Hypervalent Iodane Mediated Reactions of *N*-Acetyl Enamines for the Synthesis of Oxazoles and Imidazoles

Supporting Information

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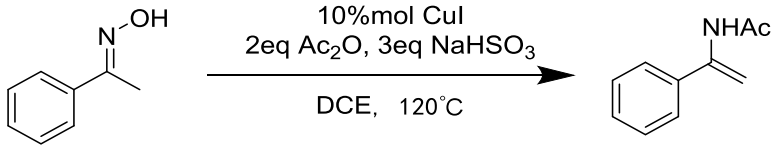
1. General

General Experimental Methods. Unless otherwise noted, all chemicals were purchased from commercial suppliers and used without further purification. All reactions were performed by standard Schlenk techniques in oven-dried reaction vessels under air. Flash column chromatography was carried out using commercially available 300−400 mesh under pressure unless otherwise indicated. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV-300 (300 MHz) or AV-400 (400 MHz) NMR spectrometers. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm). High Resolution Mass measurement was performed on an Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source. Anhydrous acetonitrile (MeCN) was distilled and stored over molecular sieves.

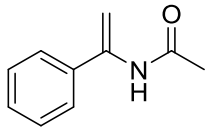
2.Preparation of Substrate 2a-2y, 4a-4j

2. 1 Typical Procedure for the Synthesis of Enamides **2a-2m.**[1]



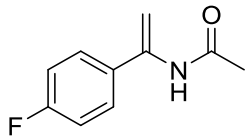
The mixture of ketoxime (0.5 mmol), acetic anhydride (1.0 mmol, 102.0 mg),$NaHSO_3$ (1.5 mmol, 156.2 mg) and CuI (10 mol%, 9.1 mg) was stirred in 1,2-dichloroethane (DCE, 5.0 mL) at 120 ℃ under Ar, After completion of the reaction (detected by TLC), the reaction mixture was cooled to room temperature, diluted with EtOAc (25 mL) and washed with NaOH (2N, 20 mL) and brine (20 mL). The organic layers were dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by flash column chromatography on silica gel (eluent: EtOAc/Pet. Ether) to afford the corresponding enamides.

N-(1-phenylvinyl)acetamide **2a**



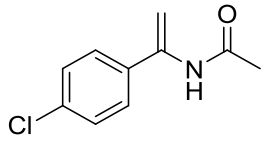
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 – 7.31 (m, 5H), 6.81 (br s, 1H),5.88 (s, 1H), 5.09 (s, 1H), 2.14 (s, 3H).

N-(1-phenylvinyl)acetamide **2b**



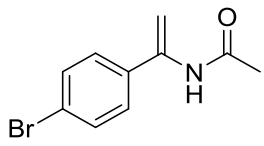
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 8.5, 5.2 Hz, 2H), 7.10 (dd, *J* = 9.8, 7.7 Hz, 2H), 6.87 (br s, 1H), 5.84 (s, 1H), 5.09 (s, 1H), 2.18 (s, 3H).

N-(1-(4-chlorophenyl)vinyl)acetamide **2c**



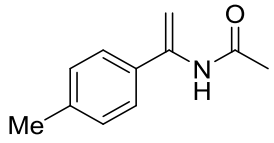
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (s, 4H), 6.99 (br s, 1H), 5.78 (s, 1H), 5.10 (s, 1H), 2.12 (s, 3H).

N-(1-(4-bromophenyl)vinyl)acetamide **2d**



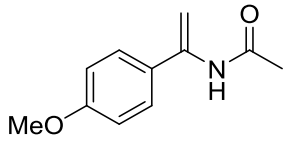
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.27 (m, 2H), 6.90 (br s, 1H), 5.84 (s, 1H), 5.14 (s, 1H), 2.17 (s, 3H).

N-(1-(4-bromophenyl)vinyl)acetamide **2e**



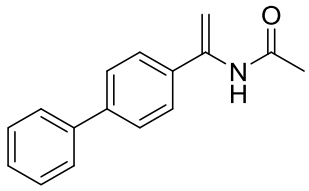
A whiye soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 6.81 ((br s, 1H), 5.88 (s, 1H), 5.10 (s, 1H), 2.41 (s, 3H), 2.18 (s, 3H).

N-(1-(4-methoxyphenyl)vinyl)acetamide **2f**



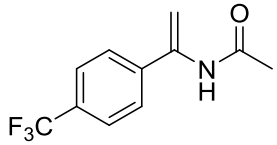
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.3 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.74 (br s, 1H), 5.78 (s, 1H), 5.02 (s, 1H), 3.83 (s, 3H), 2.14 (s, 3H).

N-(1-([1,1'-biphenyl]-4-yl)vinyl)acetamide **2g**



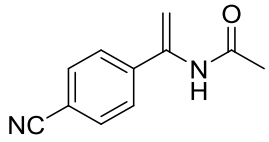
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 – 7.61 (m, 3H), 7.56 – 7.44 (m, 5H), 7.43 – 7.37 (m, 1H), 6.88 (br s, 1H), 5.91 (s, 1H), 5.19 (s, 1H), 2.19 (s, 3H).

N-(1-(4-(trifluoromethyl)phenyl)vinyl)acetamide **2h**



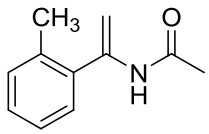
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 6.89 (br s, 1H), 5.85 (s, 1H), 5.17 (s, 1H), 2.14 (s, 3H).

N-(1-(4-cyanophenyl)vinyl)acetamide **2i**



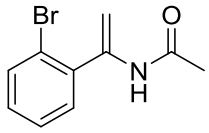
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 – 7.64 (m, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 6.96 (br s, 1H), 5.82 (s, 1H), 5.24 (s, 1H), 2.17 (s, 3H).

N-(1-(4-cyanophenyl)vinyl)acetamide **2i**



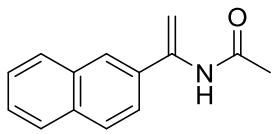
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.25 (m, 4H), 6.65 (br s, 1H), 6.11 (s, 1H), 4.75 (s, 1H), 2.40 (s, 3H), 2.10 (s, 3H).

N-(1-(2-bromophenyl)vinyl)acetamide **2k**



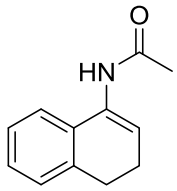
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.43 – 7.31 (m, 2H), 7.28 – 7.20 (m, 1H), 6.72 (br s, 1H), 6.03 (s, 1H), 4.84 (s, 1H), 2.10 (s, 3H).

N-(1-(naphthalen-2-yl)vinyl)acetamide **2l**



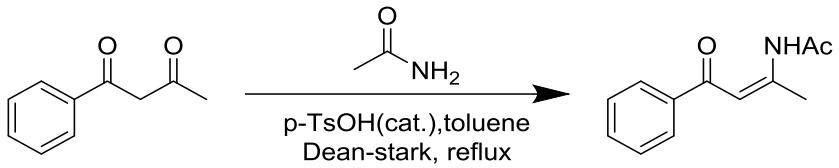
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.7 Hz, 4H), 7.62-7.49 (m, 3H), 6.96 (br s, 1H), 5.99 (s, 1H), 5.27 (s, 1H), 2.22 (s, 3H).

N-(3,4-dihydronaphthalen-1-yl)acetamide **2m**



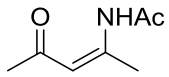
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24 – 7.16 (m, 4H), 6.79 (br s, 1H), 6.47 (t, *J* = 4.9 Hz, 1H), 2.79 (t, *J* = 7.9 Hz, 2H), 2.41 (dd, *J* = 8.1, 5.1 Hz, 2H), 2.20 (s, 3H).

2.2 Typical Procedure for the Synthesis of Enamides **2n-2y.** [2]



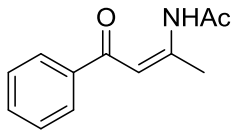
The mixture of 1,3-diketones (50 mmol), acetamide (250 mmol), and p-TsOH (10 mmol) was stirred in toluenen (150 mL) in a Dean-Stark apparatus for 24h. The reaction mixture was then cooled to room temperature, the solvent was evaporated, and the residue was purified by flash column chromatography on silica gel (eluent: EtOAc/Pet. Ether) to afford the corresponding β-ketoenamides.

(*Z*)-*N*-(4-oxopent-2-en-2-yl)acetamide **2n**



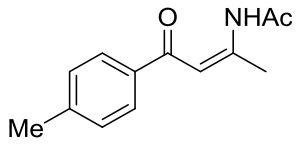
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.33 (s, 1H), 5.33 (s, 1H), 2.38 (s, 3H), 2.16 (s, 3H), 2.15 (s, 3H).

(*Z*)-*N*-(4-oxo-4-phenylbut-2-en-2-yl)acetamide **2o**



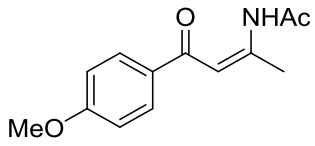
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.83 (br s, 1H), 8.07 – 7.79 (m, 2H), 7.74 – 7.37 (m, 3H), 6.06 (s, 1H), 2.54 (s, 3H), 2.25 (s, 3H).

(*Z*)-*N*-(4-oxo-4-(p-tolyl)but-2-en-2-yl)acetamide **2p**



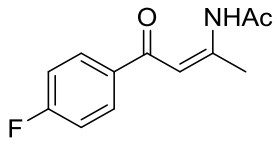
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.85 (br s, 1H), 8.01 – 7.69 (m, 2H), 7.41 – 7.17 (m, 2H), 6.05 (q, *J* = 1.0 Hz, 1H), 2.53 (s, 3H), 2.44 (s, 3H), 2.24 (s, 3H).

(*Z*)-*N*-(4-(4-methoxyphenyl)-4-oxobut-2-en-2-yl)acetamide **2q**



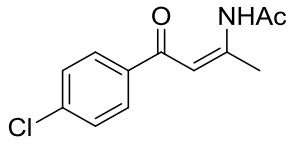
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.86 (br s, 1H), 8.04 – 7.81 (m, 2H), 7.09 – 6.88 (m, 2H), 6.03 (q, *J* = 1.0 Hz, 1H), 3.90 (s, 3H), 2.53 (s, 3H), 2.24 (s, 3H)..

(*Z*)-*N*-(4-(4-fluorophenyl)-4-oxobut-2-en-2-yl)acetamide **2r**



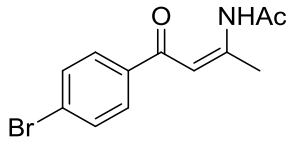
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.78 (br s, 1H), 8.06 – 7.89 (m, 2H), 7.23 – 7.03 (m, 2H), 6.01 (q, *J* = 1.0 Hz, 1H), 2.54 (s, 3H), 2.25 (s, 3H).

(*Z*)-*N*-(4-(4-chlorophenyl)-4-oxobut-2-en-2-yl)acetamide **2s**



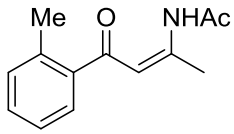
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.78 (br s, 1H), 8.00 – 7.74 (m, 2H), 7.63 – 7.40 (m, 2H), 6.01 (d, *J* = 2.0 Hz, 1H), 2.54 (s, 3H), 2.25 (s, 3H).

(*Z*)-*N*-(4-(4-bromophenyl)-4-oxobut-2-en-2-yl)acetamide **2t**



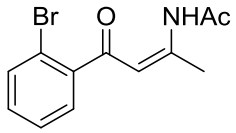
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.78 (br s, 1H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.69 – 7.49 (m, 2H), 6.00 (s, 1H), 2.54 (s, 3H), 2.25 (s, 3H).

(*Z*)-*N*-(4-oxo-4-(o-tolyl)but-2-en-2-yl)acetamide **2u**



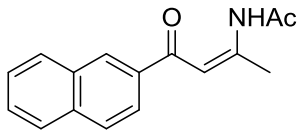
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.68 (br s, 1H), 7.47 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.35 (td, *J* = 7.4, 1.5 Hz, 1H), 7.25 (tdd, *J* = 5.6, 3.1, 1.2 Hz, 2H), 5.73 (q, *J* = 1.0 Hz, 1H), 2.54 – 2.43 (m, 6H), 2.26 (s, 3H)

(*Z*)-*N*-(4-(2-bromophenyl)-4-oxobut-2-en-2-yl)acetamide **2v**



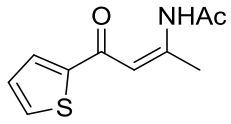
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.49 (br s, 1H), 7.63 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.46 – 7.35 (m, 2H), 7.35 – 7.29 (m, 1H), 5.71 (d, *J* = 1.1 Hz, 1H), 2.51 (s, 3H), 2.27 (s, 3H).

(*Z*)-*N*-(4-(naphthalen-2-yl)-4-oxobut-2-en-2-yl)acetamide **2w**



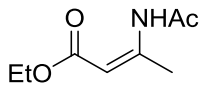
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.92 (br s, 1H), 8.45 (s, 1H), 8.01 (td, *J* = 8.3, 1.8 Hz, 2H), 7.97 – 7.88 (m, 2H), 7.66 – 7.54 (m, 2H), 6.24 (d, *J* = 1.1 Hz, 1H), 2.59 (s, 3H), 2.28 (s, 3H).

(*Z*)-*N*-(4-oxo-4-(thiophen-2-yl)but-2-en-2-yl)acetamide **2x**



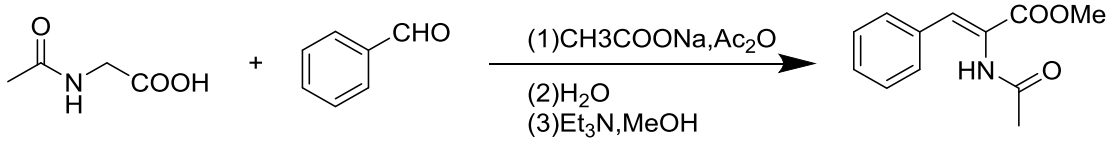
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 12.65 (br s, 1H), 7.77 (d, *J* = 3.8 Hz, 1H), 7.74 – 7.66 (m, 1H), 7.22 (t, *J* = 4.4 Hz, 1H), 5.98 (s, 1H), 2.59 (s, 3H), 2.29 (s, 3H).

Ethyl (*Z*)-3-acetamidobut-2-enoate **2y**



A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.13 (br s, 1H), 4.89 (q, *J* = 1.1 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 2.38 (s, 3H), 2.14 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H).

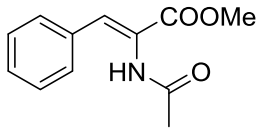
2.3 Typical Procedure for the Synthesis of Enamides **4a-4j .**[3]



To a suspension of N-acylglycine (50 mmol), sodium acetate (50 mmol), and acetic anhydride (30 mL) was added the aromatic aldehyde (50 mmol). The reaction mixture was stirred at room temperature for 1 h and then heated to 80 ℃. After 12 h, the reaction mixture was cooled down to room temperature, mixed with water (0.5 L) and stirred at room temperature for 1 h. The insoluble material was separated by filtration. The alcohol (20 mL) solution of the insoluble material (10 mol) and triethylamine (2 mL) was heated under reflux for 3 h. The solvent was evaporated, and the residue was suspended in water and extracted with EtOAc (4 × 30 mL). The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and then concentrated by a rotary

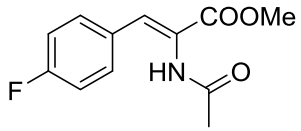
evaporator. The crude product was purified by flash column chromatography (EtOAc/PE) to give the desired compounds.

Methyl (*Z*)-2-acetamido-3-phenylacrylate **4a**



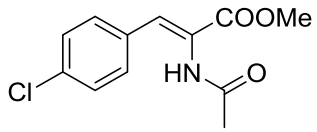
A white soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (s, 2H), 7.42 – 7.36 (m, 4H), 7.06 (br s, 1H), 3.87 (s, 3H), 2.15 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(4-fluorophenyl)acrylate **4b**



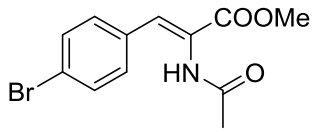
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (d, *J* = 19.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 3H), 3.87 (s, 3H), 2.16 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(4-chlorophenyl)acrylate **4c**



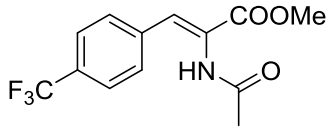
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (d, *J* = 18.9 Hz, 5H), 7.16 (br s, 1H), 3.87 (s, 3H), 2.15 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(4-bromophenyl)acrylate **4d**



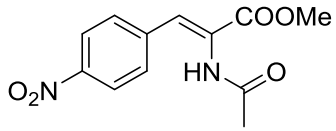
A yellow soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 10.5 Hz, 3H), 7.10 (br s, 1H), 3.88 (s, 3H), 2.16 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(4-(trifluoromethyl)phenyl)acrylate **4e**



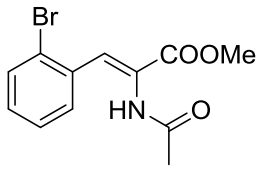
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.56 (s, 2H), 7.41 (s, 1H), 7.21 (br s, 1H), 3.90 (s, 3H), 2.15 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(4-nitrophenyl)acrylate **4f**



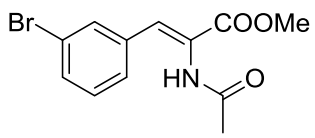
A yellow soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.18 (m, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.44 (br s, 1H), 7.41 (d, *J* = 3.3 Hz, 1H), 3.92 (s, 3H), 2.15 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(2-bromophenyl)acrylate **4g**



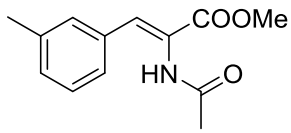
A yellow soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.1 Hz, 1H), 7.44 (d, *J* = 11.3 Hz, 2H), 7.39 – 7.26 (m, 1H), 7.26 – 7.15 (m, 1H), 7.09 (br s, 1H), 3.90 (s, 3H), 2.08 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(3-bromophenyl)acrylate **4h**



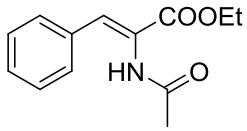
A white soild; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.38 (s, 1H), 7.34 (s, 1H), 7.26 (t, *J* = 7.8 Hz, 1H), 7.08 (br s, 1H), 3.89 (s, 3H), 2.17 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(m-tolyl)acrylate **4i**



A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.35 – 7.23 (m, 3H), 7.18 (s, 1H), 7.02 (br s, 1H), 3.87 (s, 3H), 2.37 (s, 3H), 2.15 (s, 3H).

Methyl (*Z*)-2-acetamido-3-(m-tolyl)acrylate **4j**



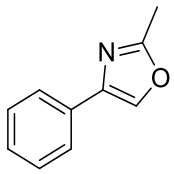
A white soild; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.2 Hz, 2H), 7.44 – 7.31 (m, 4H), 7.09 (br s, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 2.15 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H).

3. General Procedure for Intramolecular Cyclization (3a-3y)

An ovendried Schlenk tube equipped with a magnetic stir bar was charged with enamide (0.2 mmol, 1.0 equiv), fluorine reagent(0.24mmol, 1.2 equiv), 4 Å MS (60mg), CH_3CN (2 mL), BF_3·Et_2O (2.5μl, 0.02 mmol, 10 mol %) was successively added followed by stirring at room temperature for 3h. The solvent was evaporated, and the residue was purified by flash column chromatography (ethyl acetate/hexane) on silica gel and afforded corresponding oxazole **3a-3m**.

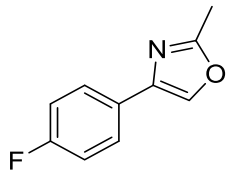
Enamide **2m-2y** was performed under the temperature of 60 ℃ to afford corresponding oxazole **3m-3y**.

2-Methyl-4-phenyloxazole **3a**



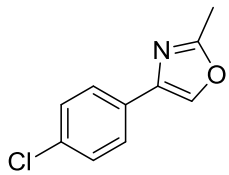
A yellow oil; 20.4mg, Yield 64 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.77 – 7.69 (m, 2H), 7.47 – 7.38 (m, 2H), 7.37 – 7.29 (m, 1H), 2.55 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 140.7, 133.2, 131.2, 128.7, 127.9, 125.4, 14.0; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{10}H_{10}NO$, 160.0762; found, 160.0758.

4-(4-Fluorophenyl)-2-methyloxazole **3b**



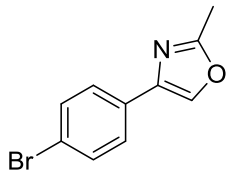
A yellow solid; mp 41-43 ℃; 15.6mg, Yield 44 %;^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.69 (dd, J = 8.7, 5.4 Hz, 2H), 7.10 (t, J = 8.7 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5 (d, $^{1}J_{C-F}$ = 246.9 Hz), 161.9, 139.9, 132.8 (d, $^{4}J_{C-F}$ = 1.6 Hz), 127.4 (d, $^{3}J_{C-F}$ = 3.3 Hz), 127.2, 127.0, 115.7 (d, $^{2}J_{C-F}$ = 21.8 Hz), 14.0; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{10}H_9FNO$, 178.0668; found, 178.0662.

4-(4-Chlorophenyl)-2-methyloxazole **3c**



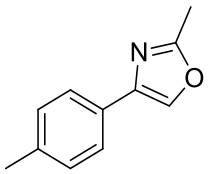
A light yellow solid; mp 87-88 ℃; 36.4mg, Yield 94 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 139.7, 133.5, 133.3, 129.7, 128.9, 126.7, 14.0; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{10}H_9ClNO$, 194.0373; found, 194.0366.

4-(4-Bromophenyl)-2-methyloxazole **3d**



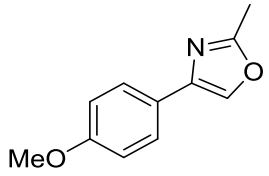
A white solid; mp 95-97 ℃; 37.6mg, Yield 79%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.55 (dd, *J* = 19.7, 8.5 Hz, 4H), 2.52 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 139.8, 133.4, 131.9, 130.1, 126.9, 121.7, 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{10}H_9BrNO$, 237.9868; found, 237.9862.

2-Methyl-4-(p-tolyl)oxazole **3e**



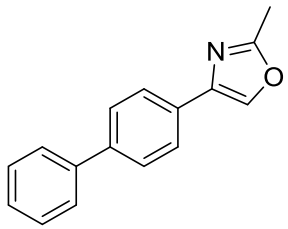
A yellow oil; 20.1mg, Yield 58 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.64 – 7.59 (m, 2H), 7.25 – 7.21 (m, 2H), 2.53 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7, 140.7, 137.7, 132.7, 129.4, 128.3, 125.3, 21.3, 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{11}H_{12}NO$, 174.0919; found, 174.0916.

4-(4-Methoxyphenyl)-2-methyloxazole **3f**



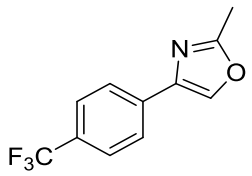
A yellow oil; 26.1mg, Yield 69 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.68 – 7.62 (m, 2H), 6.99 – 6.91 (m, 2H), 3.85 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7, 159.4, 140.5, 132.1, 126.7, 123.8, 114.1, 55.3, 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{11}H_{12}NO_2$, 190.0868; found, 190.0864.

4-([1,1'-Biphenyl]-4-yl)-2-methyloxazole **3g**



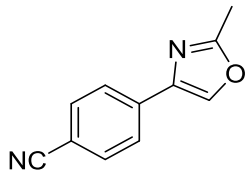
A yellow solid; mp 132-134 ℃; 22.6mg, Yield 48 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.71 – 7.62 (m, 4H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 140.6, 140.4, 133.3, 130.1, 128.8, 127.4, 127.4, 127.0, 125.8, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{14}NO$, 236.1075; found, 236.1072.

2-Methyl-4-(4-(trifluoromethyl)phenyl)oxazole **3h**



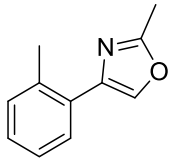
A white solid; mp 112-114 ℃; 25.0mg, Yield 55 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.83 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 3H), 2.55 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 139.5, 134.6 (q, $^{4}J_{C–F}$ = 1.5 Hz), 134.3, 129.7 (q, $^{2}J_{C–F}$ = 32.5 Hz), 125.7 (q, $^{3}J_{C–F}$ = 3.9 Hz), 125.5, 124.1 (q, $^{1}J_{C–F}$ = 271.9 Hz), 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{11}H_9F_3NO$, 228.0636; found, 228.0634.

4-(2-Methyloxazol-4-yl)benzonitrile **3i**



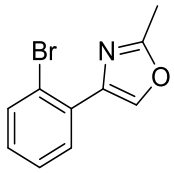
A light yellow solid; mp 102-104 ℃; 33.2mg, Yield 90 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.85 – 7.79 (m, 2H), 7.72 – 7.66 (m, 2H), 2.54 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 139.2, 135.6, 135.0, 132.6, 125.8, 118.9, 111.1, 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{11}H_9N_2O$, 185.0715; found, 185.0710.

2-Methyl-4-(o-tolyl)oxazole **3j**



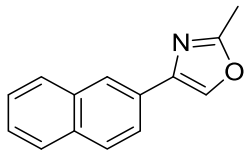
A yellow oil; 26.0mg, Yield 75 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (dt, *J* = 6.9, 1.5 Hz, 1H), 7.69 (s, 1H), 7.33 – 7.23 (m, 3H), 2.55 (s,3H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.8, 139.5, 135.3, 135.0, 130.8, 130.5, 128.4, 127.7, 126.1, 21.8, 13.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{11}H_{12}NO$, 174.0919; found, 174.0916.

4-(2-Bromophenyl)-2-methyloxazole **3k**



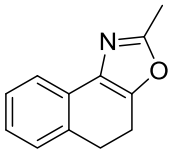
A yellow oil; 46.2mg, Yield 97 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.02 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.65 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.39 (td, *J* = 7.6, 1.3 Hz, 1H), 7.20 – 7.11 (m, 1H), 2.54 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.7, 137.9, 136.7, 133.7, 131.8, 130.3, 128.8, 127.5, 121.0, 13.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{10}H_9BrNO$, 237.9868; found, 237.9866.

2-Methyl-4-(naphthalen-2-yl)oxazole **3l**



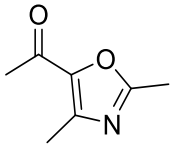
A yellow solid; mp 60-63 ℃; 32.2mg, Yield 77 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.94 (s, 1H), 7.93 – 7.82 (m, 3H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.50 (p, *J* = 7.2 Hz, 2H), 2.59 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 142.7, 140.7, 133.6, 133.6, 133.1, 128.4, 128.2, 127.7, 126.4, 126.0, 124.2, 123.4, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{14}H_{12}NO$, 210.0919; found, 210.0919.

2-Methyl-4,5-dihydronaphtho[1,2-*d*]oxazole **3m**



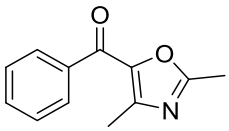
A light yellow oil; 23.3mg, Yield 53 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.5 Hz, 1H), 7.28 – 7.11 (m, 3H), 3.15 (t, *J* = 7.8 Hz, 2H), 2.97 (t, *J* = 8.1 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 147.6, 134.0, 133.2, 129.9, 127.9, 127.0, 126.5, 121.0, 29.0, 20.7, 14.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}NO$, 186.0919; found, 186.0912.

1-(2,4-Dimethyloxazol-5-yl)ethan-1-one **3n**



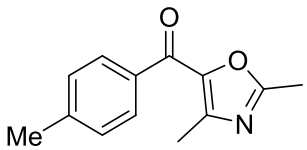
A white solid; mp 55-56 ℃; 24.8mg, Yield 89 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.50 (s, 3H), 2.45 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.5, 162.5, 145.5, 145.2, 27.5, 14.3, 13.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_7H_{10}NO_2$, 140.0712; found, 140.0706.

(2,4-Dimethyloxazol-5-yl)(phenyl)methanone **3o**



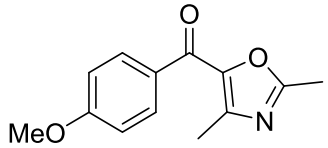
A yellow oil; 38.2mg, Yield 95 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.95 (m, 2H), 7.64 – 7.56 (m, 1H), 7.50 (t, *J* = 7.3 Hz, 2H), 2.56 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 182.7, 162.7, 147.9, 145.1, 132.7, 129.2, 128.4, 14.4, 14.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}NO_2$, 202.0868; found, 202.0864.

(2,4-Dimethyloxazol-5-yl)(p-tolyl)methanone **3p**



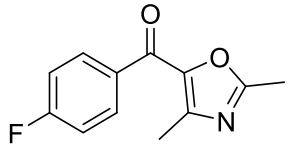
A white solid; mp 71-73 ℃; 31.4mg, Yield 73 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 2.55 (s, 3H), 2.49 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 182.4, 162.5, 147.5, 145.2, 143.6, 134.6, 129.4, 129.1, 21.7, 14.3, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{13}H_{14}NO_2$, 216.1025; found, 216.1020.

(2,4-Dimethyloxazol-5-yl)(4-methoxyphenyl)methanone **3q**



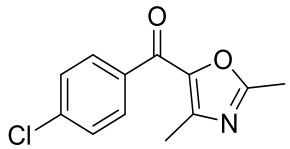
A white solid; mp 109-110 ℃; 38.9mg, Yield 84 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 – 8.01 (m, 2H), 7.02 – 6.96 (m, 2H), 3.90 (s, 3H), 2.56 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 181.2, 163.4, 162.2, 147.2, 145.2, 131.7, 129.9, 113.7, 55.5, 14.3, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{13}H_{14}NO_3$, 232.0974; found, 232.0970.

(2,4-Dimethyloxazol-5-yl)(4-fluorophenyl)methanone **3r**



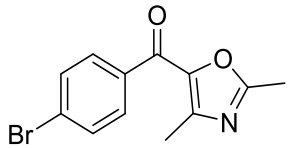
A white solid; mp 92-94 ℃; 34.6mg, Yield 79 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 – 8.01 (m, 2H), 7.26 – 7.12 (m, 2H), 2.57 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 180.9, 165.5 (d, $^1J_{C-F}$ = 254.7 Hz), 162.7, 148.2, 144.9, 133.4 (d, $^4J_{C-F}$ = 2.9 Hz), 131.9 (d, $^3J_{C-F}$ = 9.4 Hz), 115.6 (d, $^2J_{C-F}$ = 21.8 Hz), 14.4, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{11}FNO_2$, 220.0774; found, 220.0771.

(4-Chlorophenyl)(2,4-dimethyloxazol-5-yl)methanone **3s**



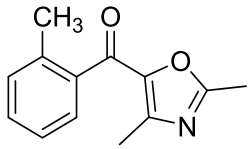
A yellow solid; mp 85-86 ℃; 36.8mg, Yield 78 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 - 7.93 (m, 2H), 7.55 – 7.44 (m, 2H), 2.56 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 181.1, 162.8, 148.5, 144.9, 139.2, 135.5, 130.7, 128.8, 14.4, 14.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{11}ClNO_2$, 236.0478; found, 236.0476.

(4-Bromophenyl)(2,4-dimethyloxazol-5-yl)methanone **3t**



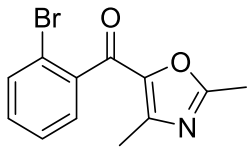
A light yellow solid; mp 66-67 ℃; 45.9mg, Yield 82 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 – 7.84 (m, 2H), 7.67 – 7.61 (m, 2H), 2.56 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 181.3, 162.8, 148.5, 144.9, 135.9, 131.7, 130.8, 127.9, 14.4, 14.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{11}BrNO_2$, 279.9973; found, 279.9972.

(2,4-Dimethyloxazol-5-yl)(o-tolyl)methanone **3u**



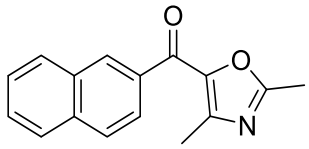
A colourless oil; 43.0mg, Yield 100 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (d, J = 8.3 Hz, 2H), 7.29 (d, J = 7.0 Hz, 2H), 2.51 (s, 3H), 2.38 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.5, 163.7, 147.5, 145.5, 137.9, 131.1, 127.8, 125.6, 19.5, 14.3, 13.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{13}H_{14}NO_2$, 216.1025; found, 216.1020.

(2-Bromophenyl)(2,4-dimethyloxazol-5-yl)methanone **3v**



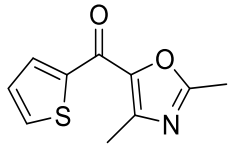
A yellow solid; mp 73-75 ℃; 48.7mg, Yield 87 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, J = 7.7 Hz, 1H), 7.52 – 7.35 (m, 3H), 2.53 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 183.0, 164.5, 148.5, 144.9, 140.0, 133.4, 131.9, 128.8, 127.7, 119.5, 14.5, 13.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{11}BrNO_2$, 279.9973; found, 279.9970.

(2,4-Dimethyloxazol-5-yl)(naphthalen-2-yl)methanone **3w**



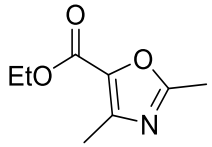
A yellow oil; 41.2mg, Yield 82 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.06 – 7.86 (m, 4H), 7.60 (t, *J* = 7.9 Hz, 2H), 2.59 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 182.6, 162.8, 147.8, 145.3, 135.4, 134.5, 132.4, 131.0, 129.6, 128.5, 128.3, 127.8, 126.8, 125.0, 14.4, 14.3; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{14}NO_2$, 252.1025; found, 252.1020.

(2,4-Dimethyloxazol-5-yl)(thiophen-2-yl)methanone **3x**



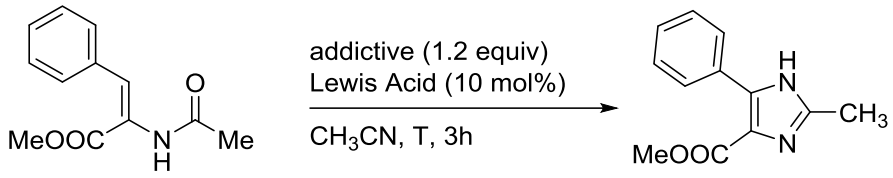
A yellow solid; mp 119-120 ℃; 41.5mg, Yield 86 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 3.8 Hz, 1H), 7.74 (d, *J* = 4.9 Hz, 1H), 7.21 (t, *J* = 4.5 Hz, 1H), 2.61 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.5, 162.3, 148.1, 144.2, 142.9, 134.3, 133.6, 128.3, 14.4, 14.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{10}H_{10}NO_2S$, 208.0432; found, 208.0427.

Ethyl 2,4-dimethyloxazole-5-carboxylate **3y**



A white solid; mp 51-52 ℃; 30.5mg, Yield 90 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 4.38 (q, *J* = 7.3 Hz, 2H), 2.50 (s, 3H), 2.44 (s, 3H), 1.39 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 158.7, 146.0, 137.5, 61.0, 14.3, 14.2, 13.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_8H_{12}NO_3$, 170.0817; found, 170.0809.

4. Optimization of Reaction Conditions of Intermolecular Cyclocondensation [a]



4a **5aa**

Entry	hypervalent iodine(III) regent	Lewis Acid	T (℃)	Yield (%)[b]
1	**1**	BF_3•OEt_2	25	<5
2	**1**	BF_3•OEt_2	60	<5
3	**1**	$AgBF_4$	60	<5
4	**1**	$ZnBF_4$	60	52
5	PIDA	$ZnBF_4$	60	6
6	PIFA	$ZnBF_4$	60	46

[a] The reactions were carried out using **4a** (0.2 mmol, 1 equiv) and hypervalent iodine(III) regent (1.2 equiv) and lewis acid (10 mol%) in MeCN (0.1 M) for 3h. [b] The yields were determined by ^{1}H NMR using 1,1,2,2-tetrachloroethane as an internal standard;

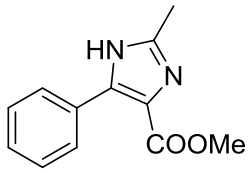
N-acetyl enamine **4a** was used as a model substrate to further optimize the reaction parameters. Initially, the optimized condition of the intramolecular cyclization was used (entry 1), the main product was unstable and gradually turned into **5aa**. The use of a higher temperature (60 ℃) did not change the result. The use of other Lewis acids like $AgBF_4$ (entry 3) still did not change the result but $ZnBF_4$ resulted in 52% (entry 4). Other hypervalent iodine(III) regents such as PIDA and PIFA (entry 5 and 6) also promoted this reaction, but with lower yields.

5. General Procedure for Intermolecular Cyclocondensation (5aa-5ac)

An ovendried Schlenk tube equipped with a magnetic stir bar was charged with enamide (0.3 mmol, 1.0 equiv), fluorine reagent(0.36mmol, 1.2 equiv), CH_3CN (3 mL), $ZnBF_4$ xH_2O (0.03 mmol, 10 mol %) was successively added followed by stirring at 60℃ for 3h. The solvent was evaporated, and the residue was purified by flash column chromatography (ethyl acetate/hexane) on silica gel and afforded corresponding imidazole.

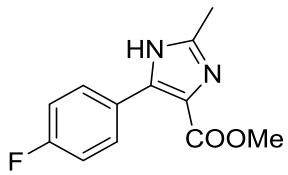
N-pentanenitrile was used as solvent to afford **5ab**. Phenylacetonitrile was used as solvent to afford **5ac**.

Methyl 2-methyl-5-phenyl-1*H*-imidazole-4-carboxylate **5aa**



A yellow oil; 22.5mg, Yield 52 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 5.1 Hz, 2H), 7.45 – 7.31 (m, 3H), 3.79 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 146.4, 142.9, 131.5, 129.1, 128.5, 128.0, 121.4, 51.6, 13.7; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{12}H_{13}N_2O_2$, 217.0977; found, 217.0968.

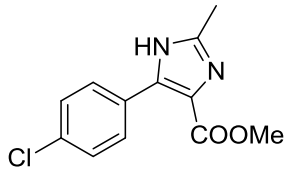
Methyl 5-(4-fluorophenyl)-2-methyl-1*H*-imidazole-4-carboxylate **5ba**



A white solid; mp 160-161 ℃; 21.1mg, Yield 45 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 – 7.66 (m, 2H), 7.06 – 6.92 (m, 2H), 3.76 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (75 MHz,

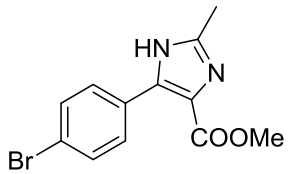
$CDCl_3$) δ 164.5, 161.5, 161.2, 146.6, 143.7 (d, $^1J_{C-F}$ = 143.2 Hz), 131.0 (d, $^3J_{C-F}$ = 8.2 Hz), 128.3, 114.9 (d, $^2J_{C-F}$ = 21.6 Hz); HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}FN_2O_2$, 235.0883; found, 235.0875.

