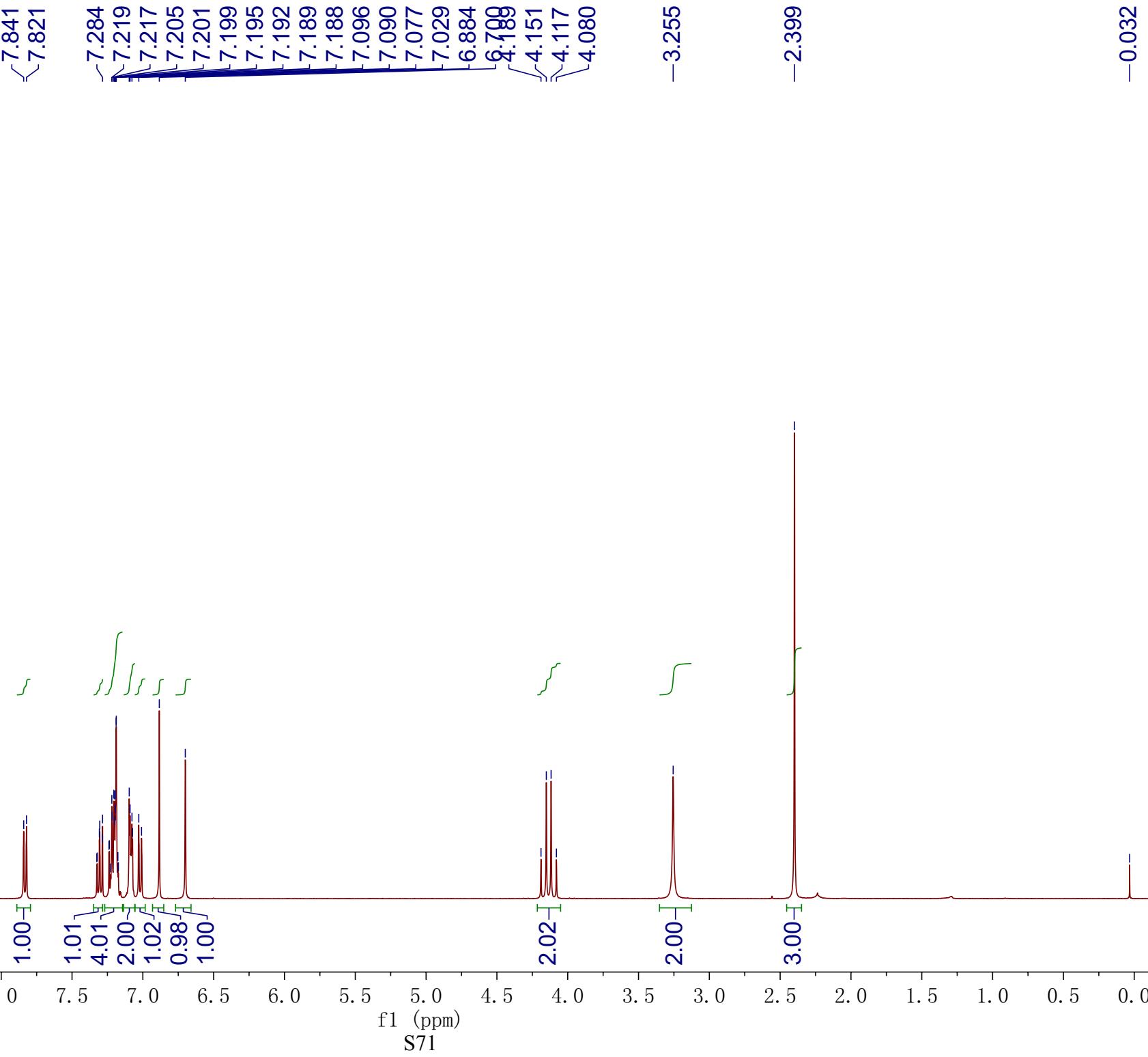


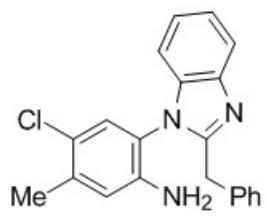
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S70



1y





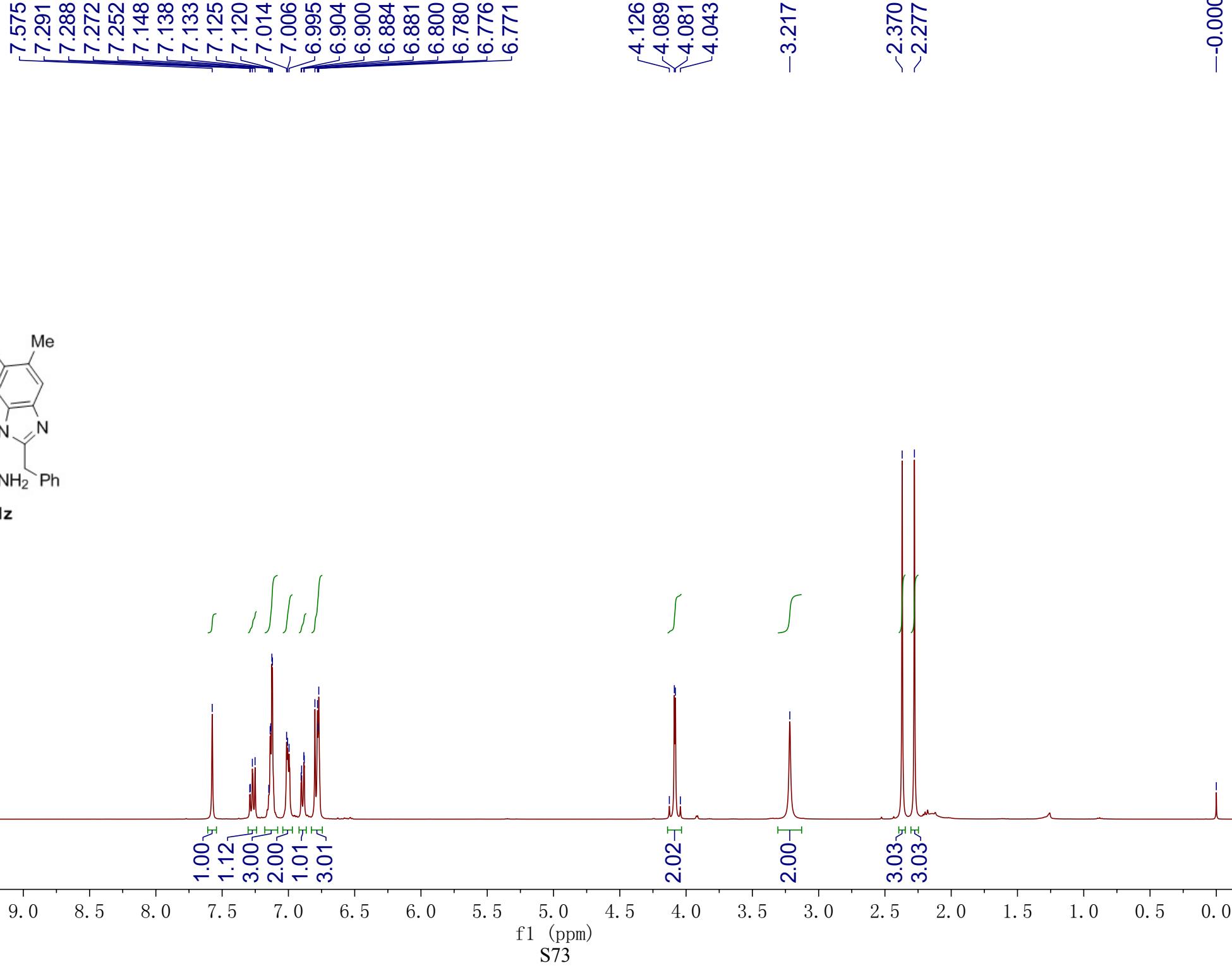
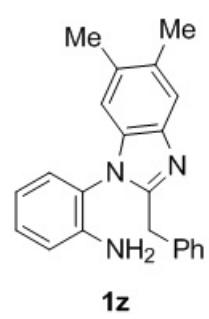
1y

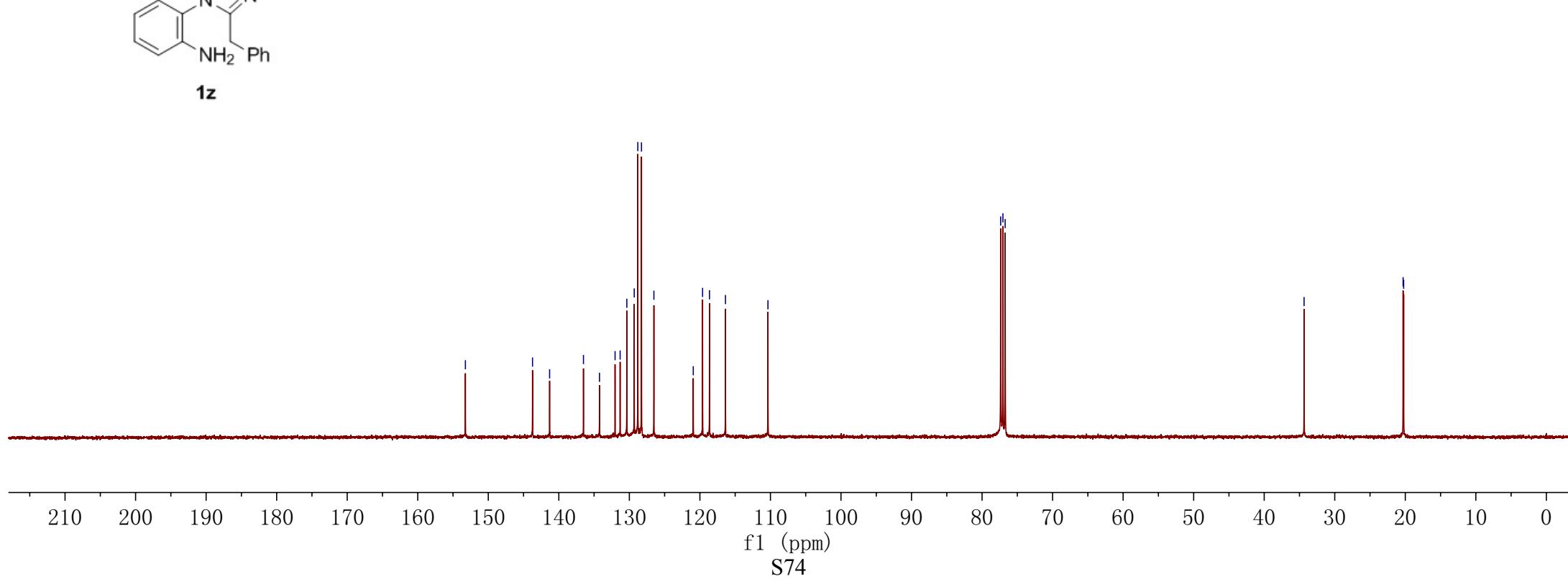
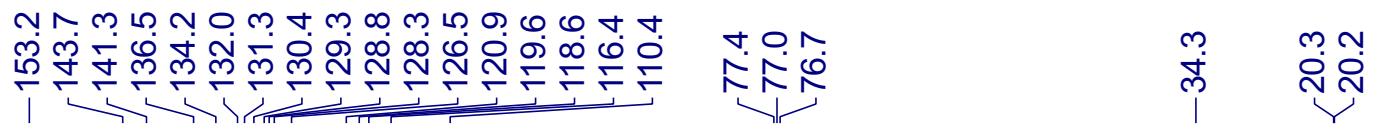
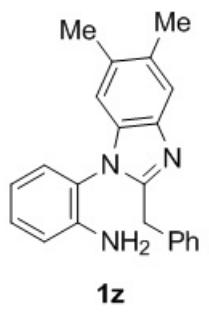
—154.1 —142.3
—136.1 —129.3
—128.9 —128.5
—126.8 —123.1
—122.7 —119.7
—118.4

—34.4
—20.1

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

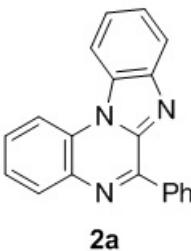
f1 (ppm)
S72



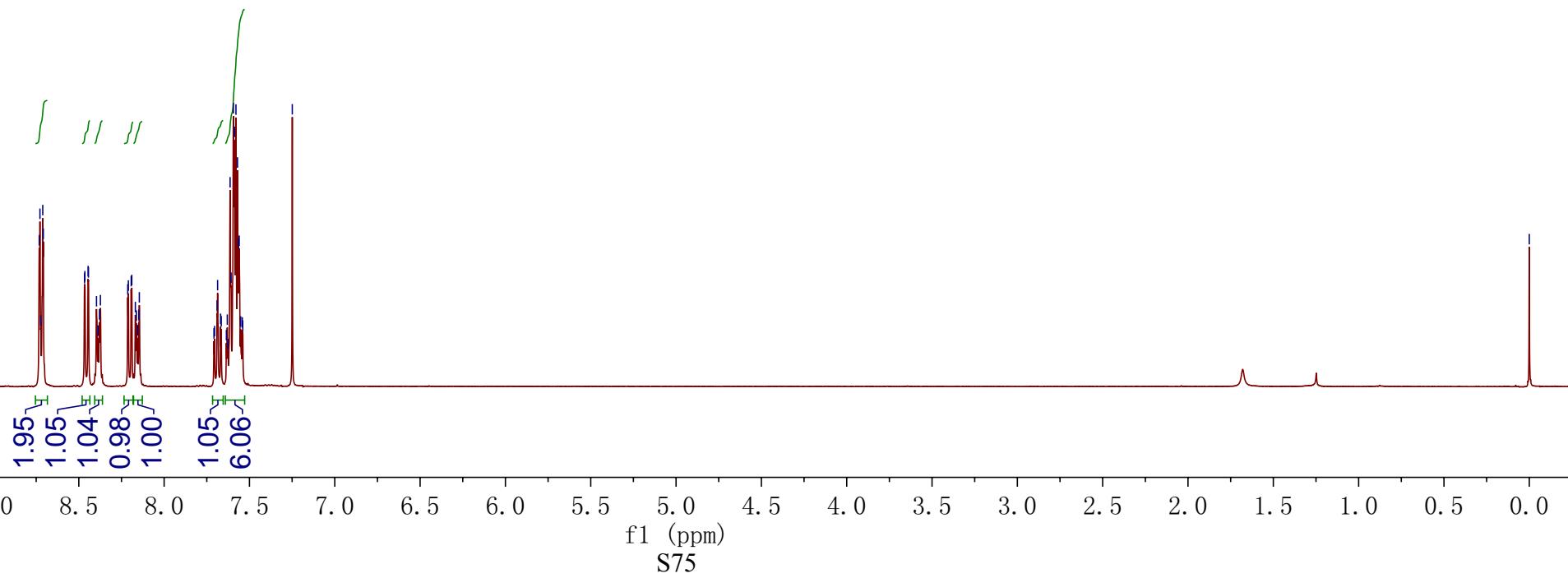


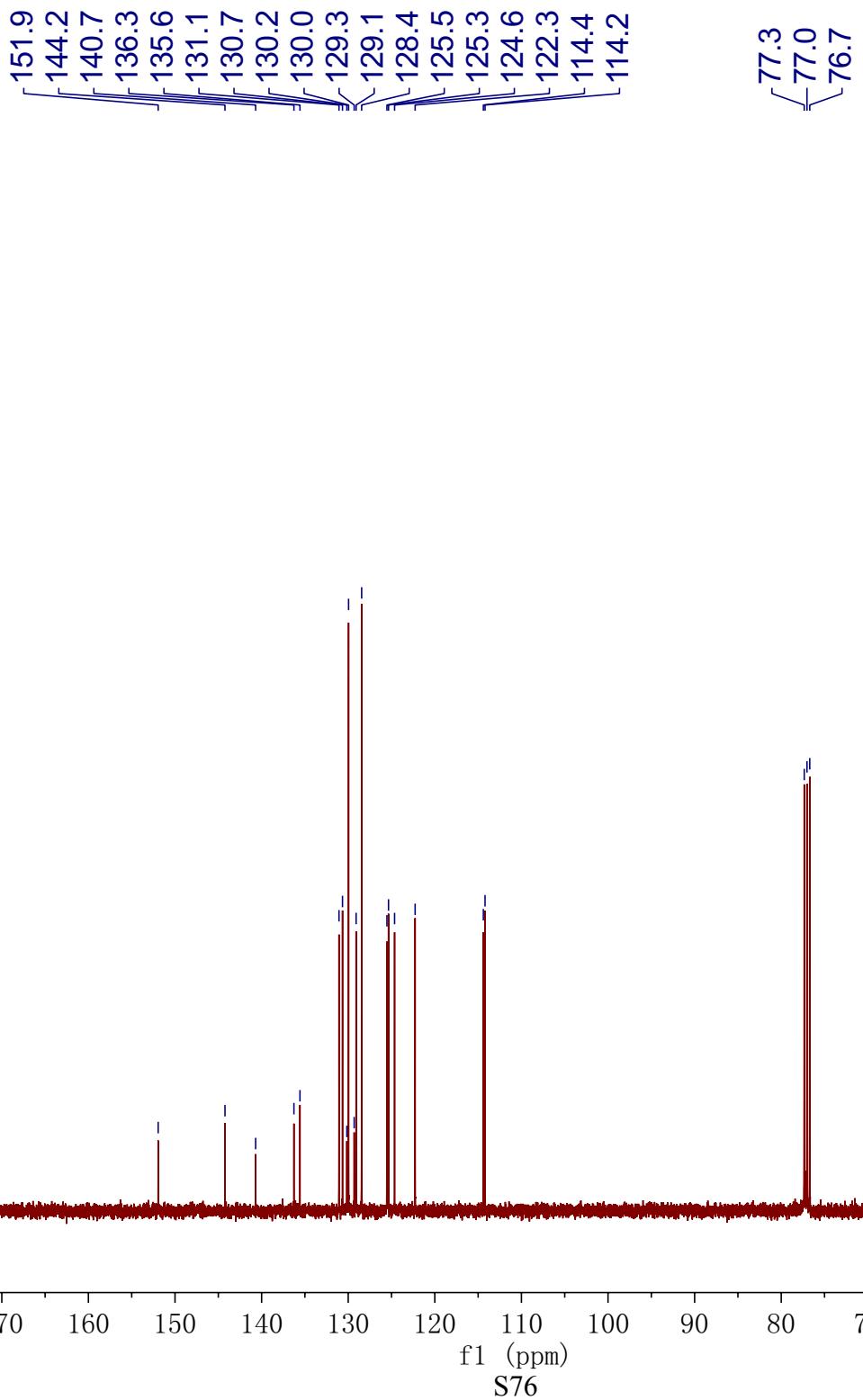
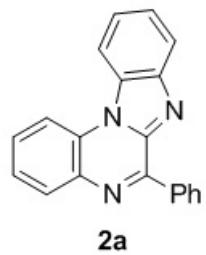
-0.000

