Supporting Information

Fe-Catalyzed Tandem Cyclization for the Synthesis of 3-Nitrofurans from Homopropargylic Alcohols and $Al(NO_3)_3 \cdot 9H_2O$

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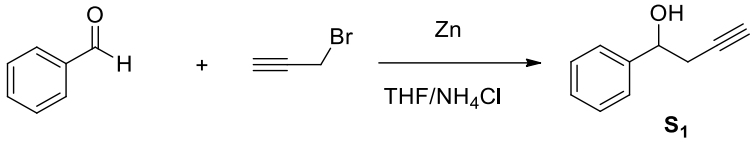
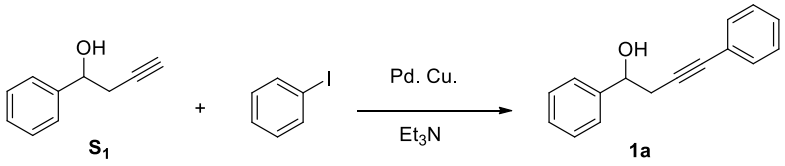
General remark

^{1}H NMR and ^{13}C NMR spectra were recorded on 400MHz and 100MHz in $CDCl_3$ (BRUKER 400M or JNM-ECS 400M). All chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Products were purified by flash chromatography on 200-300 mesh silica gels. All melting points were determined without correction. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

General procedure for the synthesis of homopropargylic alcohols[1-2]:



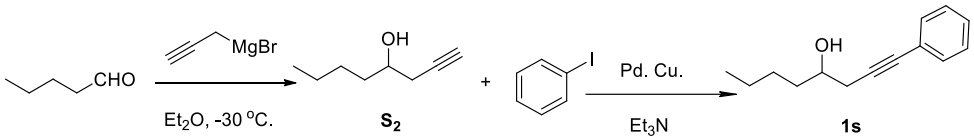
1) Aldehyde (1.0 equiv.) was dissolved in anhydrous THF. A sample was taken out for analysis and propargyl bromide (2.0 equiv.) was added. Another sample was taken out for analysis and saturated aqueous NH4Cl was added. Portions of activated zinc dust (2.0 equiv.) were added slowly on at 0℃ and the resulting suspension was stirred overnight at this temperature. The THF layer was separated from the aqueous layer, which was extracted with diethyl ether for 3 times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuum. The crude product was directly used in the next step without further purification; the residue was purified by column chromatography (silica gel, appropriate mixture of n-hexane/ethyl acetate) to obtain **S1**.



2) To a dried schlenk flask was added $Pd(PPh_3)_2Cl_2$ (0.2 mmol), CuI (0.2 mmol), iodoarene (11.0 mmol), **S1** (10.0 mmol) and freshly distilled Et_3N under argon. The resulting mixture was stirred for 16 h at rt. 50 mL of EtOAc were added and

the mixture filtered. After removal of solvent using rotary evaporator, the crude compound was purified by SiO_2 chromatography to give **1a-1q** and **1t and 1v**.

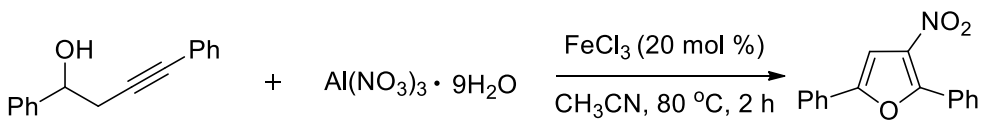
1o and 1p were prepared in the method[3]



Under an argon atmosphere, magnesium turnings (0.67 g, 27.5 mmol) and mercury chloride (0.34 g, 1.3 mmol) were mixed in dry diethyl ether (40 mL) in a 250 mL round-bottom flask. To the solution, propargyl bromide (2.0 mL, 25 mmol) was then added dropwise at 60 ^oC over about 1 h. The reaction was kept at the same temperature until the yellow solution turned cloudy. This solution was cooled to -30 ^oC and a solution of valeraldehyde (6 mmol) in Et_2O (12 ml) was added dropwise. After addition the reaction was moved to room temperature for further 30 min then quenched with sat. NH_4Cl (aq). The aqueous layer was extracted with ether and the extracts were combined with the above organic layer. The combined solution was dried over Na_2SO_4. After evaporation of the solvent the residue was purified by column chromatography (silica gel, appropriate mixture of *n*-hexane/ethyl acetate) to afford **S_2**.