Methyl 5-(4-chlorophenyl)-2-methyl-1*H*-imidazole-4-carboxylate **5ca**



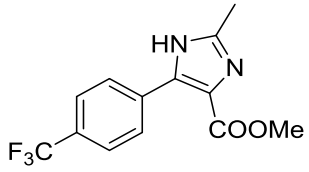
A white solid; mp 145-146 ℃; 32.1mg, Yield 64 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (s, 2H), 7.40 – 7.31 (m, 2H), 3.83 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 146.8, 143.8, 134.5, 130.8, 130.5, 128.2, 120.4, 51.8, 14.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}ClN_2O_2$, 251.0587; found, 251.0582.

Methyl 5-(4-bromophenyl)-2-methyl-1*H*-imidazole-4-carboxylate **5da**



A yellow solid; mp 144-145 ℃; 34.2mg, Yield 58 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.7 Hz, 2H), 3.84 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.5, 150.5, 146.8, 131.1, 131.0, 130.8, 130.7, 122.7, 51.7, 13.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}BrN_2O_2$, 295.0082; found, 295.0074.

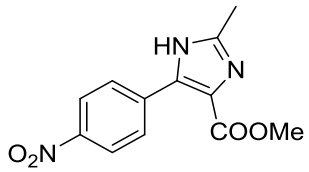
Methyl 2-methyl-5-(4-(trifluoromethyl)phenyl)-1*H*-imidazole-4-carboxylate **5ea**



A yellow oil; 19.9mg, Yield 35 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 3.88 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.0, 147.0, 144.3, 136.1, 130.2 (q, $^2J_{C-F}$ = 32.4 Hz), 129.4, 124.9 (q, $^3J_{C-F}$ = 27.8

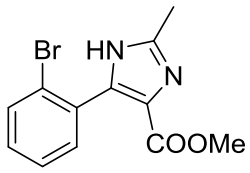
Hz), 124.9 (q, $^{4}J_{C-F}$ = 3.6 Hz), 124.2 (q, $^{1}J_{C-F}$ = 272.0 Hz), 51.9, 14.1; HRMS (ESI) m/z [M + H]$^{+}$: calcd for $C_{13}H_{12}F_3N_2O_2$, 185.0851; found, 285.0843.

Methyl 2-methyl-5-(4-nitrophenyl)-1*H*-imidazole-4-carboxylate **5fa**



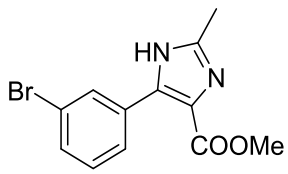
A white solid; mp 169-170 ℃; 23.0mg, Yield 44 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.37 – 8.25 (m, 2H), 8.17 (d, *J* = 8.6 Hz, 2H), 3.91 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 147.4, 144.9, 139.6, 129.9, 123.4, 123.3, 123.2, 52.0, 14.3; HRMS (ESI) m/z [M + H]$^{+}$: calcd for $C_{12}H_{12}N_3O_4$, 262.0828; found, 262.0819.

Methyl 5-(2-bromophenyl)-2-methyl-1*H*-imidazole-4-carboxylate **5ga**



A gelatineous yellow solid; 37.8mg, Yield 64 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.46 – 7.34 (m, 2H), 7.30 – 7.24 (m, 1H), 3.78 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.1, 146.5, 140.9, 133.4, 132.5, 131.9, 130.0, 126.9, 123.8, 123.4, 51.6, 13.7; HRMS (ESI) m/z [M + H]$^{+}$: calcd for $C_{12}H_{12}BrN_2O_2$, 295.0082; found, 295.0071.

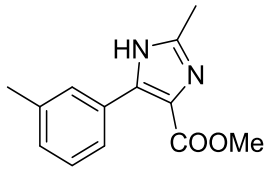
Methyl 5-(3-bromophenyl)-2-methyl-1*H*-imidazole-4-carboxylate **5ha**



A gelatineous yellow solid; 25.4mg, Yield 43 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.48 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1H), 7.30 – 7.23 (m,

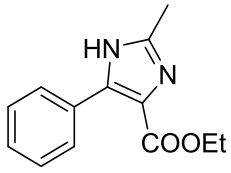
1H), 3.85 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7, 146.9, 142.5, 133.9, 132.0, 131.3, 129.4, 127.8, 121.9, 120.6, 51.8, 13.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{12}H_{12}BrN_2O_2$, 295.0082; found, 295.0071.

Methyl 2-methyl-5-(m-tolyl)-1*H*-imidazole-4-carboxylate **5ia**



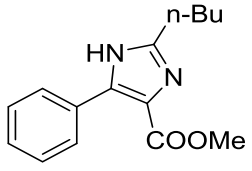
A yellow oil; 19.8mg, Yield 43 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 – 7.51 (m, 2H), 7.24 (d, *J* = 7.9 Hz, 1H), 7.18 – 7.10 (m, 1H), 3.80 (s, 3H), 2.37 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 146.2, 144.1, 137.3, 131.6, 129.6, 129.3, 127.8, 126.2, 119.6, 51.6, 21.4, 13.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{13}H_{15}N_2O_2$, 231.1134; found, 231.1124.

Ethyl 2-methyl-5-phenyl-1*H*-imidazole-4-carboxylate **5ja**



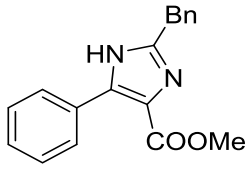
A yellow oil; 24.9mg, Yield 54 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (dt, *J* = 7.7, 1.4 Hz, 2H), 7.49 – 7.33 (m, 3H), 4.31 (q, *J* = 7.1 Hz, 2H), 2.38 (d, *J* = 2.2 Hz, 3H), 1.32 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.5, 146.4, 142.6, 132.1, 129.2, 128.4, 127.8, 120.7, 60.7, 14.2, 13.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{13}H_{15}N_2O_2$, 231.1134; found, 231.1125.

Methyl 2-butyl-5-phenyl-1*H*-imidazole-4-carboxylate **5ab**



A white solid; mp 117-118 ℃; 16.0mg, Yield 31 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.1 Hz, 2H), 7.48 – 7.36 (m, 3H), 3.87 (s, 3H), 2.77 (t, *J* = 7.9 Hz, 2H), 1.76 (p, *J* = 7.9 Hz, 2H), 1.42 (q, *J* = 8.9, 8.2 Hz, 2H), 1.01 – 0.90 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7, 150.5, 144.5, 129.1, 128.6, 128.5, 128.0, 126.9, 51.6, 30.4, 28.3, 22.4, 13.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{15}H_{19}N_2O_2$, 259.1447; found, 259.1442.

Methyl 2-benzyl-5-phenyl-1*H*-imidazole-4-carboxylate **5ac**



A gelatineous yellow solid; 23.4mg, Yield 40 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.61 (m, 2H), 7.48 – 7.29 (m, 6H), 7.24 (d, *J* = 6.4 Hz, 2H), 4.09 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 148.8, 136.1, 129.1, 129.0, 129.0, 128.9, 128.8, 128.6, 128.0, 127.3, 127.3, 51.7, 35.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_7H_{10}NO_2$, 293.1290; found, 293.1285.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_1211_3_0m

```
Bond precision:  C-C = 0.0108 A          Wavelength=0.71073

Cell:          a=5.6468(5)       b=12.0159(10)    c=14.1013(13)
               alpha=81.991(5)   beta=89.552(5)   gamma=82.145(5)
Temperature:   150 K
```

	Calculated	Reported
Volume	938.51(14)	938.51(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 H8 Br N O	C10 H8 Br N O
Sum formula	C10 H8 Br N O	C10 H8 Br N O
Mr	238.07	238.08
Dx,g cm-3	1.685	1.685
Z	4	4
Mu (mm-1)	4.335	4.335
F000	472.0	472.0
F000’	471.06	
h,k,lmax	6,14,17	6,14,17
Nref	3688	3641
Tmin,Tmax	0.541,0.707	0.434,0.745
Tmin’	0.434	

```
Correction method= # Reported T Limits: Tmin=0.434 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.987          Theta(max)= 26.021

R(reflections)= 0.0631( 2849)     wR2(reflections)= 0.1658( 3641)

S = 1.182                 Npar= 237
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01083 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      10.42 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             104.7 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2             104.1 Degree
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

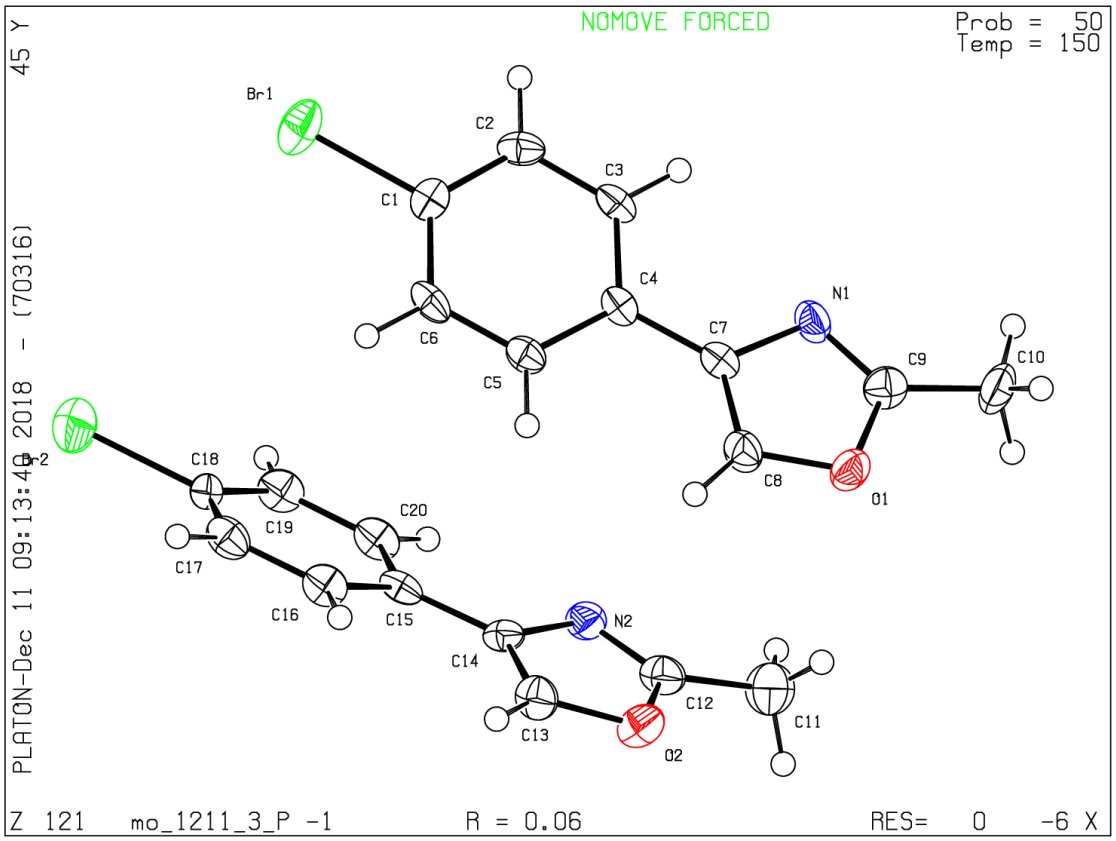
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock mo_1211_3_0m - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 22019358xj_0m

```
Bond precision:  C-C = 0.0058 A          Wavelength=0.71073

Cell:              a=9.930(3)      b=9.524(3)      c=24.977(8)
                   alpha=90        beta=90         gamma=90
Temperature:       100 K

                Calculated                Reported
Volume          2362.2(13)                2362.0(13)
Space group     P b c a                   P b c a
Hall group      -P 2ac 2ab                -P 2ac 2ab
Moiety formula  C12 H11 Br N2 O2          C12 H11 Br N2 O2
Sum formula     C12 H11 Br N2 O2          C12 H11 Br N2 O2
Mr              295.13                    295.14
Dx,g cm-3       1.660                     1.660
Z               8                         8
Mu (mm-1)       3.471                     3.471
F000            1184.0                    1184.0
F000'           1182.20
h,k,lmax        12,12,32                  12,12,32
Nref            2719                      2701
Tmin,Tmax       0.812,0.870               0.606,0.746
Tmin'           0.758

Correction method= # Reported T Limits: Tmin=0.606 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 27.533

R(reflections)= 0.0451( 1887)     wR2(reflections)= 0.1142( 2701)

S = 1.058                 Npar= 160
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         1 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

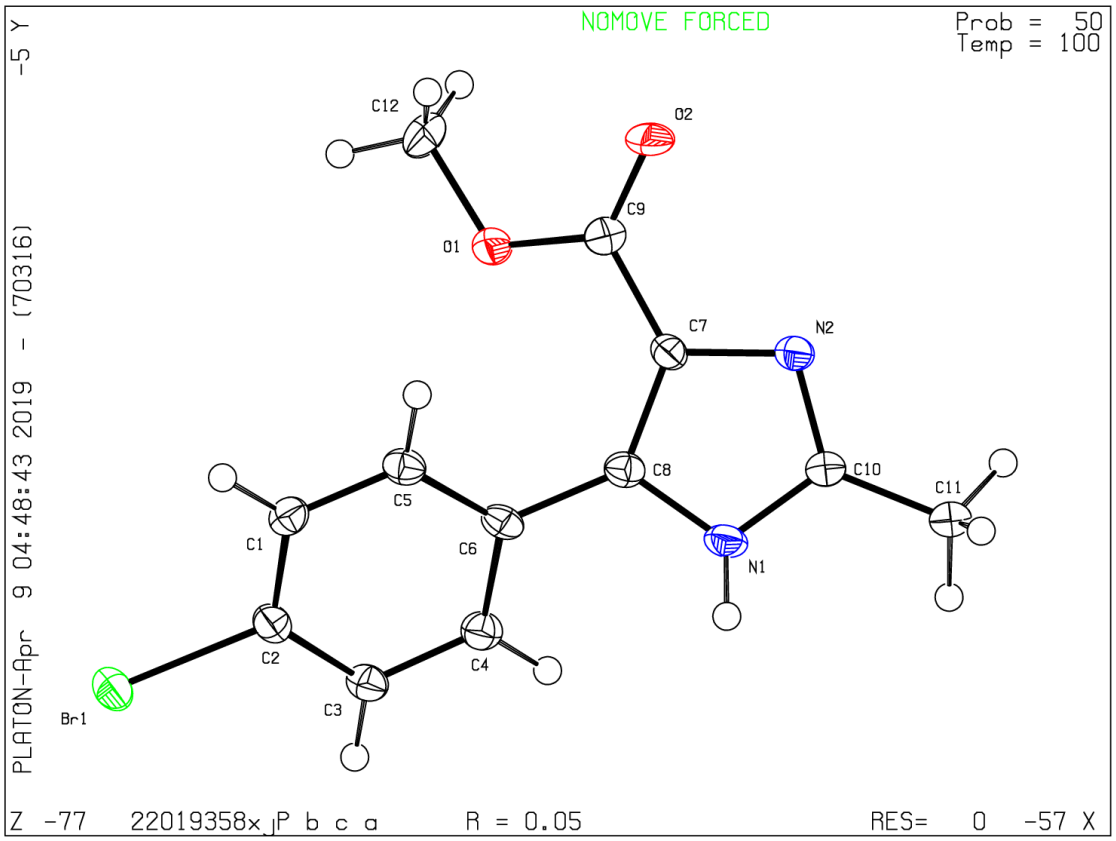
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

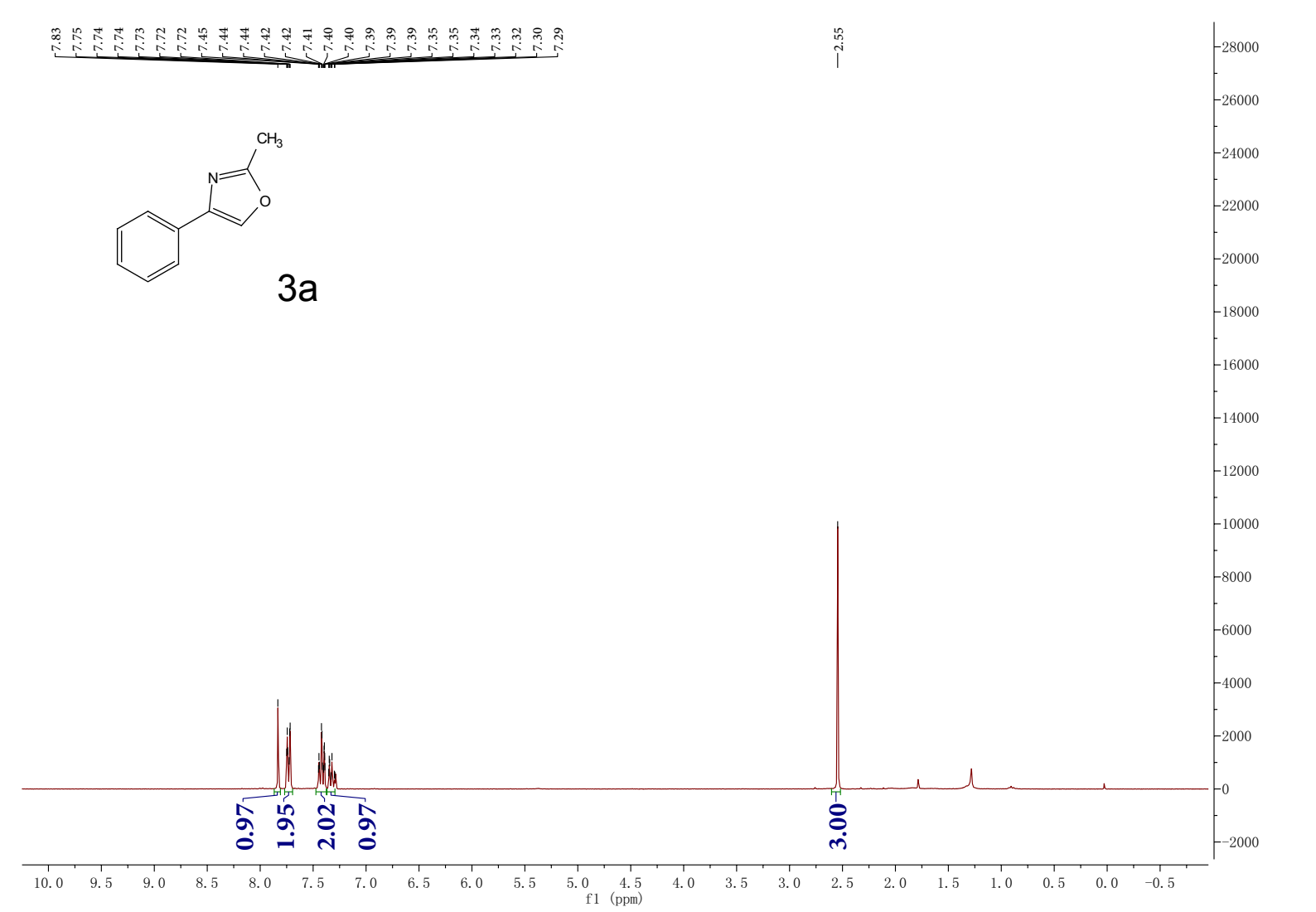
PLATON version of 17/03/2019; check.def file version of 04/03/2019