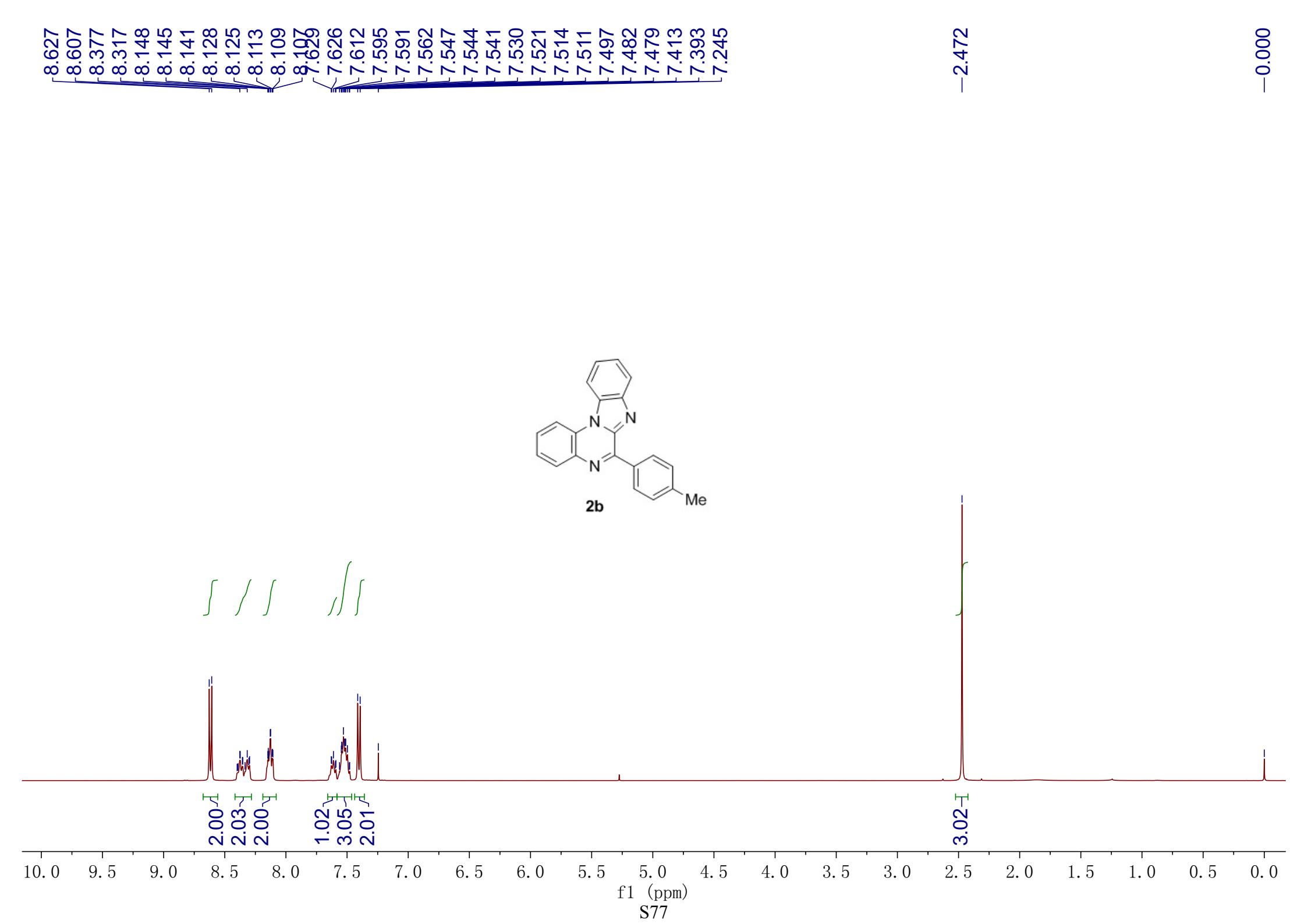
8.732
8.728
8.711
8.708
8.466
8.464
8.445
8.443
8.213
8.210
8.193
9.198
7.708
7.704
7.690
7.687
7.669
7.665
7.635
7.630
7.625
7.613
7.608
7.594
7.588
7.579
7.570
7.564
7.560
7.551
7.542
7.539
7.249

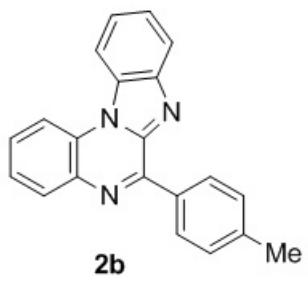


2a



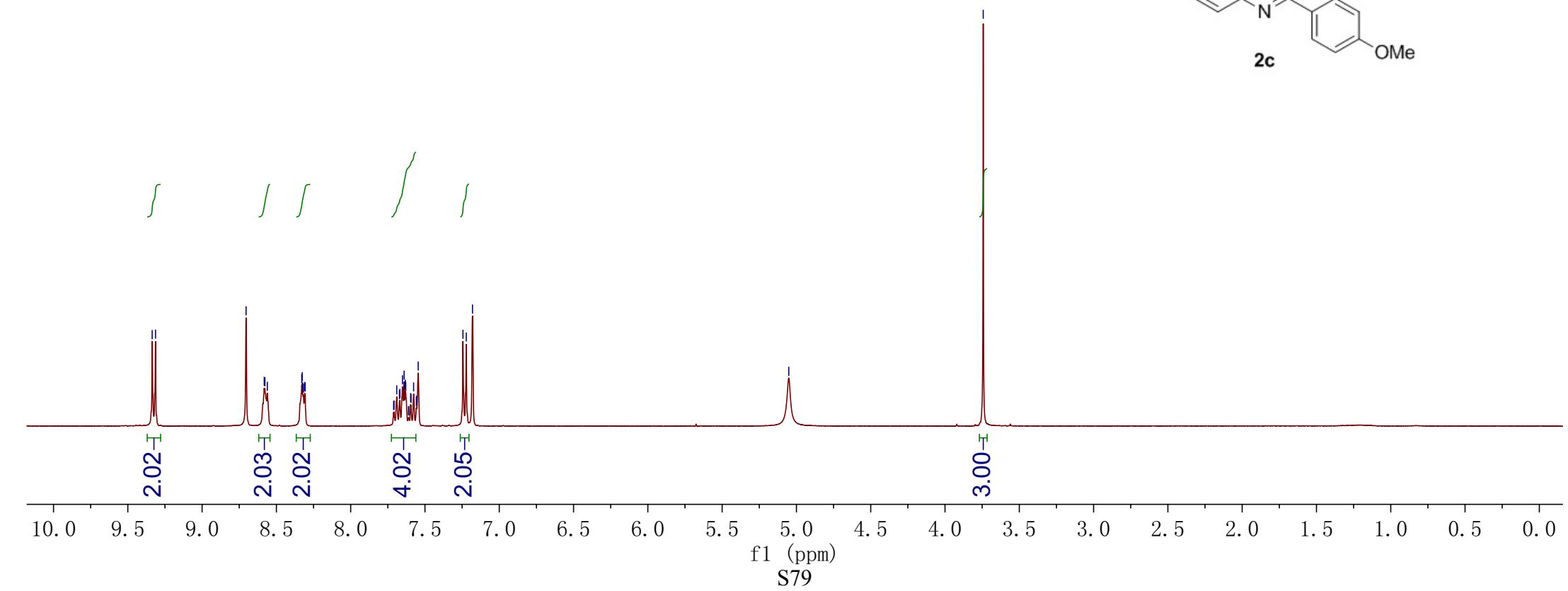
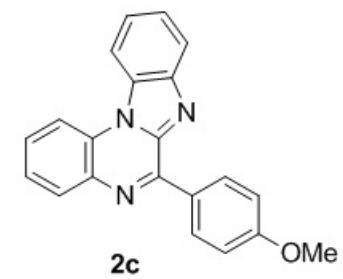


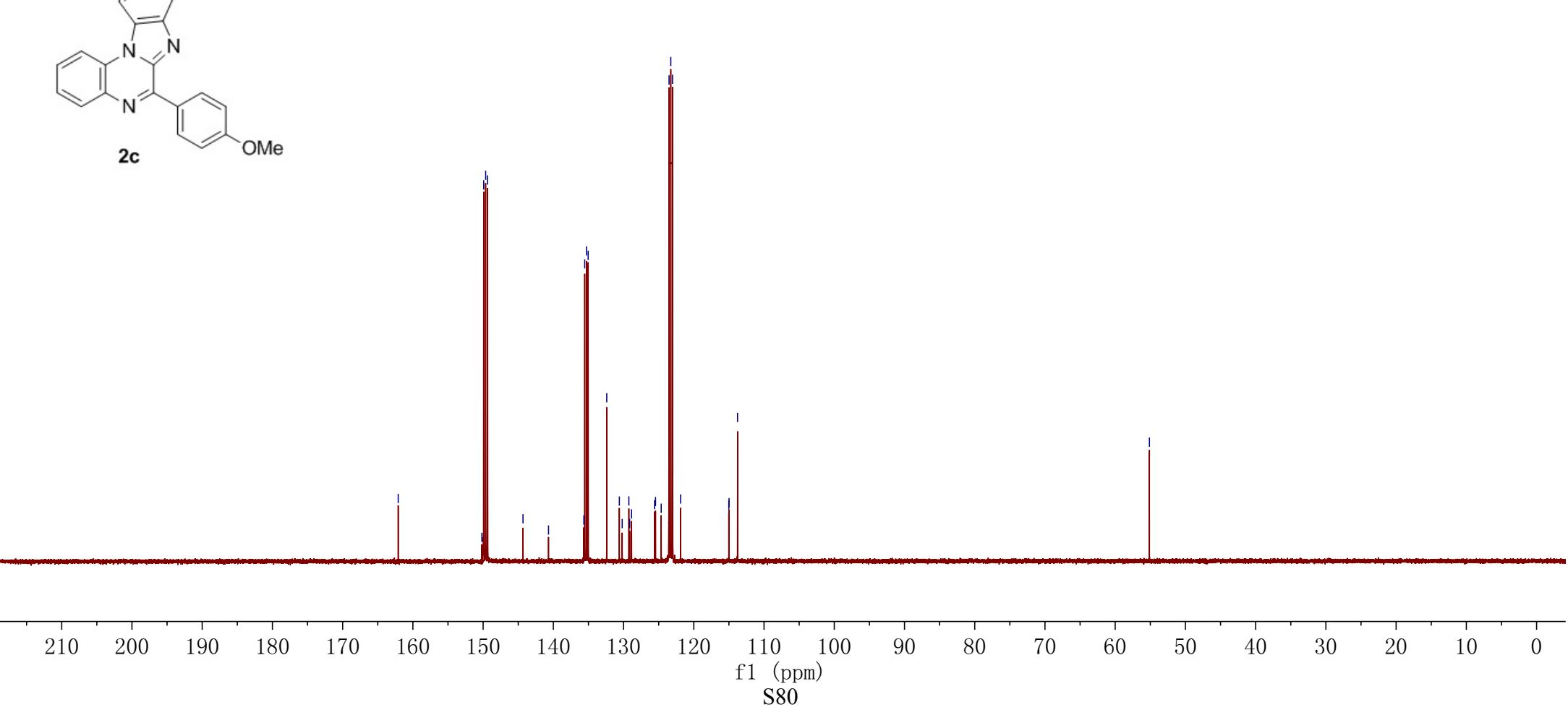
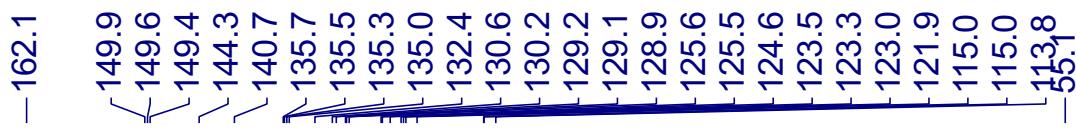
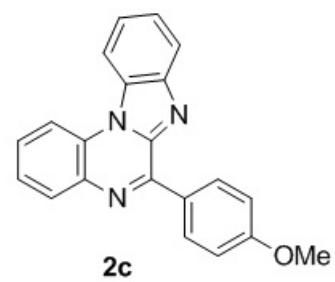


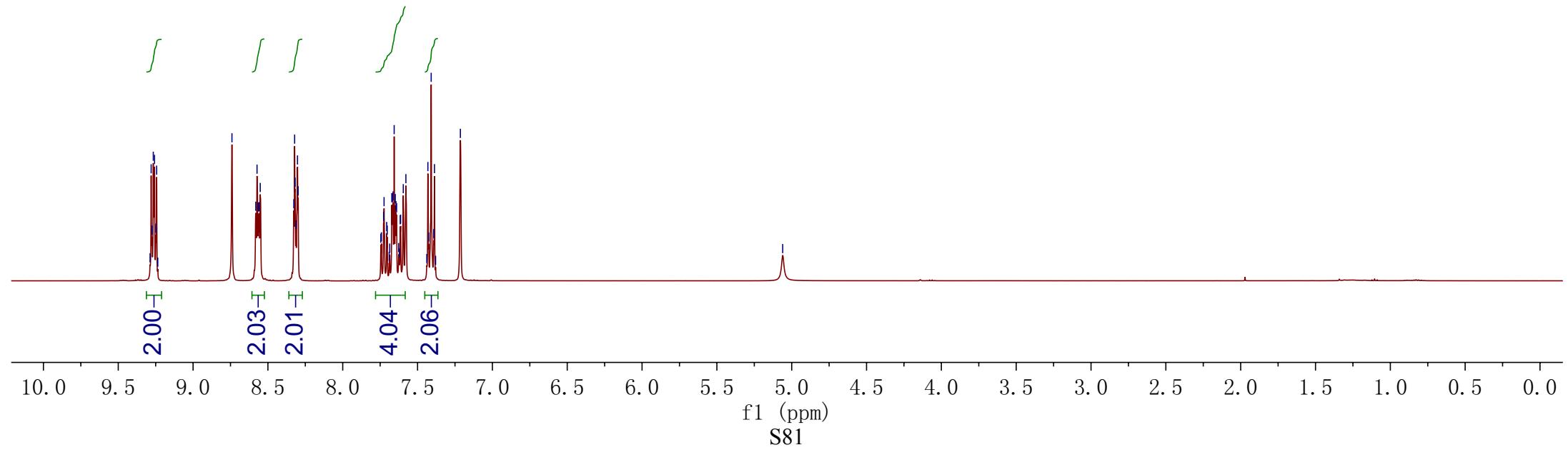
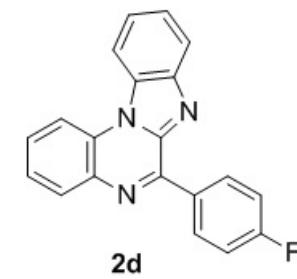
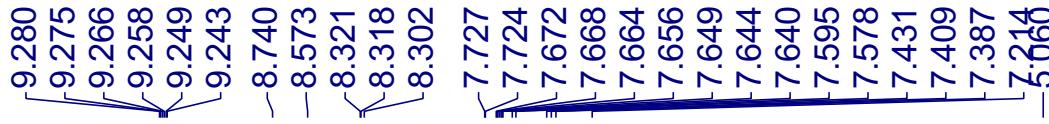


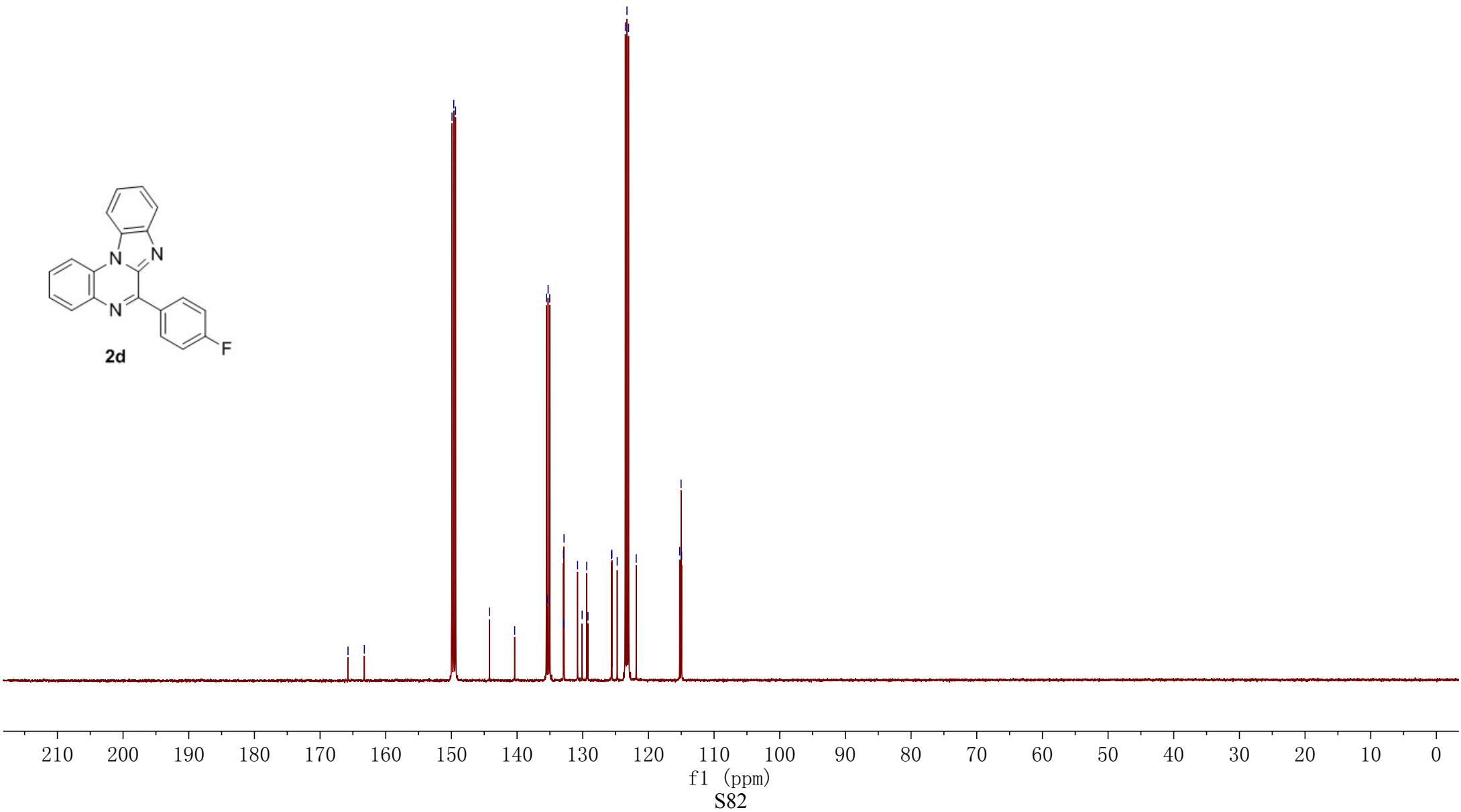
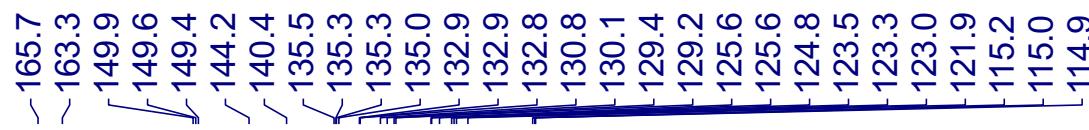
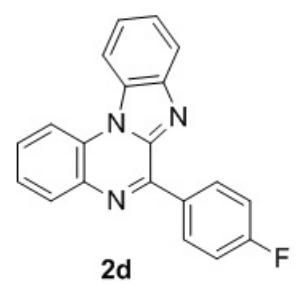
9.336
9.314
8.704
8.582
8.577
8.561
8.329
8.326
7.690
7.672
7.669
7.640
7.638
7.632
7.629
7.596
7.594
7.576
7.546
7.244
7.222
7.189
5.059