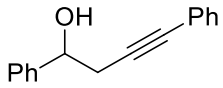
To a dried schlenk flask was added **S_2** (10.0 mmol), $Pd(PPh_3)_2Cl_2$ (0.2 mmol), CuI (0.4 mmol), iodoarene (11.0 mmol) and freshly distilled Et_3N (50 ml) under argon. The resulting mixture was stirred for 16 h at rt. The reaction mixture was quenched with sat. NH_4Cl (aq) and 50 mL of ethyl acetate were added and the mixture filtered. After removal of solvent using rotary evaporator, the crude compound was purified by column chromatography on silica gel to give **1s**.

General procedure for synthesis of 3-nitrofurans from homopropargylic alcohols and $Al(NO_3)_3$ $9H_2O$:



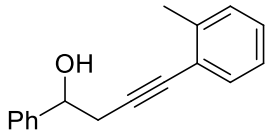
In a sealed tube, homopropargylic alcohols (44.4 mg, 0.2 mmol), $Al(NO_3)_3$ $9H_2O$ (37.5 mg, 0.15 mmol) and $FeCl_3$ (6.5 mg, 0.04 mmol) were successively added to MeCN (2.0 mL). The reactor was flushed with air. The reaction mixture was stirring at 80 ℃ for 2 hour and then the reaction mixture was cooled to room temperature. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (10:1) to afford the desired 3-(nitryl)-2,5-diphenylfuran **1a**.

The data of products:



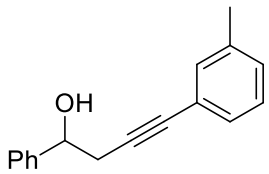
1,4-diphenylbut-3-yn-1-ol (1a)

Yellow solid (1.26 g, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.25 (m, 10 H), 4.92-4.89 (m, 1 H), 2.83-2.82 (d, *J* = 4.0 Hz, 2 H), 2.61 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.8, 131.7, 128.5, 128.3, 128.0, 127.9, 125.9, 123.3, 86.1, 83.2, 72.7, 30.6.



1-phenyl-4-(*o*-tolyl)but-3-yn-1-ol (1b)

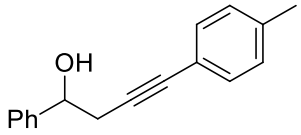
Yellow solid (1.16 g, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.44-7.42 (d, *J* = 8.0 Hz, 2 H), 7.37-7.28 (m, 3 H), 7.22-7.19 (m, 1 H), 7.17-7.10 (m, 2 H), 7.09-7.07 (m, 1 H), 4.95-4.91 (m, 1 H), 2.92-2.90 (d, *J* = 6.0 Hz, 2 H), 2.50-2.49 (d, *J* = 3.2 Hz, 1 H), 2.32 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.7, 140.2, 132.0, 129.4, 128.5, 128.0, 127.9, 125.9, 125.5, 123.1, 89.8, 82.2, 72.7, 30.6, 20.7.



1-phenyl-4-(*m*-tolyl)but-3-yn-1-ol (1c)

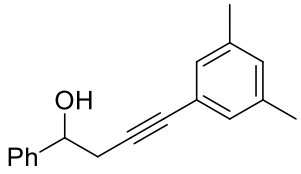
Yellow solid (1.19 g, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.37-7.35 (d,

J = 8.0 Hz, 2 H), 7.32-7.29 (m, 2 H), 7.27-7.23 (m, 1 H), 7.18-7.16 (d, *J* = 8.0 Hz, 2 H), 7.14-7.10 (m, 1 H), 7.05-7.04 (d, *J* = 4.0 Hz, 1 H), 4.86-4.82 (m, 1 H), 2.91 (s, 1 H), 2.78-2.77 (d, *J* = 4.0 Hz, 2 H), 2.25 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.6, 137.7, 132.1, 128.7, 128.6, 128.2, 128.0, 127.7, 125.7, 122.9, 85.6, 83.1, 72.4, 30.3, 21.0.



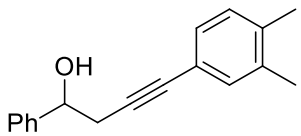
1-phenyl-4-(*p*-tolyl)but-3-yn-1-ol (1d)

Yellow solid (1.17 g, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.43-7.41 (m, 2 H), 7.38-7.34 (m, 2 H), 7.31-7.28 (m, 3 H), 7.09-7.07 (d, *J* = 8.0 Hz, 2 H), 4.94-4.90 (m, 1 H), 2.84-2.83 (d, *J* = 4.0 Hz, 2 H), 2.60-2.59 (d, *J* = 4.0 Hz, 1 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.9, 138.2, 131.7, 131.6, 129.2, 129.1, 128.6, 128.0, 125.9, 120.3, 85.3, 83.4, 72.8, 30.8, 21.6.