Datablock 22019358xj_0m - ellipsoid plot



8. Reference

1. Z. –H. Guan, Z. –Y. Zhang, Z. -H. Ren, Y. –Y. Wang and X. Zhang, *J. Org. Chem*., 2011, **76**, 339-341.
2. H. Geng, W. Zhang, J. Chen, G. Hou, L. Zhou, Y. Zou, W. Wu and X. Zhang, *Angew. Chem. Int. Ed.*, 2009, **48**, 6052 –6054.
3. Y. Zheng, X. Li, C. Ren, D. Zhang-Negrerie, Y. Du and K. Zhao, *J. Org. Chem*., 2012, **77**, 10353-10361.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7.44
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7.39
7.39
7.39
7.35
7.35
7.34
7.33
7.32
7.30
7.29
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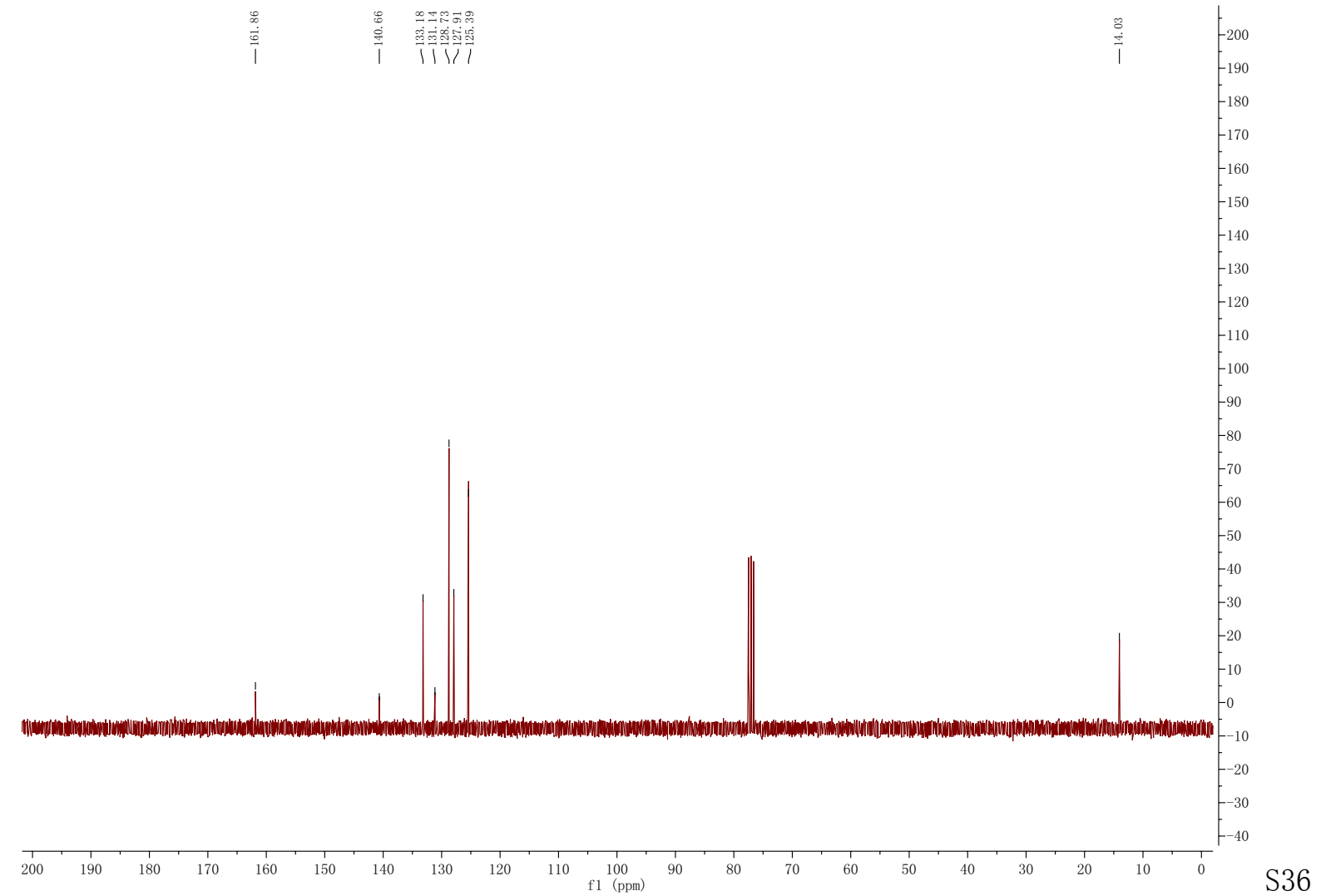
0.97
3.00
f1 (ppm)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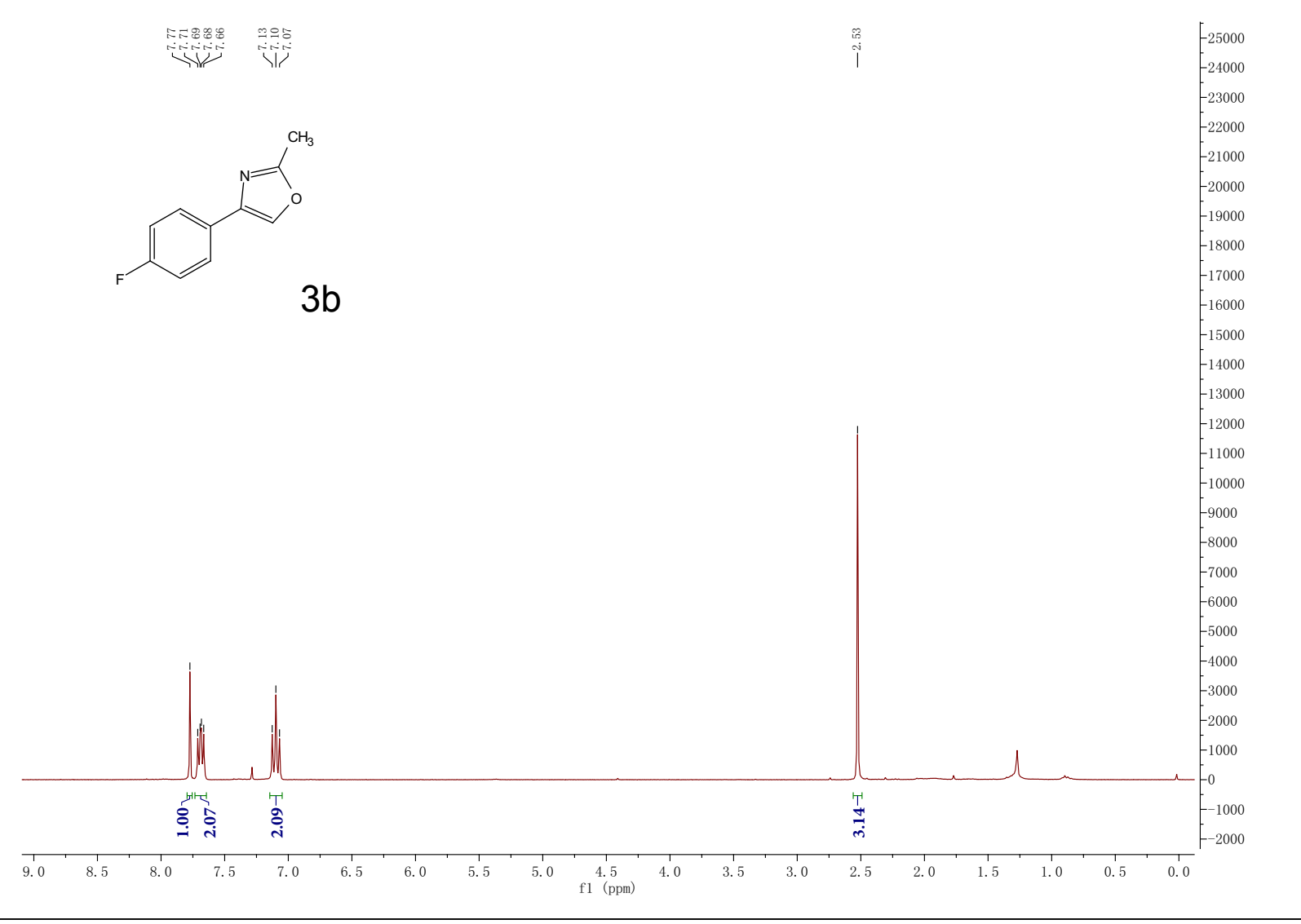
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7.66
7.13
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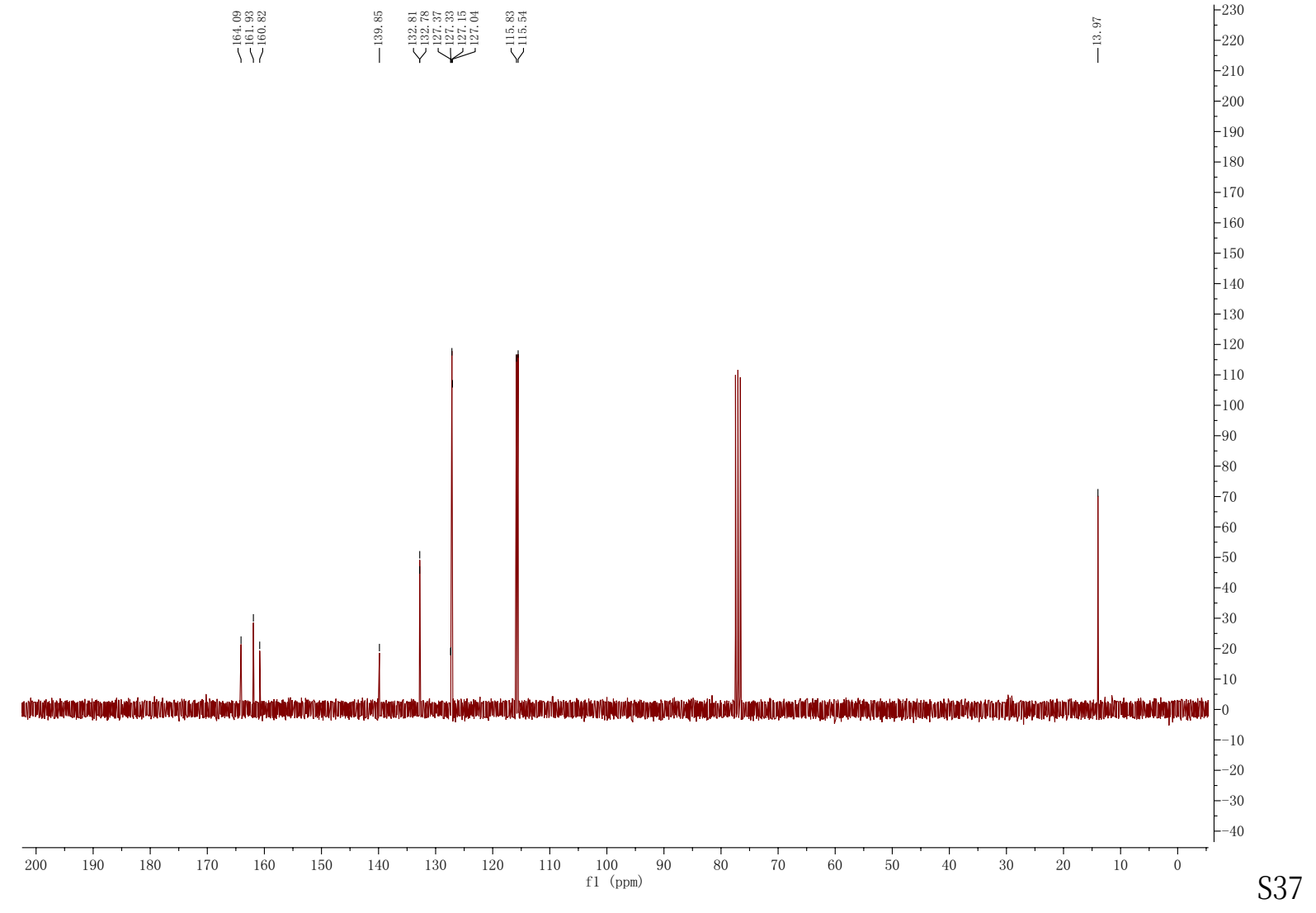
3.14
f1 (ppm)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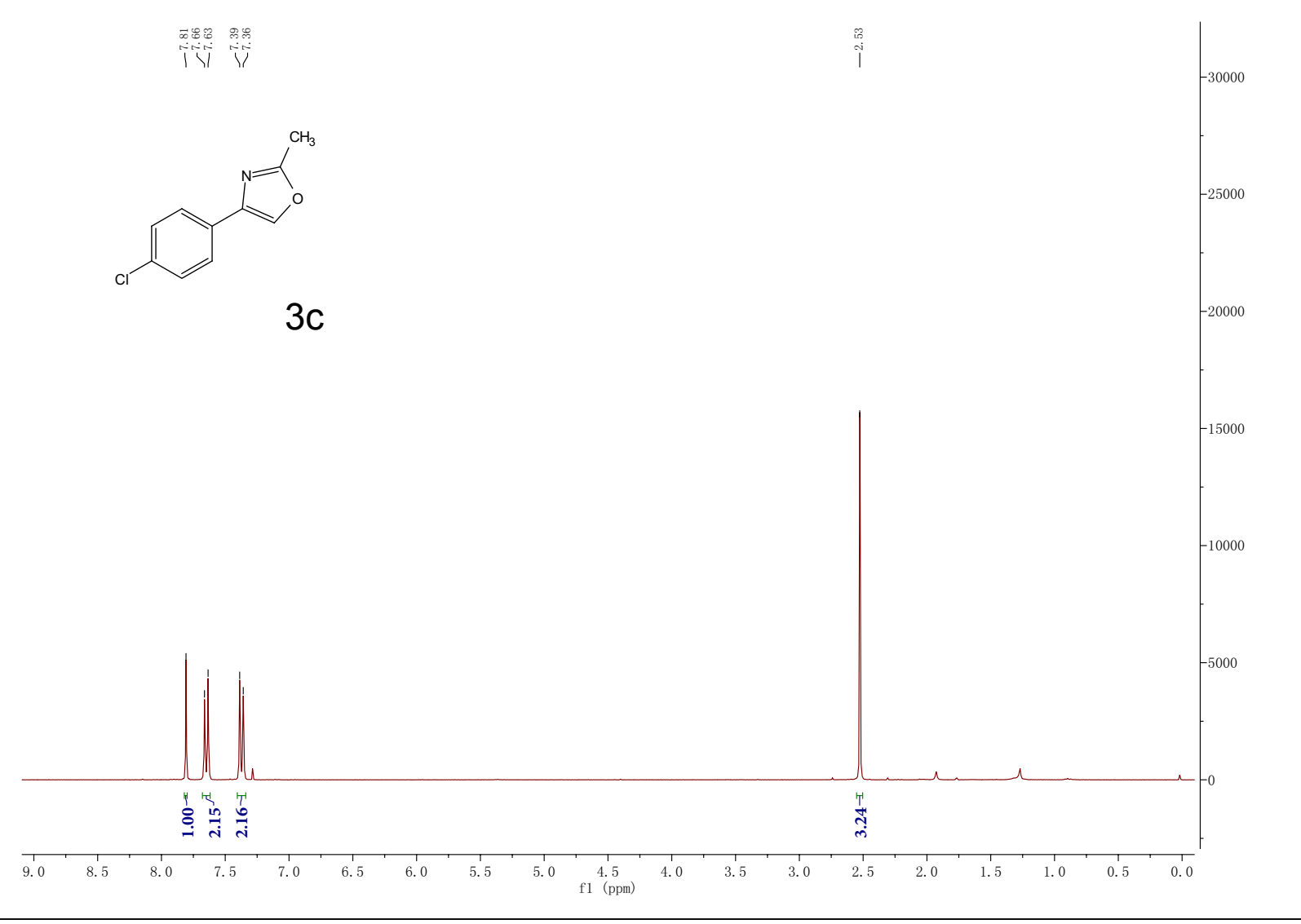
f1 (ppm)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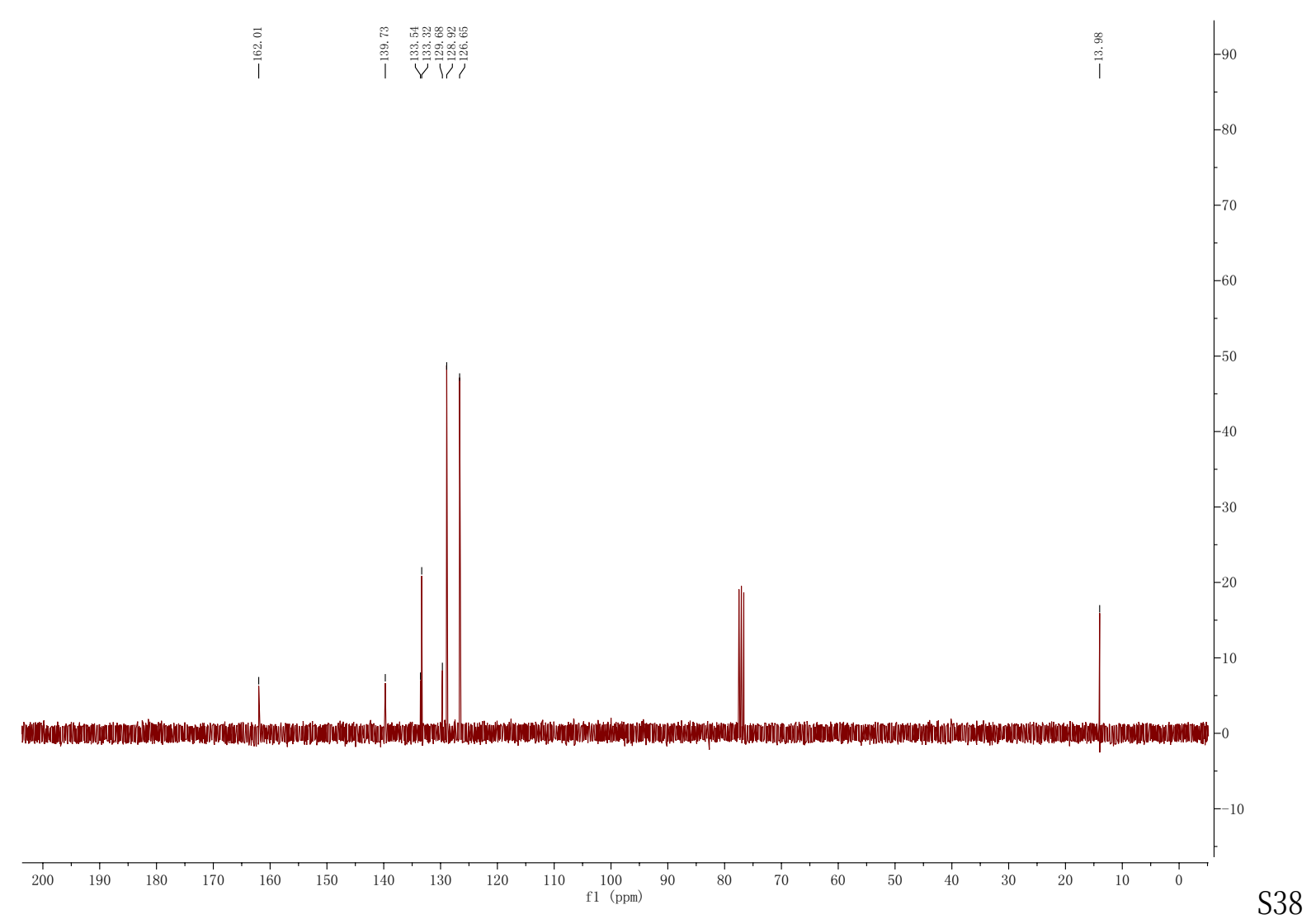
3.24
f1 (ppm)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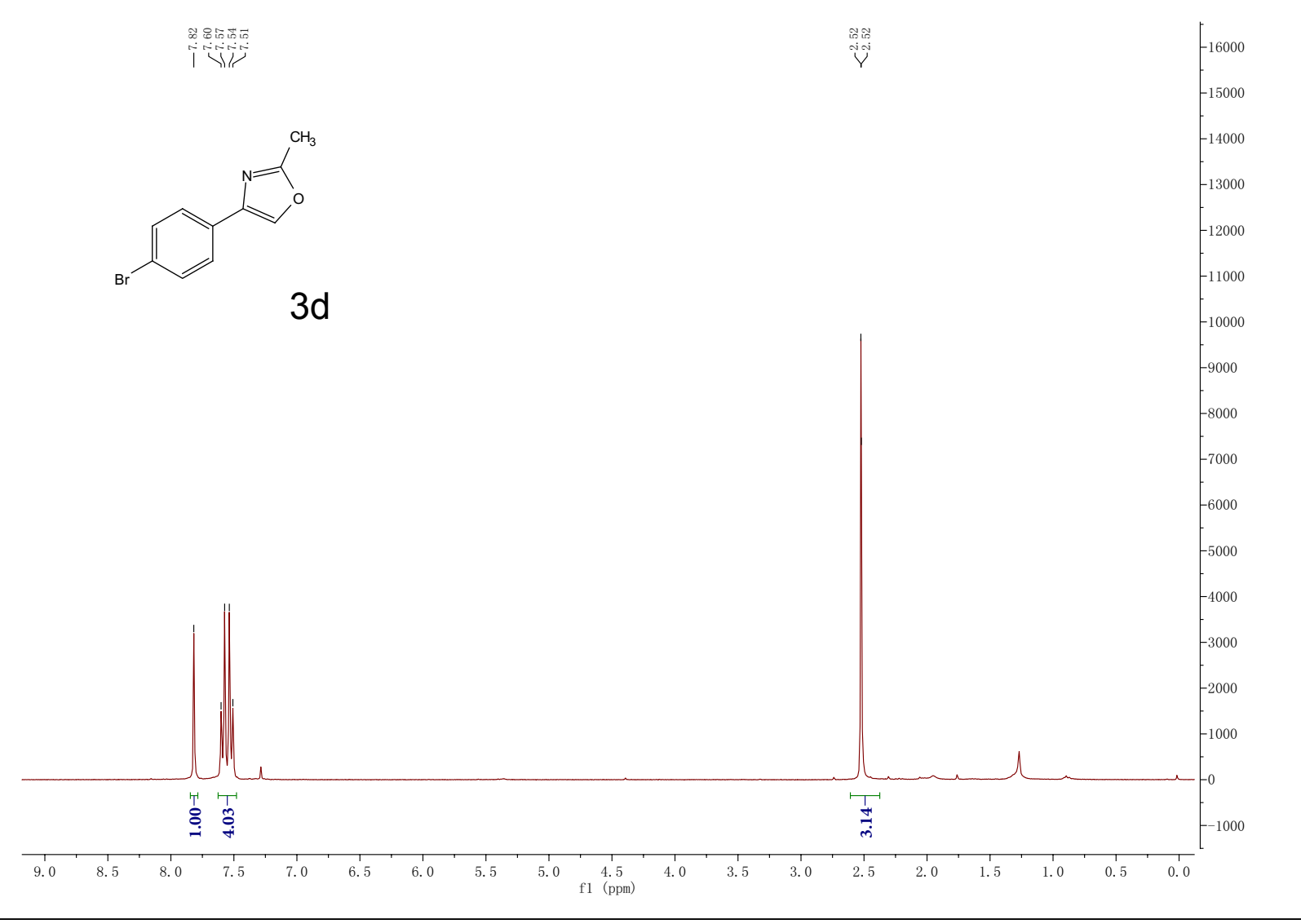
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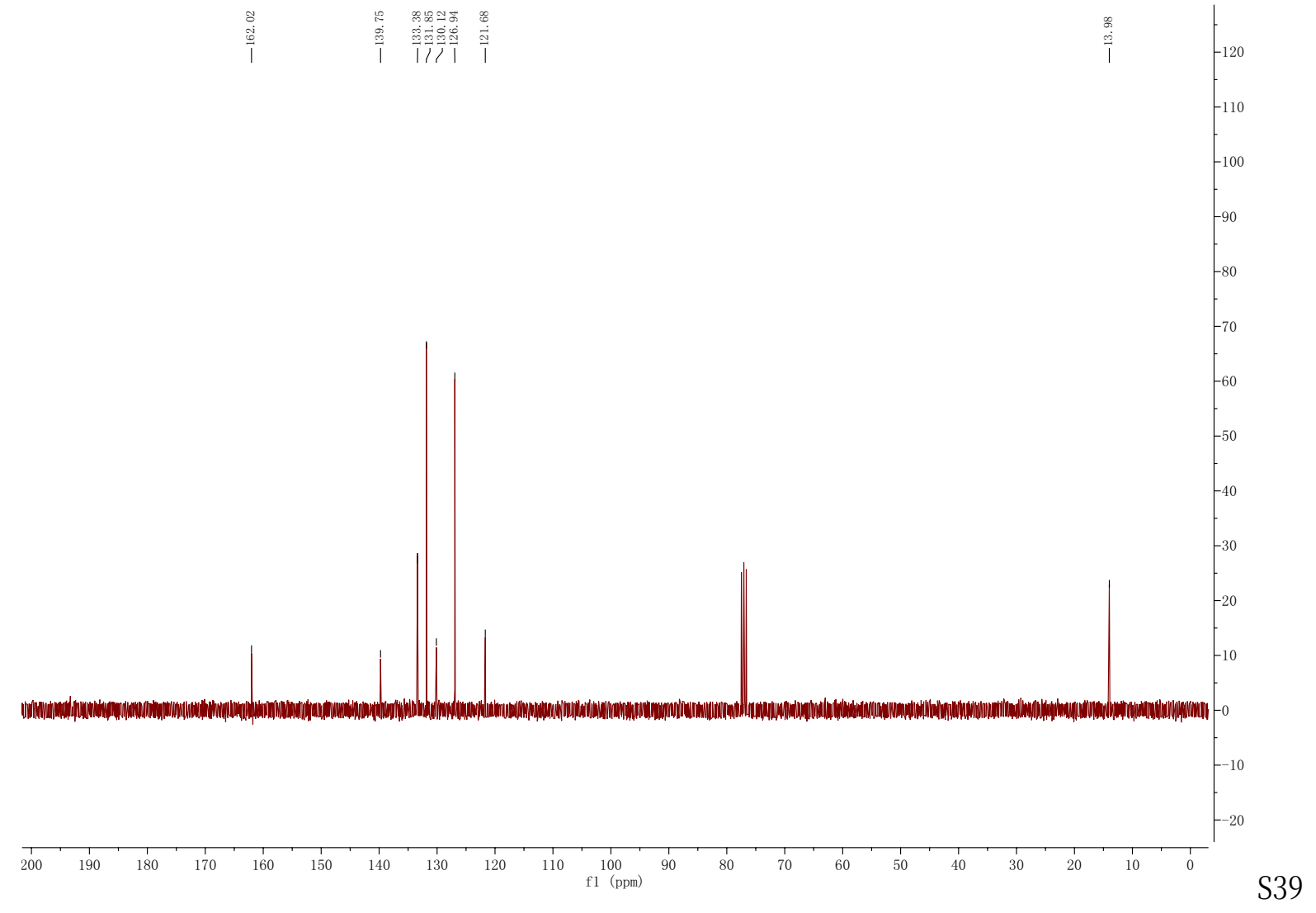
f1 (ppm)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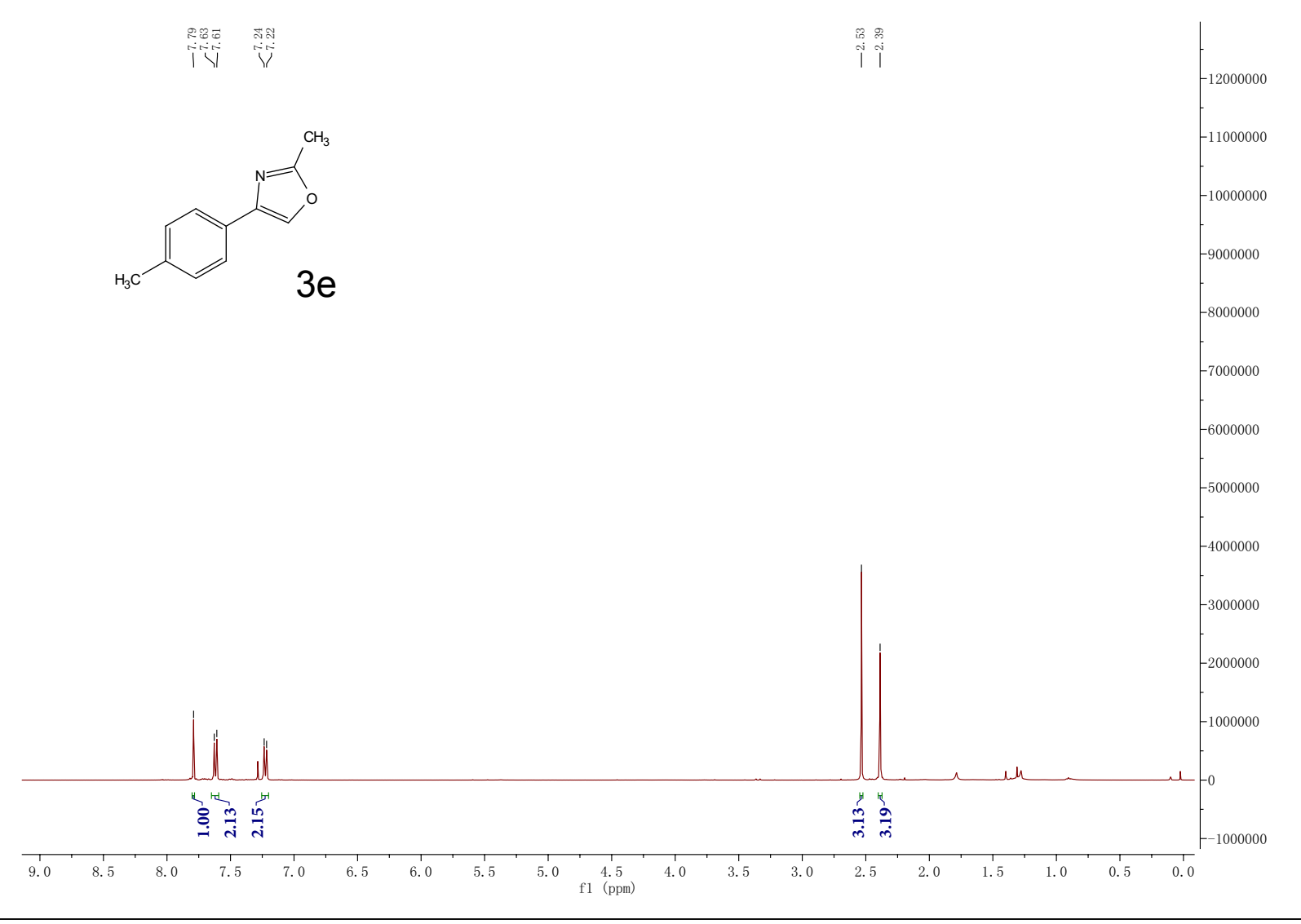
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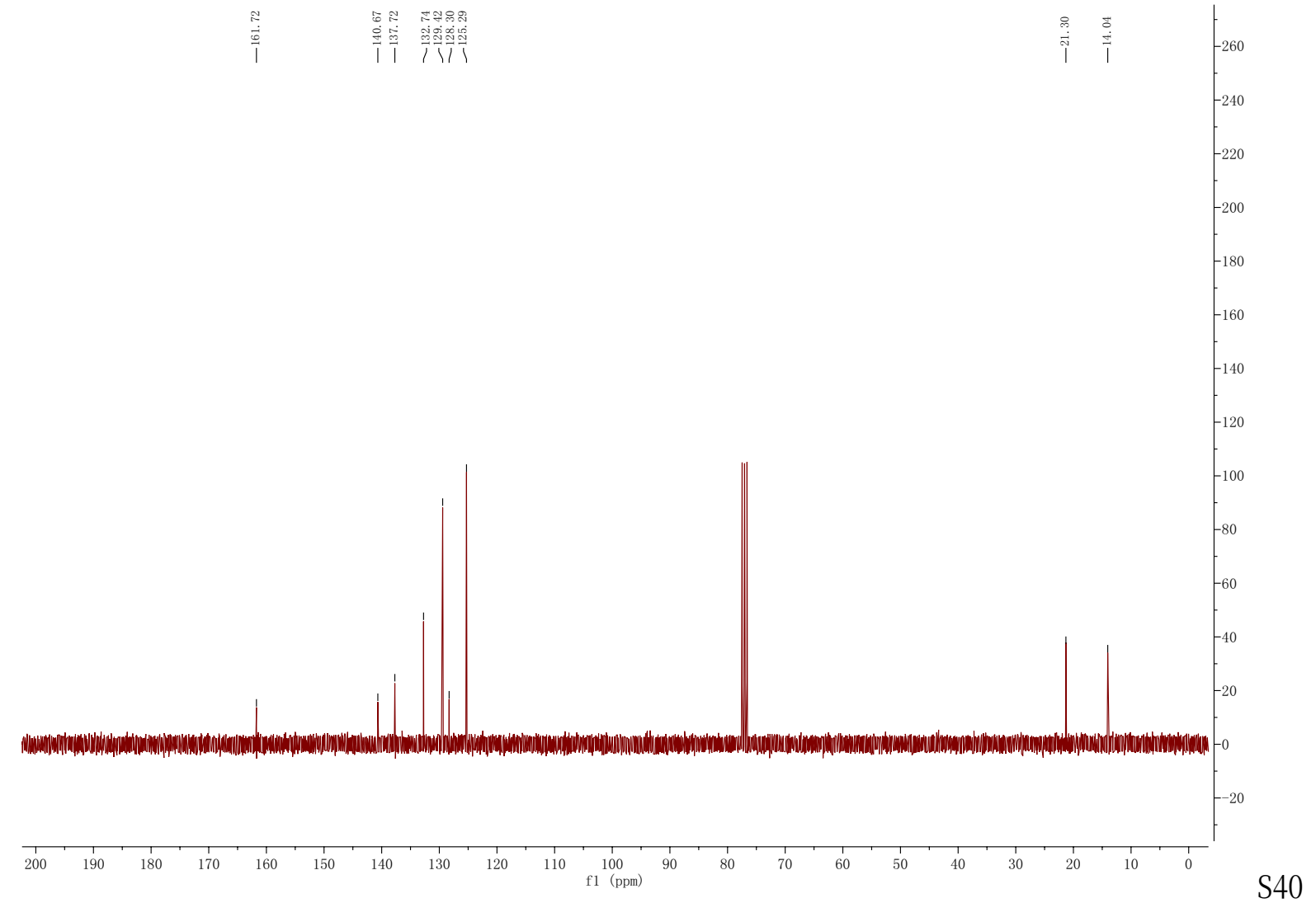
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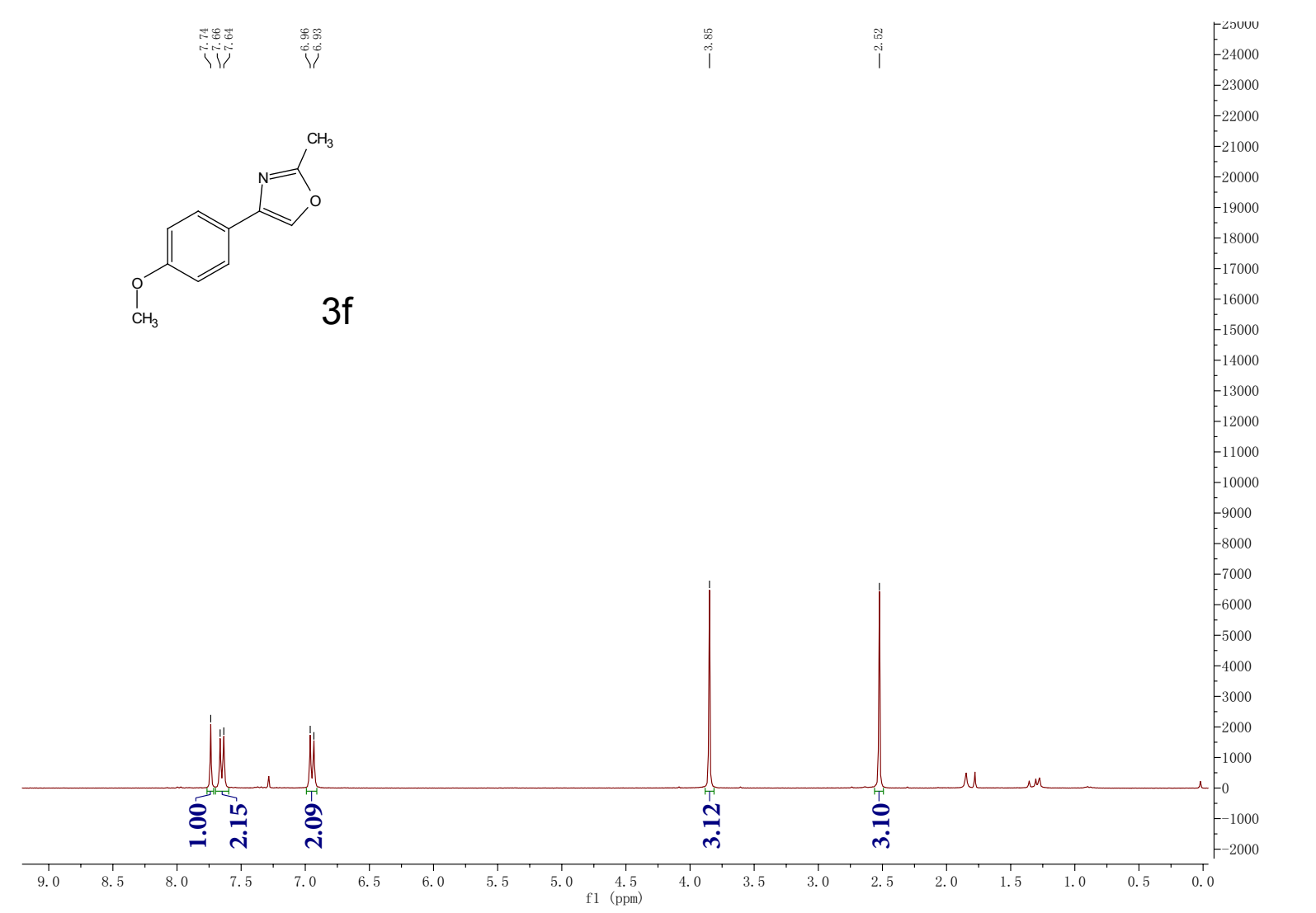
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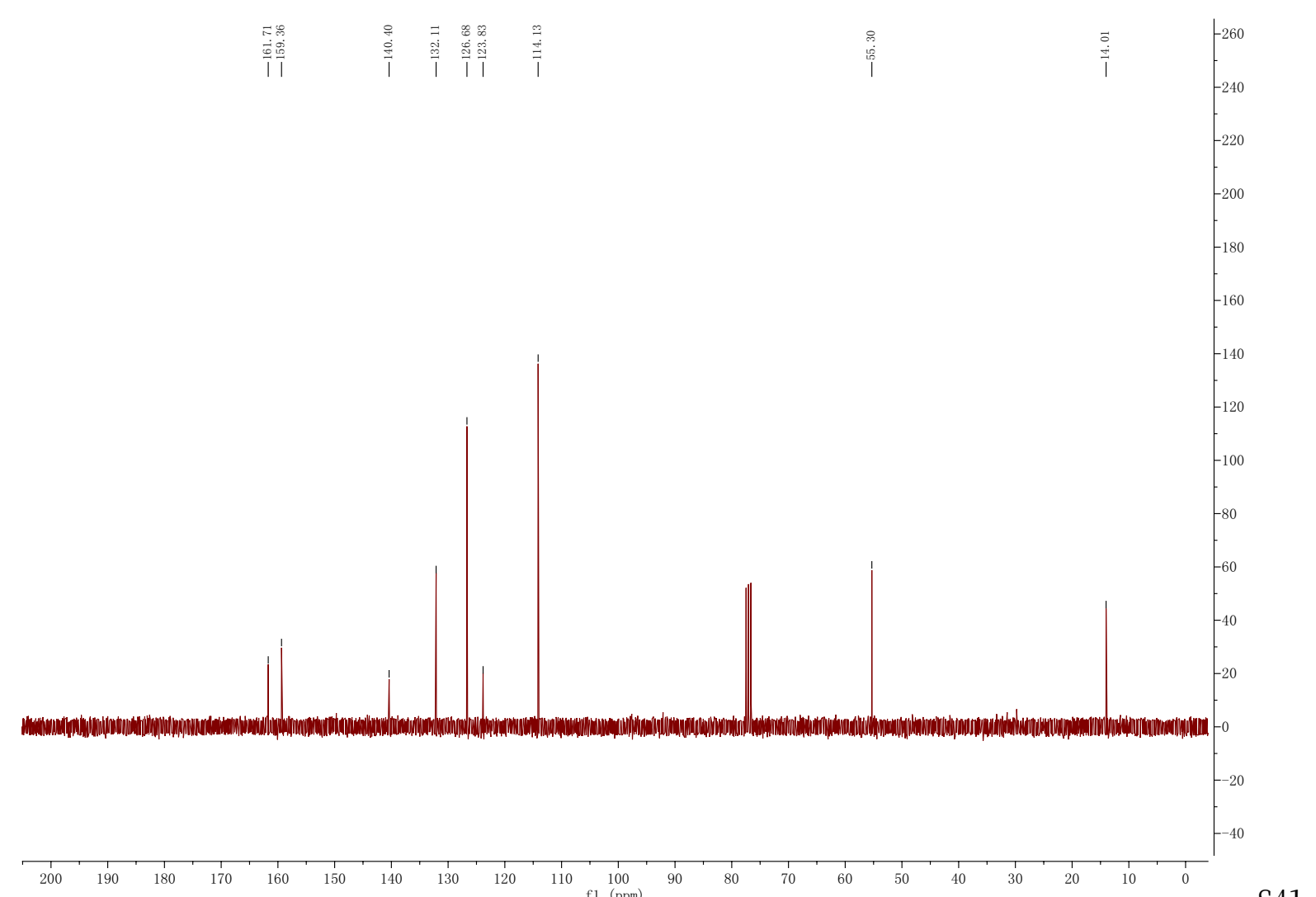
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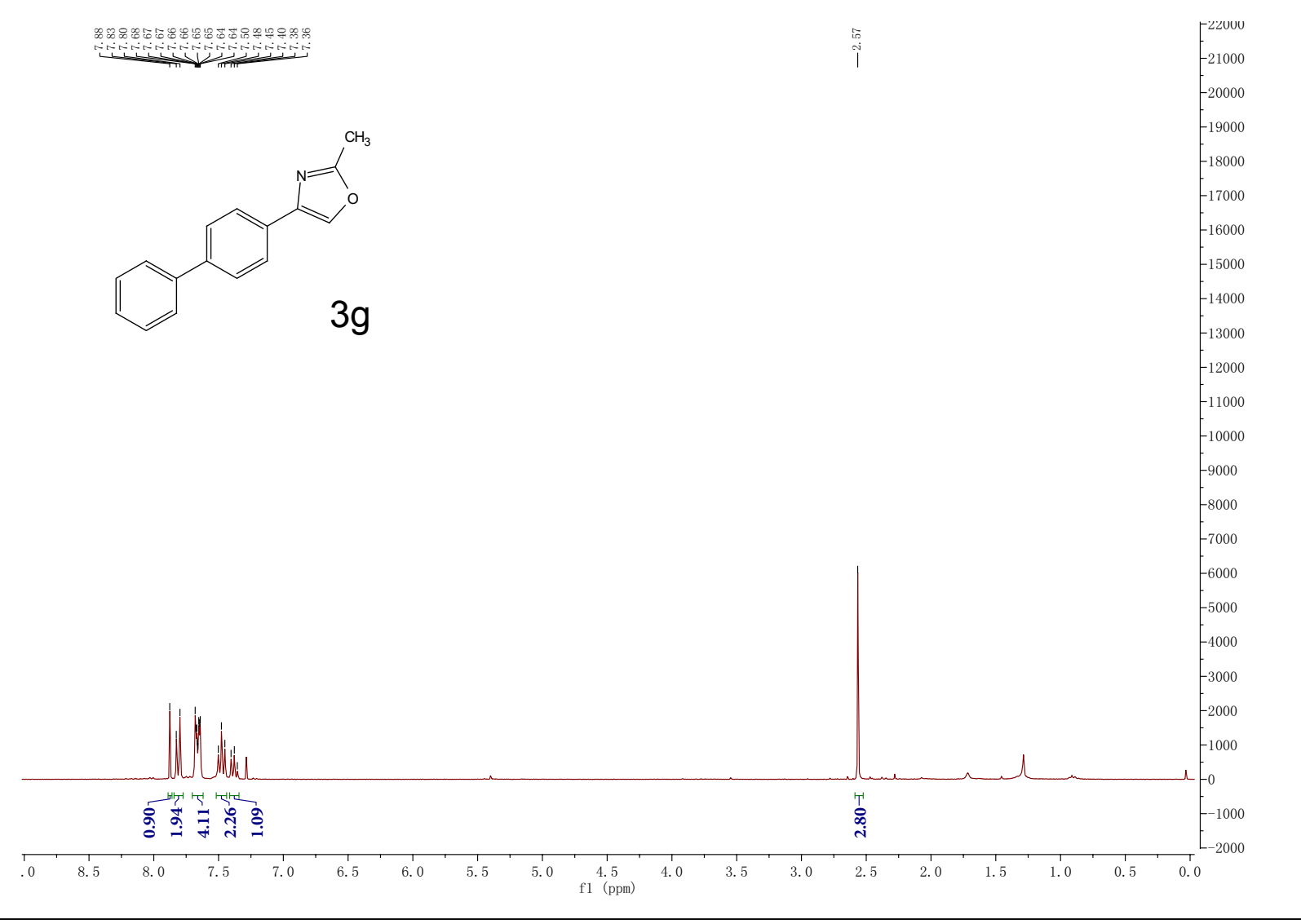
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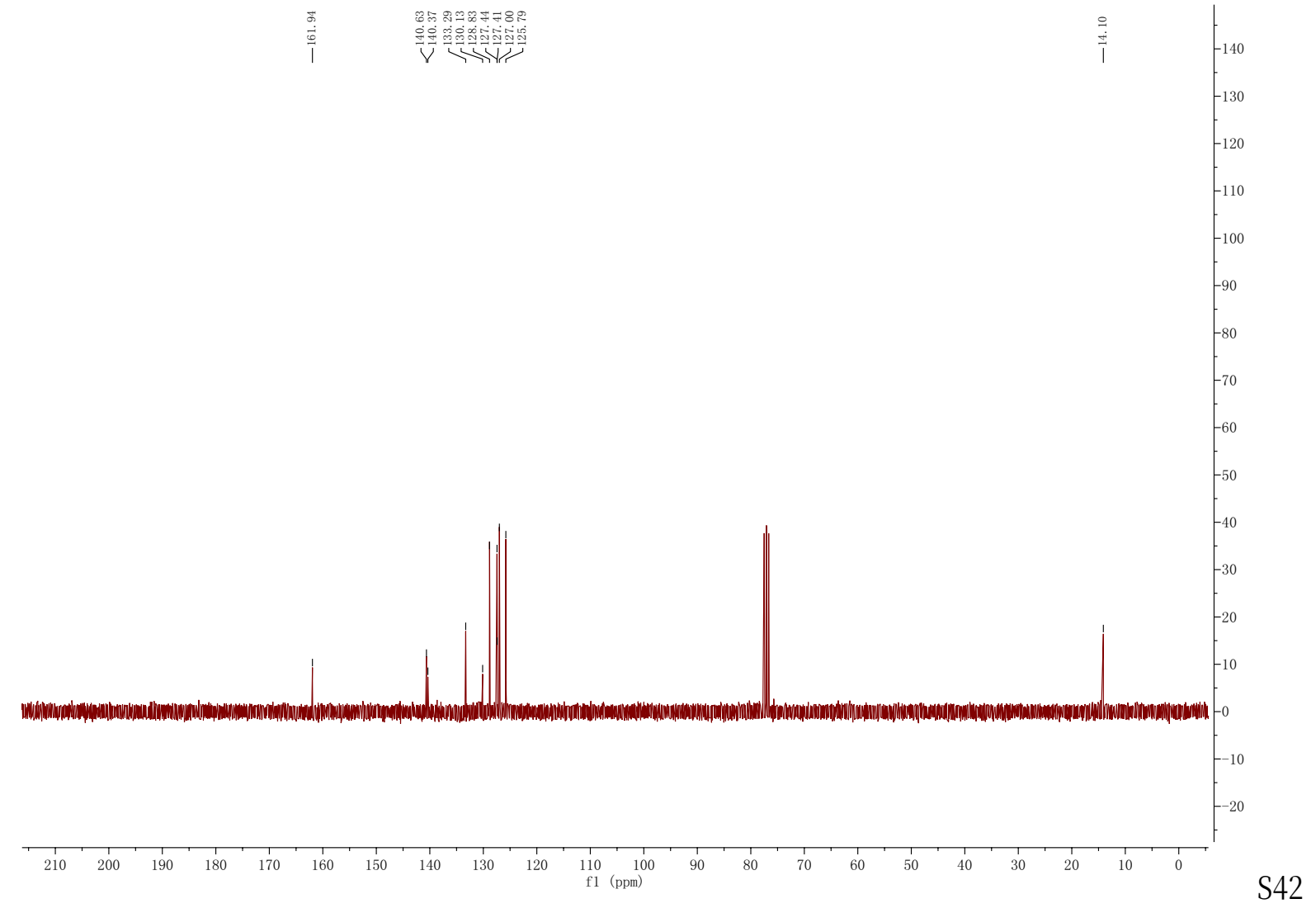
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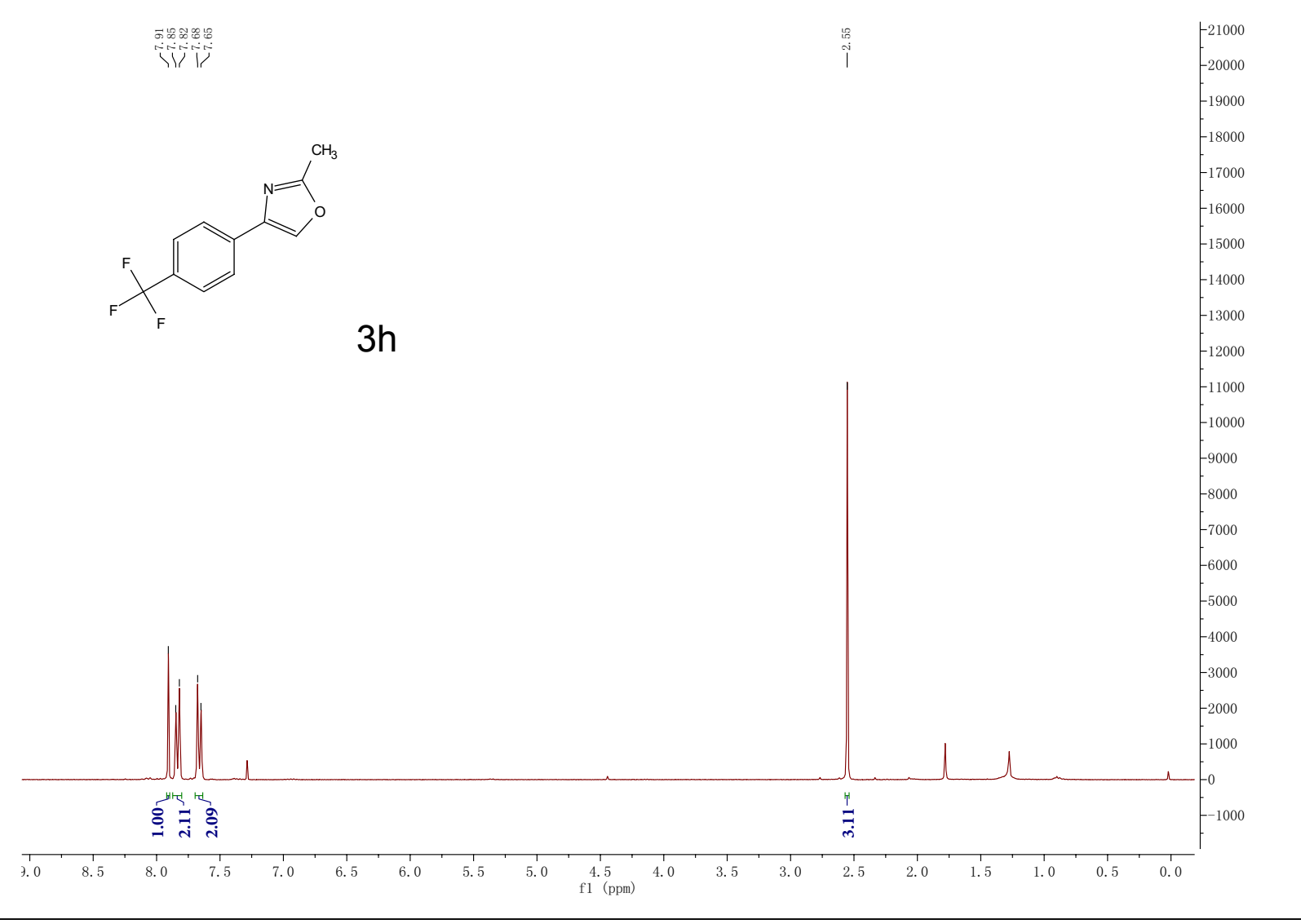
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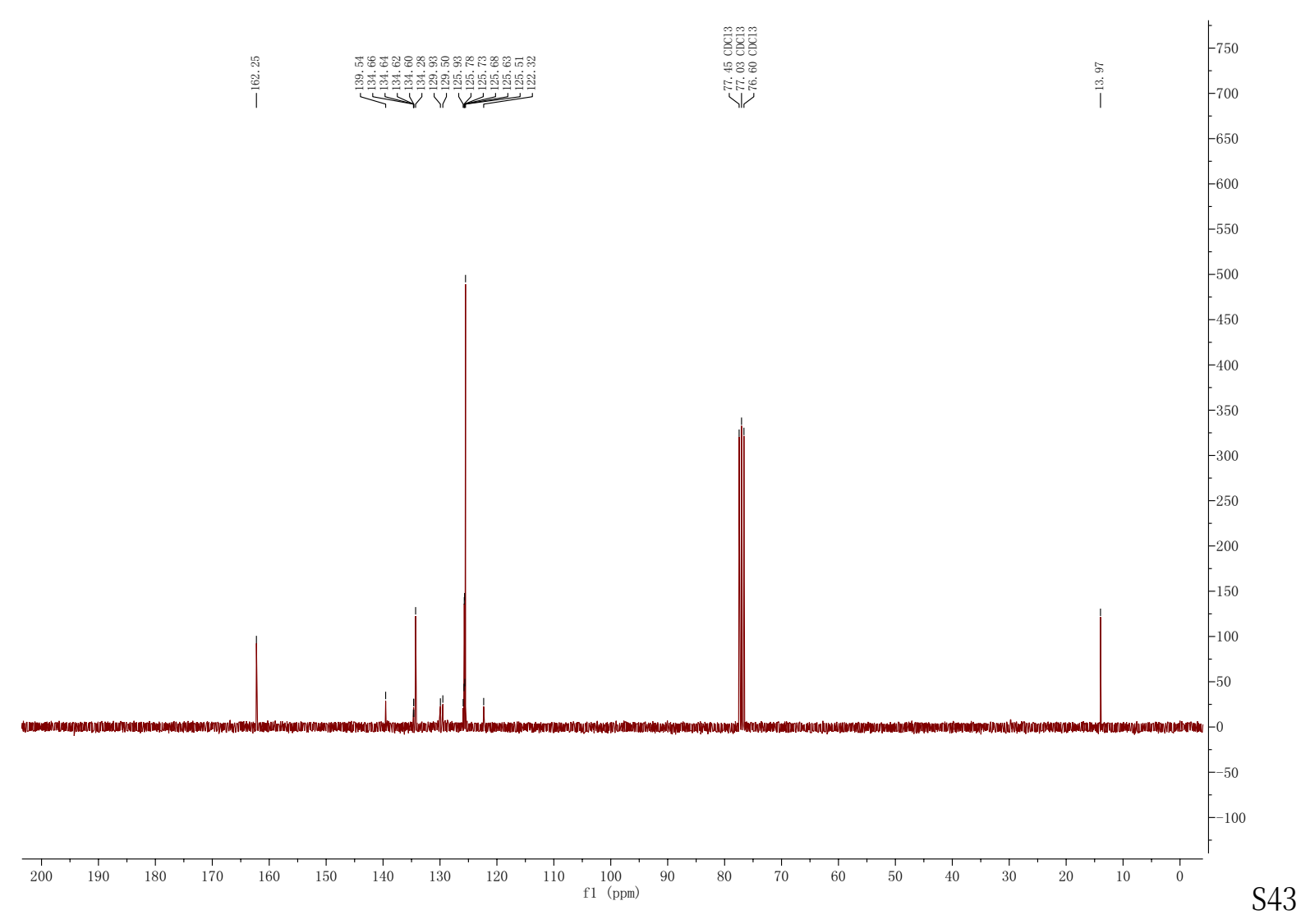
f1 (ppm)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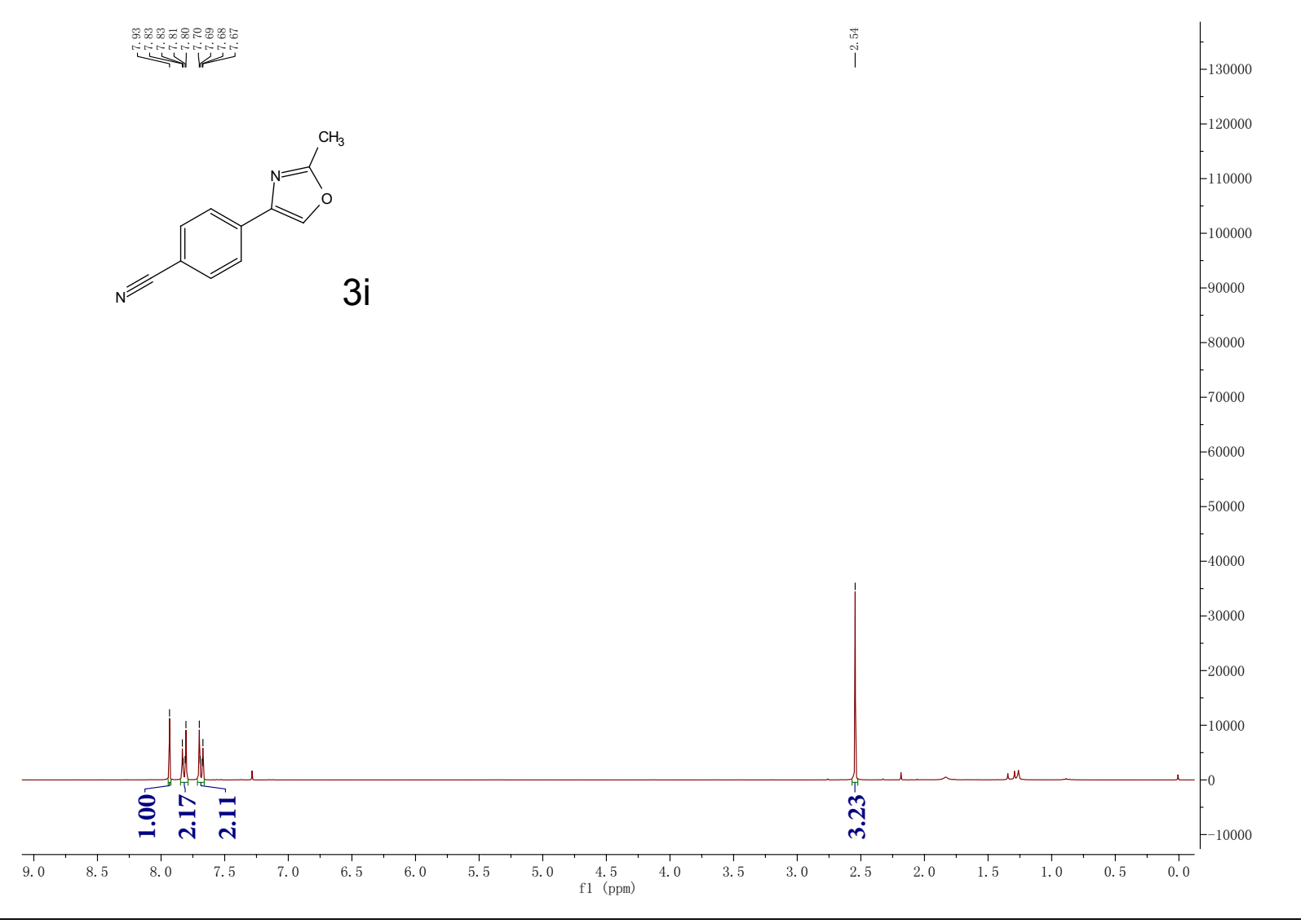
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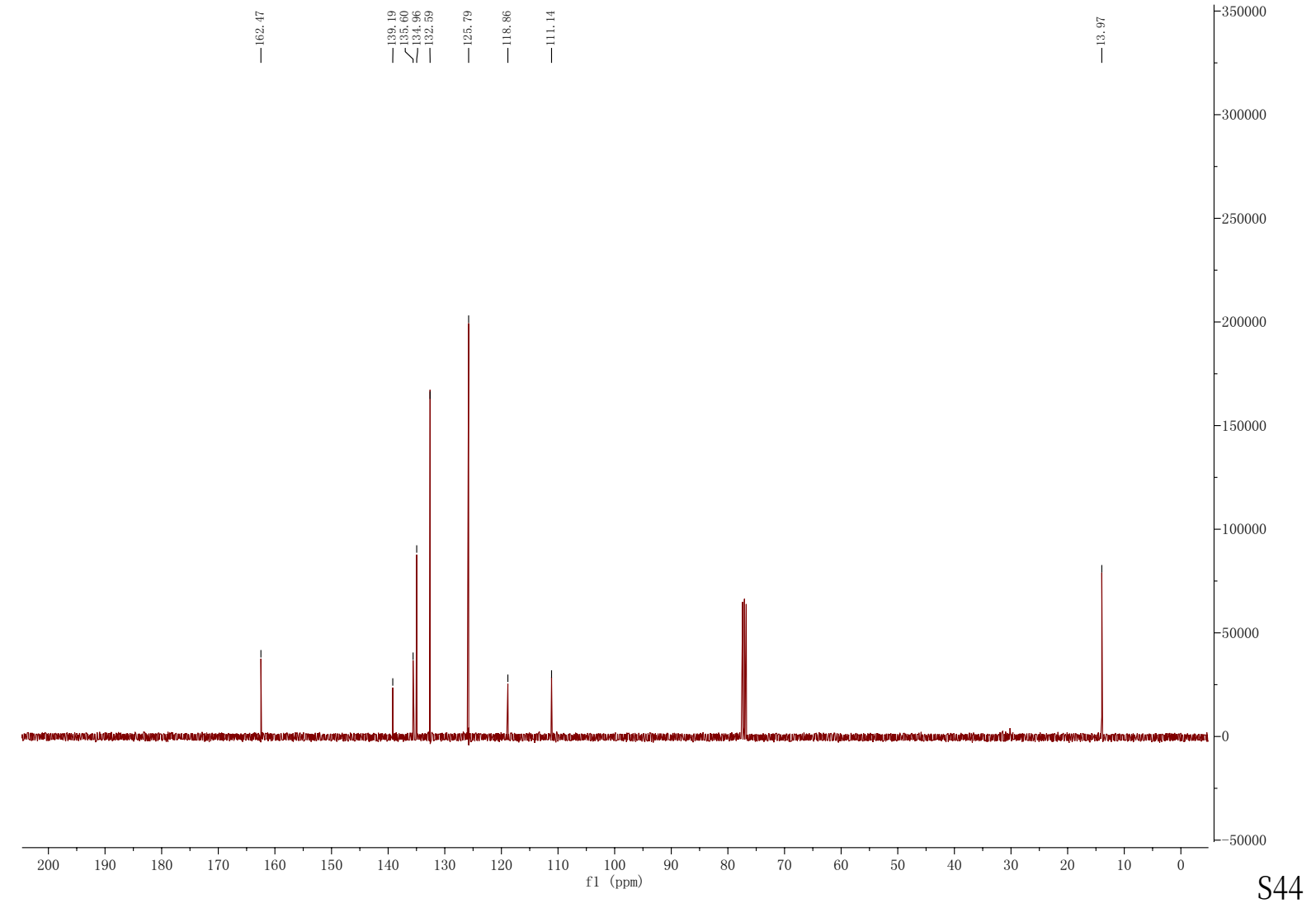
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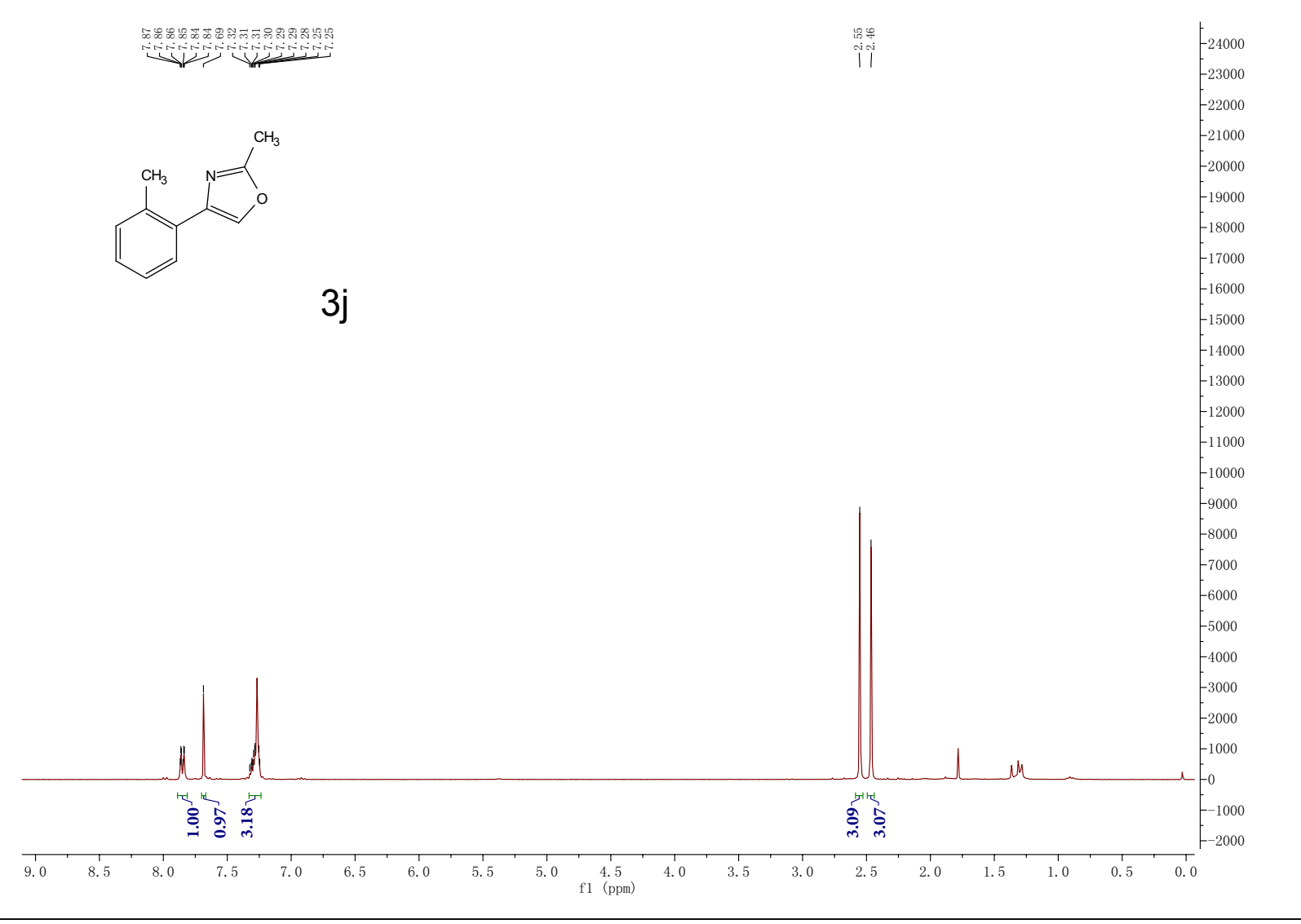
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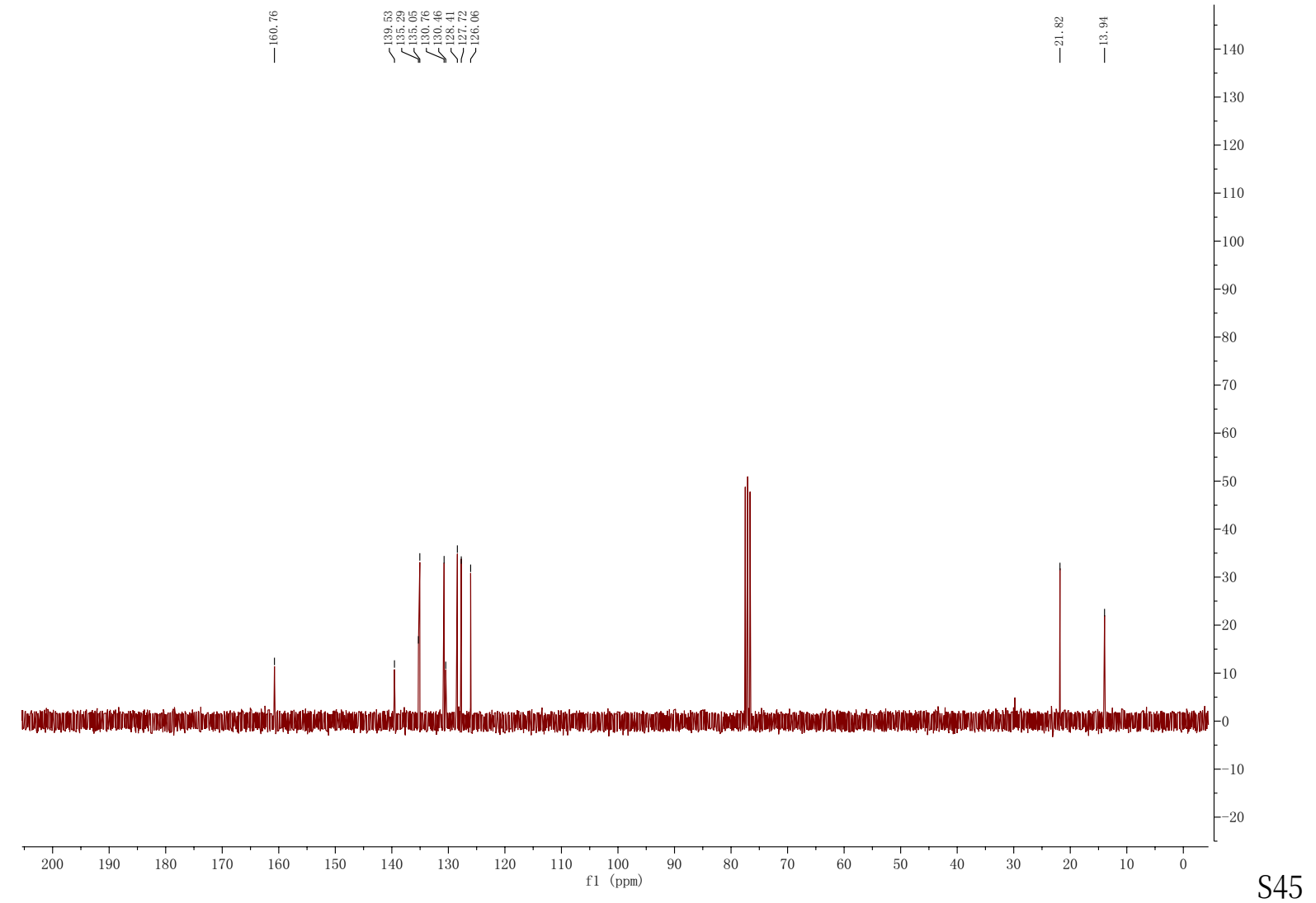
f1 (ppm)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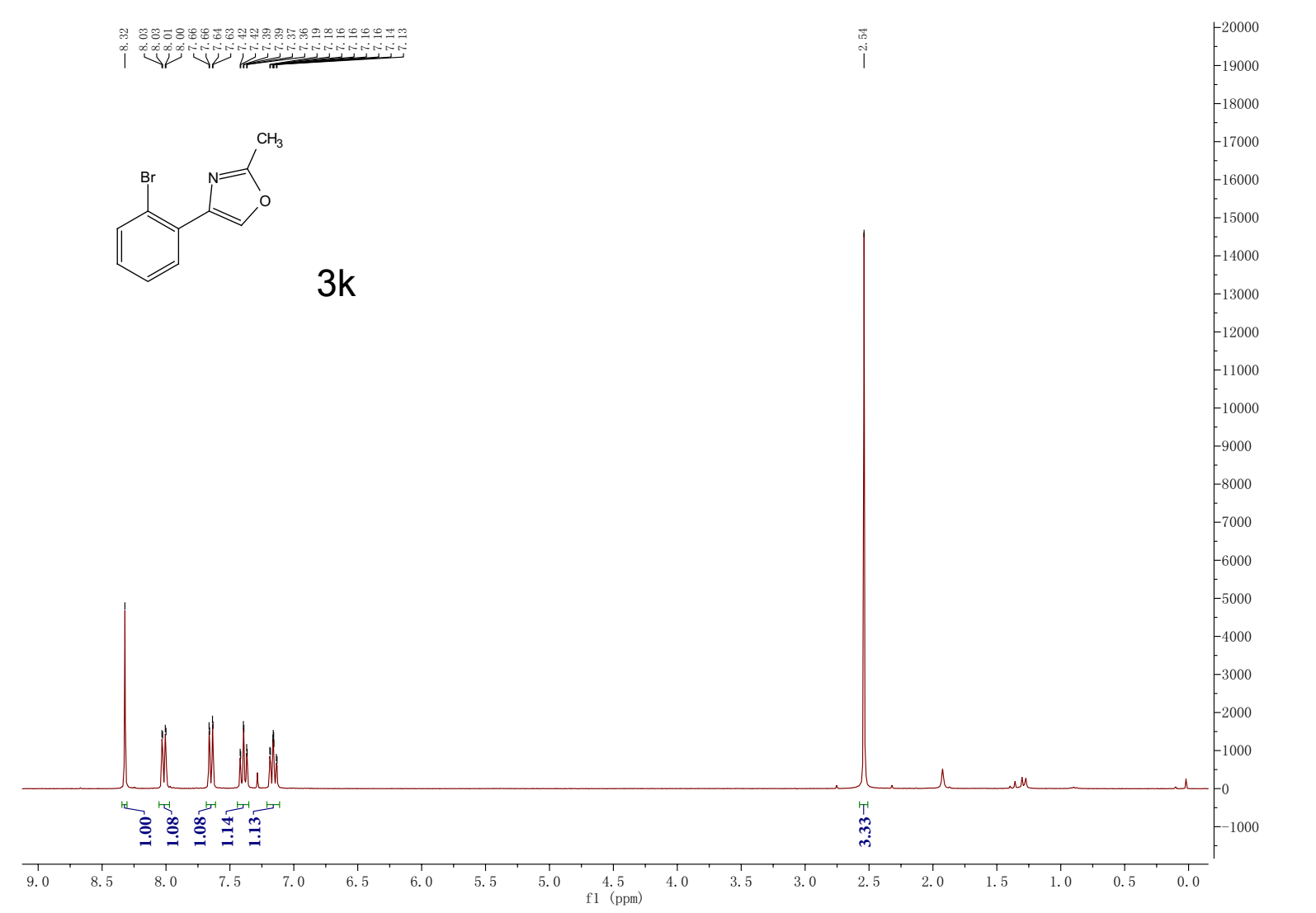
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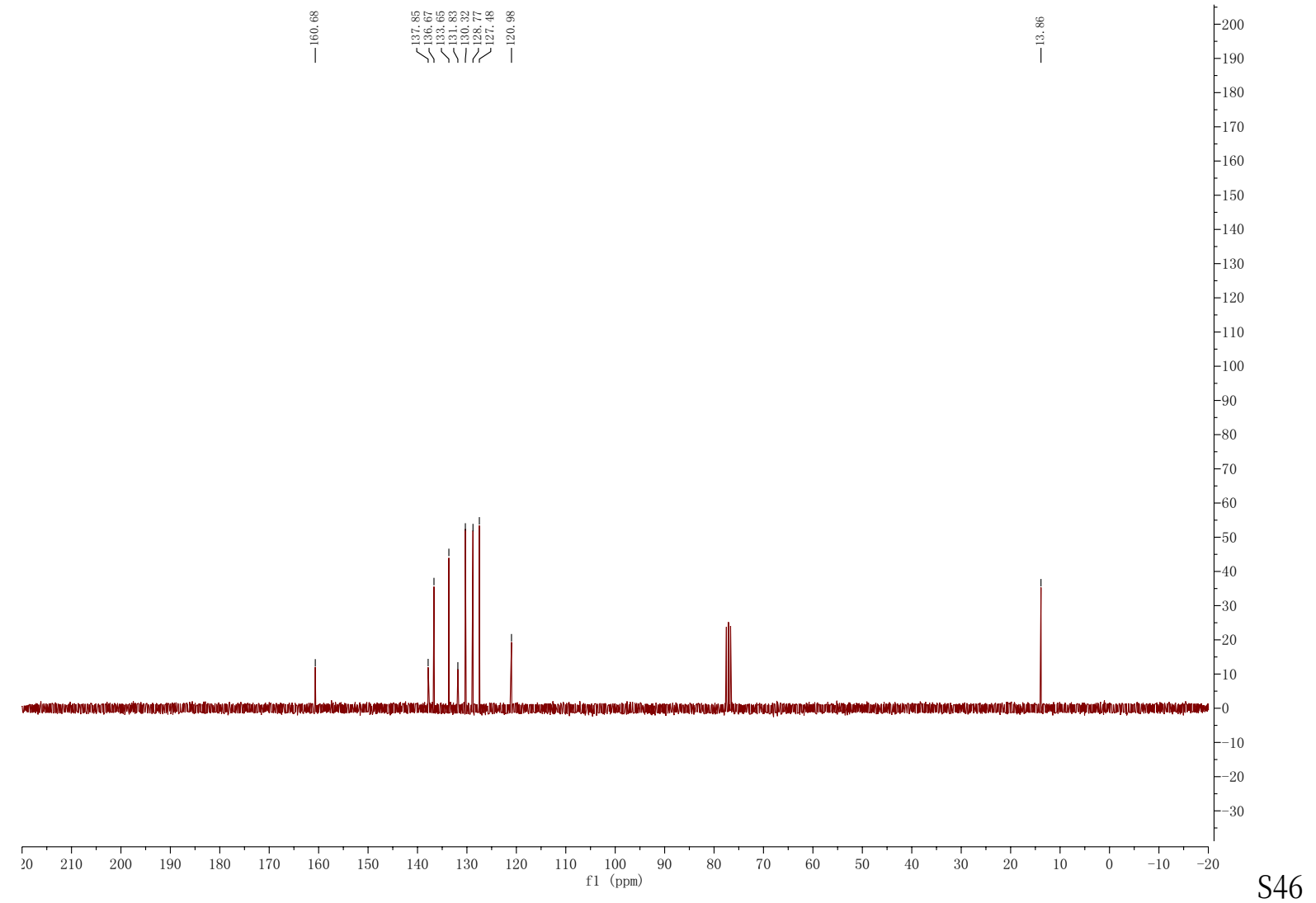
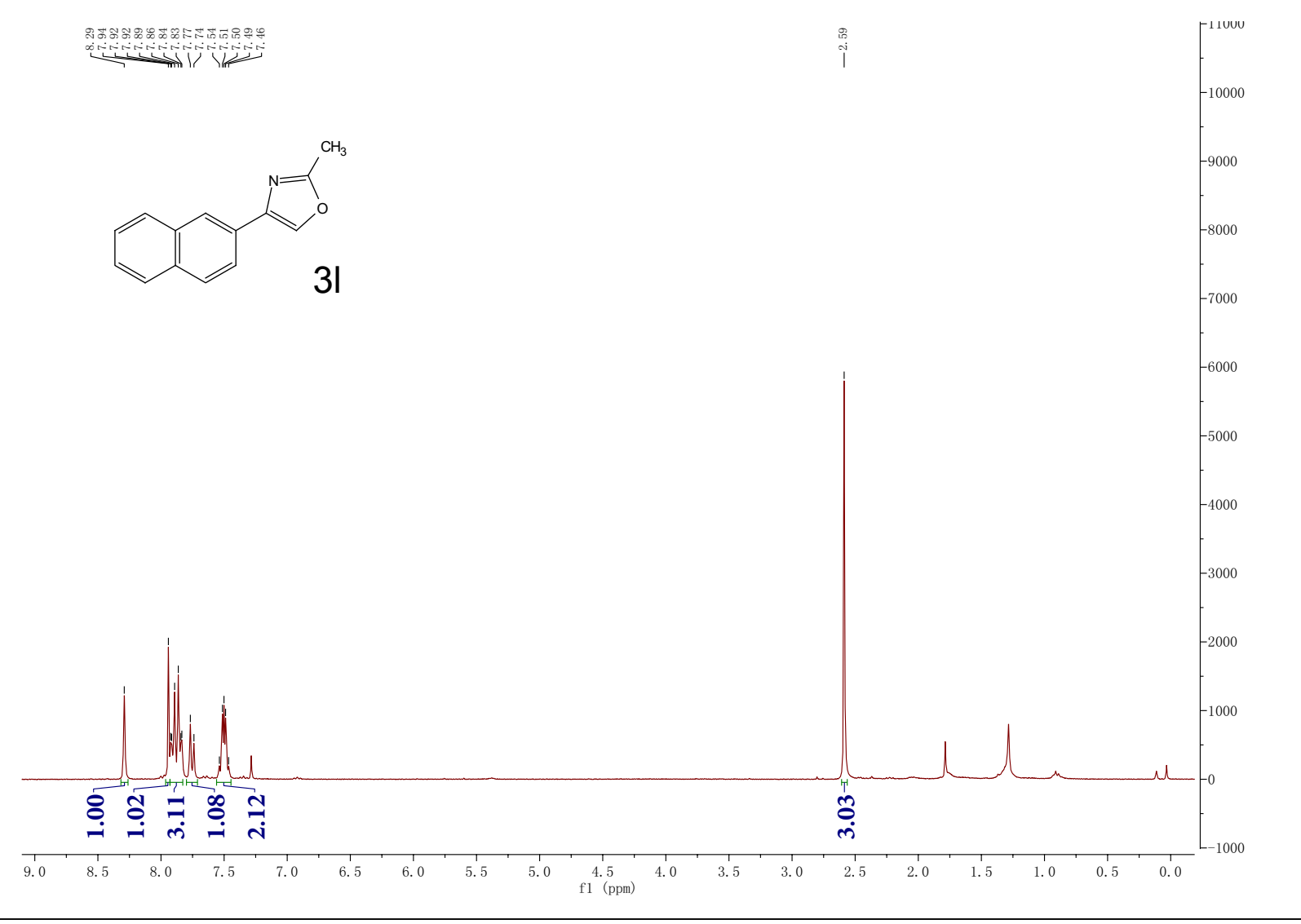
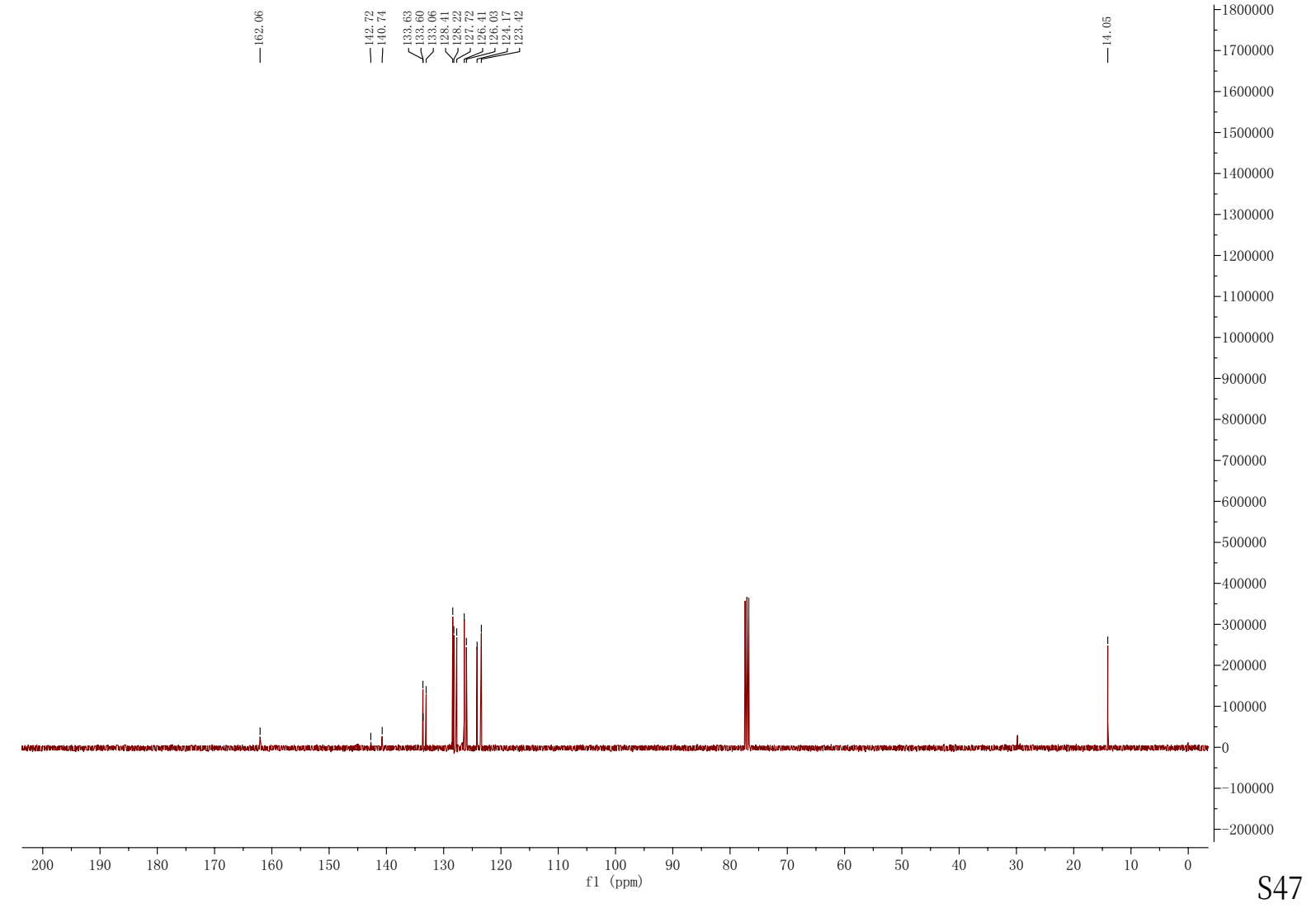
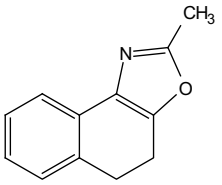
7.16
7.16
7.14
7.13
2.54
CH3
Br
N
O
3k
1.00
1.08
1.08
1.14
1.13
3.33
f1 (ppm)