-3.743



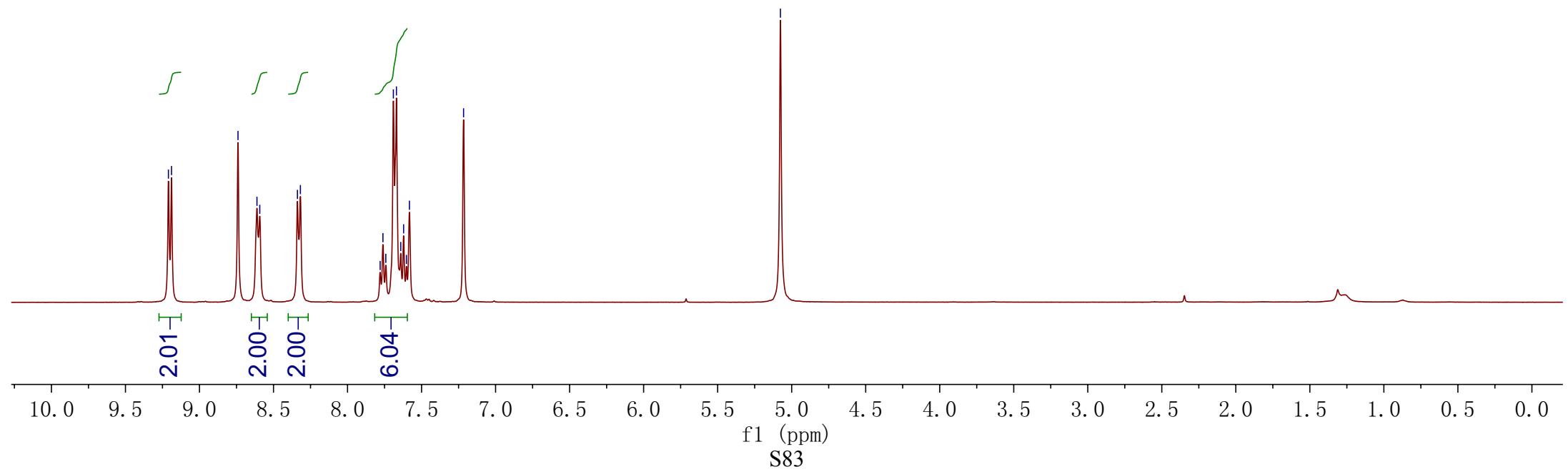
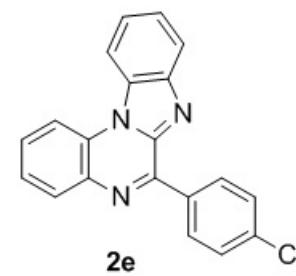


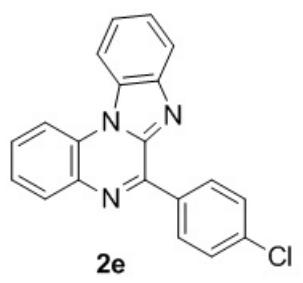




9.210
9.189
8.740
8.612
8.593
8.338
8.318
7.780
7.761
7.741
7.690
7.670
7.641
7.621
7.602
7.582
7.216

-5.076





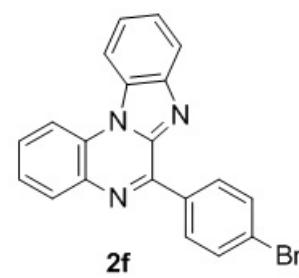
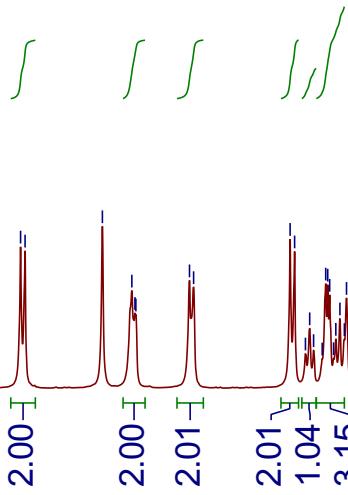
149.9
149.6
149.4
144.2
140.4
136.6
135.6
135.3
135.1
135.1
132.1
130.9
130.1
129.7
129.3
128.4
125.7
125.6
124.8
123.5
123.3
123.0
121.9
115.1
115.0

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S84

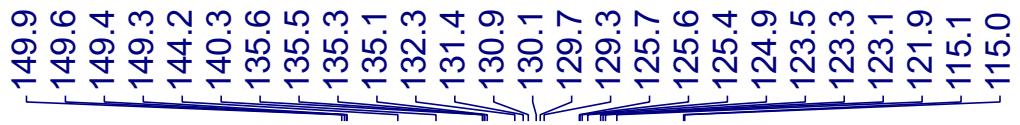
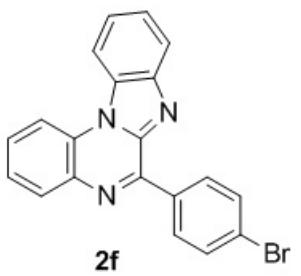
9.127
9.106
8.740
8.600
8.585
8.581
8.327
8.307
7.850
7.828
7.777
7.757
7.738
7.698
7.681
7.671
7.662
7.644
7.633
7.614
7.592
7.582
7.217

-5.067



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)
S85



A zoomed-in portion of the ¹³C NMR spectrum showing the aromatic region from approximately 110 to 150 ppm. The peaks are labeled with their corresponding chemical shifts in ppm:

- 149.9
- 149.6
- 149.4
- 149.3
- 144.2
- 140.3
- 135.6
- 135.5
- 135.3
- 135.1
- 132.3
- 131.4
- 130.9
- 130.1
- 129.7
- 129.3
- 125.7
- 125.6
- 125.4
- 124.9
- 123.5
- 123.3
- 123.1
- 121.9
- 115.1
- 115.0

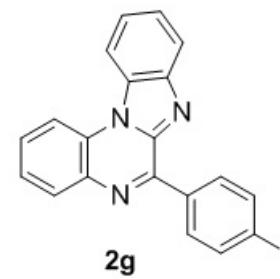
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S86

8.953
8.948
8.936
8.931
8.704
8.598
8.594
8.587
8.575
8.569
8.312
8.308
8.292
8.288
8.061
8.057
7.735
7.662
7.658
7.649
7.639
7.635
7.590
7.547
7.181
5.050

{ { { { {

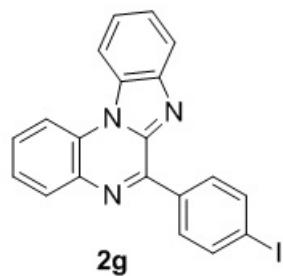
2.00
2.01
2.00
2.00
1.03
3.04



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)
S87

149.9
149.7
149.6
149.4
144.2
140.3
137.5
136.0
135.5
135.4
135.3
135.0
132.2
130.9
130.1
129.7
129.3
125.7
125.6
124.8
123.5
123.3
123.0
121.9
115.1
115.0
98.7

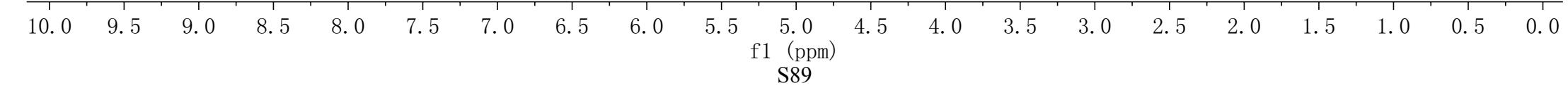
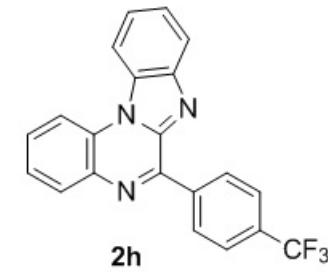
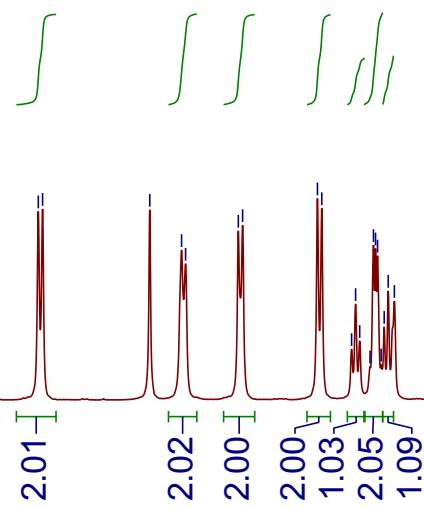


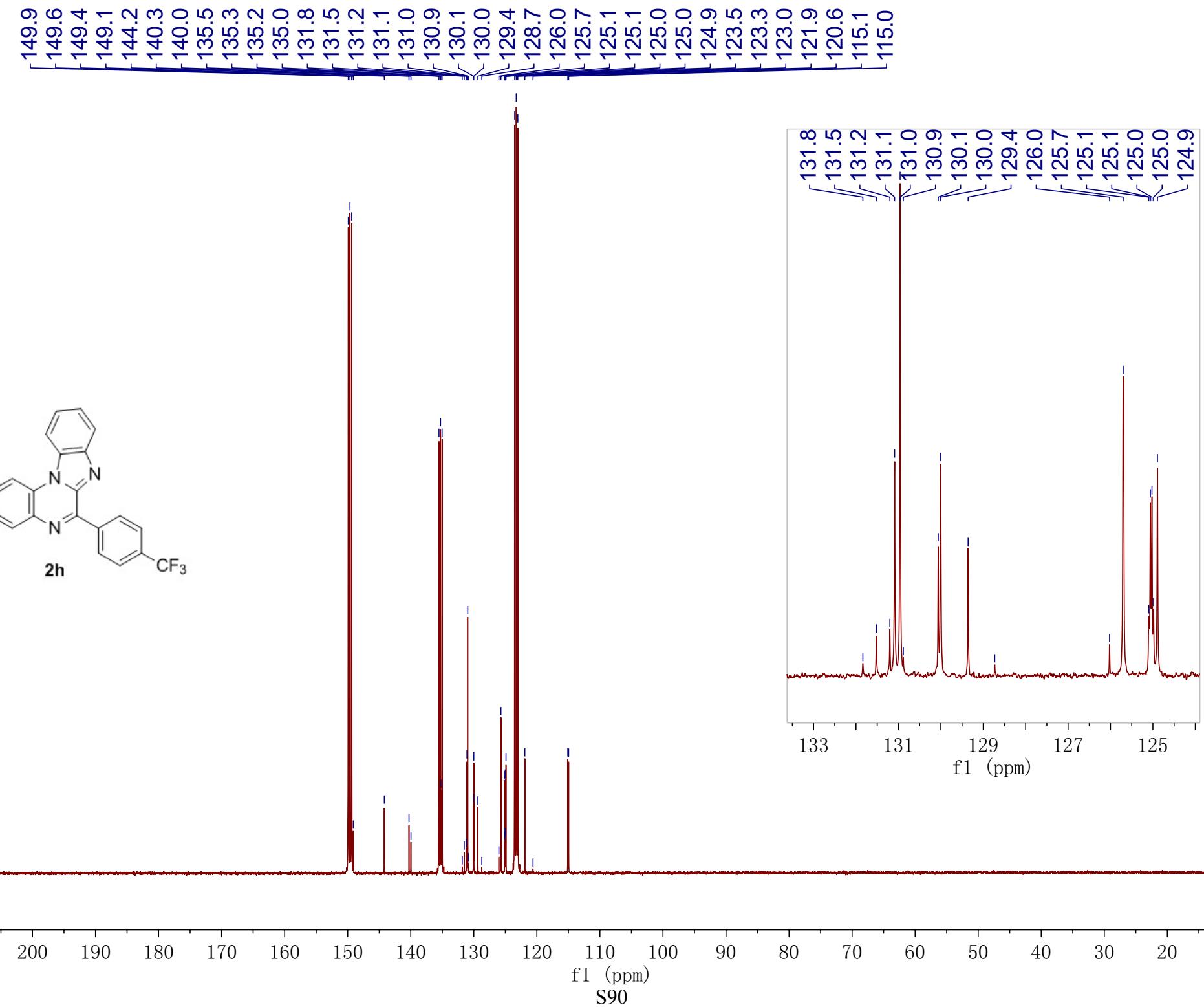
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

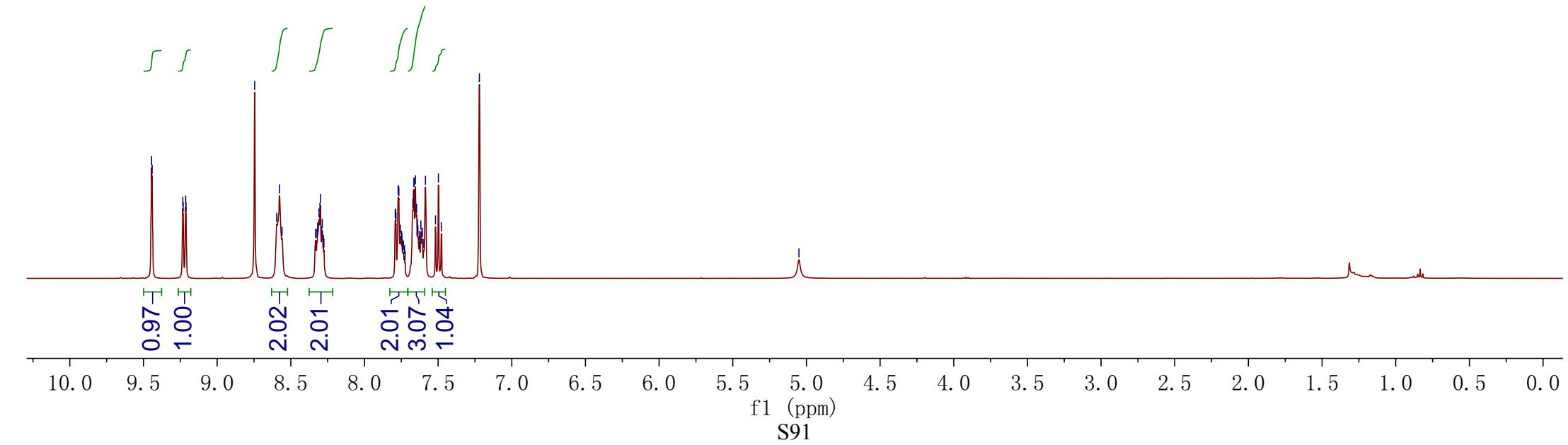
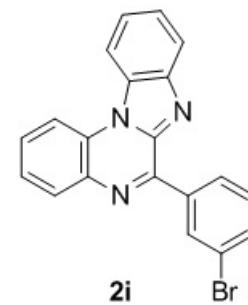
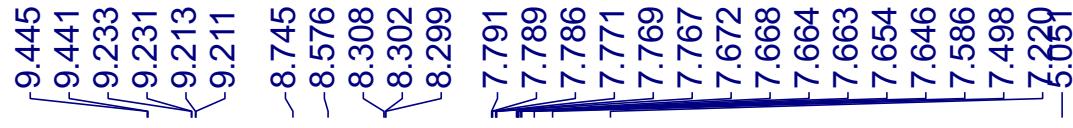
f1 (ppm)

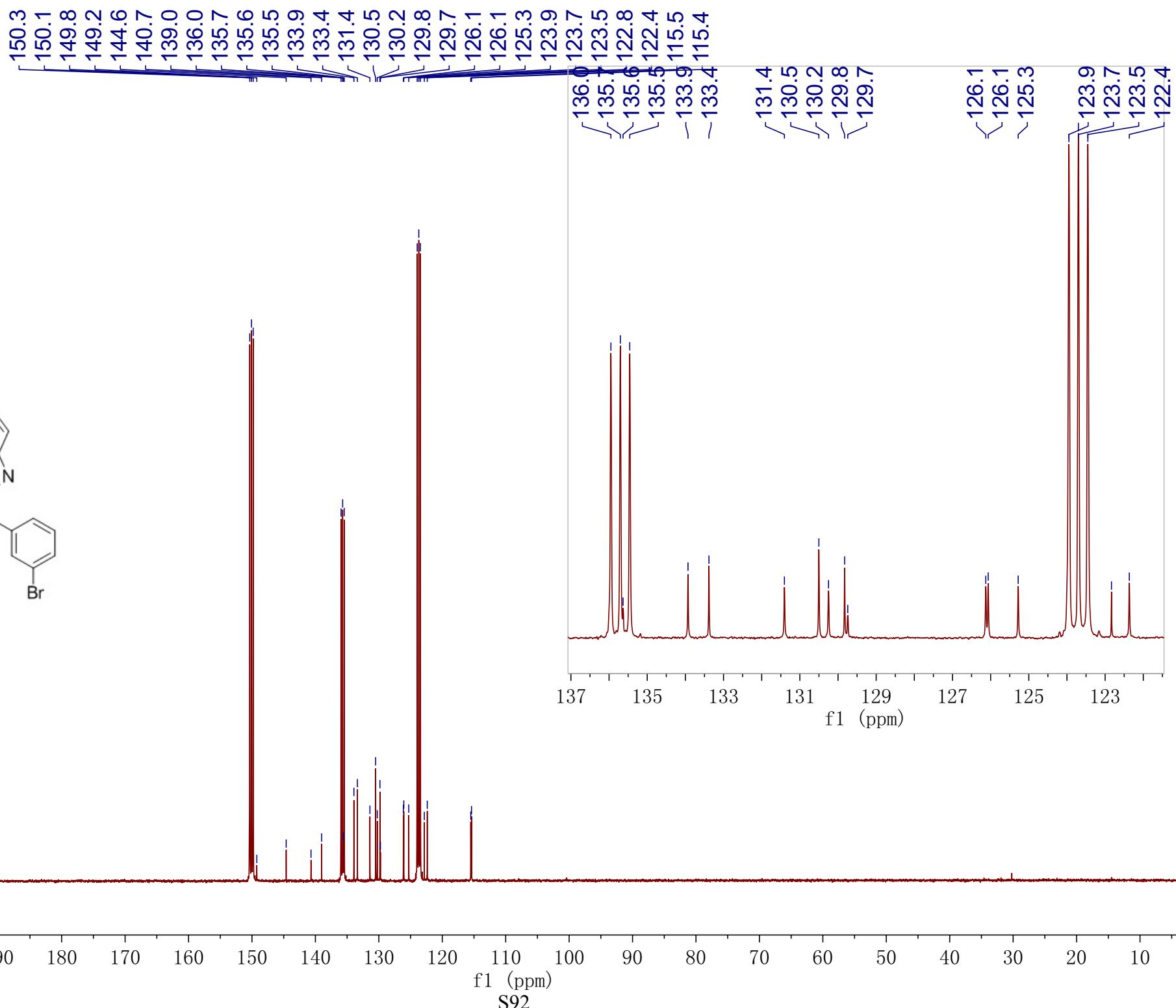
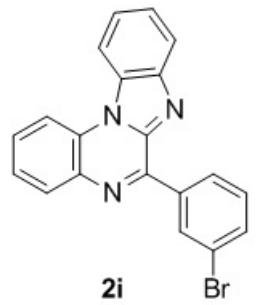
9.268
9.248
8.740
8.589
8.570
8.320
8.300
7.946
7.925
7.784
7.765
7.746
7.696
7.680
7.670
7.661
7.644
7.629
7.610
7.581
7.215

