Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

$PhI(OAc)_2$-Mediated Oxidative Rearrangement of Allylic Amides: Efficient Synthesis of Oxazoles and β-Keto Amides

Supporting Information

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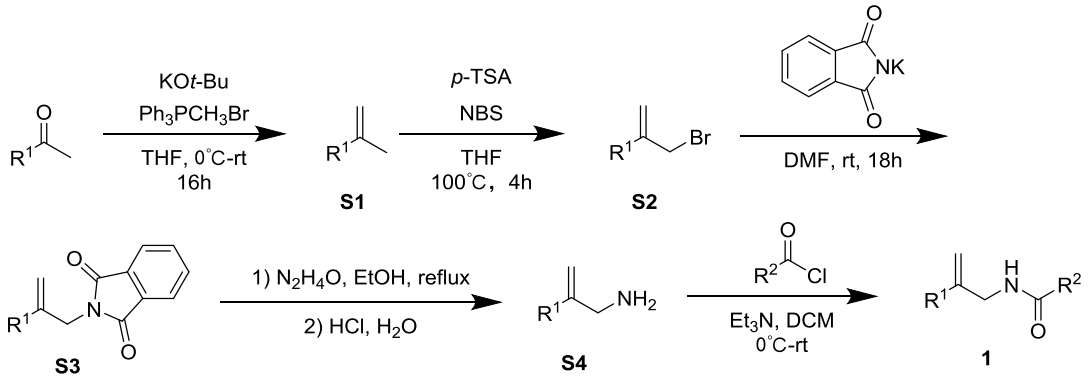
1. General

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.

2.Preparation of Substrate 1

2. 1 Typical Procedure for the Synthesis of **1**.



In an oven dried flask, methyl triphenylphosphonium bromide (1.2 equiv.) was added into THF (1.6 mL/mmol). The suspension was cooled to 0 ℃, KO*t*-Bu (1.2 equiv.) was added and the resulting yellow suspension was stirred at 0 ℃ for 45 min. To this suspension, a solution of ketone (1.0 equiv.) in THF (0.7 mL/mmol) was added dropwise and the resulting mixture was warmed gradually to r.t. and stirred at r.t. for 16 h. Reaction mixture was concentrated under reduced pressure and filtered over Celite.

The filtrate was concentrated under reduced pressure to yield a yellow oil. Purification by column chromatography over silica gel using petroleum ether as eluent afforded **S1** as a colorless oil.[S1]

In an oven dried flask S1 (1.0 eq) was added into dry THF (3.0 mL/mmol). To the resulting solution N-Bromosuccinimide (1.05 eq) and TsOH (0.1 eq) was added and the solution was refluxed at 100 ℃ for 4 h. Reaction mixture was cooled to rt and the reaction mixture was taken in petroleum ether (15 mL/mmol), washed with H_2O (3x). Organic phase was dried over Na_2SO_4, concentrated under reduced pressure to obtain a yellow oil. Purification by column chromatography over silica gel using petroleum ether as eluent afforded **S2** as a colorless oil.[S1]

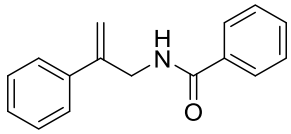
Potassium phthalimide (1.1 eq) was added to a solution of S2 (1 eq) in DMF (35 mL) at room temperature. The resulting mixture was stirred for 18 hours, after which time a dark brown colour was formed and a white precipitate observed. Dichloromethane (30 mL) was added and the mixture poured onto water (100 mL). The aqueous phase was separated and extracted with dichloromethane (3x). The combined organic extract was then washed with NaOH aq (0.2 M) and dried with anhydrous sodium sulfate. The dichloromethane was removed in vacuo and the residue purified by column chromatography (pentane : EtOAc 7 : 3) to afford the protected product **S3** as white needles.[S2]

Hydrazine hydrate (1.64 mL, 33.8 mmol, 5 eq) was added to a suspension of **S3** (1.78 g, 6.77 mmol, 1 eq) in ethanol (120 mL). The resulting mixture was heated under reflux for one hour. Then HCl aq. (2.0 M) (12 mL) was added and the reaction heated for a further one hour. The reaction mixture was then cooled to 4 ℃ and the phthalyl hydrazide removed by filtration. The ethanol was removed in vacuum and the solid residue was redissolved in 20 mL NaOH aq. (2.0 M). The solution was extracted with diethyl ether (5x) and the organic extract was dried over Na_2SO_4, filtered and the solvent removed to give the **S4** as a colourless oil.[S2]

A solution of **S4** (1.20 g, 9.0 mmol, 1.0 equiv), triethyl amine (1.04 mL, 18.0 mmol, 2.0 equiv) and a catalytic amount of DMAP in DCM (50 mL) was cooled in an ice bath. To it was added corresponding chloride (1.57 mL, 13.5 mmol, 1.5 equiv) drop wise.

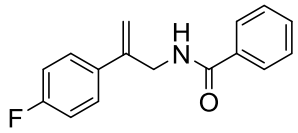
After the addition was complete, the reaction was allowed to warm to room temperature. After 2 h, the reaction was diluted with an equal amount of water and extracted with DCM (3 x 25 mL). The combined organics were washed with brine (1 x 30 mL), dried over Na_2SO_4 and concentrated under reduced pressure to give the product as a yellow solid. It was recrystallized from MeOH to obtain the pure product as a colorless solid in 1.85 g yield (87%) after collection of three crops of crystals. Compounds **1** were purified by column chromatography. [S3]

N-(2-phenylallyl)benzamide **1a**



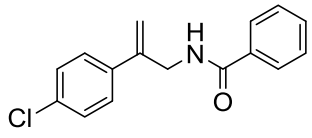
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 – 7.85 (m, 2H), 7.72 – 7.47 (m, 8H), 6.36 (brs, 1H), 5.71 (s, 1H), 5.51 (s, 1H), 4.73 (d, *J* = 5.6 Hz, 2H).

N-(2-(4-fluorophenyl)allyl)benzamide **1b**



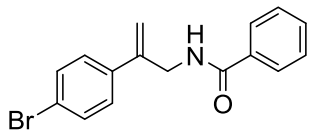
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 – 7.71 (m, 2H), 7.55 – 7.41 (m, 7.5 Hz, 5H), 7.08 (t, *J* = 8.6 Hz, 2H), 6.25 (brs, 1H), 5.51 (s, 1H), 5.35 (s, 1H), 4.56 (d, *J* = 5.7 Hz, 2H).

N-(2-(4-chlorophenyl)allyl)benzamide **1c**



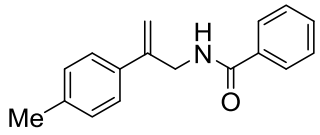
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 – 7.66 (m, 2H), 7.55 – 7.38 (m, 5H), 7.37 – 7.30 (m, 2H), 6.28 (brs, 1H), 5.52 (s, 1H), 5.35 (s, 1H), 4.53 (d, *J* = 5.7 Hz, 2H).

N-(2-(4-bromophenyl)allyl)benzamide **1d**



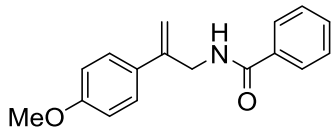
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 – 7.69 (m, 2H), 7.57 – 7.35 (m, 7H), 6.19 (brs, 1H), 5.54 (s, 1H), 5.36 (s, 1H), 4.54 (d, *J* = 5.8 Hz, 2H).

N-(2-(p-tolyl)allyl)benzamide **1e**



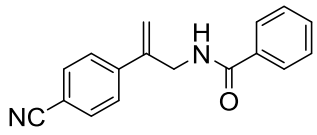
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.5 Hz, 2H), 7.52 – 7.36 (m, 5H), 7.23 – 7.14 (m, 2H), 6.20 (brs, 1H), 5.52 (s, 1H), 5.30 (s, 1H), 4.55 (d, *J* = 5.5 Hz, 2H), 2.37 (s, 3H).

N-(2-(4-methoxyphenyl)allyl)benzamide **1f**



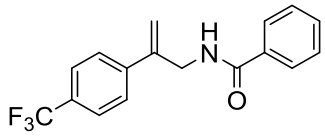
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 – 7.70 (m, 2H), 7.50 – 7.37 (m, 5H), 6.94 – 6.84 (m, 2H), 6.33 (brs, 1H), 5.46 (s, 1H), 5.24 (s, 1H), 4.52 (d, *J* = 5.6 Hz, 2H), 3.82 (s, 3H).

N-(2-(4-cyanophenyl)allyl)benzamide **1g**



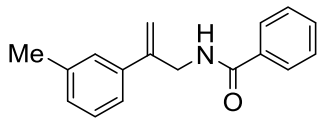
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.65 (q, *J* = 8.5 Hz, 4H), 7.60 – 7.50 (m, 1H), 7.46 (dd, *J* = 8.2, 6.8 Hz, 2H), 6.33 (brs, 1H), 5.67 (s, 1H), 5.52 (s, 1H), 4.60 (d, *J* = 5.8 Hz, 2H).

N-(2-(4-(trifluoromethyl)phenyl)allyl)benzamide **1h**



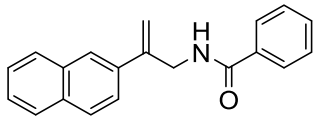
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 – 7.73 (m, 2H), 7.65 (s, 4H), 7.57 – 7.43 (m, 3H), 6.28 (brs, 1H), 5.64 (s, 1H), 5.48 (s, 1H), 4.61 (d, *J* = 5.7 Hz, 2H).

N-(2-(m-tolyl)allyl)benzamide **1i**



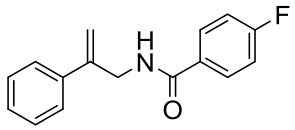
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 2H), 7.57 – 7.41 (m, 3H), 7.38 – 7.31 (m, 3H), 7.17 (d, *J* = 6.8 Hz, 1H), 6.22 (brs, 1H), 5.55 (s, 1H), 5.35 (s, 1H), 4.58 (d, *J* = 5.5 Hz, 2H), 2.41 (s, 3H).

N-(2-(naphthalen-2-yl)allyl)benzamide **1j**



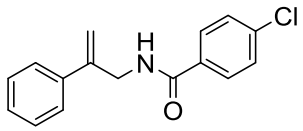
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.89 (dd, *J* = 8.8, 5.2 Hz, 3H), 7.79 – 7.61 (m, 3H), 7.56 – 7.40 (m, 5H), 6.28 (brs, 1H), 5.73 (s, 1H), 5.48 (s, 1H), 4.72 (d, *J* = 5.5 Hz, 2H).

4-fluoro-*N*-(2-phenylallyl)benzamide **1k**



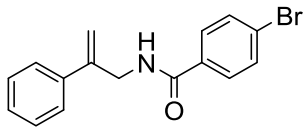
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 – 7.69 (m, 2H), 7.53 – 7.47 (m, 2H), 7.43 – 7.30 (m, 3H), 7.14 – 7.05 (m, 2H), 6.15 (brs, 1H), 5.55 (q, *J* = 0.8 Hz, 1H), 5.34 (td, *J* = 1.4, 0.8 Hz, 1H), 4.56 (ddd, *J* = 5.6, 1.4, 0.7 Hz, 2H).

4-chloro-*N*-(2-phenylallyl)benzamide **1l**



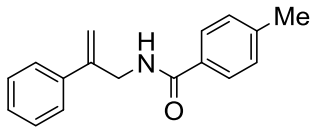
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 7.4 Hz, 2H), 7.48 – 7.34 (m, 5H), 6.17 (brs, 1H), 5.58 (s, 1H), 5.37 (s, 1H), 4.59 (d, *J* = 5.6 Hz, 2H).

4-bromo-*N*-(2-phenylallyl)benzamide **1m**



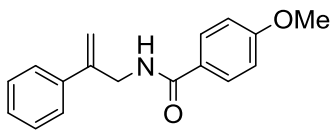
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 – 7.43 (m, 6H), 7.36 (t, *J* = 7.5 Hz, 3H), 6.38 (brs, 1H), 5.53 (d, *J* = 5.6 Hz, 1H), 5.31 (d, *J* = 5.6 Hz, 1H), 4.52 (d, *J* = 12.4 Hz, 2H).

4-methyl-*N*-(2-phenylallyl)benzamide **1n**



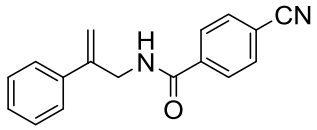
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.9 Hz, 2H), 7.61 – 7.52 (m, 2H), 7.49 – 7.37 (m, 3H), 7.28 (d, *J* = 7.8 Hz, 2H), 6.23 (brs, 1H), 5.60 (s, 1H), 5.40 (s, 1H), 4.62 (d, *J* = 5.6 Hz, 2H), 2.46 (s, 3H).

4-methoxy-*N*-(2-phenylallyl)benzamide **1o**



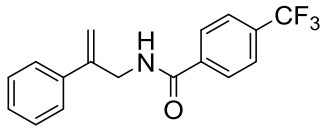
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 2H), 7.55 – 7.47 (m, 2H), 7.42 – 7.31 (m, 3H), 7.03 – 6.79 (m, 2H), 6.11 (brs, 1H), 5.54 (d, *J* = 0.8 Hz, 1H), 5.34 (d, *J* = 1.1 Hz, 1H), 4.55 (d, *J* = 5.7 Hz, 2H), 3.85 (s, 3H).

4-cyano-*N*-(2-phenylallyl)benzamide **1p**



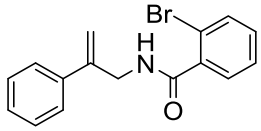
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 – 7.69 (m, 4H), 7.52 – 7.46 (m, 2H), 7.43 – 7.33 (m, 3H), 6.23 (brs, 1H), 5.57 (q, *J* = 0.7 Hz, 1H), 5.35 (q, *J* = 1.3 Hz, 1H), 4.58 (d, *J* = 5.0 Hz, 2H).

N-(2-phenylallyl)-4-(trifluoromethyl)benzamide **1q**



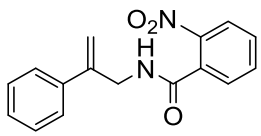
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 – 7.81 (m, 2H), 7.76 – 7.67 (m, 2H), 7.57 – 7.49 (m, 2H), 7.46 – 7.35 (m, 3H), 6.26 (brs, 1H), 5.59 (d, *J* = 0.9 Hz, 1H), 5.38 (d, *J* = 1.0 Hz, 1H), 4.61 (d, *J* = 5.0 Hz, 2H).

2-bromo-*N*-(2-phenylallyl)benzamide **1r**



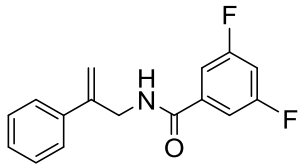
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 – 7.49 (m, 3H), 7.48 – 7.32 (m, 5H), 7.30 – 7.22 (m, 1H), 6.22 (brs, 1H), 5.56 (s, 1H), 5.41 (s, 1H), 4.57 (d, *J* = 4.9 Hz, 2H).

2-nitro-*N*-(2-phenylallyl)benzamide **1s**



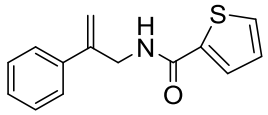
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.70 – 7.48 (m, 4H), 7.47 – 7.35 (m, 4H), 6.10 (brs, 1H), 5.58 (s, 1H), 5.42 (s, 1H), 4.57 (d, *J* = 5.6 Hz, 2H).

3,5-difluoro-*N*-(2-phenylallyl)benzamide **1t**



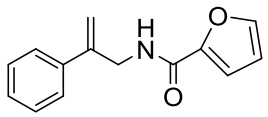
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.43 (m, 4H), 7.43 – 7.31 (m, 3H), 7.07 (dd, *J* = 5.0, 3.8 Hz, 1H), 6.08 (brs, 1H), 5.55 (q, *J* = 0.8 Hz, 1H), 5.34 (q, *J* = 1.2 Hz, 1H), 4.54 (ddd, *J* = 5.8, 1.5, 0.8 Hz, 2H).

N-(2-phenylallyl)thiophene-2-carboxamide **1u**



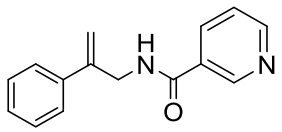
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.43 – 7.33 (m, 3H), 7.26 – 7.19 (m, 2H), 6.95 (tt, *J* = 8.6, 2.3 Hz, 1H), 6.13 (brs, 1H), 5.56 (d, *J* = 0.8 Hz, 1H), 5.34 (d, *J* = 1.1 Hz, 1H), 4.56 (dd, *J* = 5.6, 1.3 Hz, 2H).

N-(2-phenylallyl)furan-2-carboxamide **1v**



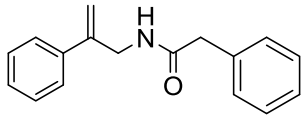
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 – 7.49 (m, 2H), 7.48 – 7.34 (m, 4H), 7.17 (dd, *J* = 3.5, 0.8 Hz, 1H), 6.58 – 6.52 (m, 1H), 6.51 (brs, 1H), 5.57 (s, 1H), 5.36 (s, 1H), 4.55 (d, *J* = 5.9 Hz, 2H).

N-(2-phenylallyl)nicotinamide **1w**



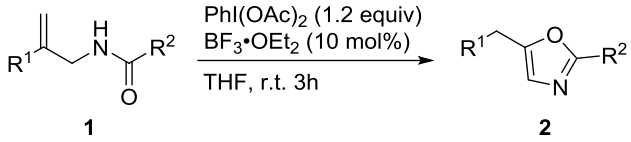
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.89 (d, *J* = 2.3 Hz, 1H), 8.69 (dd, *J* = 4.9, 1.7 Hz, 1H), 8.08 (ddd, *J* = 8.0, 2.3, 1.7 Hz, 1H), 7.54 – 7.43 (m, 2H), 7.42 – 7.31 (m, 4H), 6.50 (brs, 1H), 5.54 (d, *J* = 0.8 Hz, 1H), 5.34 (d, *J* = 0.9 Hz, 1H), 4.57 (dd, *J* = 5.6, 0.7 Hz, 2H).

2-phenyl-*N*-(2-phenylallyl)acetamide **1x**



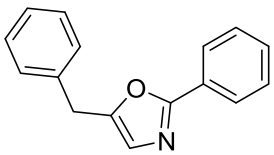
A white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 – 7.28 (m, 7H), 7.27 (d, *J* = 1.5 Hz, 1H), 7.19 – 7.11 (m, 2H), 5.46 (brs, 1H), 5.38 (q, *J* = 0.9 Hz, 1H), 5.10 (td, *J* = 1.5, 0.8 Hz, 1H), 4.31 (dt, *J* = 5.8, 1.2 Hz, 2H), 3.58 (s, 2H).

3. General Procedure for Cyclization of allylic amides (2a-2x)



An ovendried Schlenk tube equipped with a magnetic stir bar was charged with allylic amides (0.3 mmol, 1.0 equiv), $PhI(OAc)_2$ (0.36 mmol, 1.2 equiv), BF_3·Et_2O (3.7μl, 0.03 mmol, 10 mol %) and THF (3 mL), followed by stirring at room temperature for 3h. The solvent was evaporated, and the residue was purified by flash column chromatography (hexane/ethyl acetate) on silica gel and afforded corresponding oxazole **2a-2x**.

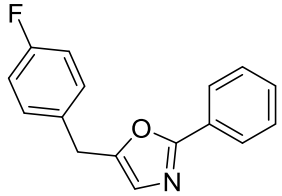
5-benzyl-2-phenyloxazole **2a**



A yellow oil; 58.0mg, Yield 82 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.94 (m, 2H), 7.46 – 7.37 (m, 3H), 7.36 – 7.22 (m, 5H), 6.86 (t, *J* = 1.1 Hz, 1H), 4.04 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 151.5, 136.7, 130.1, 130.0, 128.8, 128.3, 127.7, 127.0, 126.1, 124.9, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{10}H_{10}NO$, 236.1075; found,

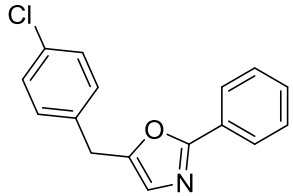
236.1068.

5-(4-fluorobenzyl)-2-phenyloxazole **2b**



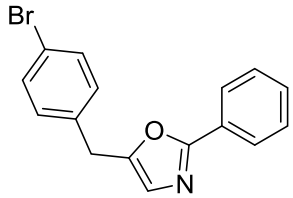
A colorless oil; 67.6mg, Yield 89 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 – 7.99 (m, 2H), 7.51 – 7.45 (m, 3H), 7.30 (dd, *J* = 5.8, 3.0 Hz, 2H), 7.16 – 7.01 (m, 2H), 6.90 (s, 1H), 4.08 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9 (d, $^{1}J_{C–F}$ = 244.9 Hz), 161.4, 151.2, 132.3 (d, $^{4}J_{C–F}$ = 2.8 Hz), 130.2 (d, $^{3}J_{C–F}$ = 3.8 Hz), 130.2, 128.8, 128.3 (d, $^{2}J_{C–F}$ = 122.2 Hz), 126.1, 124.8, 115.6 (d, *J* = 21.4 Hz), 31.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}FNO$, 254.0981; found, 254.0981.

5-(4-chlorobenzyl)-2-phenyloxazole **2c**



A yellow oil; 80.1mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.51 – 7.44 (m, 3H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 8.5 Hz, 2H), 6.92 (s, 1H), 4.06 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.5, 150.9, 135.1, 132.9, 130.3, 130.1, 128.9, 128.8, 127.5, 126.2, 124.9, 31.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}ClNO$, 270.0686; found, 270.0682.

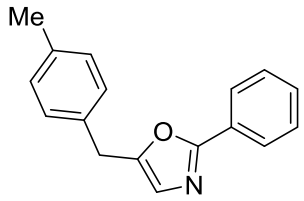
5-(4-bromobenzyl)-2-phenyloxazole **2d**



A yellow oil; 93.8mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.78 – 7.38 (m, 5H), 7.14 (d, *J* = 8.3 Hz, 2H), 6.85 (s, 1H), 3.99 (s, 2H); ^{13}C

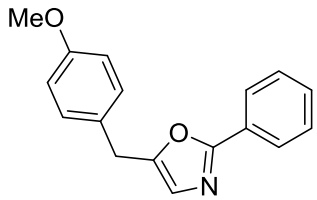
NMR (75 MHz, $CDCl_3$) δ 161.5, 150.7, 135.7, 131.8, 130.4, 130.2, 128.8, 127.5, 126.1, 125.0, 120.9, 31.6; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}BrNO$, 314.0181; found, 314.0178.

5-(4-methylbenzyl)-2-phenyloxazole **2e**



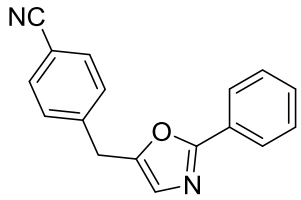
A colorless oil; 67.9mg, Yield 91 %; ^1H NMR (300 MHz, $CDCl_3$) δ 8.02 – 7.93 (m, 2H), 7.40 (dq, *J* = 4.0, 2.0 Hz, 3H), 7.21 – 7.08 (m, 4H), 6.84 (s, 1H), 4.01 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.2, 151.8, 136.6, 133.6, 130.1, 129.4, 128.7, 128.6, 127.6, 126.1, 124.7, 31.8, 21.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO$, 250.1232; found, 250.1228.

5-(4-methoxybenzyl)-2-phenyloxazole **2f**



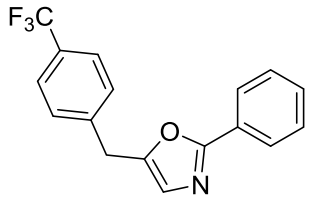
A yellow oil; 68.5mg, Yield 86 %; ^1H NMR (300 MHz, $CDCl_3$) δ 8.07 – 7.97 (m, 2H), 7.51 – 7.40 (m, 3H), 7.26 – 7.19 (m, 2H), 6.94 – 6.87 (m, 2H), 6.86 (t, *J* = 1.1 Hz, 1H), 4.03 (s, 2H), 3.82 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.2, 158.6, 152.0, 130.1, 129.8, 128.7, 128.7, 127.7, 126.1, 124.6, 114.2, 55.3, 31.3; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO_2$, 266.1181; found, 266.1172.

4-((2-phenyloxazol-5-yl)methyl)benzonitrile **2g**



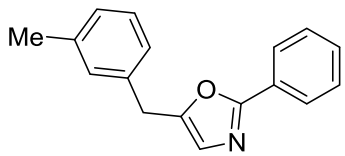
A white solid; mp 106-110 ℃; 51.8mg, Yield 66 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (p, *J* = 3.7 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.47 (dt, *J* = 6.5, 2.7 Hz, 5H), 6.97 (s, 1H), 4.18 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.8, 149.5, 142.2, 132.6, 130.4, 129.5, 128.8, 127.3, 126.2, 125.5, 118.7, 111.1, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{13}N_2O$, 261.1028; found, 261.1028.

2-phenyl-5-(4-(trifluoromethyl)benzyl)oxazole **2h**



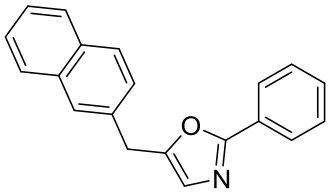
A colorless oil; 77.6mg, Yield 85 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dq, *J* = 5.8, 3.6, 2.6 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.54 – 7.40 (m, 5H), 6.96 (s, 1H), 4.18 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.6, 150.2, 140.7, 130.3, 129.8 (q, $^2J_{C–F}$ = 29.7 Hz), 129.0, 128.8, 128.3 (q, $^1J_{C–F}$ = 132.5 Hz), 126.2, 125.7 (q, $^4J_{C–F}$ = 3.8 Hz), 125.2, 122.4 (q, $^3J_{C–F}$ = 6.3 Hz), 31.9; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{13}F_3NO$, 304.0949; found, 304.0941.

5-(3-methylbenzyl)-2-phenyloxazole **2i**



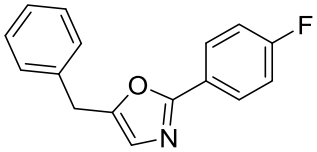
A yellow oil; 74.3mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ8.05 – 7.94 (m, 2H), 7.45 – 7.35 (m, 3H), 7.28 – 7.17 (m, 1H), 6.86 (t, 1H), 4.02 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3, 151.6, 138.4, 136.6, 130.1, 129.5, 128.7, 128.6, 127.7, 126.1, 125.8, 124.8, 32.1, 21.4; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO$, 250.1232; found, 250.1223.

5-(naphthalen-2-ylmethyl)-2-phenyloxazole **2j**



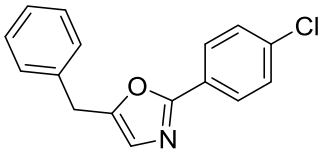
A white solid; mp 57-58 ℃; 84.9mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11 – 7.99 (m, 2H), 7.85 (dt, *J* = 6.6, 3.9 Hz, 3H), 7.76 (s, 1H), 7.57 – 7.40 (m, 6H), 6.94 (d, *J* = 1.1 Hz, 1H), 4.25 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 151.3, 134.1, 133.5, 132.4, 130.1, 128.7, 128.4, 127.7, 127.6, 127.2, 126.9, 126.3, 126.1, 125.8, 125.0, 32.3; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{16}NO$, 286.1232; found, 286.1225.

5-benzyl-2-(4-fluorophenyl)oxazole **2k**



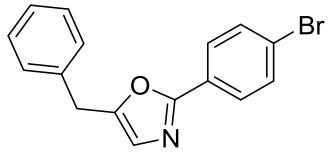
A colorless oil; 69.5mg, Yield 92 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 – 7.97 (m, 2H), 7.45 – 7.28 (m, 5H), 7.22 – 7.11 (m, 2H), 6.90 (t, *J* = 1.1 Hz, 1H), 4.11 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.5, 161.4 (d, $^{1}J_{C-F}$ = 130.5 Hz), 151.5, 136.6, 128.7 (d, $^{3}J_{C-F}$ = 4.5 Hz), 128.3, 128.2, 127.0, 124.8, 124.0 (d, $^{4}J_{C-F}$ = 3.0 Hz), 115.9 (d, $^{2}J_{C-F}$ = 22.1 Hz), 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}FNO$, 254.0981; found, 254.0973.

5-benzyl-2-(4-chlorophenyl)oxazole **2l**



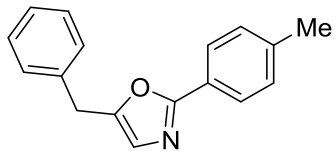
A white solid; mp 83-84 ℃; 80.1mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.93 (m, 2H), 7.50 – 7.28 (m, 7H), 6.91 (t, *J* = 1.1 Hz, 1H), 4.11 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 151.7, 136.5, 136.1, 129.0, 128.8, 128.7, 127.4, 127.0, 126.1, 125.0, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}ClNO$, 270.0686; found, 270.0675.

5-benzyl-2-(4-bromophenyl)oxazole **2m**



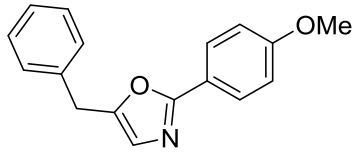
A light yellow solid; mp 87-88 ℃; 93.6mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 – 7.85 (m, 2H), 7.67 – 7.57 (m, 2H), 7.47 – 7.28 (m, 5H), 6.92 (t, *J* = 1.1 Hz, 1H), 4.11 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 151.8, 136.5, 132.0, 128.8, 128.7, 127.6, 127.1, 126.6, 125.1, 124.5, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}BrNO$, 314.0181; found, 314.0172.

5-benzyl-2-(p-tolyl)oxazole **2n**



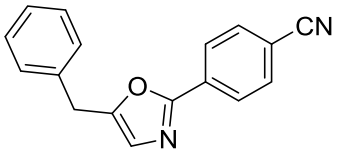
A white solid; mp 82-83 ℃; 60.0mg, Yield 80 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.2, 2.4 Hz, 2H), 7.46 – 7.23 (m, 7H), 6.89 (t, 1H), 4.12 (s, 2H), 2.44 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.5, 151.1, 140.3, 136.8, 129.4, 128.7, 126.9, 126.1, 125.0, 124.7, 32.2, 21.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO$, 250.1232; found, 250.1223.

5-benzyl-2-(4-methoxyphenyl)oxazole **2o**



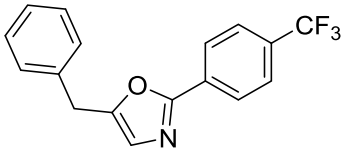
A colorless oil; 52.1mg, Yield 65 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.90 (m, 2H), 7.41 – 7.25 (m, 5H), 7.01 – 6.92 (m, 2H), 6.85 (t, *J* = 1.1 Hz, 1H), 4.07 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4, 161.1, 150.8, 136.8, 128.7, 127.8, 126.9, 124.5, 120.5, 114.1, 55.3, 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO_2$, 266.1181; found, 266.1171.

4-(5-benzyloxazol-2-yl)benzonitrile **2p**



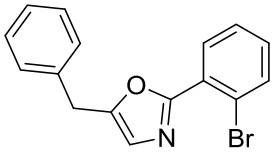
A white solid; mp 113-114 ℃; 65.0mg, Yield 83 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 – 8.03 (m, 2H), 7.75 – 7.65 (m, 2H), 7.44 – 7.24 (m, 5H), 7.00 – 6.92 (m, 1H), 4.10 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 152.9, 136.2, 132.6, 131.3, 128.9, 128.7, 127.2, 126.4, 125.7, 118.4, 113.2, 32.2, 29.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{13}N_2O$, 261.1028; found, 261.1019.

5-benzyl-2-(4-(trifluoromethyl)phenyl)oxazole **2q**



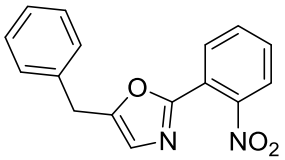
A yellow oil; 84.6mg, Yield 93 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (dd, J = 8.9, 0.8 Hz, 2H), 7.71 (dd, J = 8.9, 0.7 Hz, 2H), 7.45 – 7.27 (m, 5H), 6.95 (t, J = 1.1 Hz, 1H), 4.11 (d, J = 1.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.9, 152.4, 136.4, 131.6 (q, $^2J_{C–F}$ = 32.8 Hz), 130.8, 129.3, 128.8, 128.7, 126.3, 126.2 (q, $^1J_{C–F}$ = 133.1 Hz), 125.8 (q, $^3J_{C–F}$ = 3.9 Hz), 122.1, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{13}F_3NO$, 304.0949; found, 304.0939.

5-benzyl-2-(2-bromophenyl)oxazole **2r**



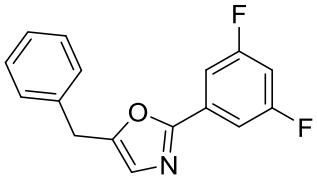
A yellow oil; 85.8mg, Yield 91 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (dd, J = 7.8, 1.8 Hz, 1H), 7.73 (dd, J = 8.0, 1.2 Hz, 1H), 7.49 – 7.24 (m, 7H), 7.01 (t, 1H), 4.13 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 152.0, 136.5, 134.5, 131.1, 131.0, 128.8, 128.8, 128.5, 127.4, 127.0, 124.7, 120.9, 32.2; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}BrNO$, 314.0181; found, 314.0173.

5-benzyl-2-(2-nitrophenyl)oxazole **2s**



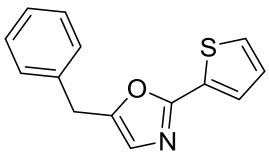
A yellow oil; 83.5mg, Yield 99 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 7.7, 1.6 Hz), 7.78 (dd, *J* = 7.8, 1.4 Hz), 7.63 (dtd, *J* = 23.1, 7.6, 1.5 Hz), 7.46 – 7.27 (m), 6.96 (t, *J* = 1.1 Hz), 4.09 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.6, 153.1, 148.5, 136.2, 132.0, 130.8, 130.2, 128.8, 128.7, 127.1, 125.3, 123.8, 121.1, 32.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{13}N_2O_3$, 281.0926; found, 281.0918.

5-benzyl-2-(3,5-difluorophenyl)oxazole **2t**



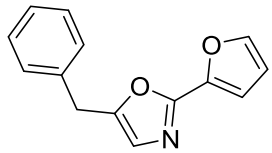
A white solid; mp 62-63 ℃; 73.2mg, Yield 90 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 – 7.49 (m, 2H), 7.42 – 7.35 (m, 2H), 7.35 – 7.27 (m, 3H), 6.92 (t, *J* = 1.1 Hz, 1H), 6.87 (tt, *J* = 8.8, 2.4 Hz, 1H), 4.09 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.8 (d, *J* = 12.5 Hz), 161.5 (d, *J* = 12.5 Hz), 159.1 (dd, *J* = 3.9, 3.4), 152.4, 136.2, 130.4 (dd, *J* = 11.2, 10.6 Hz), 128.8 (d, *J* = 9.3 Hz), 126.2 (d, *J* = 136.9 Hz), 109.1 (d, *J* = 27.3 Hz), 109.1 (d, *J* = 9.2 Hz), 105.3 (dd, *J* = 26.7, 25.4 Hz), 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{12}F_2NO$, 272.0887; found, 272.0877.

5-benzyl-2-(thiophen-2-yl)oxazole **2u**



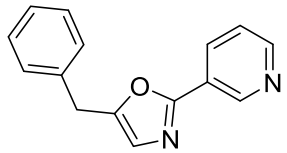
A yellow oil; 61.4mg, Yield 85 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.46 – 7.26 (m, 6H), 7.11 (dd, *J* = 5.0, 3.7 Hz, 1H), 6.85 (d, *J* = 1.2 Hz, 1H), 4.08 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.5, 151.0, 136.5, 130.2, 128.8, 128.7, 127.9, 127.3, 127.0, 124.7, 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{14}H_{12}NOS$, 242.0640; found, 242.0630.

5-benzyl-2-(furan-2-yl)oxazole **2v**



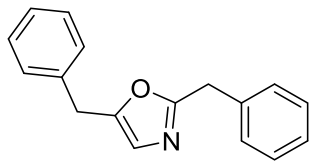
A yellow oil; 59.0mg, Yield 73 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 (d, *J* = 1.7 Hz, 1H), 7.45 – 7.26 (m, 5H), 7.00 (d, *J* = 3.5 Hz, 1H), 6.88 (d, *J* = 1.1 Hz, 1H), 6.56 (dd, *J* = 3.5, 1.8 Hz, 1H), 4.10 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.1, 151.1, 144.1, 143.1, 136.4, 128.8, 128.7, 127.0, 124.7, 111.7, 110.9, 32.0; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{14}H_{12}NO_2$, 226.0868; found, 226.0858.

5-benzyl-2-(pyridin-3-yl)oxazole **2w**



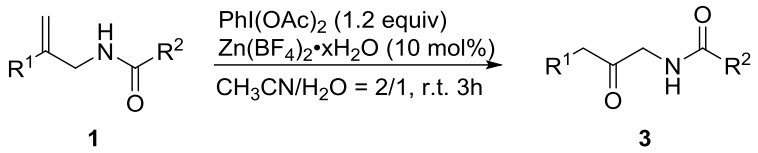
A white solid; mp 57-58 ℃; 54.5mg, Yield 77 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (d, *J* = 2.1 Hz, 1H), 8.65 (dd, *J* = 4.8, 1.7 Hz, 1H), 8.25 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.46 – 7.21 (m, 6H), 6.92 (d, *J* = 1.1 Hz, 1H), 4.09 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 152.3, 150.7, 147.4, 136.3, 133.2, 128.8, 128.7, 127.1, 125.1, 123.8, 123.5, 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{15}H_{13}N_2O$, 237.1028; found, 237.1020.

2,5-dibenzyloxazole **2x**



A colorless oil; 60.7mg, Yield 81 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 – 7.22 (m, 10H), 6.71 (s, 1H), 4.13 (s, 2H), 4.00 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 151.5, 136.8, 135.7, 128.9, 128.7, 128.7, 127.0, 126.9, 123.5, 34.7, 32.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{16}NO$, 250.1232; found, 250.1222.

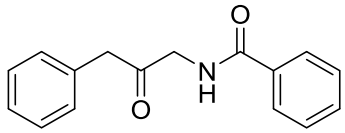
4. General Procedure for Synthesis of *β*-Keto Amides (3a-3x)



1 3

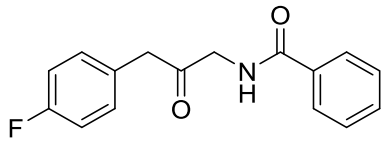
An ovendried Schlenk tube equipped with a magnetic stir bar was charged with allylic amides (0.2 mmol, 1.0 equiv), $PhI(OAc)_2$ (0.24 mmol, 1.2 equiv), ZnBF4•xH2O (0.02 mmol, 10 mol %), CH_3CN/H_2O (2 mL/1mL) was successively added followed by stirring at room temperature for 3h. The solvent was evaporated, and the residue was purified by flash column chromatography (hexane/ethyl acetate) on silica gel and afforded corresponding β-keto amides **3a-3x**.

N-(2-oxo-3-phenylpropyl)benzamide **3a**



A white solid; mp 99-101 ℃; 44.9 mg, Yield 89 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.0 Hz, 2H), 7.61 – 7.24 (m, 8H), 7.03 (brs, 1H), 4.42 (d, *J* = 4.4 Hz, 2H), 3.84 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.3, 167.3, 133.7, 132.9, 131.8, 129.4, 129.0, 128.6, 127.6, 127.1, 49.2, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{16}NO_2$, 254.1181; found, 254.1180.

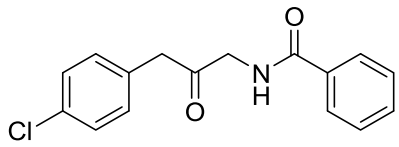
N-(3-(4-fluorophenyl)-2-oxopropyl)benzamide **3b**



A white solid; mp 121-122 ℃; 34.4 mg, Yield 63 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (dt, *J* = 8.6, 1.9 Hz, 2H), 7.62 – 7.42 (m, 3H), 7.24 (dd, *J* = 8.5, 5.5 Hz, 2H), 7.08 (td, *J* = 8.8, 2.2 Hz, 2H), 7.03 (brs, 1H), 4.42 (d, *J* = 4.6 Hz, 2H), 3.82 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.0, 167.4, 162.2 (d, $^1J_{C-F}$ = 246.2 Hz), 153.7, 133.6, 131.9, 131.0

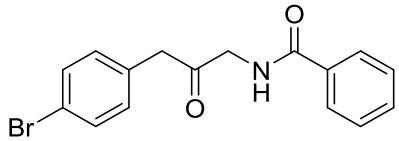
(d, $^{3}J_{C-F}$ = 8.2 Hz), 128.7, 127.1, 115.9 (d, $^{2}J_{C-F}$ = 21.4 Hz), 49.2, 46.6; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}FNO_2$, 272.1087; found, 272.1087.

N-(3-(4-chlorophenyl)-2-oxopropyl)benzamide **3c**



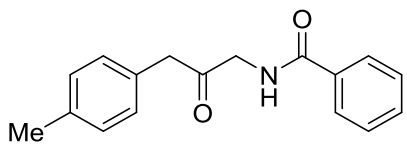
A white solid; mp 135-136 ℃; 36.9 mg, Yield 64 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 – 7.77 (m, 2H), 7.57 – 7.49 (m, 1H), 7.49 – 7.40 (m, 2H), 7.37 – 7.30 (m, 2H), 7.24 – 7.14 (m, 2H), 7.00 (brs, 1H), 4.39 (d, *J* = 4.6 Hz, 2H), 3.79 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.7, 167.4, 133.6 133.5, 131.9, 131.3, 130.8, 129.1, 128.7, 127.1, 49.3, 46.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}ClNO_2$, 288.0791; found, 288.0789.

N-(3-(4-bromophenyl)-2-oxopropyl)benzamide **3d**



A white solid; mp 148-150 ℃; 40.4 mg, Yield 61 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 – 7.76 (m, 2H), 7.62 – 7.40 (m, 5H), 7.20 – 7.07 (m, 2H), 6.97 (brs, 1H), 4.40 (d, *J* = 4.6 Hz, 2H), 3.78 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.5, 167.4, 133.6, 132.1, 131.9, 131.8, 131.1, 128.7, 127.1, 121.6, 49.3, 46.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}BrNO_2$, 332.0286; found, 332.0284.

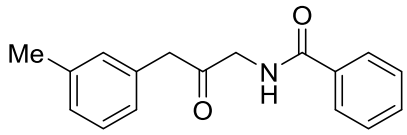
N-(2-oxo-3-(p-tolyl)propyl)benzamide **3e**



A white solid; mp 121-122 ℃; 52.4 mg, Yield 98 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 – 7.77 (m, 2H), 7.56 – 7.38 (m, 3H), 7.22 – 7.11 (m, 4H), 7.04 (brs, 1H), 4.37 (d, *J* = 4.5 Hz, 2H), 3.77 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.5, 167.3,

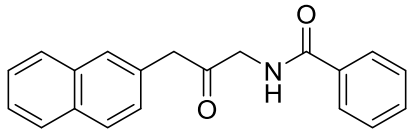
137.2, 133.7, 131.8 129.8, 129.7, 129.3, 128.6, 127.1, 49.1, 47.4, 21.1; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{18}NO_2$, 268.1338; found, 268.1333.

N-(2-oxo-3-(m-tolyl)propyl)benzamide **3i**



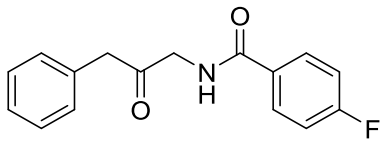
A white solid; mp 85-86 ℃; 38.8 mg, Yield 73 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 – 7.79 (m, 2H), 7.73 – 7.40 (m, 3H), 7.40 – 7.24 (m, 1H), 7.21 – 7.06 (m, 3H), 7.03 (brs, 1H), 4.41 (d, *J* = 4.3 Hz, 2H), 3.80 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.4, 167.3, 138.8, 133.8, 132.8, 131.8, 130.1, 128.9, 128.6, 128.3, 127.1, 126.4, 49.1, 47.8, 21.4; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{18}NO_2$, 268.1338; found, 268.1337.

N-(3-(naphthalen-2-yl)-2-oxopropyl)benzamide **3j**



A white solid; mp 110-112 ℃; 55.7 mg, Yield 92 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 – 7.78 (m, 5H), 7.75 (s, 1H), 7.54 (ddp, *J* = 7.1, 2.6, 1.3 Hz, 3H), 7.49 – 7.34 (m, 3H), 7.04 (brs, 1H), 4.45 (d, *J* = 4.5 Hz, 2H), 3.99 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.3, 167.4, 133.7, 133.6, 132.6, 131.8, 130.4, 128.8, 128.6, 128.4, 127.8, 127.7, 127.2, 127.1, 126.5, 126.2, 49.2, 47.9; HRMS (ESI) m/z $[M + Na]^+$: calcd for $C_{20}H_{18}NO_2$, 326.1157; found, 326.1152.

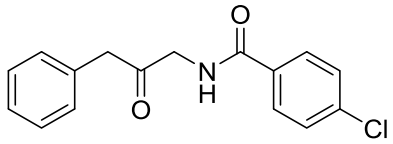
4-fluoro-*N*-(2-oxo-3-phenylpropyl)benzamide **3k**



A white solid; mp 134-136 ℃; 39.4 mg, Yield 73 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 – 7.75 (m, 2H), 7.40 – 7.27 (m, 3H), 7.26 – 7.22 (m, 2H), 7.16 – 7.05 (m, 2H),

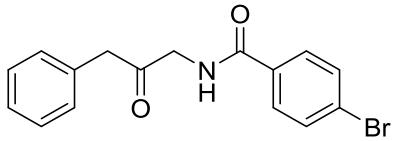
6.86 (brs, 1H), 4.37 (d, J = 4.5 Hz, 2H), 3.81 (s, 2H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.1, 166.2, 164.9 (d, $^1J_{C–F}$ = 252.3 Hz), 132.8 (d, $^4J_{C–F}$ = 1.5 Hz), 129.9, 129.4 (d, $^3J_{C–F}$ = 9.1 Hz), 129.4, 129.1, 127.6, 115.7 (d, $^2J_{C–F}$ = 21.9 Hz), 49.1, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}FNO_2$, 272.1087; found, 272.1080.

4-chloro-*N*-(2-oxo-3-phenylpropyl)benzamide **3l**



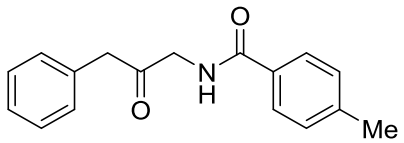
A white solid; mp 152-155 ℃; 39.8 mg, Yield 69 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 – 7.70 (m, 2H), 7.45 – 7.36 (m, 3H), 7.36 – 7.29 (m, 2H), 7.28 – 7.23 (m, 2H), 6.97 (brs, 1H), 4.38 (d, J = 4.5 Hz, 2H), 3.82 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.1, 166.2, 138.1, 132.8, 132.0, 129.4, 129.0, 128.9, 128.5, 127.6, 49.1, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}ClNO_2$, 310.0611; found, 310.0602.

4-bromo-*N*-(2-oxo-3-phenylpropyl)benzamide **3m**



A white solid; mp 164-166 ℃; 64.7 mg, Yield 97 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 – 7.53 (m, 4H), 7.43 – 7.30 (m, 3H), 7.26 (dd, J = 7.9, 1.7 Hz, 2H), 6.95 (brs, 1H), 4.38 (d, J = 4.4 Hz, 2H), 3.82 (s, 2H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.1, 166.3, 132.7, 132.5, 131.9, 129.4, 129.1, 128.7, 127.6, 126.6, 49.1, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}BrNO_2$, 332.0286; found, 332.0277.

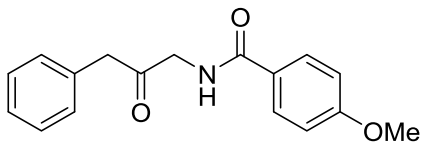
4-methyl-*N*-(2-oxo-3-phenylpropyl)benzamide **3n**



A white solid; mp 113-115 ℃; 41.0 mg, Yield 77 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, J = 8.1 Hz, 2H), 7.44 – 7.33 (m, 3H), 7.31 – 7.24 (m, 4H), 6.96 (brs, 1H), 4.41

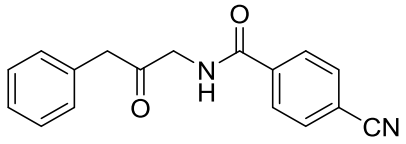
(d, J = 4.4 Hz, 2H), 3.84 (s, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.3, 167.3, 142.3, 132.9, 130.9, 129.4, 129.3, 129.0, 127.55, 127.1, 49.2, 47.8, 21.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{18}NO_2$, 268.1338; found, 268.1333.

4-methoxy-*N*-(2-oxo-3-phenylpropyl)benzamide **3o**



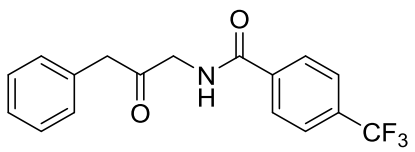
A white solid; mp 130-132 ℃; 44.2 mg, Yield 78 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 – 7.72 (m, 2H), 7.42 – 7.19 (m, 5H), 6.97 (brs, 1H), 6.94 – 6.85 (m, 2H), 4.36 (d, J = 4.6 Hz, 2H), 3.83 (s, 3H), 3.80 (s, 2H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.5, 166.9, 162.4, 133.0, 129.4, 129.0, 128.9, 127.5, 125.9, 113.8, 55.4, 49.2, 47.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{18}NO_3$, 284.1287; found, 284.1279.

4-cyano-*N*-(2-oxo-3-phenylpropyl)benzamide **3p**



A white solid; mp 123-126 ℃; 47 mg, Yield 73%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 – 7.83 (m, 2H), 7.77 – 7.66 (m, 2H), 7.41 – 7.29 (m, 3H), 7.28 – 7.21 (m, 2H), 7.09 (brs, 1H), 4.38 (d, J = 4.5 Hz, 2H), 3.82 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.9, 165.5, 137.5, 132.7, 132.5, 129.4, 129.1, 127.8, 127.7, 118.0, 115.3, 49.1, 47.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{15}N_2O_2$, 279.1134; found, 279.1127.