160.68
137.85
136.67
133.65
131.83
130.32
128.77
127.48
120.98
13.86
f1 (ppm)

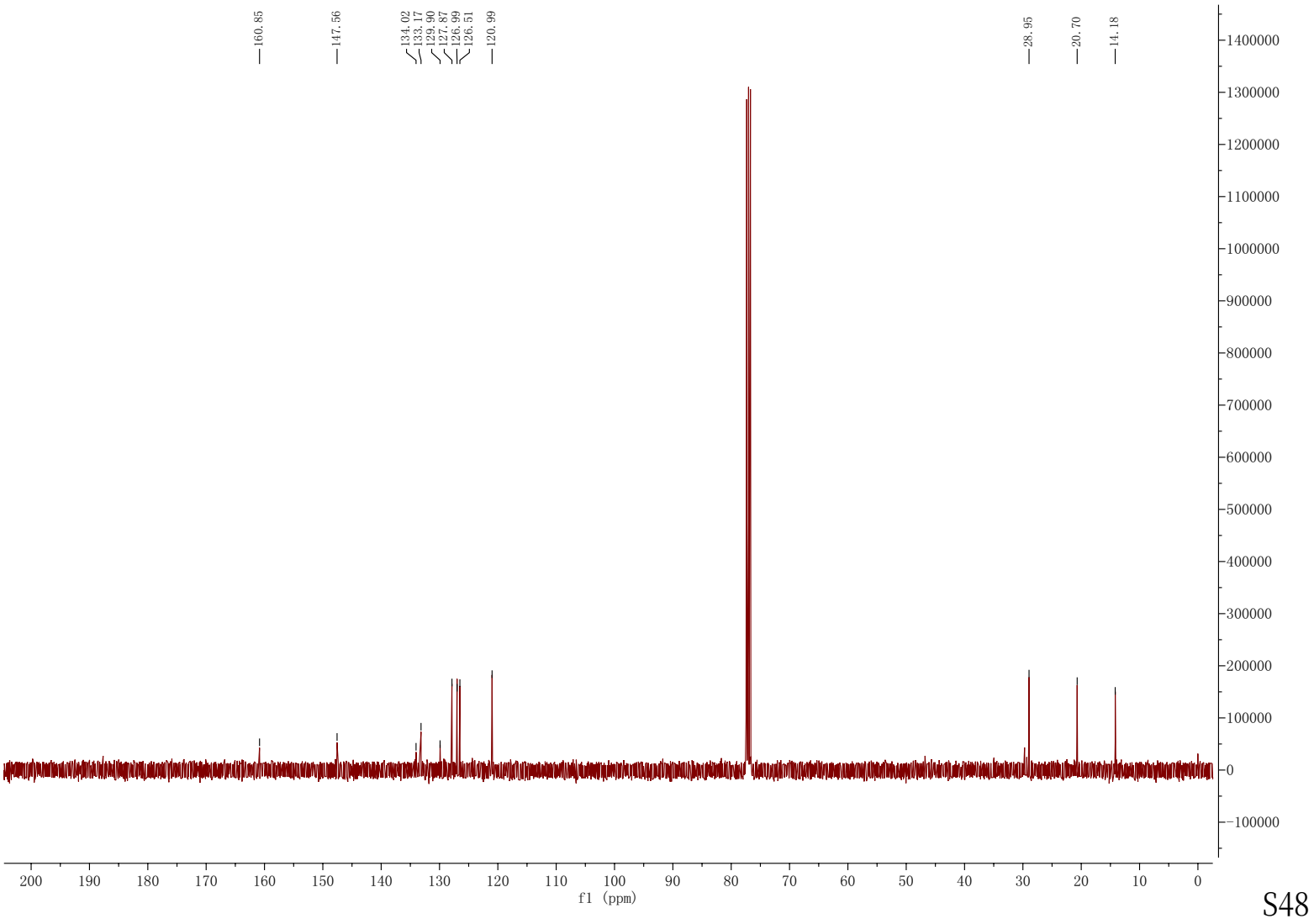

8.29
7.94
7.92
7.92
7.89
7.86
7.84
7.83
7.77
7.74
7.54
7.51
7.50
7.49
7.46
2.59
CH3
N
O
3l
1.00
1.02
3.11
1.08
2.12
3.03
f1 (ppm)

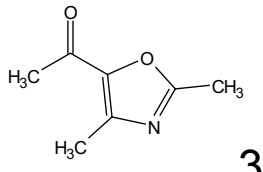

162.06
142.72
140.74
133.63
133.60
133.06
128.41
128.22
127.72
126.41
126.03
124.17
123.42
14.05
f1 (ppm)


CH3
N
O

3m

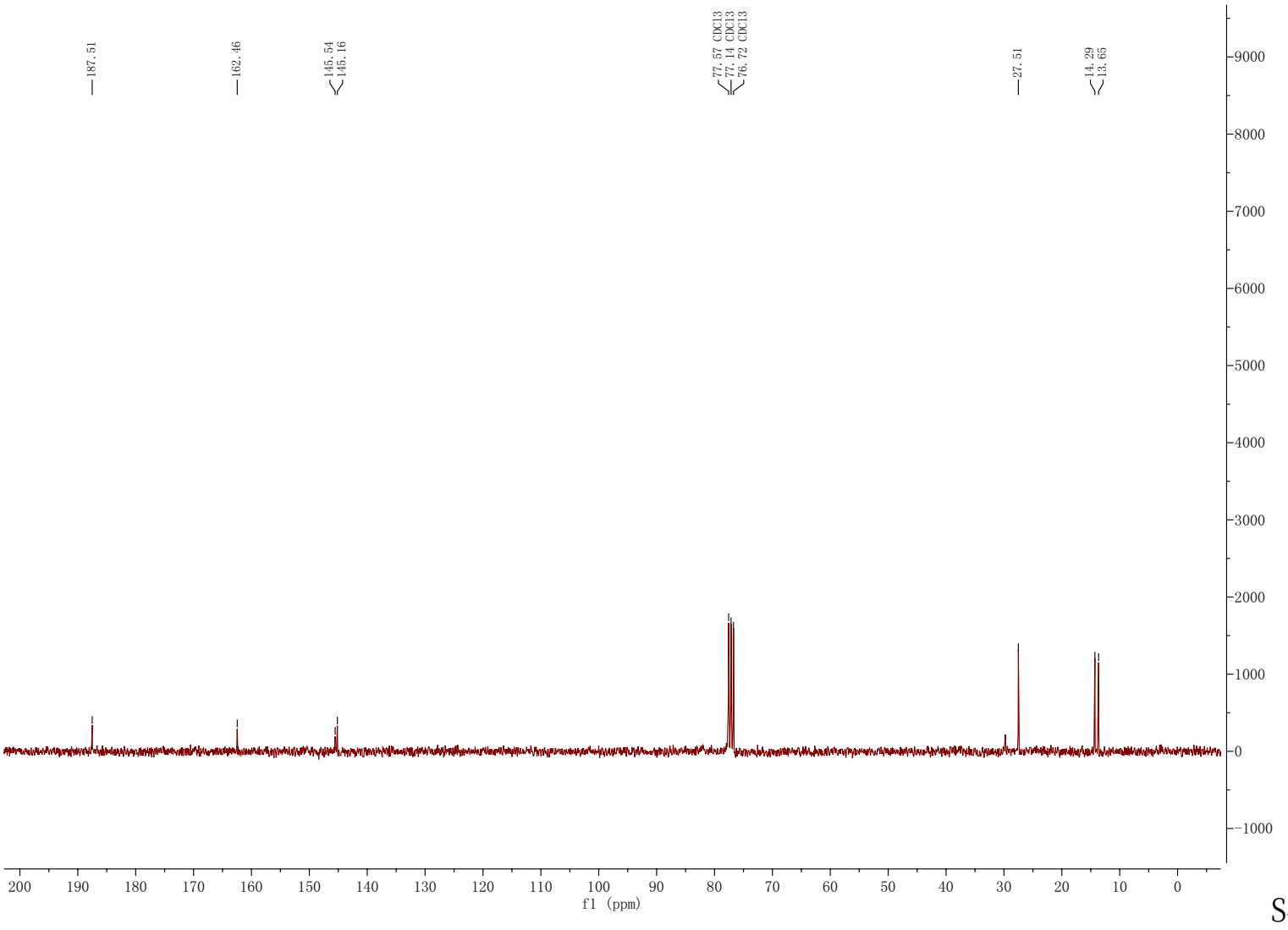
7.62
7.59
7.27
7.24
7.19
7.18
7.18
7.17
7.15
3.18
3.15
3.13
2.99
2.97
2.94
2.53
1.00
2.97
2.11
2.09
3.01
f1 (ppm)


160.85
147.56
134.02
133.17
129.90
127.87
126.99
126.51
120.99
28.95
20.70
14.18
f1 (ppm)


O
H_3C
O
CH_3
N
H_3C

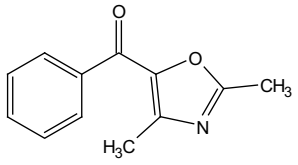
3n

2.50
2.45
3.00
6.08
f1 (ppm)


187.51
162.46
145.54
145.16
77.57 CDCl3
77.14 CDCl3
76.72 CDCl3
27.51
14.29
13.65
f1 (ppm)


7.99
7.99
7.98
7.97
7.96
7.96
7.63
7.62
7.62
7.61
7.60
7.59
7.58
7.58
7.57
7.53
7.50
7.48