4-(3,5-dimethylphenyl)-1-phenylbut-3-yn-1-ol (1e)

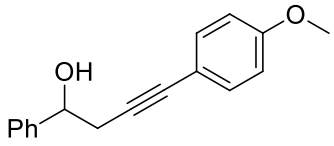
Yellow solid (1.08 g, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.41 (d, *J* = 4.0 Hz, 2 H), 7.37-7.34 (m, 2 H), 7.31-7.29 (m, 1 H), 7.02 (s, 2 H), 6.91 (s, 1 H), 4.92-4.84 (m, 1 H), 2.83-2.82 (d, *J* = 4.0 Hz, 2 H), 2.58-2.55 (m, 1 H), 2.26 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.8, 137.9, 130.0, 129.5, 128.5, 128.0, 125.9, 122.9, 85.3, 83.6, 72.8, 30.8, 21.2.



4-(3,4-dimethylphenyl)-1-phenylbut-3-yn-1-ol (1f)

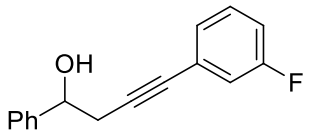
Yellow solid (1.11 g, 80% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.44-7.41 (m, 2 H), 7.38-7.36 (m, 2 H), 7.35-7.30 (m, 1 H), 7.17-7.10 (m, 1 H), 7.14-7.12 (m, 1 H) 7.05-7.03 (d, *J* = 8.0 Hz, 1 H), 4.93-4.91 (m, 1 H), 2.84-2.82 (m, 2 H), 2.57 (s, 1 H),

2.24 (s, 3 H), 2.21 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.9, 137.0, 136.7, 132.8, 129.7, 129.2, 128.5, 128.0, 125.9, 120.5, 85.0, 83.6, 72.8, 30.8, 19.8, 19.7.



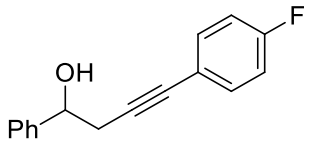
4-(4-methoxyphenyl)-1-phenylbut-3-yn-1-ol (1g)

Yellow solid (1.03 g, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.43-7.41 (m, 2 H), 7.37-7.32 (m, 2 H), 7.30-7.23 (m, 3 H), 6.81-6.79 (d, *J* = 8.8 Hz, 2 H), 4.93-4.89 (m, 1 H), 3.77 (s, 3 H) 2.83-2.81 (m, 2 H), 2.55-2.54 (d, *J* = 3.2 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.4, 142.8, 133.1, 128.4, 127.9, 125.8, 115.4, 113.9, 84.4, 83.1, 72.7, 55.3, 30.7.



4-(3-fluorophenyl)-1-phenylbut-3-yn-1-ol (1h)

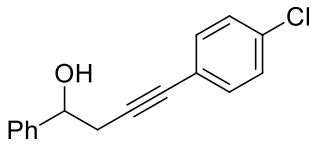
Yellow solid (0.97 g, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.43-7.37 (m, 4 H), 7.35-7.31 (m, 1 H), 7.29-7.20 (m, 1 H), 7.16-7.14 (d, *J* = 8.0 Hz, 1 H), 7.08-7.05 (d, *J* = 2.4 Hz, 1 H) 7.01-6.97 (m, 1 H), 4.95-4.91 (m, 1 H), 2.86-2.84 (d, *J* = 8.0 Hz, 2 H), 2.60 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.4 (d, *J* = 245.0 Hz, 1 C), 142.7, 129.9, 128.6, 128.1, 127.6, 125.9, 125.3 (d, *J* = 10.0 Hz, 1 C), 118.7, 118.6, 118.5 (d, *J* = 10.0 Hz, 1 C), 115.5 (d, *J* = 25.0 Hz, 1 C), 87.4, 82.0, 72.7 (d, *J* = 5.0 Hz, 1 C), 30.5.