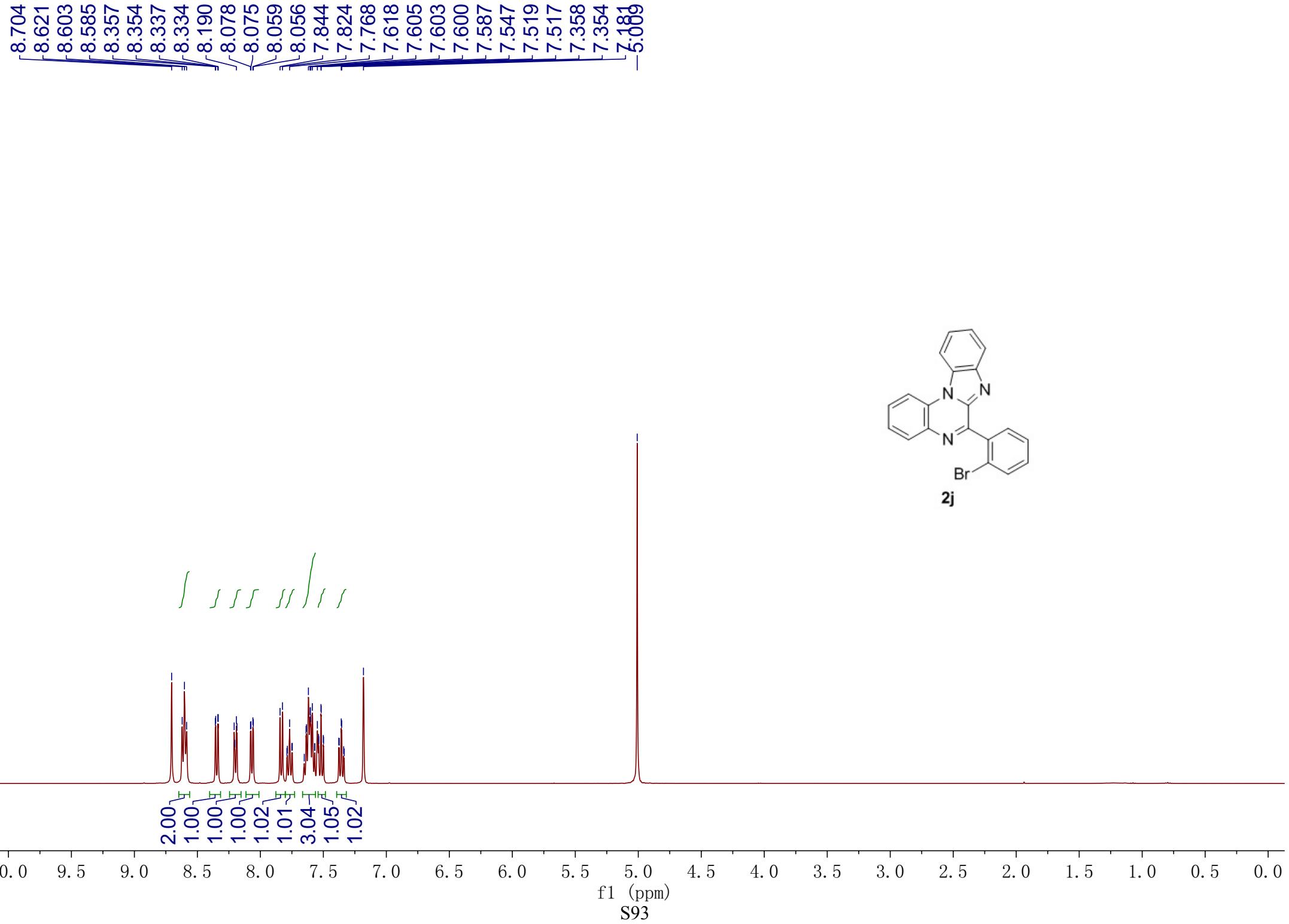
-5.058



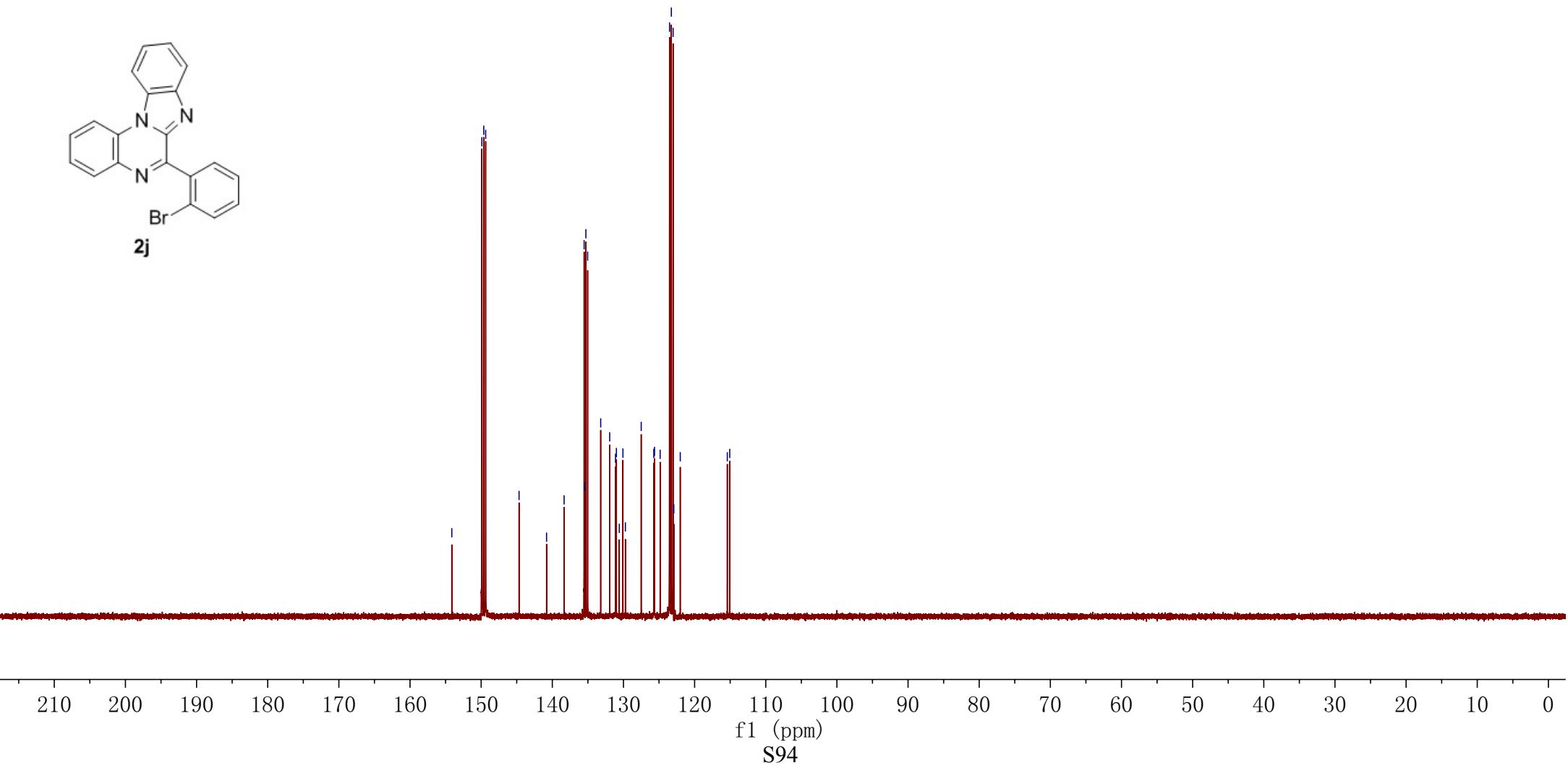
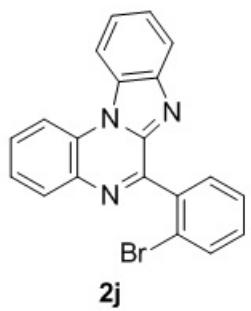


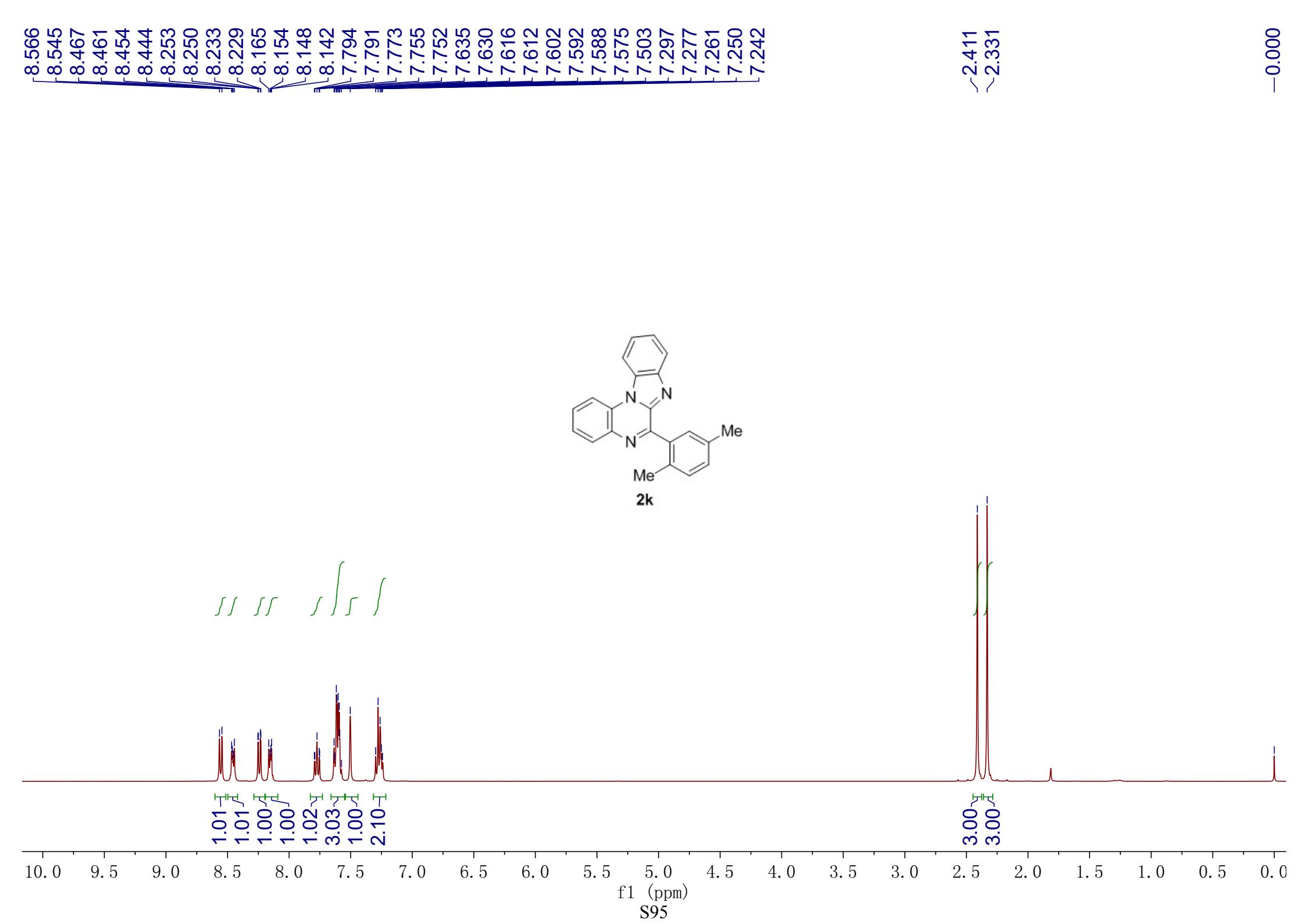


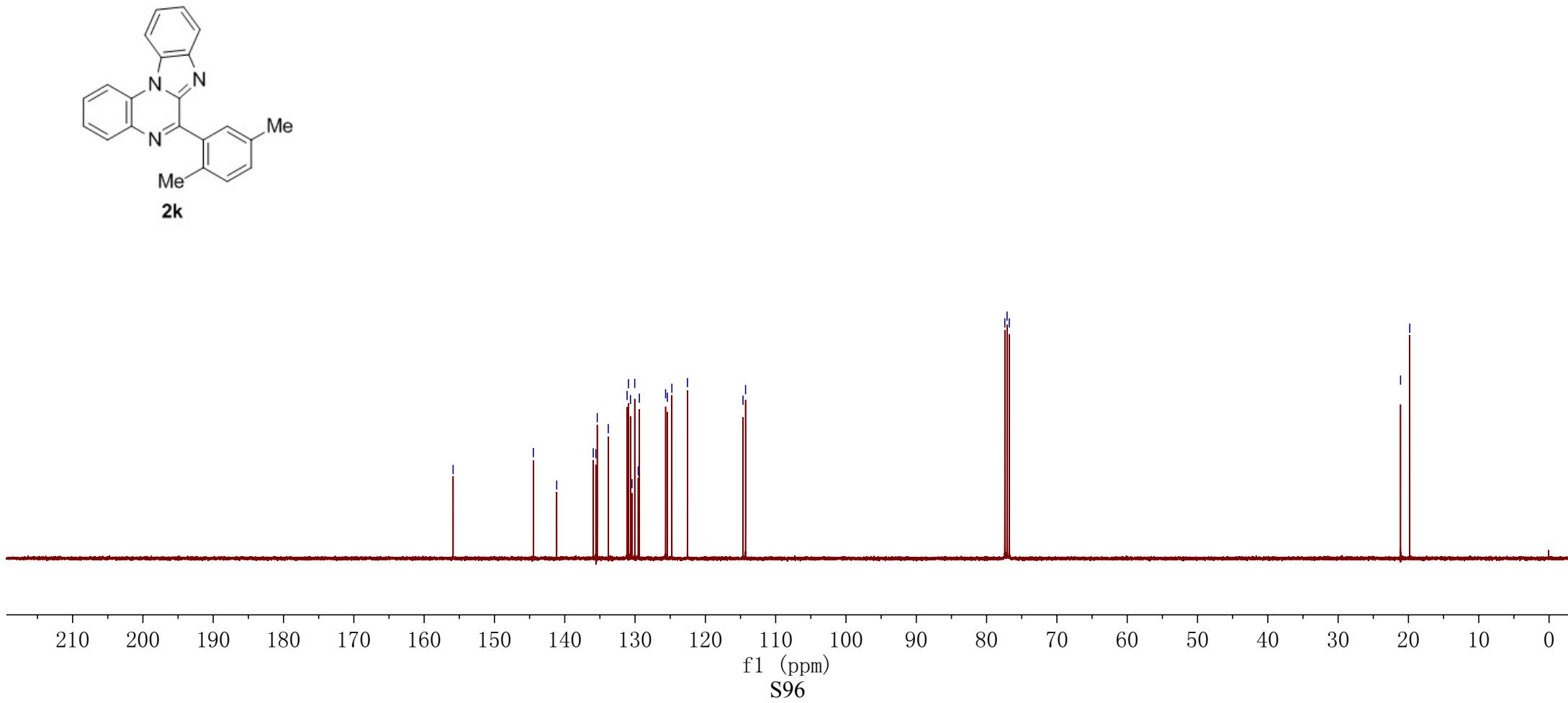
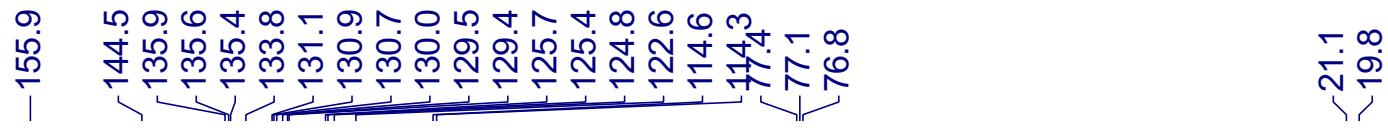
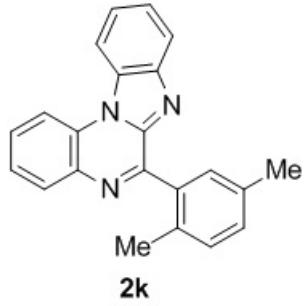




154.1
149.9
149.6
149.4
144.7
140.8
138.3
135.5
135.5
135.3
135.0
133.2
131.9
131.1
131.0
130.6
130.1
129.7
127.5
125.7
125.6
124.8
123.5
123.3
123.0
122.9
122.0
115.4
115.1