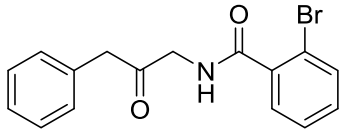
N-(2-oxo-3-phenylpropyl)-4-(trifluoromethyl)benzamide **3q**



A white solid; mp 132-133 ℃; 53.9 mg, Yield 84 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (dt, J = 8.0, 0.8 Hz, 2H), 7.70 (dt, J = 8.2, 0.7 Hz, 2H), 7.42 – 7.29 (m, 3H), 7.29 – 7.24 (m, 2H), 7.04 (brs, 1H), 4.41 (d, J = 4.5 Hz, 2H), 3.84 (s, 2H); ^{13}C NMR (75

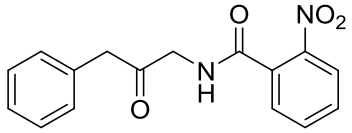
MHz, $CDCl_3$) δ 203.0, 166.0, 136.9, 133.5 (q, $^2J_{C–F}$ = 32.8 Hz), 132.7, 129.4, 129.1, 127.7, 127.6, 125.7 (q, $^3J_{C–F}$, J = 3.7 Hz), 123.6 (q, $^1J_{C–F}$ = 272.5 Hz), 49.1, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{15}F_3NO_2$, 332.1055; found, 332.1053.

2-bromo-*N*-(2-oxo-3-phenylpropyl)benzamide **3r**



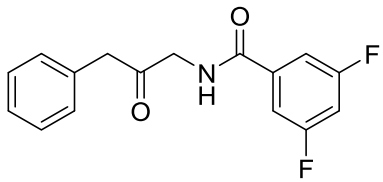
A gelatinous solid; 38.7 mg, Yield 64 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 – 7.57 (m, 1H), 7.57 – 7.50 (m, 1H), 7.42 – 7.23 (m, 7H), 6.86 (brs, 1H), 4.40 (d, J = 4.6 Hz, 2H), 3.83 (s, 2H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.6, 167.5, 136.9, 133.5, 132.8, 131.5, 129.6, 129.4, 129.0, 127.6, 127.5, 119.4, 49.2, 47.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}BrNO_2$, 332.0286; found, 332.0277.

2-nitro-*N*-(2-oxo-3-phenylpropyl)benzamide **3s**



A white solid; mp 156-160 ℃; 39.8 mg, Yield 67 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, J = 8.1, 1.3 Hz, 1H), 7.73 – 7.50 (m, 3H), 7.43 – 7.29 (m, 3H), 7.28 – 7.23 (m, 2H), 6.70 (brs, 1H), 4.40 (d, J = 4.6 Hz, 2H), 3.83 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.6, 166.4, 133.7, 132.7, 132.3, 130.7, 129.4, 129.4, 129.1, 128.7, 127.6, 124.6, 77.5, 77.1, 76.6, 49.2, 47.7; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{16}H_{15}N_2O_4$, 299.1032; found, 299.1025.

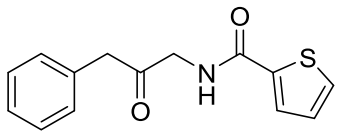
3,5-difluoro-*N*-(2-oxo-3-phenylpropyl)benzamide **3t**



A white solid; mp 93-95 ℃; 31.1 mg, Yield 54 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42

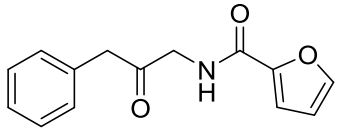
– 7.29 (m, 5H), 7.28 – 7.22 (m, 2H), 6.97 (ddt, J = 10.9, 8.6, 2.3 Hz, 2H), 4.37 (d, J = 4.5 Hz, 2H), 3.82 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.8, 164.9 (dd, $^2J_{C–F}$ = 25.5, $^3J_{C–F}$ = 7.9 Hz), 163.0 (d, $^1J_{C–F}$ = 274.6 Hz), 136.9 (d, $^4J_{C–F}$ = 7.3 Hz), 132.7, 129.4, 129.1, 127.7, 110.4 (dd, $^2J_{C–F}$ = 26.1, $^3J_{C–F}$ = 8.6 Hz), 107.2 (dd, $^2J_{C–F}$ = 25.2, $^2J_{C–F}$ = 25.4 Hz), 49.1, 47.8.; HRMS (ESI) m/z [M + Na]$^+$: calcd for $C_{16}H_{14}F_2NO_2$, 312.0812; found, 312.0802.

N-(2-oxo-3-phenylpropyl)thiophene-2-carboxamide **3u**



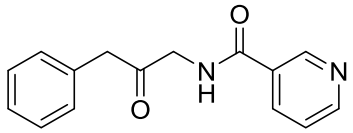
A white solid; mp 130-132 ℃; 41.1 mg, Yield 79 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 (dd, J = 3.8, 1.2 Hz, 1H), 7.49 (dd, J = 5.0, 1.2 Hz, 1H), 7.40 – 7.29 (m, 3H), 7.28 – 7.21 (m, 2H), 7.07 (dd, J = 5.0, 3.7 Hz, 1H), 6.88 (brs, 1H), 4.36 (d, J = 4.6 Hz, 2H), 3.81 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.1, 161.8, 138.1, 132.9, 130.4, 129.4, 129.0, 128.6, 127.7, 127.5, 49.0, 47.7; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{14}H_{14}NO_2S$, 260.0745; found, 260.0741.

N-(2-oxo-3-phenylpropyl)furan-2-carboxamide **3v**



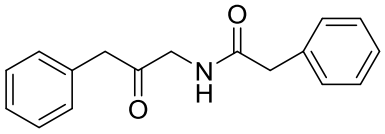
A white solid; mp 75-76 ℃; 33.5 mg, Yield 69 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (dd, J = 1.8, 0.8 Hz, 1H), 7.40 – 7.29 (m, 3H), 7.28 – 7.22 (m, 2H), 7.12 (dd, J = 3.5, 0.8 Hz, 1H), 7.08 (brs, 1H), 6.50 (dd, J = 3.5, 1.8 Hz, 1H), 4.35 (d, J = 4.7 Hz, 2H), 3.81 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.8, 158.3, 147.4, 144.3, 133.0, 129.4, 129.0, 127.5, 114.7, 112.1, 48.3, 47.7; HRMS (ESI) m/z [M + H]$^+$: calcd for $C_{14}H_{14}NO_3$, 244.0974; found, 244.0970.

N-(2-oxo-3-phenylpropyl)nicotinamide **3w**



A white solid; mp 104-106 ℃; 24.5 mg, Yield 48 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.02 (dd, *J* = 2.3, 0.9 Hz, 1H), 8.72 (dd, *J* = 4.9, 1.7 Hz, 1H), 8.11 (ddd, *J* = 8.0, 2.3, 1.7 Hz, 1H), 7.42 – 7.30 (m, 4H), 7.28 – 7.23 (m, 2H), 7.12 (brs, 1H), 4.39 (d, *J* = 4.6 Hz, 2H), 3.83 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.9, 165.5, 152.5, 148.2, 135.1, 132.7, 129.5, 129.4, 129.1, 127.7, 123.5, 49.0, 47.8; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{15}H_{15}N_2O_2$, 255.1134; found, 255.1127.

N-(2-oxo-3-phenylpropyl)-2-phenylacetamide **3x**



A white solid; mp 120-122 ℃; 46.9 mg, Yield 88 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.24 (m, 8H), 7.22 – 7.14 (m, 2H), 6.26 (brs, 1H), 4.15 (d, *J* = 4.7 Hz, 2H), 3.71 (s, 2H), 3.60 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.0, 171.2, 134.6, 132.9, 129.5, 129.1, 129.0, 128.7, 127.5, 127.5, 48.8, 47.6, 43.5; HRMS (ESI) m/z $[M + H]^+$: calcd for $C_{17}H_{18}NO_2$, 268.1338; found, 268.1332.

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: 22019781dzh_0m

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Bond precision:  C-C = 0.0026 A          Wavelength=0.71073

Cell:           a=10.2125(19)    b=11.318(2)         c=11.717(2)
                alpha=90         beta=100.447(6)     gamma=90
Temperature:    303 K

                Calculated                Reported
Volume          1331.9(4)                 1332.0(4)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C17 H12 N2 O              C17 H12 N2 O
Sum formula     C17 H12 N2 O              C17 H12 N2 O
Mr              260.29                    260.29
Dx,g cm-3       1.298                     1.298
Z               4                         4
Mu (mm-1)       0.082                     0.082
F000            544.0                     544.0
F000'           544.21
h,k,lmax        12,14,14                  12,14,14
Nref            2753                      2734
Tmin,Tmax       0.988,0.993               0.661,0.745
Tmin'           0.985

Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 26.467

R(reflections)= 0.0460( 1788)     wR2(reflections)= 0.1182( 2734)

S = 1.051                 Npar= 181
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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

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PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C14      --C17      .        5.3 s.u.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             104.9 Degree
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   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
   3 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   0 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

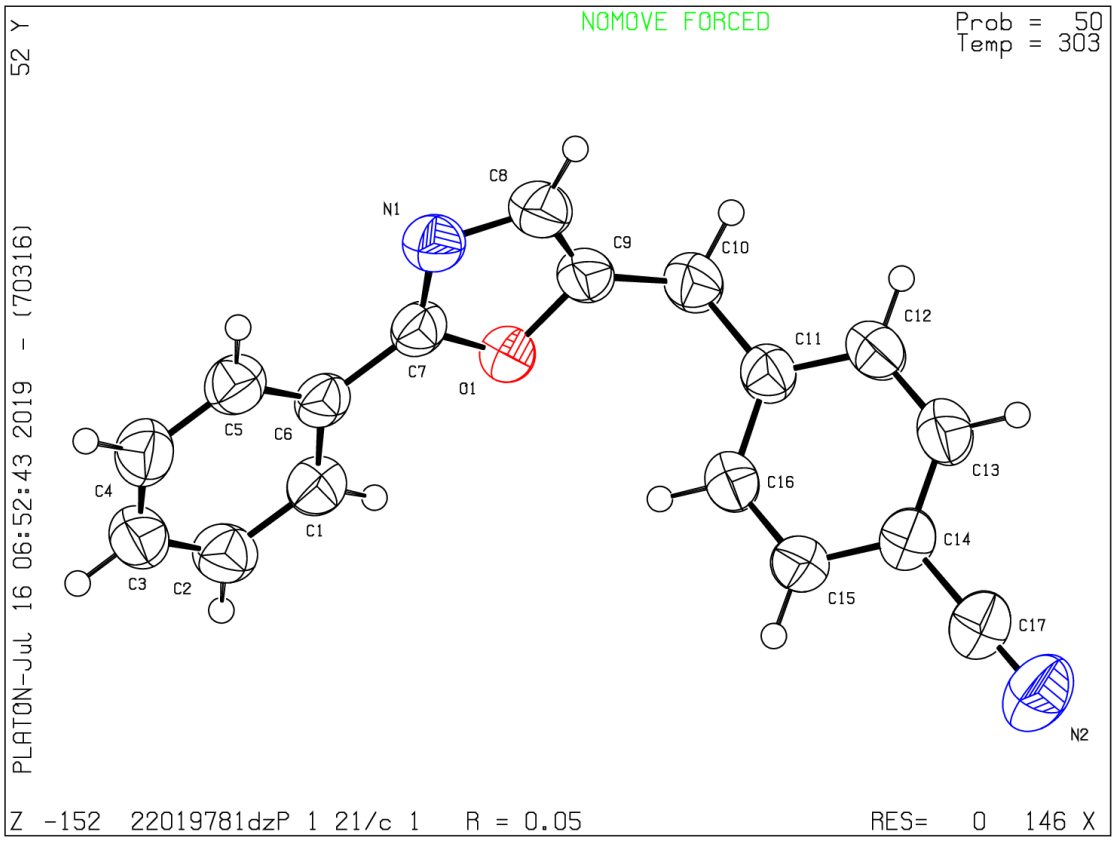
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/05/2019; check.def file version of 29/04/2019

Datablock 22019781dzh_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: 22019736dzh_0m

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Cell:            a=32.857(4)    b=5.0957(6)          c=8.5639(9)
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Temperature:     100 K

                Calculated                Reported
Volume          1403.3(3)                 1403.3(3)
Space group     C c                       C 1 c 1
Hall group      C -2yc                    C -2yc
Moiety formula  C16 H14 Cl N O2           C16 H14 Cl N O2
Sum formula     C16 H14 Cl N O2           C16 H14 Cl N O2
Mr              287.73                    287.73
Dx,g cm-3       1.362                     1.362
Z               4                         4
Mu (mm-1)       0.272                     0.272
F000            600.0                     600.0
F000'           600.84
h,k,lmax        40,6,10                   40,6,10
Nref            2917[ 1460]               2456
Tmin,Tmax       0.984,0.995               0.685,0.745
Tmin'           0.978

Correction method= # Reported T Limits: Tmin=0.685 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.84      Theta(max)= 26.438

R(reflections)= 0.0453( 1838)     wR2(reflections)= 0.1089( 2456)

S = 1.016                 Npar= 181
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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

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PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00694 Ang.
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  Cc              Ia Note
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```
   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
   3 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   1 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

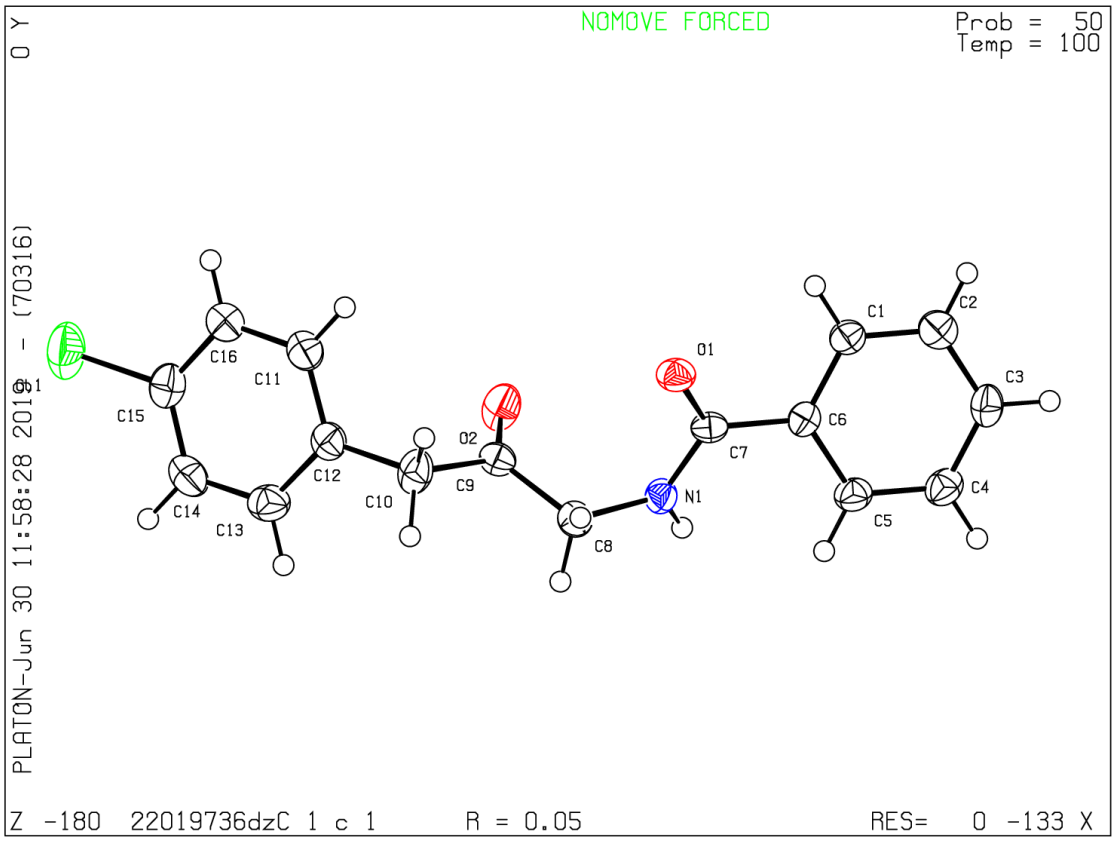
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

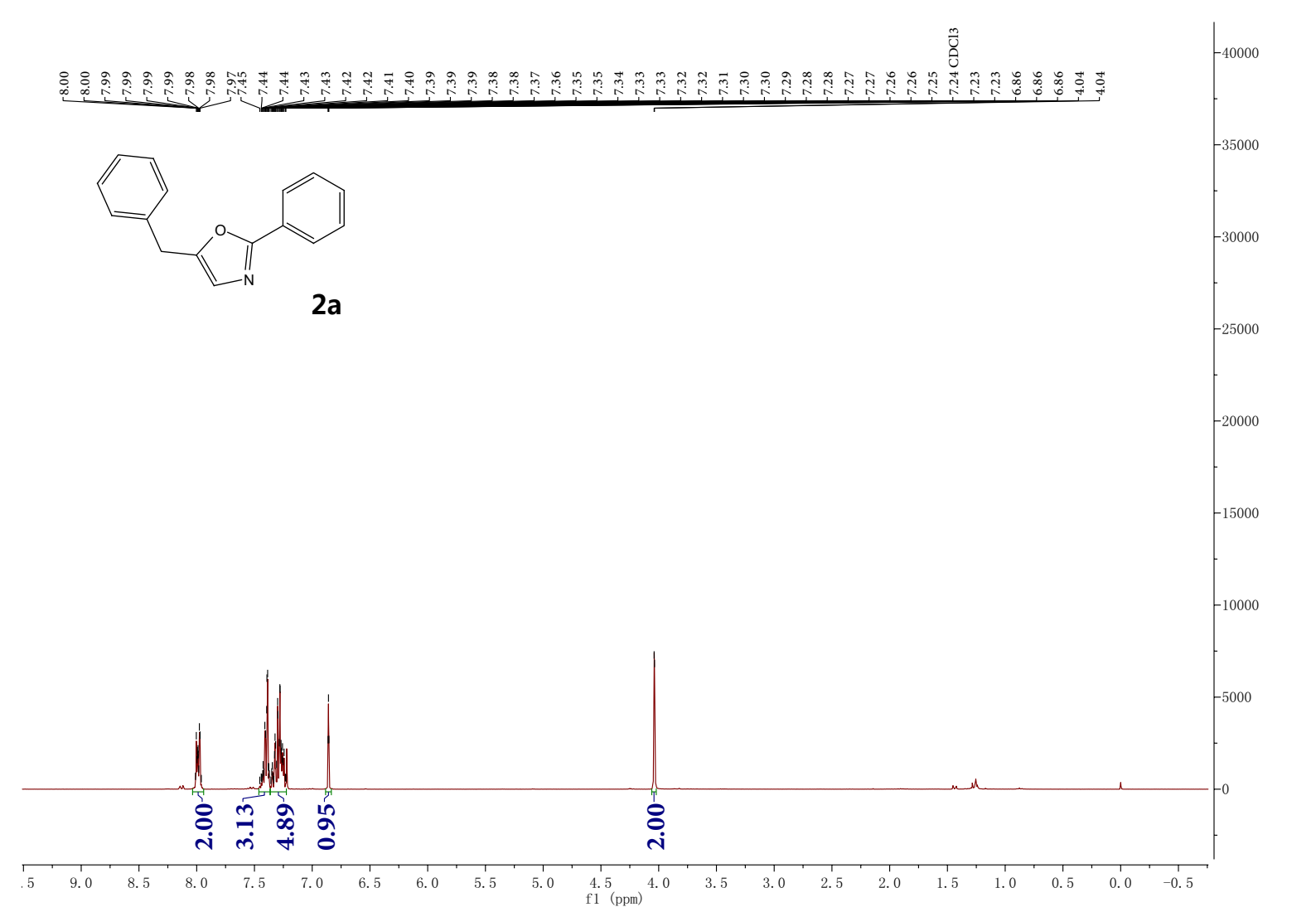
PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock 22019736dzh_0m - ellipsoid plot



7. Reference

S1. C. B. Tripathi, S. Mukherjee, *Angew*. *Chem*. *Int*. *Ed.*, 2013, **52** ,8450-8453
S2. D. A. Fort, T. J. Woltering, M. Nettekoven, H. Knustb, T. Bach, *Chem*. *Commun*., 2013, **49**, 2989-2991
S3. A. Jaganathan, A. Garzan, D. C. Whitehead, R. J. Staples, B. Borhan, *Angew*. *Chem. Int*. *Ed.*, 2011, **50**, 2593-2596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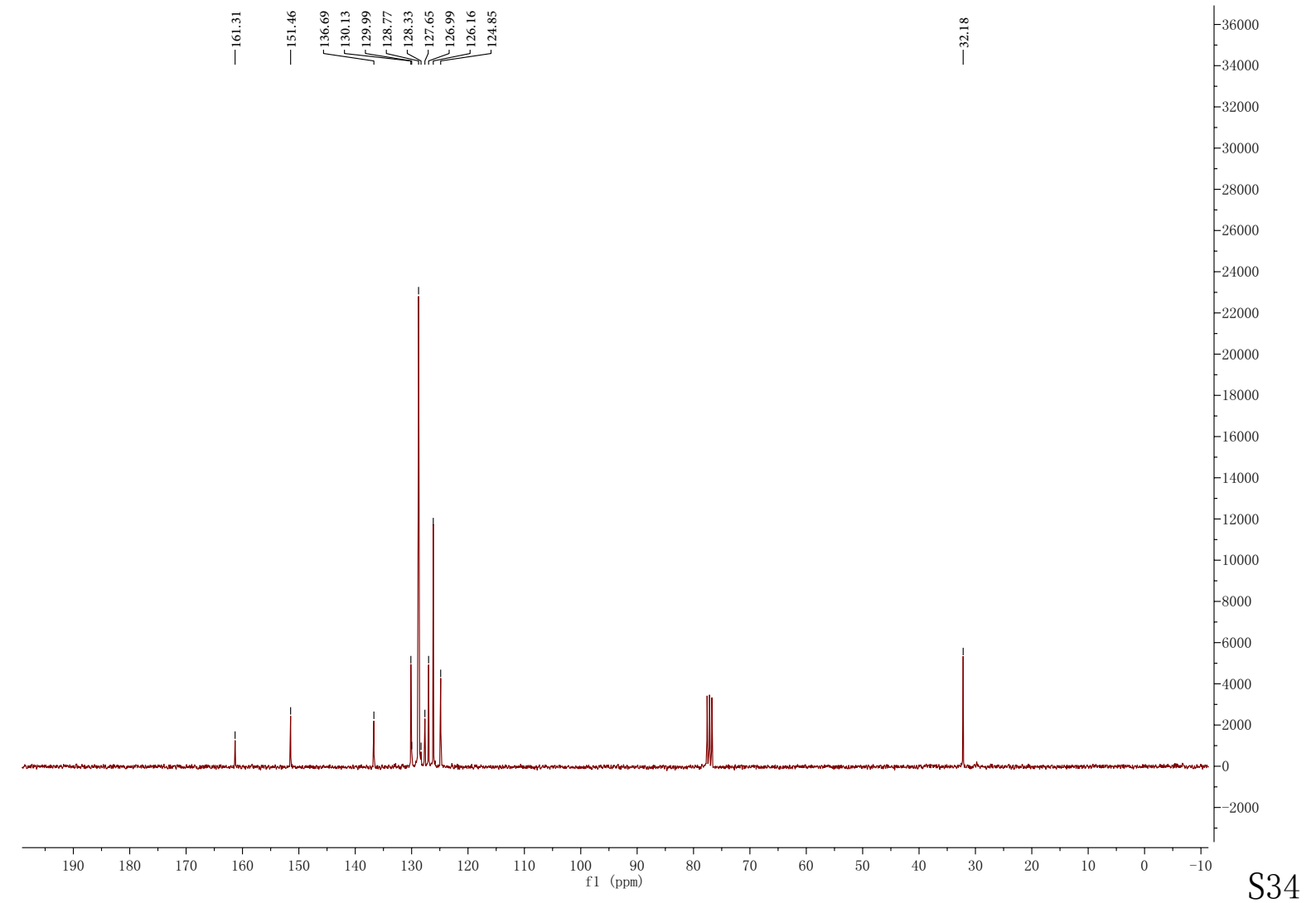
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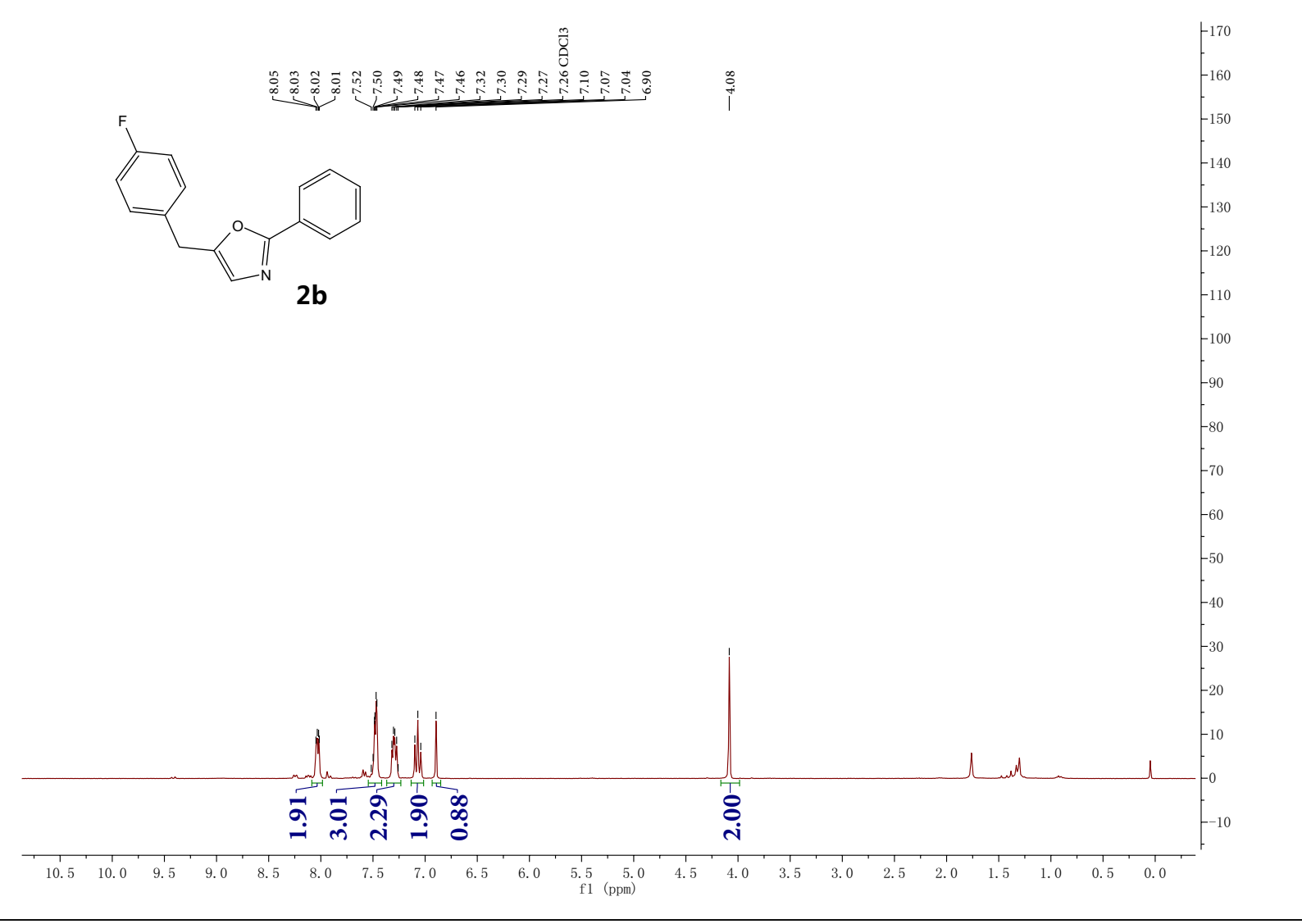
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7.27
7.26 CDCl3
7.10
7.07
7.04
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N
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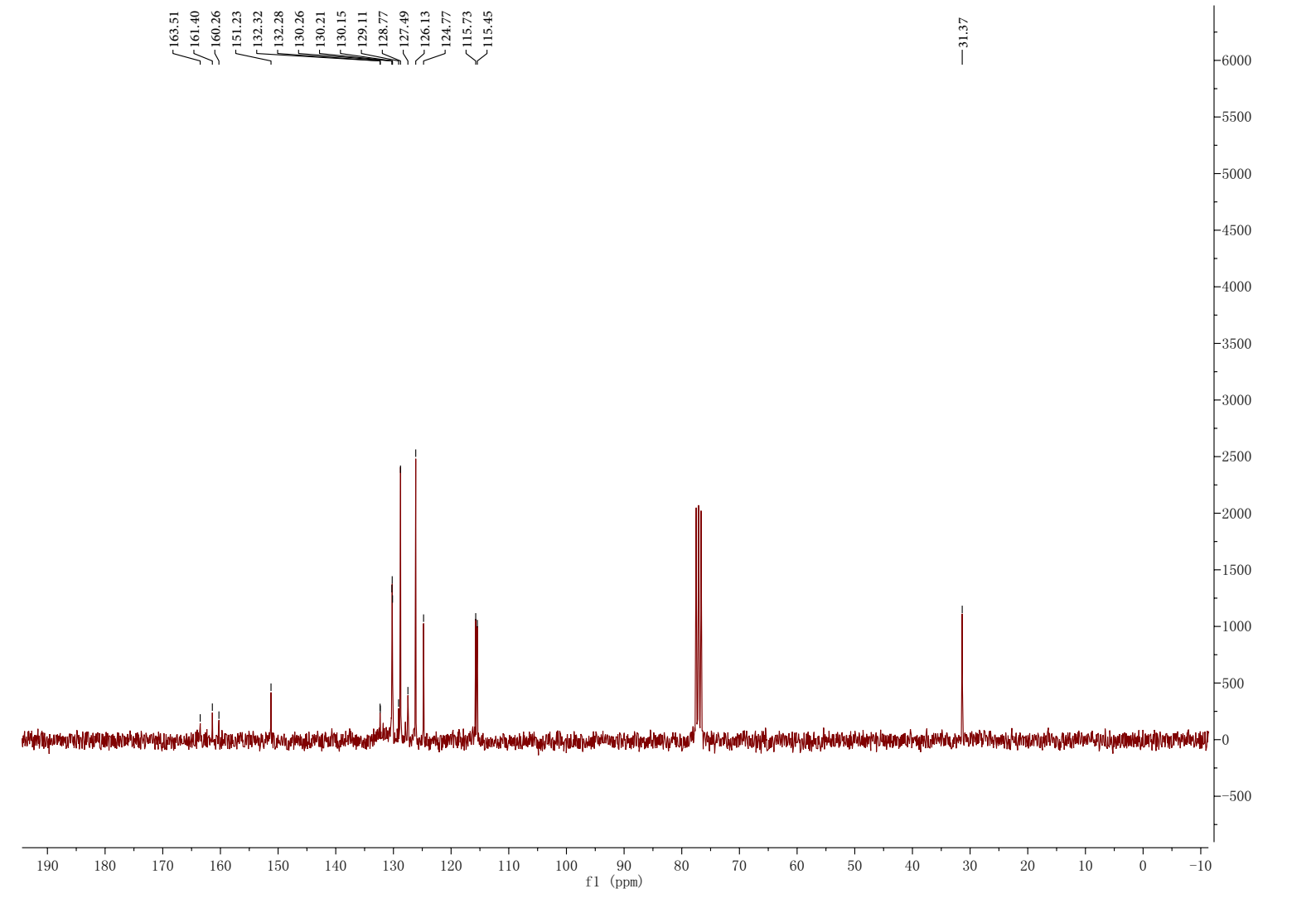
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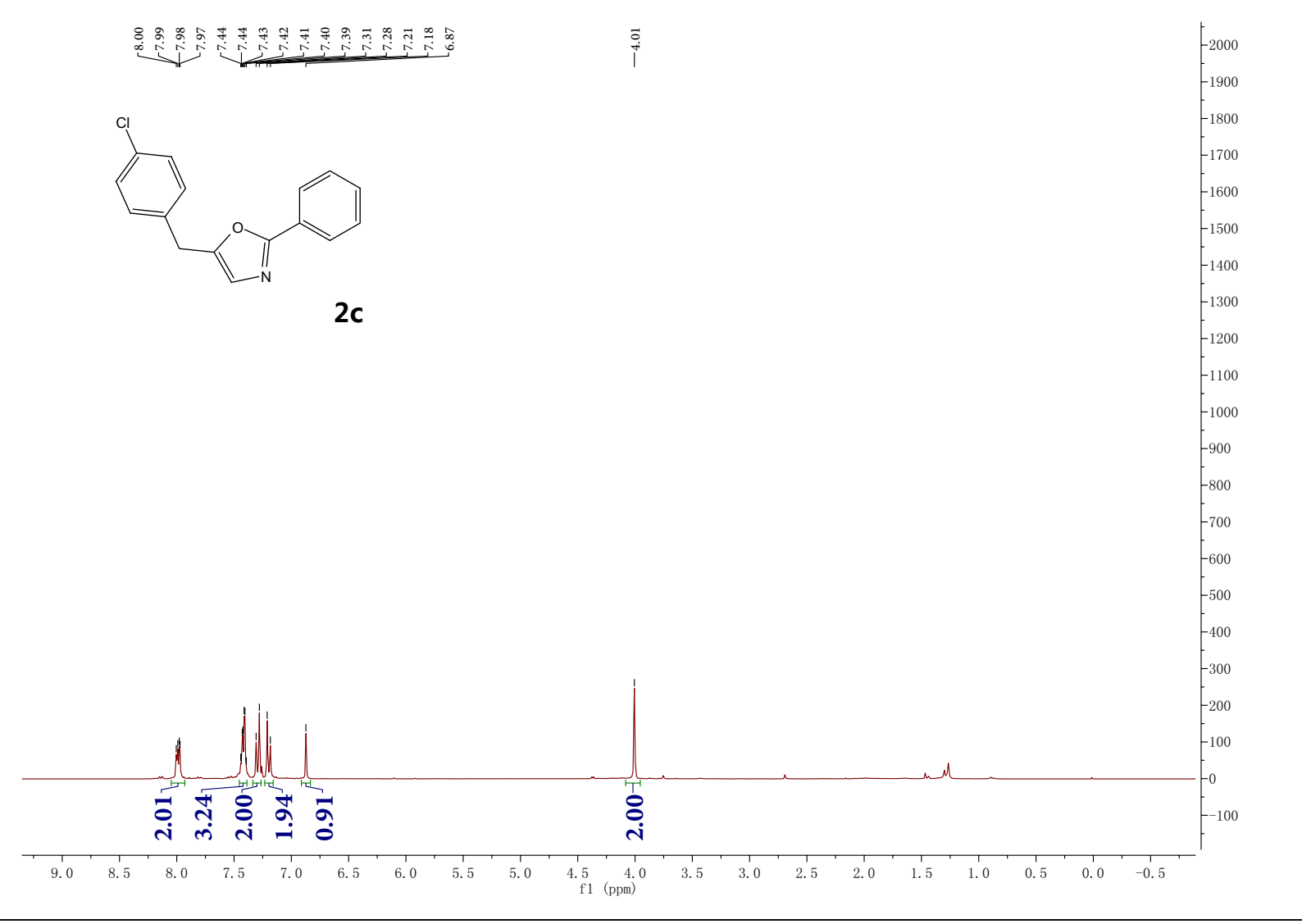
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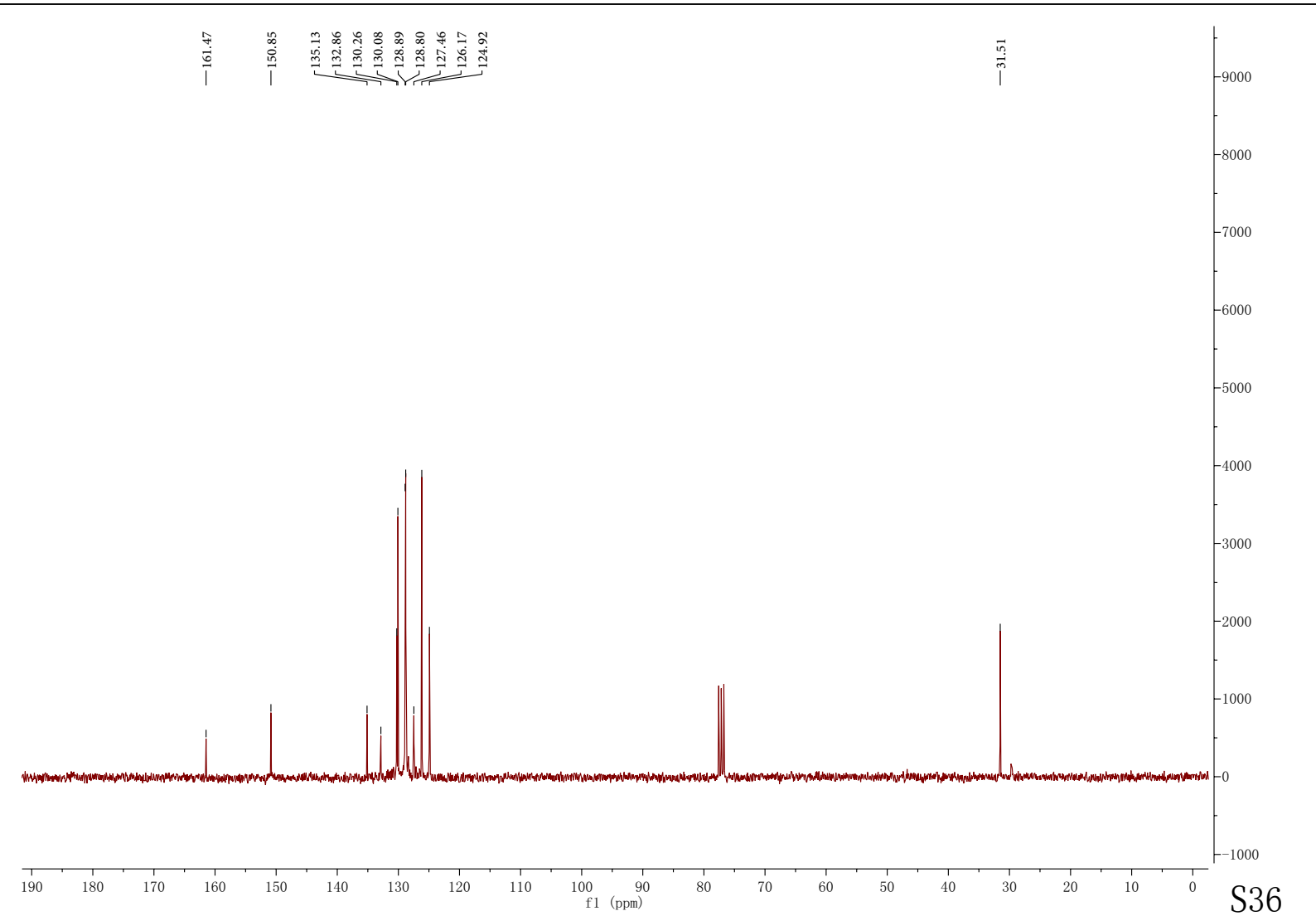
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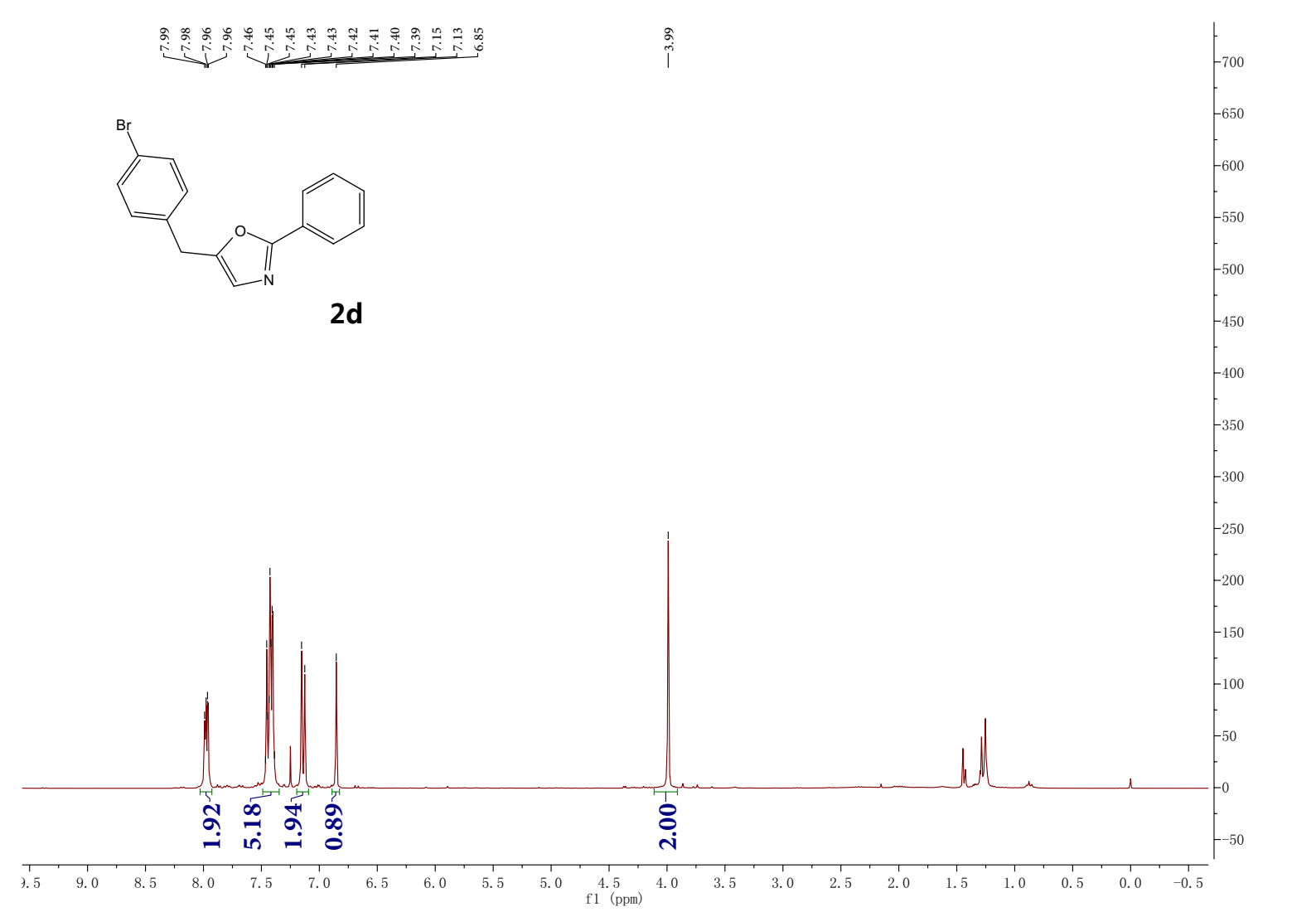
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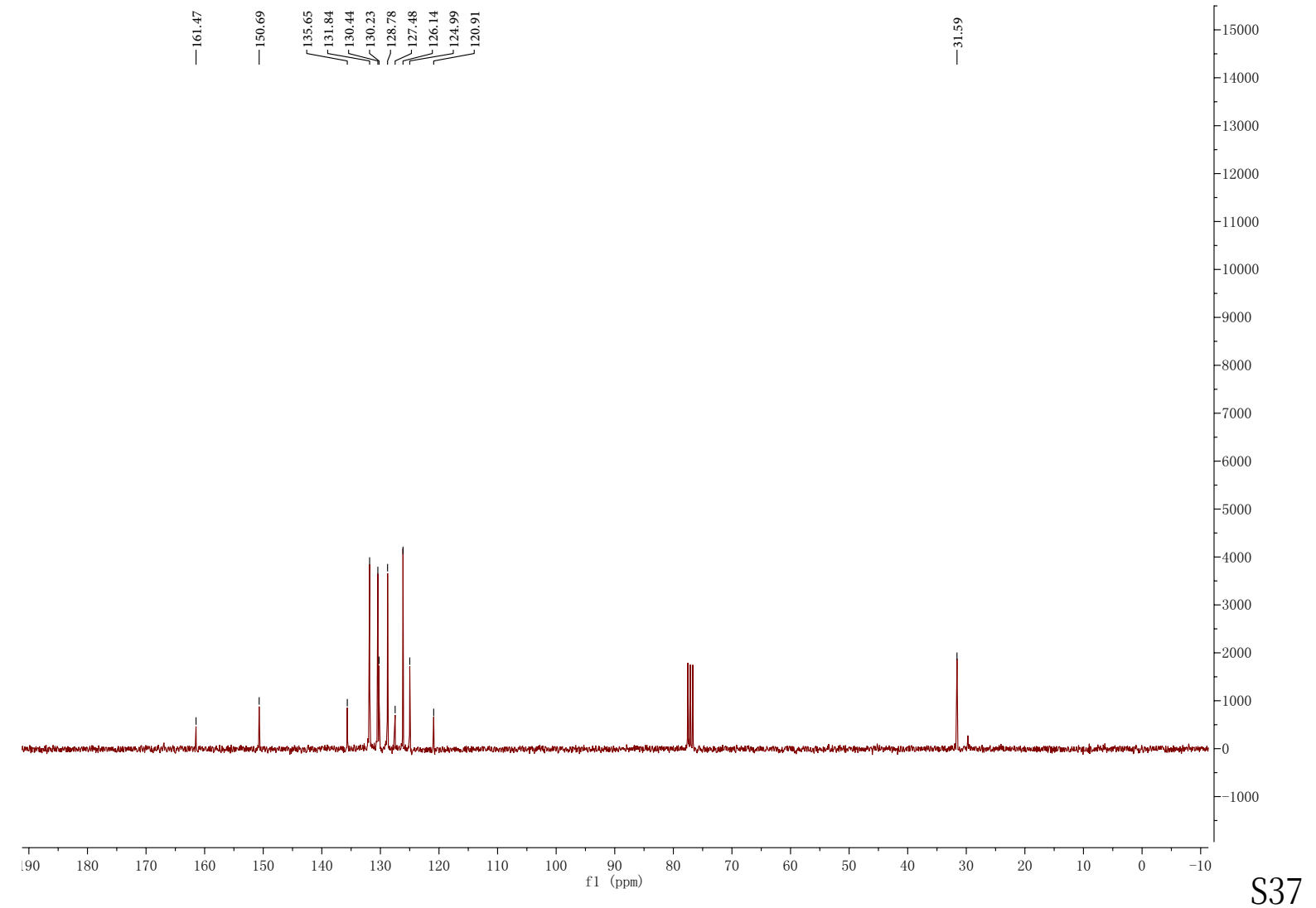
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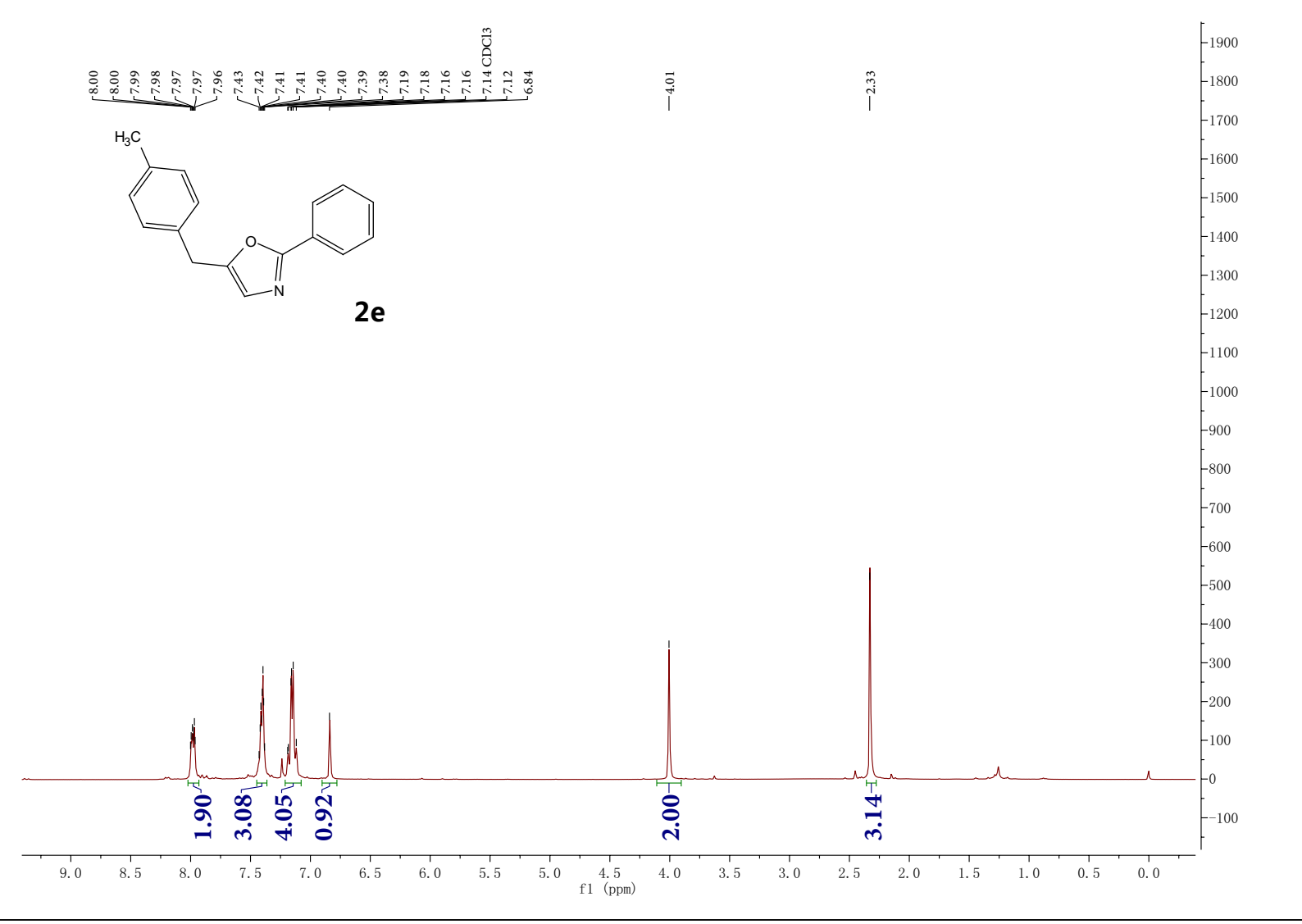
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7.16
7.14 CDCl3
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6.84
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O
N
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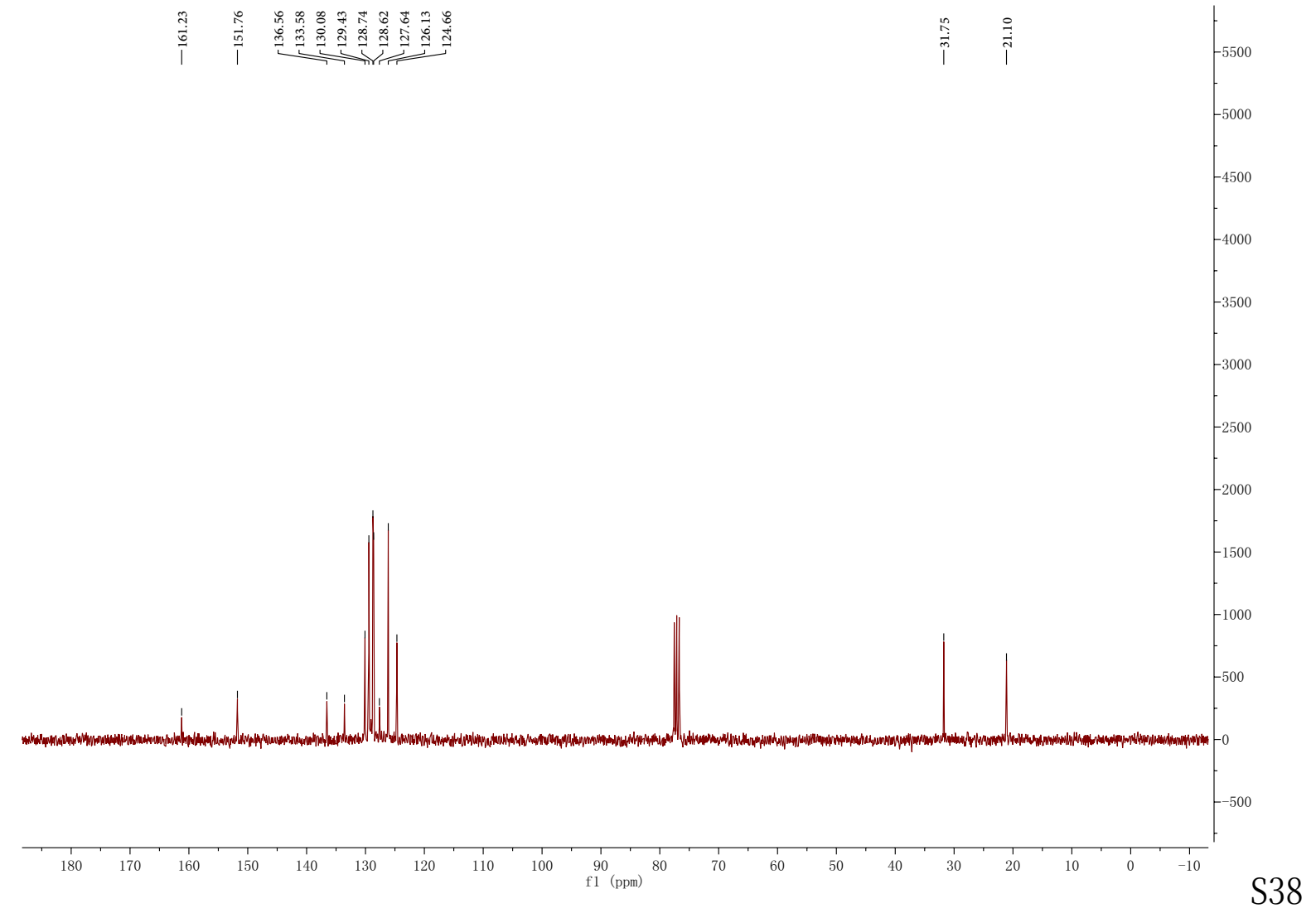
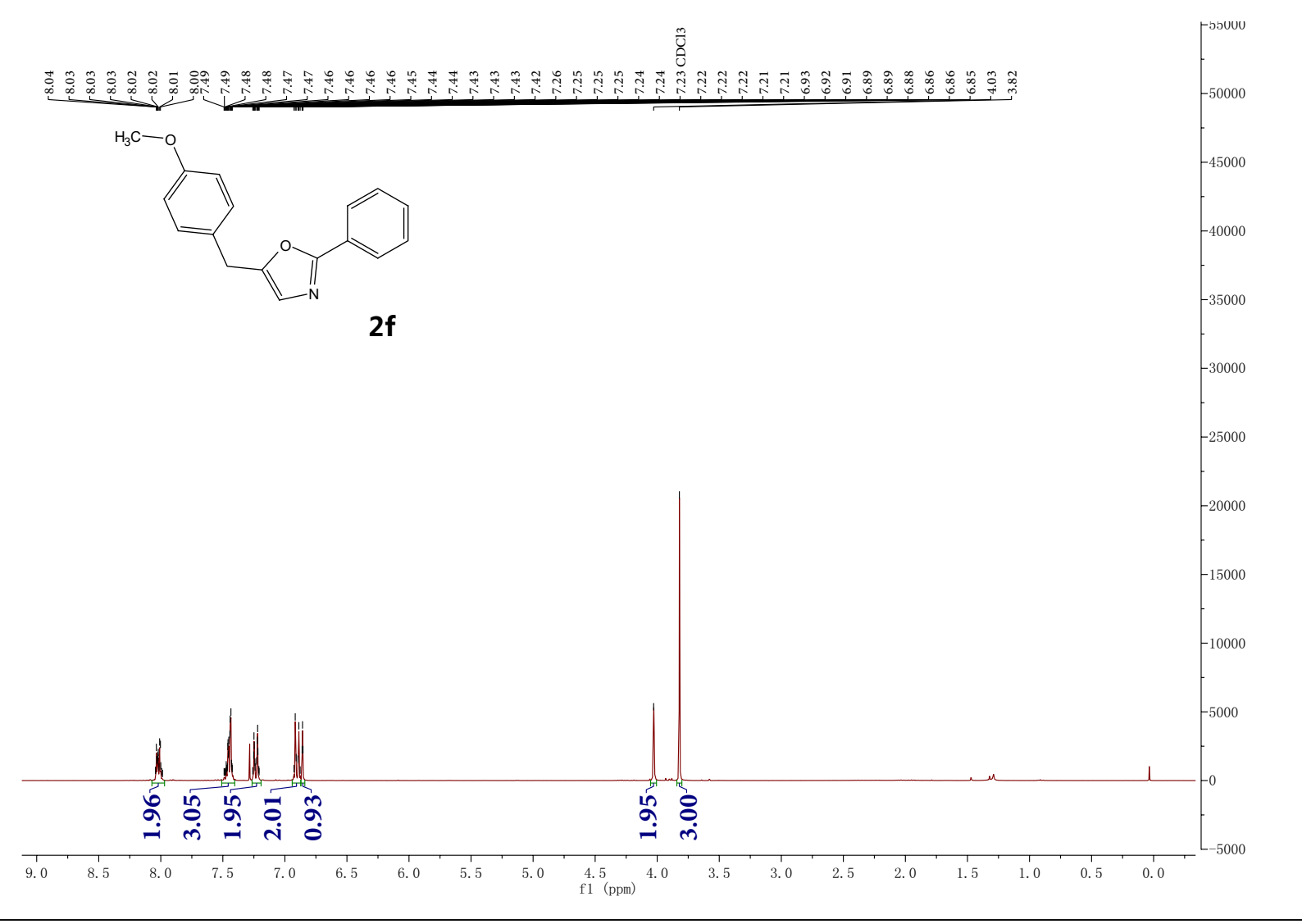
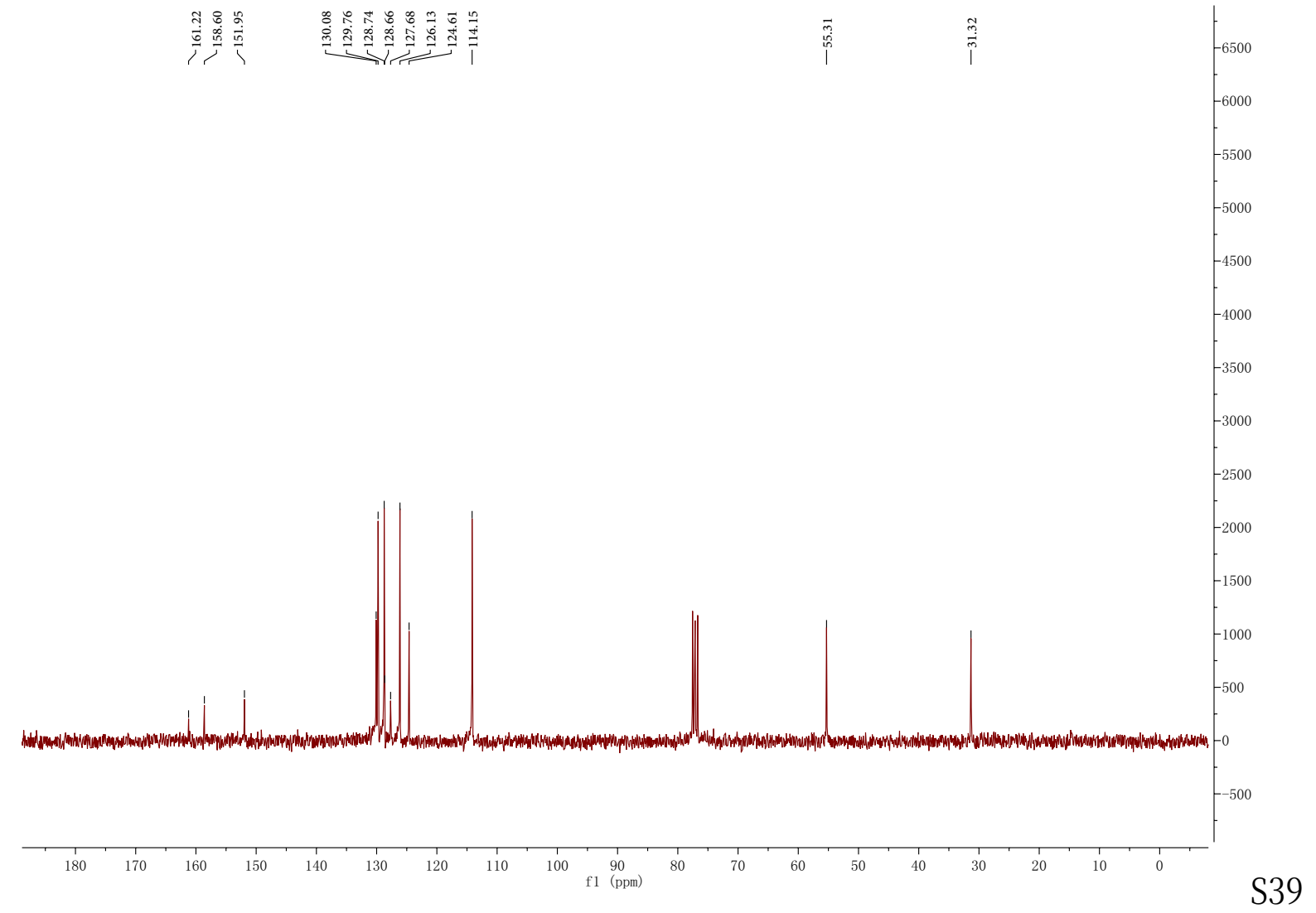
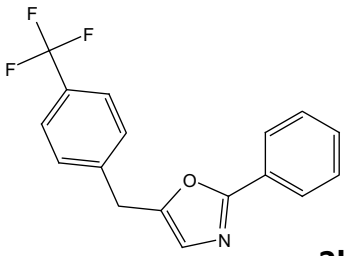
4.05
0.92
2.00
3.14
f1 (ppm)