2.56
2.49


O
O
CH3
N
H3C

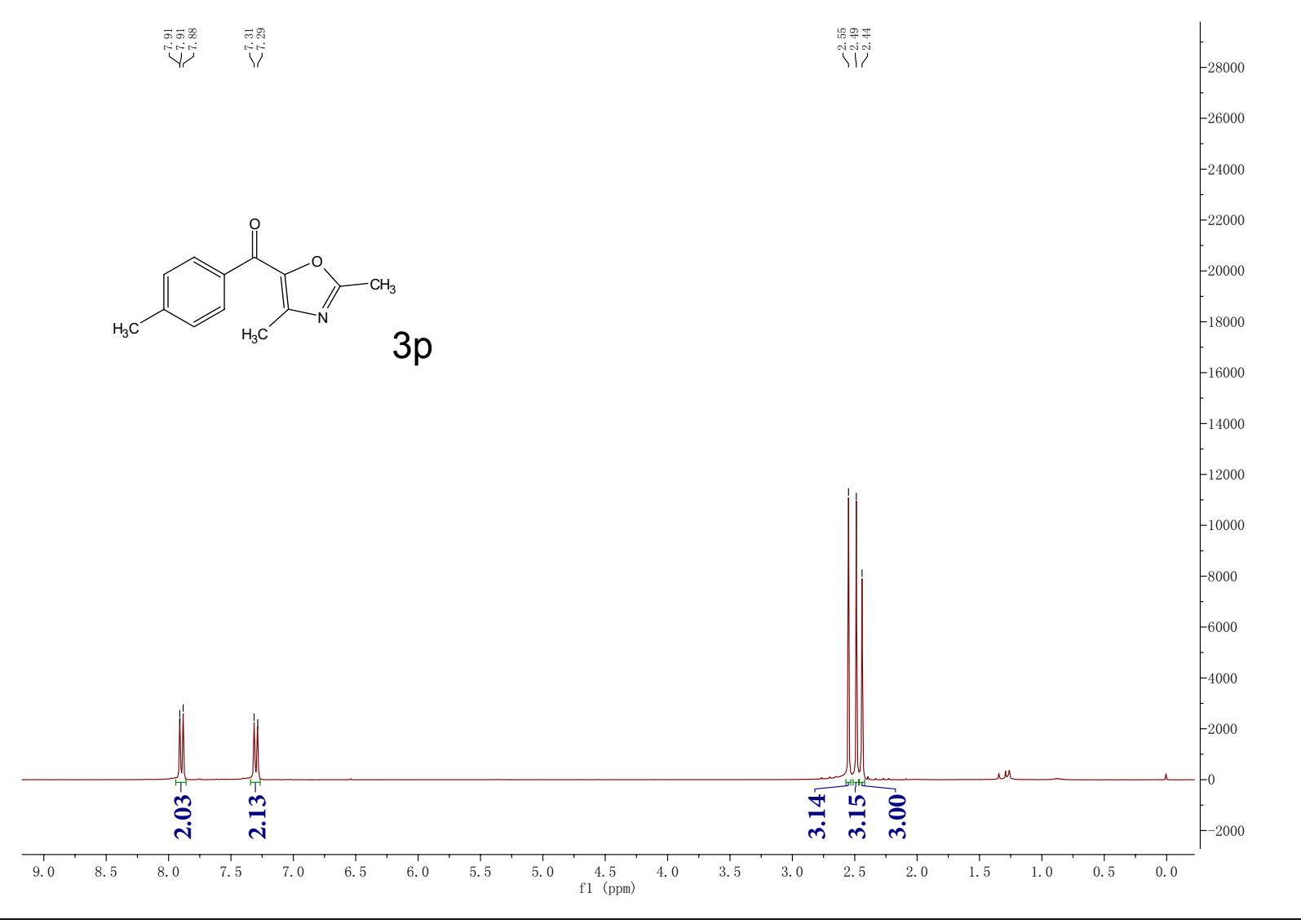
3o

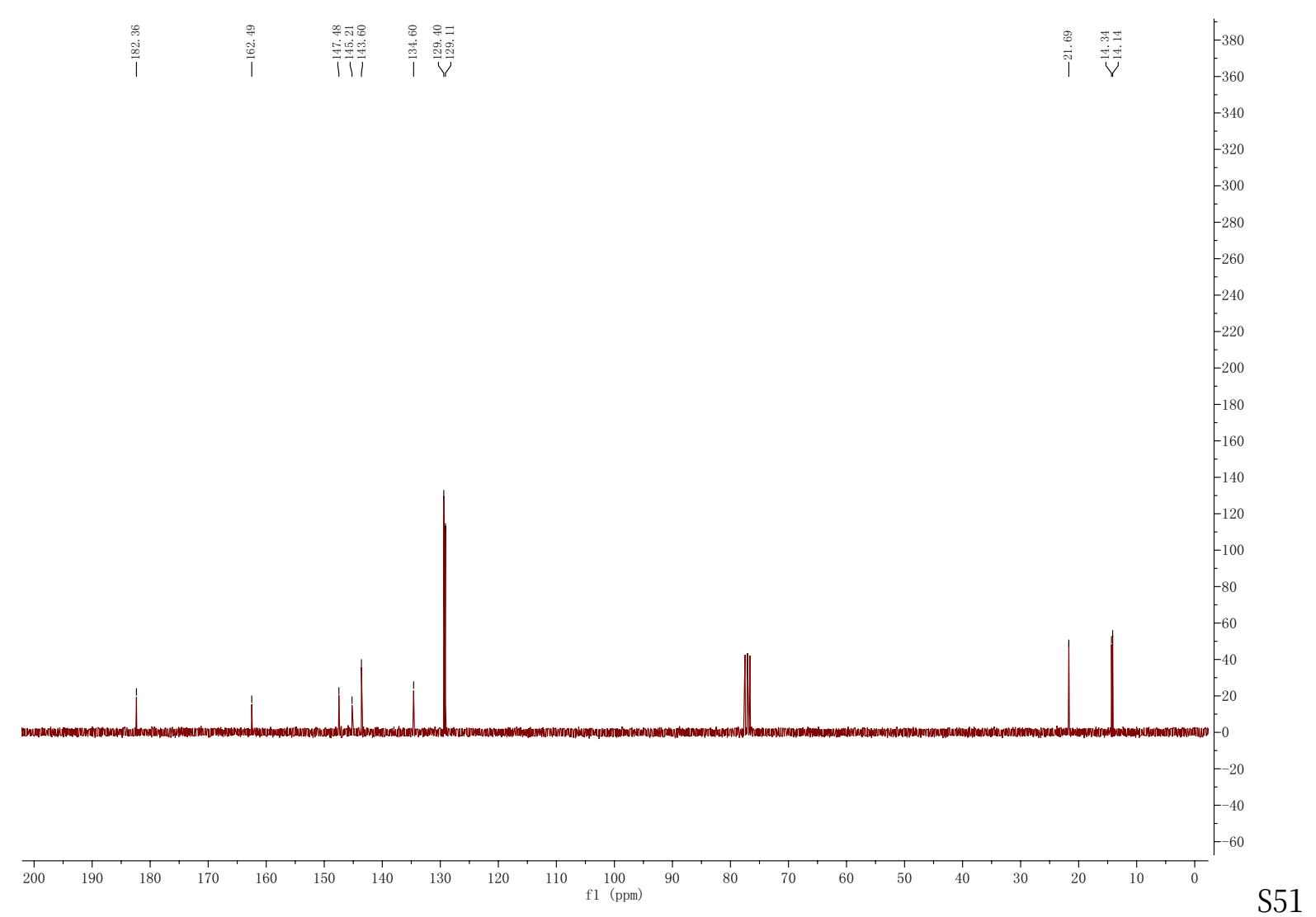
1.98
1.03
2.09
3.00
2.99
f1 (ppm)

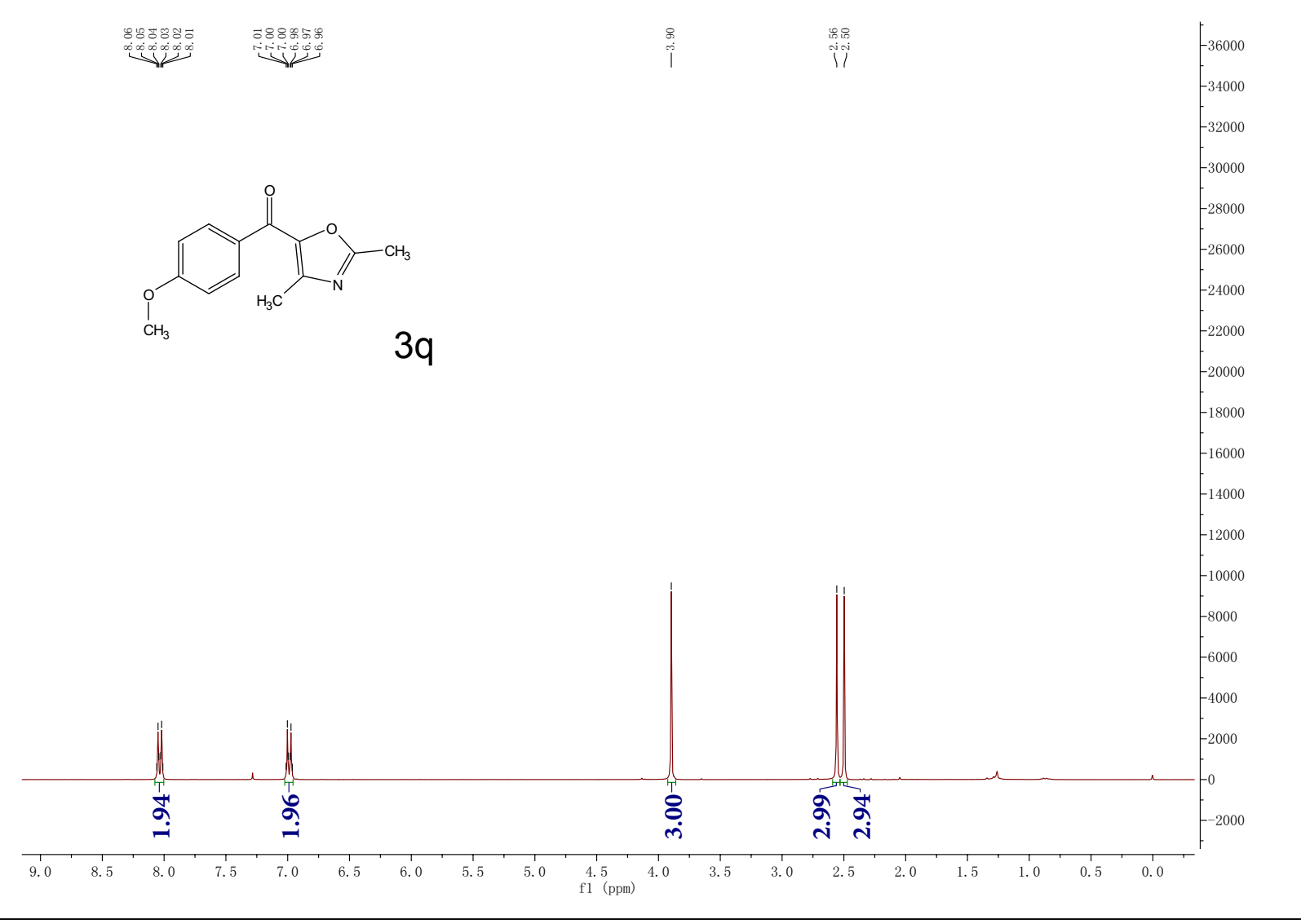

182.69
162.74
147.89
145.13
132.74
129.22
128.41

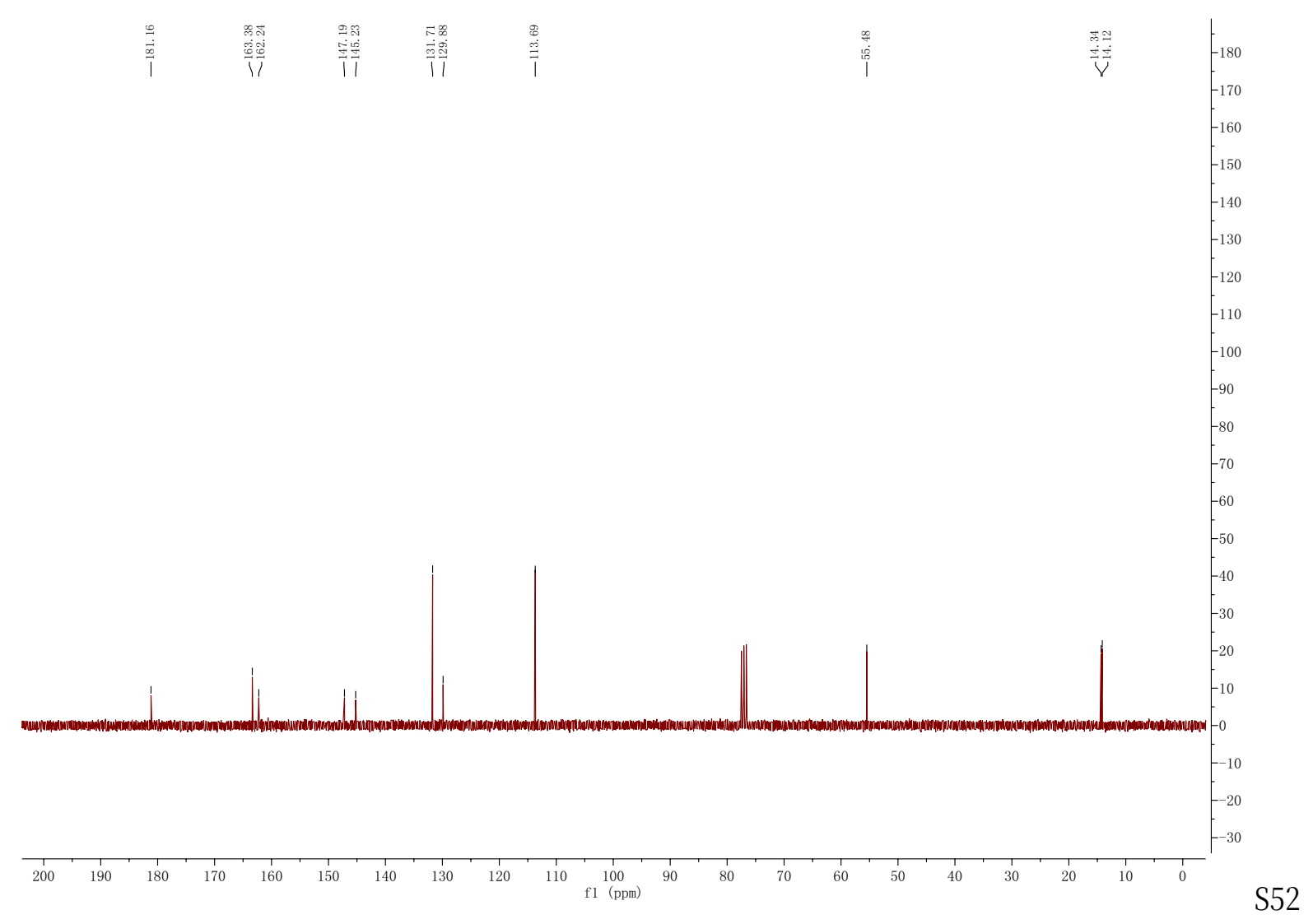

14.36
14.16

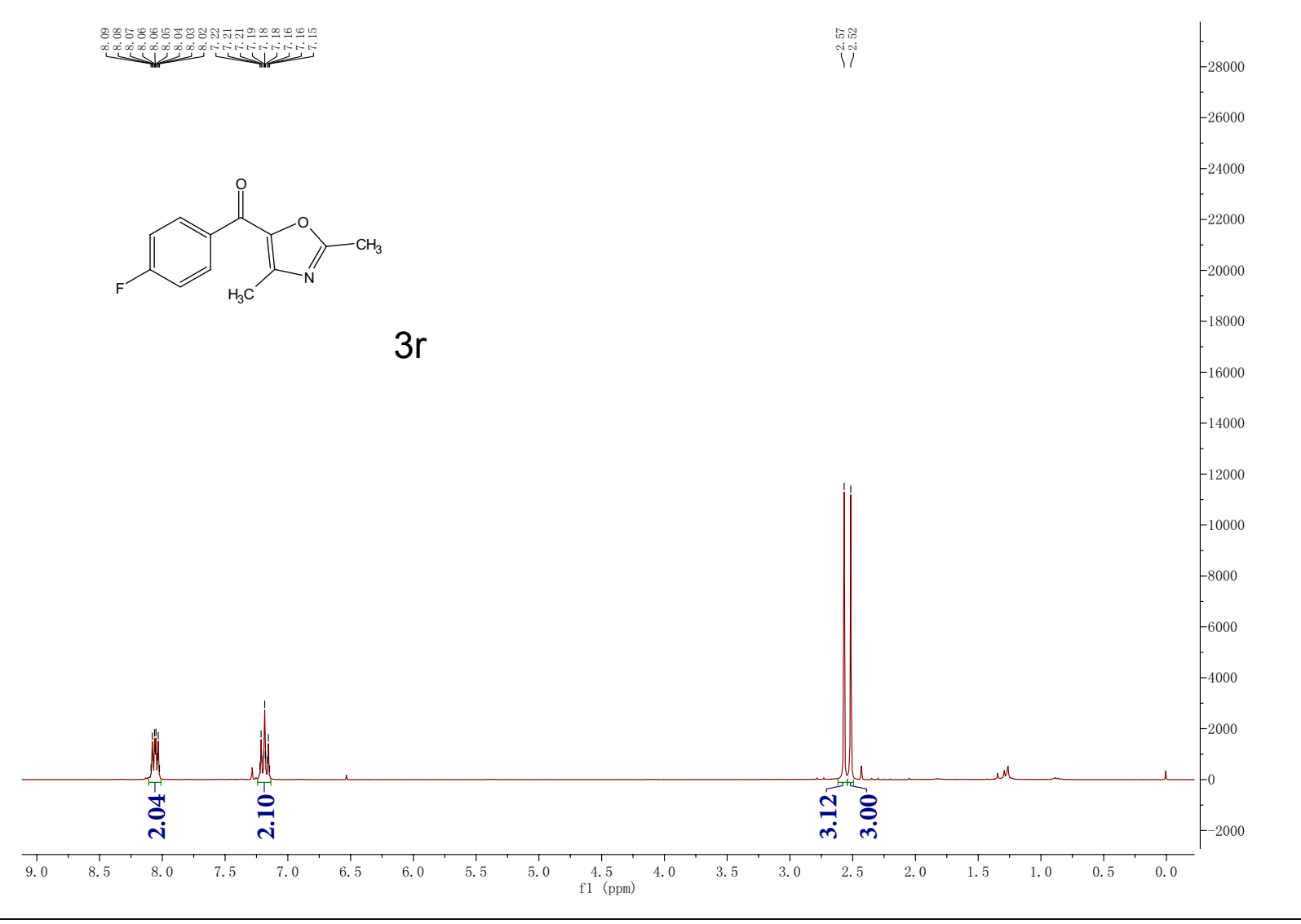
f1 (ppm)

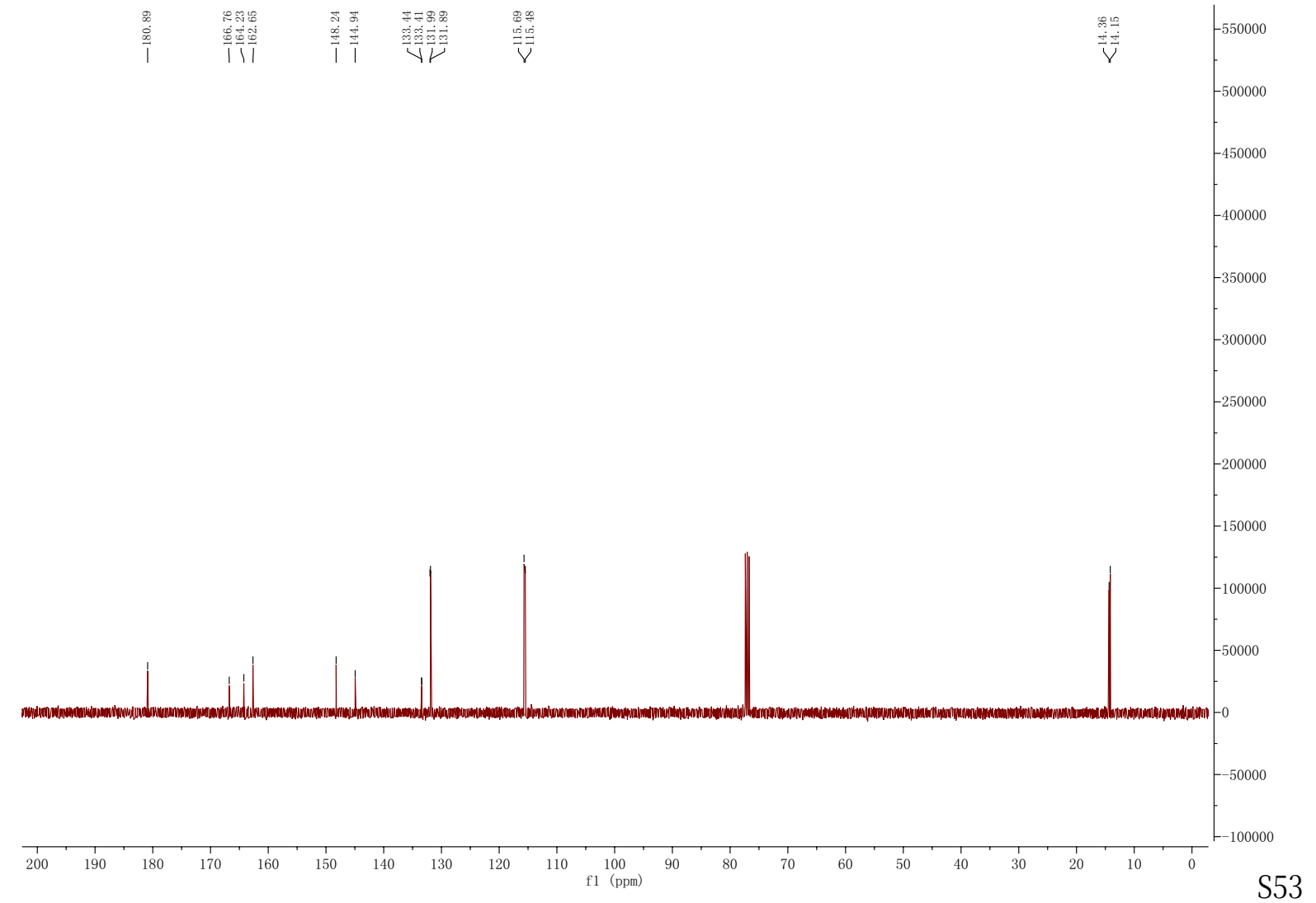

7.91
7.91
7.88
7.31
7.29
2.55
2.49
2.44
O
O
CH3
H3C
N
H3C
3p
2.03
2.13
3.14
3.15
3.00
f1 (ppm)


182.36
162.49
147.48
145.21
143.60
134.60
129.40
129.11
21.69
14.34
14.14
f1 (ppm)

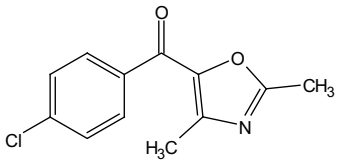

8.06
8.05
8.04
8.03
8.02
8.01
7.01
7.00
7.00
6.98
6.97
6.96
3.90
2.56
2.50
O
O
CH3
N
H3C
O
CH3
3q
1.94
1.96
3.00
2.99
2.94
f1 (ppm)


181.16
163.38
162.24
147.19
145.23
131.71
129.88
113.69
55.48
14.34
14.12
f1 (ppm)

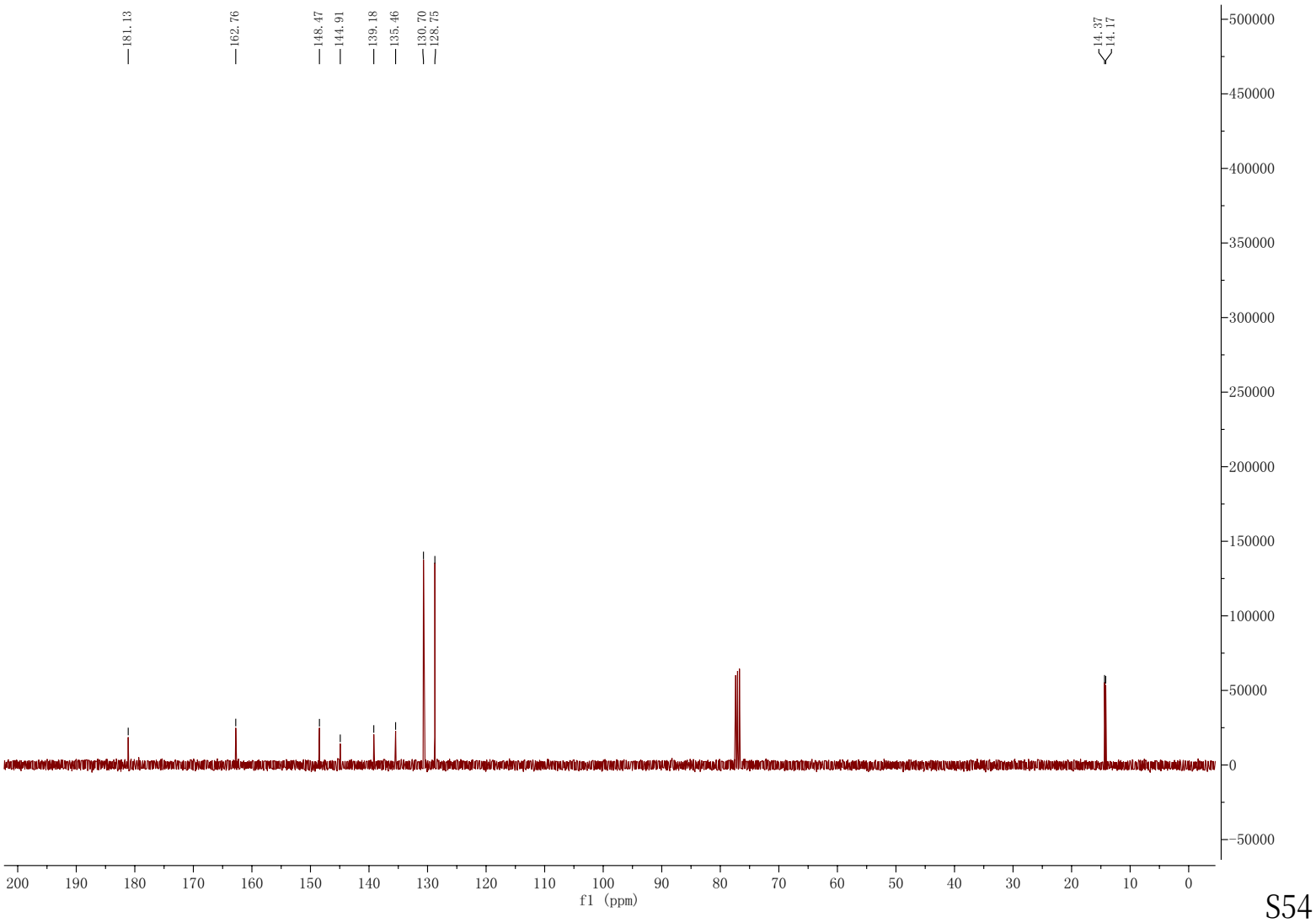

8.09
8.08
8.07
8.06
8.06
8.05
8.04
8.03
8.02
7.22
7.21
7.21
7.19
7.18
7.18
7.16
7.16
7.15
2.57
2.52
O
O
CH3
N
F
H3C
3r
2.04
2.10
3.12
3.00
f1 (ppm)

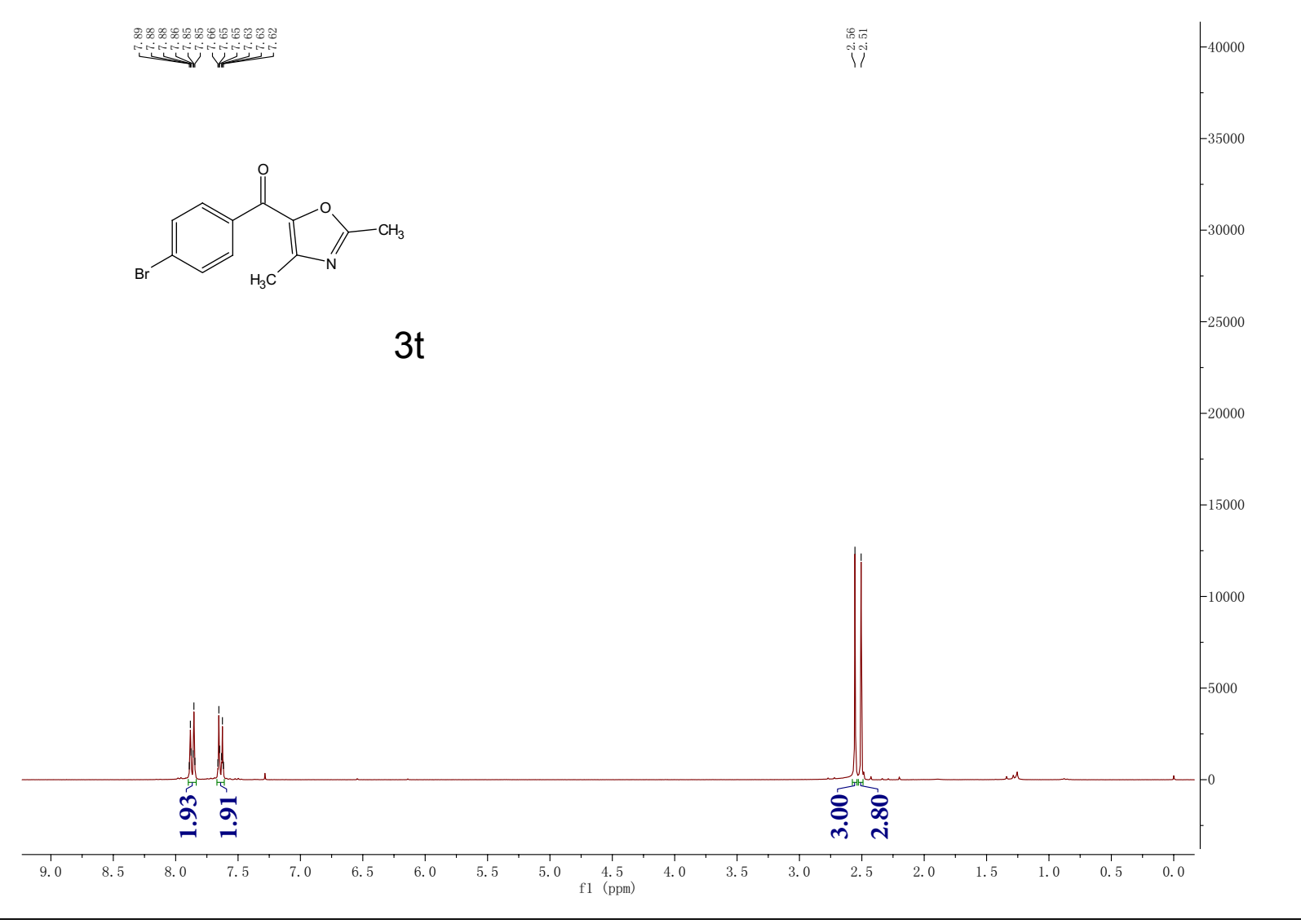

180.89
166.76
164.23
162.65
148.24
144.94
133.44
133.41
131.99
131.89
115.69
115.48
14.36
14.15
f1 (ppm)

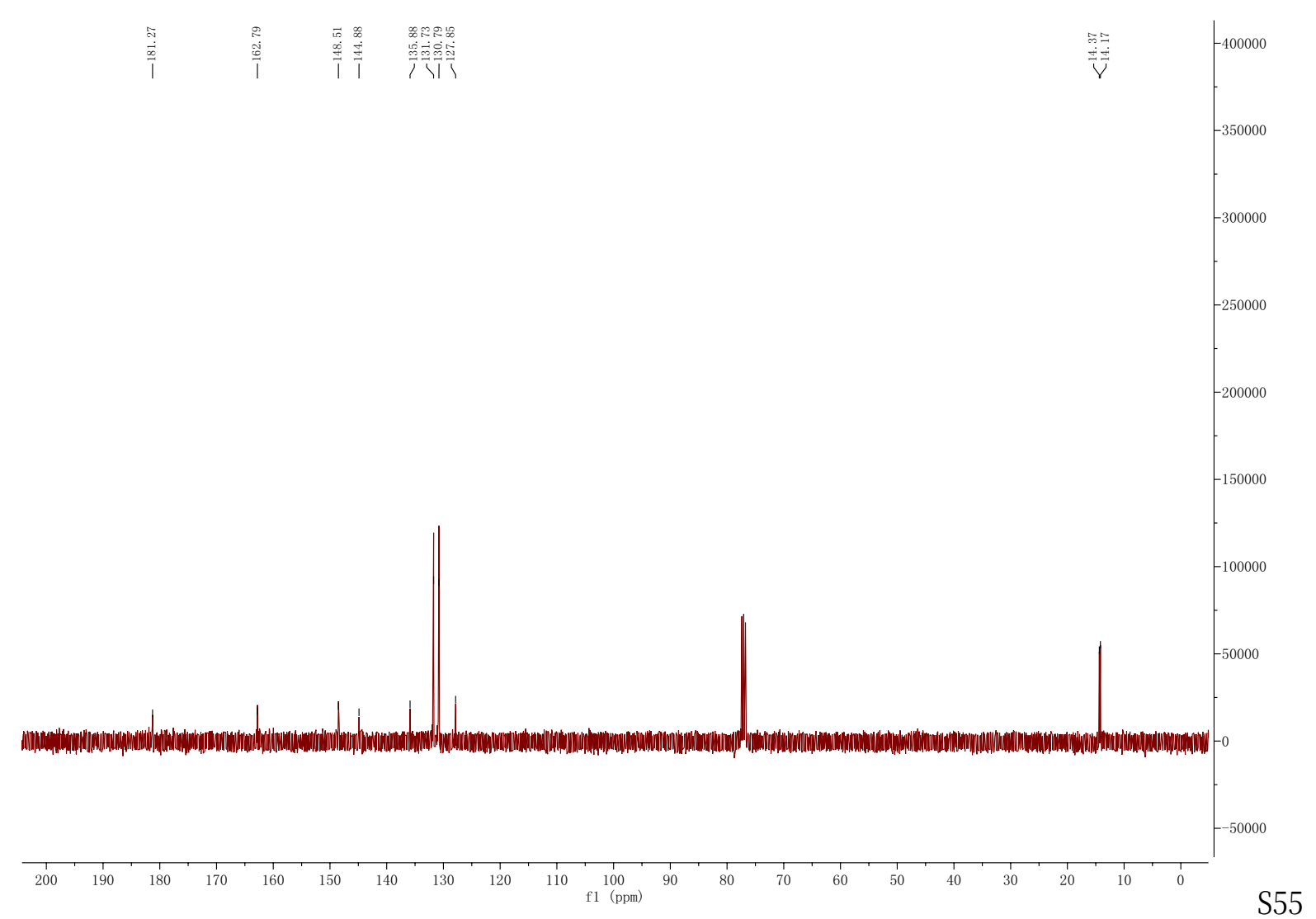
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.99 – 7.93 (m, 1H).