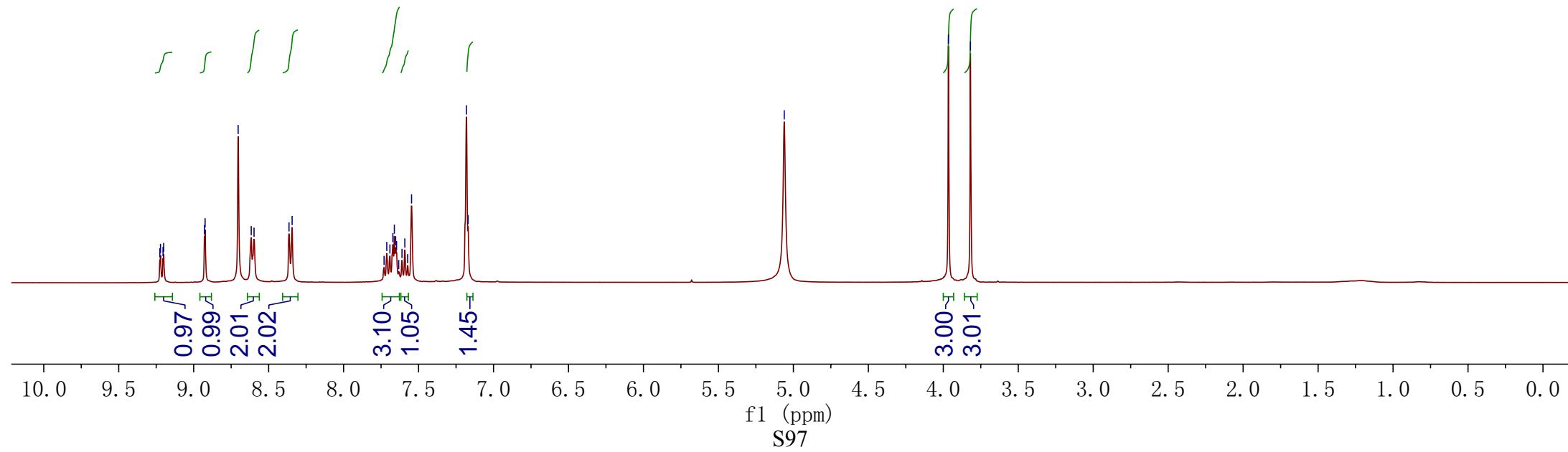
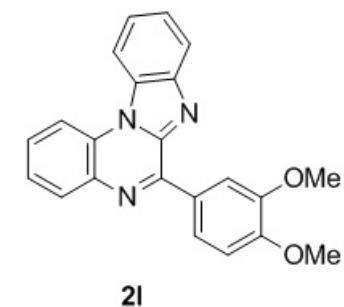


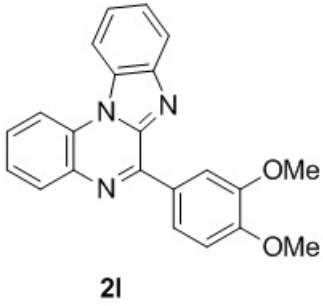


9.226
9.221
9.204
9.200
8.928
8.924
8.703
8.616
8.597
8.364
8.343
7.730
7.712
7.691
7.671
7.662
7.653
7.647
7.632
7.611
7.592
7.573
7.547
7.181
7.170

-5.061

-3.966
-3.819



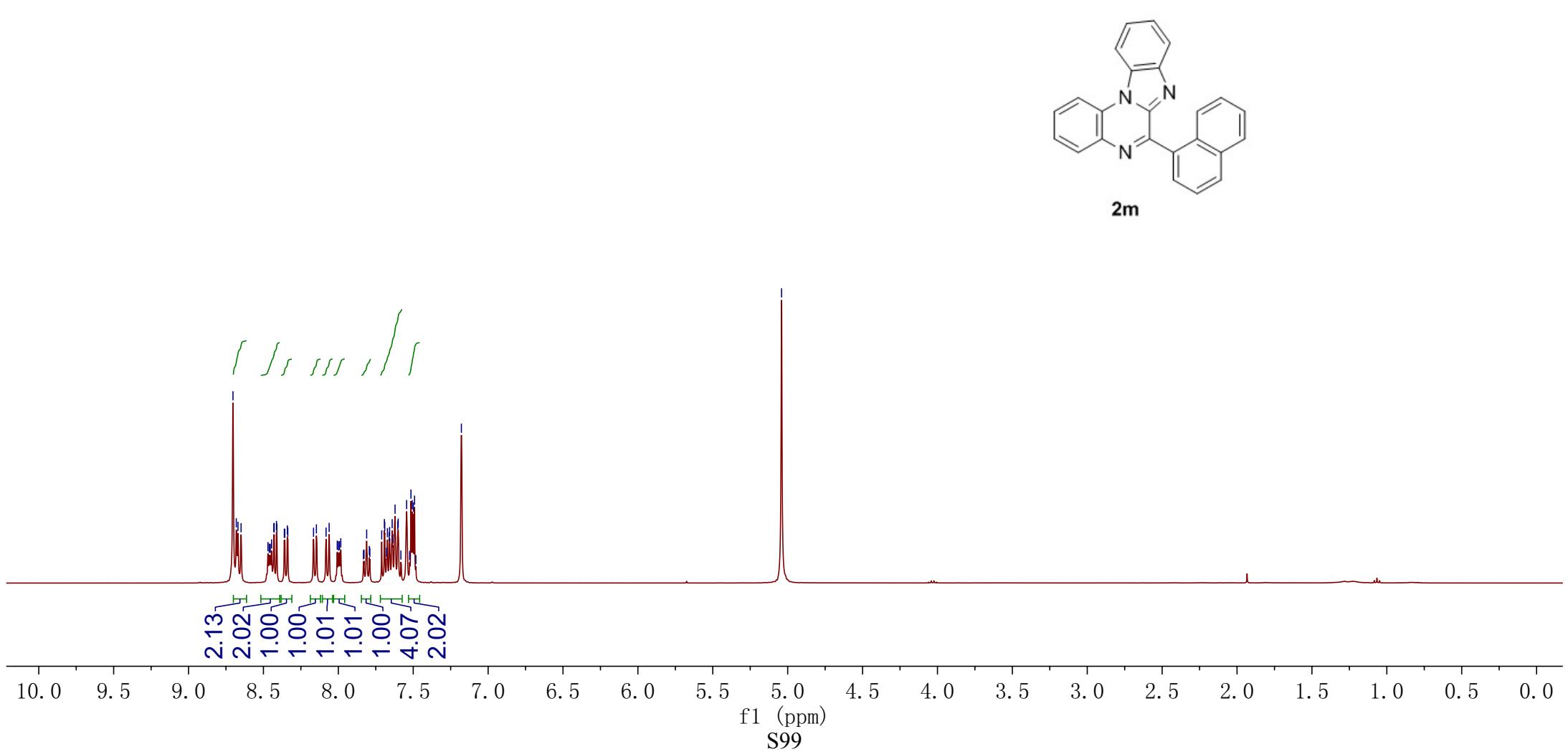
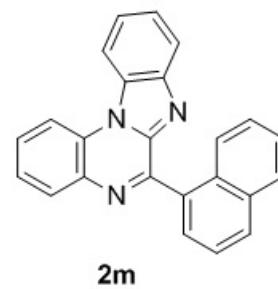


152.3
150.1
149.9
149.6
149.4
149.3
144.3
140.8
135.6
135.5
135.3
135.0
135.3
130.6
130.2
129.4
129.2
128.9
125.6
125.5
125.0
124.7
123.5
123.3
123.0
122.0
115.1
115.0
113.8
111.2

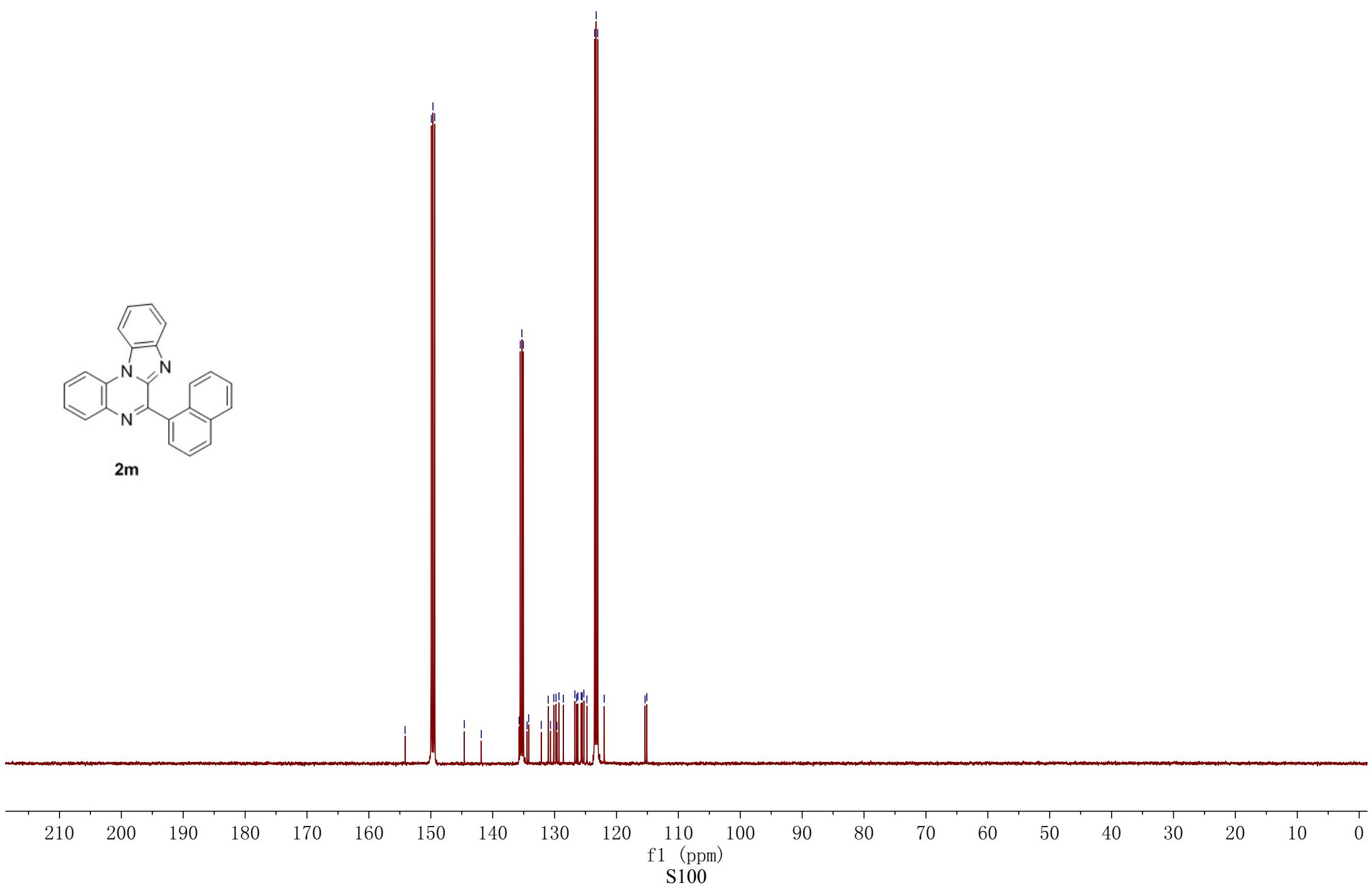
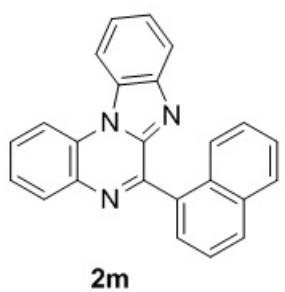
55.8
55.6

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

8.703
8.681
8.670
8.649
8.431
8.428
8.413
8.341
8.337
8.166
8.146
8.082
8.061
7.692
7.690
7.658
7.641
7.621
7.603
7.600
7.544
7.515
7.507
7.499
7.491
7.178



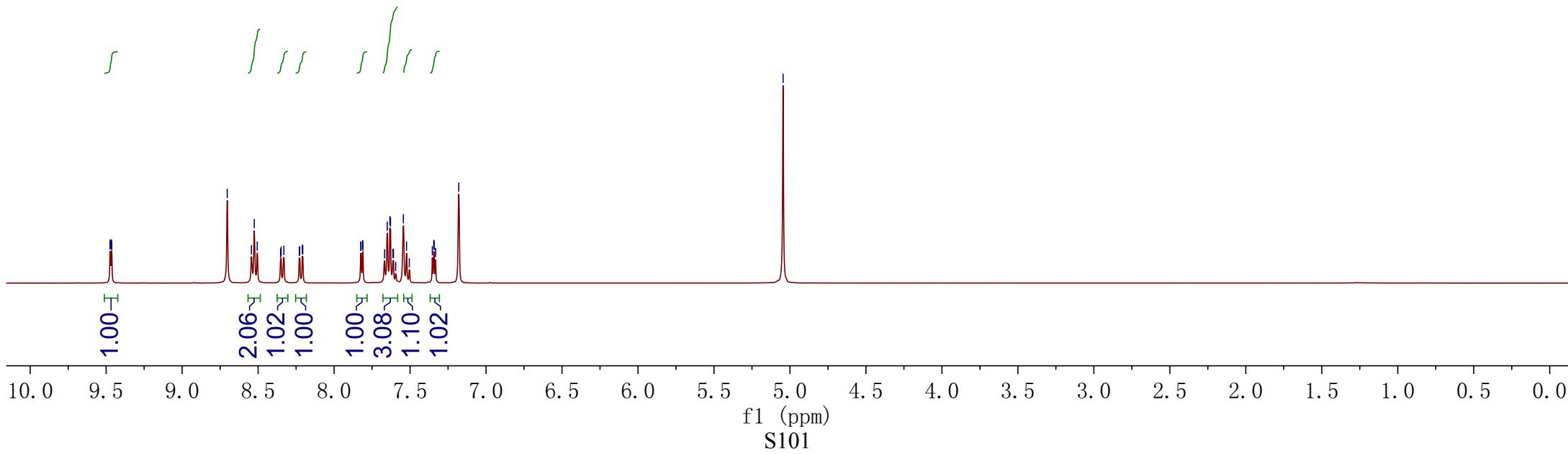
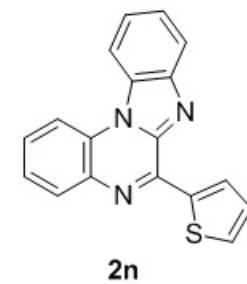
154.2
149.9
149.6
149.4
144.6
141.8
135.7
135.5
135.3
135.0
134.4
134.2
132.2
131.0
130.7
130.1
129.8
129.6
129.3
128.6
126.7
126.4
126.2
125.7
125.5
125.3
124.8
123.5
123.3
123.0
122.0
115.4
115.1



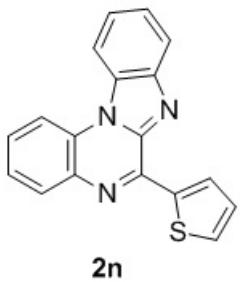
9.474
9.472
9.465
9.463

8.703
8.544
8.525
8.506
8.209

7.825
7.823
7.812
7.810
7.650
7.633
7.629
7.613
7.544
7.523
7.354
7.344
7.341
7.332
5.180
5.045



149.9
149.6
149.4
145.9
144.3
141.4
139.3
135.5
135.4
135.3
135.0
133.9
131.5
130.3
130.2
129.0
128.7
125.7
125.6
124.8
123.5
123.3
123.0
121.9
115.1
115.0

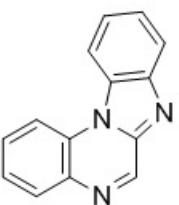


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

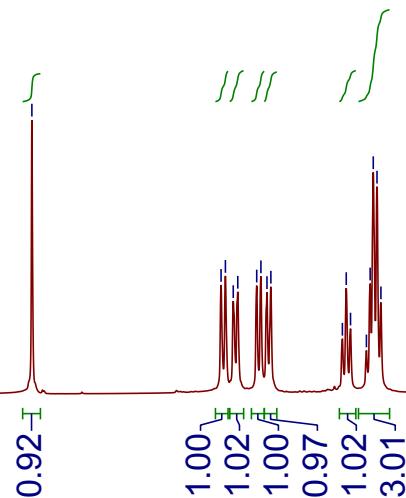
f1 (ppm)
S102

-9.118
8.215
8.194
8.156
8.135
8.044
8.024
7.995
7.977
7.635
7.617
7.596
7.520
7.503
7.488
7.470
7.451
7.295