161.23
151.76
136.56
133.58
130.08
129.43
128.74
128.62
127.64
126.13
124.66
31.75
21.10
f1 (ppm)


8.04 8.03 8.03 8.03 8.02 8.02 8.01 8.00 7.49 7.49 7.48 7.48 7.47 7.47 7.46 7.46 7.46 7.46 7.45 7.44 7.44 7.43 7.43 7.43 7.42 7.26 7.25 7.25 7.25 7.24 7.24 7.23 CDCl3 7.22 7.22 7.22 7.21 7.21 6.93 6.92 6.91 6.89 6.89 6.88 6.86 6.86 6.85 4.03 3.82
H3C O
O
N
2f
1.96 3.05 1.95 2.01 0.93 1.95 3.00
f1 (ppm)


161.22 158.60 151.95 130.08 129.76 128.74 128.66 127.68 126.13 124.61 114.15 55.31 31.32
f1 (ppm)



2h

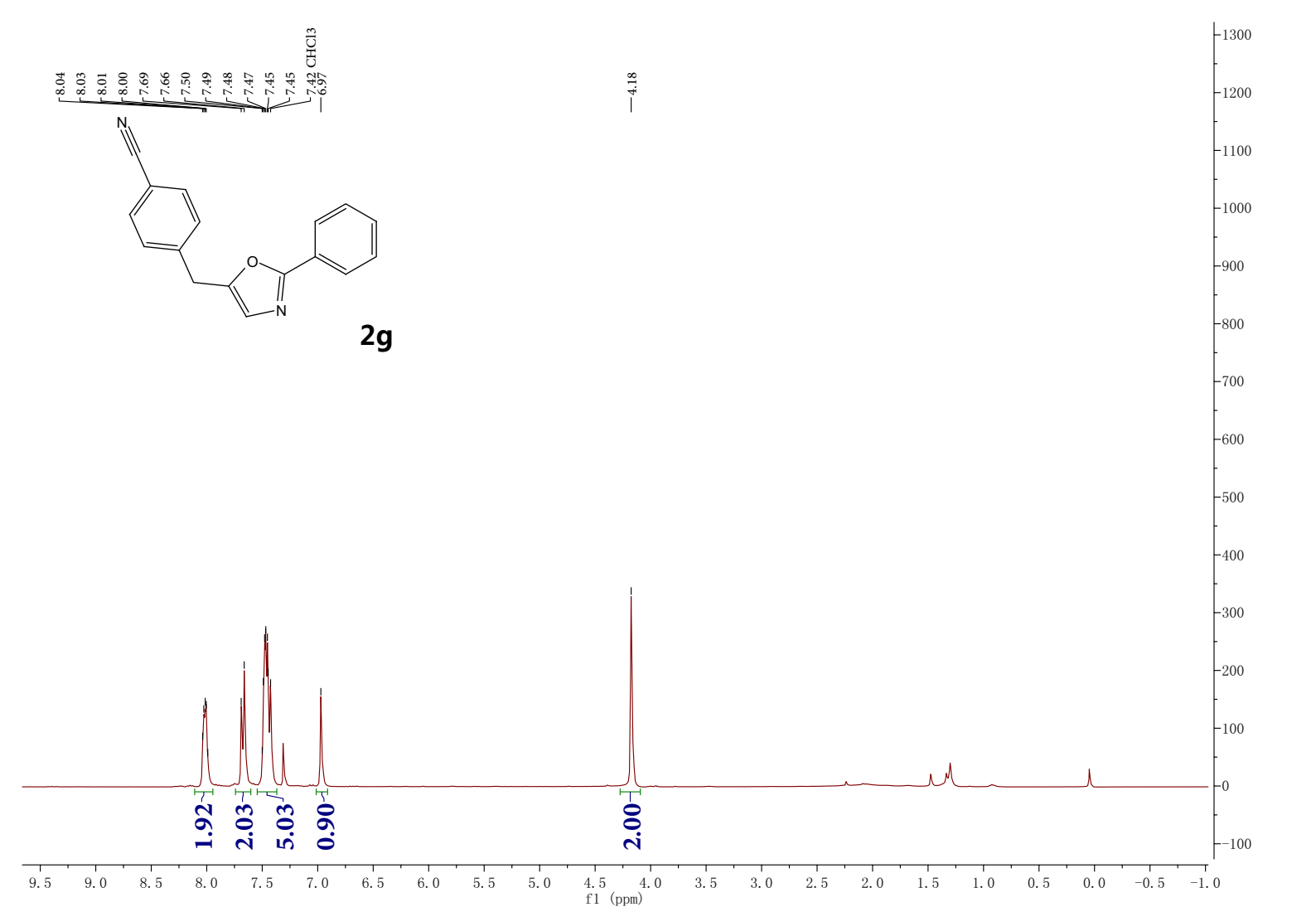
8.05 8.04 8.03 8.02 8.01 8.00 7.66 7.64 7.51 7.49 7.48 7.47 7.44 6.96 4.18

1.80 1.93 5.08 0.92 2.00

f1 (ppm)

161.61 150.19 140.74 130.30 129.99 129.60 129.16 129.03 128.78 127.40 126.16 125.78 125.72 125.67 125.62 125.18 122.43 122.34 31.92

f1 (ppm)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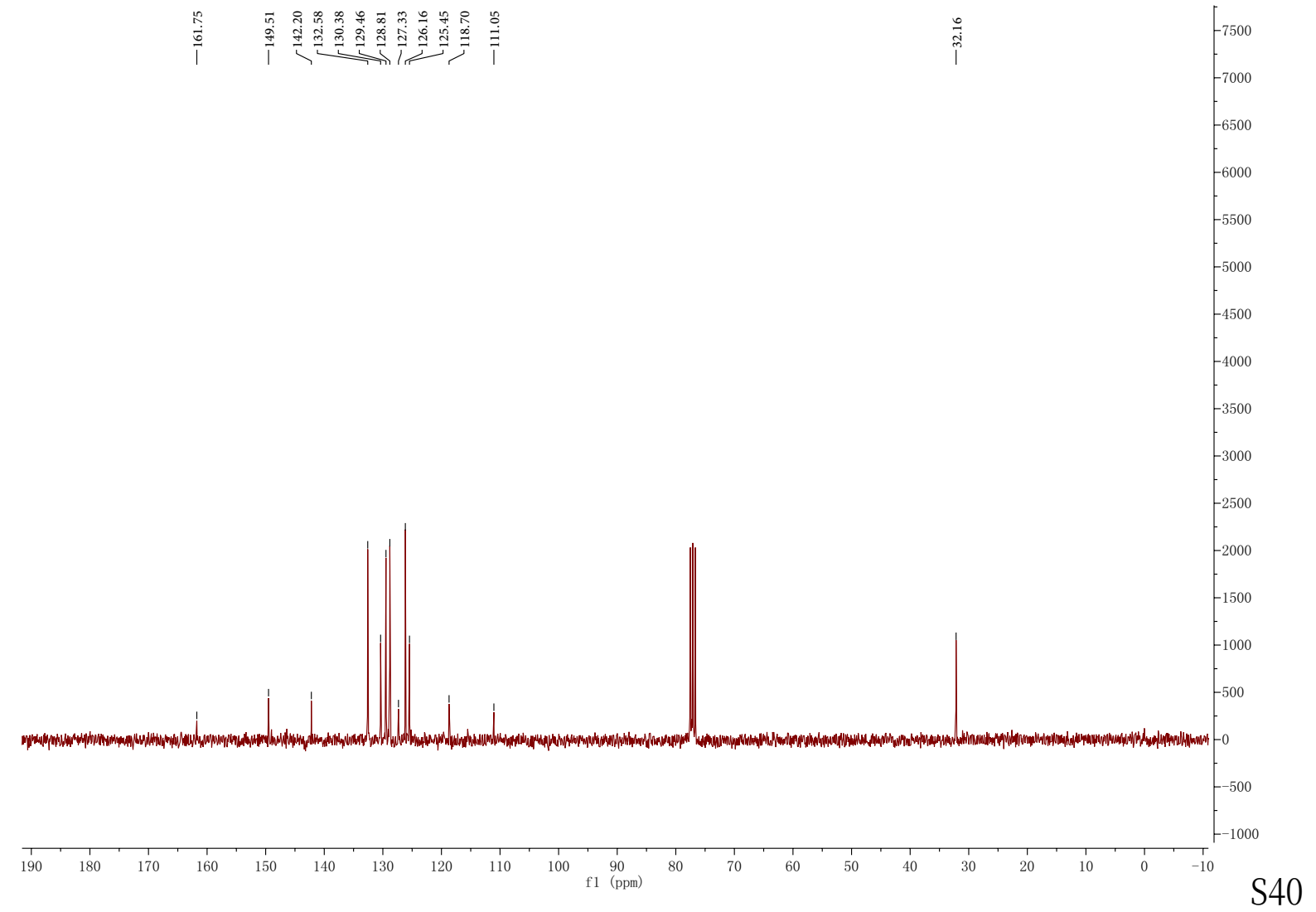
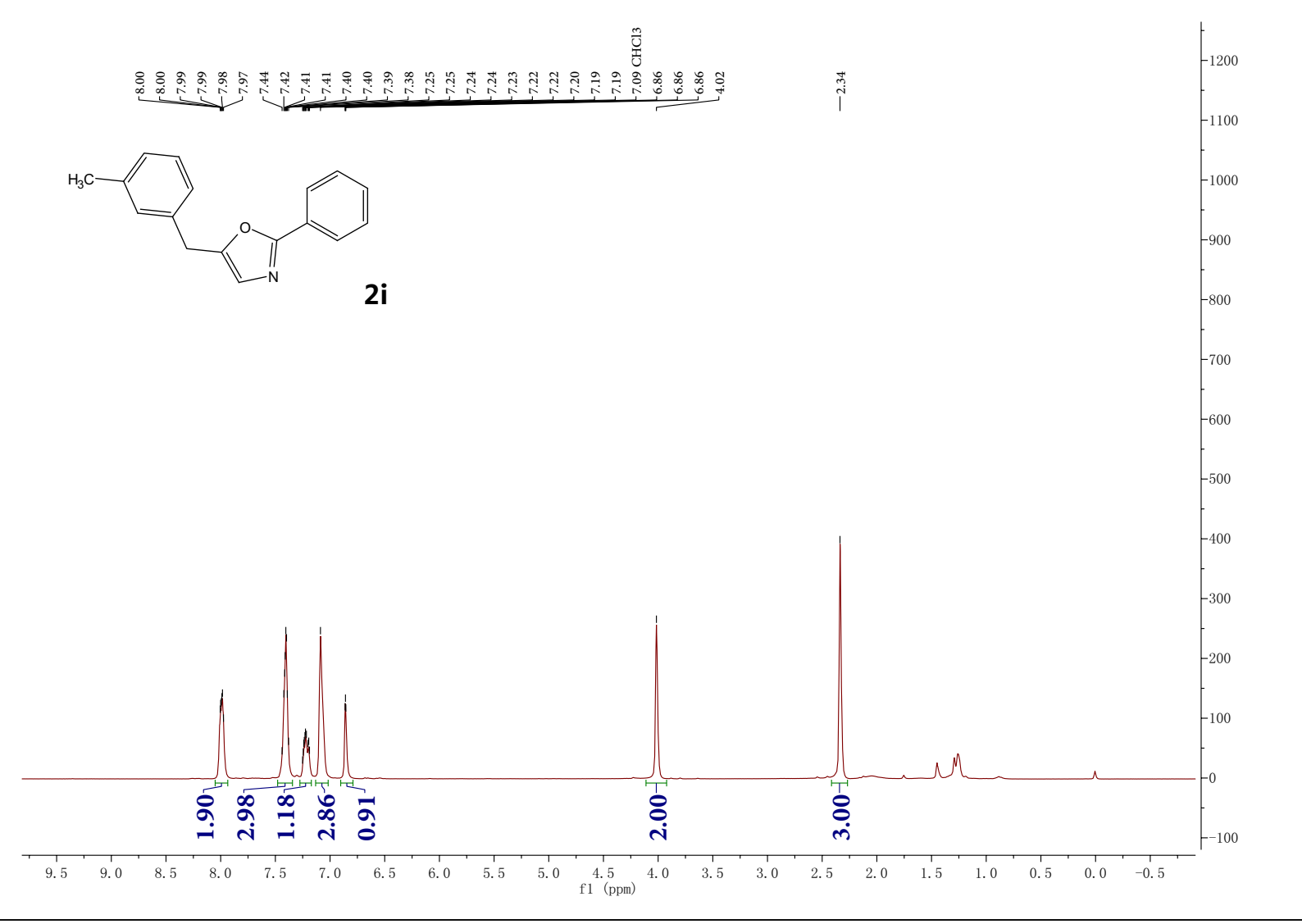
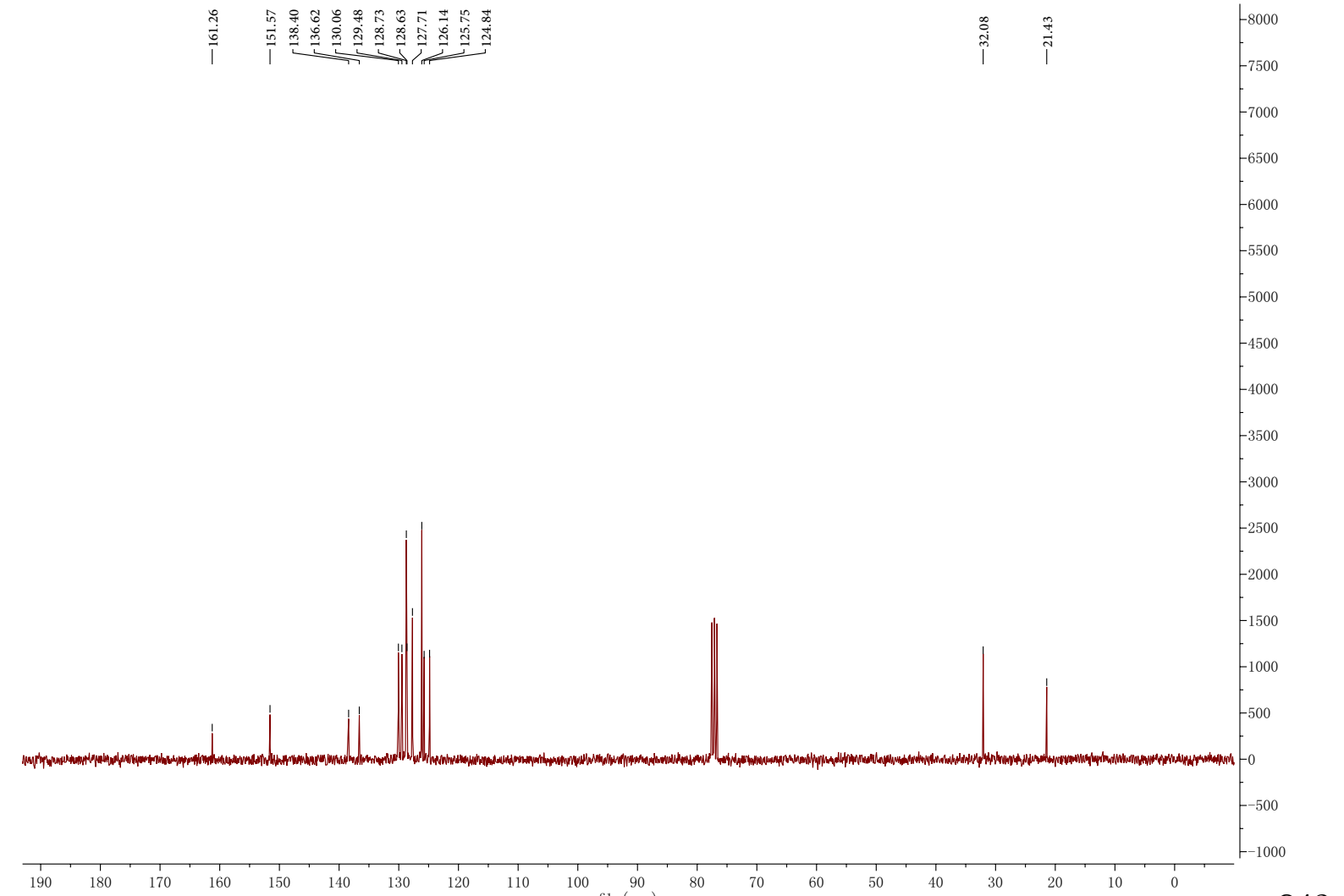
8.03
8.01
8.00
7.69
7.66
7.50
7.49
7.48
7.47
7.45
7.45
7.42
CHCl3
6.97
4.18
N
O
N
1.92
2.03
5.03
0.90
2.00
f1 (ppm)

2g


161.75
149.51
142.20
132.58
130.38
129.46
128.81
127.33
126.16
125.45
118.70
111.05
32.16
f1 (ppm)


8.00
8.00
7.99
7.99
7.98
7.97
7.44
7.42
7.41
7.41
7.40
7.40
7.39
7.38
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.20
7.19
7.19
7.09 CHCl3
6.86
6.86
6.86
4.02
2.34
H3C
O
N
2i
1.90
2.98
1.18
2.86
0.91
2.00
3.00
f1 (ppm)


161.26
151.57
138.40
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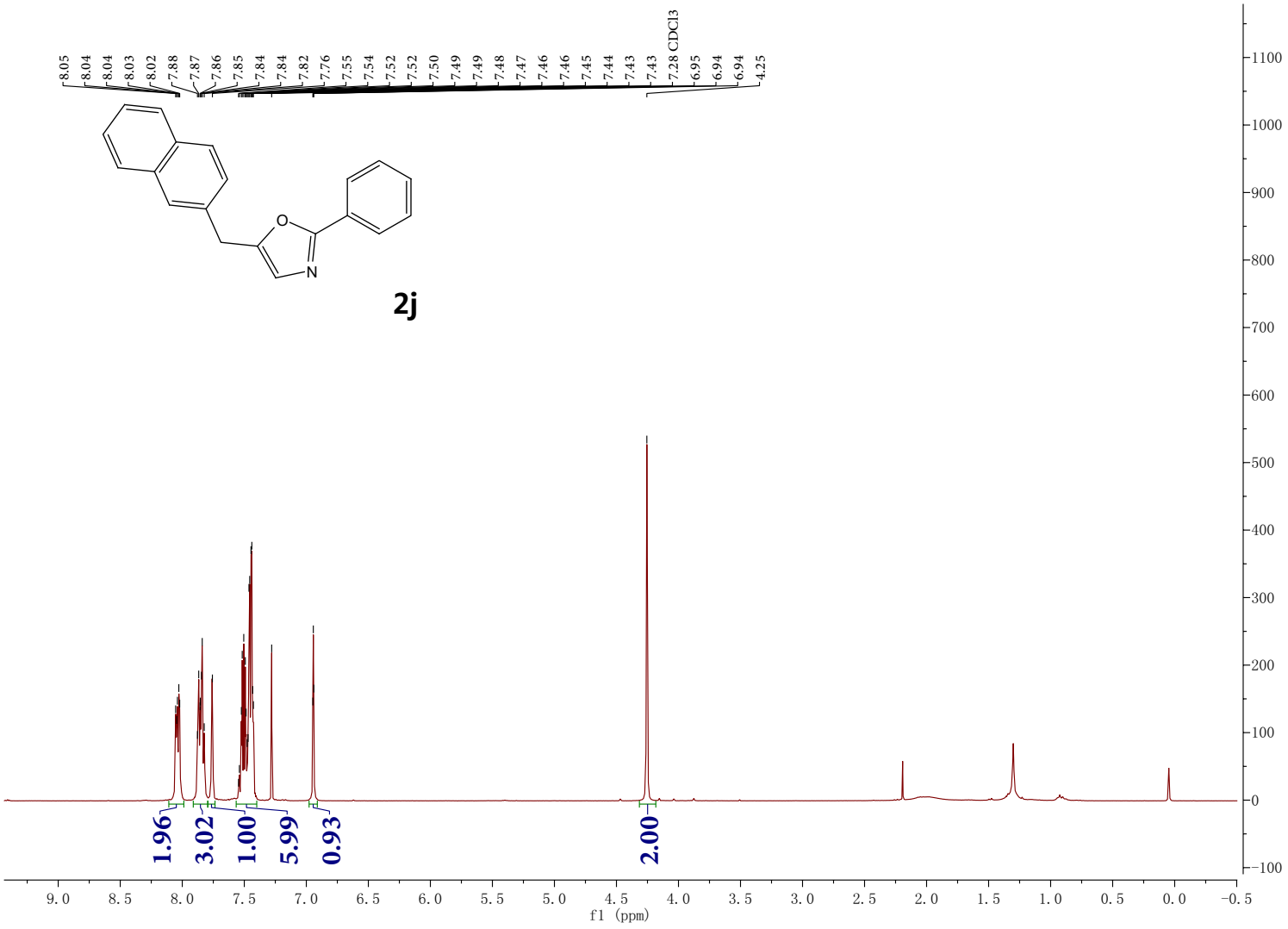
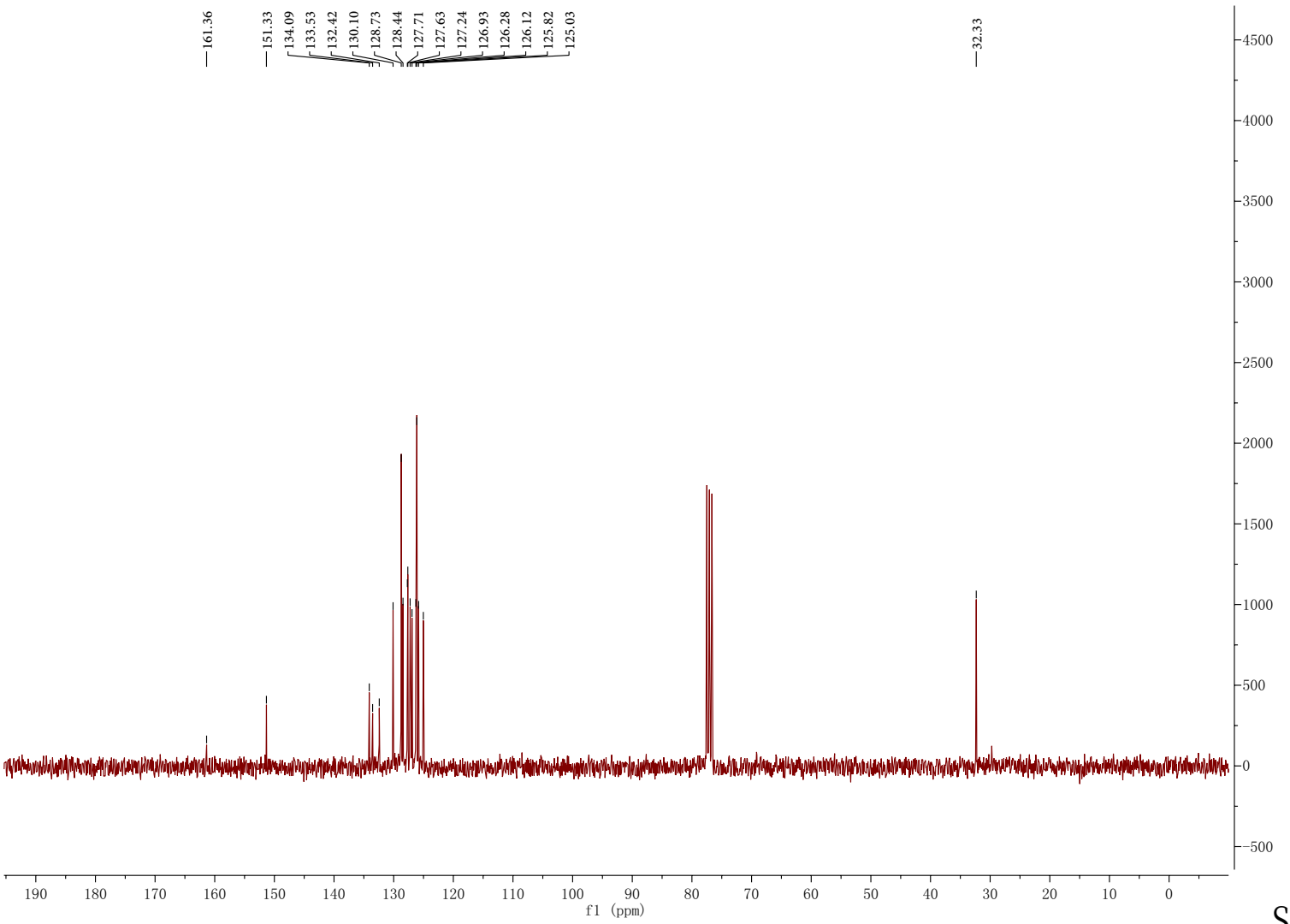
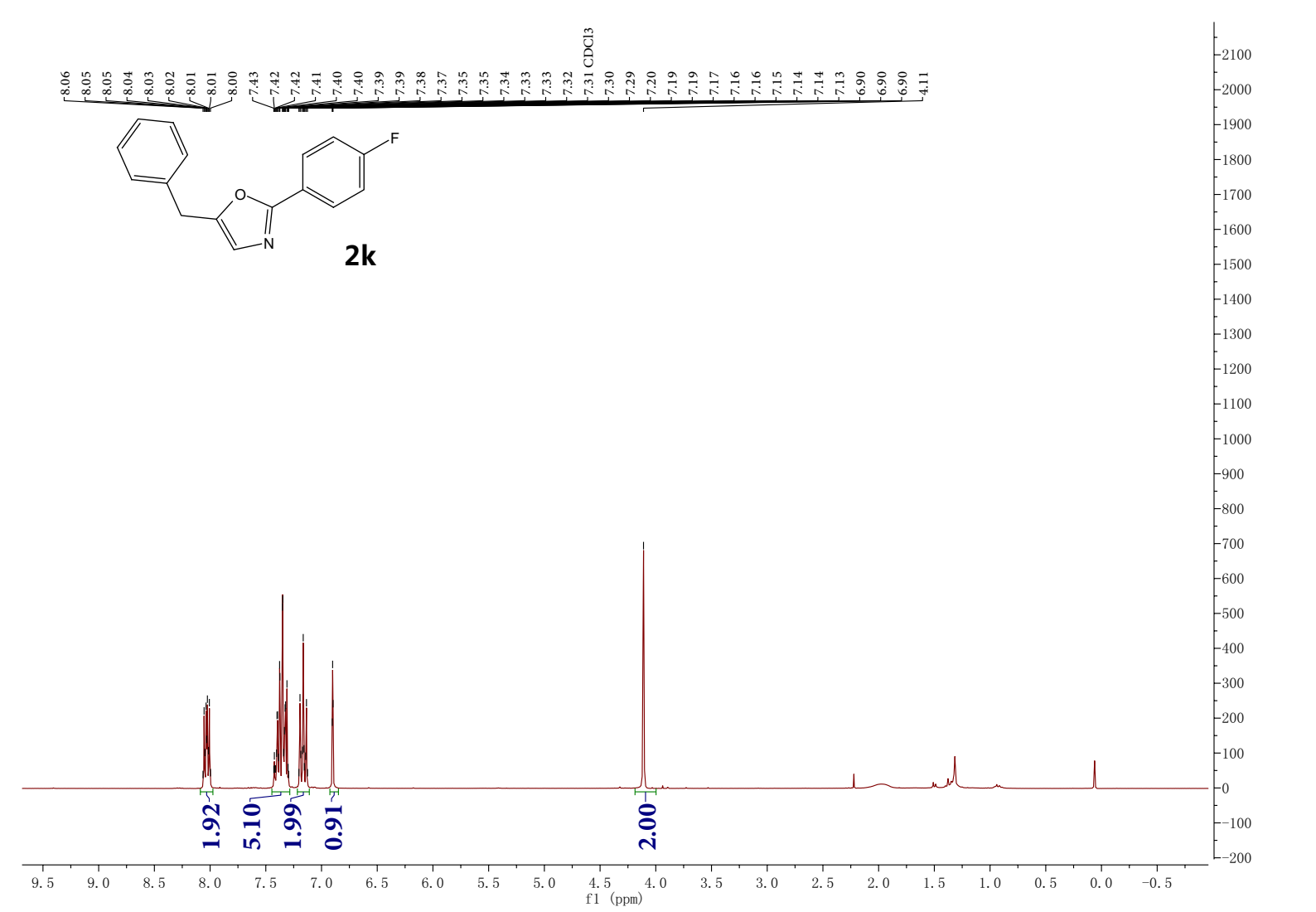
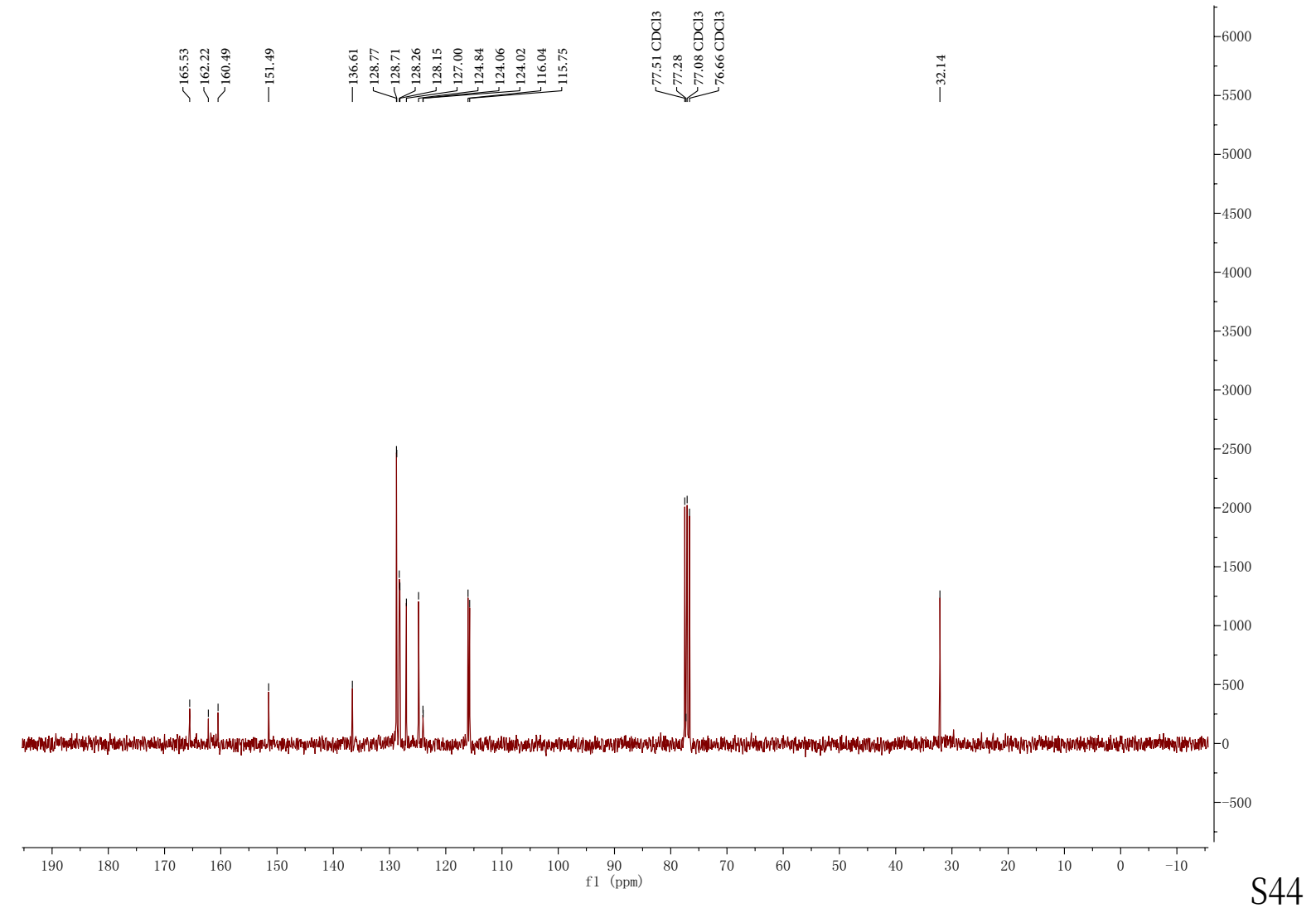
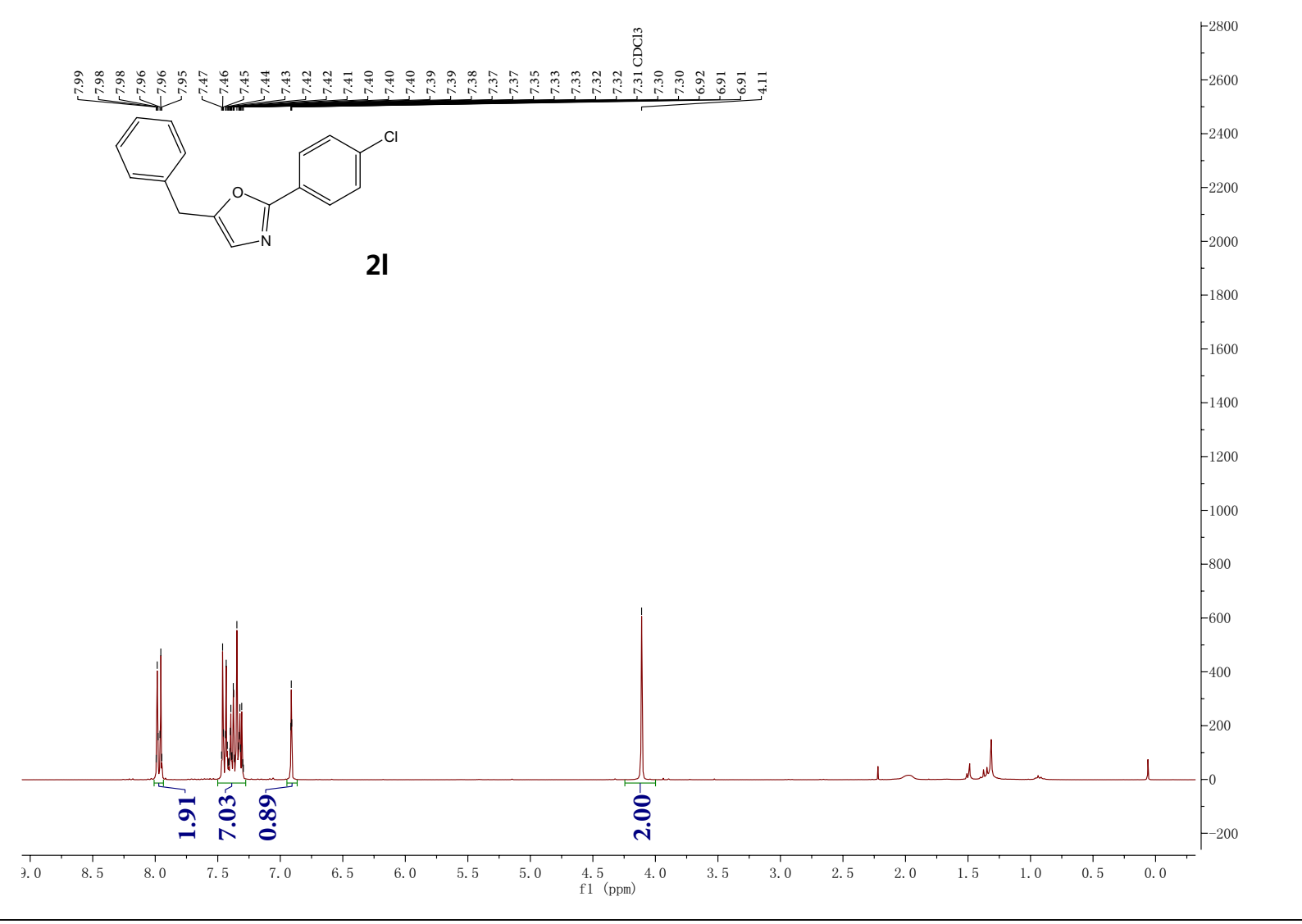
128.73
128.63
127.71
126.14
125.75
124.84
32.08
21.43
f1 (ppm)

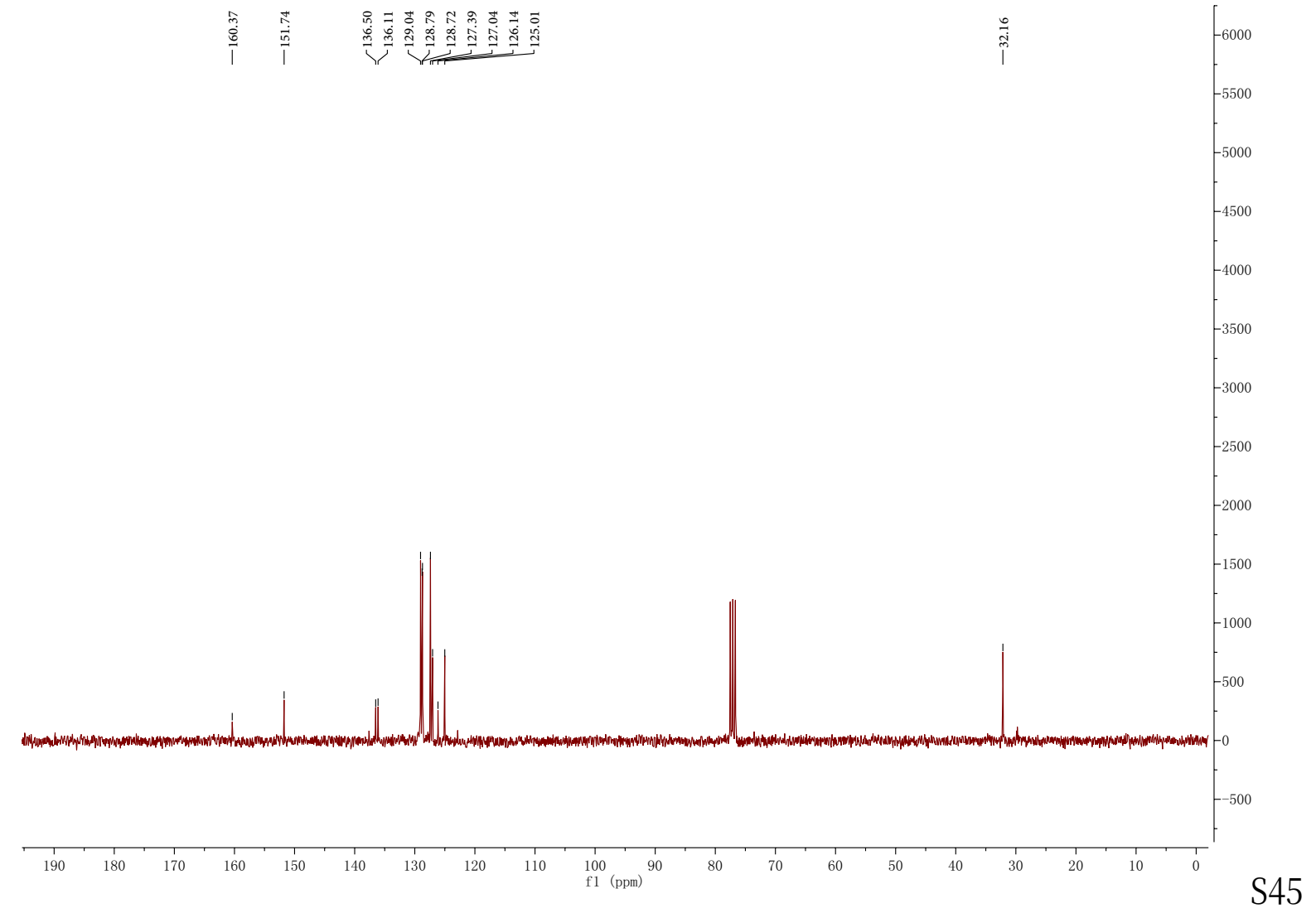

8.05 8.04 8.04 8.03 8.02 7.88 7.87 7.86 7.85 7.84 7.84 7.82 7.76 7.55 7.54 7.52 7.52 7.50 7.49 7.49 7.48 7.47 7.46 7.46 7.45 7.44 7.43 7.43 7.28 CDCl3 6.95 6.94 6.94 4.25
O
N
2j
1.96
3.02
1.00
5.99
0.93
2.00
f1 (ppm)