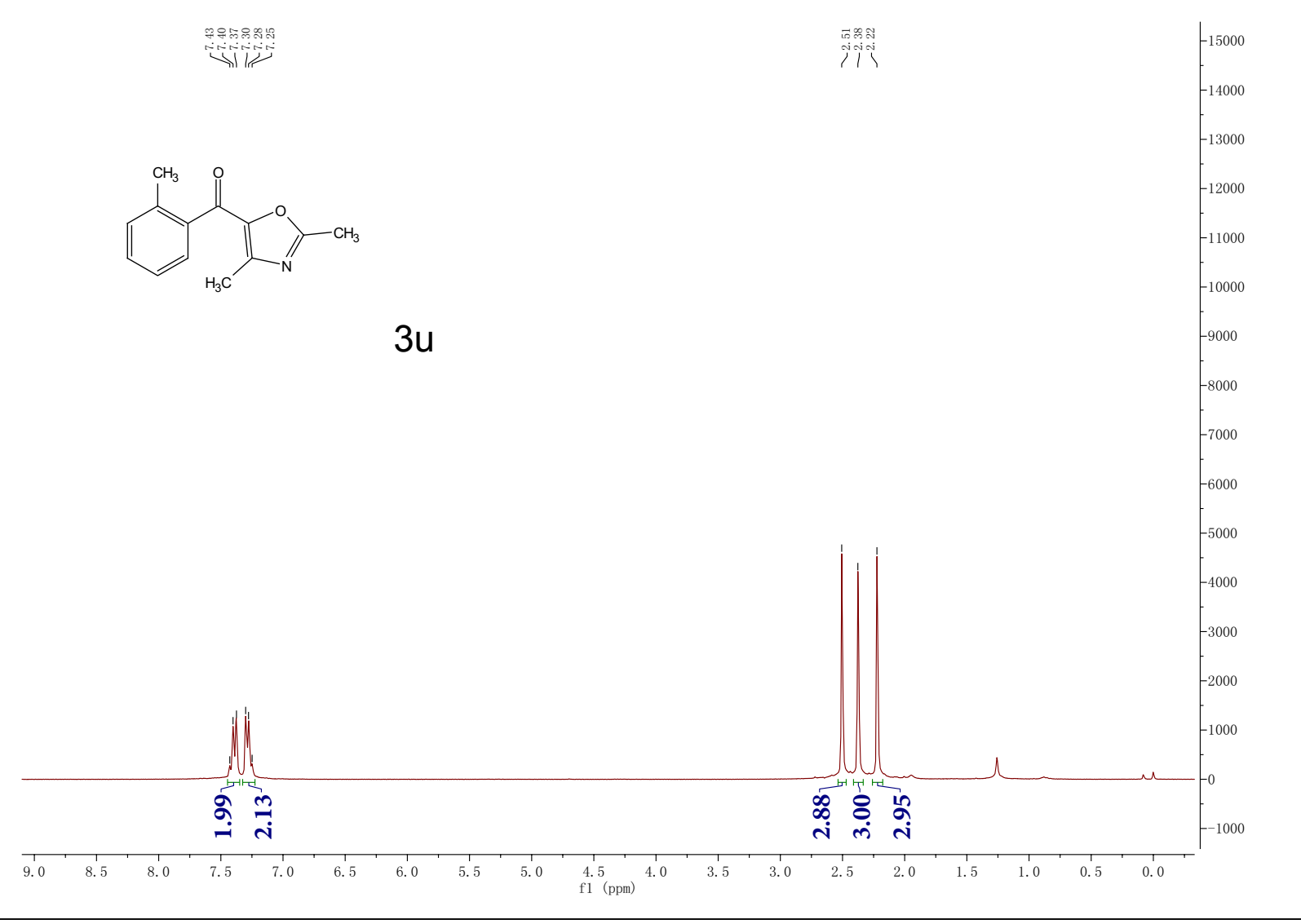


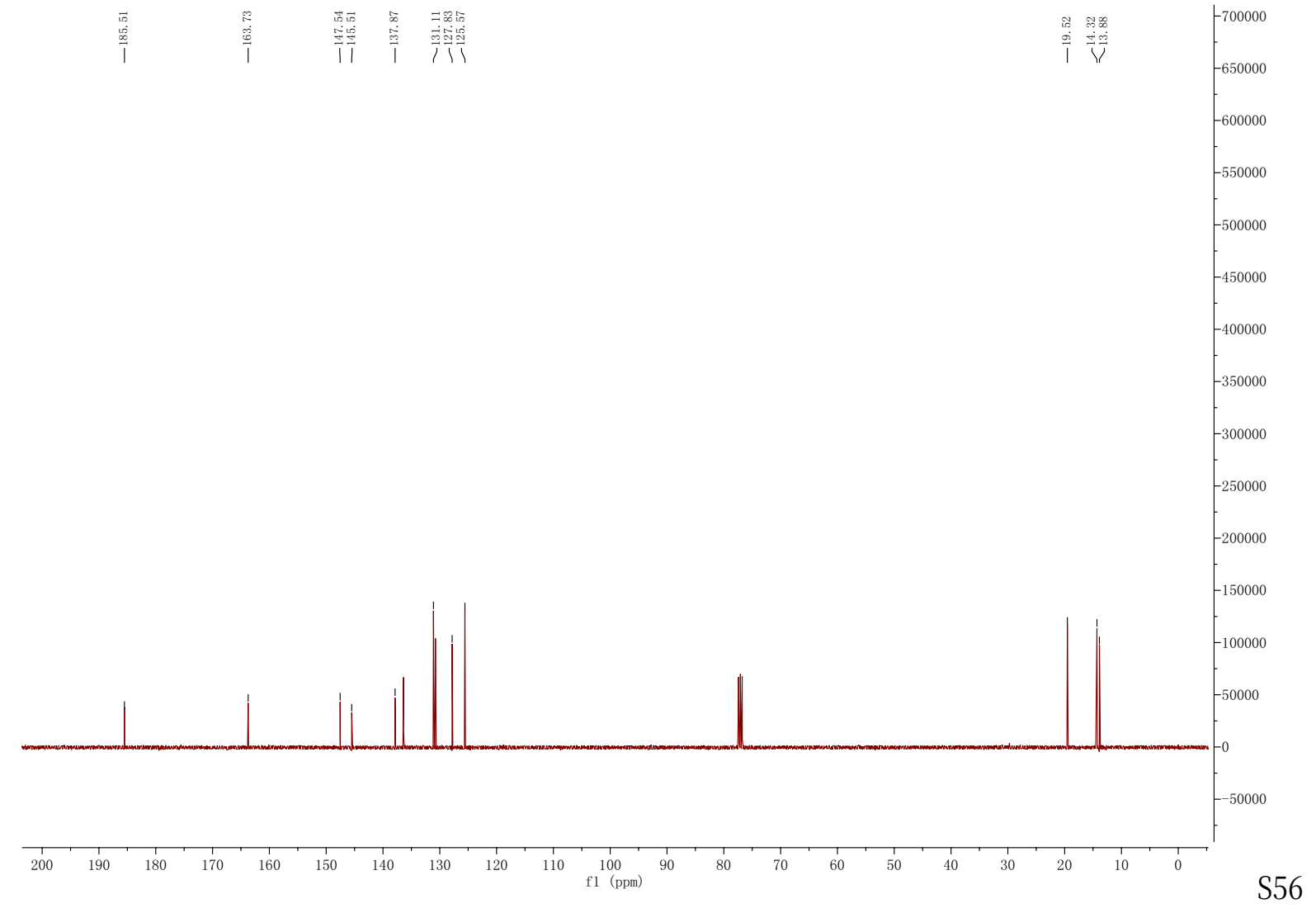
3s

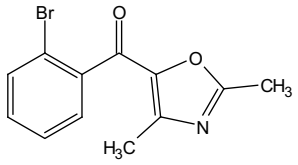



7.89
7.88
7.88
7.86
7.85
7.85
7.66
7.65
7.65
7.63
7.63
7.62
2.56
2.51
O
O
CH3
N
H3C
Br
3t
1.93
1.91
3.00
2.80
f1 (ppm)


181.27
162.79
148.51
144.88
135.88
131.73
130.79
127.85
14.37
14.17
f1 (ppm)

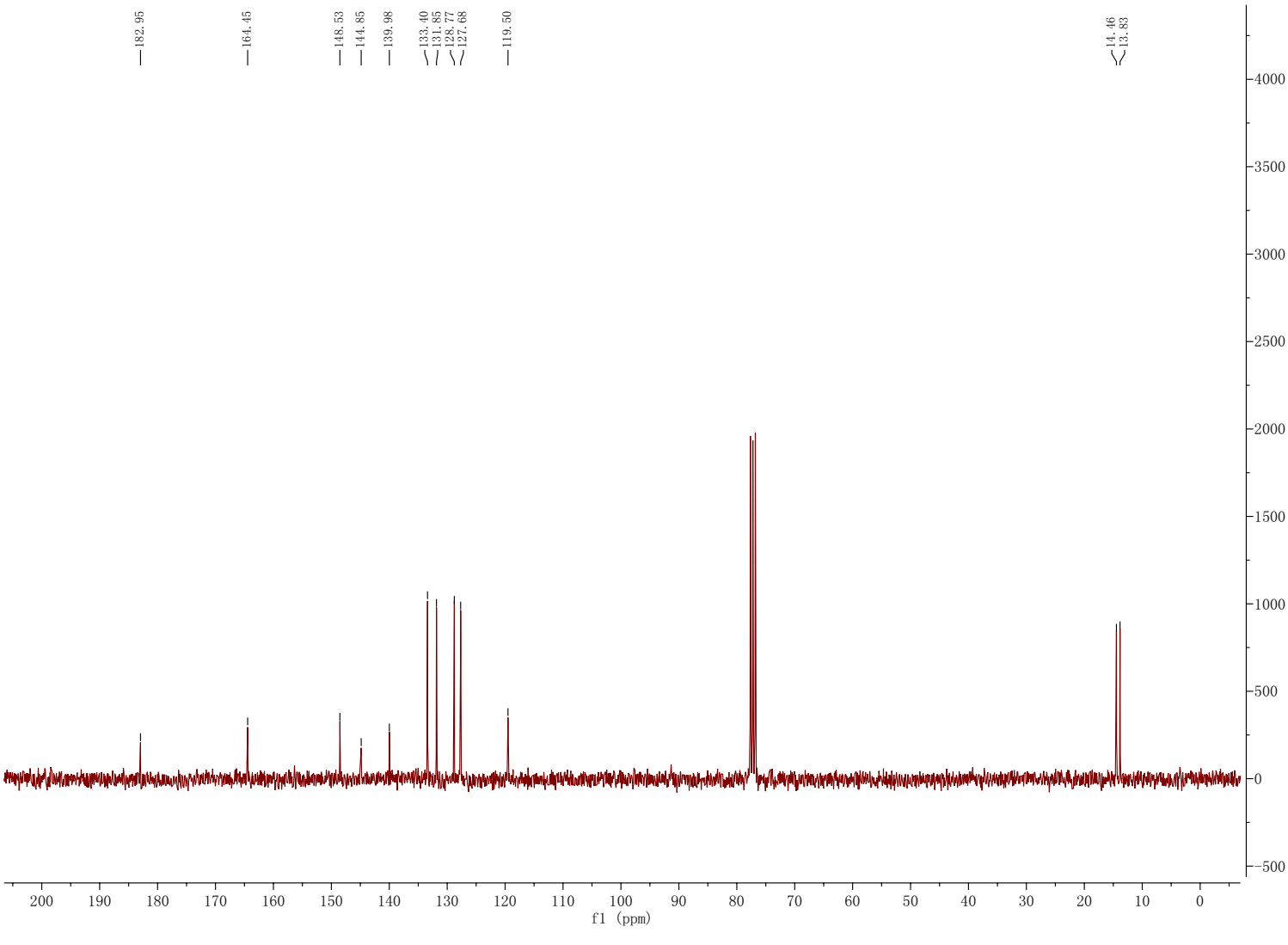

7.43
7.40
7.37
7.30
7.28
7.25
2.51
2.38
2.22
CH3
O
O
CH3
N
H3C
3u
1.99
2.13
2.88
3.00
2.95
f1 (ppm)

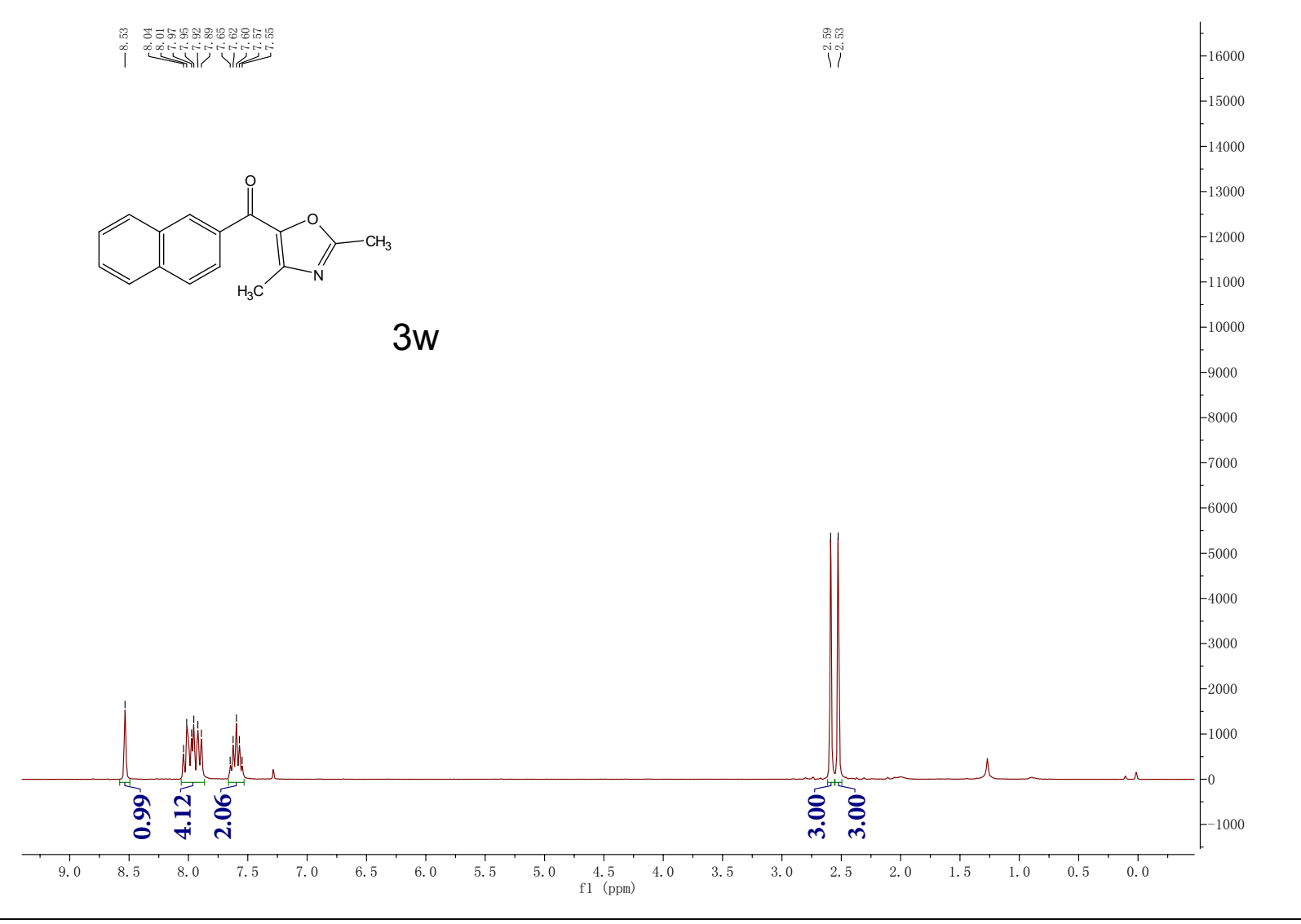

185.51
163.73
147.54
145.51
137.87
131.11
127.83
125.57
19.52
14.32
13.88
f1 (ppm)

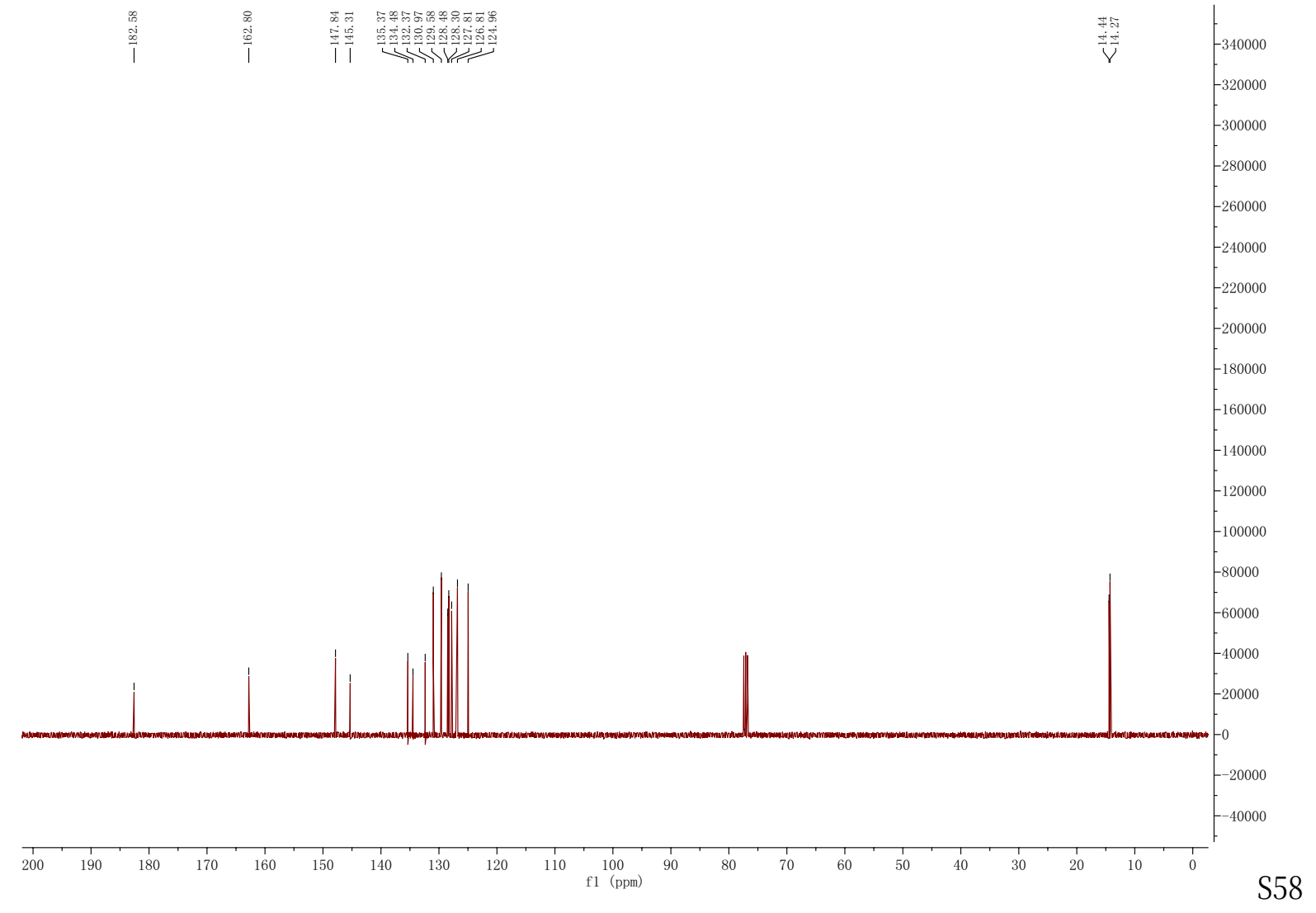

Br
O
O
CH3
N
H3C

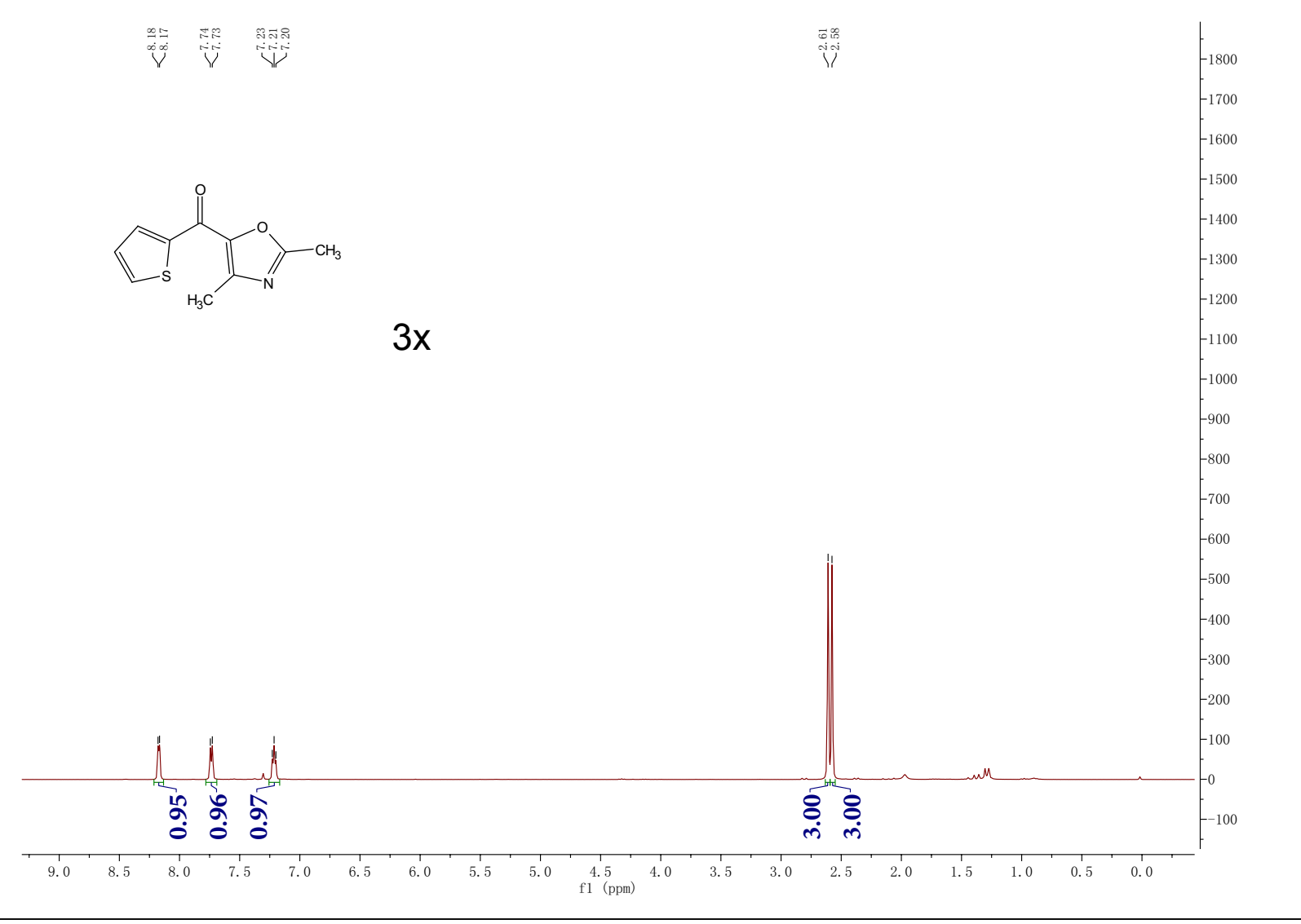
3v

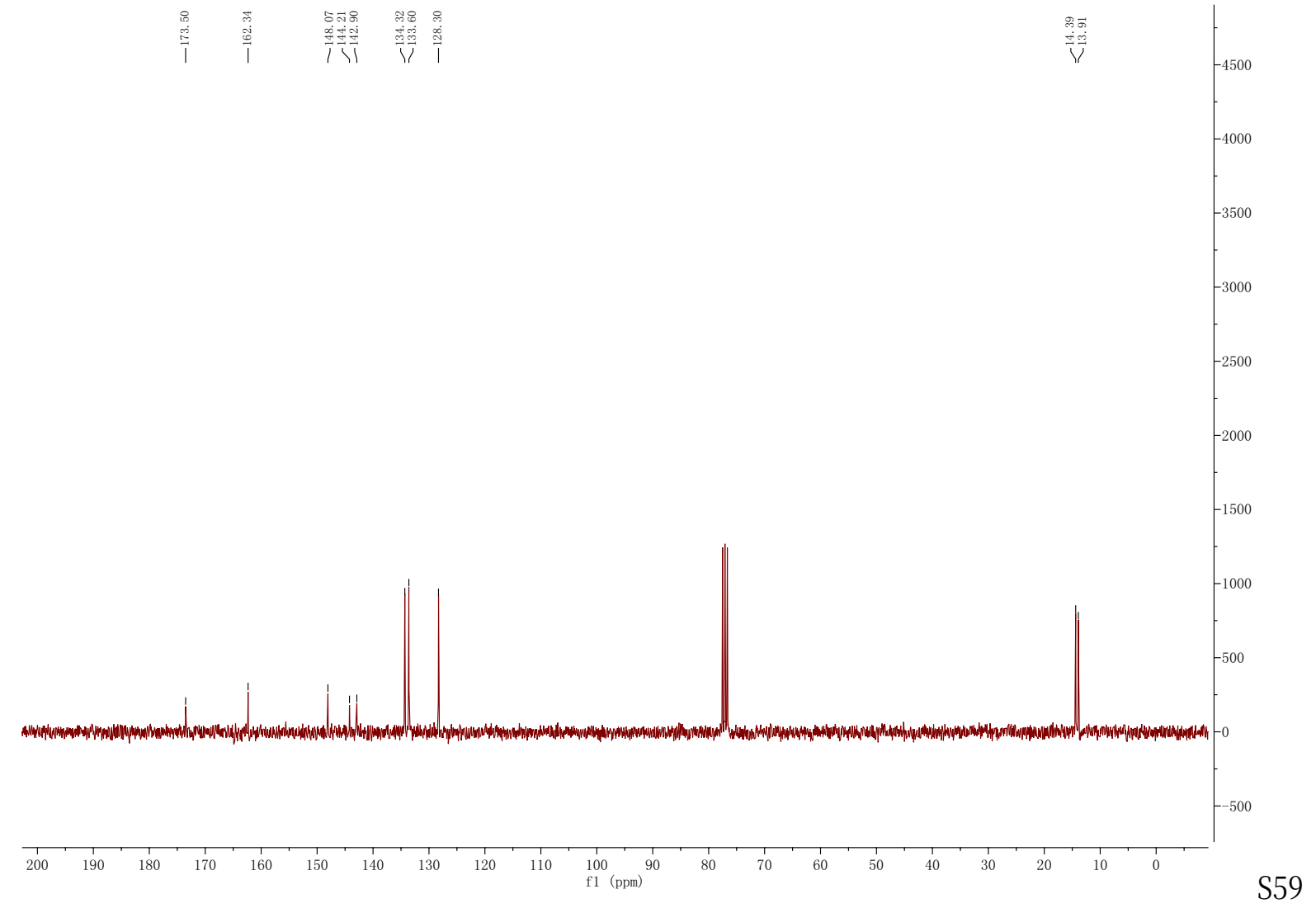
1.03
3.09
3.04
3.00
f1 (ppm)

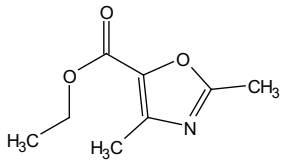

182.95
164.45
148.53
144.85
139.98
133.40
131.85
128.77
127.68
119.50
14.46
13.83
f1 (ppm)


8.53
8.04
8.01
7.97
7.95
7.92
7.89
7.65
7.62
7.60
7.57
7.55
2.59
2.53
O
O
CH3
N
H3C
3w
0.99
4.12
2.06
3.00
3.00
f1 (ppm)


182.58
162.80
147.84
145.31
135.37
134.48
132.37
130.97
129.58
128.48
128.30
127.81
126.81
124.96
14.44
14.27
f1 (ppm)

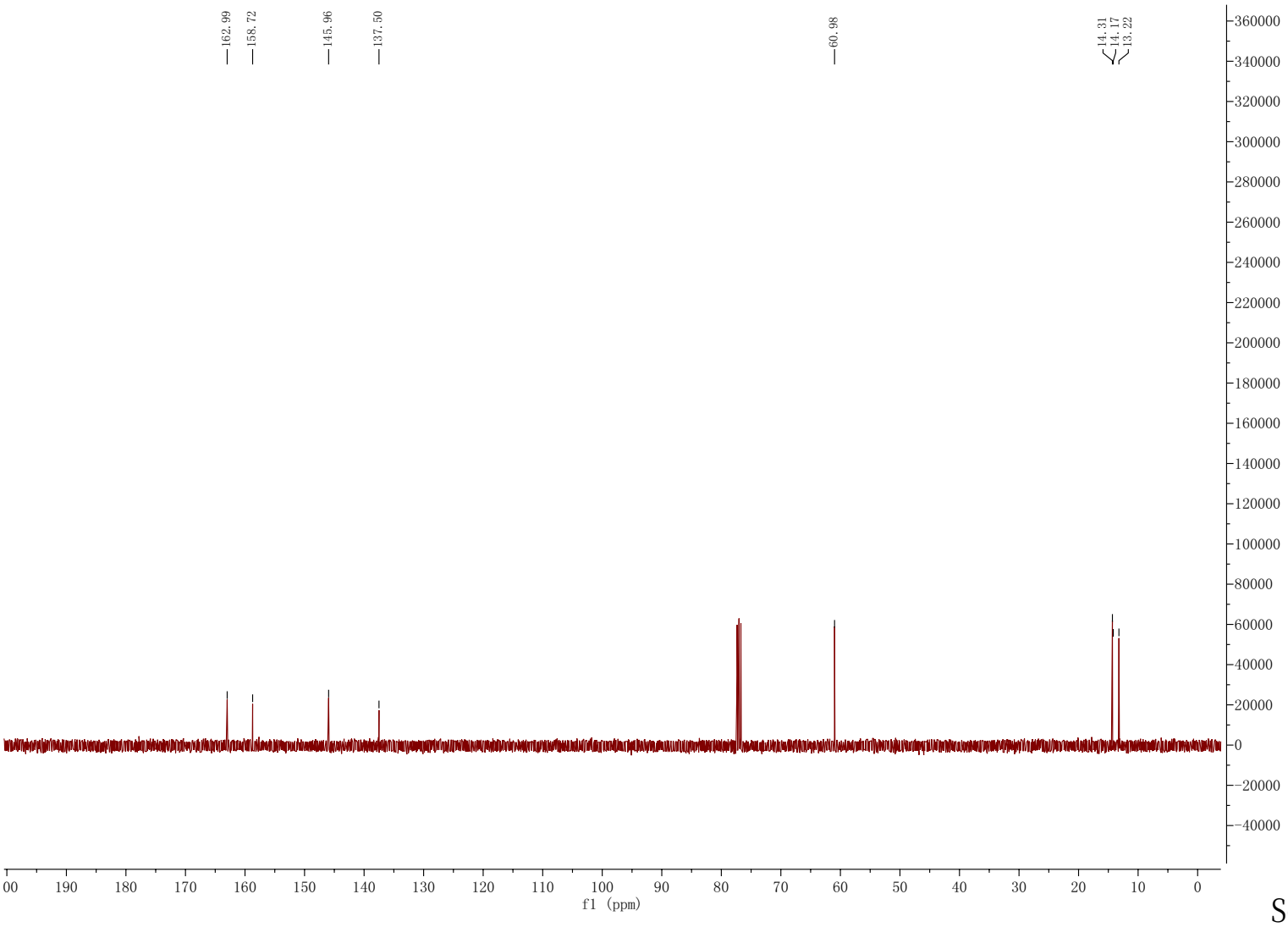

8.18
8.17
7.74
7.73
7.23
7.21
7.20
2.61
2.58
O
O
S
N
CH3
H3C
3x
0.95
0.96
0.97
3.00
3.00
f1 (ppm)

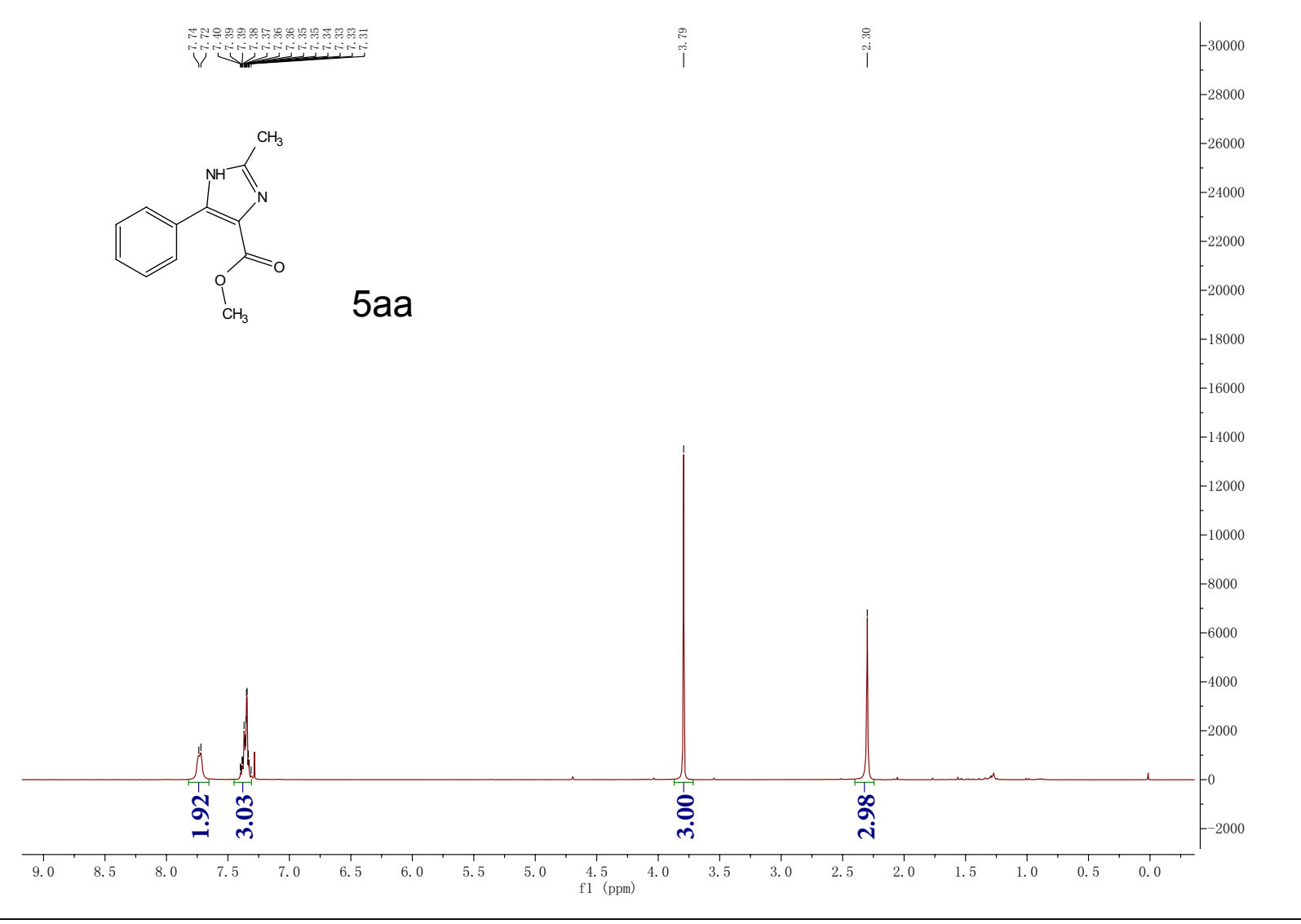

173.50
162.34
148.07
144.21
142.90
134.32
133.60
128.30
14.39
13.91
f1 (ppm)

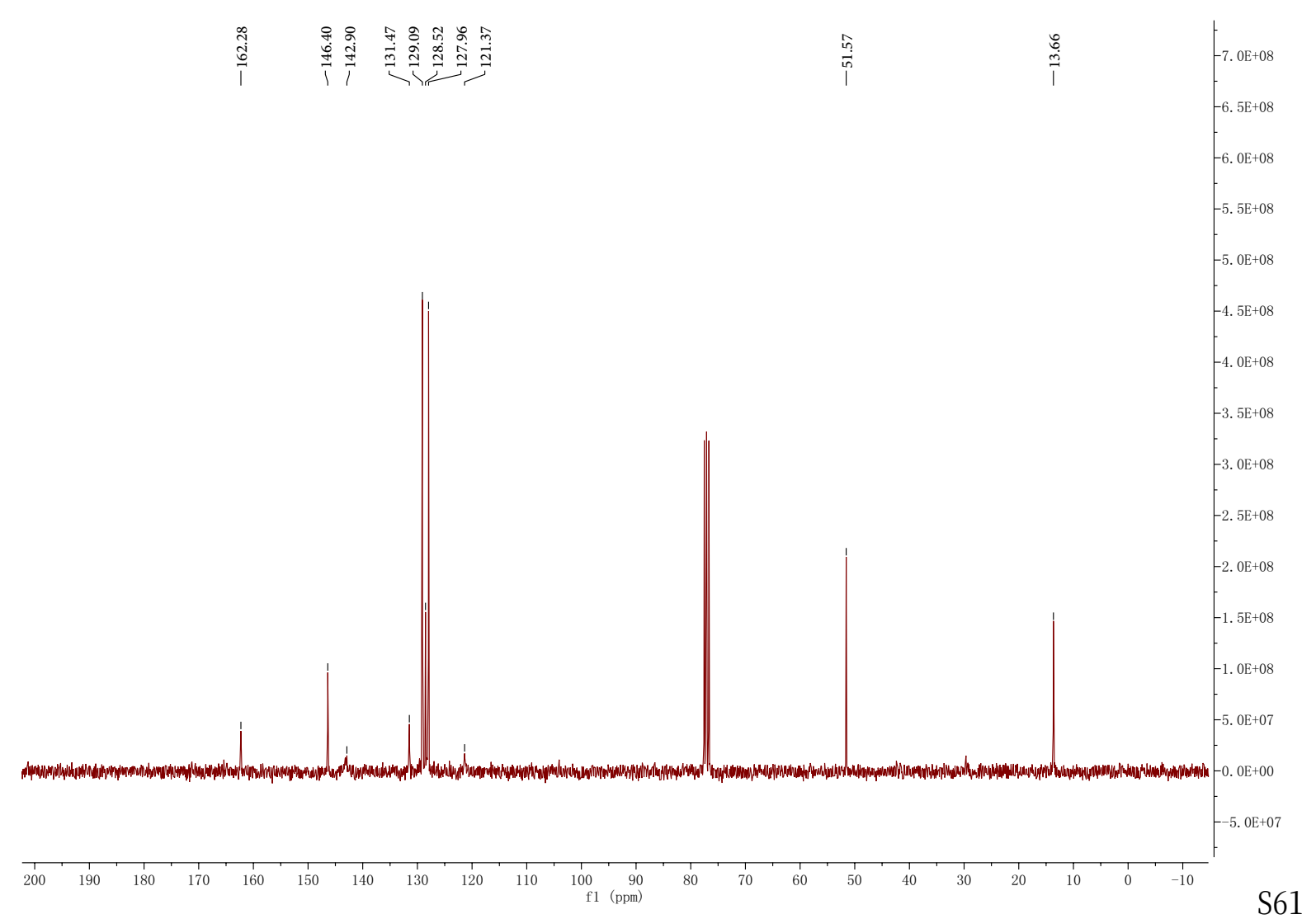

O
O
O
CH3
H3C
N
H3C

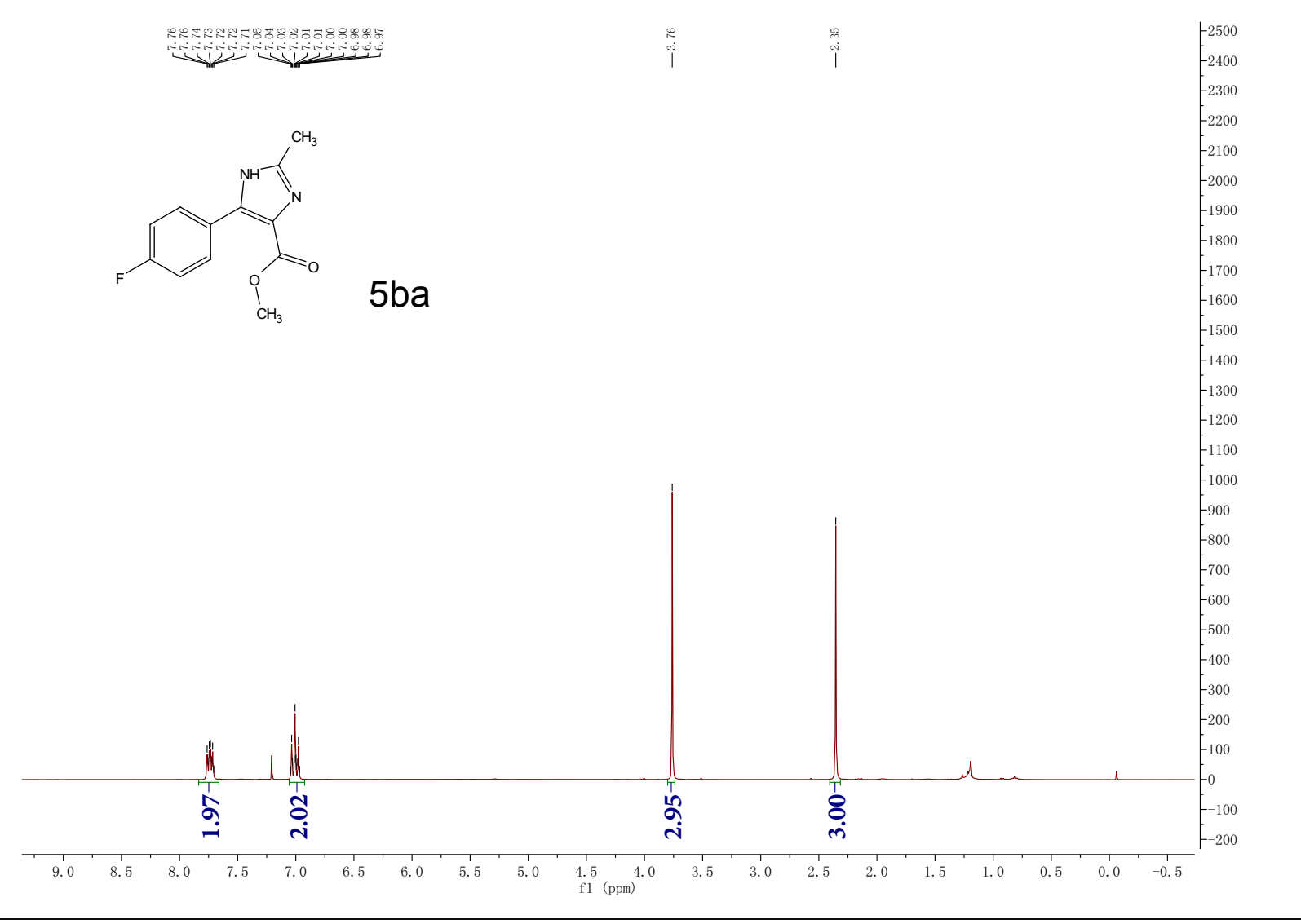
3y

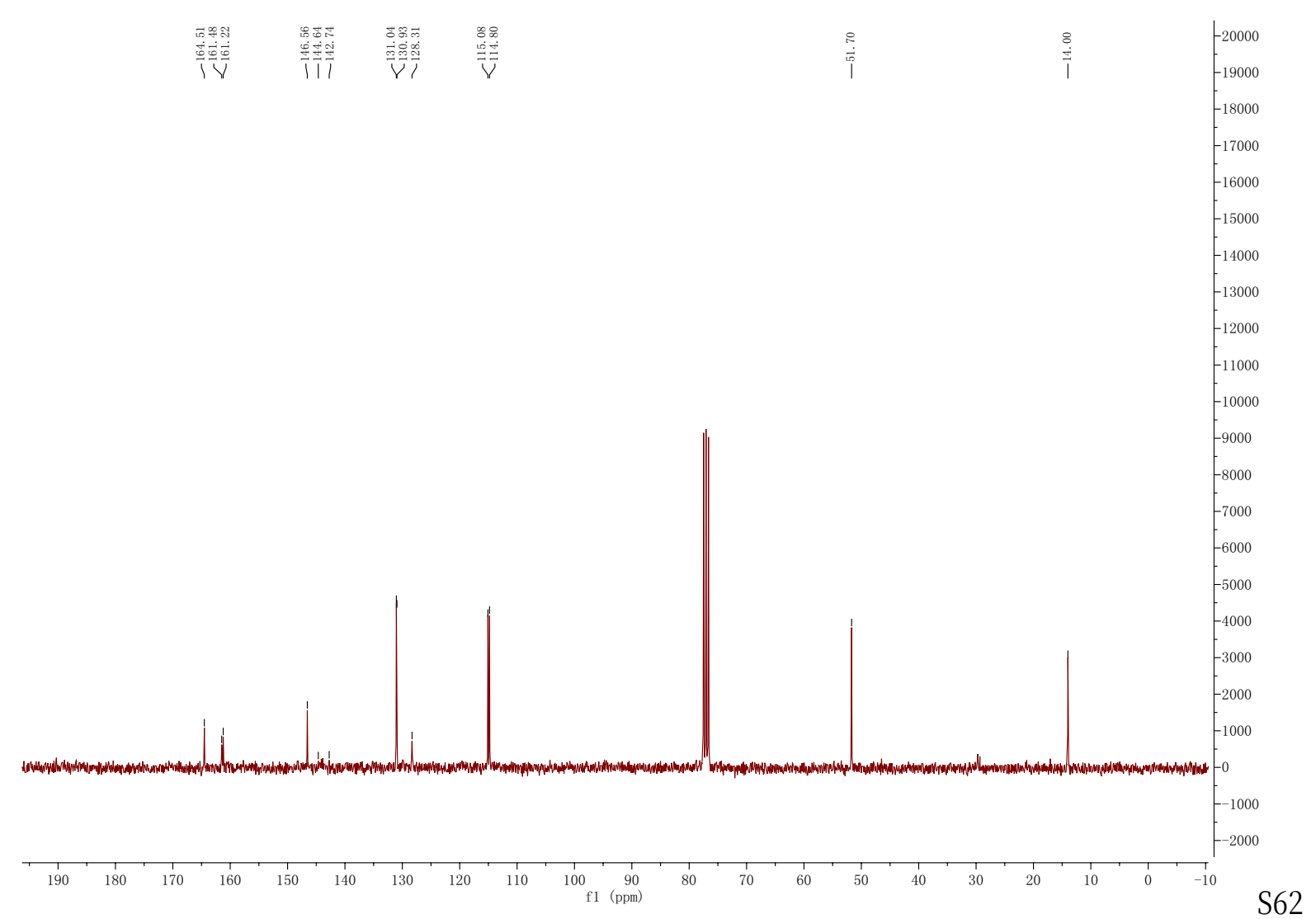
4.41
4.39
4.37
4.34
2.50
2.44
1.42
1.39
1.37
1.97
2.96
2.97
3.00
f1 (ppm)