--0.000



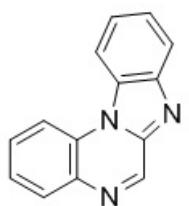
2o



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

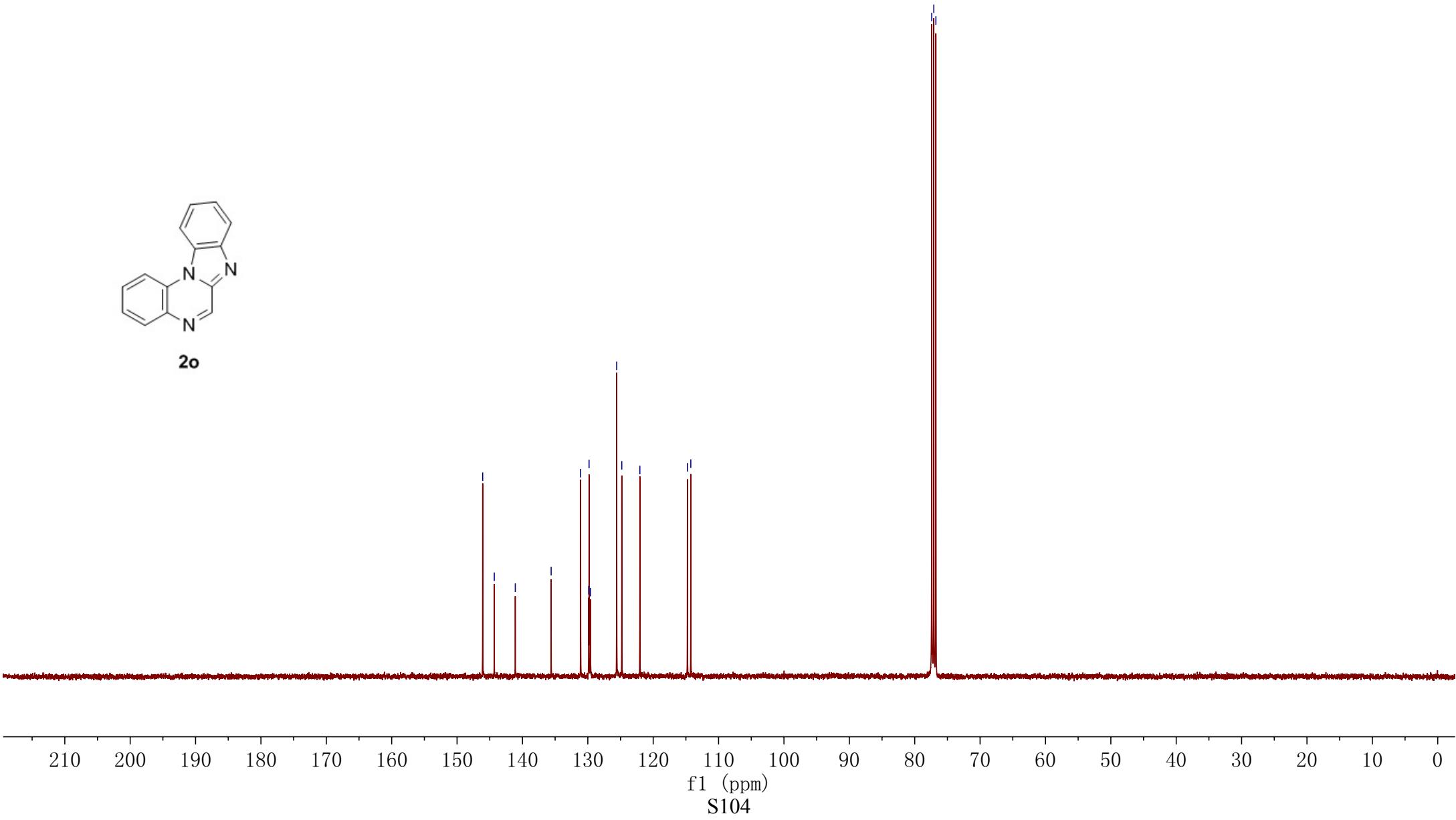
S103

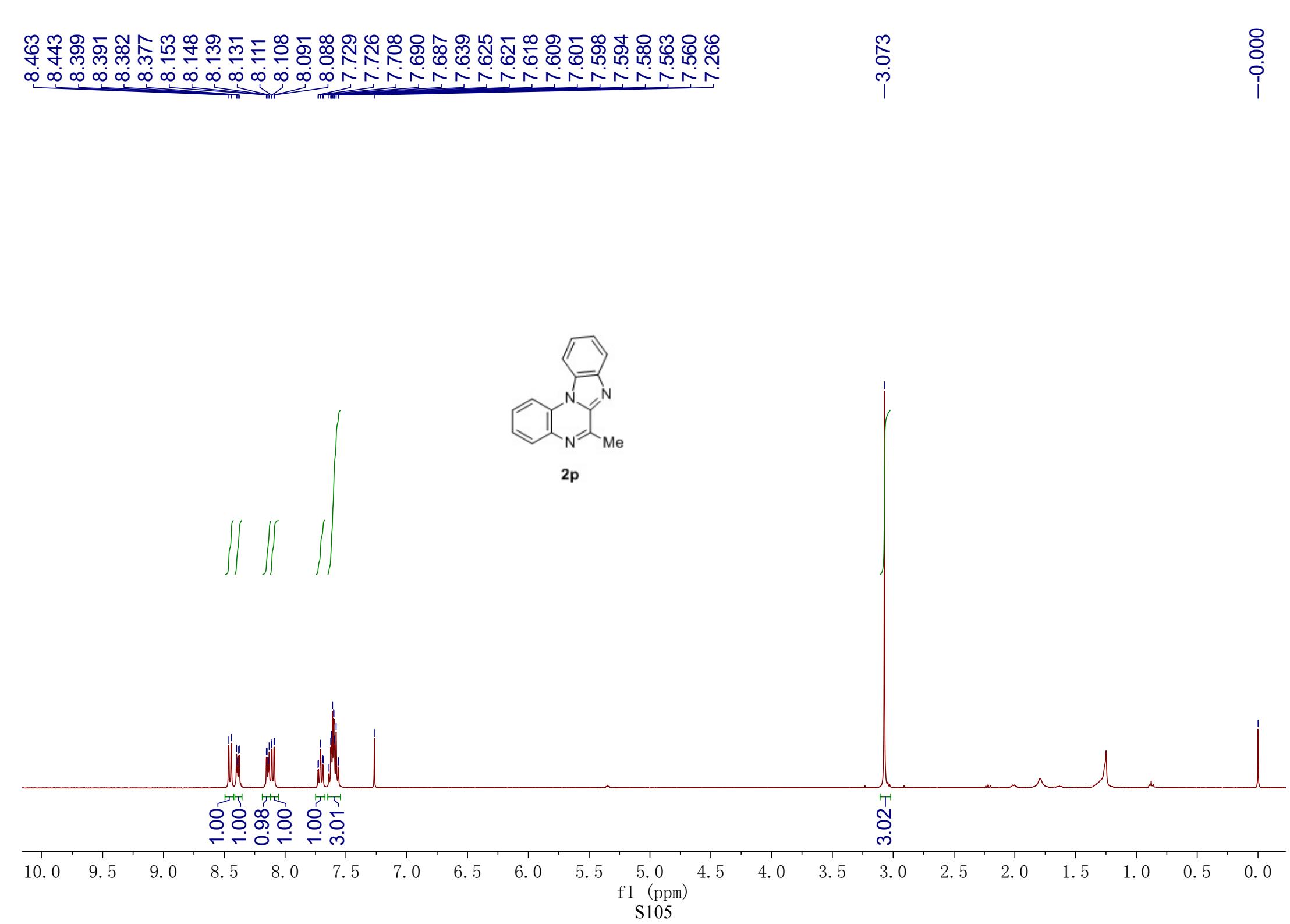


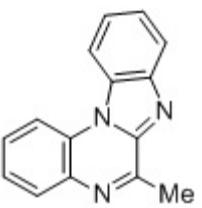
2o

146.1
144.3
141.1
135.6
131.1
129.9
129.8
129.6
125.6
124.8
122.0
114.8
114.2

77.4
77.1
76.8



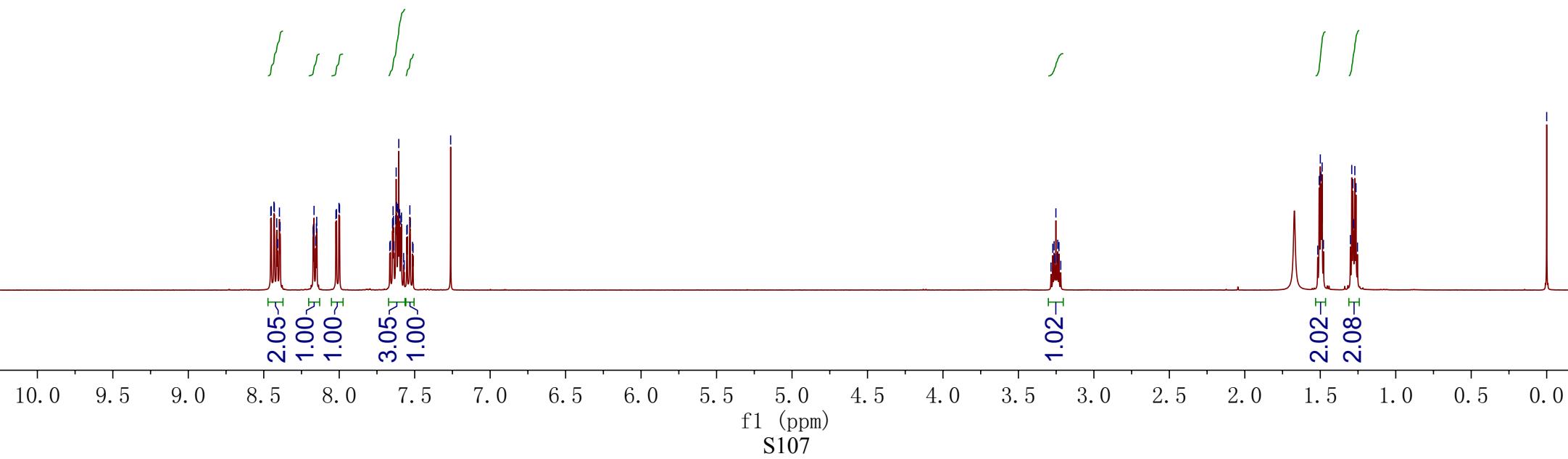
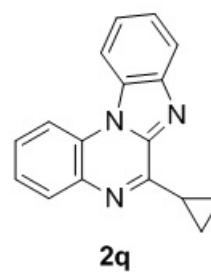


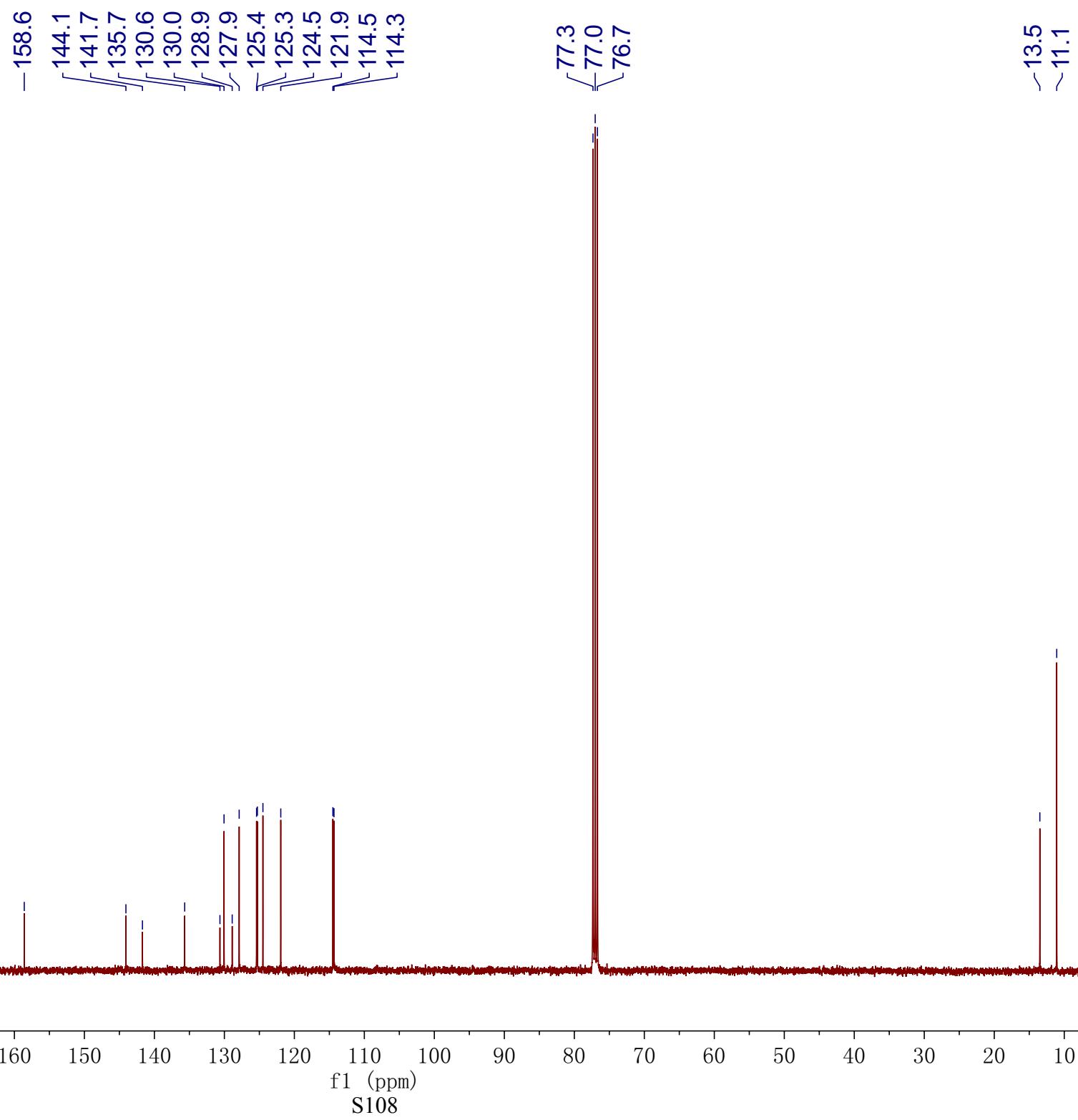
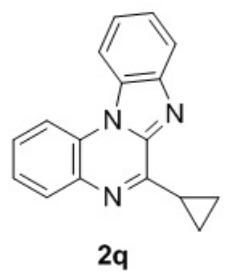


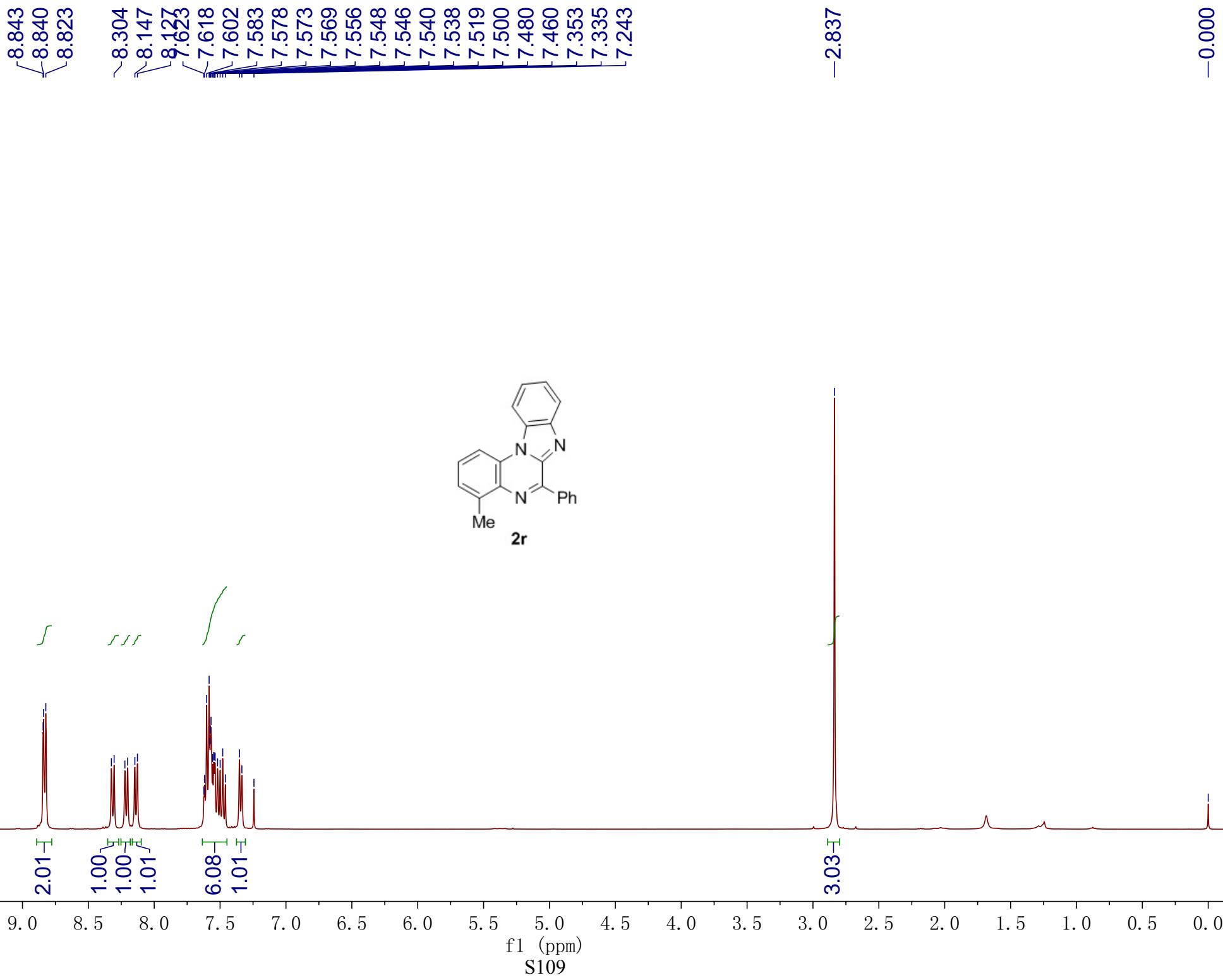
2p

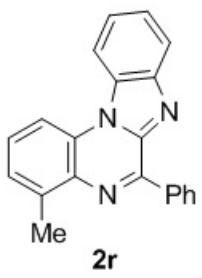


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0



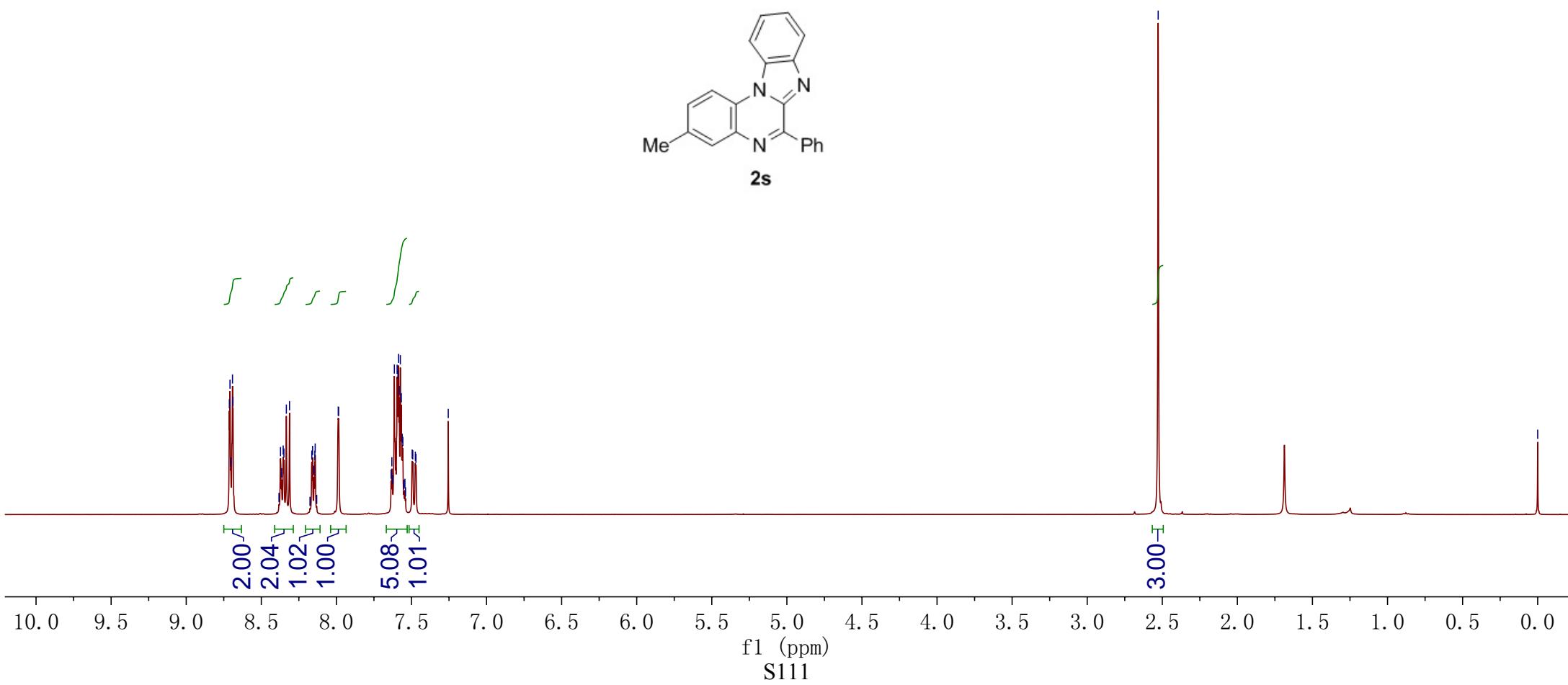
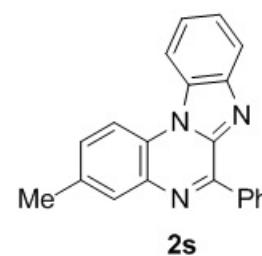
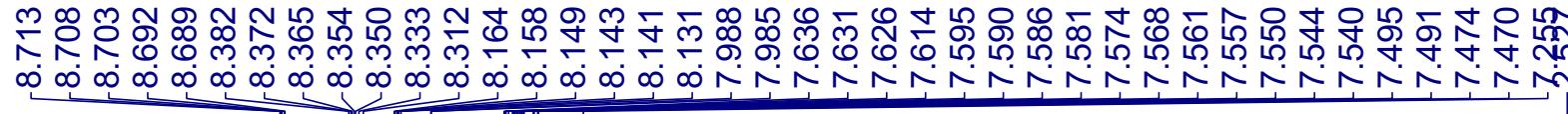