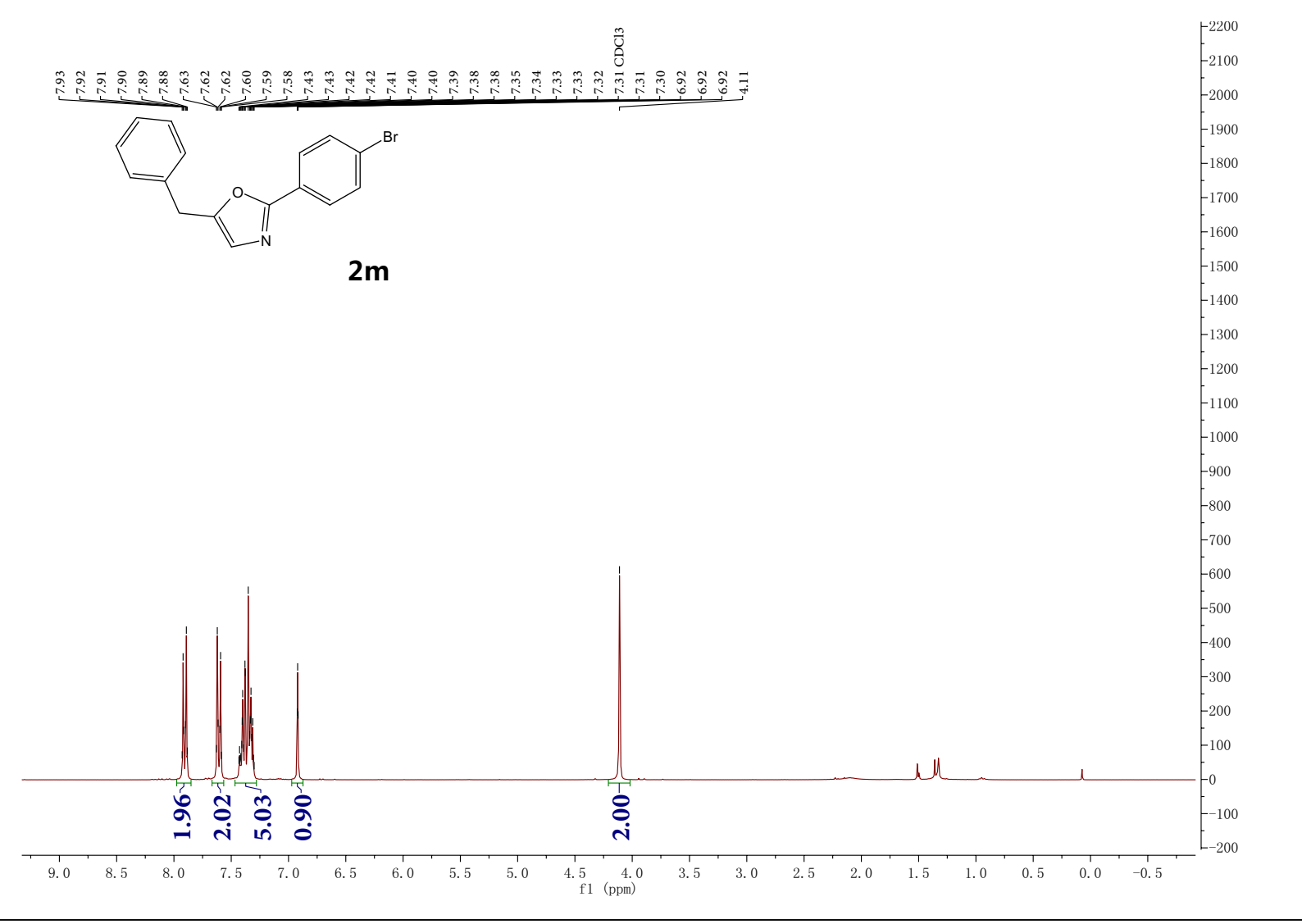

161.36 151.33 134.09 133.53 132.42 130.10 128.73 128.44 127.71 127.63 127.24 126.93 126.28 126.12 125.82 125.03
32.33
f1 (ppm)

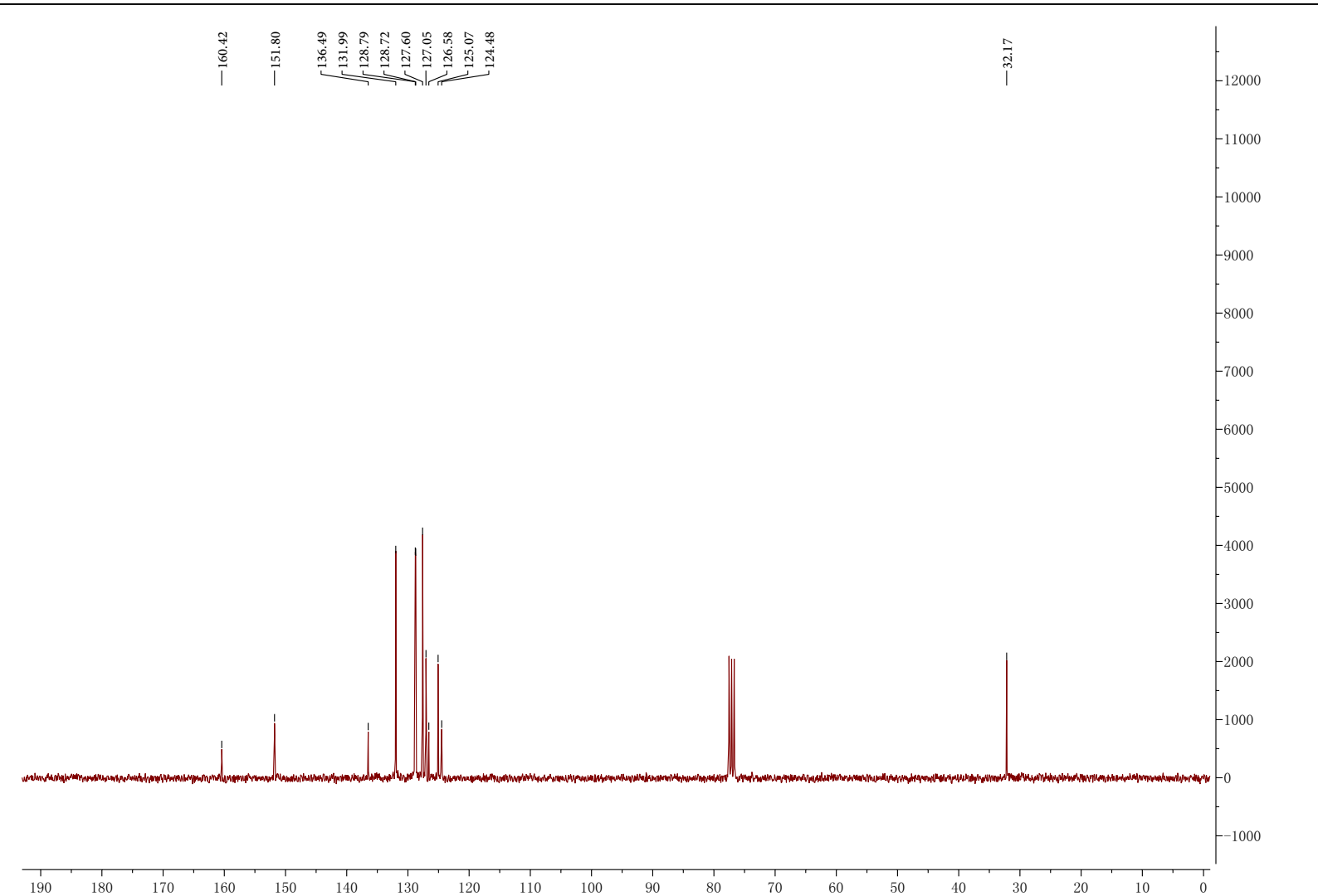

8.06 8.05 8.05 8.04 8.03 8.02 8.01 8.01 8.00
7.43 7.42 7.42 7.41 7.40 7.40 7.39 7.39 7.38 7.37 7.35 7.35 7.34 7.33 7.33 7.32 7.31 CDCl3 7.30 7.29 7.20 7.19 7.19 7.17 7.16 7.16 7.15 7.14 7.14 7.13 6.90 6.90 6.90 4.11
F
O
N
2k
1.92
5.10
1.99
0.91
2.00
f1 (ppm)


165.53 162.22 160.49 151.49 136.61 128.77 128.71 128.26 128.15 127.00 124.84 124.06 124.02 116.04 115.75
77.51 CDCl3 77.28 77.08 CDCl3 76.66 CDCl3
32.14
f1 (ppm)


7.99 7.98 7.98 7.96 7.96 7.95 7.47 7.46 7.45 7.44 7.43 7.42 7.42 7.41 7.40 7.40 7.40 7.39 7.39 7.38 7.37 7.37 7.35 7.33 7.33 7.32 7.32 7.31 CDCl3 7.30 7.30 6.92 6.91 6.91 4.11
Cl
O
N
2l
1.91
7.03
0.89
2.00
f1 (ppm)


160.37 151.74 136.50 136.11 129.04 128.79 128.72 127.39 127.04 126.14 125.01 32.16
f1 (ppm)


7.93
7.92
7.91
7.90
7.89
7.88
7.63
7.62
7.62
7.60
7.59
7.58
7.43
7.43
7.42
7.42
7.41
7.40
7.40
7.39
7.38
7.38
7.35
7.34
7.33
7.33
7.32
7.31 CDCl3
7.31
7.30
6.92
6.92
6.92
4.11
Br
O
N
2m
1.96
2.02
5.03
0.90
2.00
f1 (ppm)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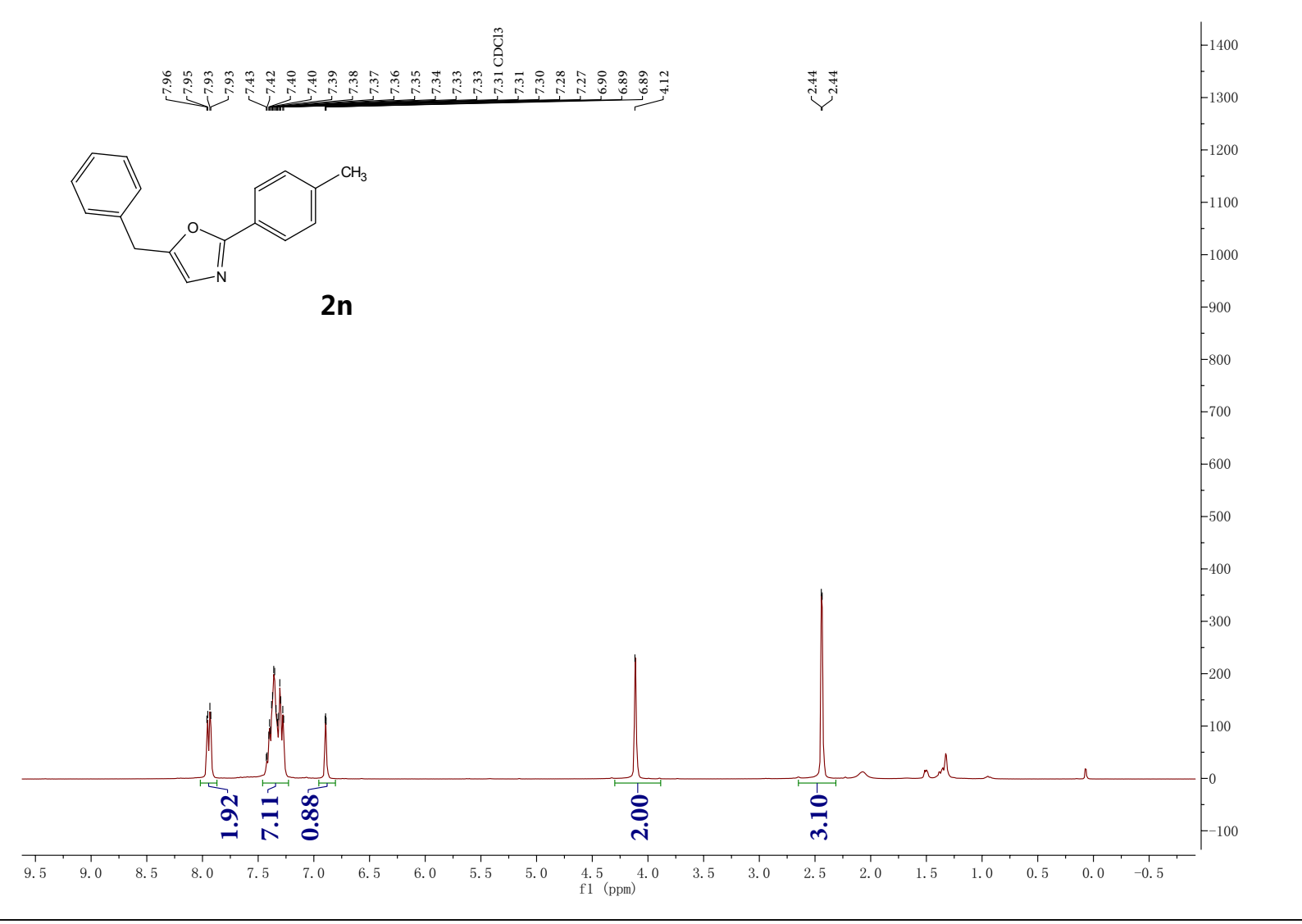
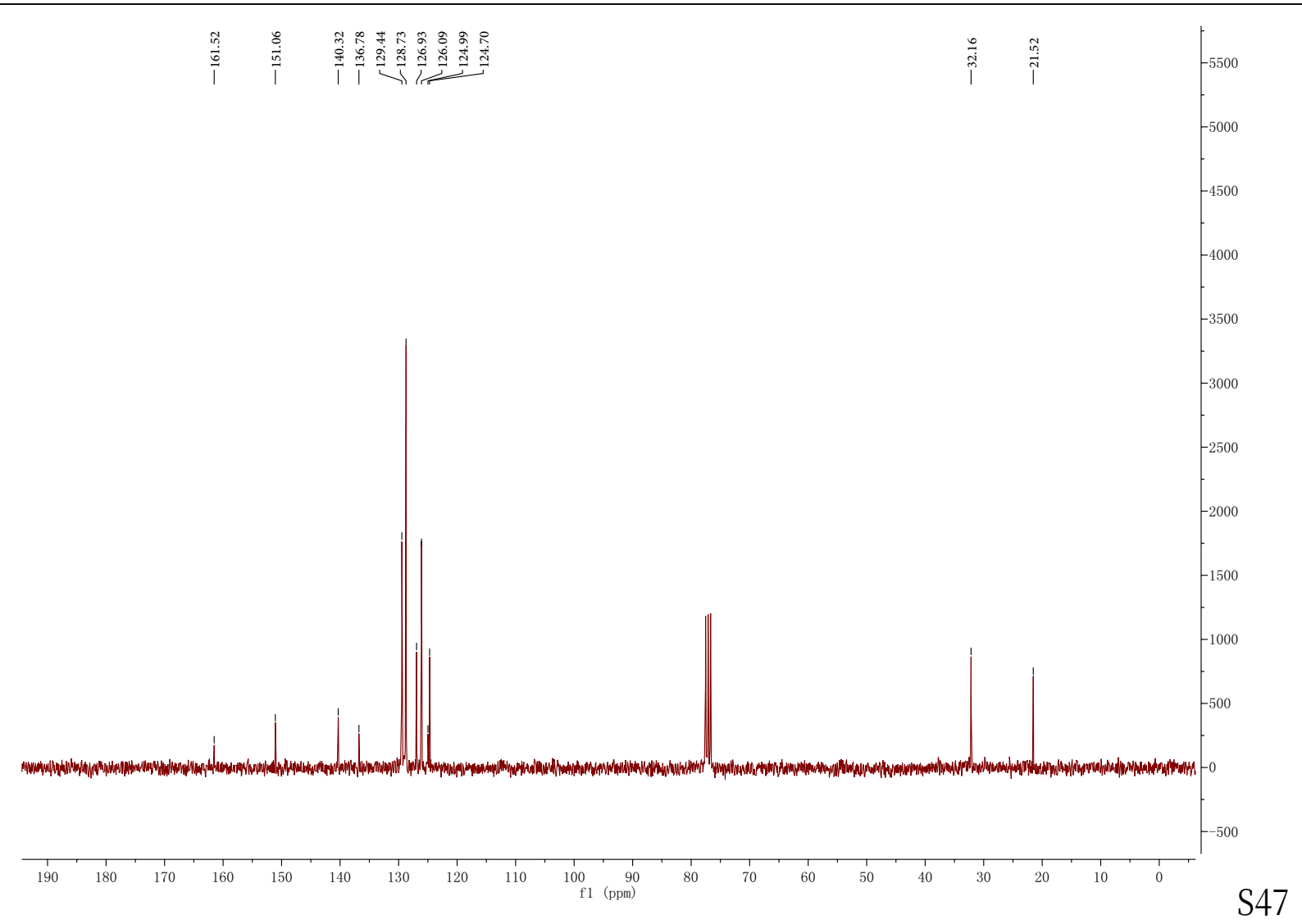
151.80
136.49
131.99
128.79
128.72
127.60
127.05
126.58
125.07
124.48
32.17
f1 (ppm)


7.96
7.95
7.93
7.93
7.43
7.42
7.40
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.33
7.31 CDCl3
7.31
7.30
7.28
7.27
6.90
6.89
6.89
4.12
2.44
2.44
CH3
O
N
2n
1.92
7.11
0.88
2.00
3.10
f1 (ppm)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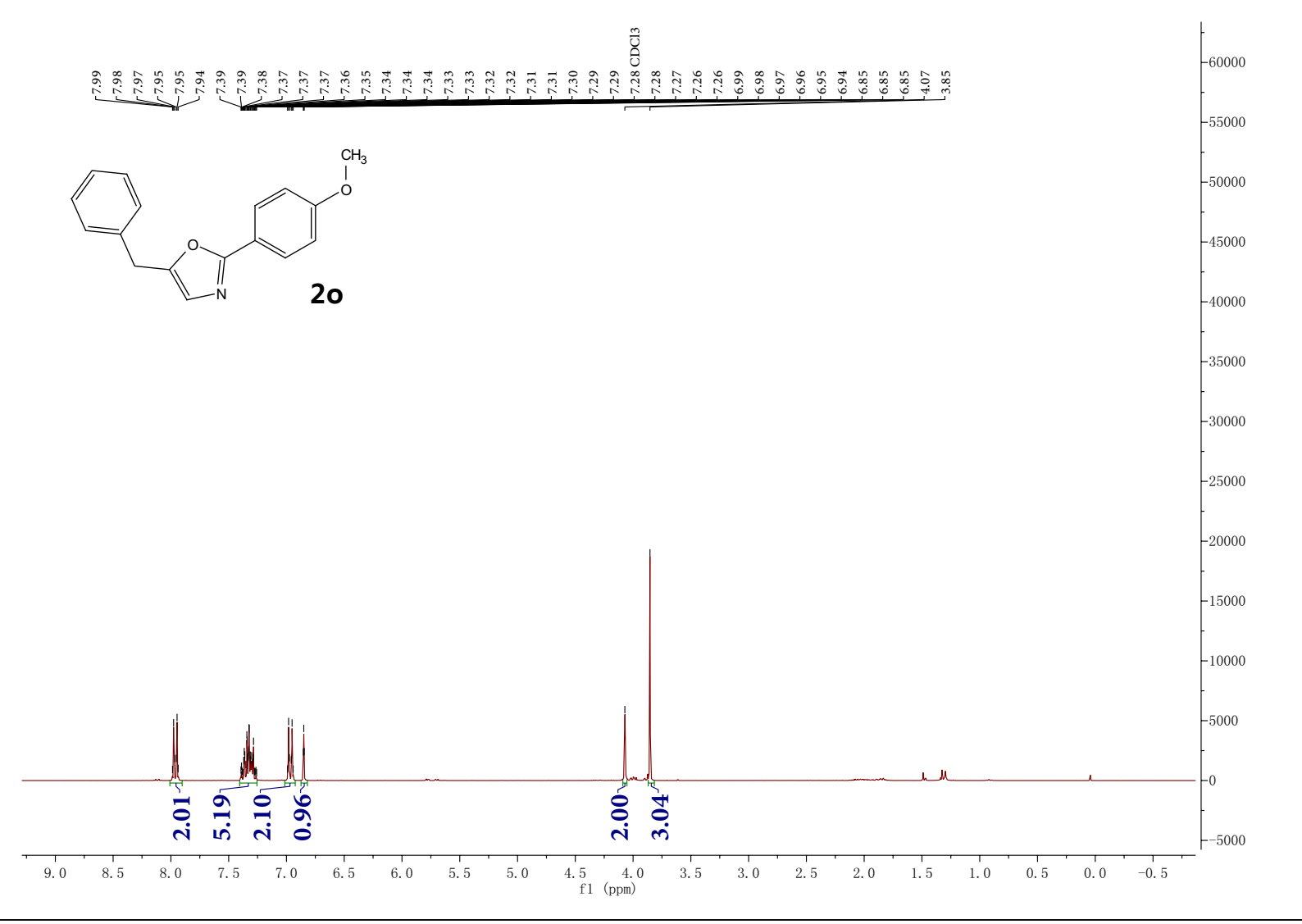
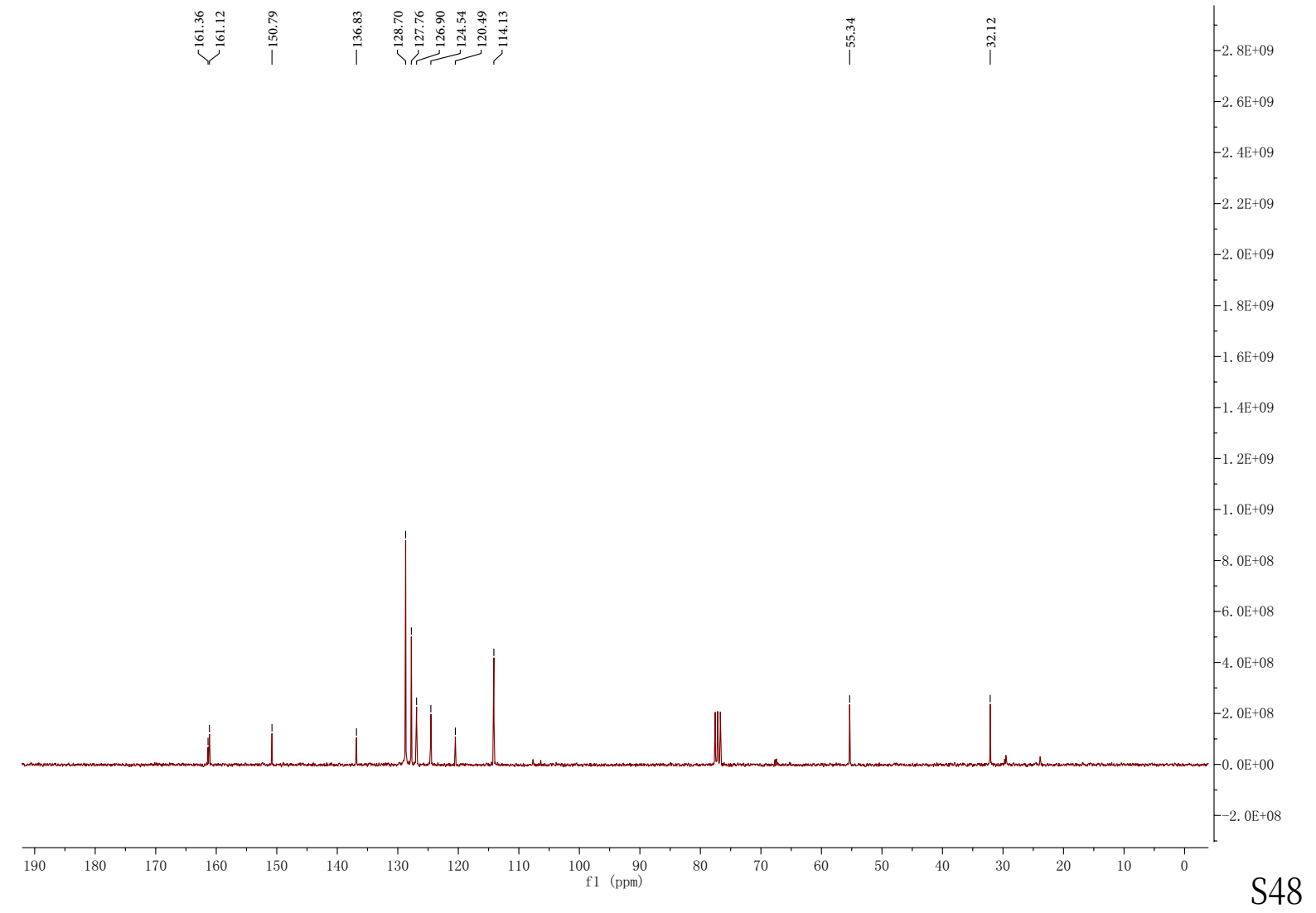
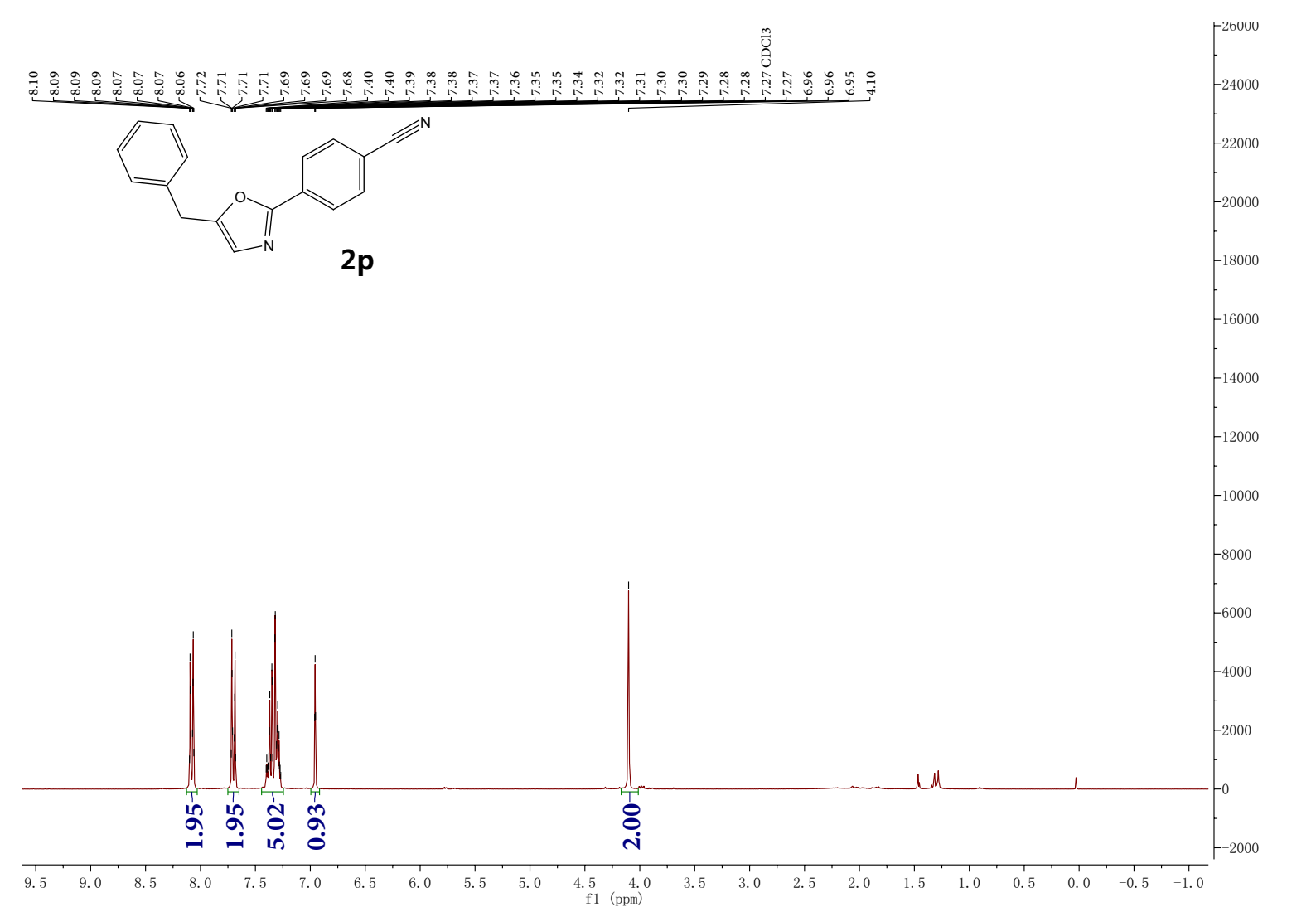
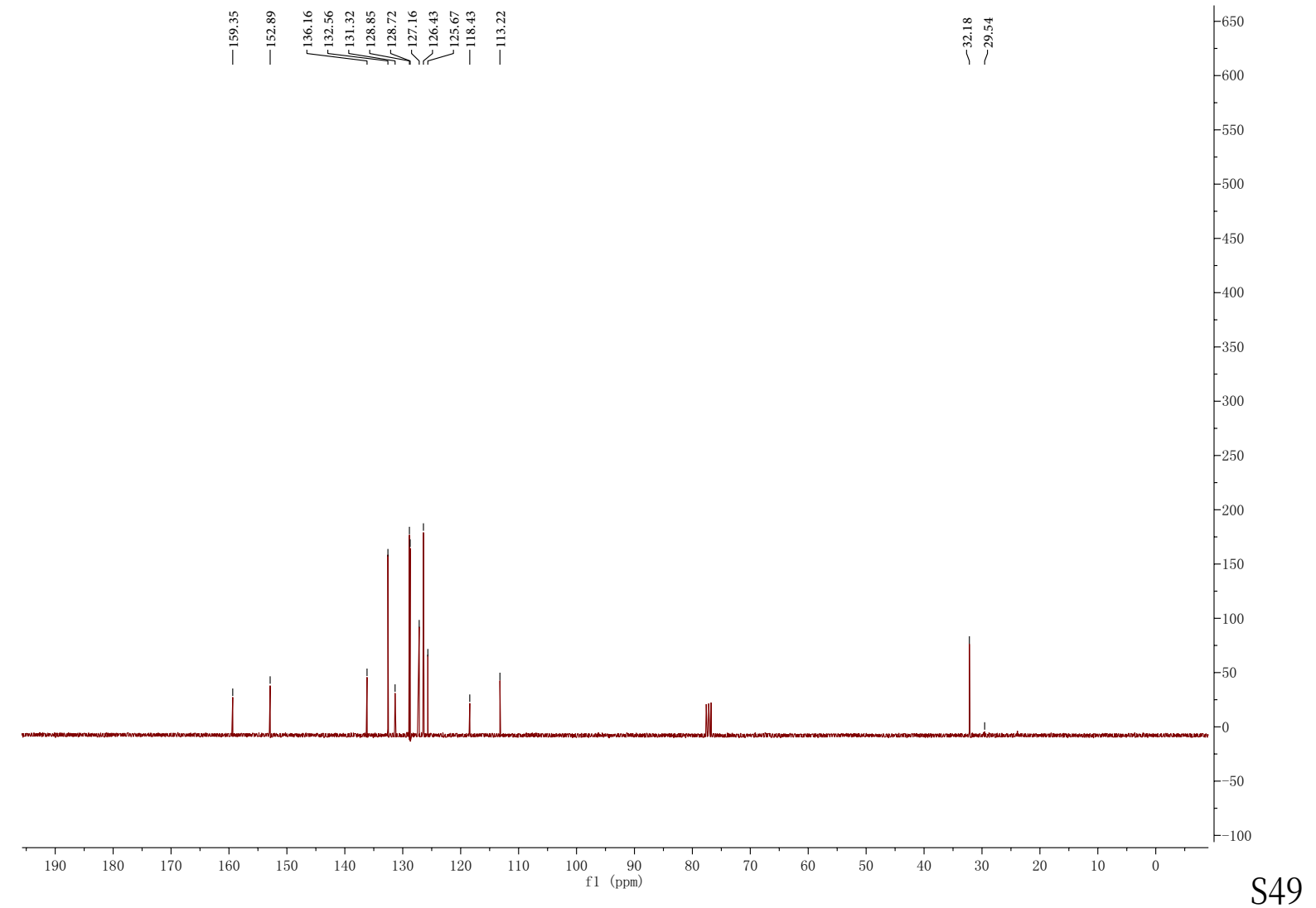
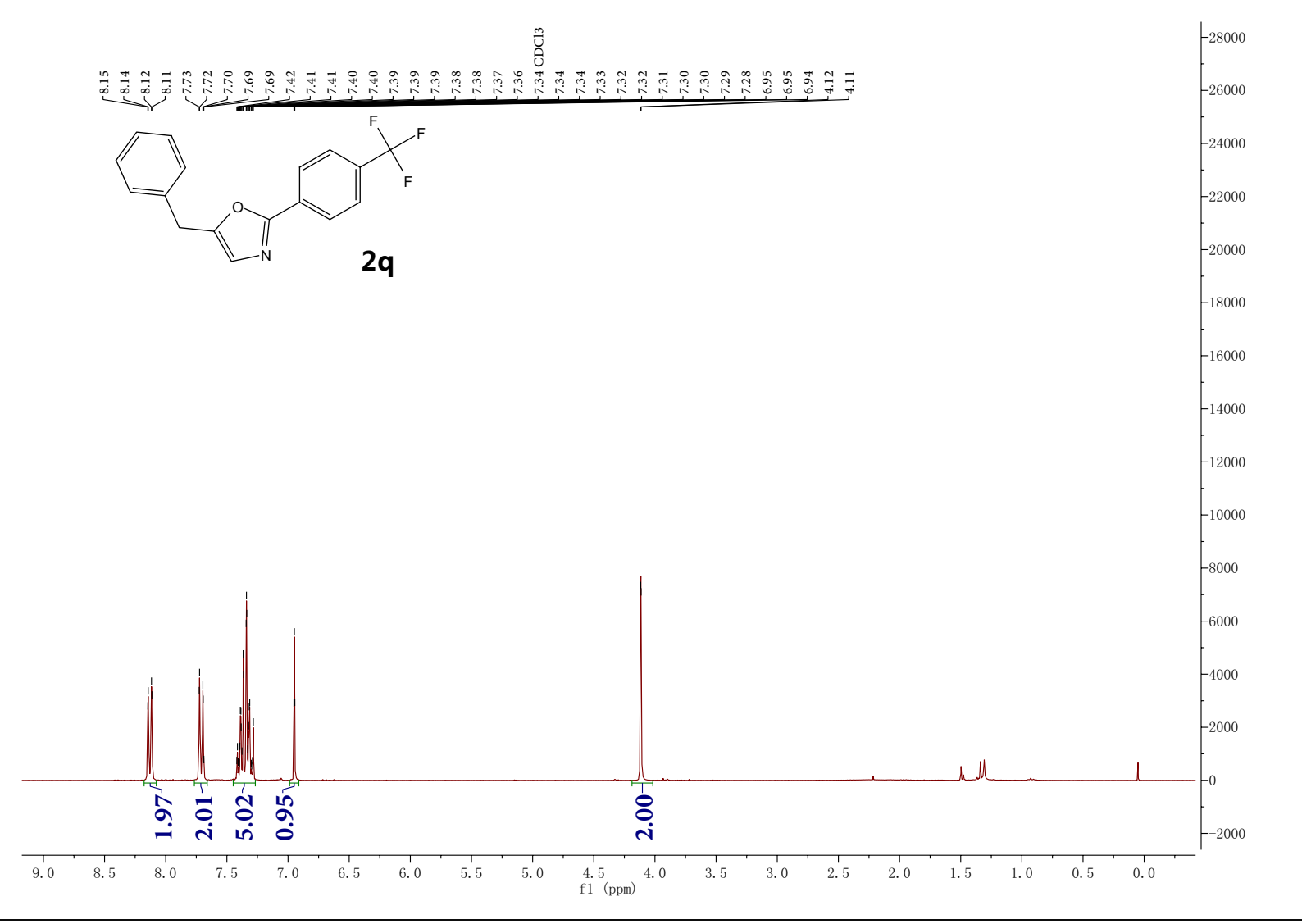
151.06
140.32
136.78
129.44
128.73
126.93
126.09
124.99
124.70
32.16
21.52
f1 (ppm)


7.99 7.98 7.97 7.95 7.95 7.94 7.39 7.39 7.38 7.37 7.37 7.37 7.36 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.29 7.28 CDCl3 7.28 7.27 7.26 7.26 6.99 6.98 6.97 6.96 6.95 6.94 6.85 6.85 6.85 4.07 3.85
CH3
O
O
N
2o
2.01
5.19
2.10
0.96
2.00
3.04
f1 (ppm)


161.36 161.12 150.79 136.83 128.70 127.76 126.90 124.54 120.49 114.13 55.34 32.12
f1 (ppm)


8.10 8.09 8.09 8.09 8.07 8.07 8.07 8.06 7.72 7.71 7.71 7.71 7.69 7.69 7.69 7.68 7.40 7.40 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.34 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.28 7.27 CDCl3 7.27 6.96 6.96 6.95 4.10
N
O
N
2p
1.95
1.95
5.02
0.93
2.00
f1 (ppm)


159.35 152.89 136.16 132.56 131.32 128.85 128.72 127.16 126.43 125.67 118.43 113.22 32.18 29.54
f1 (ppm)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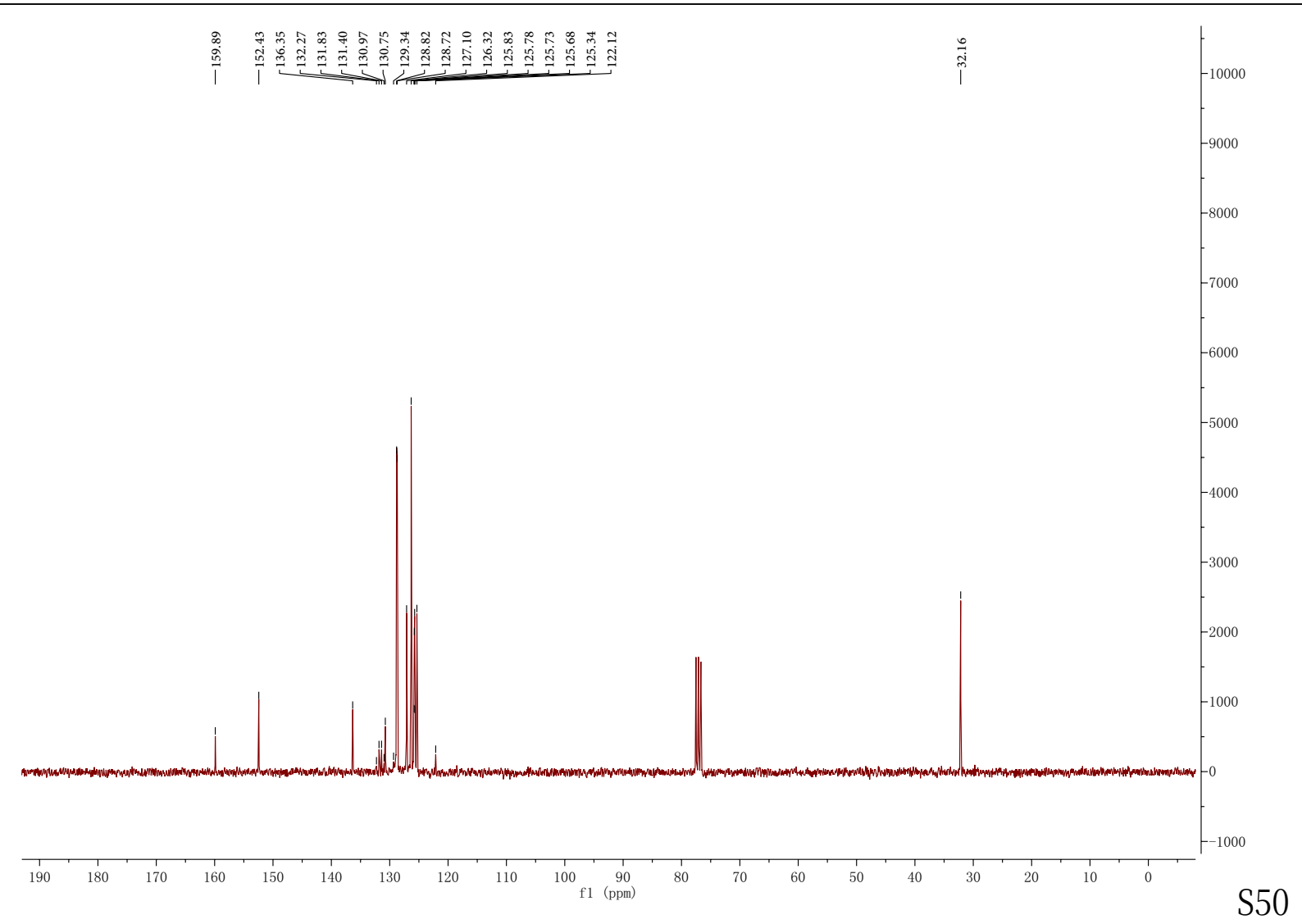
8.14
8.12
8.11
7.73
7.72
7.70
7.69
7.69
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.39
7.38
7.38
7.37
7.36
7.34 CDCl3
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.28
6.95
6.95
6.94
4.12
4.11
F
F
F
O
N
2q
1.97
2.01
5.02
0.95
2.00
f1 (ppm)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130.75
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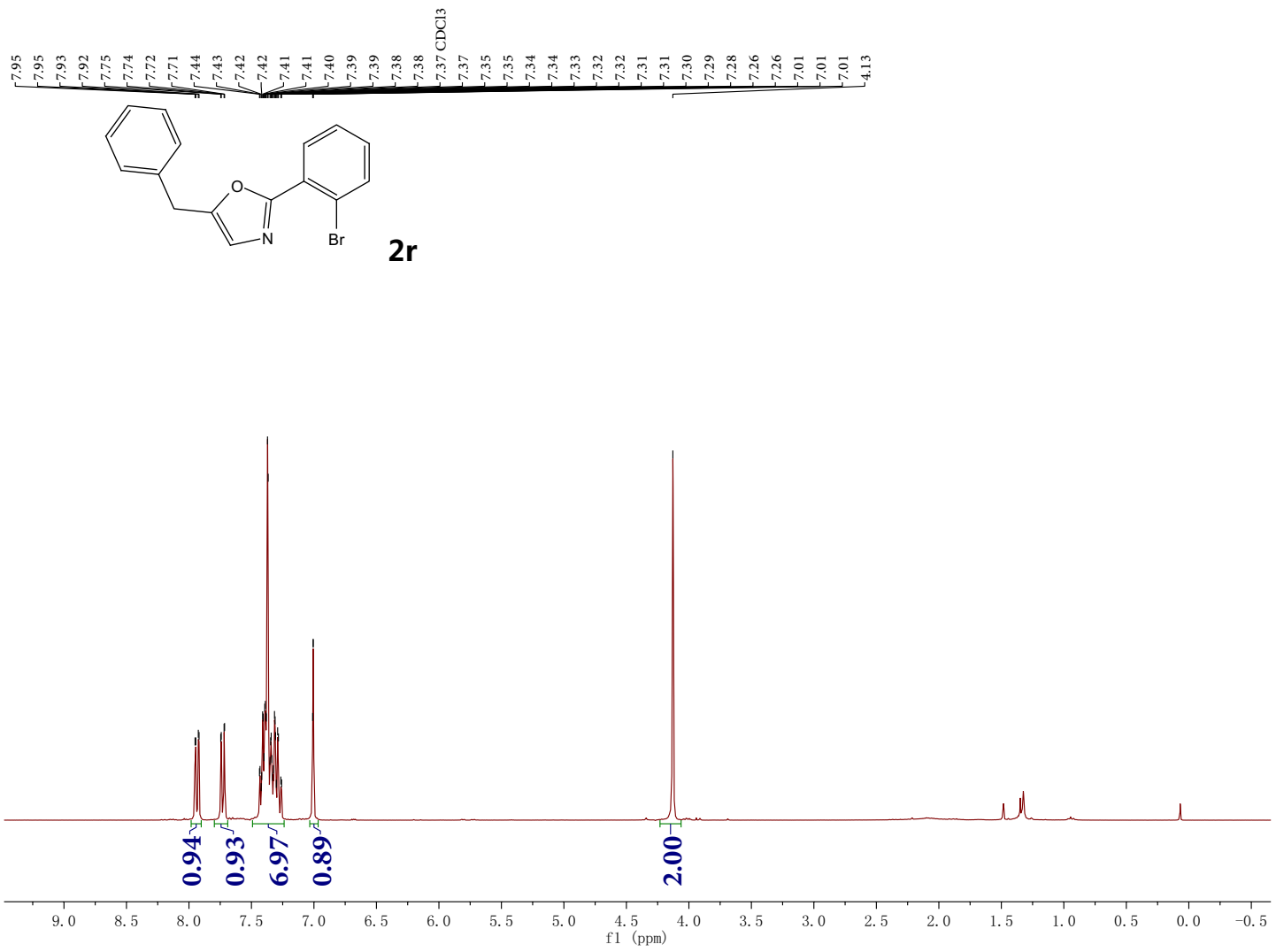
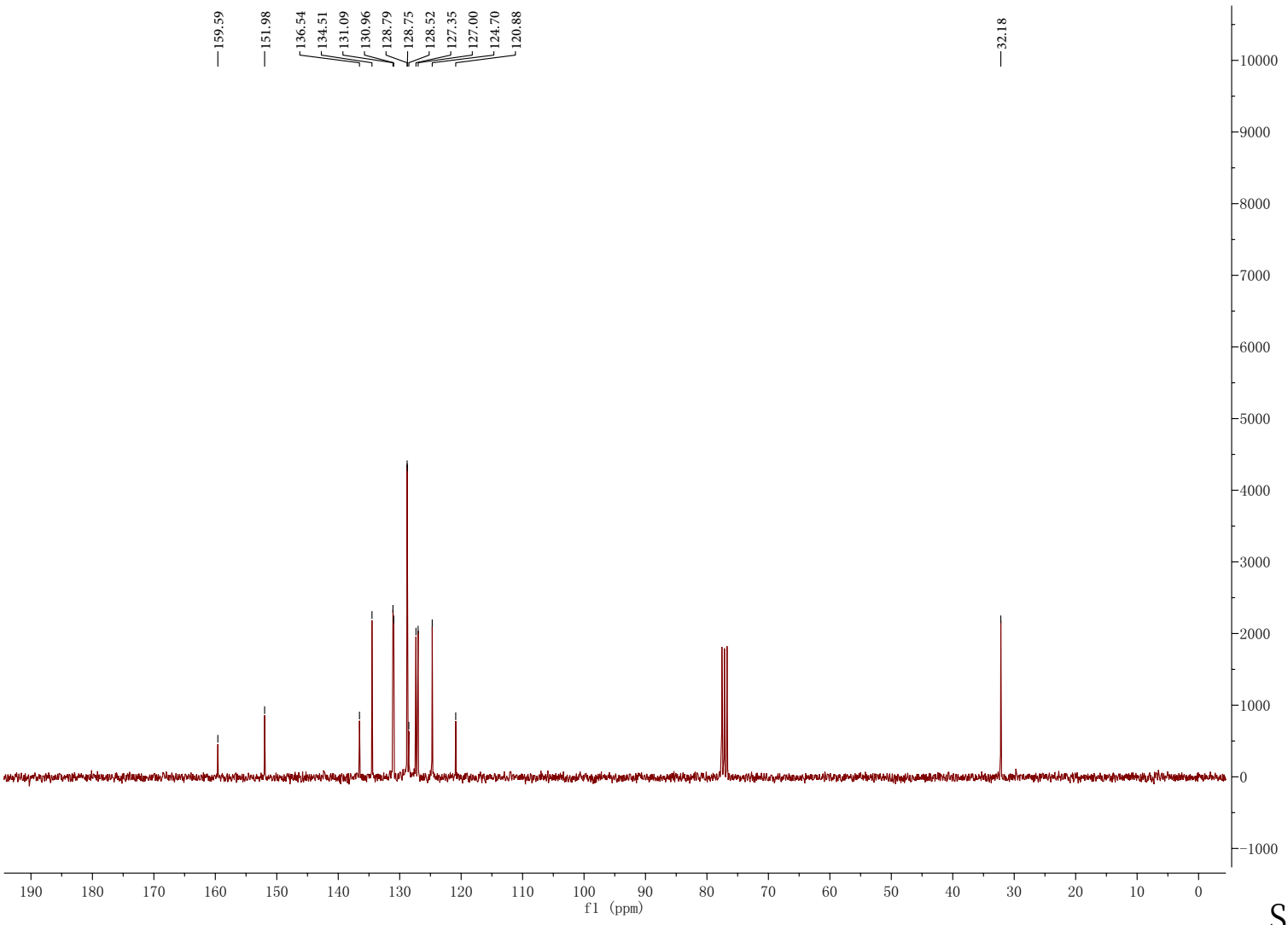
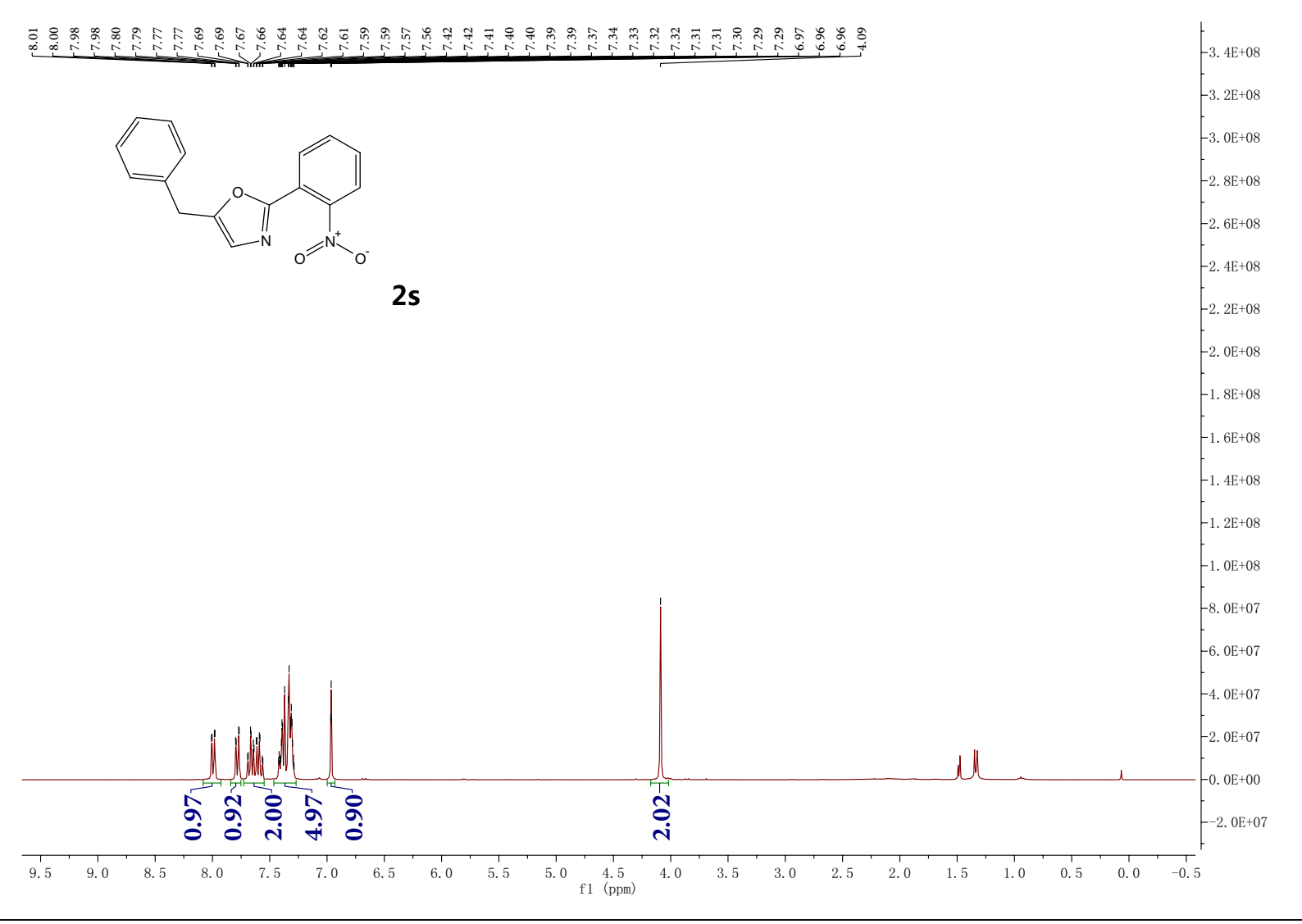
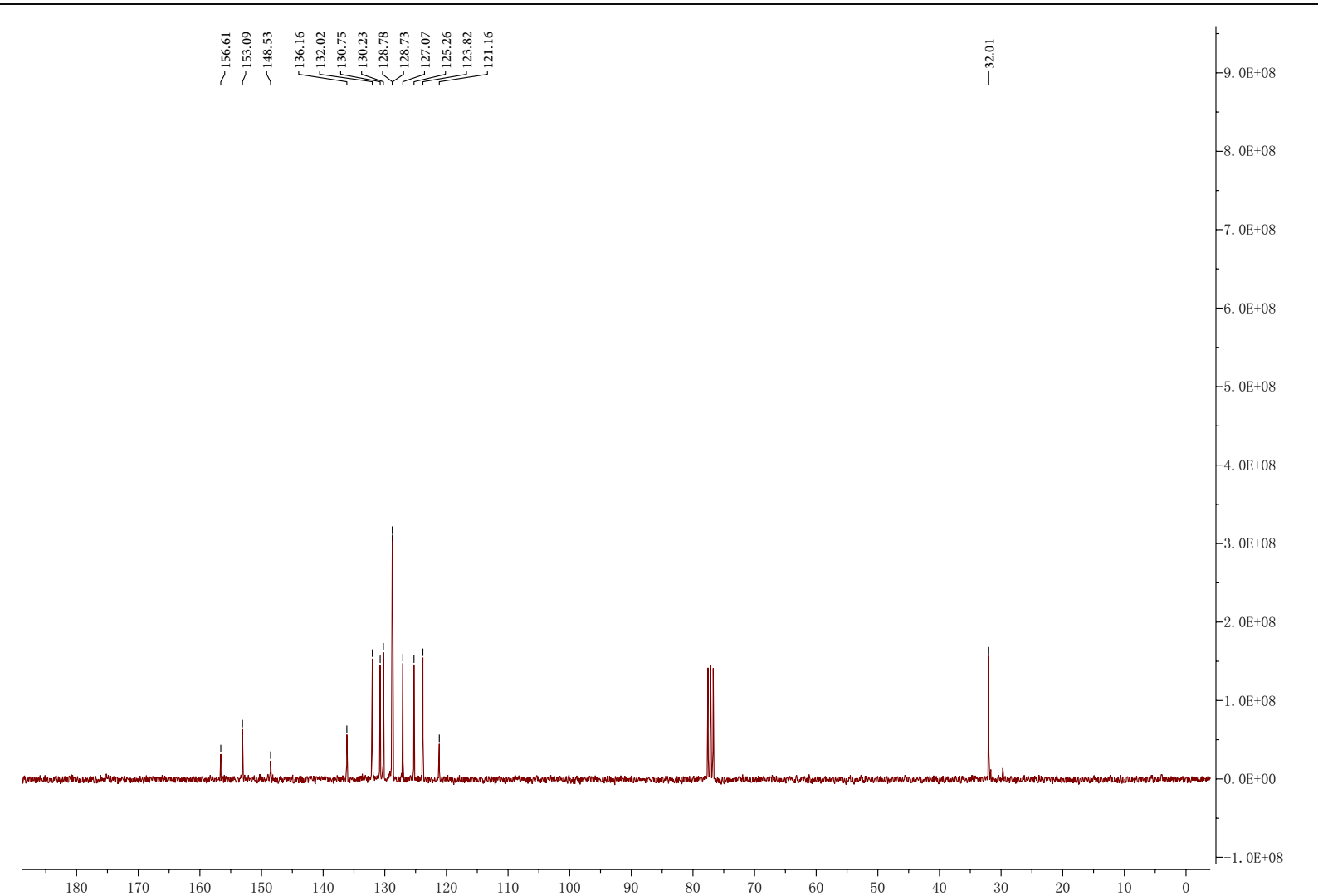
128.72
127.10
126.32
125.83
125.78
125.73
125.68
125.34
122.12
32.16
f1 (ppm)