4-(4-fluorophenyl)-1-phenylbut-3-yn-1-ol (1i)

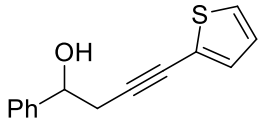
Yellow solid (0.99 g, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.45-7.31 (m, 7 H), 7.01- 6.96 (m, 2 H), 4.97-4.93 (m, 1 H), 2.86-2.85 (d, *J* = 6.4 Hz, 2 H), 2.48-2.47 (d, *J* = 2.4 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.4 (d, *J* = 248.0 Hz, 1 C), 142.7, 133.6 (d, *J* = 8.0 Hz, 1 C), 128.5, 128.0, 125.8, 119.4 (d, *J* =

3.0 Hz, 1 C), 115.5 (d, *J* = 23.0 Hz, 1 C), 85.7 (d, J = 2.0 Hz, 1 C), 82.1, 72.6, 30.5.



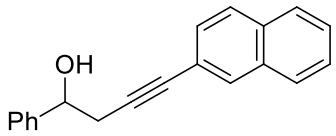
4-(4-chlorophenyl)-1-phenylbut-3-yn-1-ol (1j)

Yellow solid (0.93 g, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.35 (m, 4 H), 7.33-7.29 (m, 2 H), 7.28-7.21 (m, 4 H), 4.93-4.89 (m, 1 H), 2.83-2.81 (d, *J* = 8.0 Hz, 2 H), 2.58 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.6, 133.9, 132.8, 128.5, 128.4, 127.9, 125.7, 121.7, 87.1, 81.9, 72.5, 30.4.



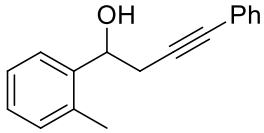
1-phenyl-4-(thiophen-2-yl)but-3-yn-1-ol (1k)

Yellow solid (0.91 g, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.44-7.31 (m, 5 H), 7.20-7.14 (m, 2 H), 6.95-6.93 (m, 1 H), 4.94-4.92 (m, 1 H), 2.88-2.86 (d, *J* =6.0 Hz, 1 H), 2.54 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.6, 131.6, 128.5, 128.0, 126.9, 126.5, 125.8, 95.2, 90.2, 72.6, 30.9.



4-(naphthalen-2-yl)-1-phenylbut-3-yn-1-ol (1l)

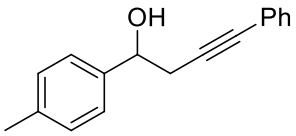
Yellow solid (0.95 g, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.11-8.09 (d, *J* = 8.0 Hz, 1 H), 7.79-7.73 (m, 2 H), 7.61-7.57 (m, 1 H), 7.48-7.44 (m, 4 H), 7.37-7.30 (m, 4 H), 5.00-4.97 (m, 1 H), 3.01-2.99 (d, *J* = 8.0 Hz, 1 H), 2.75 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.7, 133.4, 133.1, 130.2, 128.4, 128.3, 128.1, 127.9, 126.6, 126.2, 125.9, 125.1, 120.9, 90.9, 81.1, 72.7, 30.6.



4-phenyl-1-(*o*-tolyl)but-3-yn-1-ol (1m)

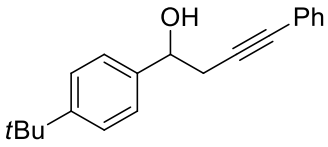
Yellow solid (1.15 g, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.47-7.45 (d, *J* = 8.0 Hz, 1 H), 7.31-7.29 (m, 2 H), 7.19-7.04 (m, 6 H), 5.09-5.06 (m, 1 H),

2.73-2.72 (d, *J* = 4.0 Hz, 2 H), 2.51 (s, 1 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.9, 134.8, 131.9, 131.7, 130.6, 130.4, 128.3, 126.4, 125.4, 125.4, 86.4, 83.1, 69.3, 29.5, 19.3.



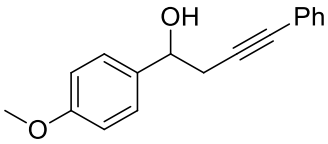
4-phenyl-1-(p-tolyl)but-3-yn-1-ol (1n)

Yellow solid (1.16 g, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.37 (m, 2 H), 7.33-7.31 (d, *J* = 8.0 Hz, 2 H), 7.29-7.27 (m, 3 H), 7.24-7.17 (m, 2 H), 4.94-4.92 (m, 1 H), 2.85-2.83 (d, *J* = 8.0 Hz, 2 H), 2.43-2.42 (d, *J* = 4.0 Hz, 1 H), 2.35 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.85, 137.72, 131.93, 131.59, 129.45, 128.99, 128.55, 128.13, 127.85, 126.02, 125.64, 123.39, 86.21, 83.21, 72.82, 30.69.