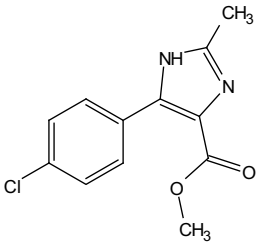

162.99
158.72
145.96
137.50
60.98
14.31
14.17
13.22
f1 (ppm)


7.74
7.72
7.40
7.39
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.31
3.79
2.30
CH3
NH
N
O
O
CH3
5aa
1.92
3.03
3.00
2.98
f1 (ppm)


162.28
146.40
142.90
131.47
129.09
128.52
127.96
121.37
51.57
13.66
f1 (ppm)

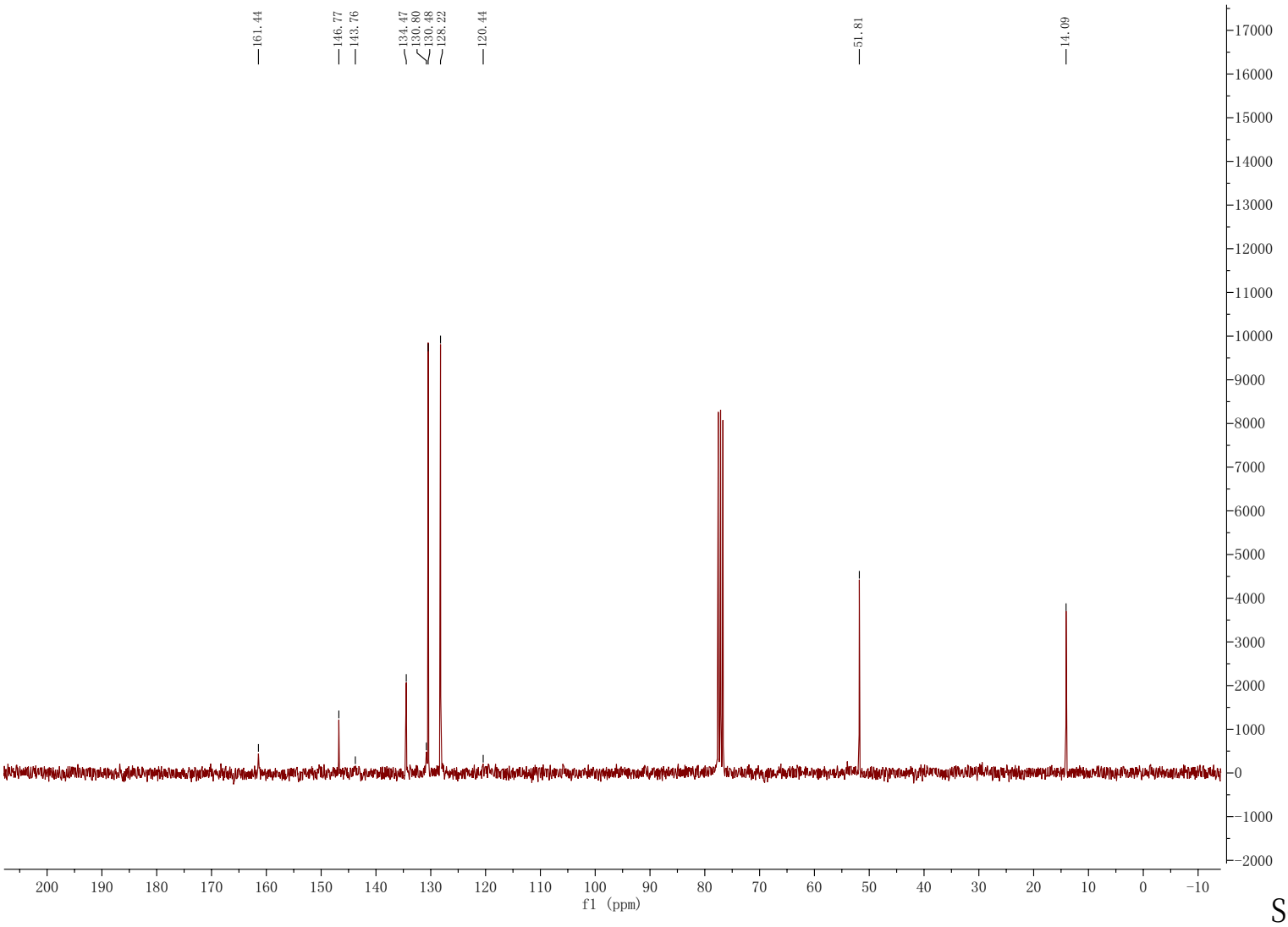

7.76
7.76
7.74
7.73
7.72
7.72
7.71
7.05
7.04
7.03
7.02
7.01
7.01
7.00
7.00
6.98
6.98
6.97
3.76
2.35
CH3
NH
N
F
O
O
CH3
5ba
1.97
2.02
2.95
3.00
f1 (ppm)

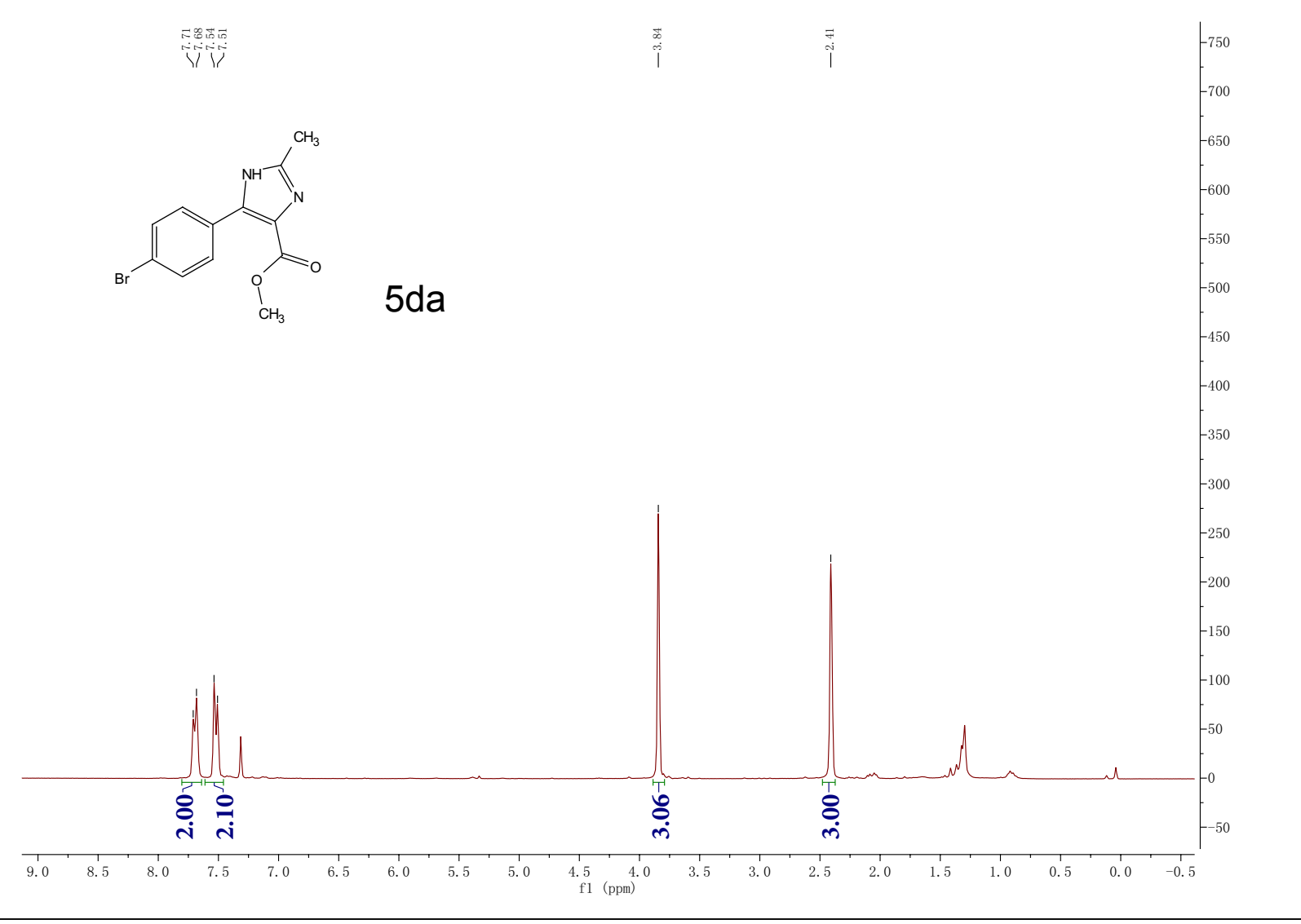

164.51
161.48
161.22
146.56
144.64
142.74
131.04
130.93
128.31
115.08
114.80
51.70
14.00
f1 (ppm)

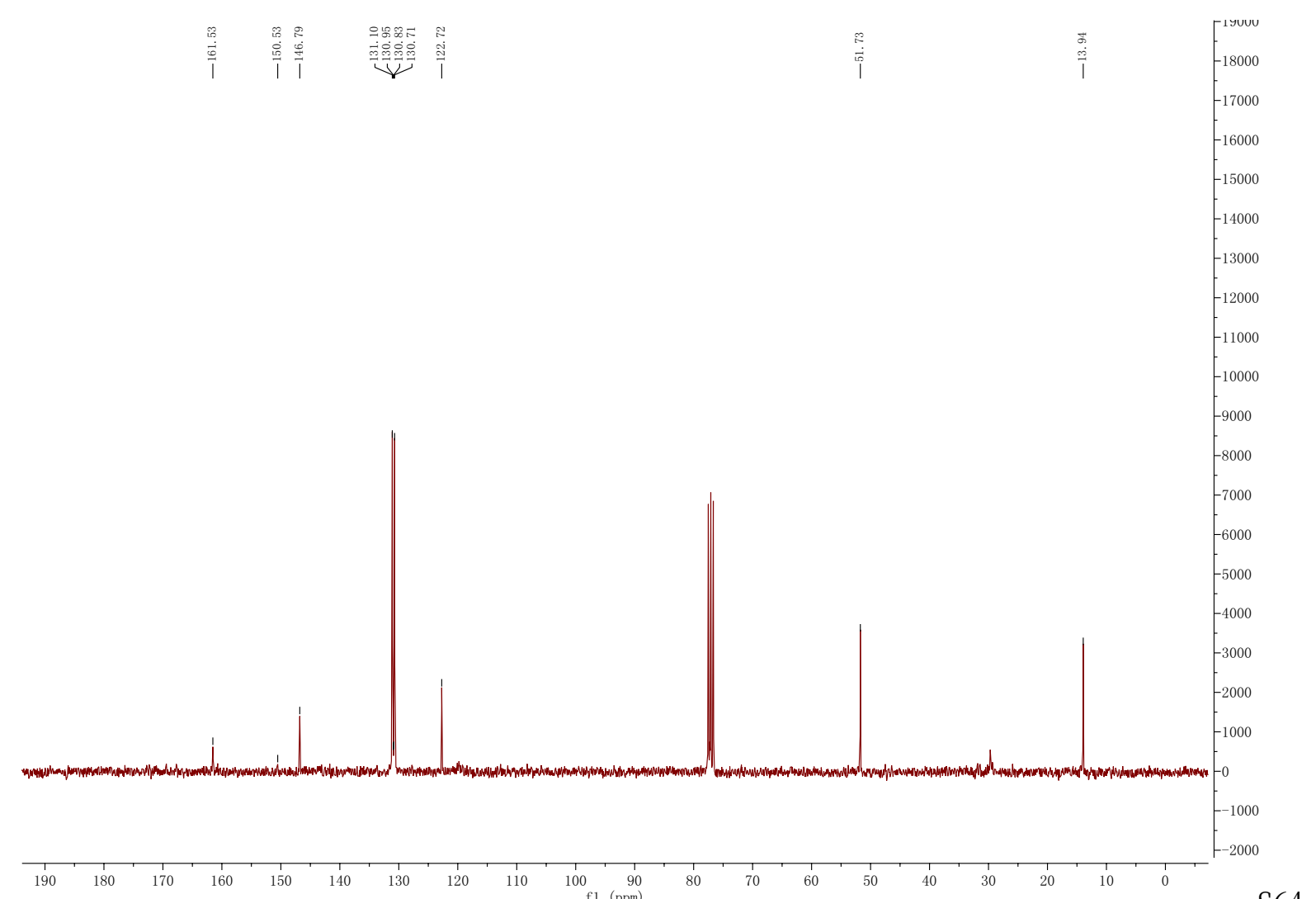

CH3
NH
N
O
Cl
O
CH3

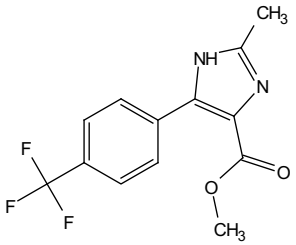
5ca

7.77
7.38
7.37
7.36
7.36
7.35
7.34
7.33
3.83
2.42
2.01
2.00
3.04
3.06
f1 (ppm)


161.44
146.77
143.76
134.47
130.80
130.48
128.22
120.44
51.81
14.09
f1 (ppm)

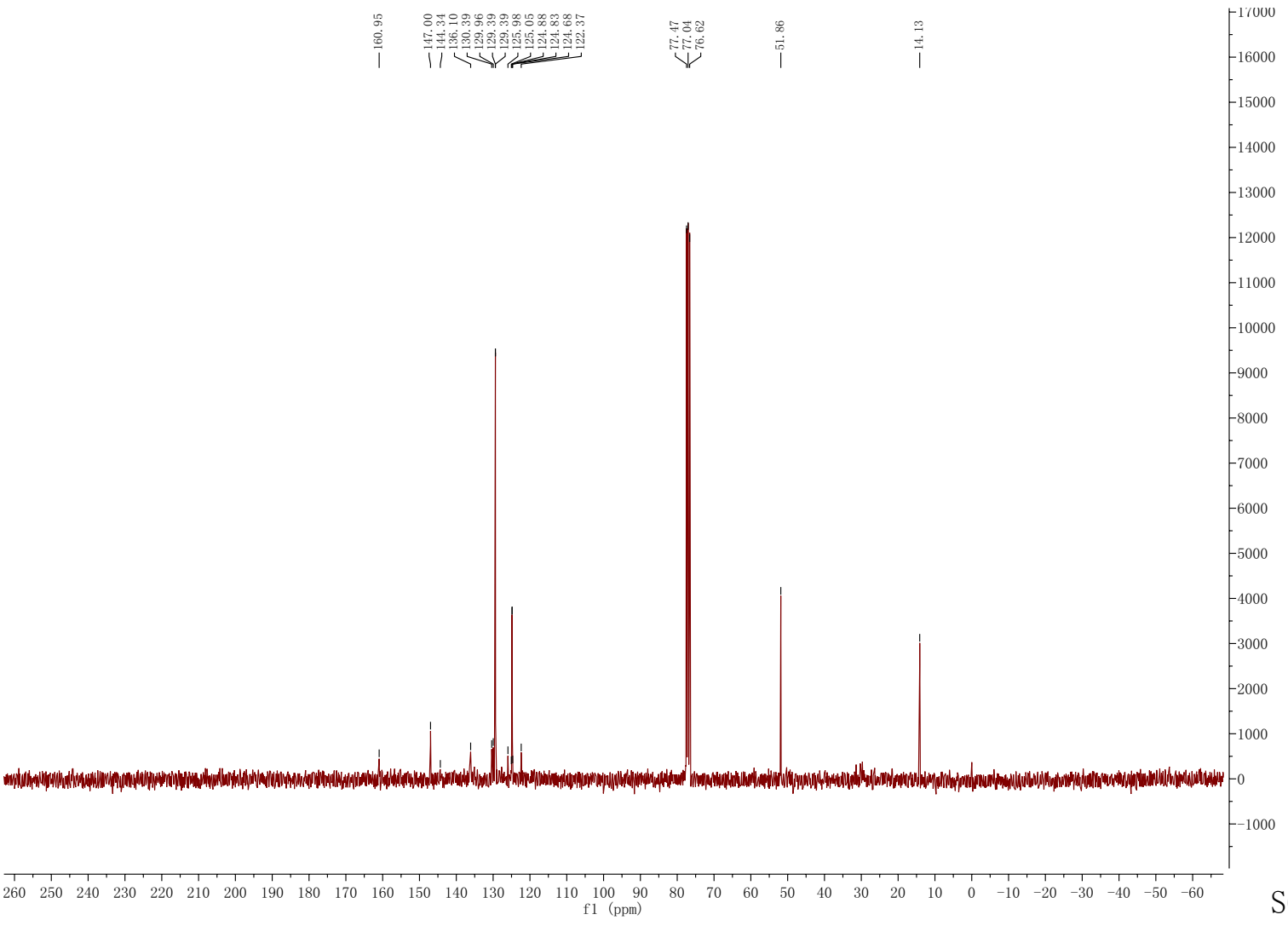

7.71
7.68
7.54
7.51
3.84
2.41
CH3
NH
N
Br
O
O
CH3
5da
2.00
2.10
3.06
3.00
f1 (ppm)

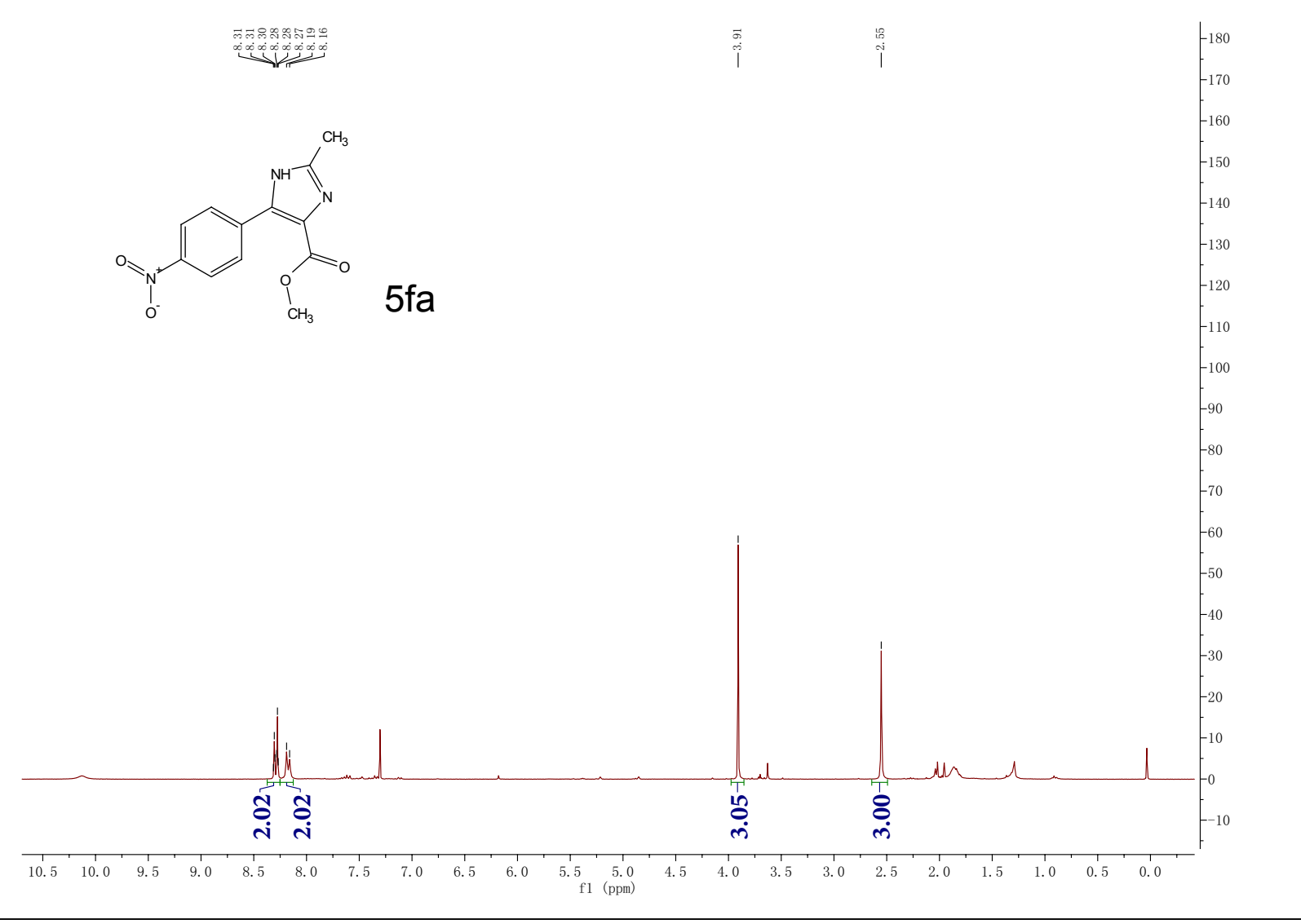

161.53
150.53
146.79
131.10
130.95
130.83
130.71
122.72
51.73
13.94
f1 (ppm)


CH3
NH
N
F
F
F
O
O
CH3

5ea

8.01
7.99
7.69
7.66
3.88
2.50
1.95
2.12
3.07
3.00
f1 (ppm)