7.95 7.95 7.93 7.92 7.75 7.74 7.72 7.71 7.44 7.43 7.42 7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.38 7.37 CDCl3 7.37 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.28 7.26 7.26 7.01 7.01 7.01 4.13
O
N
Br
2r
0.94
0.93
6.97
0.89
2.00
f1 (ppm)


159.59 151.98 136.54 134.51 131.09 130.96 128.79 128.75 128.52 127.35 127.00 124.70 120.88
32.18
f1 (ppm)


8.01 8.00 7.98 7.98 7.80 7.79 7.77 7.77 7.69 7.69 7.67 7.66 7.64 7.64 7.62 7.61 7.59 7.59 7.57 7.56 7.42 7.42 7.41 7.40 7.40 7.39 7.39 7.37 7.34 7.33 7.32 7.32 7.31 7.31 7.30 7.29 7.29 6.97 6.96 6.96 4.09
O
N
O
N+
O-
0.97
0.92
2.00
4.97
0.90
2.02
f1 (ppm)

2s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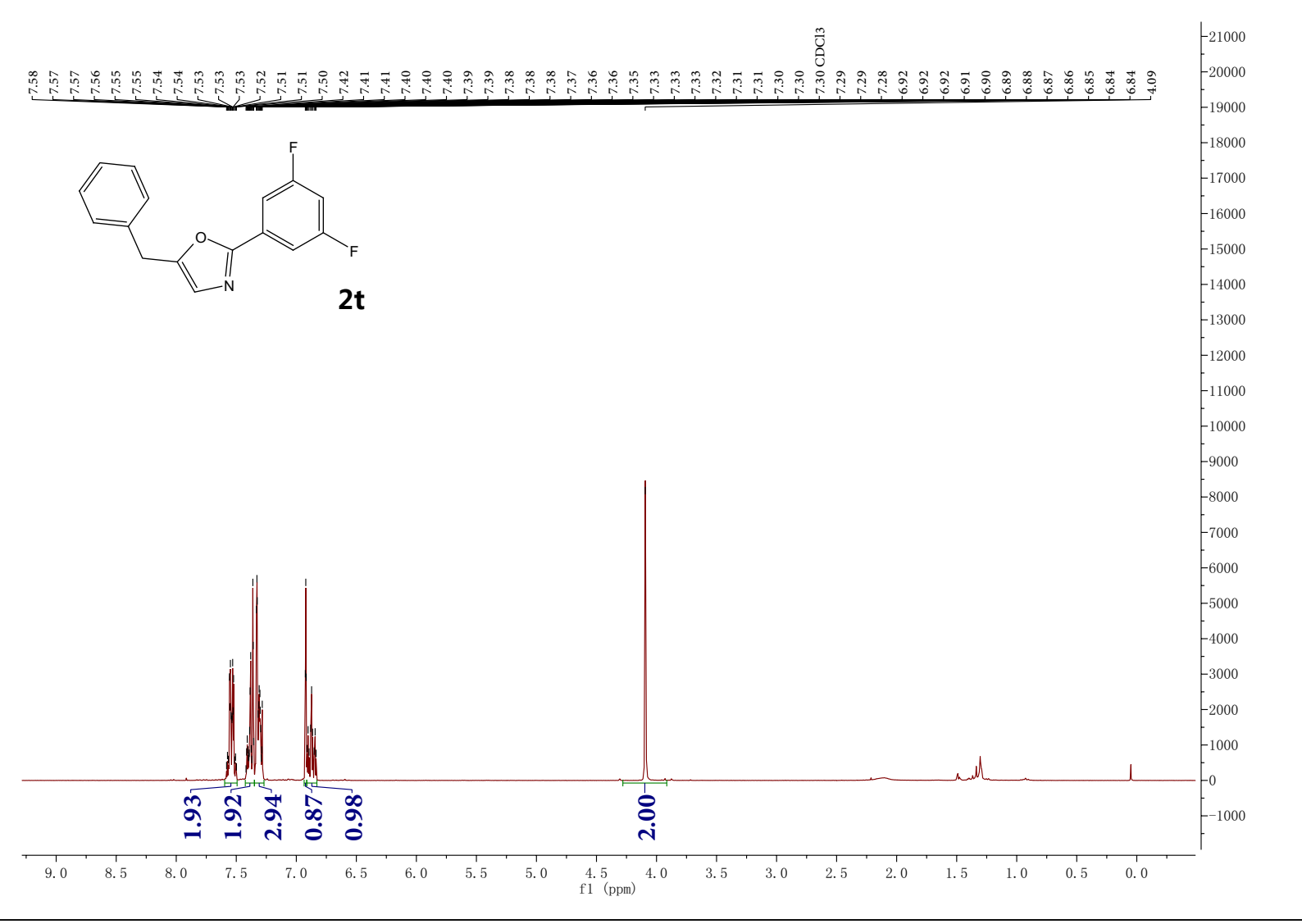
32.01
f1 (ppm)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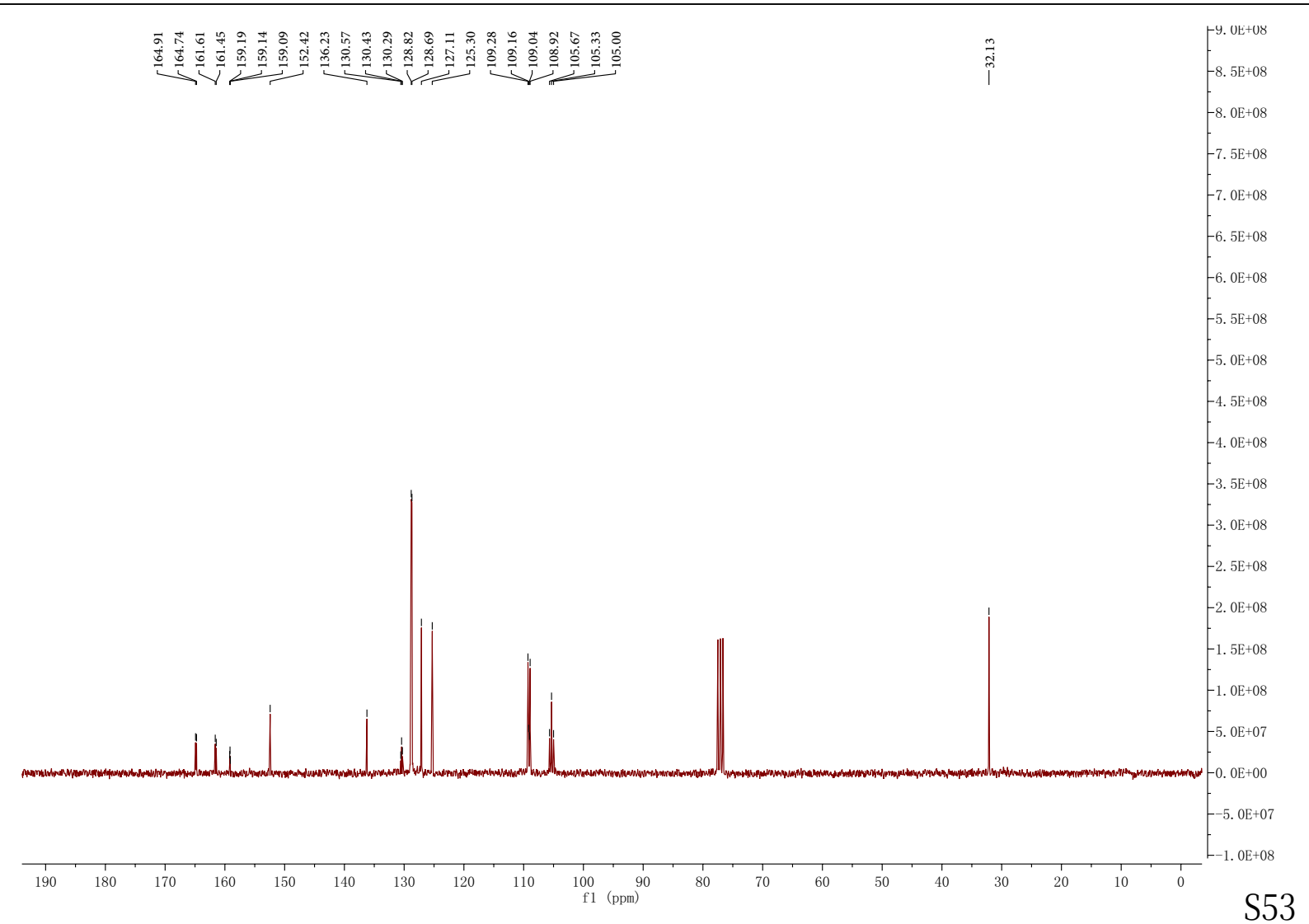
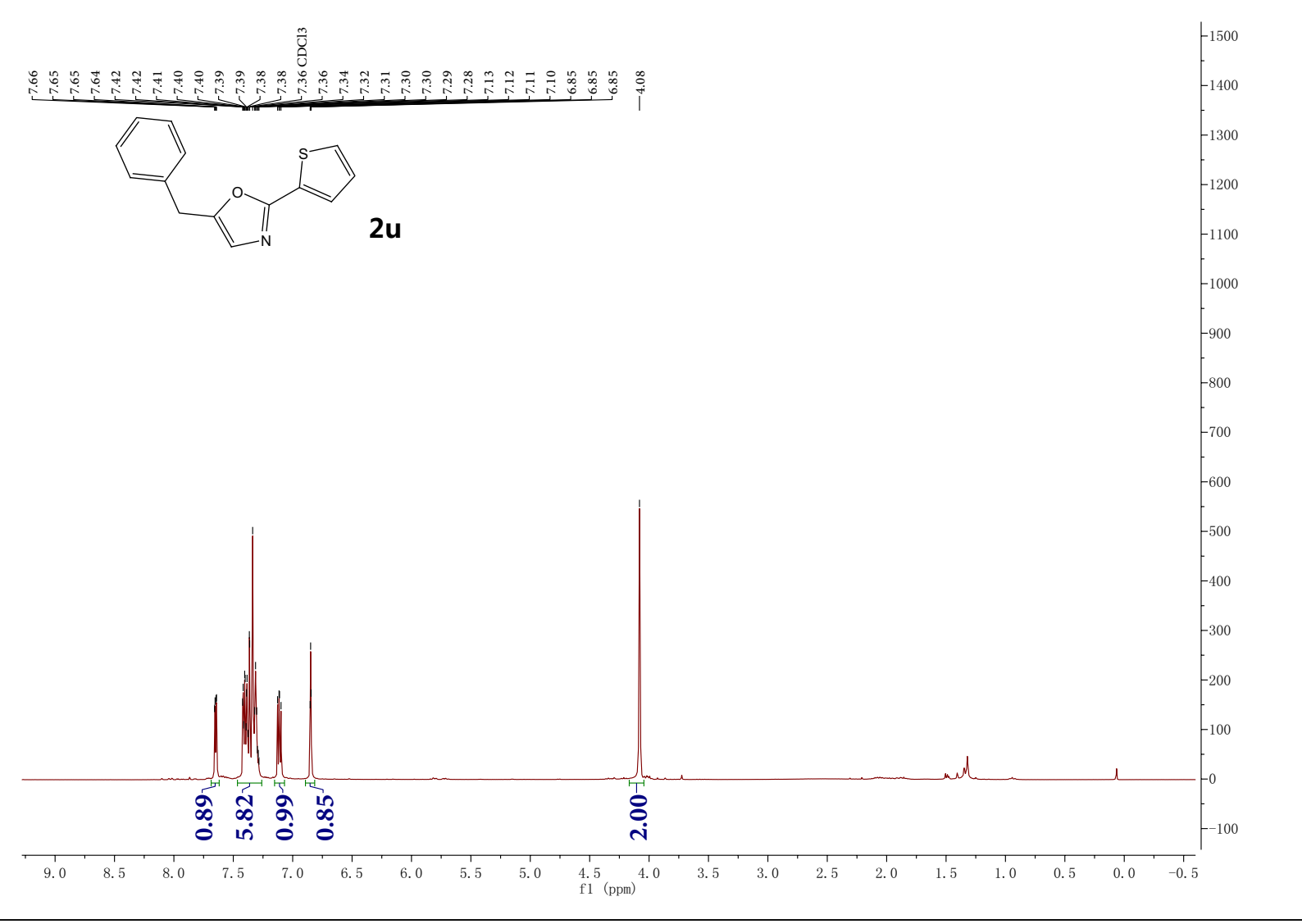
F
O
N
F
2t
1.93
1.92
2.94
0.87
0.98
2.00
f1 (ppm)


164.91 164.74 161.61 161.45 159.19 159.14 159.09 152.42 136.23 130.57 130.43 130.29 128.82 128.69 127.11 125.30 109.28 109.16 109.04 108.92 105.67 105.33 105.00
32.13
f1 (ppm)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7.65
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7.42
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7.40
7.40
7.39
7.39
7.38
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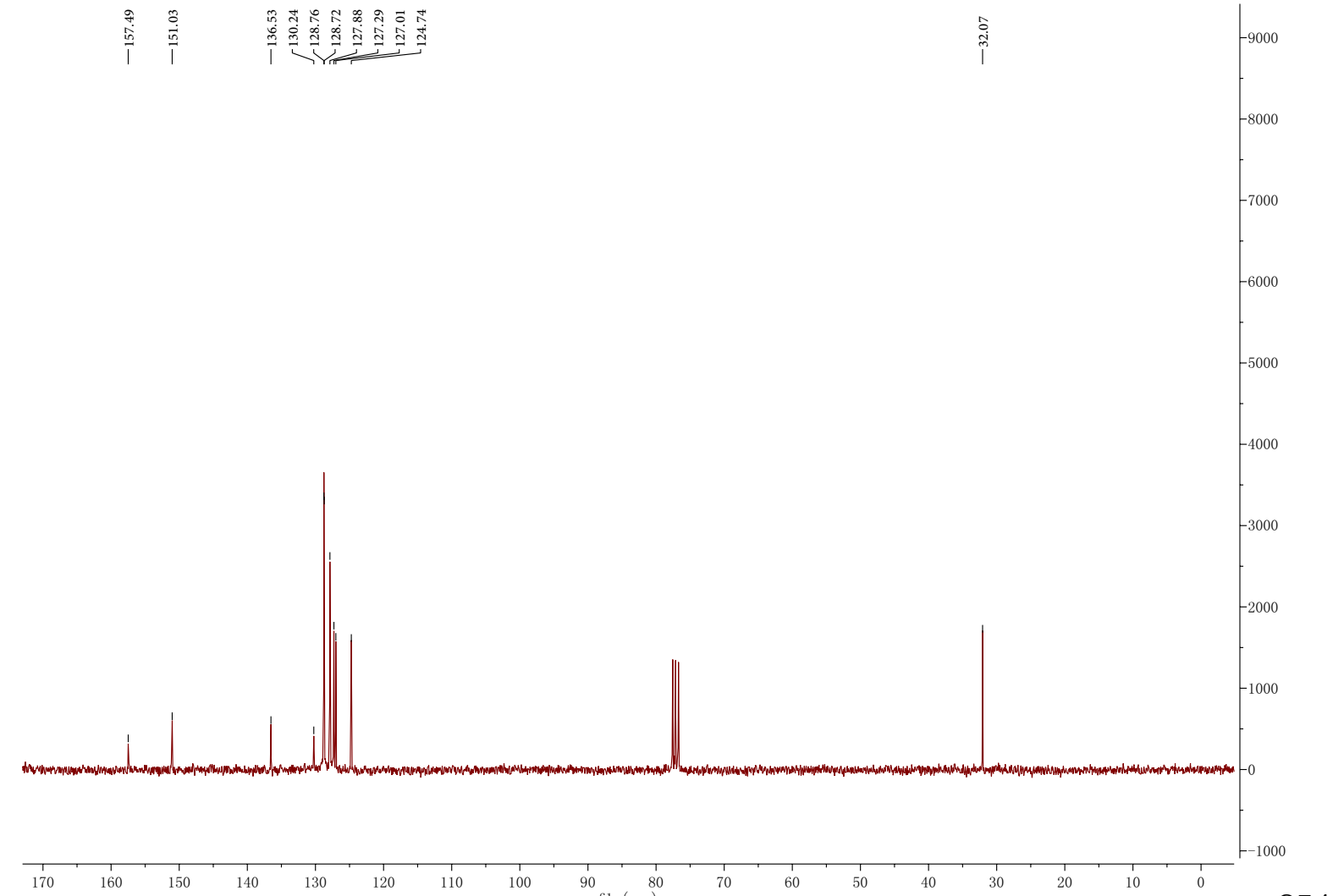
7.36
7.34
7.32
7.31
7.30
7.30
7.29
7.28
7.13
7.12
7.11
7.10
6.85
6.85
6.85
4.08
S
O
N
2u
0.89
5.82
0.99
0.85
2.00
f1 (ppm)


157.49
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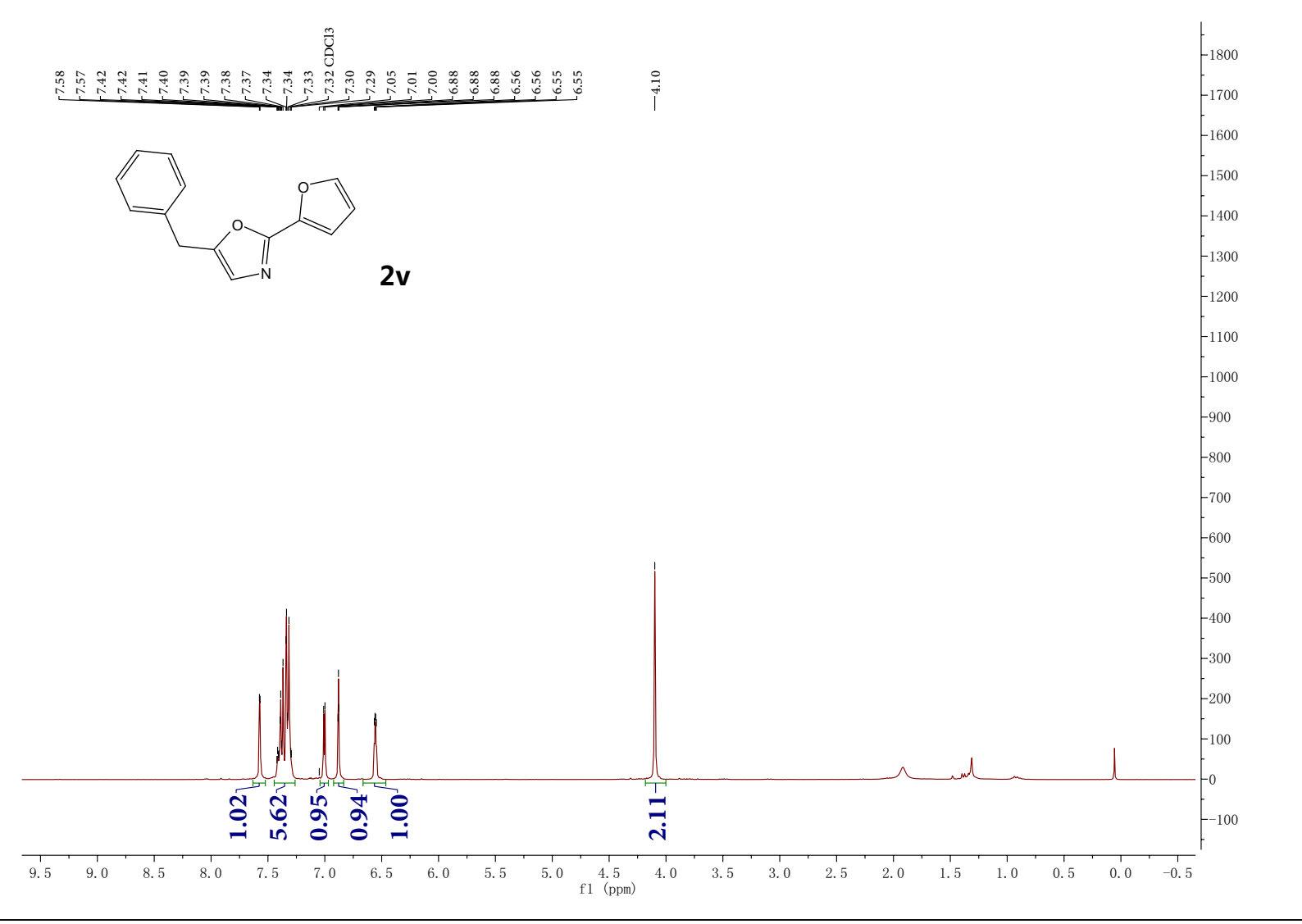
136.53
130.24
128.76
128.72
127.88
127.29
127.01
124.74
32.07
f1 (ppm)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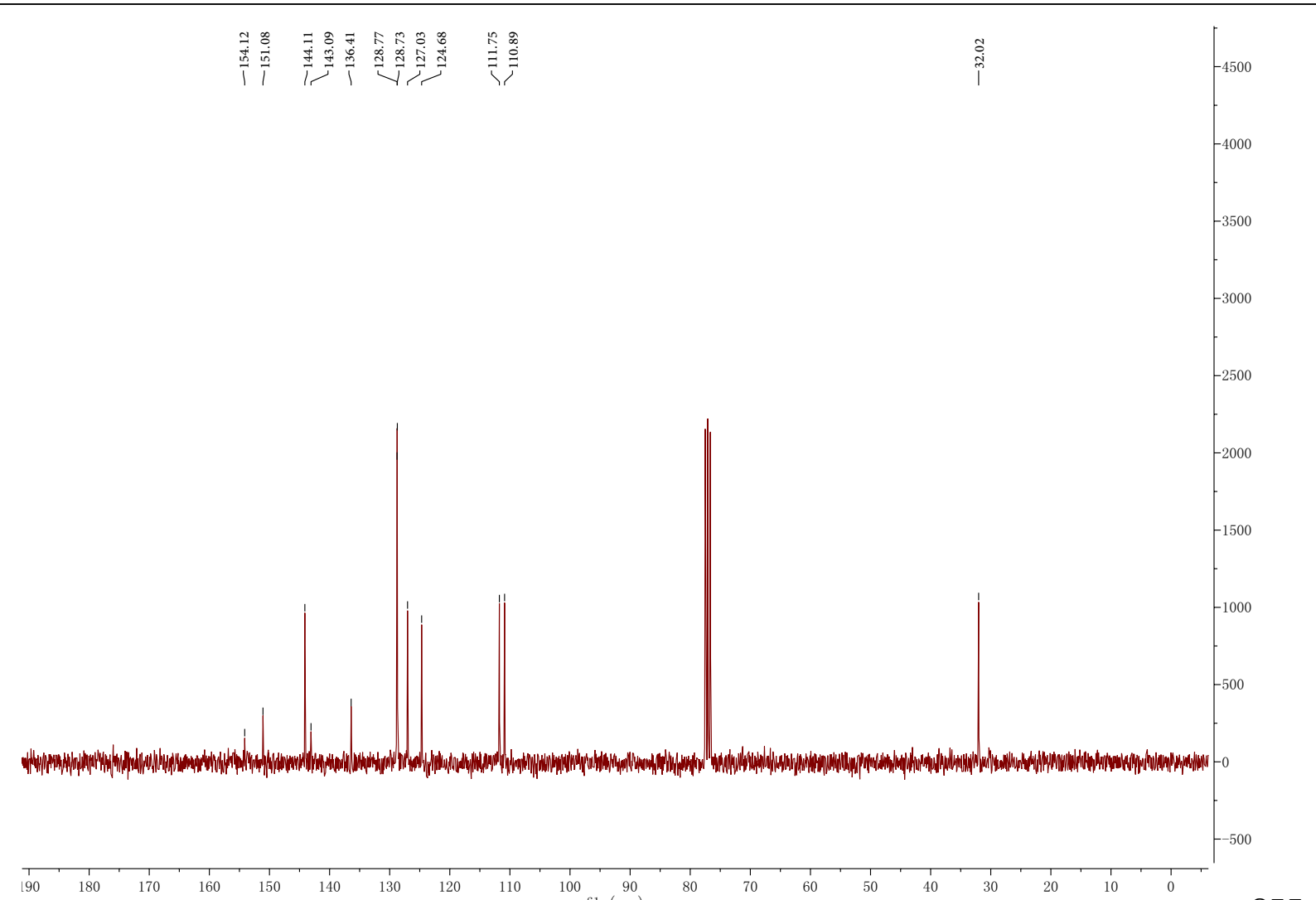
7.57
7.42
7.42
7.41
7.40
7.39
7.39
7.38
7.37
7.34
7.34
7.33
7.32 CDCl3
7.30
7.29
7.05
7.01
7.00
6.88
6.88
6.88
6.56
6.56
6.55
6.55
4.10
O
O
N
2v
1.02
5.62
0.95
0.94
1.00
2.11
f1 (ppm)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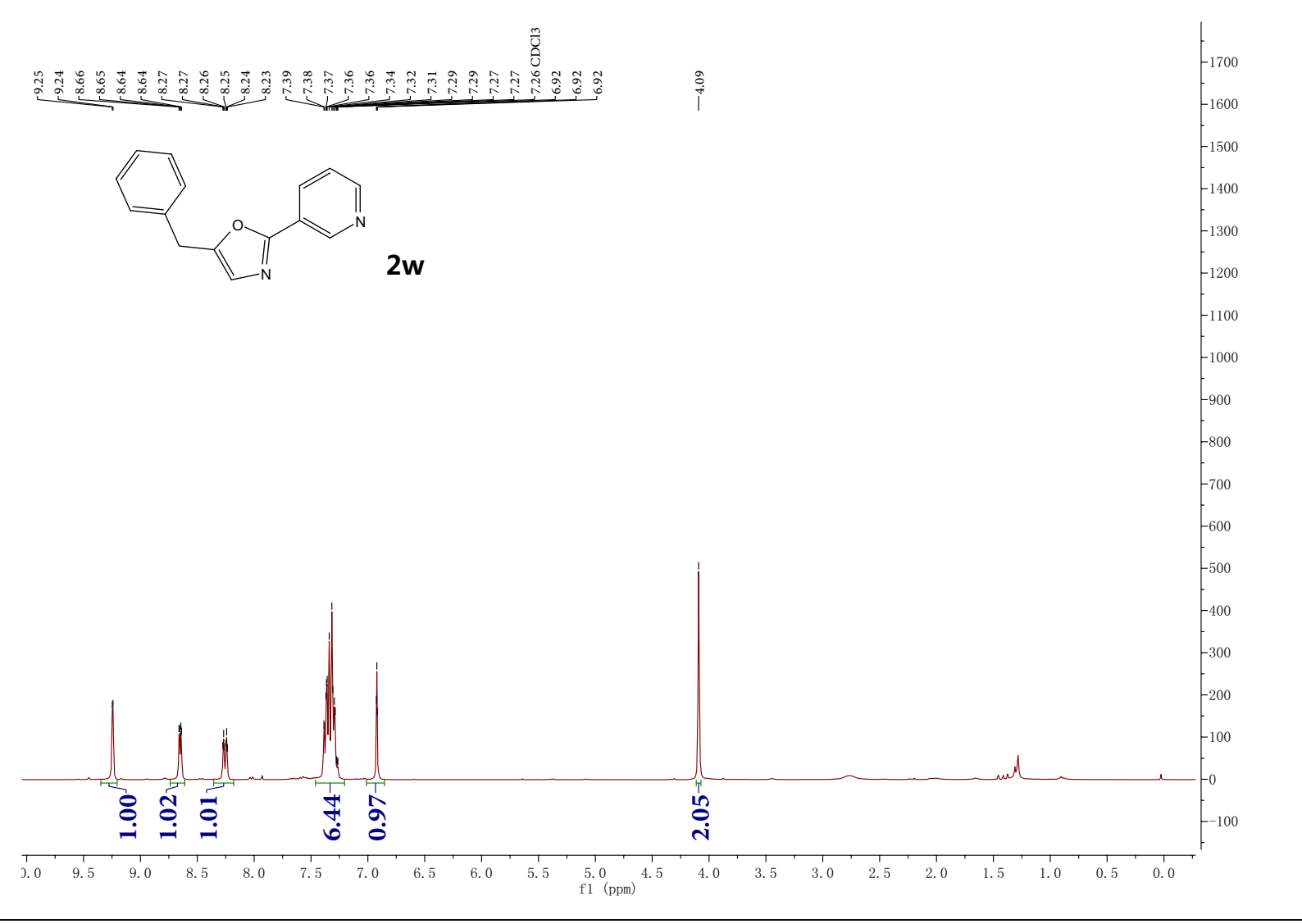
151.08
144.11
143.09
136.41
128.77
128.73
127.03
124.68
111.75
110.89
32.02
f1 (ppm)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9.24
8.66
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8.64
8.27
8.27
8.26
8.25
8.24
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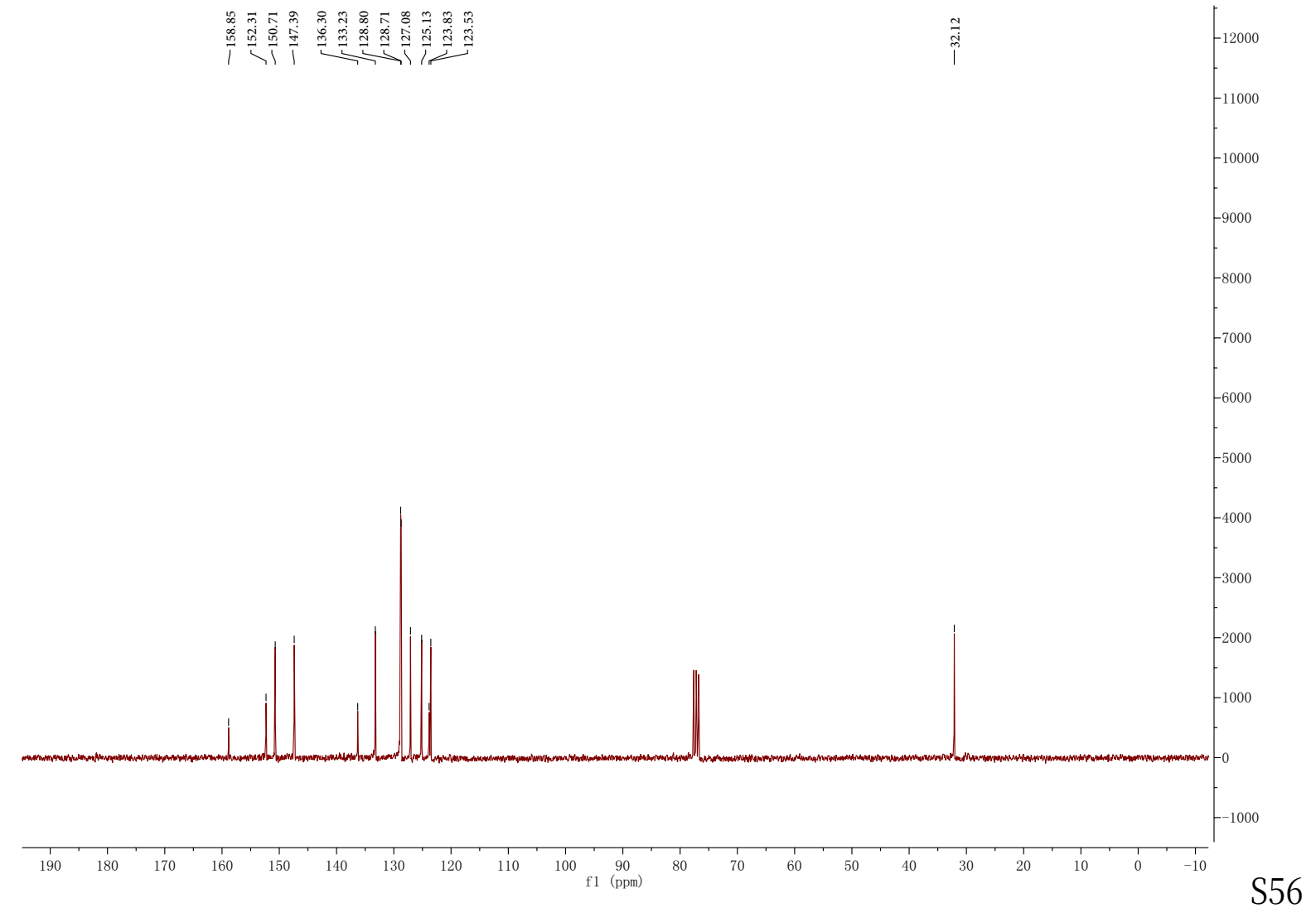
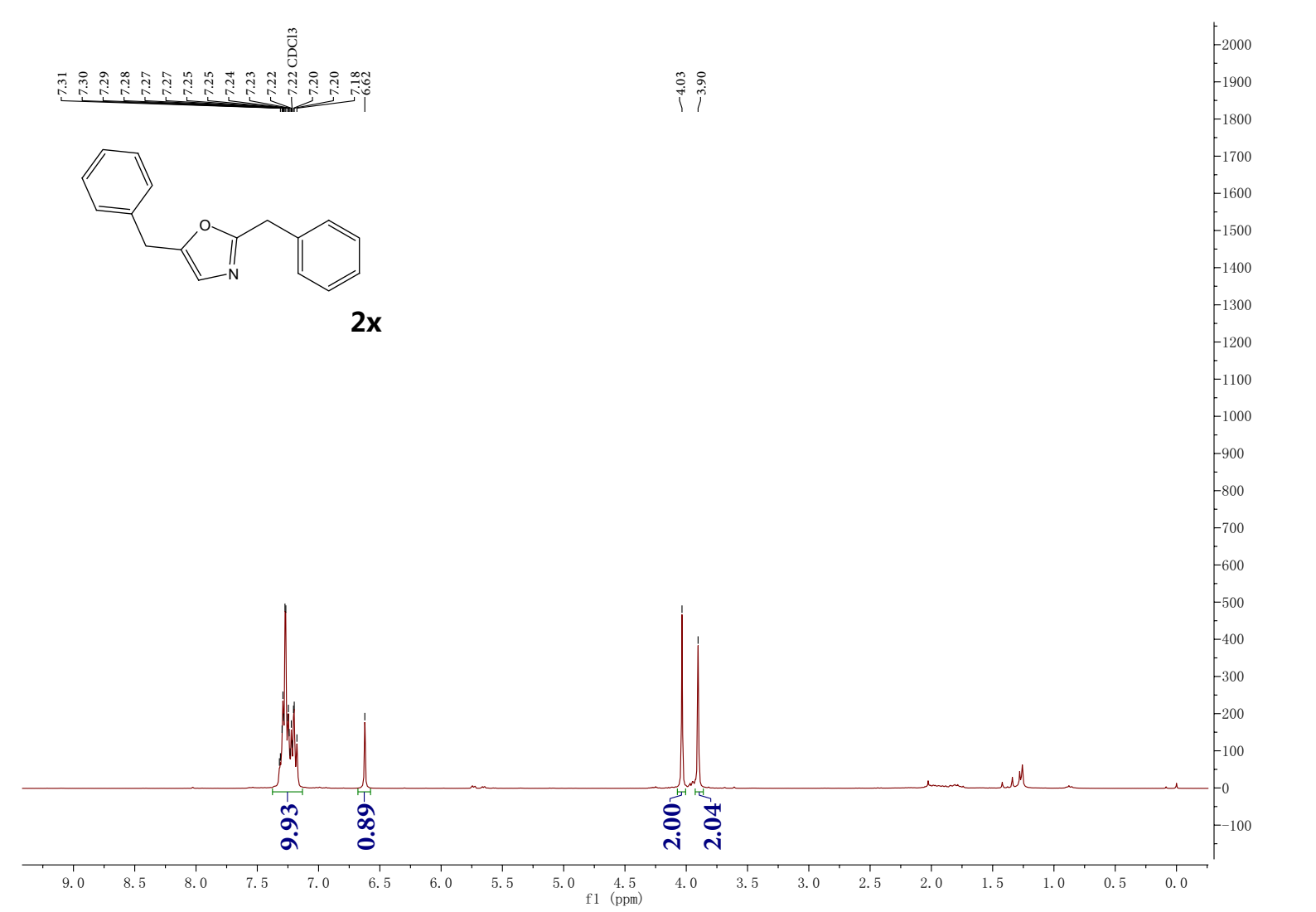
7.39
7.38
7.37
7.36
7.36
7.34
7.32
7.31
7.29
7.29
7.27
7.27
7.26 CDCl3
6.92
6.92
6.92
4.09
O
N
N
2w
1.00
1.02
1.01
6.44
0.97
2.05
f1 (ppm)


158.85
152.31
150.71
147.39
136.30
133.23
128.80
128.71
127.08
125.13
123.83
123.53
32.12
f1 (ppm)


7.31
7.30
7.29
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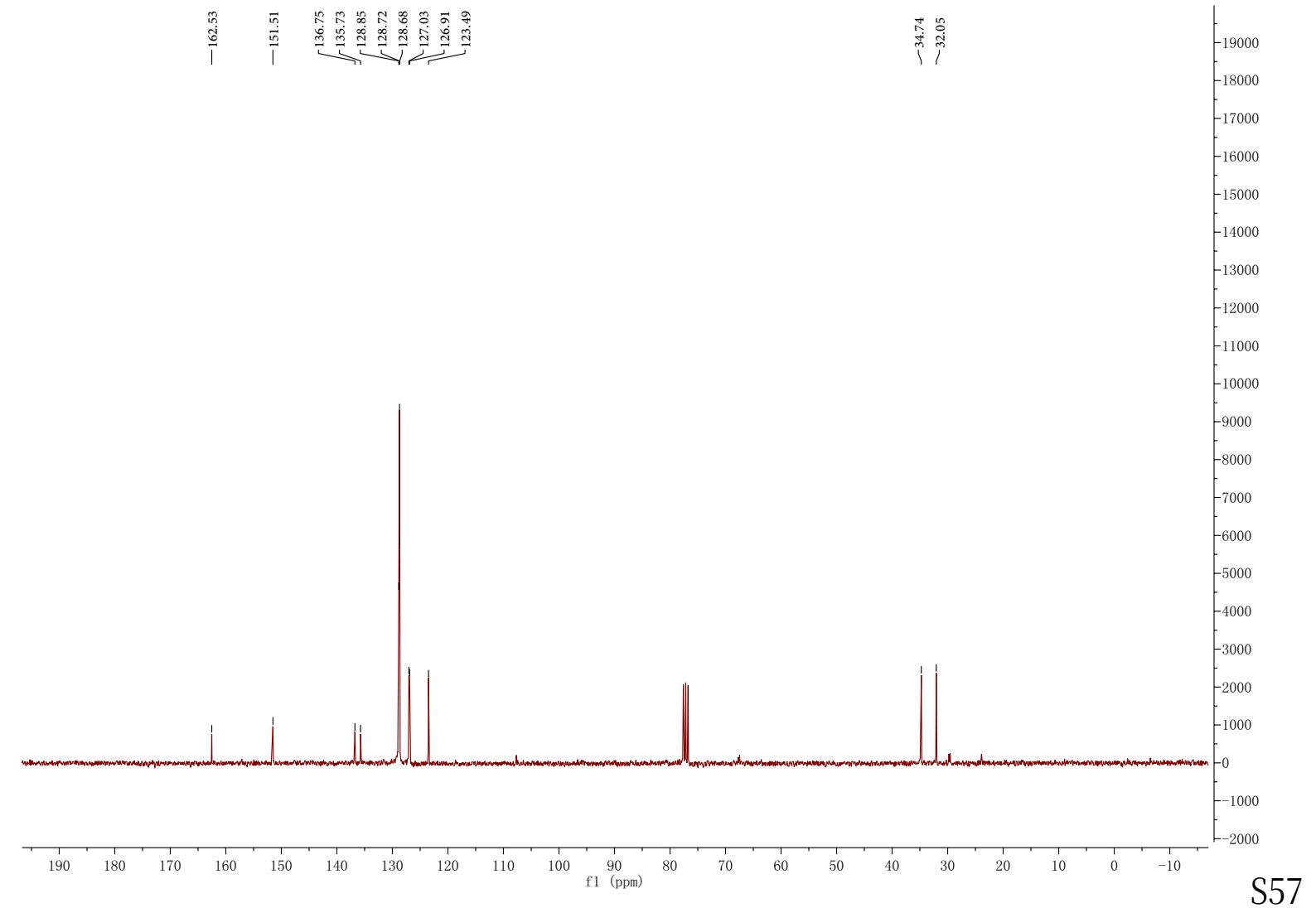
7.27
7.27
7.25
7.25
7.24
7.23
7.22
7.22 CDCl3
7.20
7.20
7.18
6.62
4.03
3.90
O
N
2x
9.93
0.89
2.00
2.04
f1 (ppm)