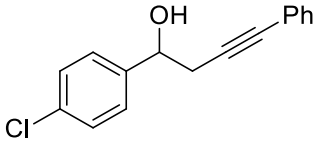
1-(4-(*tert*-butyl)phenyl)-4-phenylbut-3-yn-1-ol (1o)

Yellow solid (0.97 g, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.41-7.36 (m, 6 H), 7.29-7.27 (m, 3 H), 4.95-4.91 (m, 1 H), 2.87-2.85 (d, *J* = 6.4 Hz, 2 H), 2.41-2.40 (d, *J* = 3.6 Hz, 1 H), 1.32 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.9, 139.3, 131.7, 128.2, 128.0, 125.6, 125.4, 123.3, 86.3, 83.1, 72.5, 34.6, 31.4, 30.5.



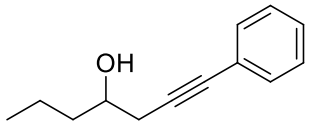
1-(4-methoxyphenyl)-4-phenylbut-3-yn-1-ol (1p)

Yellow solid (0.96 g, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.35 (m, 4 H), 7.29-7.27 (m, 3 H), 6.92-6.89 (m, 2 H), 4.93-4.89 (m, 1 H), 3.81(s, 3 H), 2.85-2.83 (m, 2 H), 2.41 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.4, 135.0, 131.8, 128.4, 127.2, 127.1, 114.0, 113.9, 86.2, 83.2, 72.5, 55.5, 30.7.



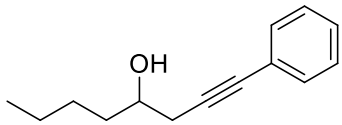
1-(4-chlorophenyl)-4-phenylbut-3-yn-1-ol (1q)

Yellow solid (0.94 g, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.36-7.26 (m, 9 H), 4.90-4.87 (m, 1 H), 2.81-2.79 (d, *J* = 6.4 Hz, 2 H), 2.68-2.67 (d, *J* = 2.0 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 141.2, 133.6, 131.7, 128.6, 128.3, 128.2, 127.3, 123.1, 85.5, 83.5, 71.9, 30.6.



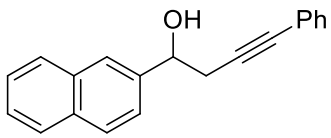
1-phenylhept-1-yn-4-ol (1r)

Colorless oil (0.41g, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.40 (m, 2 H), 7.29-7.27 (m, 3 H), 3.84 (s, 1 H), 2.67-2.51 (m, 2 H), 2.08 (s, 1 H), 1.61-1.54 (m, 2 H), 1.51-1.38 (m, 2 H), 0.97-0.94 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.7, 128.3, 127.9, 123.4, 86.3, 83.0, 70.2, 36.1, 28.4, 27.8, 22.7, 14.0.



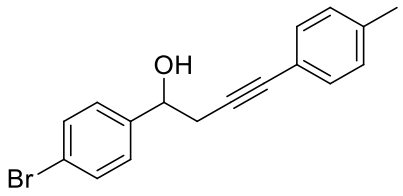
1-phenyloct-1-yn-4-ol (1s)

Colorless oil (0.39 g, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.39 (m, 2 H), 7.29-7.25 (m, 3 H), 3.85-3.80 (m, 1 H), 2.67-2.51 (m, 2 H), 2.06 (s, 1 H), 1.63-1.57 (m, 2 H), 1.48-1.33 (m, 4 H), 0.94-0.90 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 131.7, 128.3, 127.9, 123.4, 86.3, 83.0, 70.0, 38.6, 28.4, 18.9, 14.0.



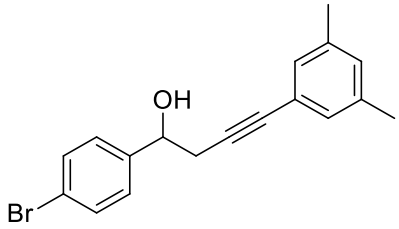
1-(naphthalen-2-yl)-4-phenylbut-3-yn-1-ol (1t)

Yellow solid (0.94 g, 75% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.07-8.04 (d, *J* = 9.0 Hz, 1 H), 7.85-7.82 (m, 1 H), 7.77-7.70 (m, 2 H), 7.50-7.42 (m, 3 H), 7.37-7.32 (m, 2 H), 7.25-7.21 (m, 2 H), 5.67-4.65 (m, 1 H), 3.10-3.02 (m, 1 H), 2.96-2.88 (m, 1 H), 2.78-2.77 (d, *J* = 3.0 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 138.1, 133.7, 131.6, 130.2, 128.9, 128.3, 128.2, 127.9, 126.1, 125.5, 125.3, 123.2, 122.9, 86.3, 83.4, 69.3, 29.7.