160.95
147.00
144.34
136.10
130.39
129.96
129.39
129.39
125.98
125.05
124.88
124.83
124.68
122.37
77.47
77.04
76.62
51.86
14.13
f1 (ppm)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8.31
8.30
8.28
8.28
8.27
8.19
8.16
3.91
2.55
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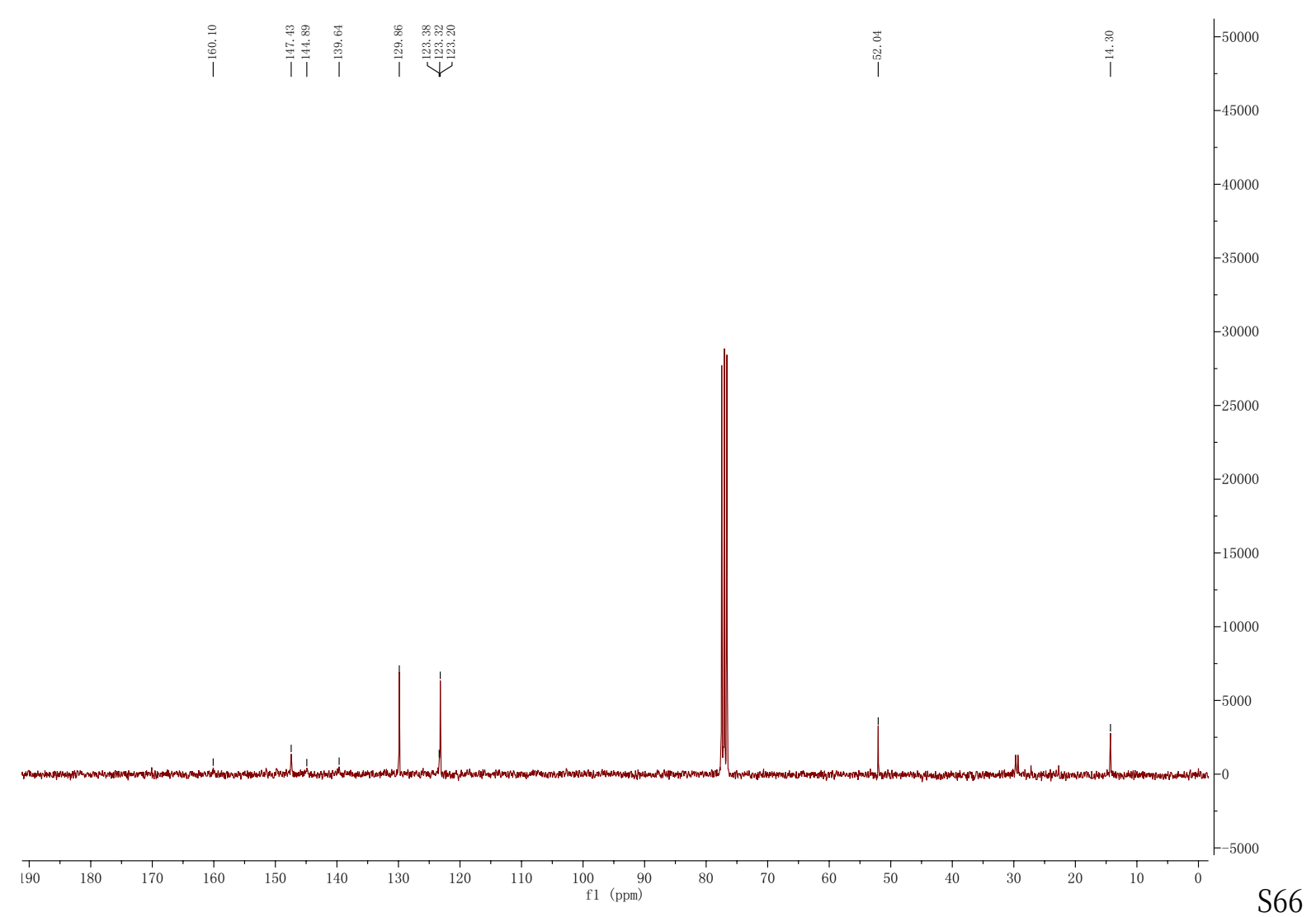
O
N+
O-
O
O
CH3
5fa
2.02
2.02
3.05
3.00
f1 (ppm)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123.38
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123.20
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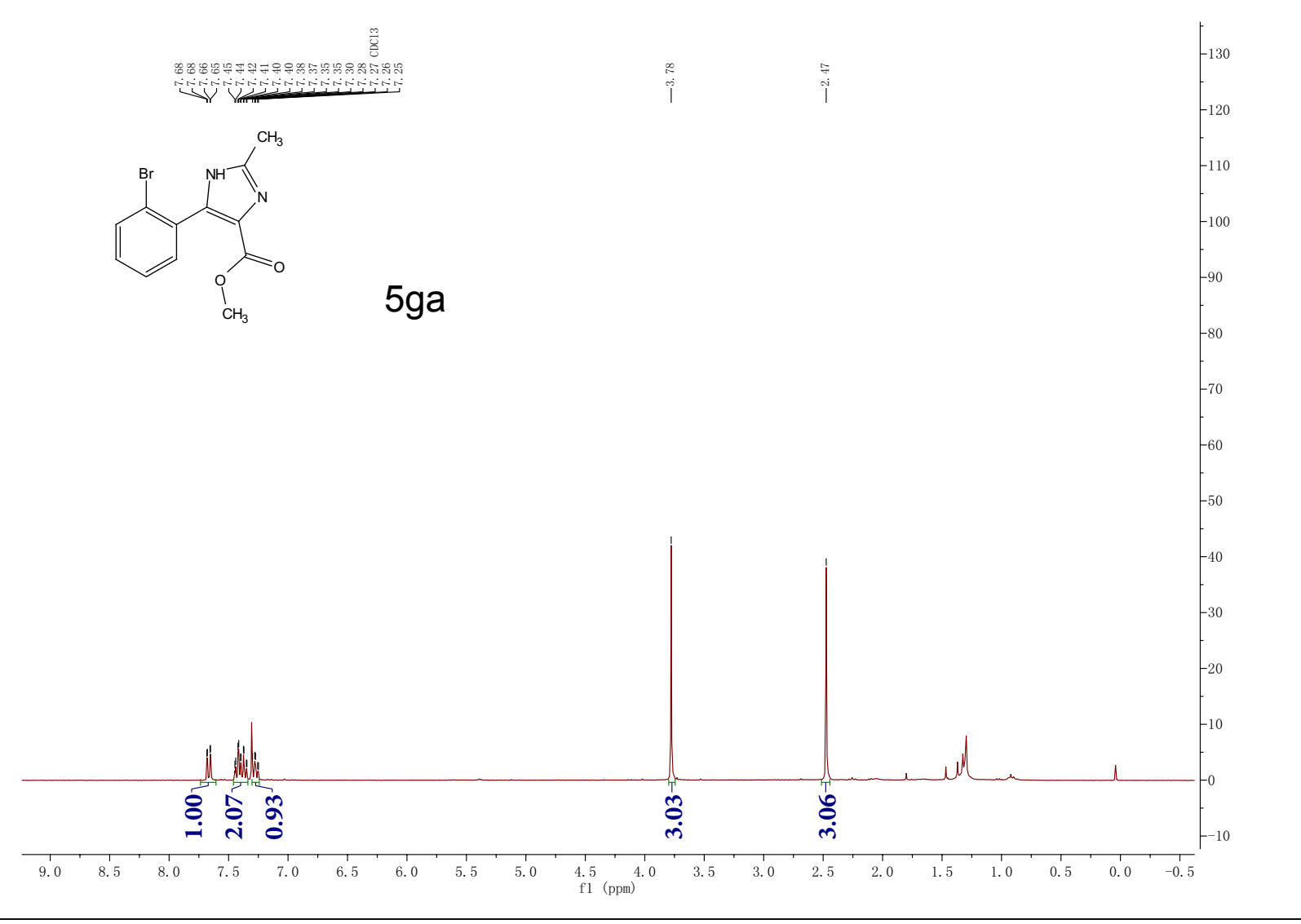
14.30
f1 (ppm)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7.44
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7.41
7.40
7.40
7.38
7.37
7.35
7.30
7.28
CDCl3
7.27
7.26
7.25
3.78
2.47
Br
NH
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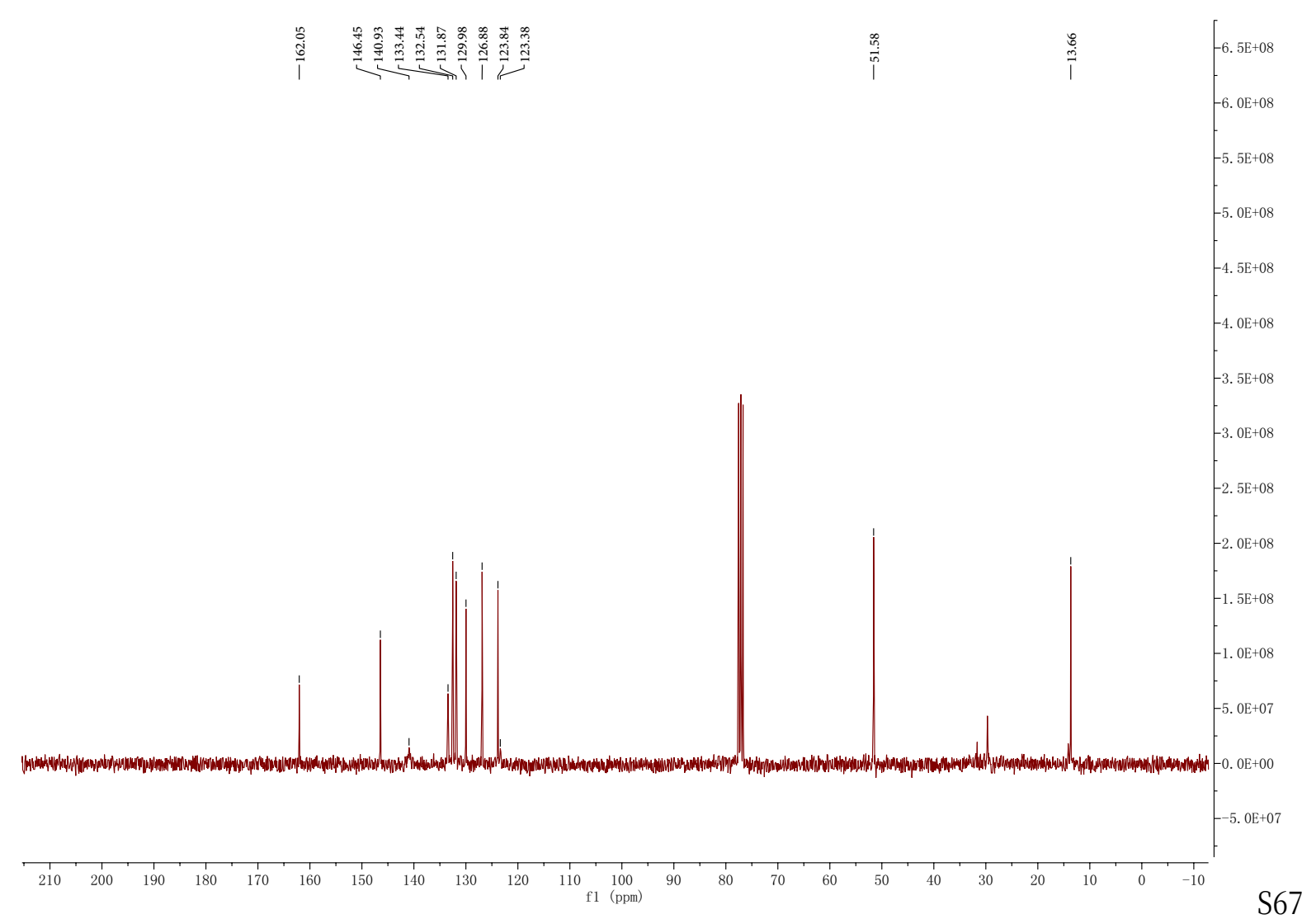
CH3
O
O
CH3
5ga
1.00
2.07
0.93
3.03
3.06
f1 (ppm)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140.93
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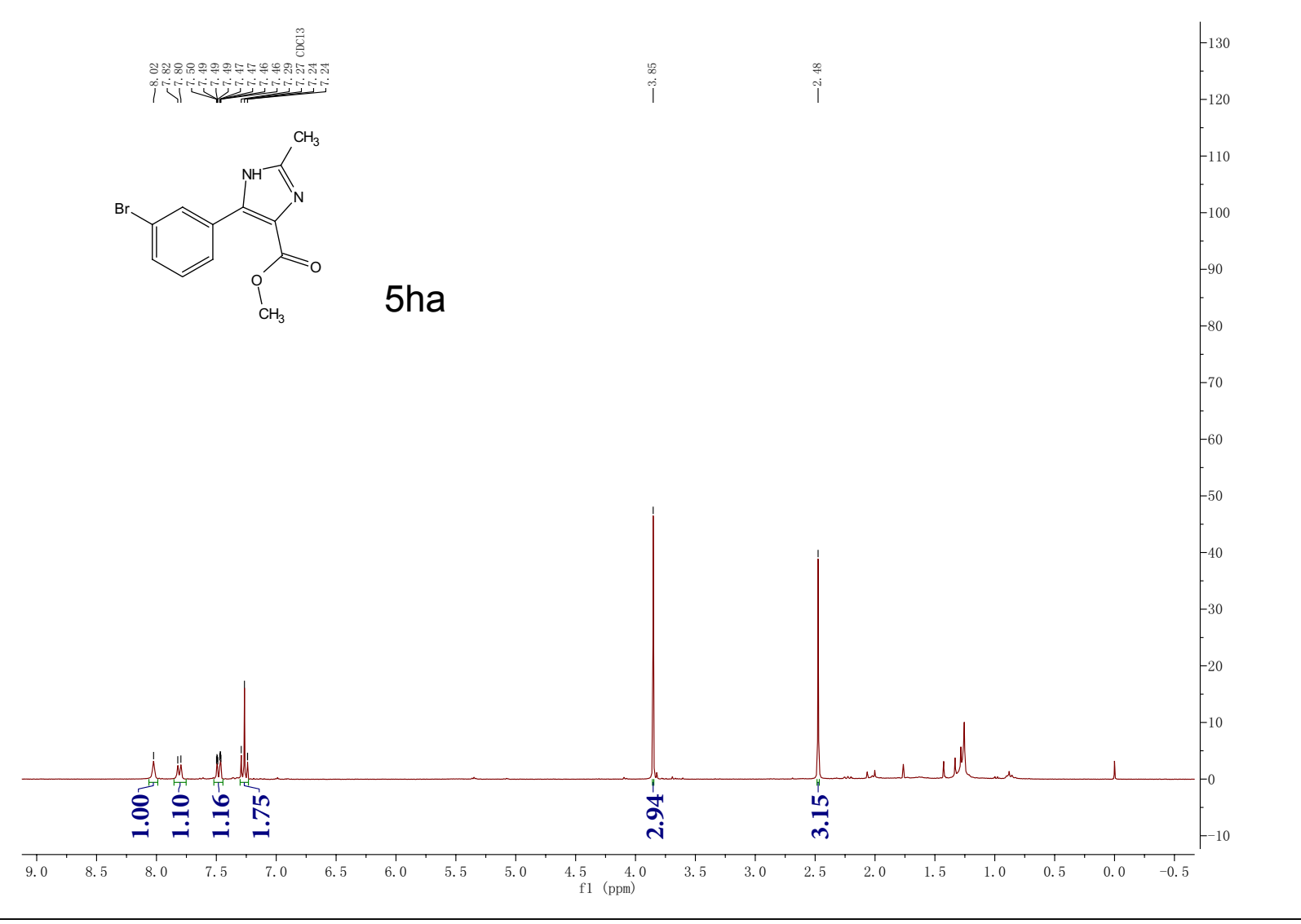
132.54
131.87
129.98
126.88
123.84
123.38
51.58
13.66
f1 (ppm)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7.80
7.50
7.49
7.49
7.49
7.47
7.47
7.46
7.46
7.29
CDCl3
7.27
7.24
7.24
3.85
2.48
CH3
NH
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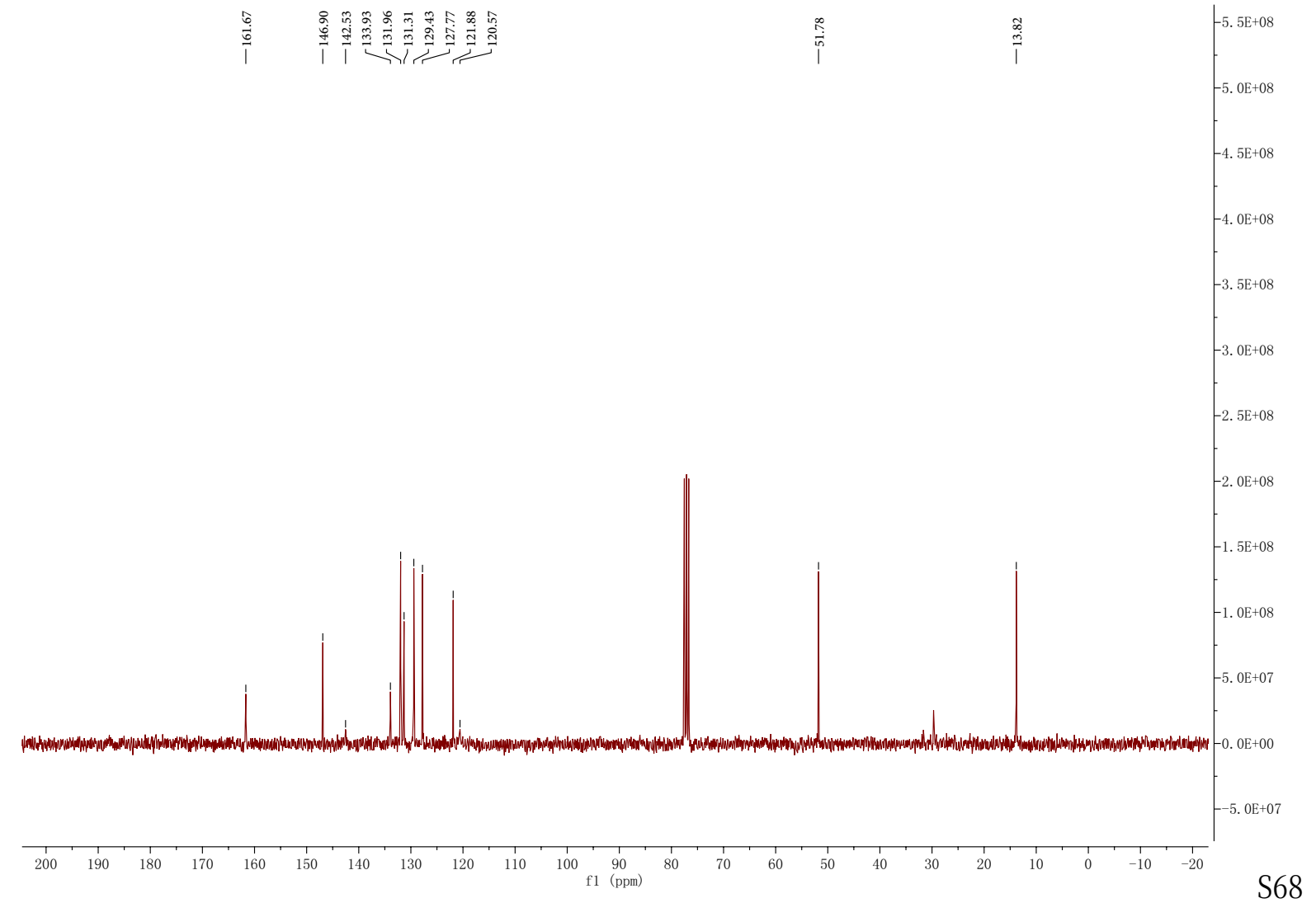
Br
O
O
CH3
5ha
1.00
1.10
1.16
1.75
2.94
3.15
f1 (ppm)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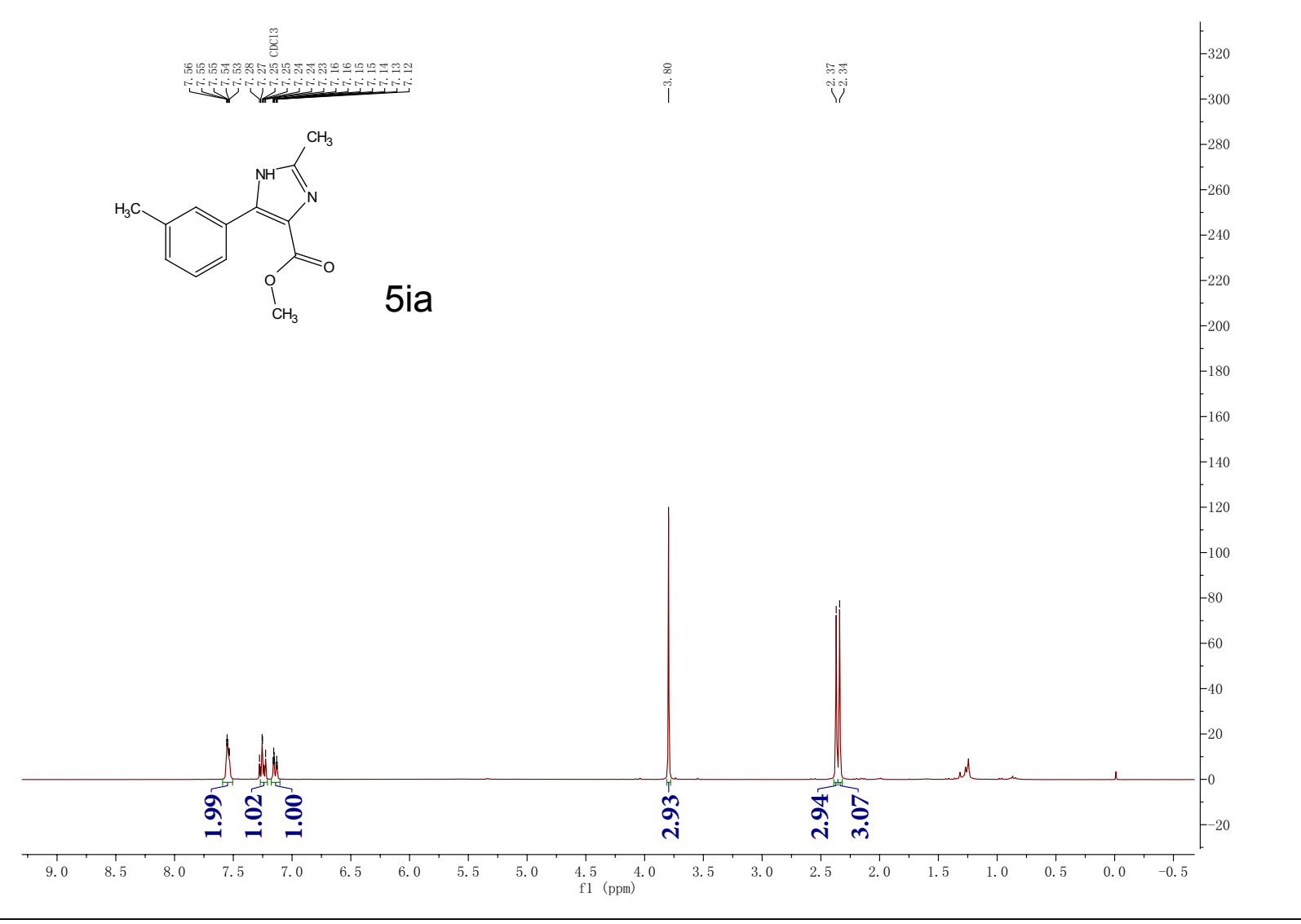
129.43
127.77
121.88
120.57
51.78
13.82
f1 (ppm)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7.55
7.55
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7.28
CDCl3
7.27
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7.25
7.24
7.24
7.23
7.16
7.15
7.15
7.14
7.13
7.12
3.80
2.37
2.34
CH3
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H3C
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O
CH3
5ia
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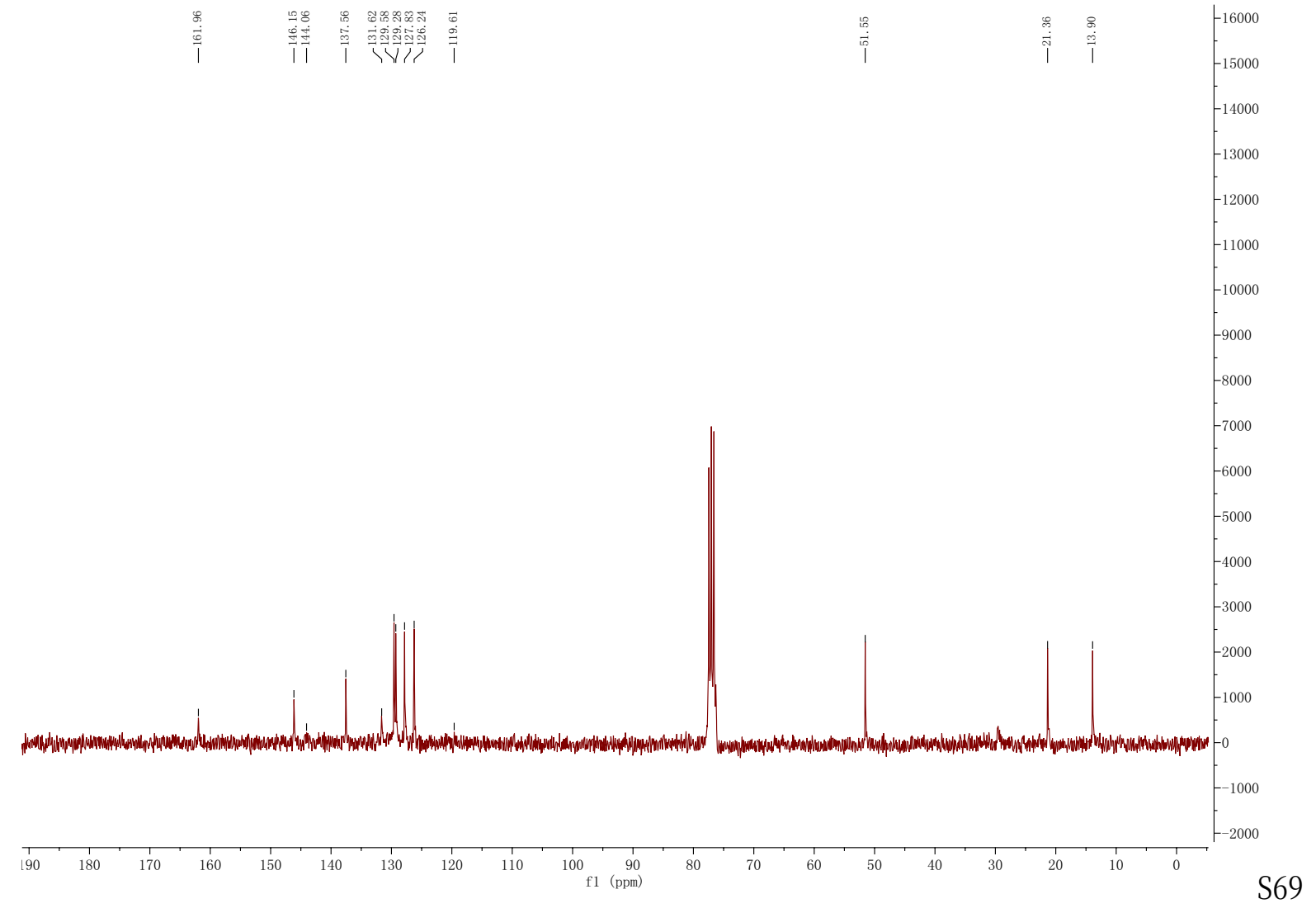
1.02
1.00
2.93
2.94
3.07
f1 (ppm)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144.06
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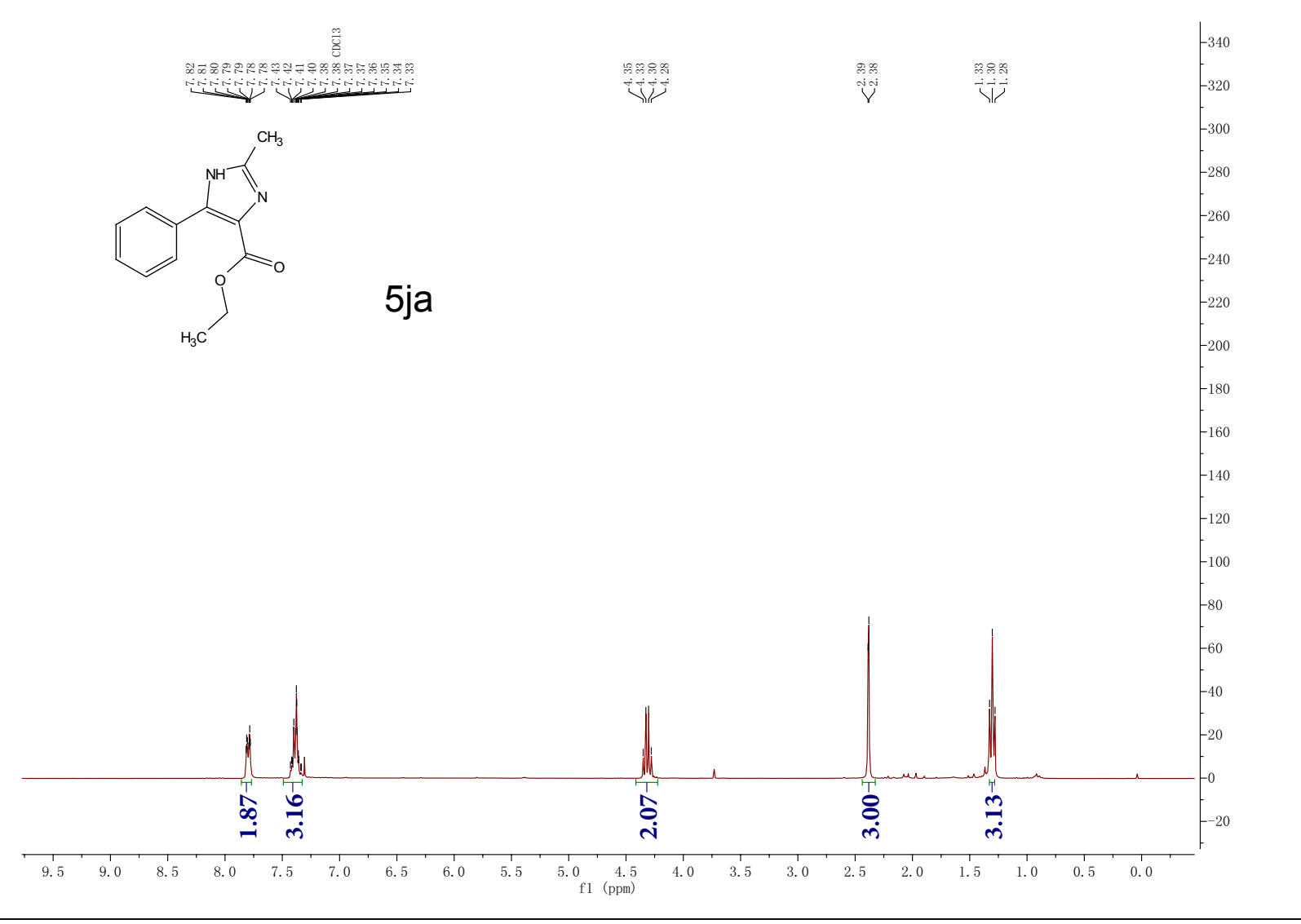
129.58
129.28
127.83
126.24
119.61
51.55
21.36
13.90
f1 (ppm)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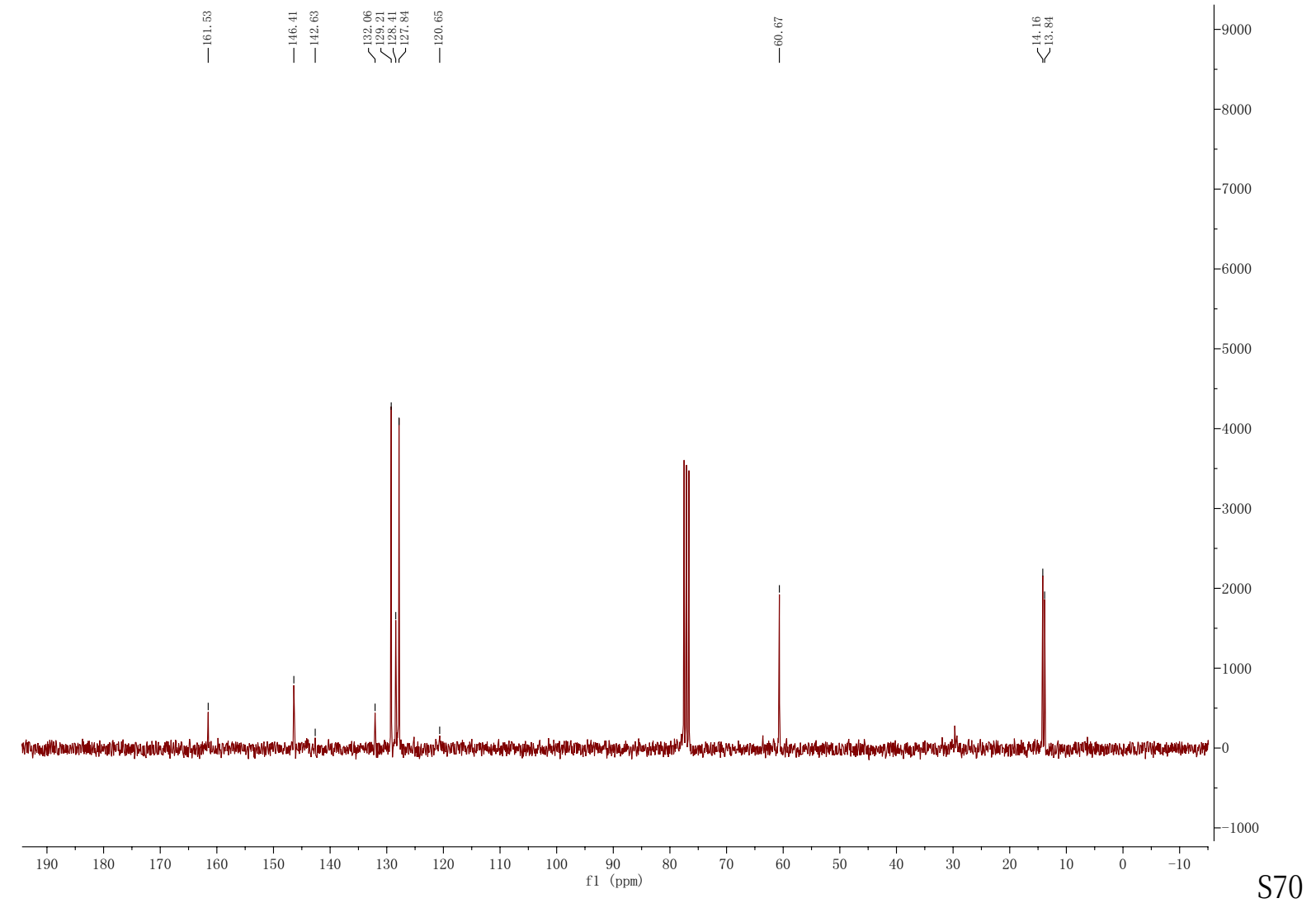
7.81
7.80
7.79
7.79
7.78
7.78
7.43
7.42
7.41
7.40
7.38
CDCl3
7.38
7.37
7.37
7.36
7.35
7.34
7.33
4.35
4.33
4.30
4.28
2.39
2.38
1.33
1.30
1.28
CH3
NH
N
O
O
H3C
5ja
1.87
3.16
2.07
3.00
3.13
f1 (ppm)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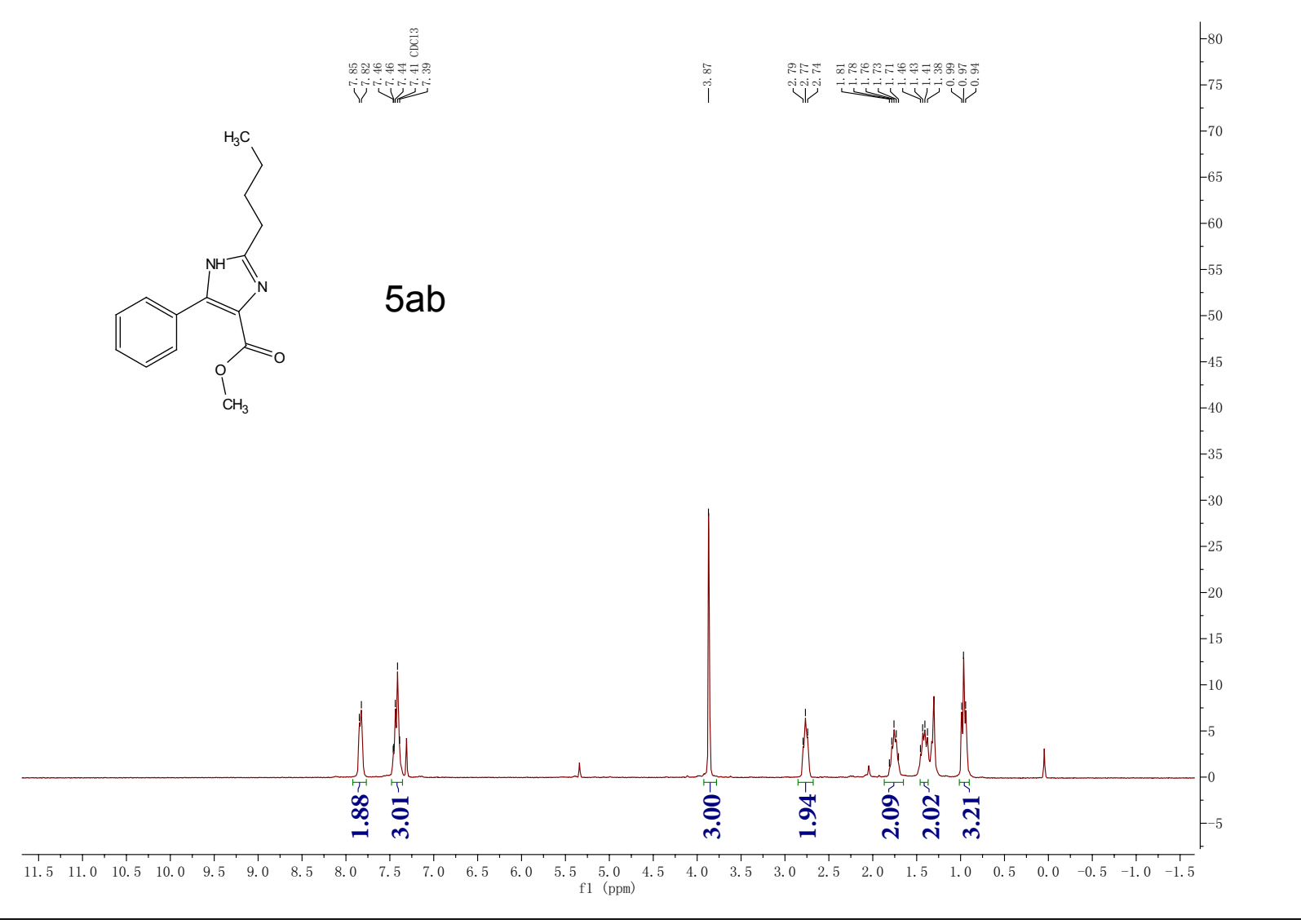
120.65
60.67
14.16
13.84
f1 (ppm)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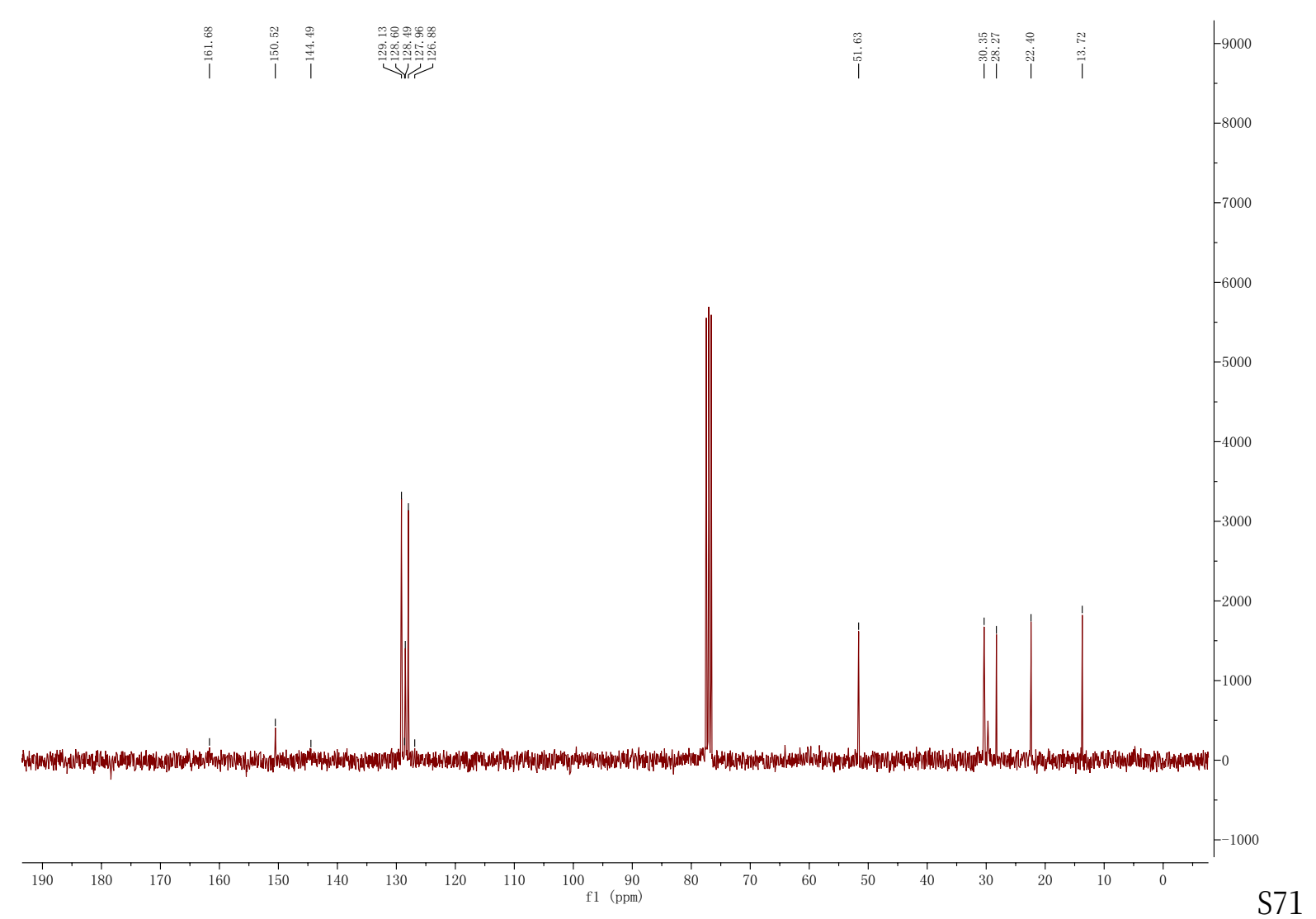
7.41
CDCl3
7.39
3.87
2.79
2.77
2.74
1.81
1.78
1.76
1.73
1.71
1.46
1.43
1.41
1.38
0.99
0.97
0.94
H3C
NH
N
O
O
CH3
5ab
1.88
3.01
3.00
1.94
2.09
2.02
3.21
f1 (ppm)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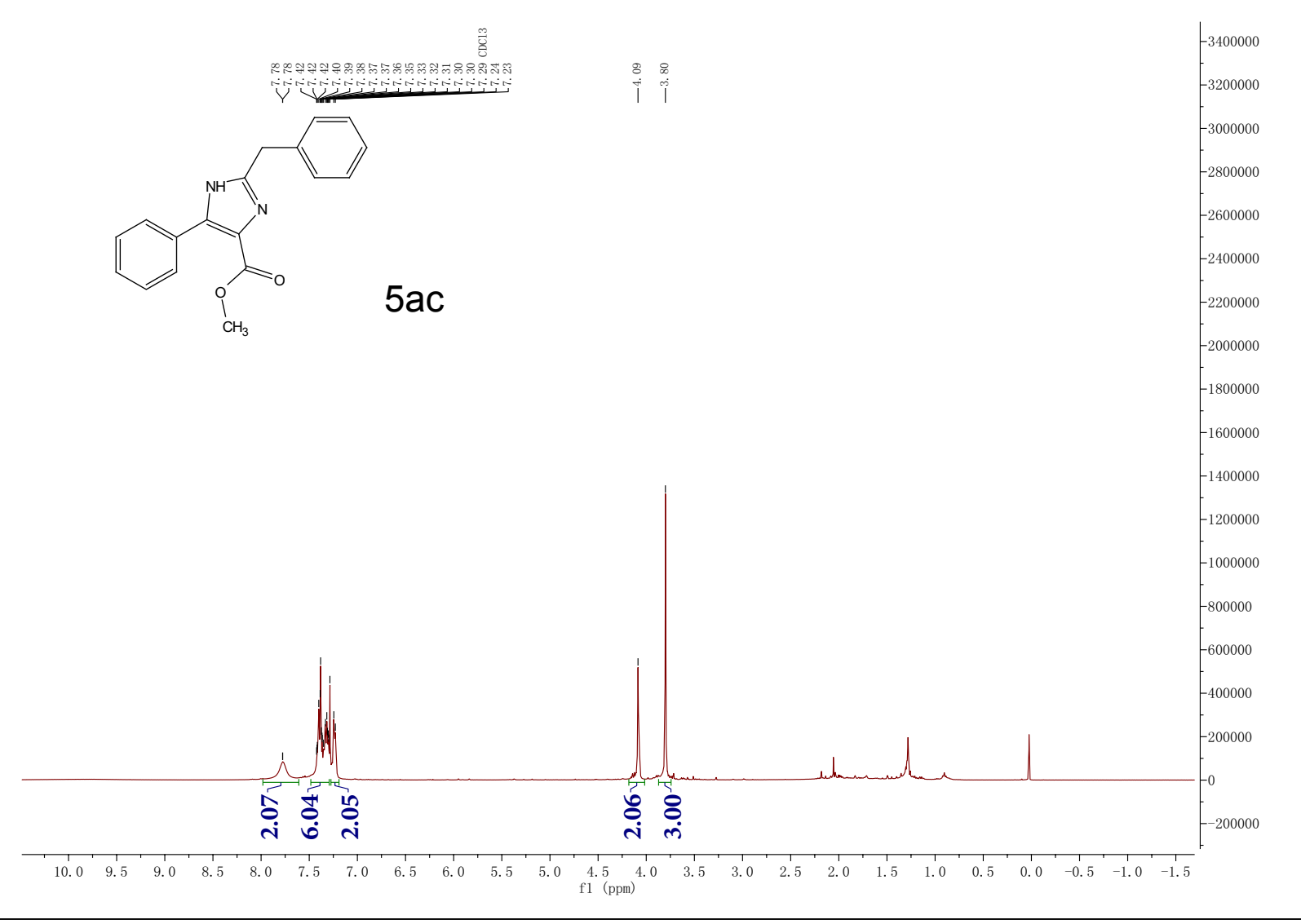
126.88
51.63
30.35
28.27
22.40
13.72
f1 (ppm)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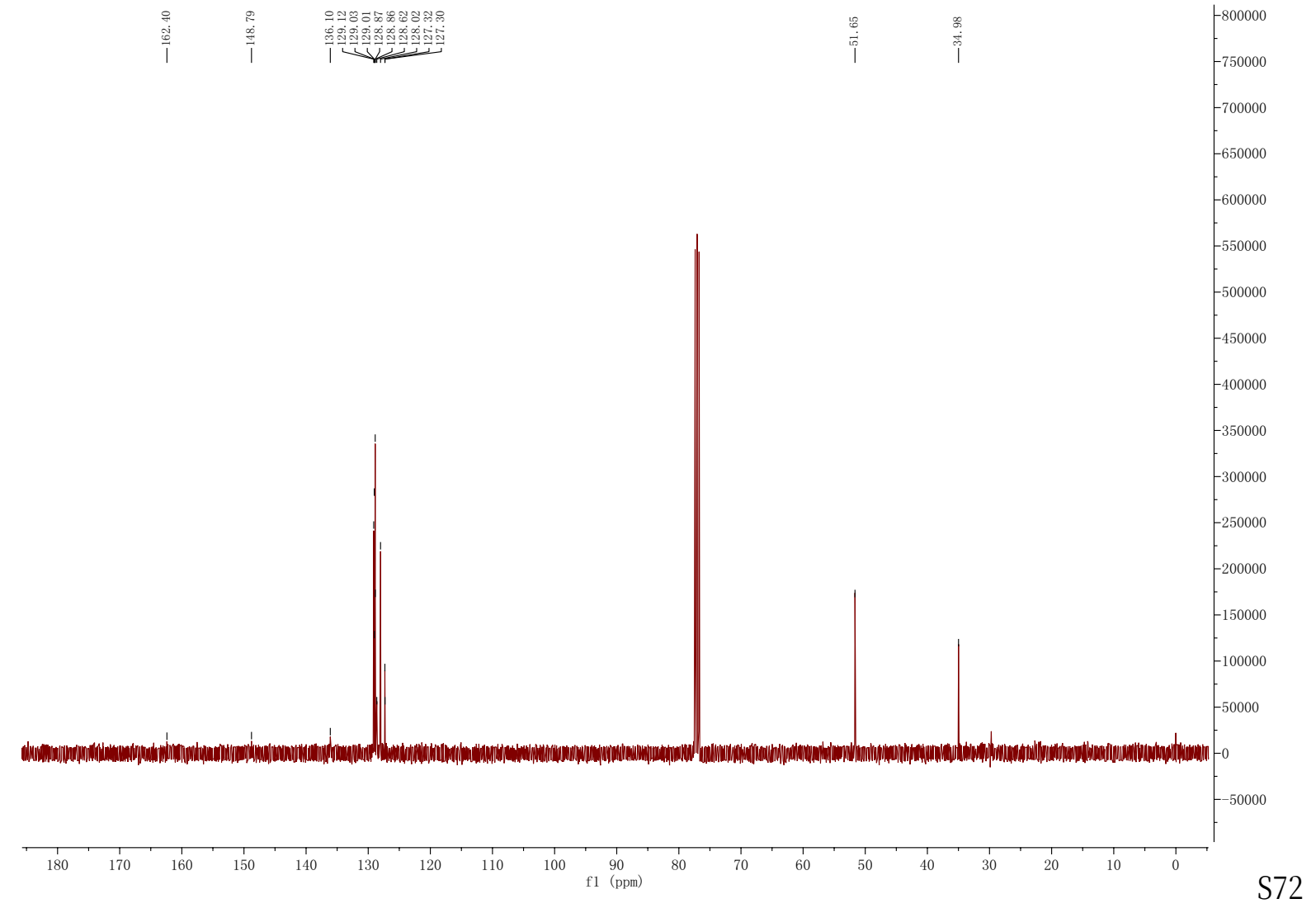
7.78
7.42
7.42
7.42
7.40
7.39
7.38
7.37
7.37
7.36
7.35
7.33
7.32
7.31
7.30
7.30
7.29 CDCl3
7.24
7.23
4.09
3.80
NH
N
O
O
CH3
5ac
2.07
6.04
2.05
2.06
3.00
f1 (ppm)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136.10
129.12
129.03
129.01
128.87
128.86
128.62
128.02
127.32
127.30
51.65
34.98
f1 (ppm)