162.53
151.51
136.75
135.73
128.85
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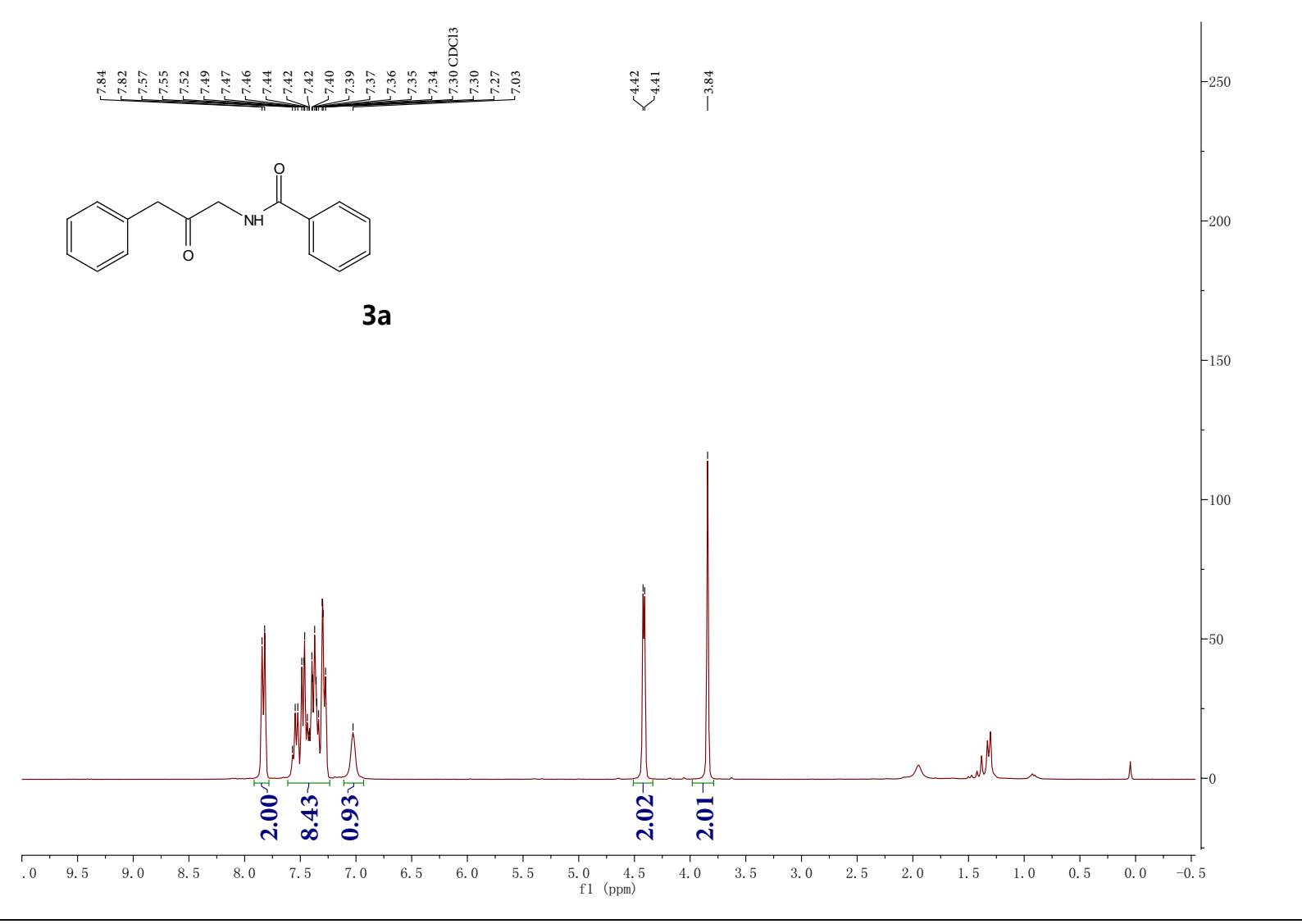
128.68
127.03
126.91
123.49
34.74
32.05
f1 (ppm)


7.84
7.82
7.57
7.55
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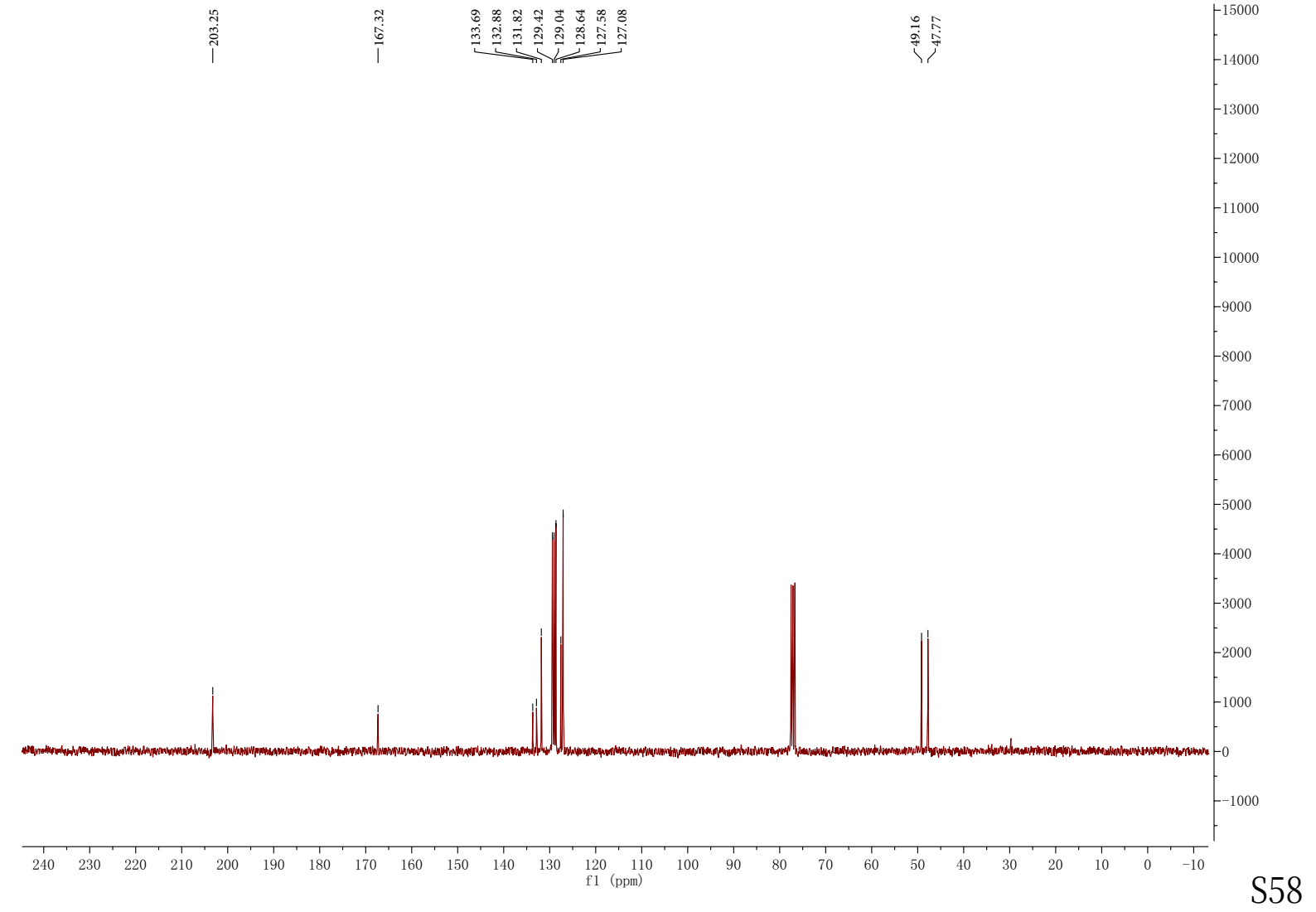
7.49
7.47
7.46
7.44
7.42
7.42
7.40
7.39
7.37
7.36
7.35
7.34
7.30 CDCl3
7.30
7.27
7.03
4.42
4.41
3.84
O
NH
O
2.00
8.43
0.93
2.02
2.01
f1 (ppm)

3a


203.25
167.32
133.69
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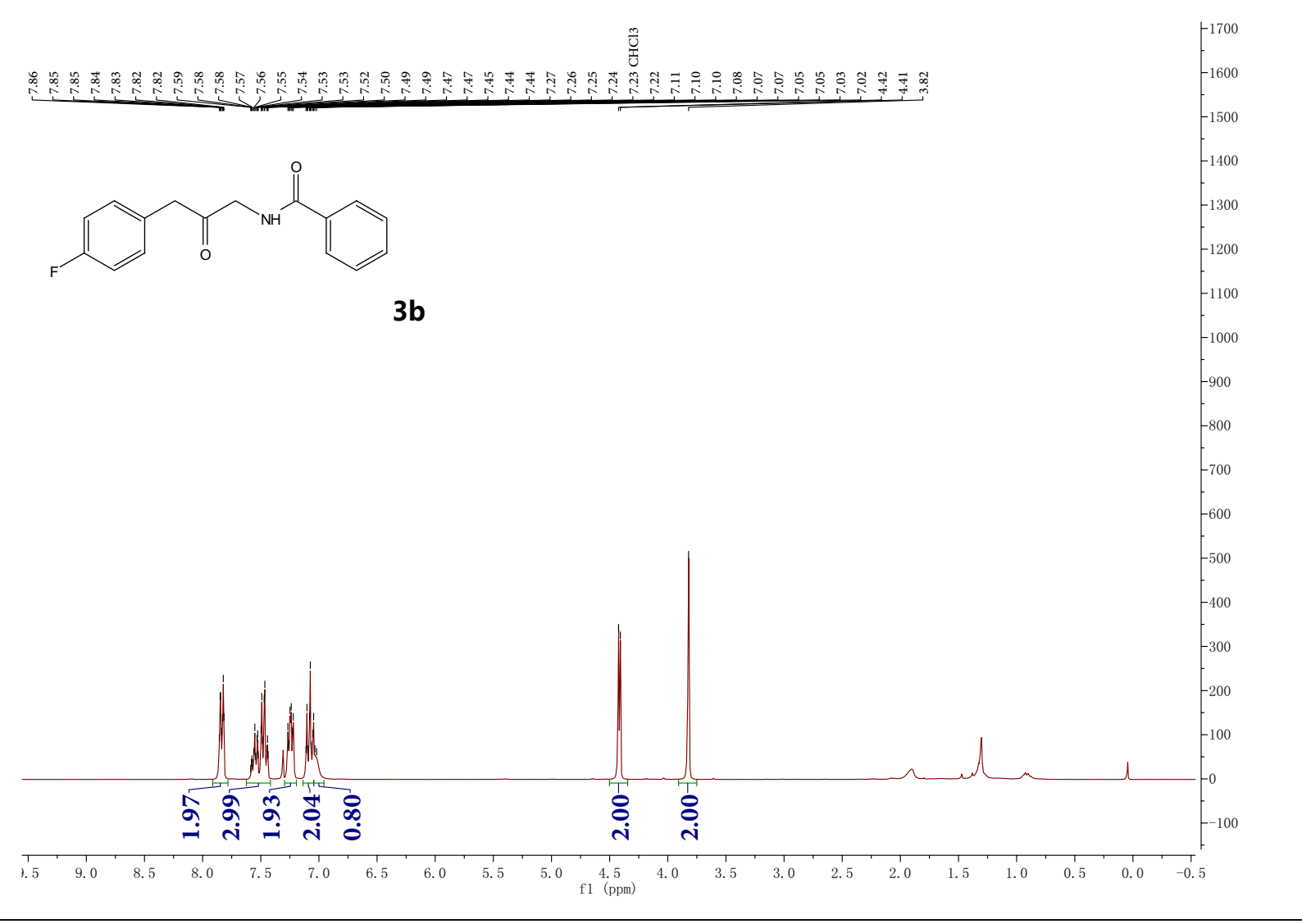
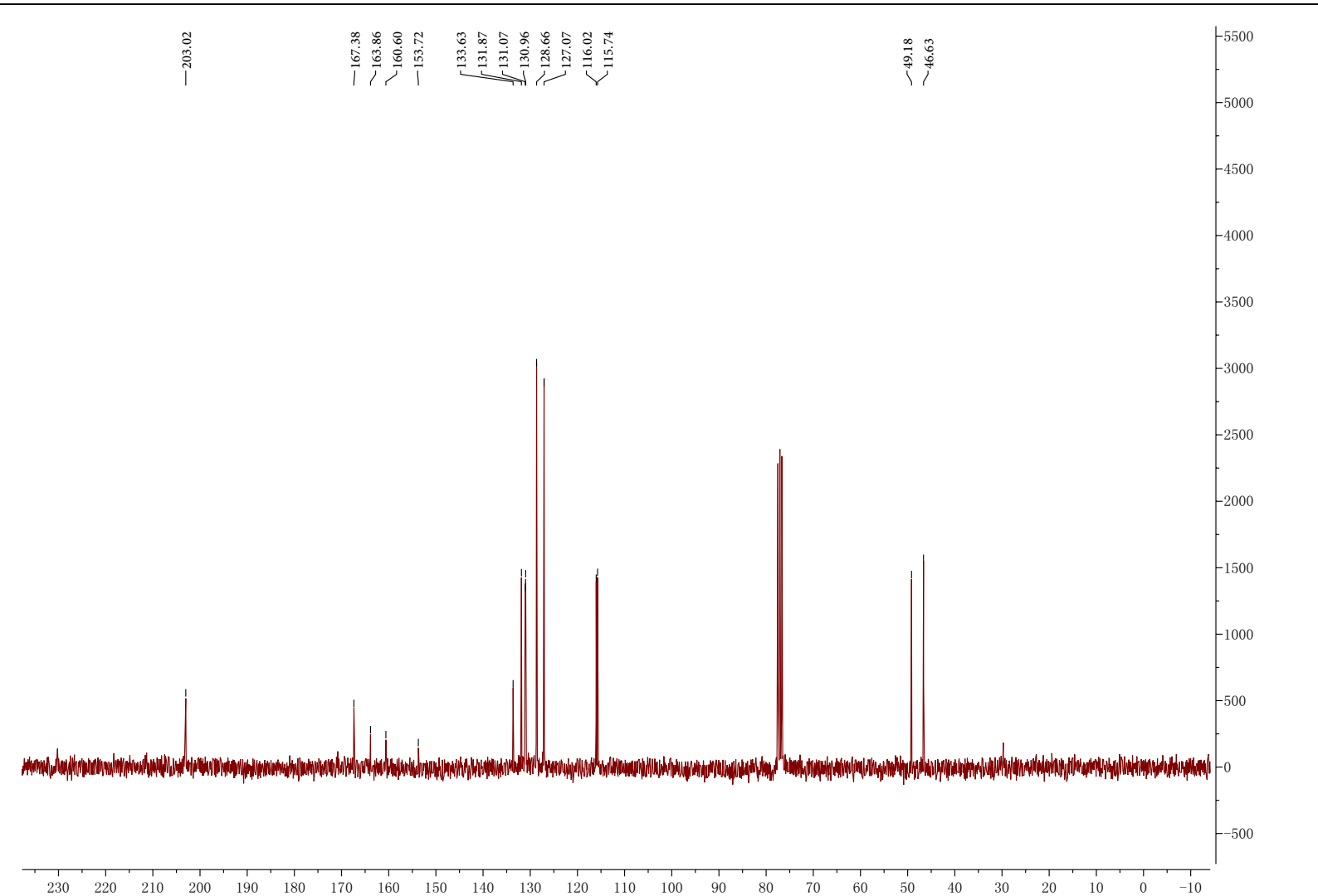
131.82
129.42
129.04
128.64
127.58
127.08
49.16
47.77
f1 (ppm)


7.86 7.85 7.85 7.84 7.83 7.82 7.82 7.59 7.58 7.58 7.57 7.56 7.55 7.54 7.53 7.53 7.52 7.50 7.49 7.49 7.47 7.47 7.45 7.44 7.44 7.27 7.26 7.25 7.24 7.23 CHCl3 7.22 7.11 7.10 7.10 7.08 7.07 7.07 7.05 7.05 7.03 7.02 4.42 4.41 3.82
O
NH
O
F
3b
1.97
2.99
1.93
2.04
0.80
2.00
2.00
f1 (ppm)


203.02
167.38
163.86
160.60
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133.63
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131.07
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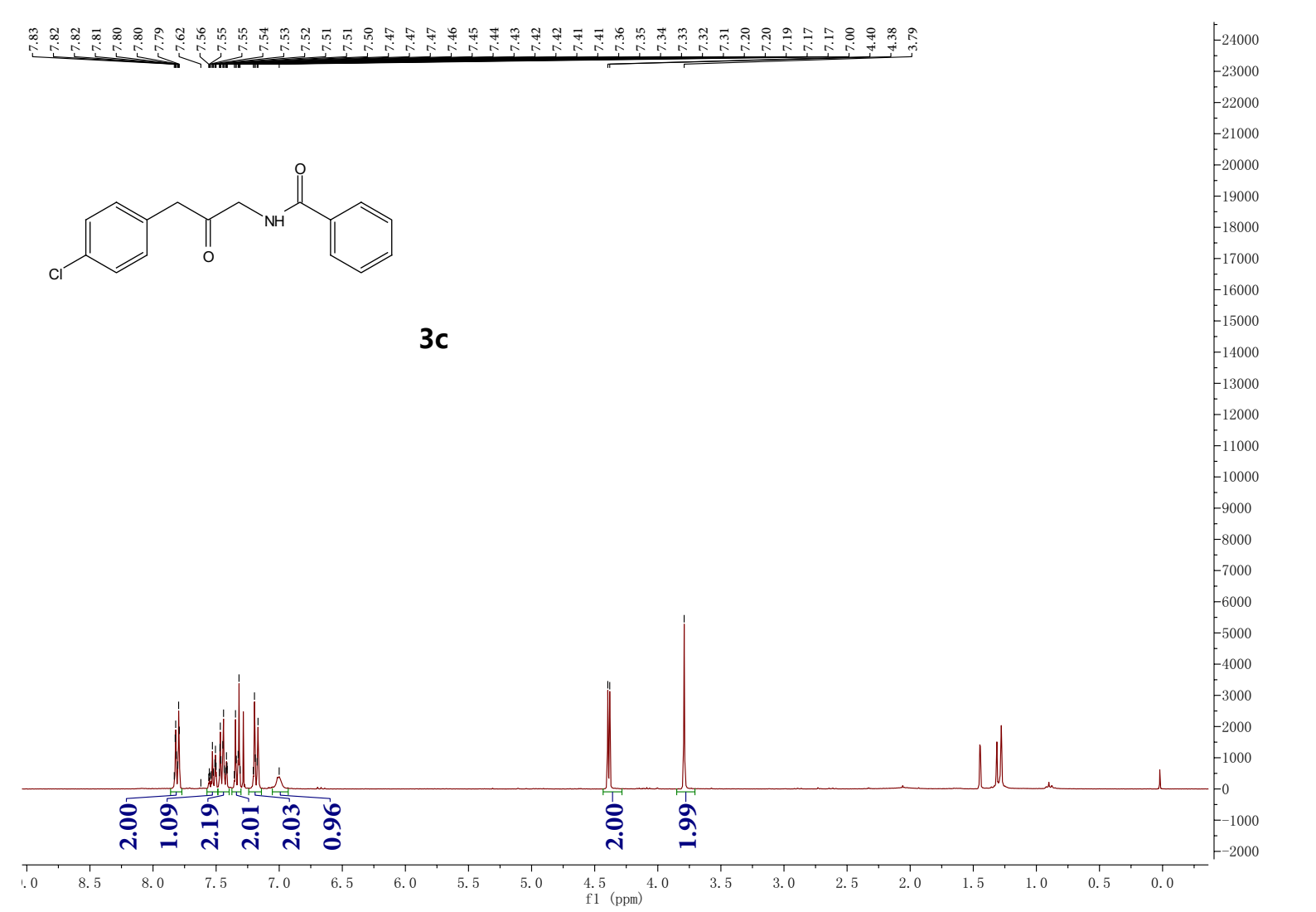
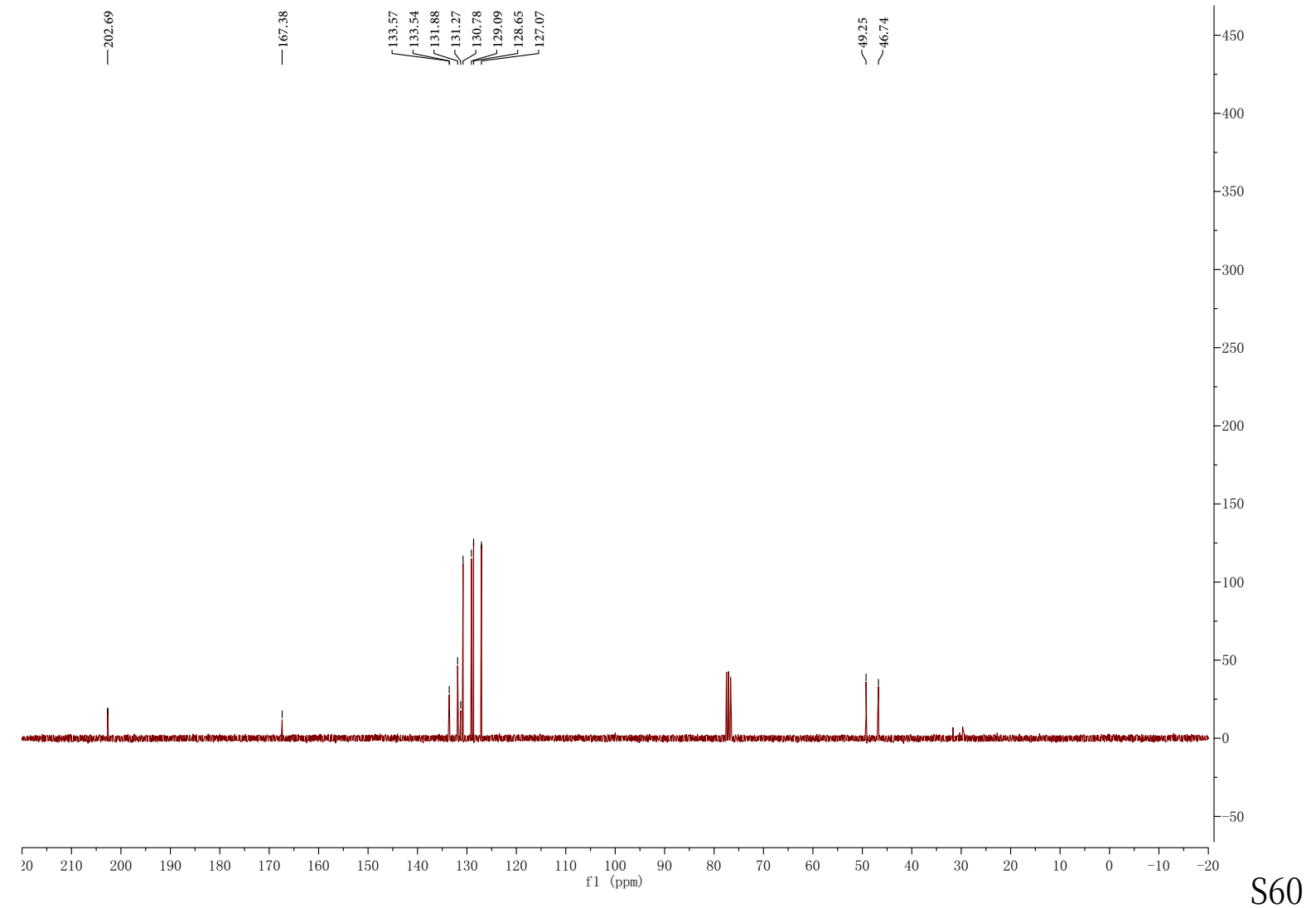
128.66
127.07
116.02
115.74
49.18
46.63
f1 (ppm)


7.83 7.82 7.82 7.81 7.80 7.80 7.79 7.62 7.56 7.55 7.55 7.54 7.53 7.52 7.51 7.51 7.50 7.47 7.47 7.47 7.46 7.45 7.44 7.43 7.42 7.42 7.41 7.41 7.36 7.35 7.34 7.33 7.32 7.31 7.20 7.20 7.19 7.17 7.17 7.00 4.40 4.38 3.79
O
NH
O
Cl
3c
2.00
1.09
2.19
2.01
2.03
0.96
2.00
1.99
f1 (ppm)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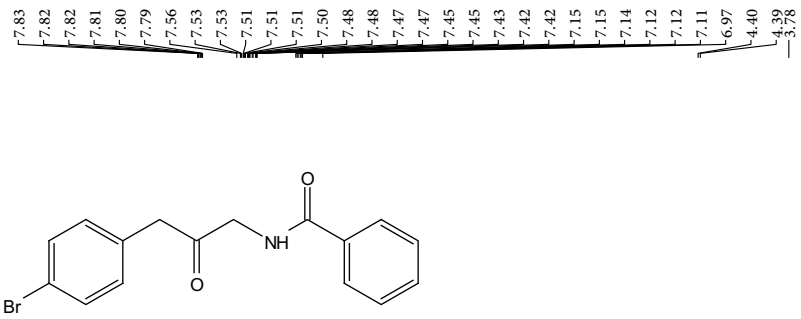
167.38
133.57
133.54
131.88
131.27
130.78
129.09
128.65
127.07
49.25
46.74
f1 (ppm)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7.82
7.82
7.81
7.80
7.79
7.56
7.53
7.53
7.51
7.51
7.51
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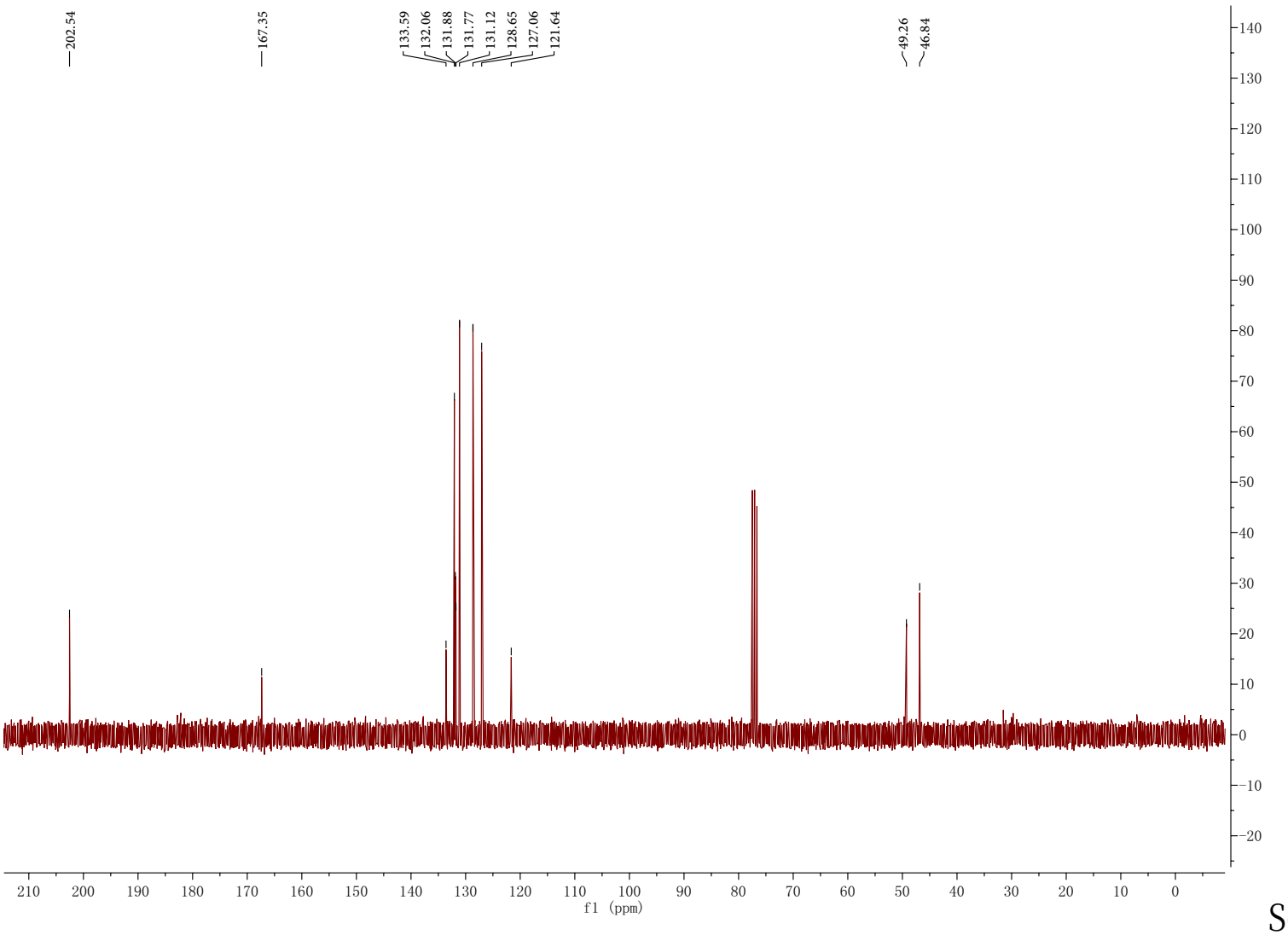
7.48
7.48
7.47
7.47
7.45
7.45
7.43
7.42
7.42
7.15
7.15
7.14
7.12
7.12
7.11
6.97
4.40
4.39
3.78
O
NH
O
Br

3d

1.98
5.03
2.03
1.00
1.97
2.00
f1 (ppm)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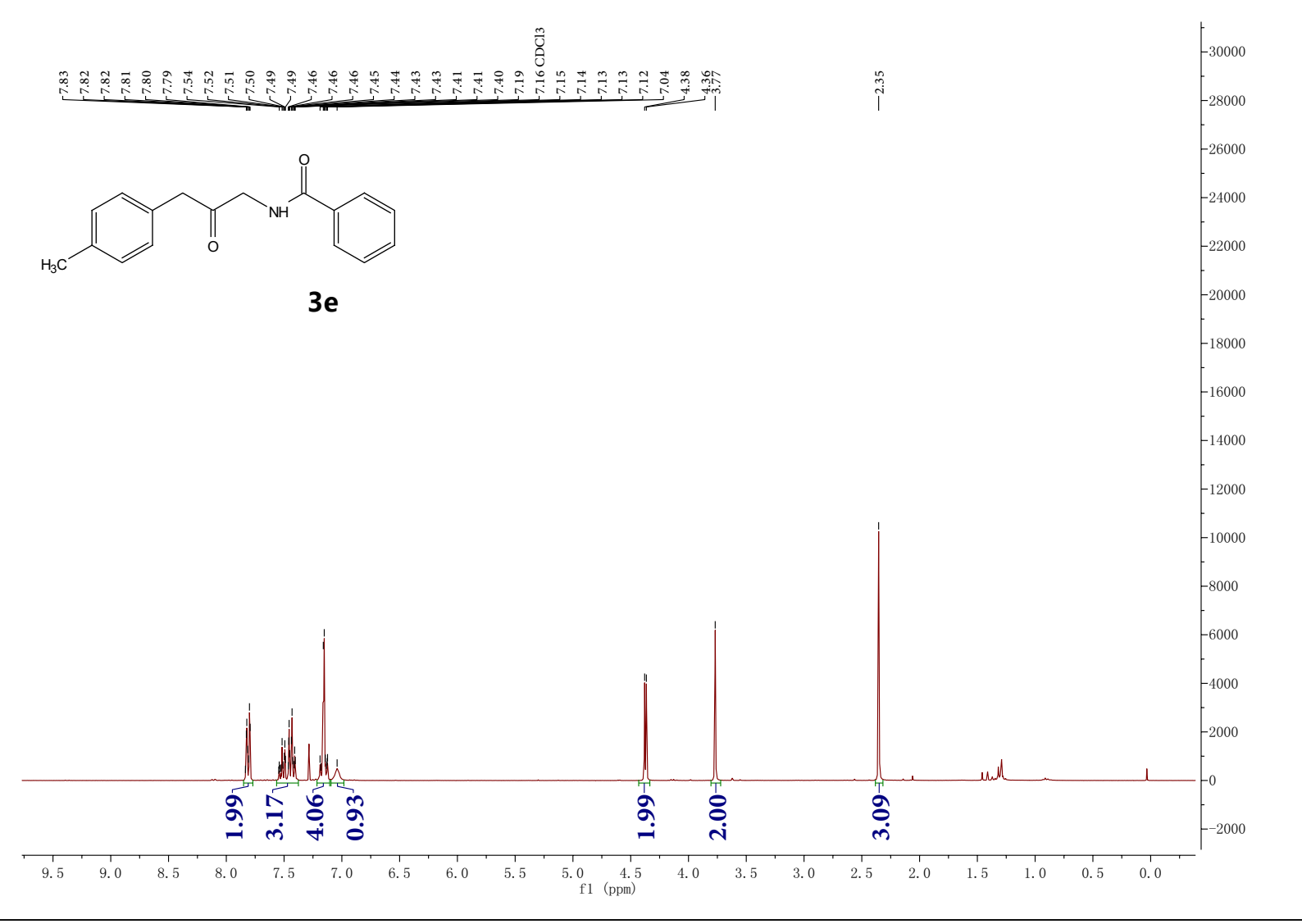
131.12
128.65
127.06
121.64
49.26
46.84
f1 (ppm)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7.82
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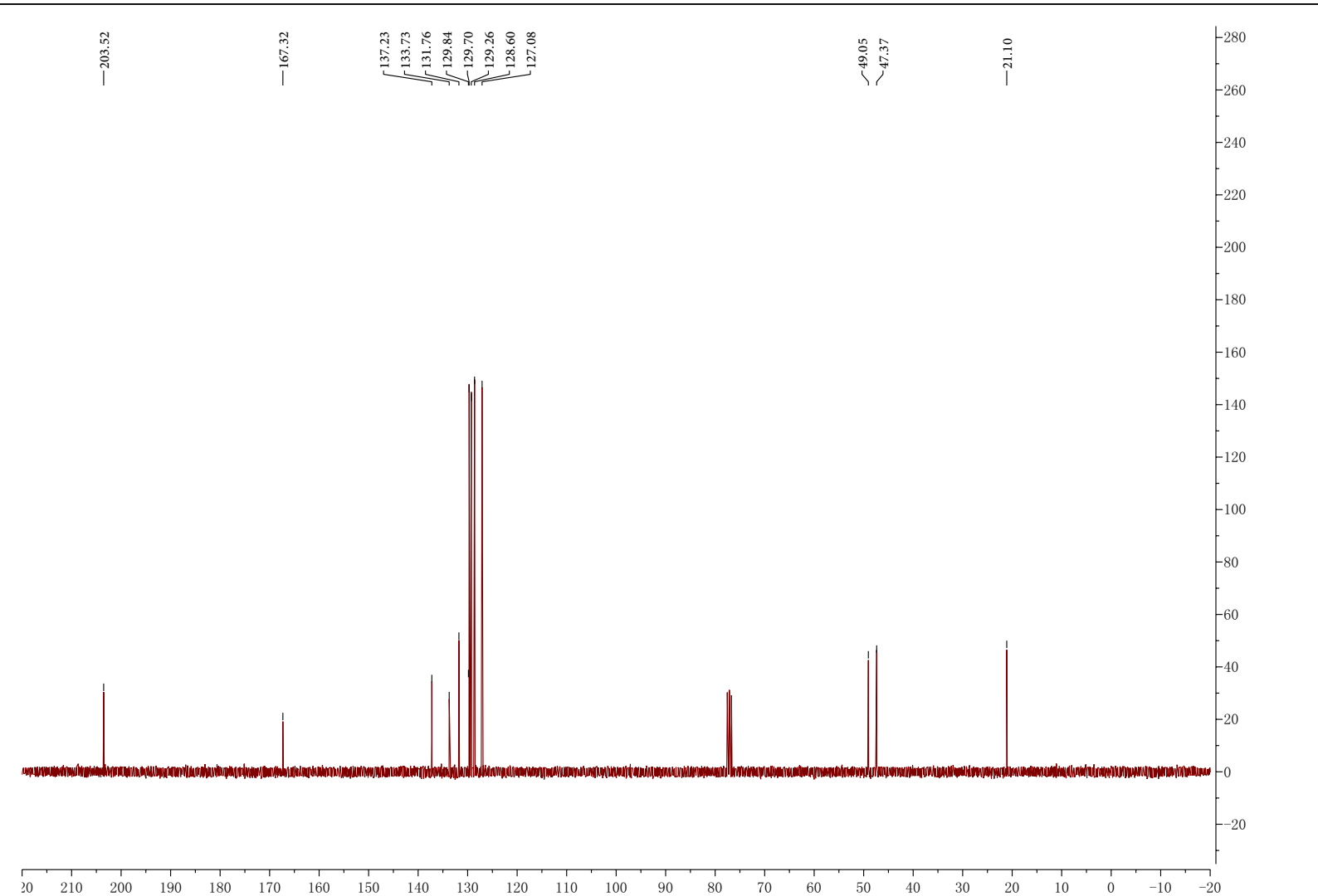
7.80
7.79
7.54
7.52
7.51
7.50
7.49
7.49
7.46
7.46
7.46
7.45
7.44
7.43
7.43
7.41
7.41
7.40
7.19
7.16 CDCl3
7.15
7.14
7.13
7.13
7.12
7.04
4.38
4.36
3.77
2.35
O
NH
O
H3C
3e
1.99
3.17
4.06
0.93
1.99
2.00
3.09
f1 (ppm)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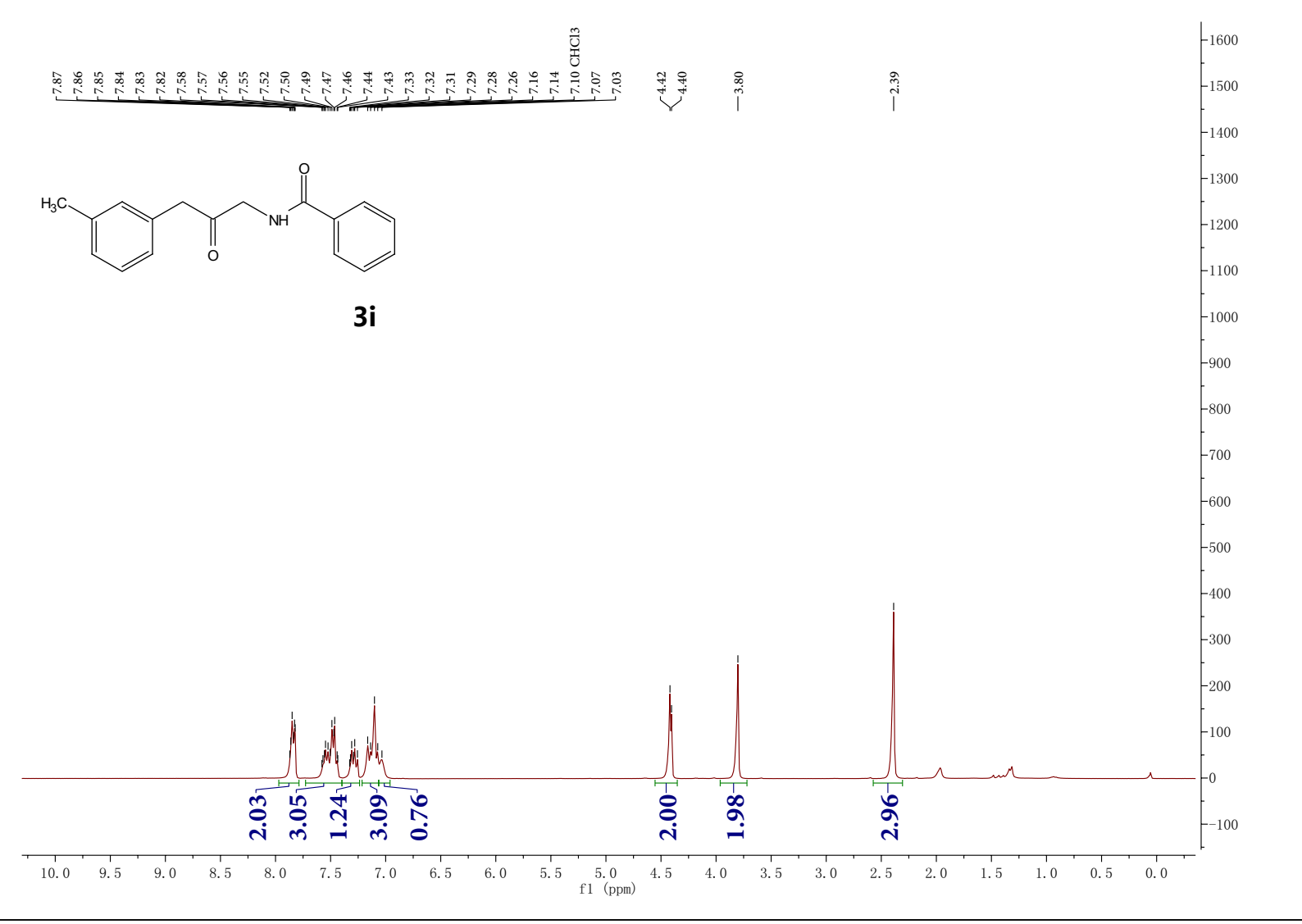
129.26
128.60
127.08
49.05
47.37
21.10
f1 (ppm)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7.56
7.55
7.52
7.50
7.49
7.47
7.46
7.44
7.43
7.33
7.32
7.31
7.29
7.28
7.26
7.16
7.14
7.10 CHCl3
7.07
7.03
4.42
4.40
3.80
2.39
H3C
NH
O
O
O
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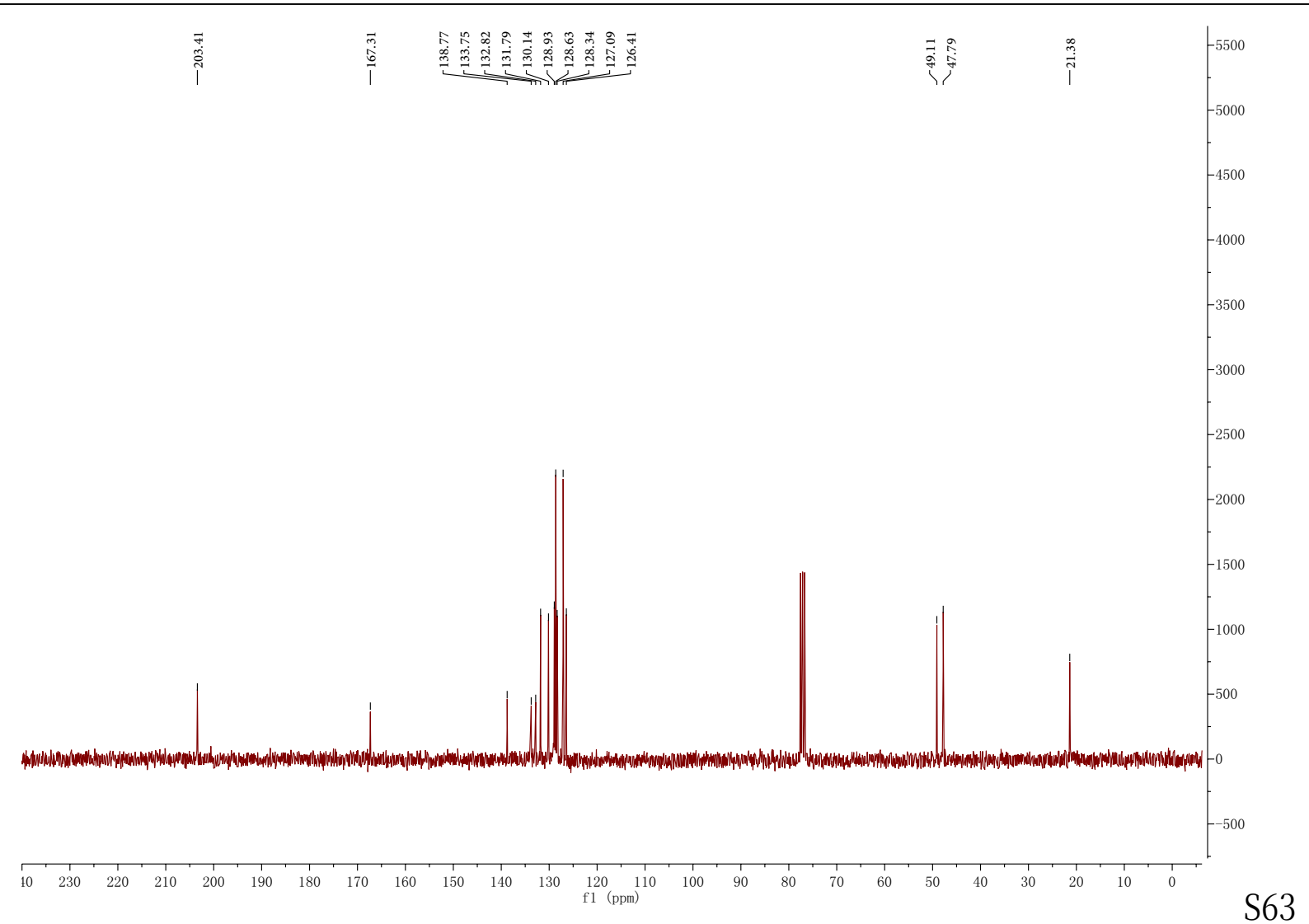
2.03
3.05
1.24
3.09
0.76
2.00
1.98
2.96
f1 (ppm)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132.82
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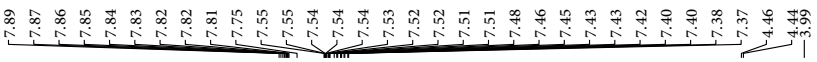
130.14
128.93
128.63
128.34
127.09
126.41
49.11
47.79
21.38
f1 (ppm)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7.86
7.85
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7.82
7.81
7.75
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7.55
7.54
7.54
7.54
7.53
7.52
7.52
7.51
7.51
7.48
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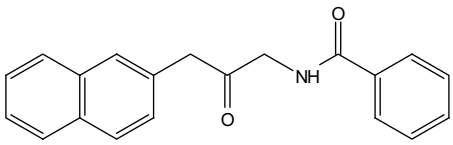
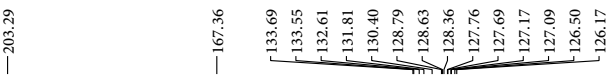
7.40
7.38
7.37
4.46
4.44
3.99