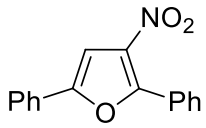
1-(4-bromophenyl)-4-(*p*-tolyl)but-3-yn-1-ol (1u)

Yellow solid (0.83 g, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.63-7.61 (d, *J* = 8.0 Hz, 1 H), 7.46-7.45 (d, *J* = 4.0 Hz, 2 H), 7.27-7.24(m, 1 H), 7.21-7.19 (d, *J* = 8.0 Hz, 2 H), 7.05-7.03 (d, *J* = 8.0 Hz, 2 H), 2.96-2.86 (m, 2 H), 2.38 (s, 1 H), 2.30 (s, 3 H), 2.28-2.26 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.8, 137.9, 131.5, 128.8, 127.9, 126.7, 125.6, 120.1, 84.9, 84.0, 76.0, 34.2.



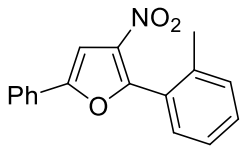
1-(4-bromophenyl)-4-(3,5-dimethylphenyl)but-3-yn-1-ol (1v)

Yellow solid (0.79 g, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.46-7.44 (d, *J* = 8.0 Hz, 2 H), 7.7.27-7.25 (d, *J* = 8.0 Hz, 2 H), 6.99 (s, 2 H), 6.91 (s, 1 H), 4.85-4.83 (m, 1 H), 2.78 (s, 1 H), 2.76-2.75 (d, *J* = 8.0 Hz, 1 H), 2.25 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 141.6, 137.7, 131.4, 130.0, 129.3, 127.5, 122.5, 121.5, 84.6, 83.7, 71.9, 30.4, 21.0.



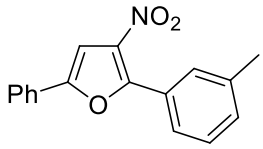
3-nitro-2,5-diphenylfuran (3a)

Yellow solid (34.5 mg, 65% yield), melting point: 78-80 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.36-8.34 (m, 2 H), 7.86-7.84 (m, 2 H), 7.68-7.64 (m, 1 H), 7.56-7.48 (m, 5 H), 7.05 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.8, 170.7, 162.4, 135.7, 134.0, 130.7, 129.1, 128.6, 126.7, 126.0, 100.2; HRMS calcd for $C_{16}H_{12}NO_3$ $[M+H]^+$ 266.0812; found: 266.0816.



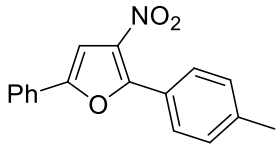
3-nitro-5-phenyl-2-(*o*-tolyl)furan (3b)

Yellow solid (26.2 mg, 47% yield), melting point: 115-118 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.40-8.37 (d, *J* = 12.0 Hz, 2 H), 7.90-7.84 (m, 2 H), 7.50-7.49 (d, *J* = 4.0 Hz, 2 H), 7.01-7.00 (m, 3 H), 3.90 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 186.0, 170.6, 162.4, 138.4, 135.7, 134.9, 131.0, 130.7, 129.1, 128.4, 127.1, 126.7, 125.9, 100.2, 21.3; HRMS calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$ 280.0968; found: 280.0971.



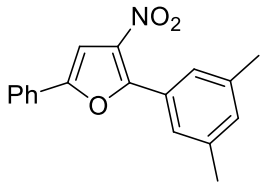
3-nitro-5-phenyl-2-(*m*-tolyl)furan (3c)

Yellow solid (26.8 mg, 48% yield), melting point: 127-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.16-8.13 (m, 2 H), 7.86-7.84 (d, *J*=8.0 Hz, 2 H), 7.52-7.48 (m, 3 H), 7.46-7.40 (m, 2 H), 7.04 (s, 1 H), 2.45 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 186.0, 170.6, 162.4, 138.4, 135.7, 134.9, 131.0, 130.7, 129.1, 128.4, 128.0, 126.7, 125.9, 100.2, 21.4; HRMS calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$ 280.0968; found: 280.0973.