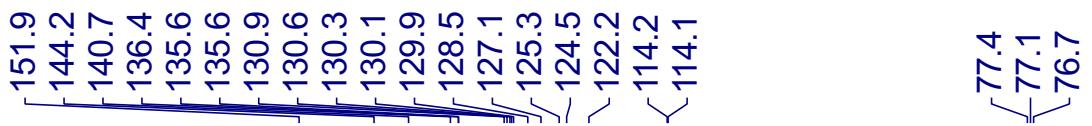
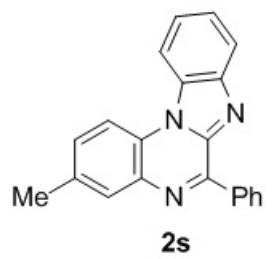




210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S110





-21.1

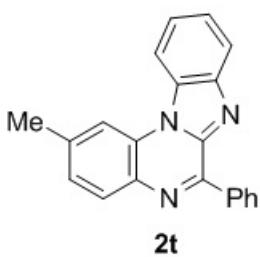
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S112

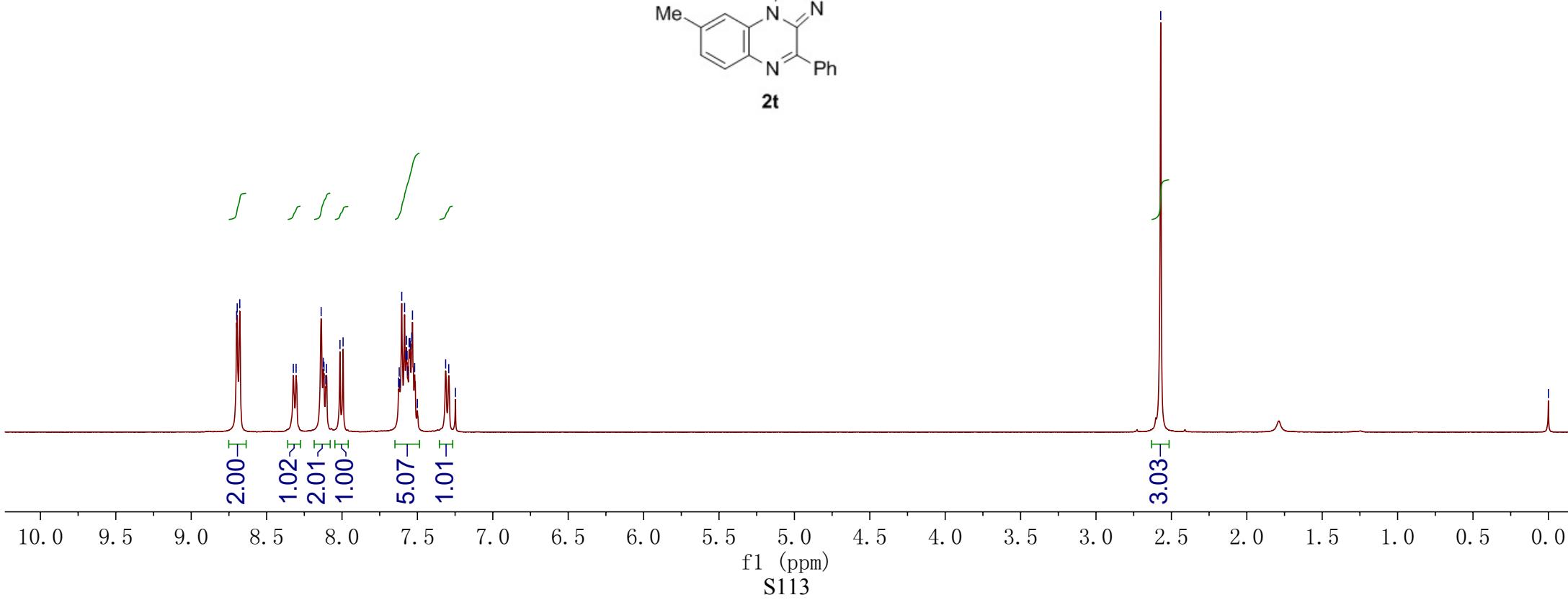
8.699
8.695
8.678
8.323
8.304
8.138
8.125
8.120
8.108
8.103
8.013
7.993
7.625
7.621
7.616
7.604
7.585
7.573
7.569
7.565
7.555
7.550
7.547
7.538
7.533
7.518
7.501
7.313
7.292
7.248

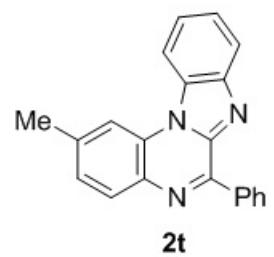
-2.571

-0.000



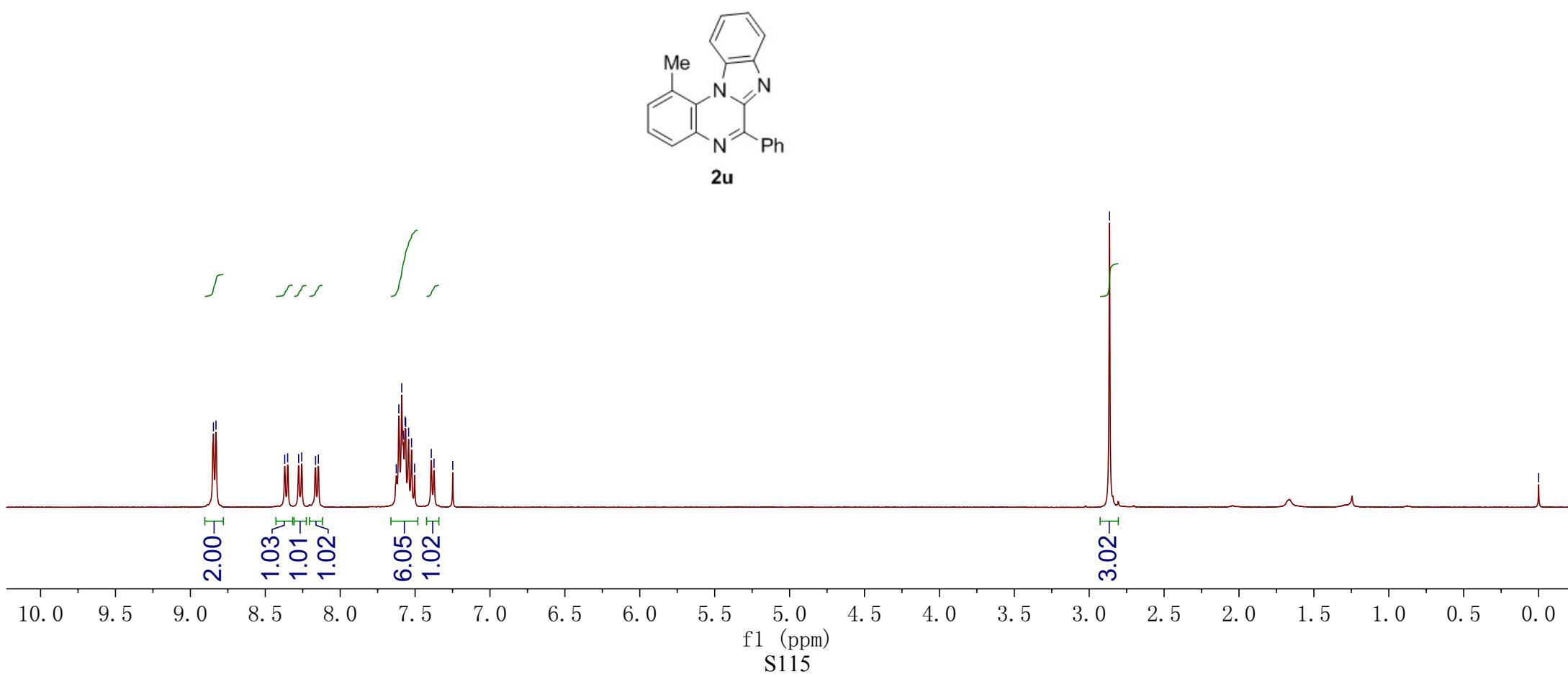
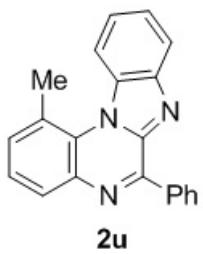
2t

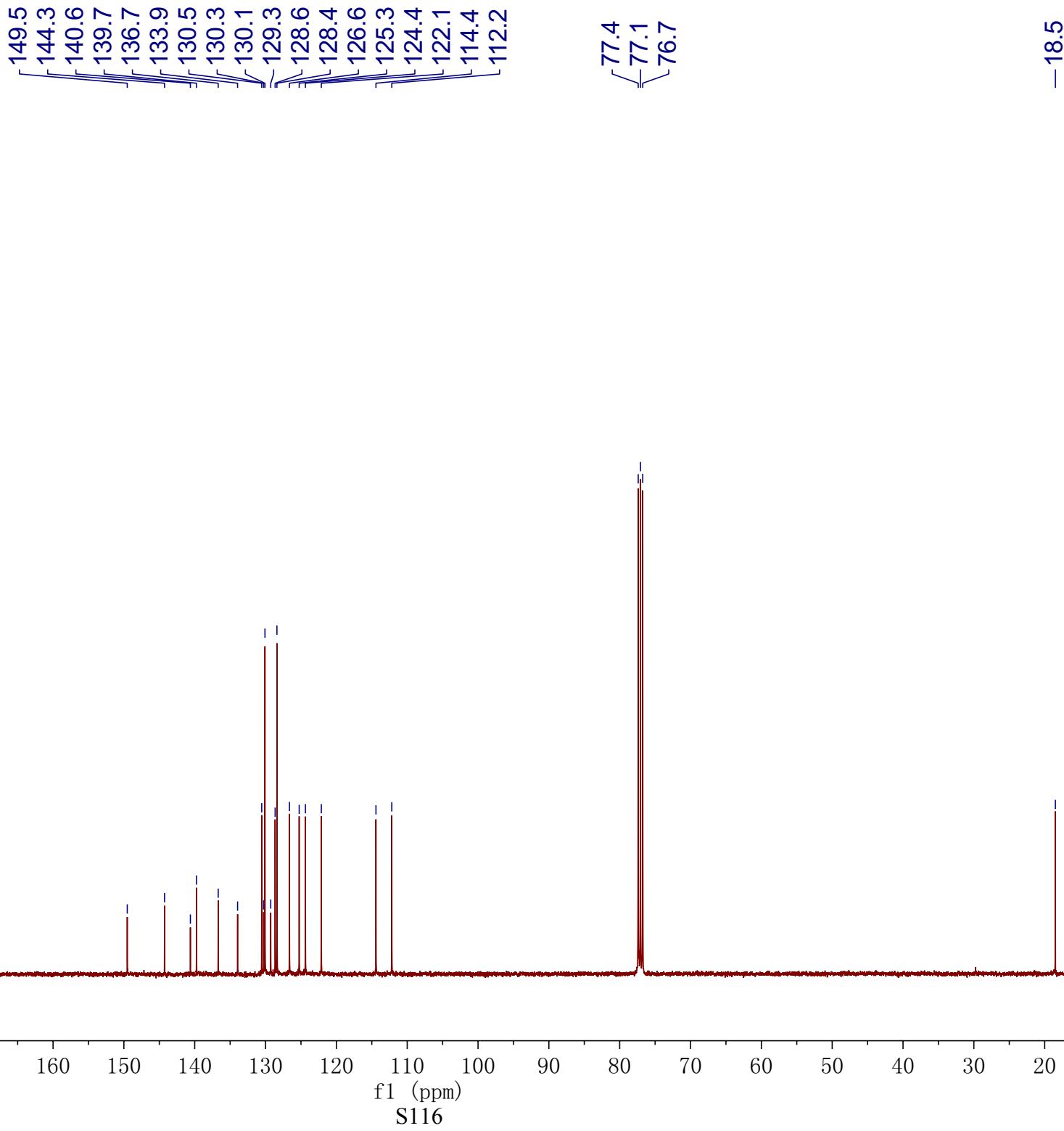
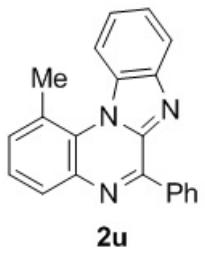




210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

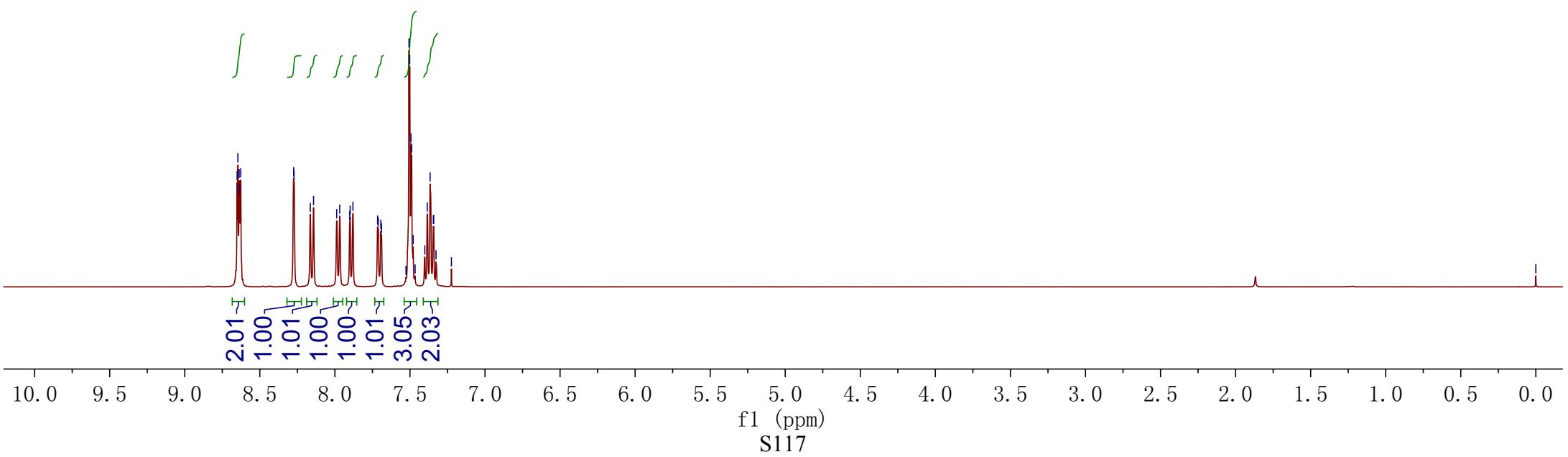
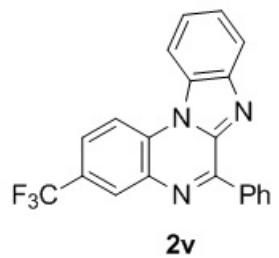
8.846
8.829
8.351
8.277
8.257
8.146
7.625
7.608
7.589
7.579
7.566
7.563
7.543
7.524
7.503
7.392
7.374
7.249
-2.864
-0.000

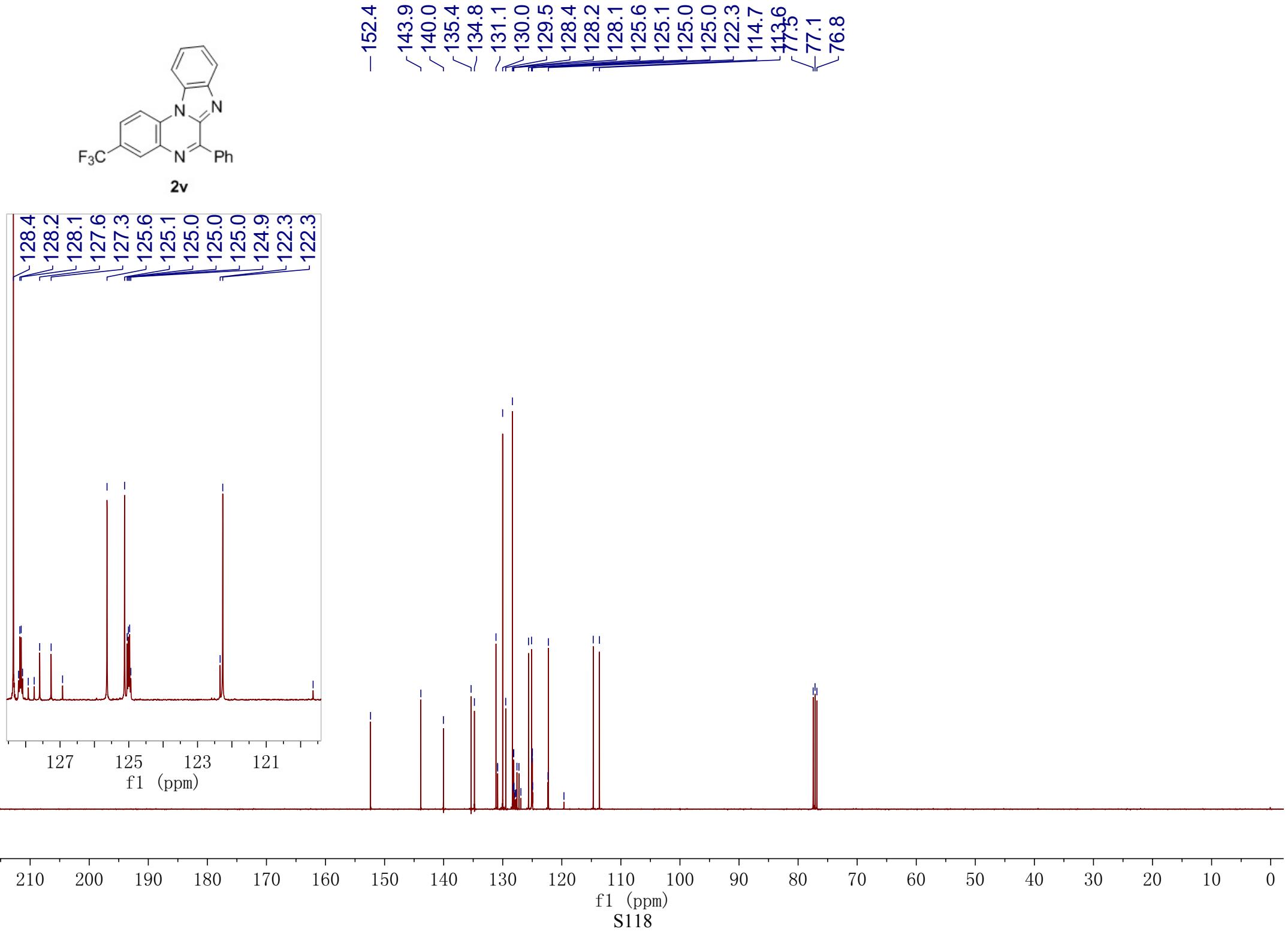
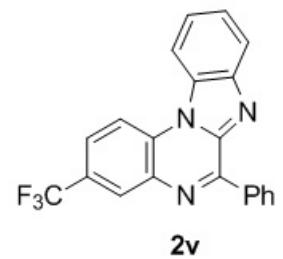