O
NH
O

3j

4.96
1.00
2.93
3.20
0.94
2.00
2.00
f1 (ppm)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130.40
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128.63
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127.76
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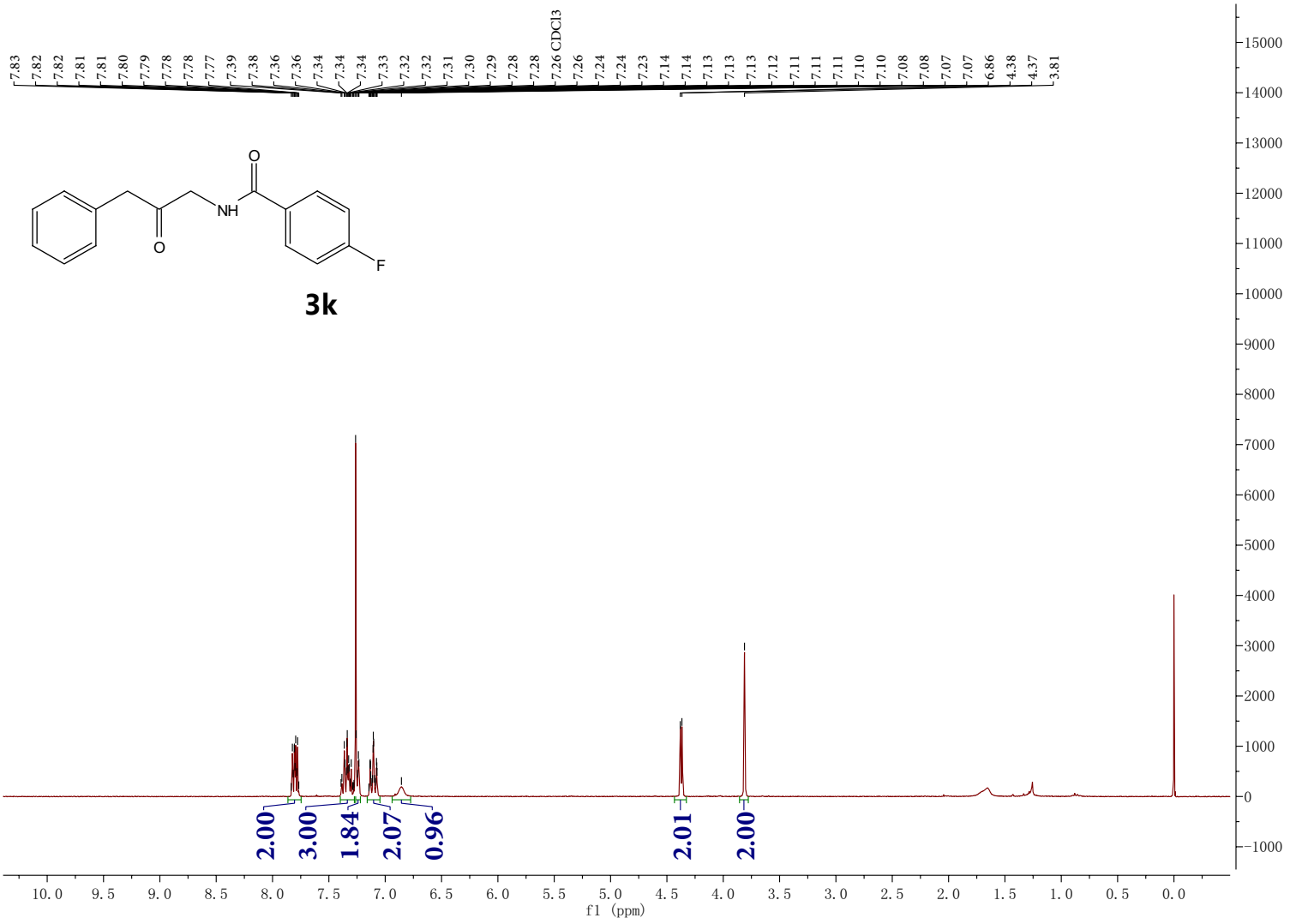
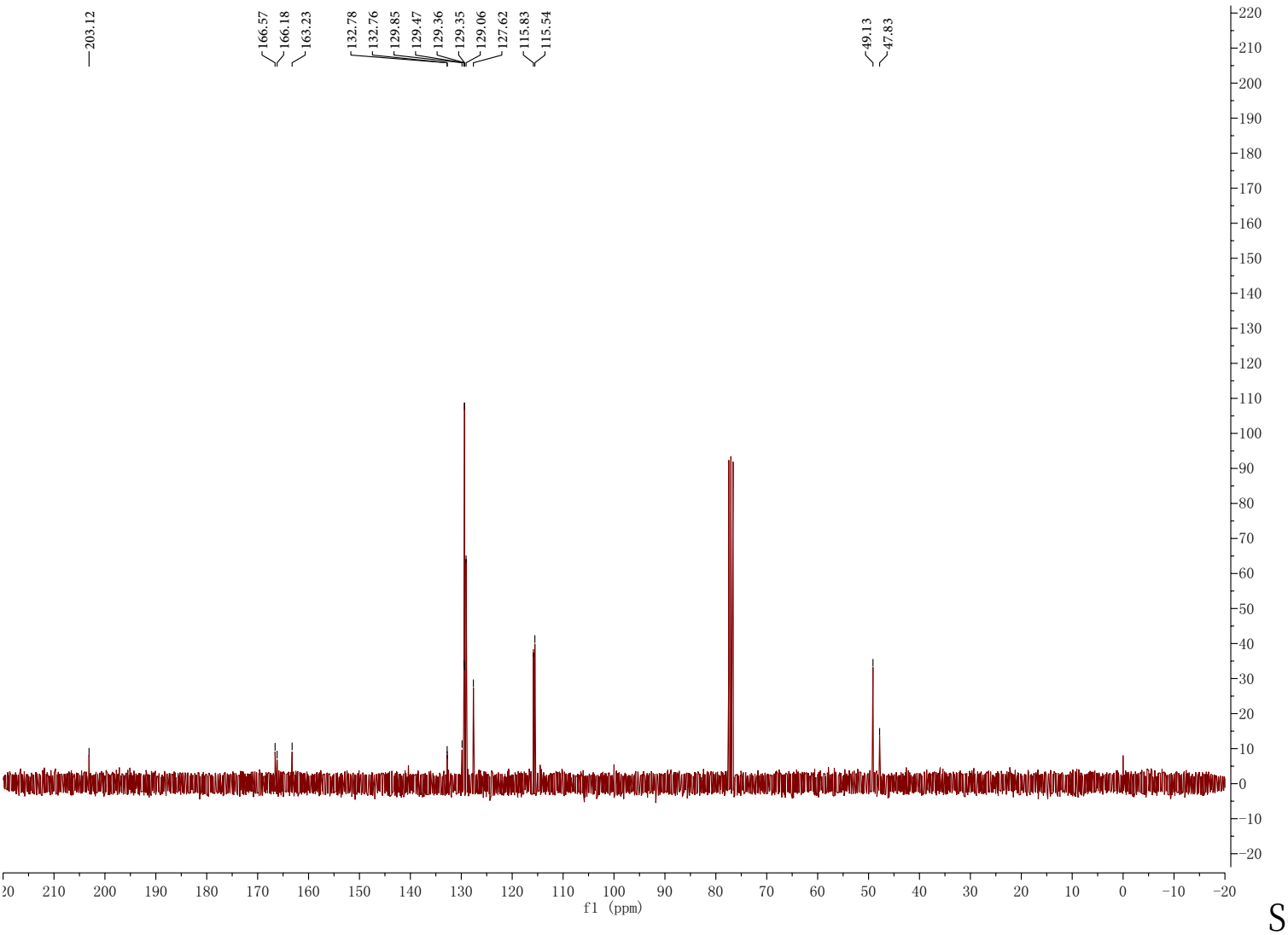
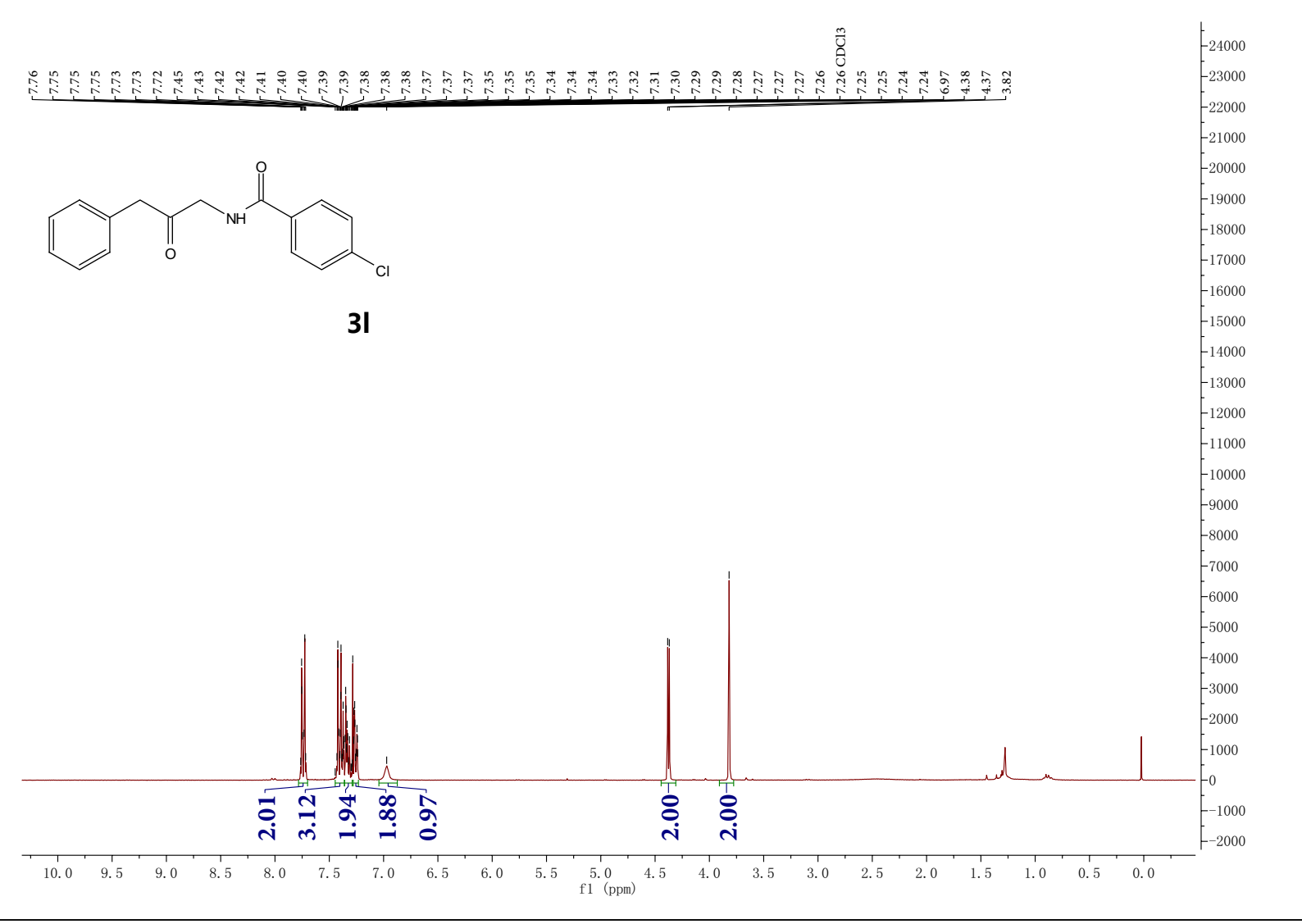
127.09
126.50
126.17
49.24
47.88

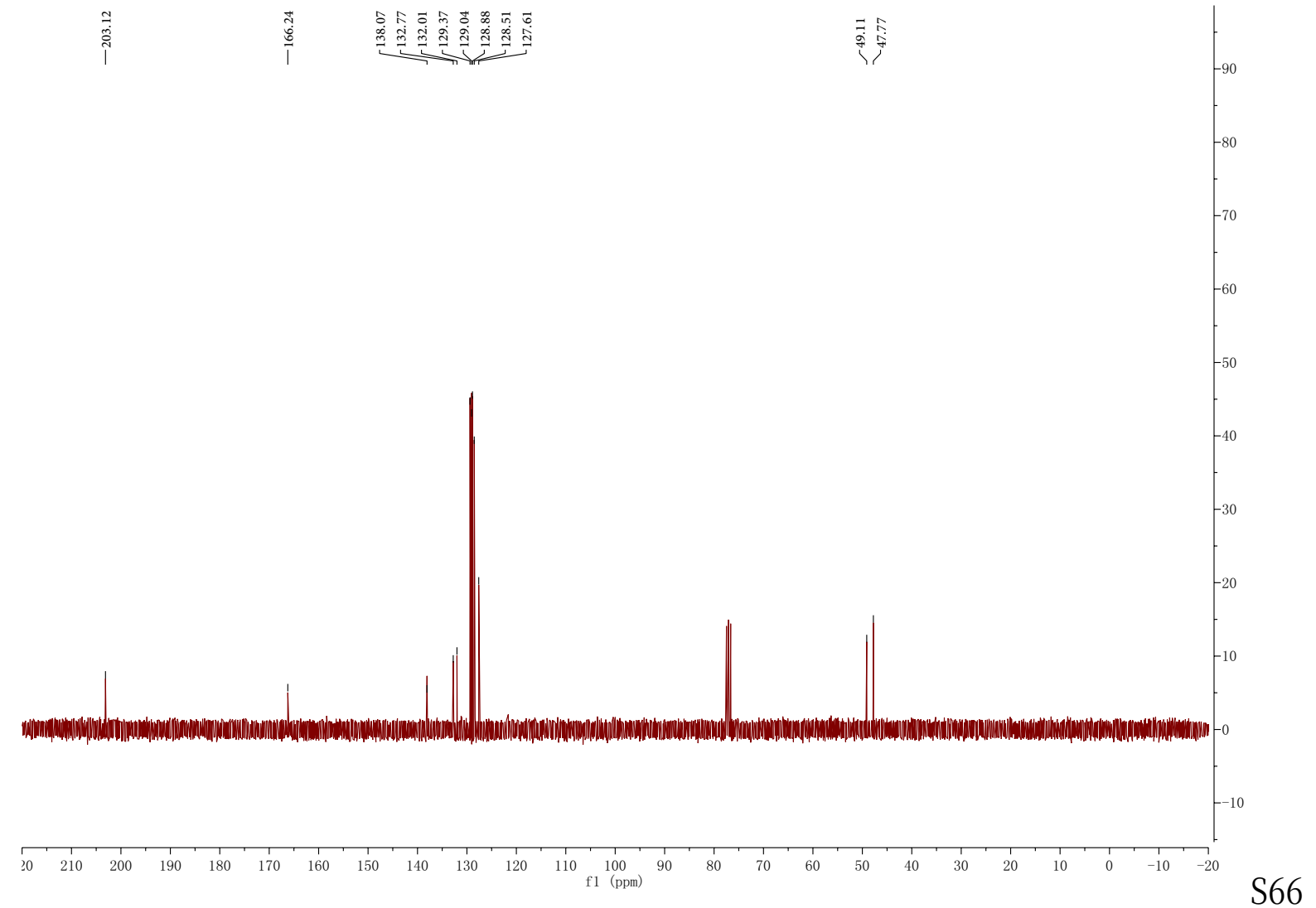
f1 (ppm)


7.83 7.82 7.82 7.81 7.81 7.80 7.79 7.78 7.78 7.77 7.39 7.38 7.36 7.36 7.34 7.34 7.34 7.33 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.26 CDCl3 7.26 7.24 7.24 7.23 7.14 7.14 7.13 7.13 7.13 7.12 7.11 7.11 7.11 7.10 7.10 7.08 7.08 7.07 7.07 6.86 4.38 4.37 3.81
O
NH
O
F
3k
2.00
3.00
1.84
2.07
0.96
2.01
2.00
f1 (ppm)


203.12
166.57 166.18 163.23
132.78 132.76 129.85 129.47 129.36 129.35 129.06 127.62
115.83 115.54
49.13 47.83
f1 (ppm)


7.76 7.75 7.75 7.75 7.73 7.73 7.72 7.45 7.43 7.42 7.42 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.35 7.35 7.34 7.34 7.34 7.33 7.32 7.31 7.30 7.29 7.29 7.28 7.27 7.27 7.27 7.26 7.26 CDCl3 7.25 7.25 7.24 7.24 6.97 4.38 4.37 3.82
O
NH
O
Cl
2.01
3.12
1.94
1.88
0.97
2.00
2.00
f1 (ppm)

3l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129.04
128.88
128.51
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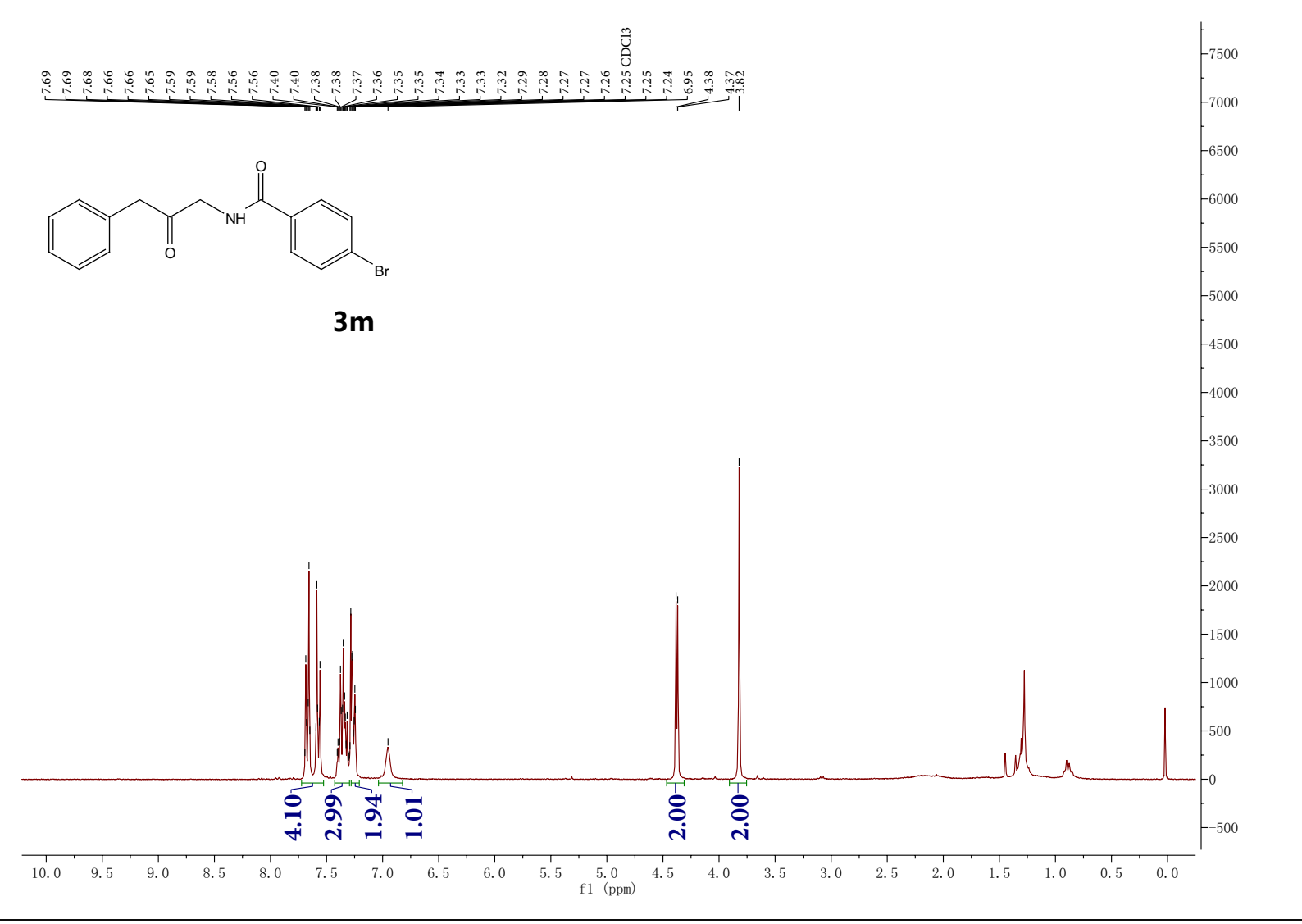
47.77
f1 (ppm)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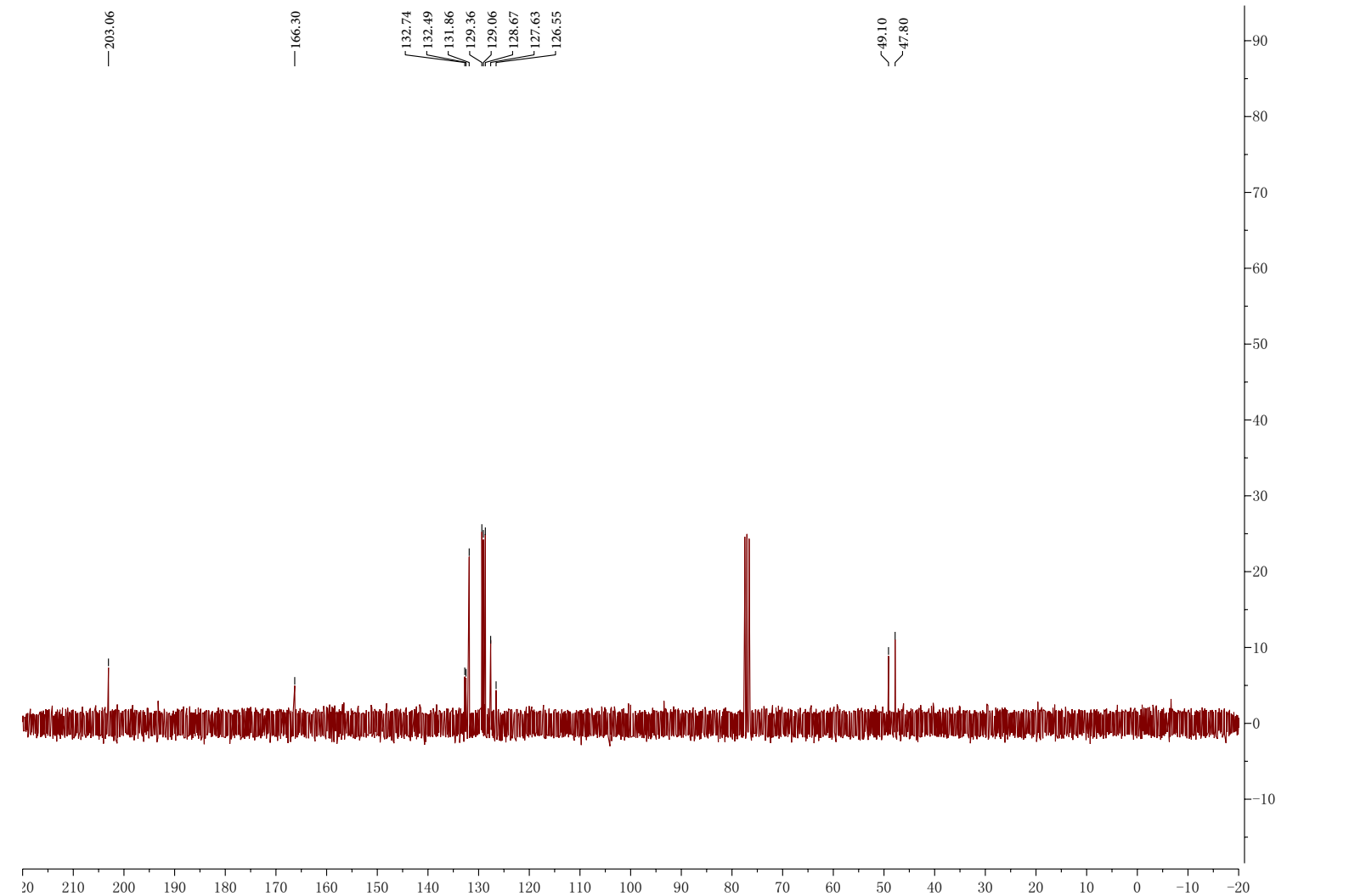
O
NH
O
Br
3m
4.10
2.99
1.94
1.01
2.00
2.00
f1 (ppm)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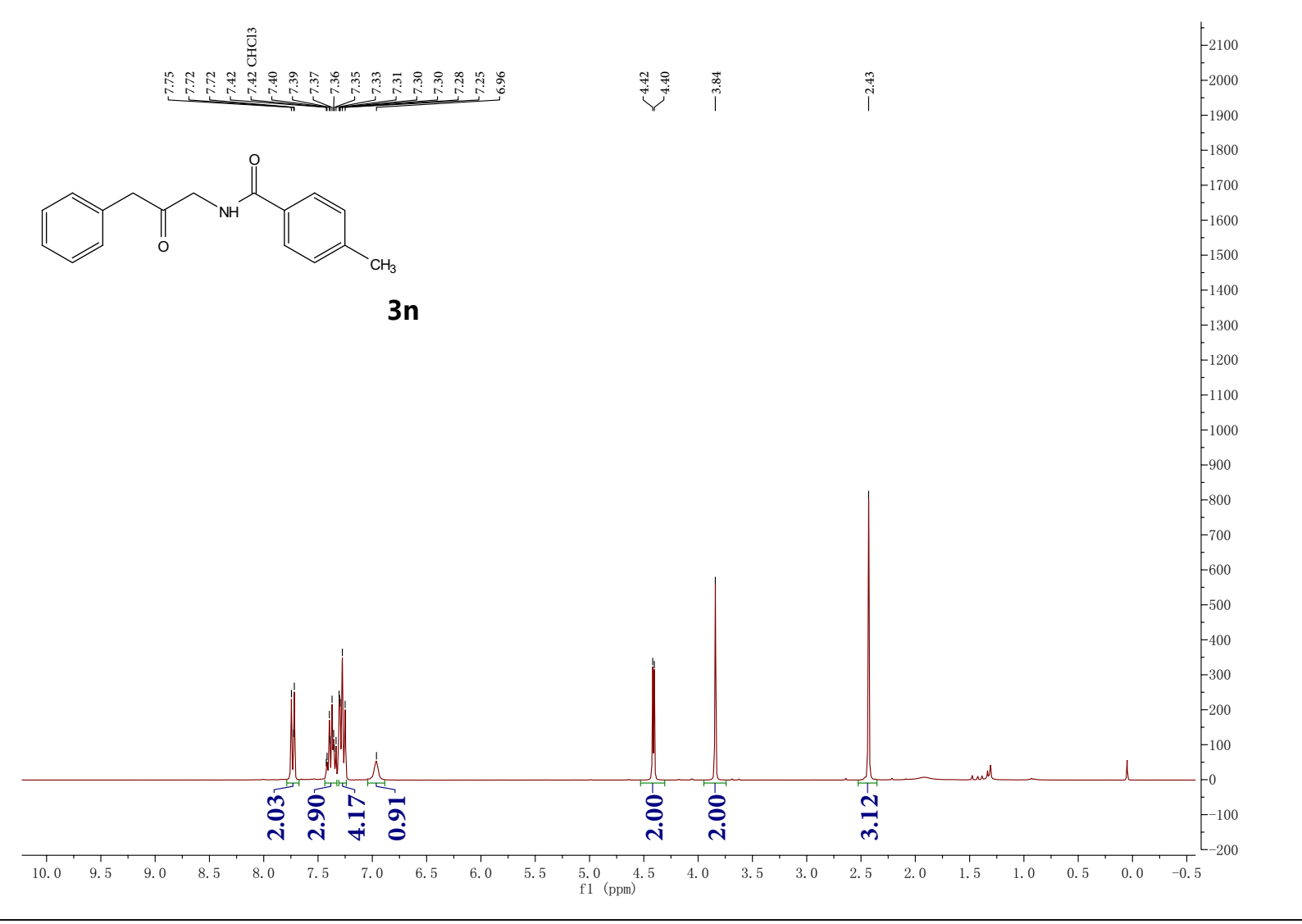
49.10 47.80
f1 (ppm)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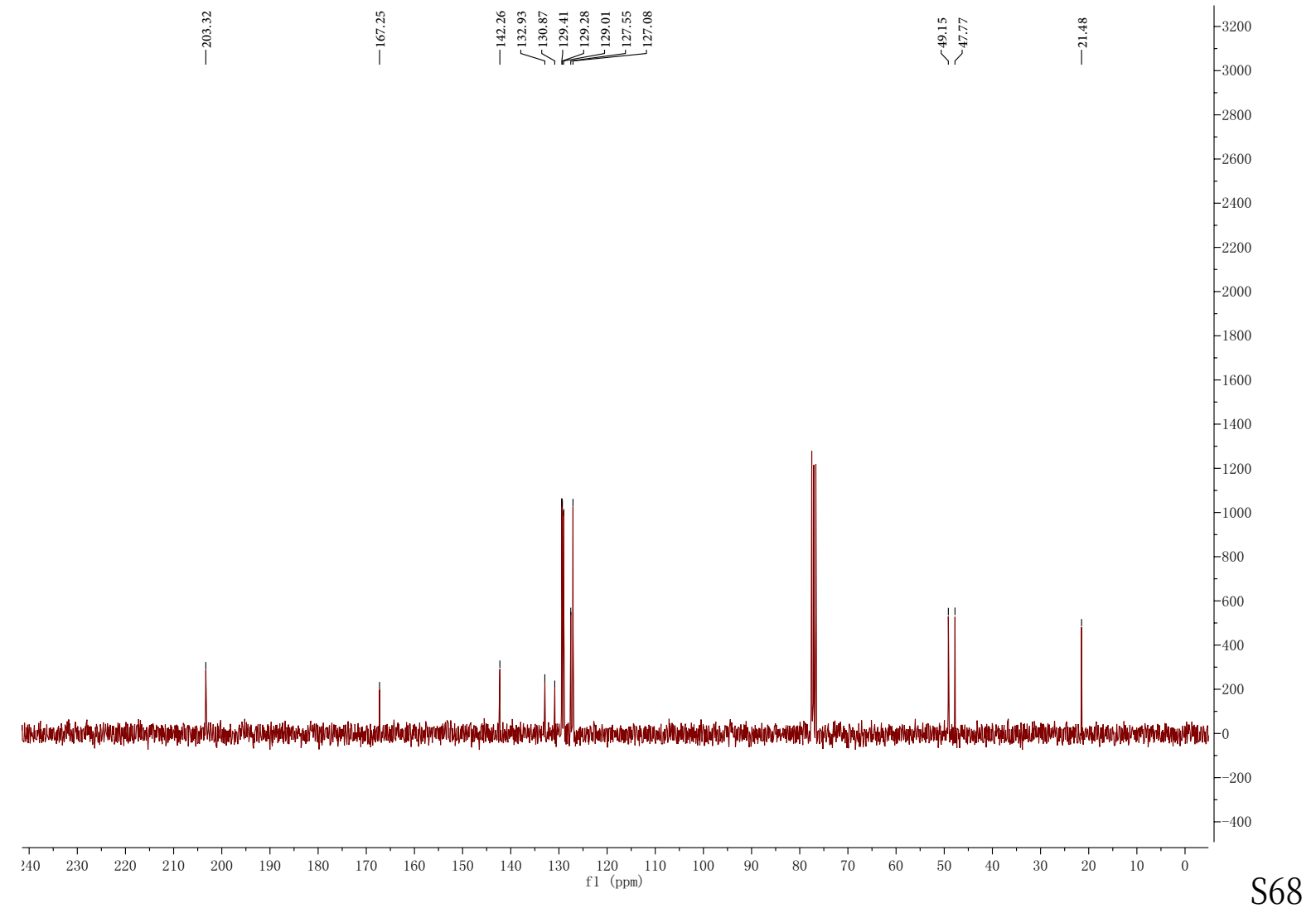
7.35
7.33
7.31
7.30
7.30
7.28
7.25
6.96
4.42
4.40
3.84
2.43
O
NH
O
CH3
2.03
2.90
4.17
0.91
2.00
2.00
3.12
f1 (ppm)

3n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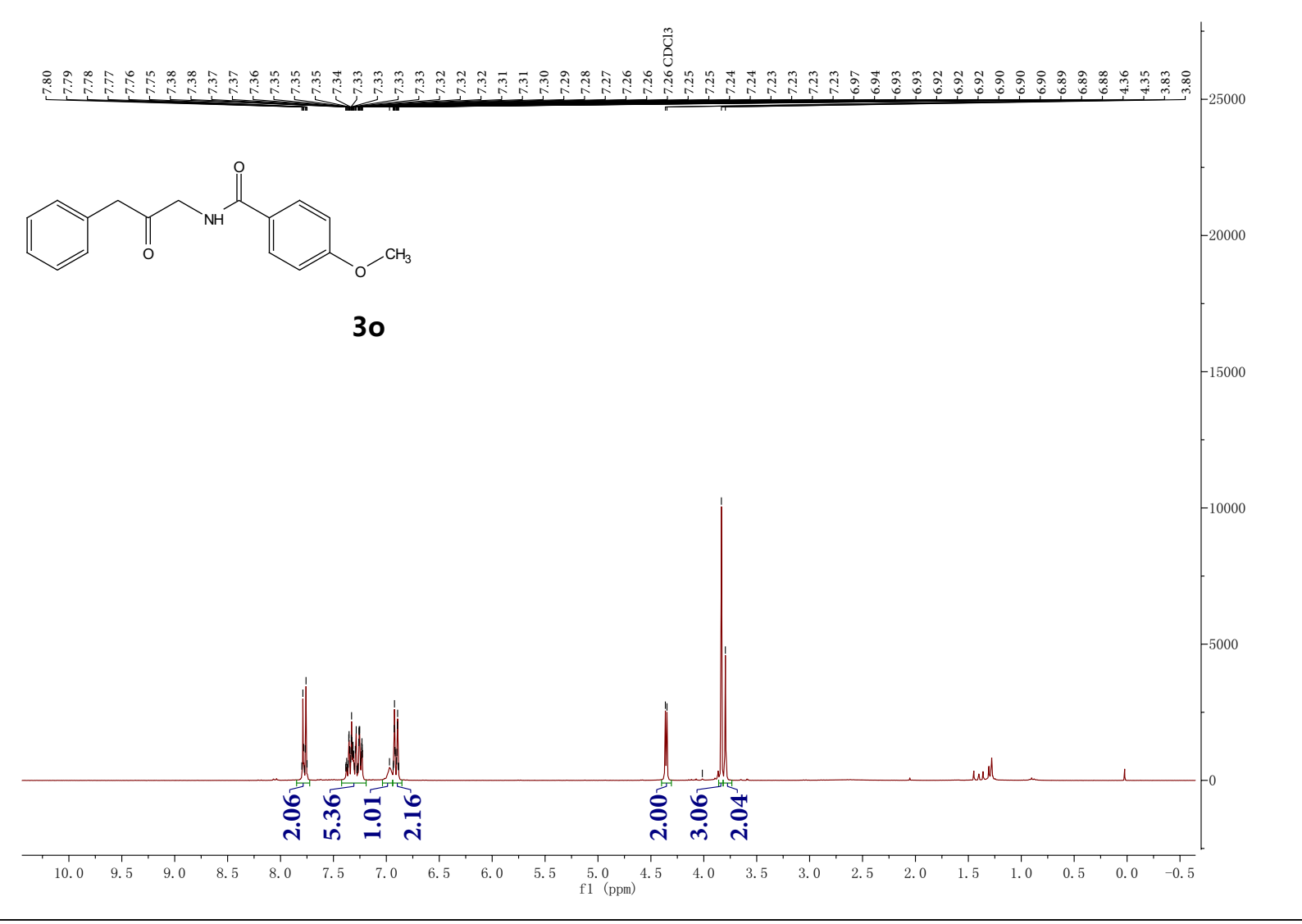
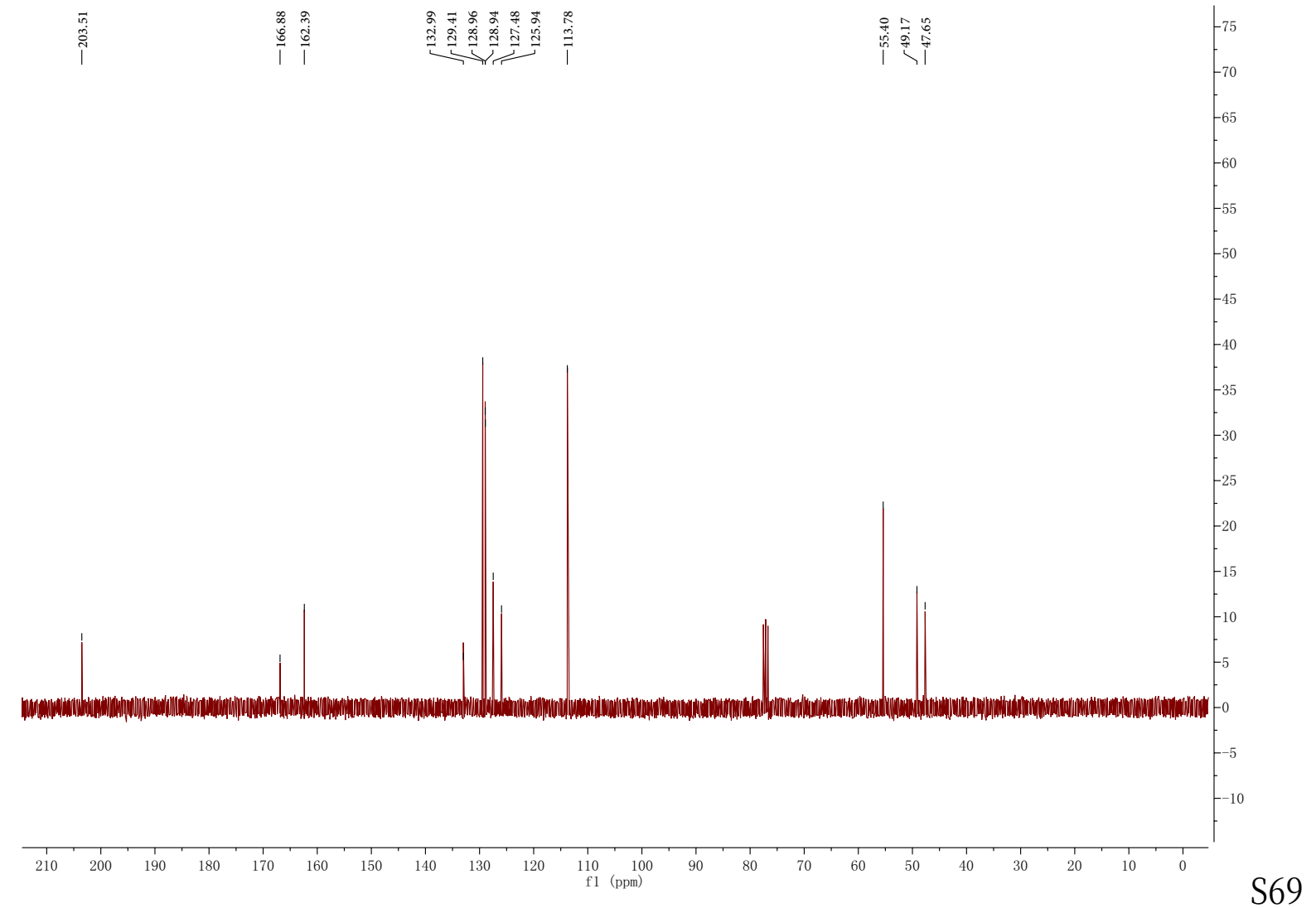
142.26
132.93
130.87
129.41
129.28
129.01
127.55
127.08
49.15
47.77
21.48
f1 (ppm)


7.80 7.79 7.78 7.77 7.76 7.75 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.35 7.34 7.33 7.33 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.29 7.28 7.27 7.26 7.26 CDCl3 7.25 7.25 7.24 7.24 7.23 7.23 7.23 7.23 6.97 6.94 6.93 6.93 6.92 6.92 6.92 6.90 6.90 6.90 6.89 6.89 6.88 4.36 4.35 3.83 3.80
O
NH
O
O
CH3
3o
2.06
5.36
1.01
2.16
2.00
3.06
2.04
f1 (ppm)


203.51
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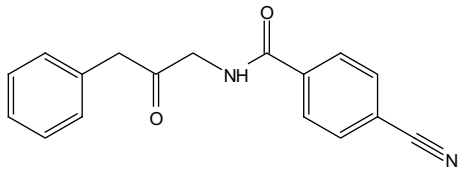
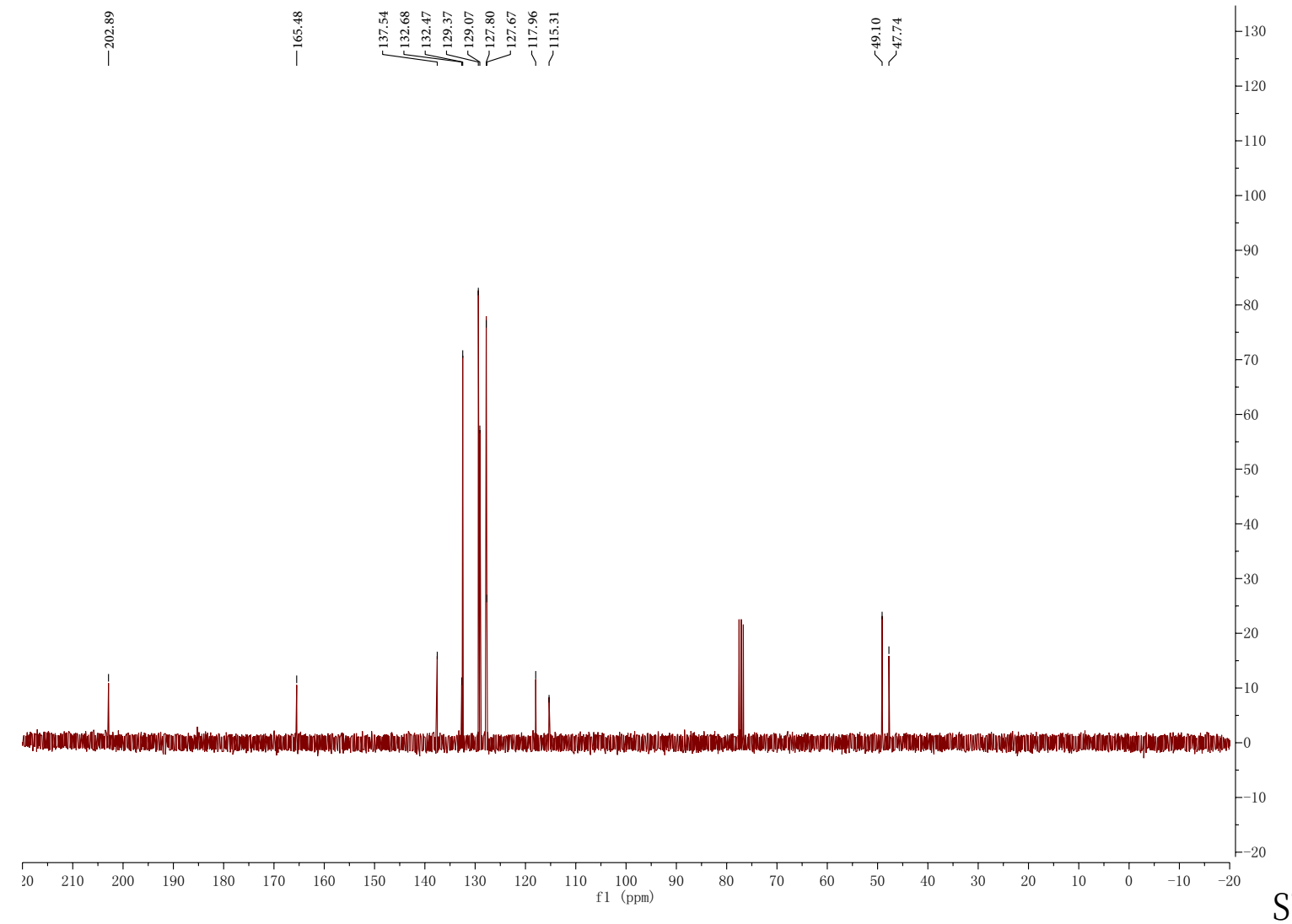
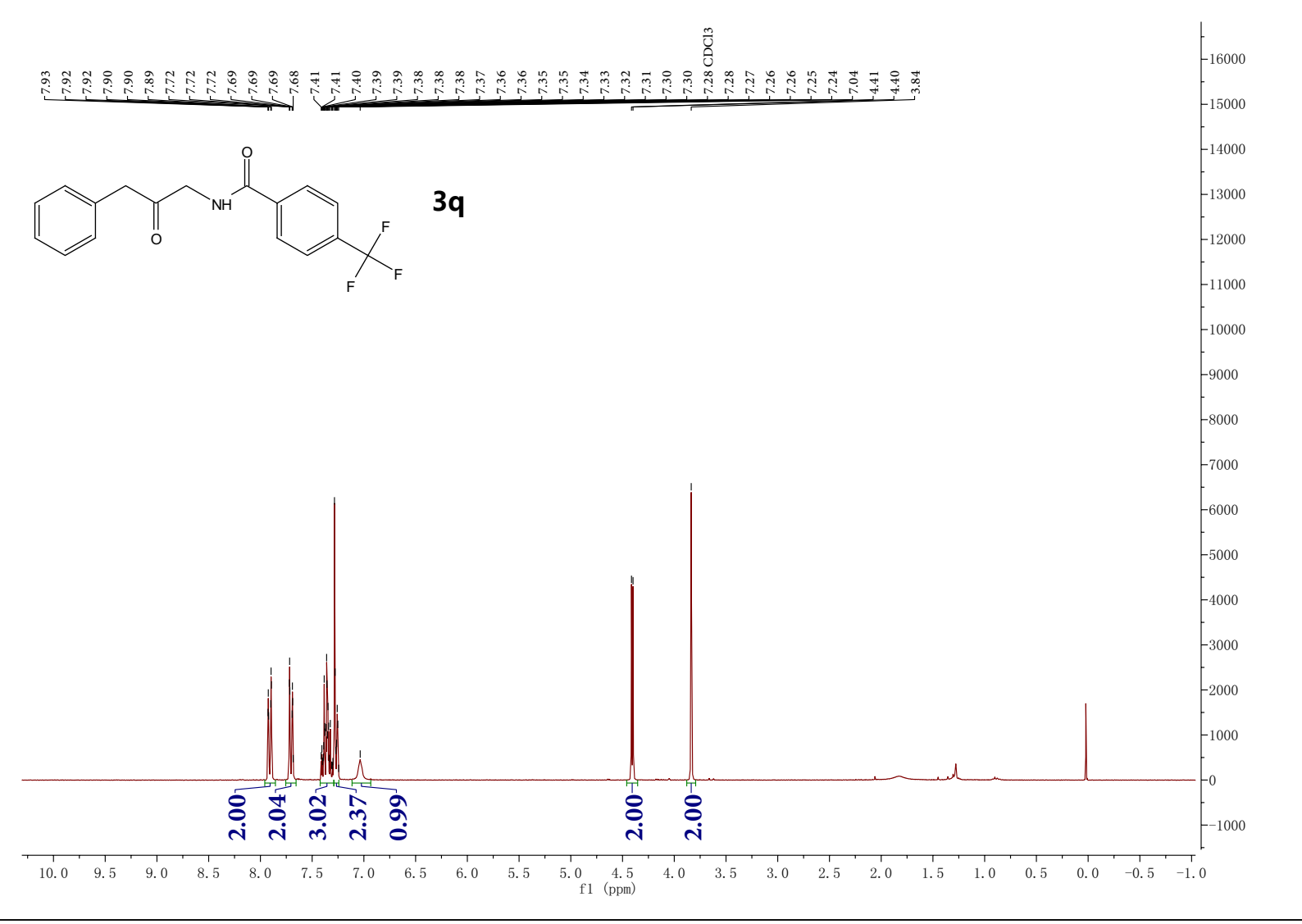
132.99
129.41
128.96
128.94
127.48
125.94
113.78
55.40
49.17
47.65
f1 (ppm)

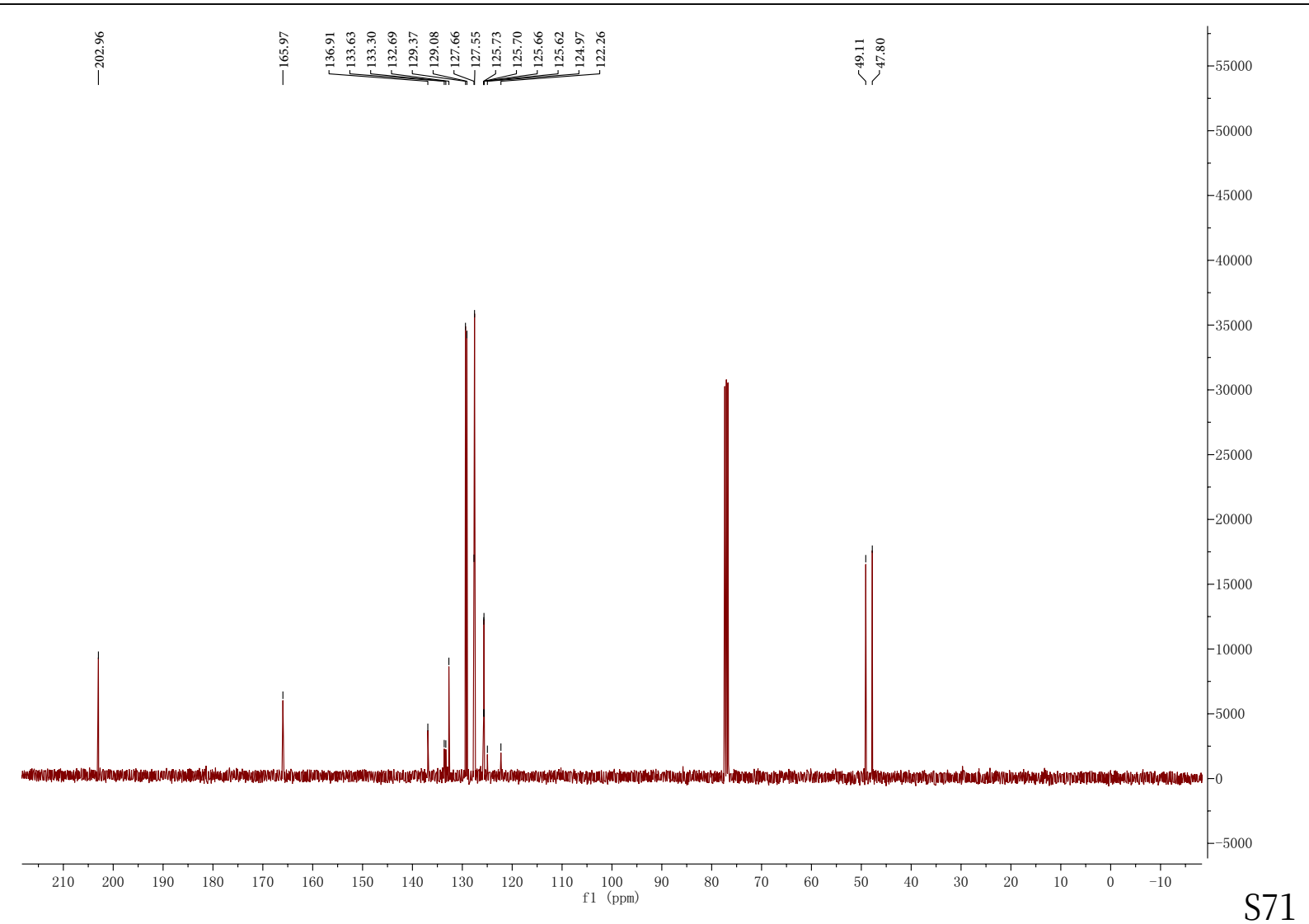

O
NH
O
N

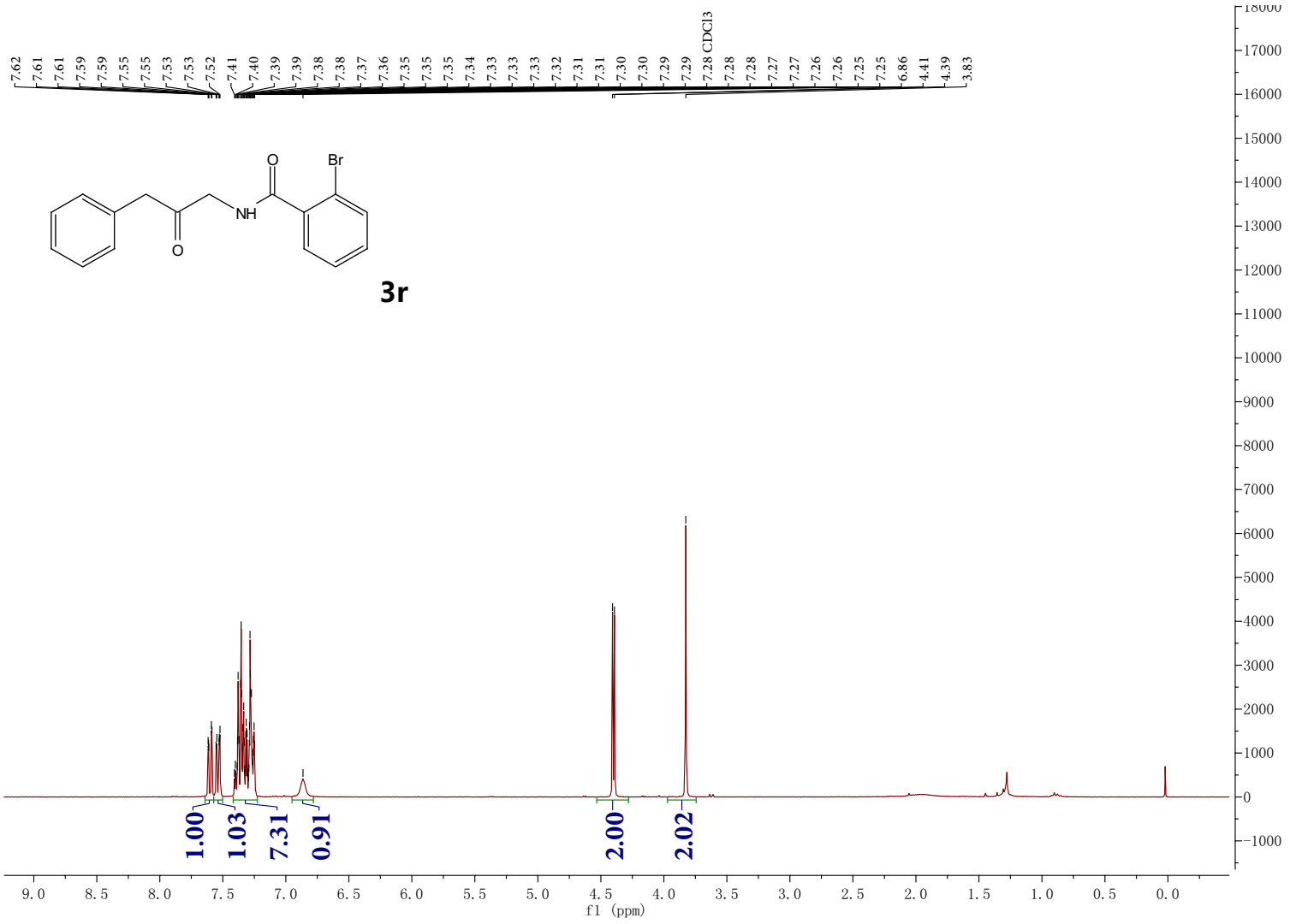
3p

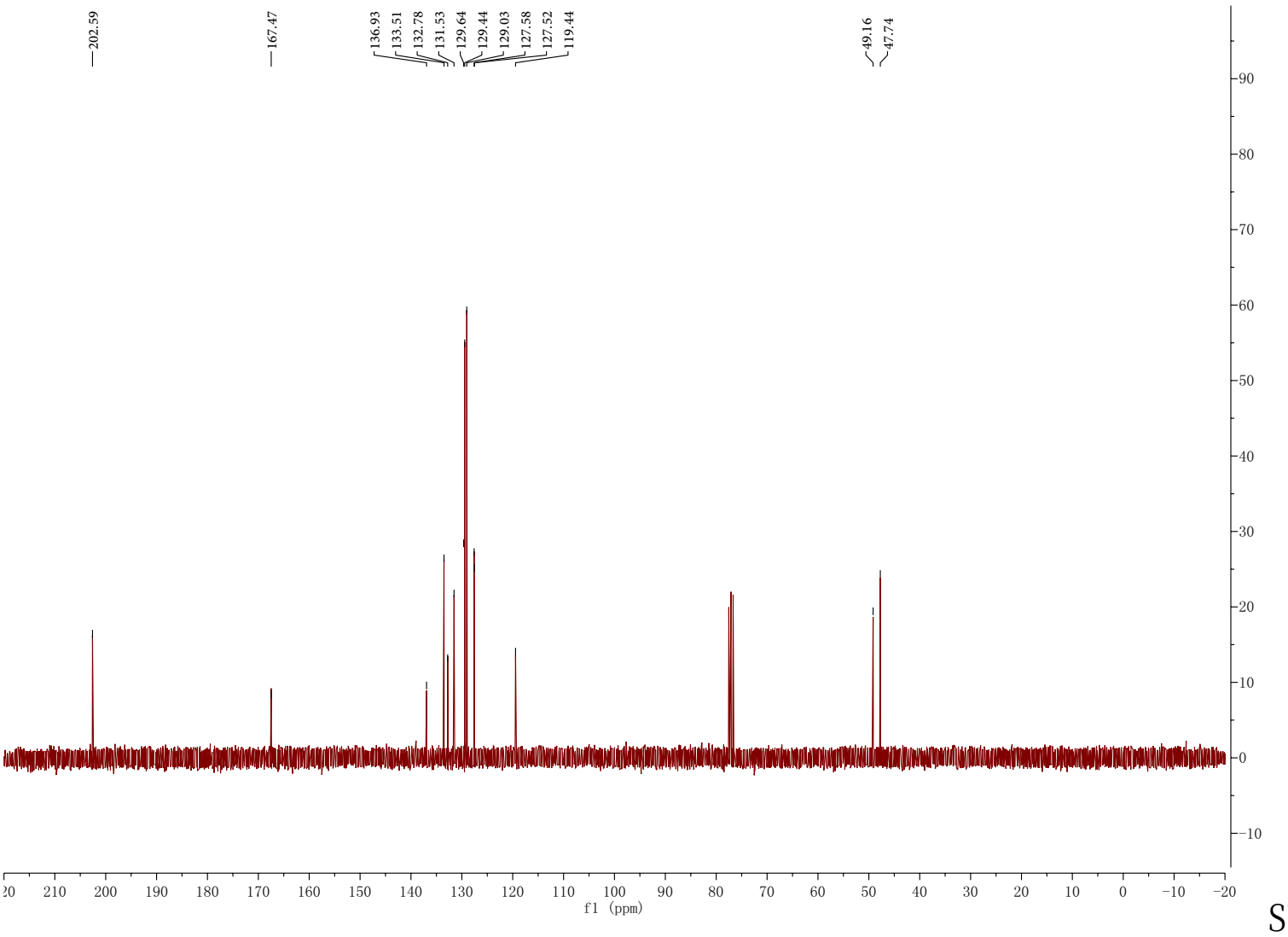
2.01
2.05
2.92
1.95
0.99
1.99
2.00
f1 (ppm)