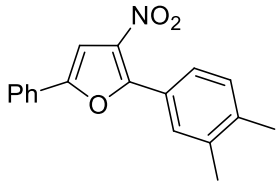
3-nitro-5-phenyl-2-(p-tolyl)furan (3d)

Yellow solid (33.5 mg, 60% yield), melting point: 104-106 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.27-8.25 (d, *J* = 8.0 Hz, 2 H), 7.86-7.84 (m, 2 H), 7.51-7.49 (d, J=8.0 Hz, 3 H), 7.35-7.33 (d, *J* = 8.0 Hz, 2 H), 7.04 (s, 1 H), 2.46 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.3, 170.6, 162.5, 145.2, 133.2, 130.8, 130.7, 129.3, 129.1, 126.7, 126.0, 100.3, 21.8; HRMS calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$ 280.0968; found: 280.0972.



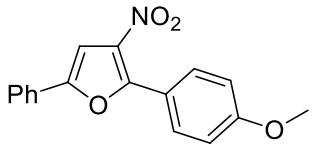
2-(3,5-dimethylphenyl)-3-nitro-5-phenylfuran (3e)

Yellow solid (27.0 mg, 46% yield), melting point: 62-64 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.93 (s, 2 H), 7.87-7.84 (m, 2 H), 7.53-7.48 (m, 3 H), 7.30 (s, 1 H), 7.03 (s, 1 H), 2.42 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 186.2, 170.6, 162.5, 138.3, 135.8, 135.7, 130.7, 129.1, 128.4, 126.7, 125.9, 100.2, 21.3; HRMS calcd for $C_{18}H_{16}NO_3$ $[M+H]^+$ 294.1125; found: 284.1129.



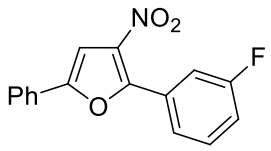
2-(3,4-dimethylphenyl)-3-nitro-5-phenylfuran (3f)

Yellow solid (28.1 mg, 48% yield), melting point: 106-109 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.11-8.09 (d, *J* = 8.0 Hz, 2 H), 7.85-7.83 (m, 2 H), 7.50-7.48 (m, 3 H), 7.29-7.27 (d, *J* = 8.0 Hz, 1 H), 7.02 (s, 1 H), 2.35 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.5, 170.5, 162.5, 143.9, 137.0, 133.6, 131.5, 130.6, 129.8, 129.1, 128.6, 126.7, 125.9, 100.2, 20.2, 19.8; HRMS calcd for $C_{18}H_{16}NO_3$ $[M+H]^+$ 294.1125; found: 284.1130.



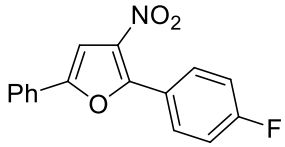
2-(4-methoxyphenyl)-3-nitro-5-phenylfuran (3g)

Yellow solid (29.5 mg, 50% yield), melting point: 107-109 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.40-8.38 (d, *J* = 8.0 Hz, 2 H), 7.86-7.84 (m, 2 H), 7.51-7.49 (d, *J* = 8.0 Hz, 3 H), 7.03-7.00 (m, 3 H), 3.91 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 183.9, 170.5, 164.4, 162.7, 133.2, 130.6, 129.1, 128.6, 126.7, 125.9, 113.9, 100.3, 55.5; HRMS calcd for $C_{17}H_{14}NO_4$ $[M+H]^+$ 296.0918; found: 296.0923.



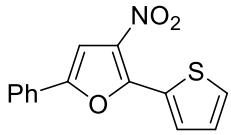
2-(3-fluorophenyl)-3-nitro-5-phenylfuran (3h)

Yellow solid (26.6 mg, 47% yield), melting point: 109-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.20-8.18 (d, *J* = 8.0 Hz, 1 H), 8.07-8.05 (d, *J* = 8.0 Hz, 1 H), 7.86-7.84 (m, 2 H), 7.52-7.49 (m, 4 H), 7.38-7.33 (m, 1 H), 7.05 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 184.4, 171.0, 163.8, 162.2, 161.4, 137.5 (d, *J* = 7.0 Hz, 1 C), 130.8, 130.2 (d, *J* = 8.0 Hz, 1 C), 129.2, 126.6 (d, *J* = 2.0 Hz, 1 C), 126.0, 121.1 (d, *J* = 21.0 Hz, 1 C), 117.3 (d, *J* = 23.0 Hz, 1 C), 100.3; HRMS calcd for $C_{16}H_{11}FNO_3$ $[M+H]^+$ 284.0718; found: 284.0721.