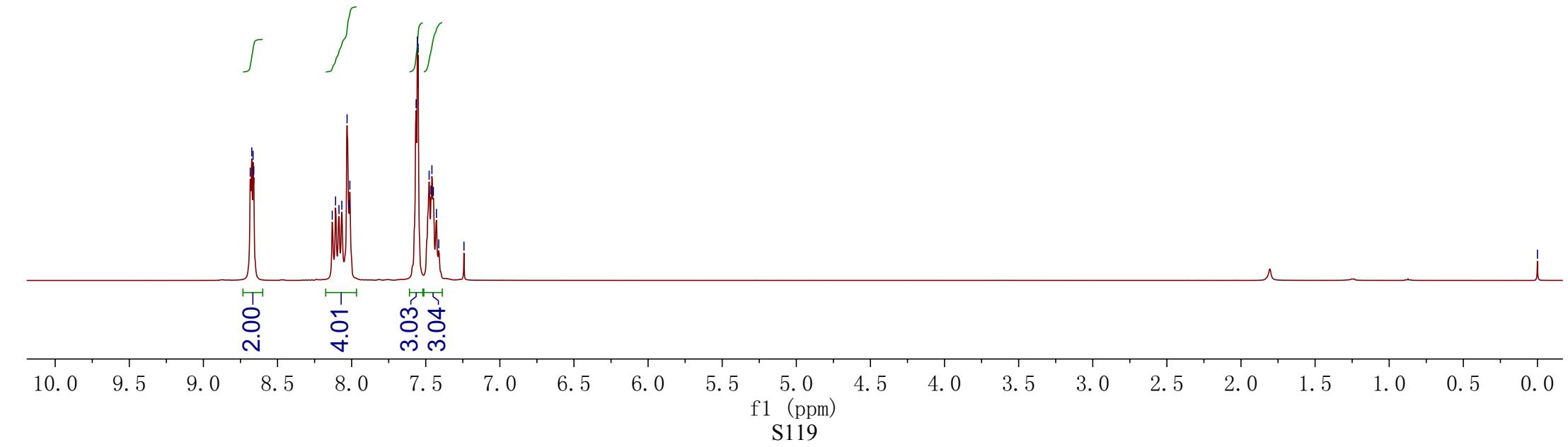
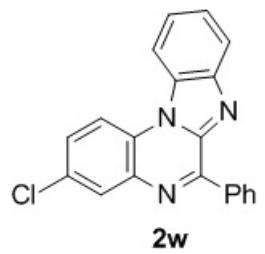


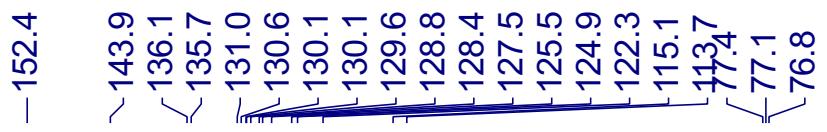
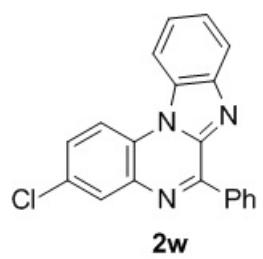
-0.000

8.651
8.646
8.638
8.627
8.622
8.275
8.272
8.164
8.142
7.988
7.968
7.901
7.898
7.880
7.716
7.711
7.694
7.690
7.526
7.506
7.502
7.493
7.489
7.479
7.466
7.401
7.385
7.366
7.344
7.342
7.326
7.224







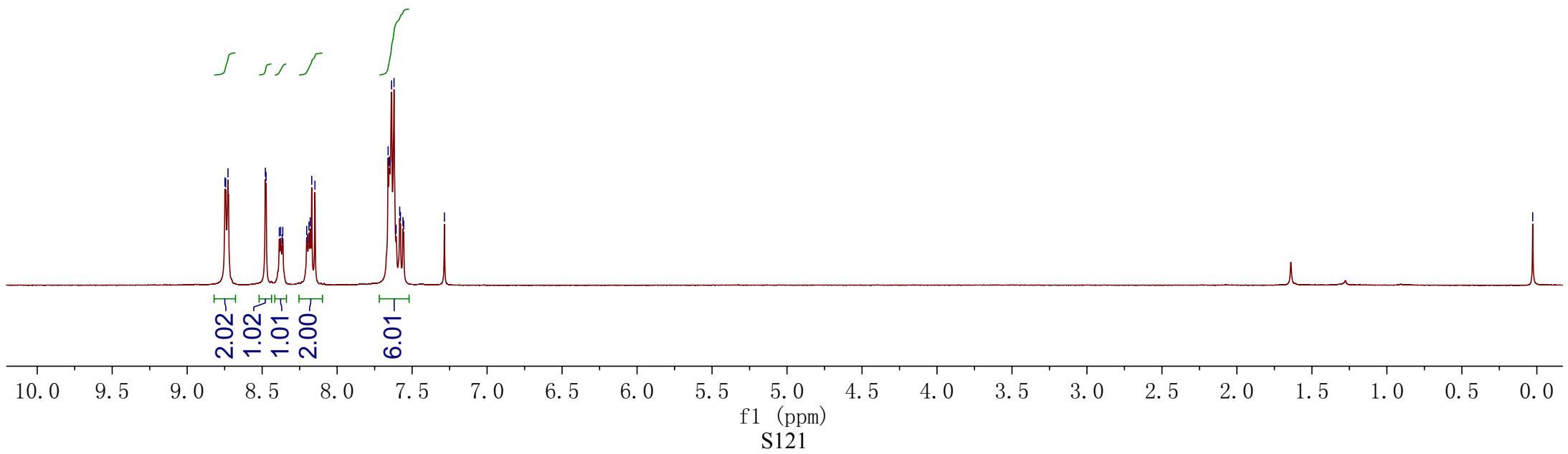
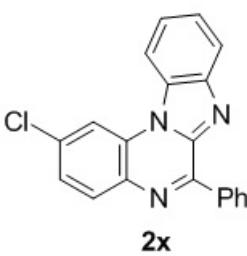


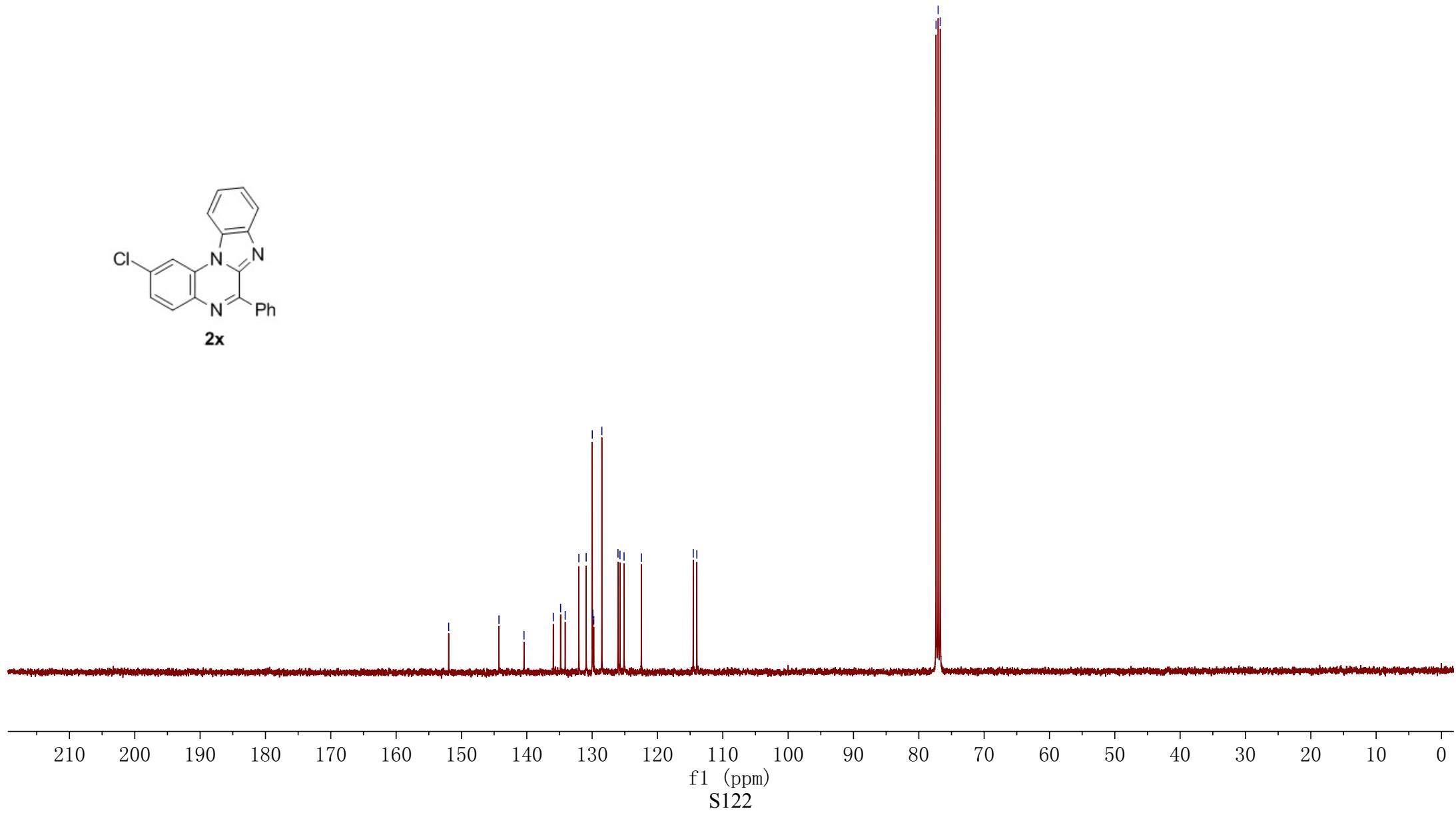
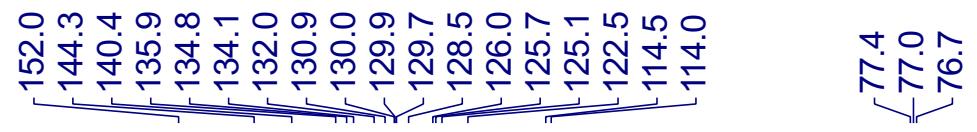
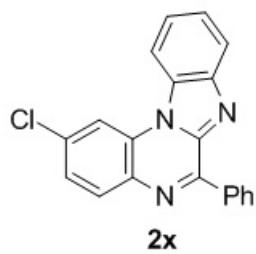
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S120

-0.028

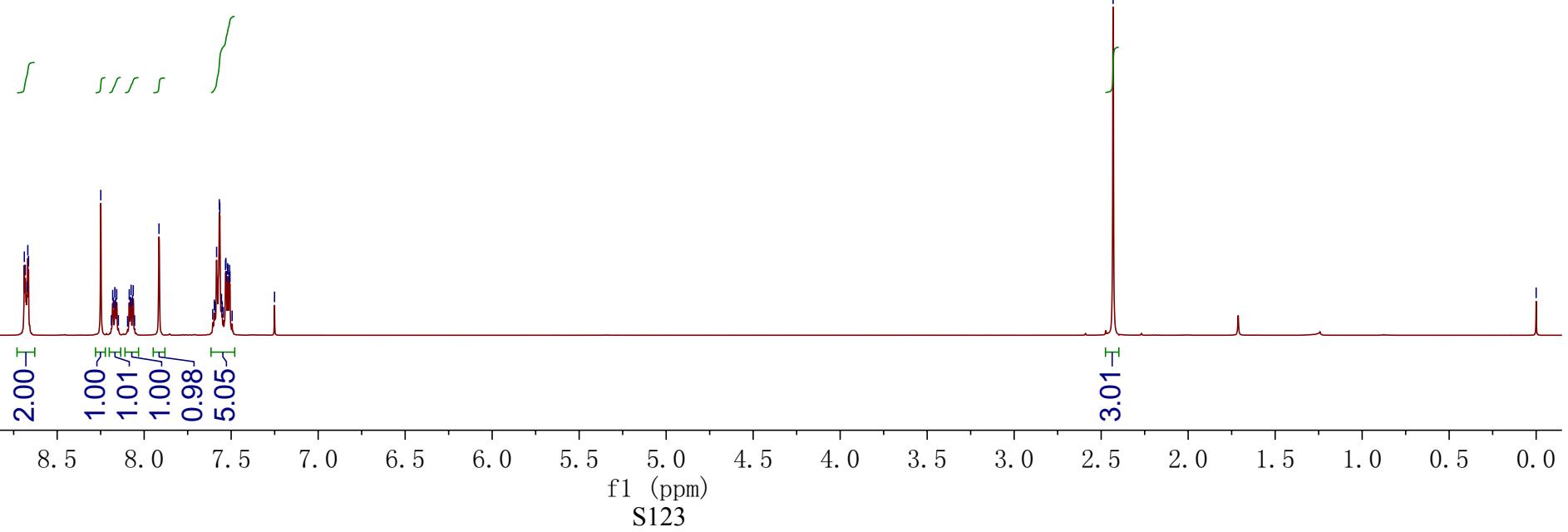
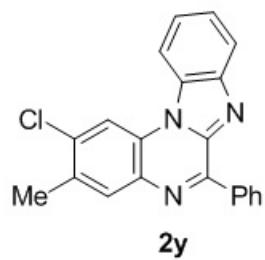
8.748
8.743
8.728
8.479
8.474
8.377
8.362
8.203
8.188
8.179
8.169
8.148
7.660
7.654
7.651
7.637
7.621
7.607
7.583
7.578
7.561
7.556
7.285

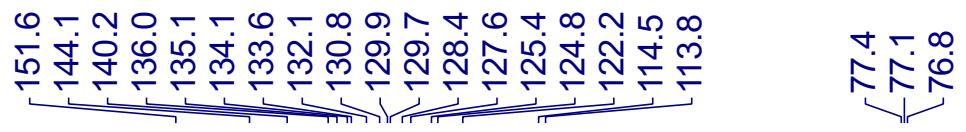
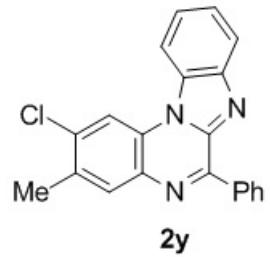




8.689
8.683
8.673
8.669
8.665

8.249
8.181
8.177
8.168
8.164
8.158
8.086
8.079
8.075
8.067
8.063
7.915
7.606
7.597
7.592
7.584
7.568
7.565
7.556
7.551
7.545
7.532
7.531
7.519
7.509
7.507
7.494
7.251
-0.000



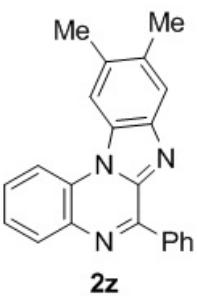
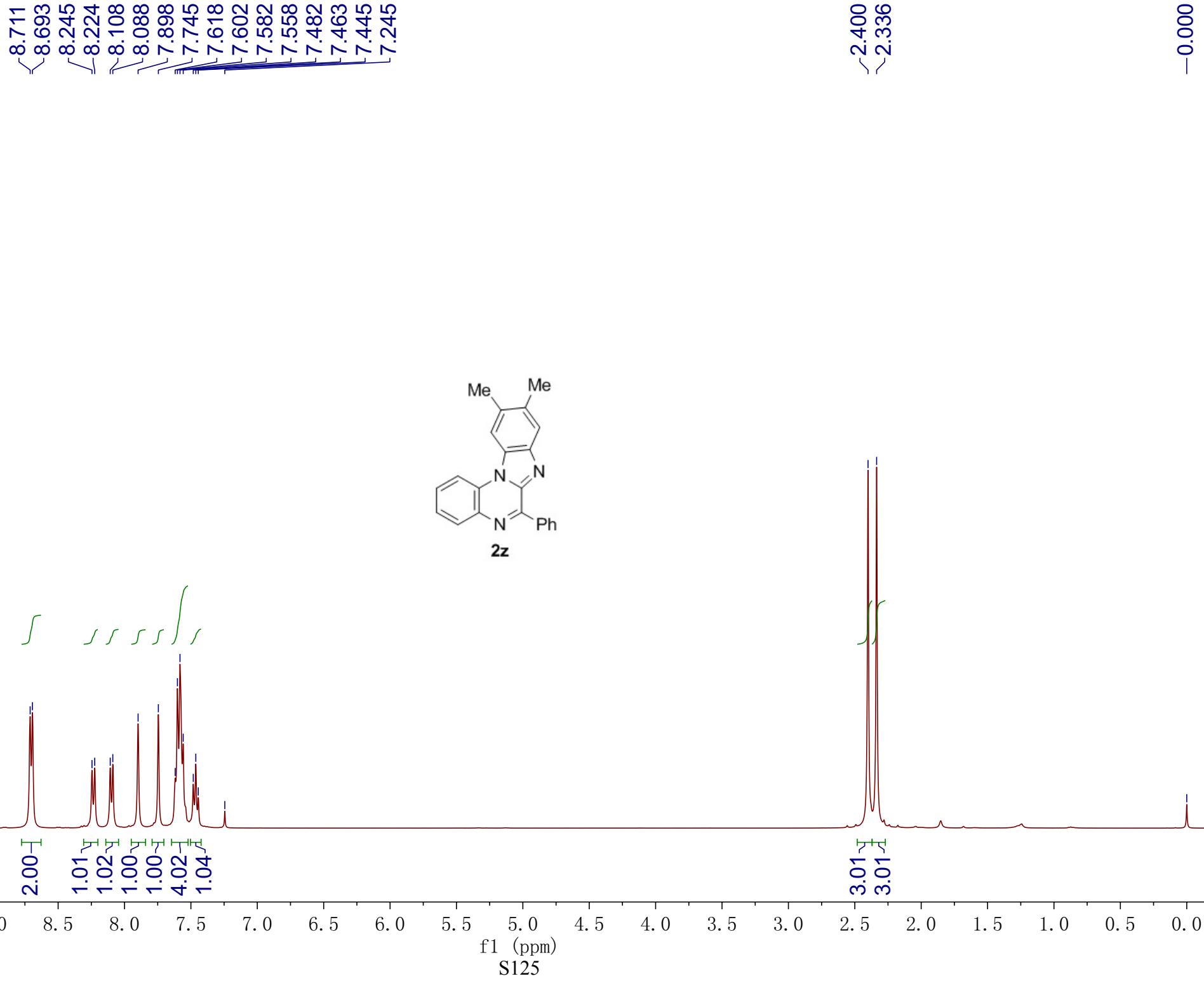


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)
S124

- 19.8

77.4
77.1
76.8



f1 (ppm)
S125