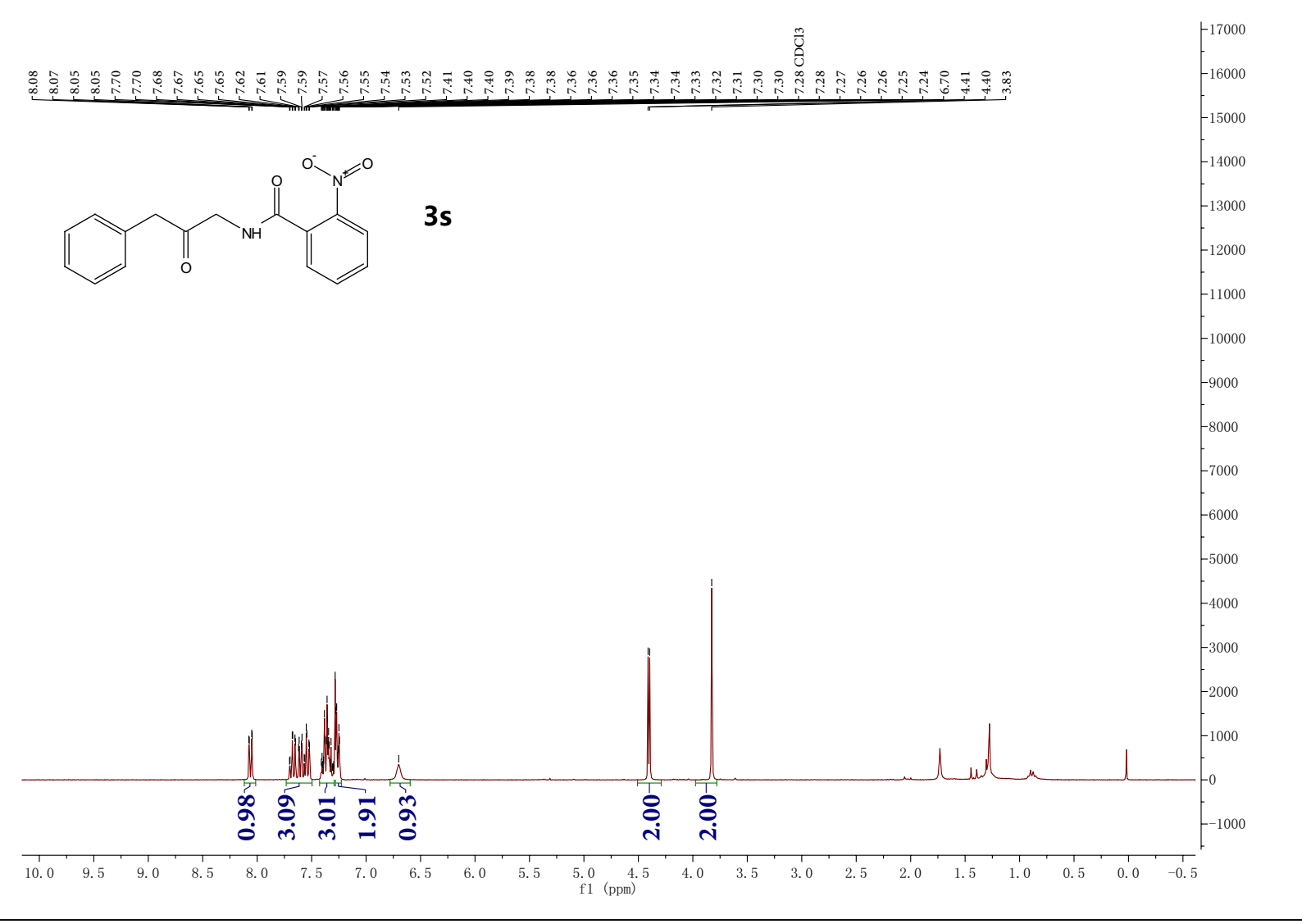

202.89
165.48
137.54
132.68
132.47
129.37
129.07
127.80
127.67
117.96
115.31
49.10
47.74
f1 (ppm)

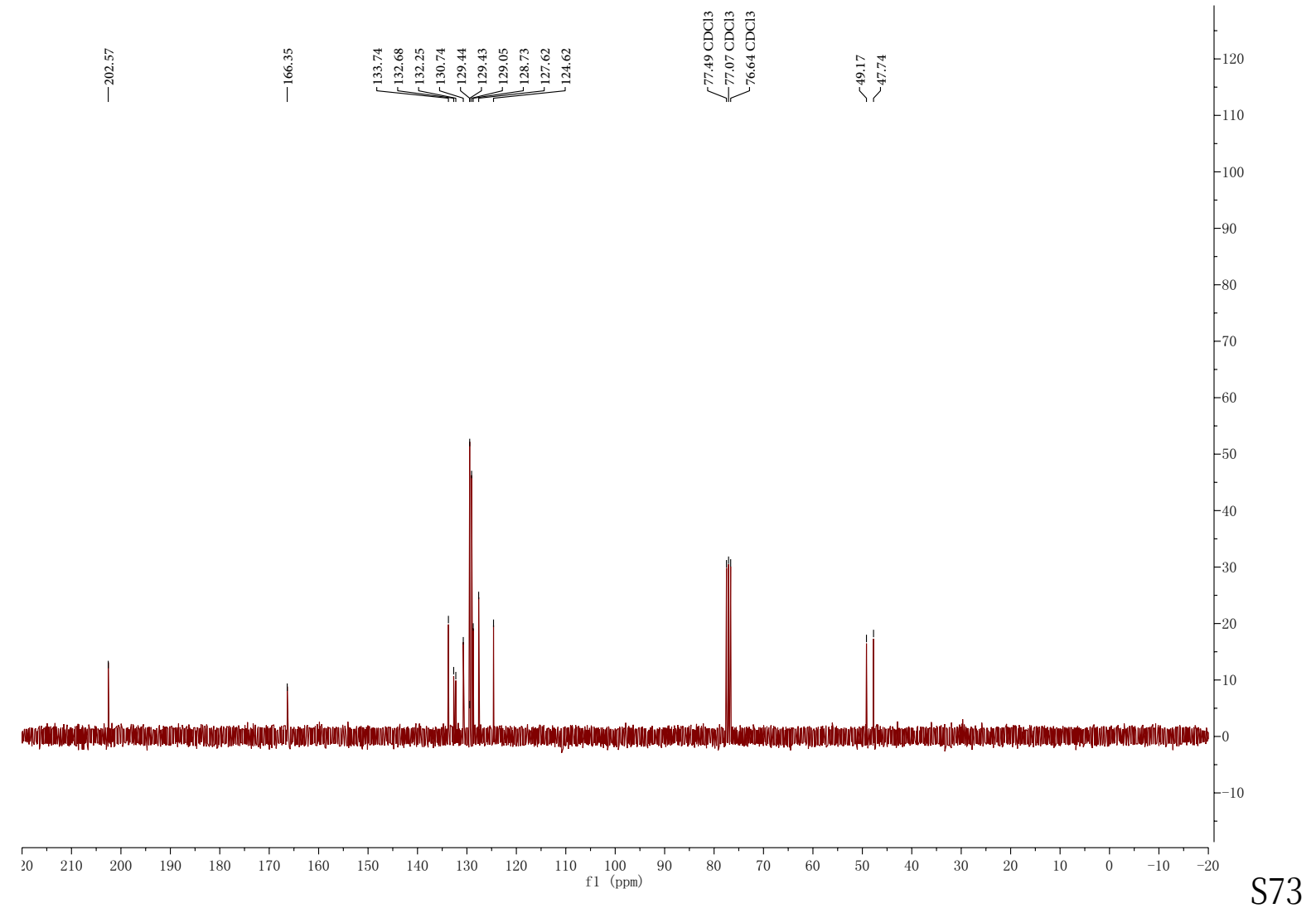

7.93 7.92 7.92 7.90 7.90 7.89 7.72 7.72 7.72 7.69 7.69 7.69 7.68 7.41 7.41 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.32 7.31 7.30 7.30 7.28 CDCl3 7.28 7.27 7.26 7.26 7.25 7.24 7.04 4.41 4.40 3.84
O
NH
O
F
F
F
3q
2.00 2.04 3.02 2.37 0.99 2.00 2.00
f1 (ppm)

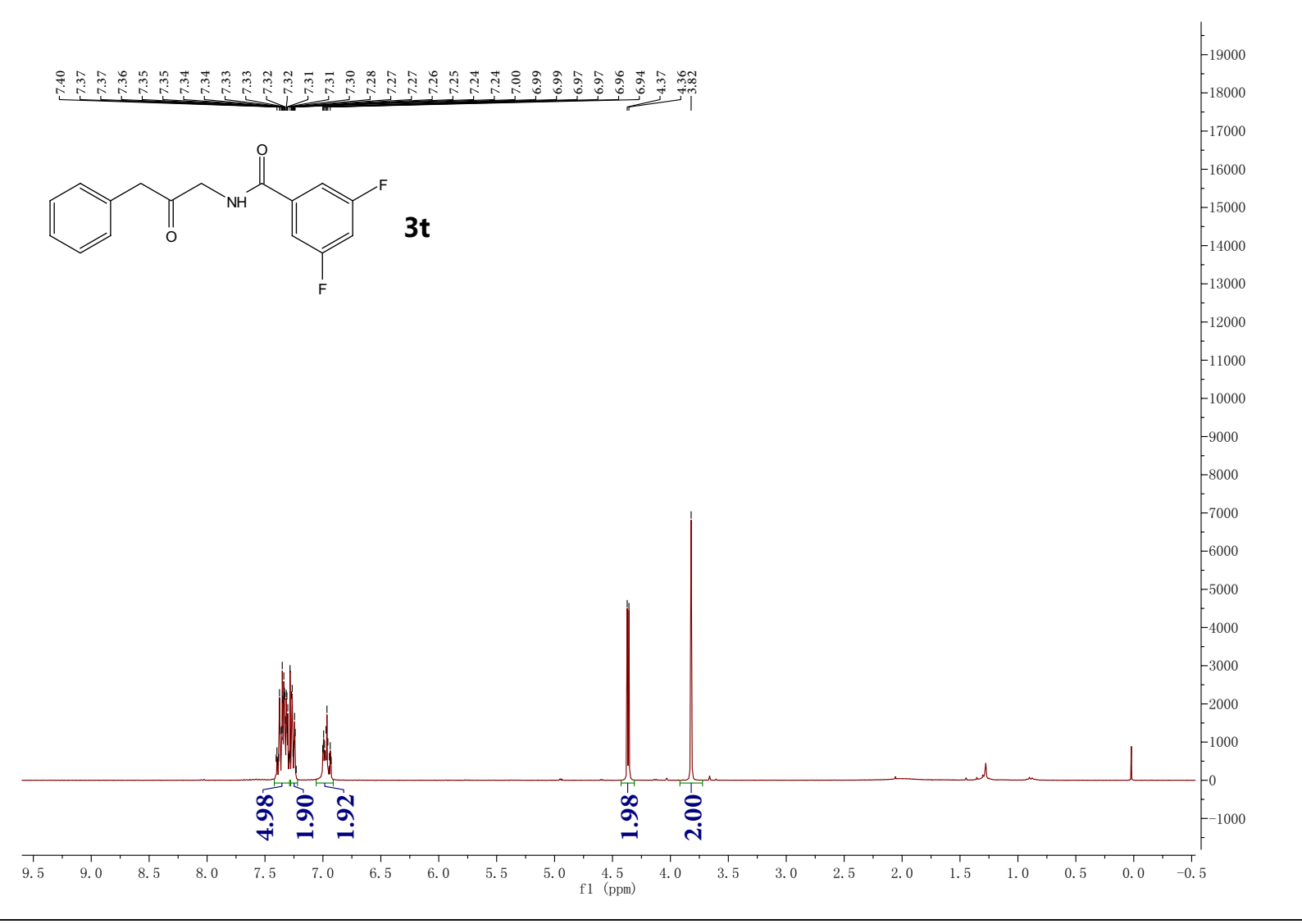

202.96 165.97 136.91 133.63 133.30 132.69 129.37 129.08 127.66 127.55 125.73 125.70 125.66 125.62 124.97 122.26 49.11 47.80
f1 (ppm)

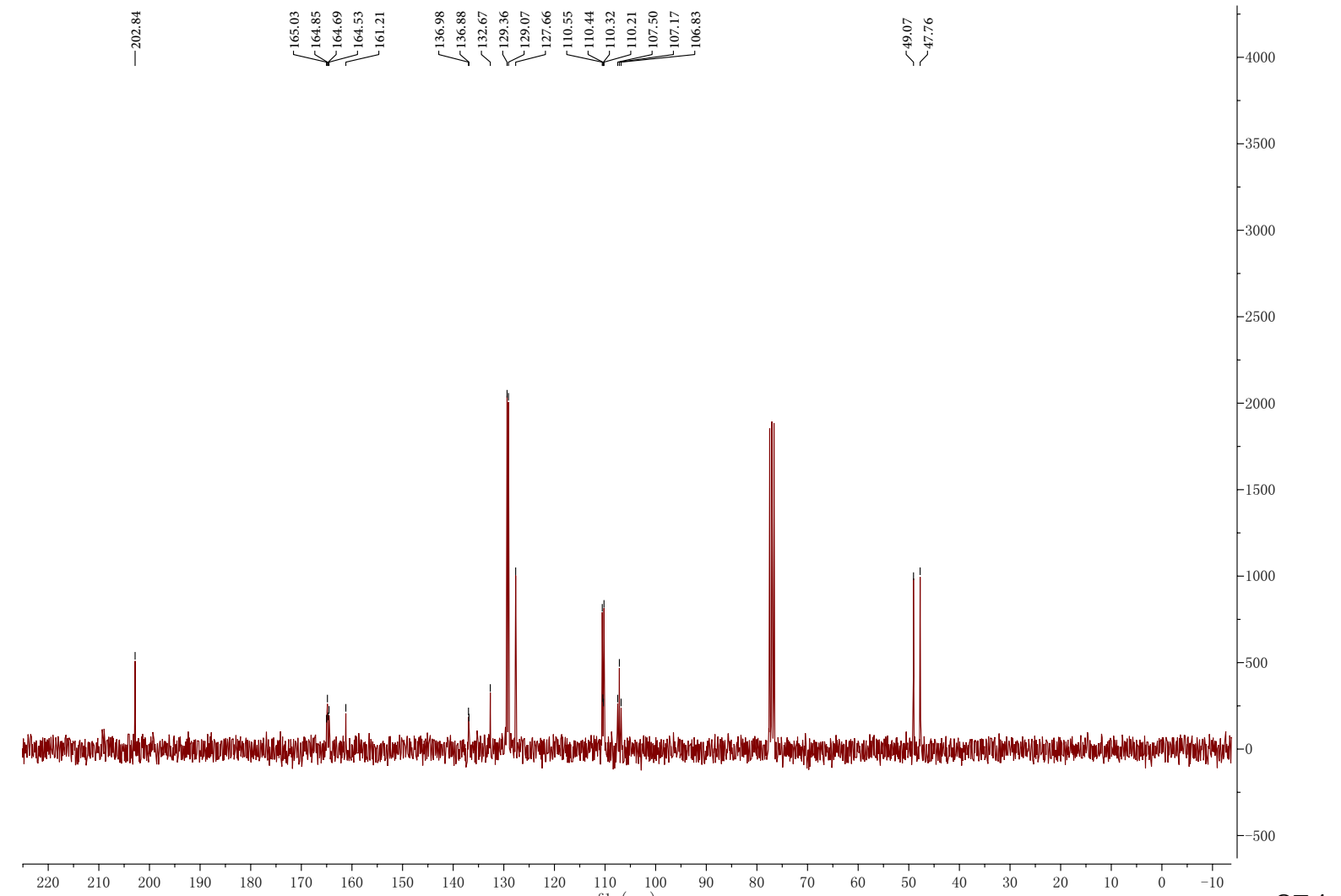

7.62 7.61 7.61 7.59 7.59 7.55 7.55 7.53 7.53 7.52 7.41 7.40 7.39 7.39 7.38 7.38 7.37 7.36 7.35 7.35 7.35 7.34 7.33 7.33 7.33 7.32 7.31 7.31 7.30 7.30 7.29 7.29 7.28 CDCl3 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.25 6.86 4.41 4.39 3.83
O
Br
NH
O
3r
1.00
1.03
7.31
0.91
2.00
2.02
f1 (ppm)


202.59
167.47
136.93
133.51
132.78
131.53
129.64
129.44
129.03
127.58
127.52
119.44
49.16
47.74
f1 (ppm)


8.08 8.07 8.05 8.05 7.70 7.70 7.68 7.67 7.65 7.65 7.62 7.61 7.59 7.59 7.57 7.56 7.55 7.54 7.53 7.52 7.41 7.40 7.40 7.39 7.38 7.38 7.36 7.36 7.36 7.35 7.34 7.34 7.33 7.32 7.31 7.30 7.30 7.28 CDCl3 7.28 7.27 7.26 7.26 7.25 7.24 6.70 4.41 4.40 3.83
O
N
O
NH
O
3s
0.98
3.09
3.01
1.91
0.93
2.00
2.00
f1 (ppm)


202.57
166.35
133.74
132.68
132.25
130.74
129.44
129.43
129.05
128.73
127.62
124.62
77.49 CDCl3
77.07 CDCl3
76.64 CDCl3
49.17
47.74
f1 (ppm)


7.40
7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.28
7.27
7.27
7.26
7.25
7.24
7.24
7.00
6.99
6.99
6.97
6.97
6.96
6.94
4.37
4.36
3.82
O
NH
O
F
F
3t
4.98
1.90
1.92
1.98
2.00
f1 (ppm)


202.84
165.03
164.85
164.69
164.53
161.21
136.98
136.88
132.67
129.36
129.07
127.66
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110.44
110.32
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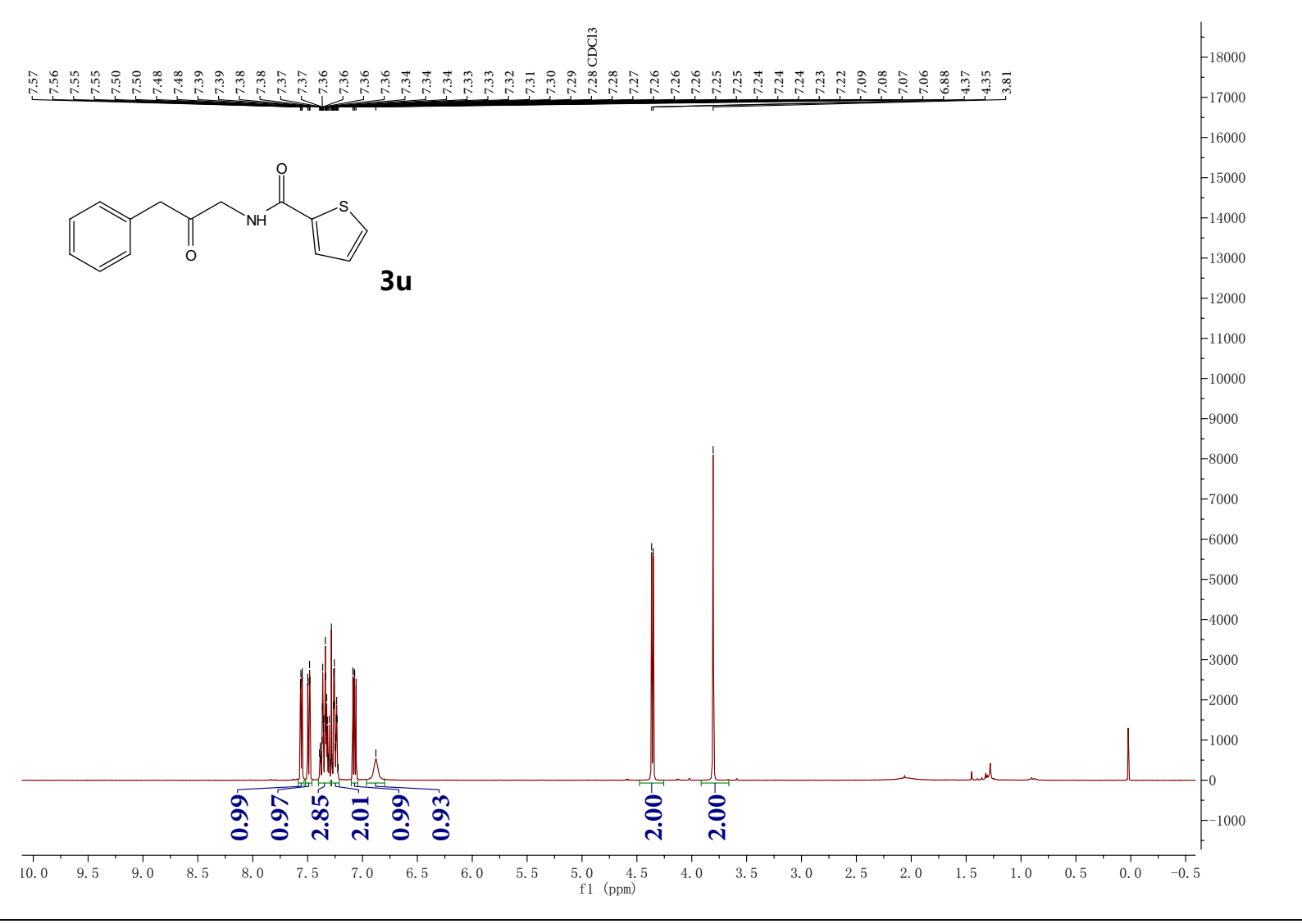
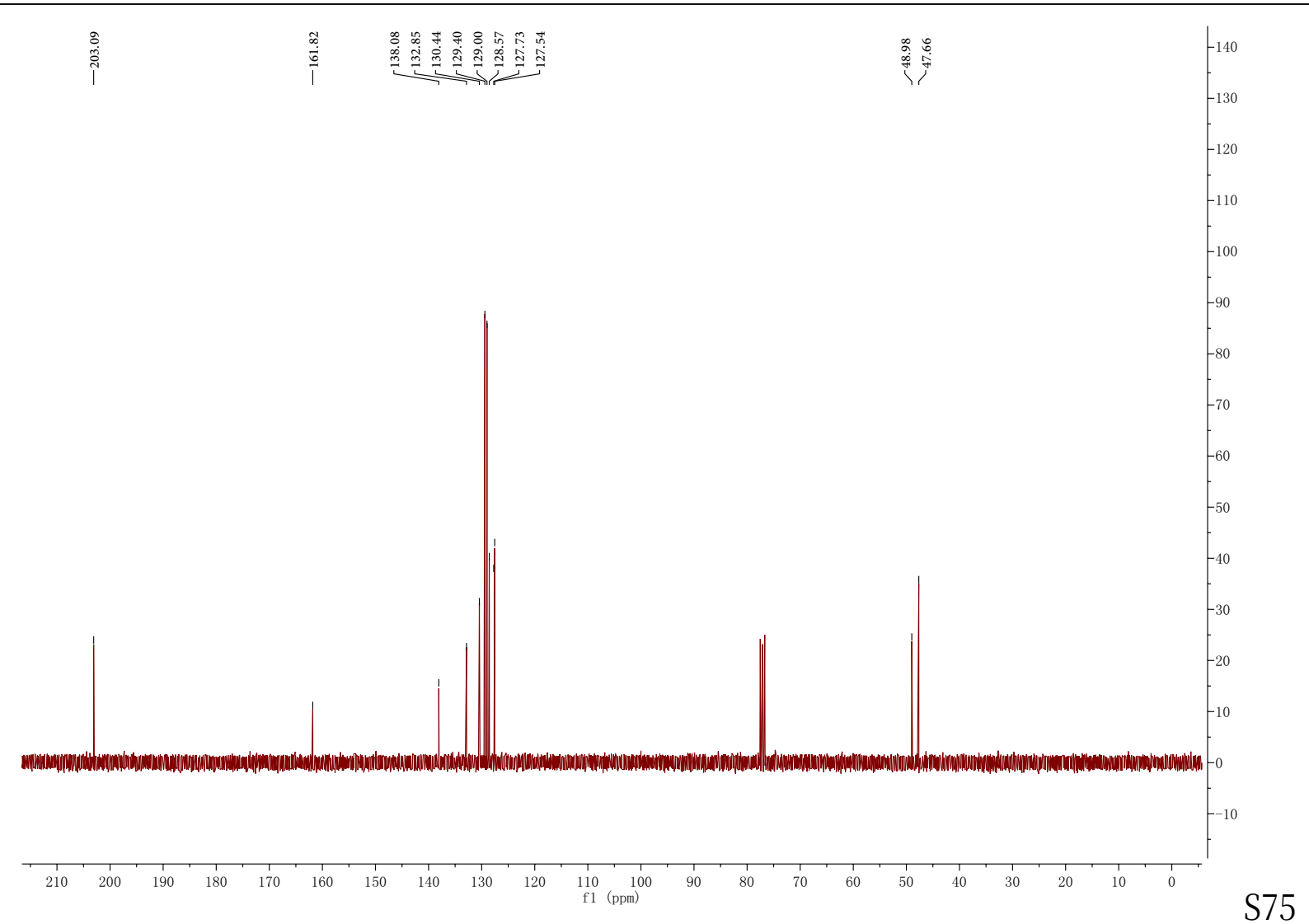
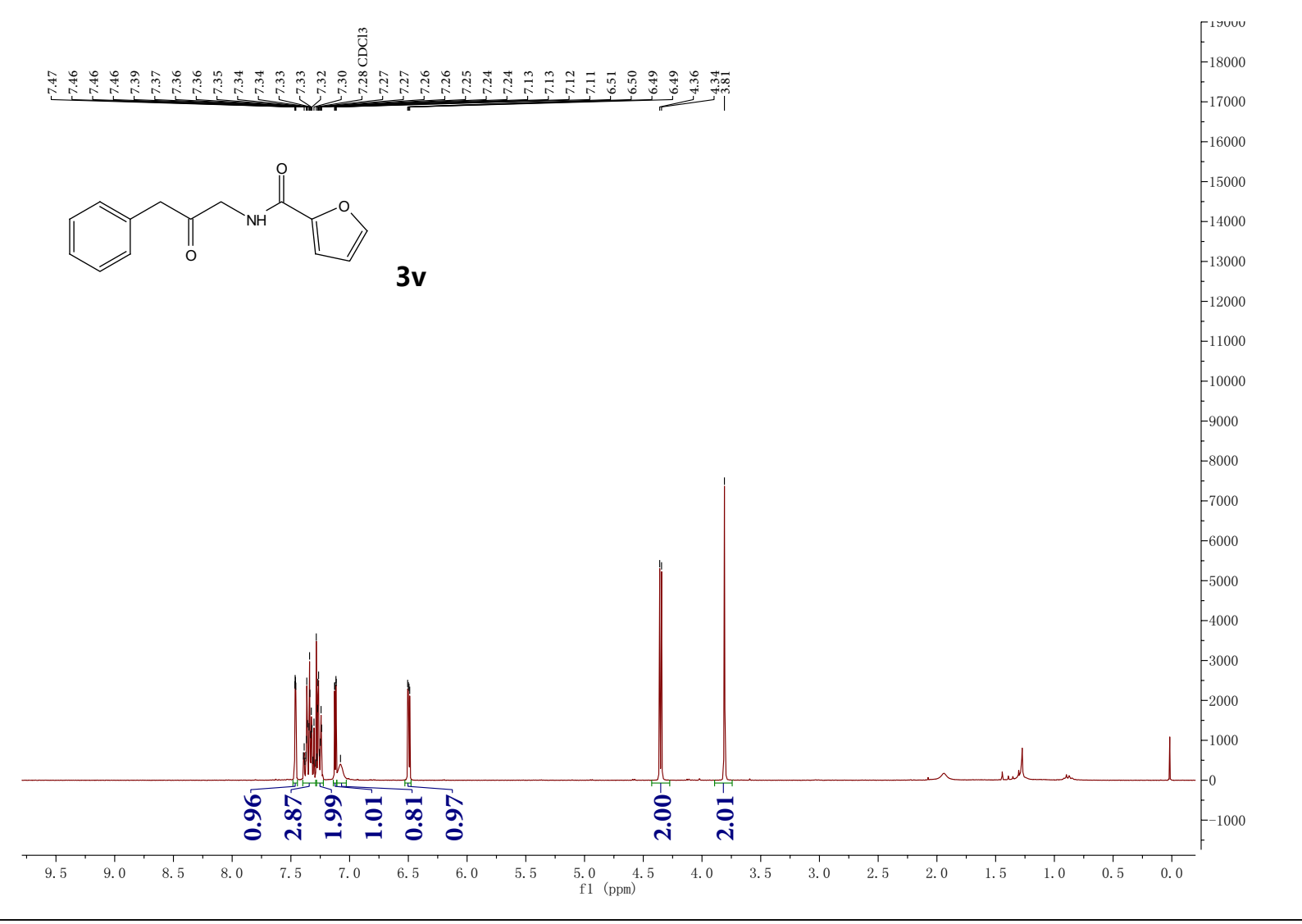
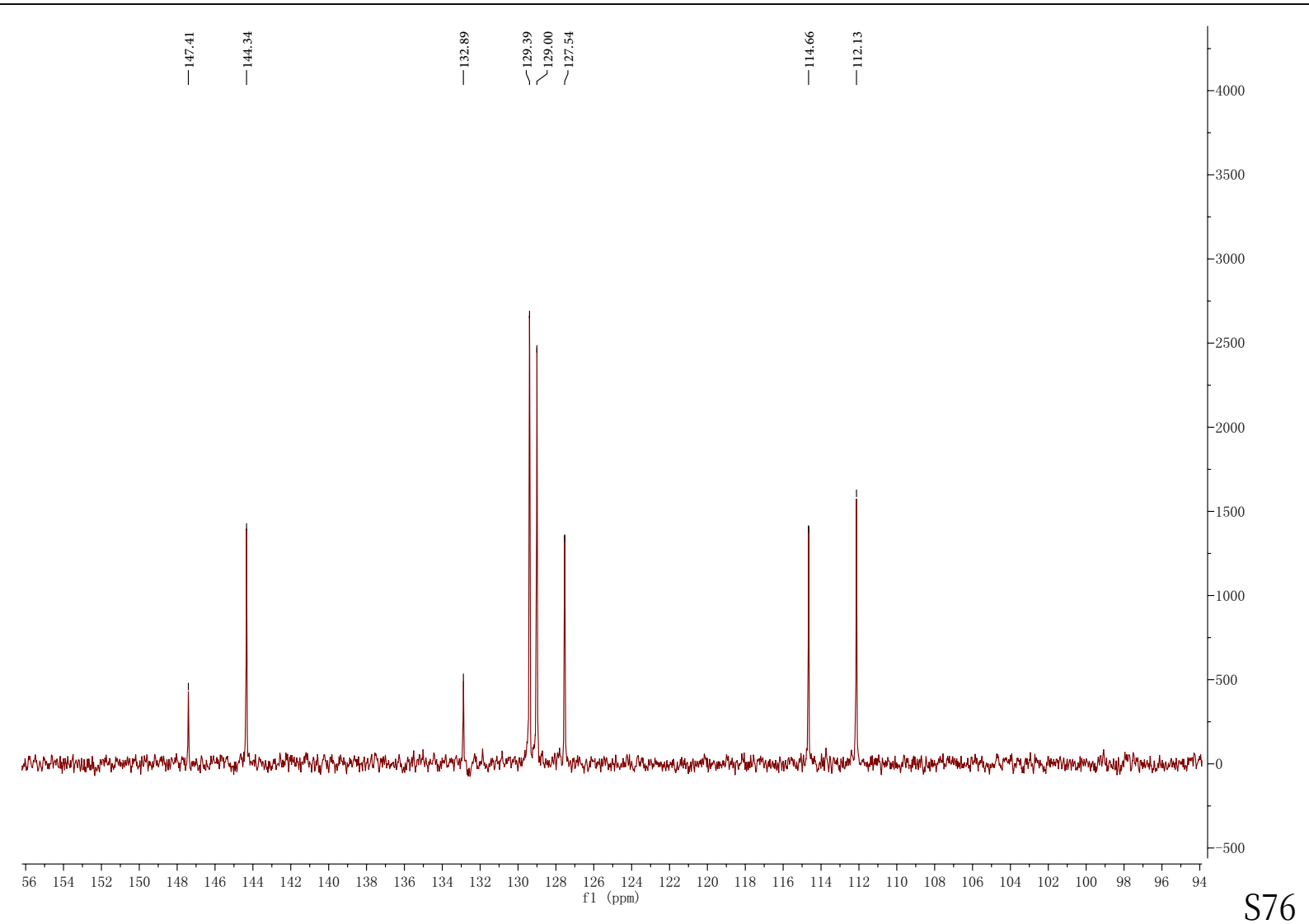
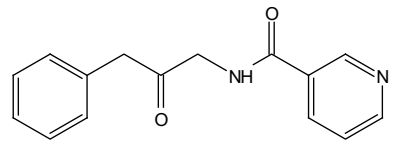
107.17
106.83
49.07
47.76
f1 (ppm)


7.57 7.56 7.55 7.55 7.50 7.50 7.48 7.48 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.36 7.36 7.34 7.34 7.34 7.33 7.33 7.32 7.31 7.30 7.29 7.28 CDCl3 7.28 7.27 7.26 7.26 7.26 7.25 7.25 7.24 7.24 7.24 7.23 7.22 7.09 7.08 7.07 7.06 6.88 4.37 4.35 3.81
O
NH
S
O
3u
0.99
0.97
2.85
2.01
0.99
0.93
2.00
2.00
f1 (ppm)


203.09
161.82
138.08
132.85
130.44
129.40
129.00
128.57
127.73
127.54
48.98
47.66
f1 (ppm)

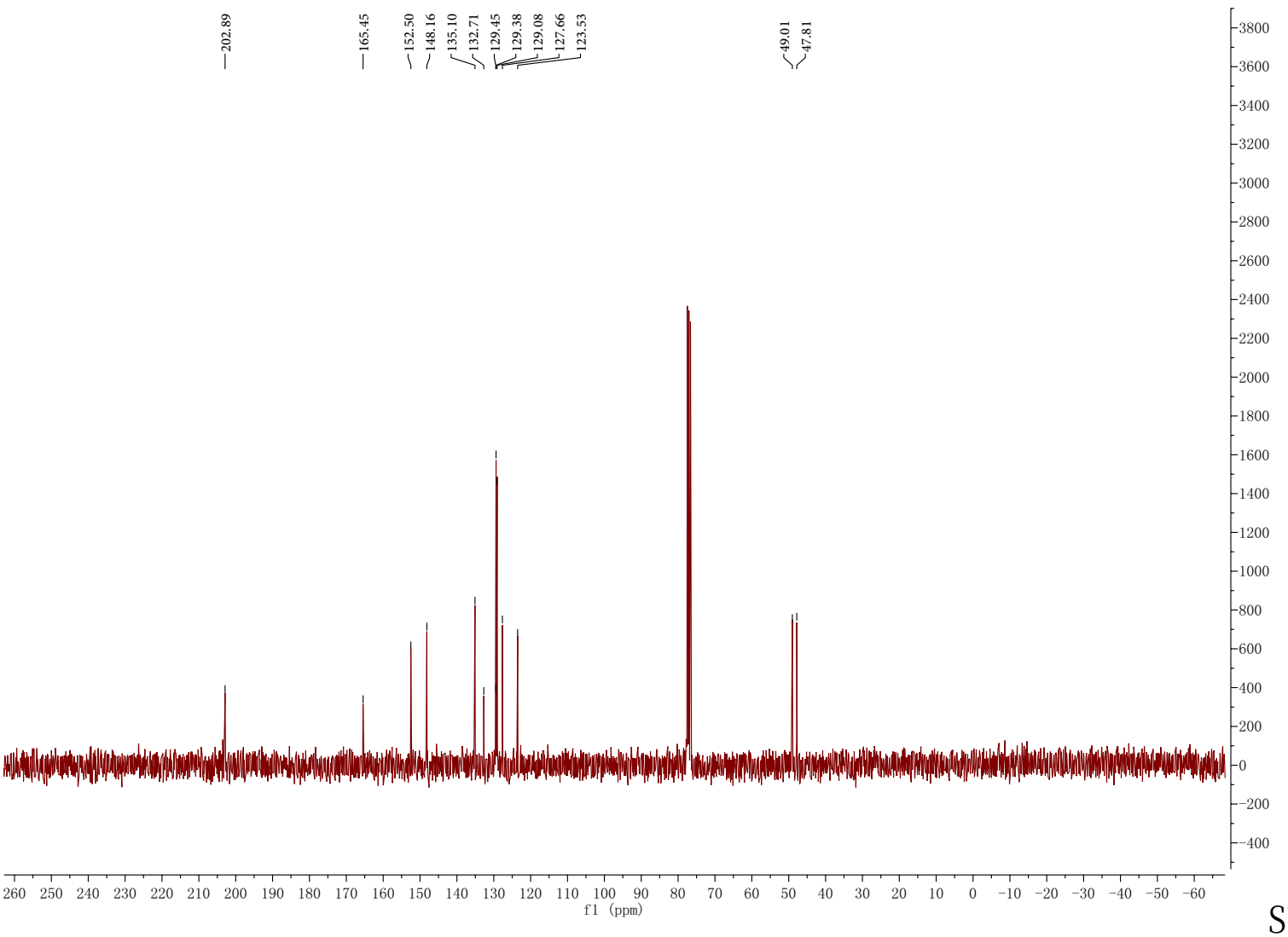

7.47 7.46 7.46 7.46 7.39 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.30 7.28 CDCl3 7.27 7.27 7.26 7.26 7.25 7.24 7.24 7.13 7.13 7.12 7.11 6.51 6.50 6.49 6.49 4.36 4.34 3.81
O
NH
O
O
3v
0.96
2.87
1.99
1.01
0.81
0.97
2.00
2.01
f1 (ppm)

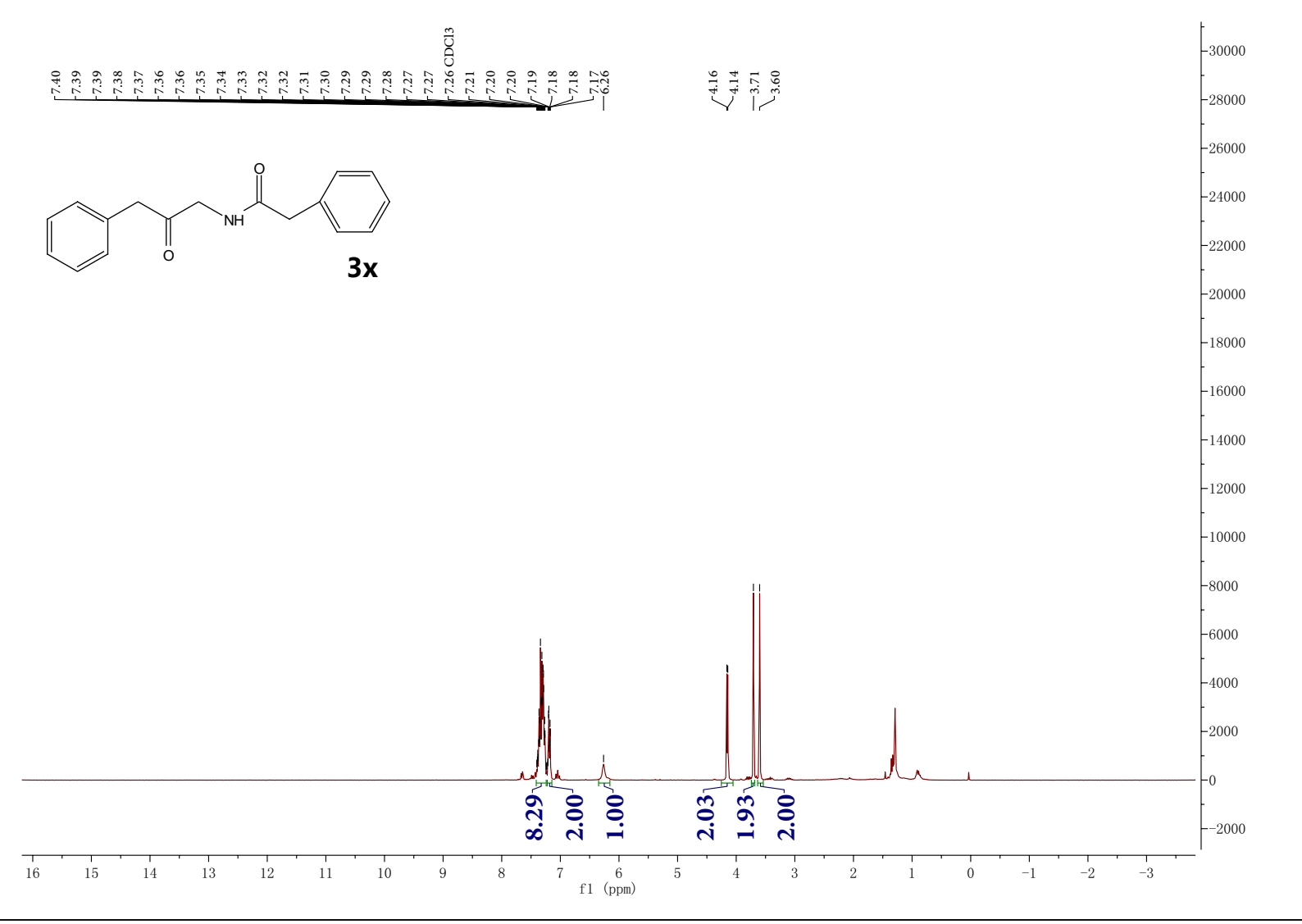

147.41
144.34
132.89
129.39
129.00
127.54
114.66
112.13
f1 (ppm)

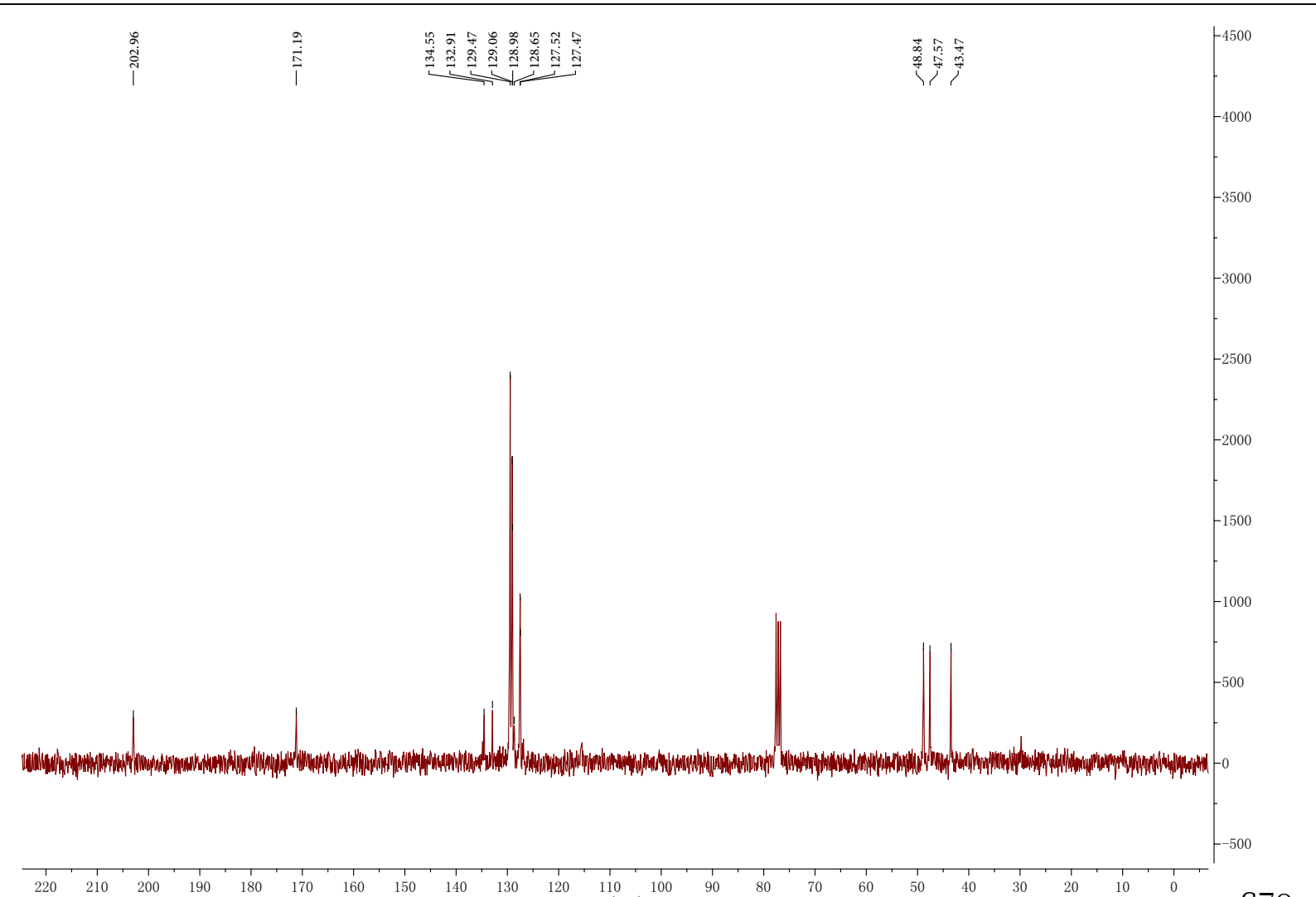

O
NH
N
O

3w

0.96
1.00
0.99
3.88
1.96
0.92
1.98
2.00
f1 (ppm)


202.89
165.45
152.50
148.16
135.10
132.71
129.45
129.38
129.08
127.66
123.53
49.01
47.81
f1 (ppm)


7.40
7.39
7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.26 CDCl3
7.21
7.20
7.20
7.19
7.18
7.18
7.17
6.26
4.16
4.14
3.71
3.60
O
NH
O
3x
8.29
2.00
1.00
2.03
1.93
2.00
f1 (ppm)


202.96
171.19
134.55
132.91
129.47
129.06
128.98
128.65
127.52
127.47
48.84
47.57
43.47
f1 (ppm)