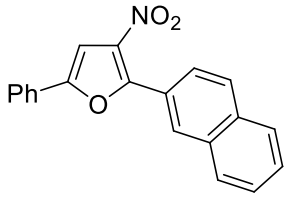
2-(4-fluorophenyl)-3-nitro-5-phenylfuran (3i)

Yellow solid (25.5 mg, 45% yield), melting point: 107-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.45-8.42 (m, 2 H), 7.86-7.83 (m, 2 H), 7.51-7.49 (m, 3 H), 7.23-7.18 (m, 2 H), 7.05 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 184.0, 170.8, 167.7, 165.1, 162.4, 133.5 (d, *J* = 10.0 Hz, 1 C), 130.8, 129.1, 126.6, 126.0, 115.8 (d, *J* = 22.0 Hz, 1 C), 100.2; HRMS calcd for $C_{16}H_{11}FNO_3$ $[M+H]^+$ 284.0718; found: 284.0723.



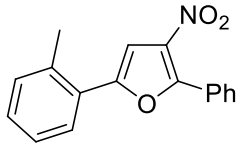
3-nitro-5-phenyl-2-(thiophen-2-yl)furan (3k)

Yellow solid (32.5 mg, 60% yield), melting point: 118-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.52-8.50 (m, 1 H), 7.86-7.84 (m, 3 H), 7.51-7.49 (m, 3 H), 7.26-7.23 (m, 1 H), 7.05 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 177.0, 170.9, 162.2, 141.6, 136.7, 136.1, 130.1, 129.1, 128.6, 126.6, 125.9, 99.7; HRMS calcd for $C_{14}H_{10}NO_3S$ $[M+H]^+$ 272.0376; found: 272.0380.



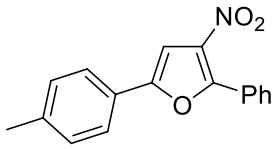
2-(naphthalen-2-yl)-3-nitro-5-phenylfuran (3l)

Yellow solid (25.2 mg, 40% yield), melting point: 128-130 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.61-8.59 (d, *J* = 8.0 Hz, 1 H), 8.20-8.18 (d, *J* = 8.0 Hz, 1 H), 8.09-8.07 (d, *J* = 8.0 Hz, 1 H), 7.93-7.91 (d, *J* = 8.0 Hz, 1 H), 7.86-7.84 (m, 2 H), 7.64-7.60 (m, 1 H), 7.58-7.54 (m, 2 H), 7.50-7.48 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 188.1, 171.1, 163.5, 133.8, 133.7, 133.1, 131.8, 130.8, 130.7, 129.1, 128.6, 128.2, 126.7, 126.6, 125.9, 125.3, 124.2, 100.0; HRMS calcd for $C_{20}H_{14}NO_3$ $[M+H]^+$ 316.0968; found: 316.0974.



3-nitro-2-phenyl-5-(*o*-tolyl)furan (3m)

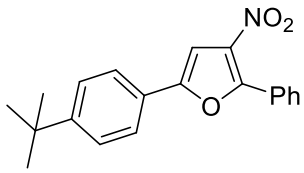
Yellow oil (27.9 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.38-8.36 (d, *J* = 8.0 Hz, 2 H), 7.80-7.78 (d, *J* = 8.0 Hz, 1 H), 7.67-7.64 (m, 1 H), 7.56-7.52 (m, 2 H), 7.39-7.32 (m, 3 H), 6.91 (s, 1 H), 2.56 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.8, 170.7, 162.1, 136.4, 135.7, 134.0, 131.5, 130.6, 130.5, 128.5, 128.4, 126.4, 126.2, 103.2, 21.5; HRMS calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$ 280.0968; found: 280.0973.



3-nitro-2-phenyl-5-(*p*-tolyl)furan (3n)

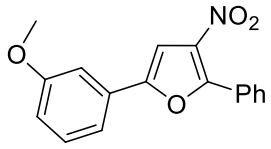
Yellow solid (20.6 mg, 37% yield), melting point: 63-65 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.36-8.33 (m, 2 H), 7.75-7.72 (m, 2 H), 7.68-7.62 (m, 1 H), 7.56-7.51 (m, 2 H), 7.32-7.29 (d, *J* = 9.0 Hz, 2 H), 6.99 (s, 1 H), 2.42 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 185.9, 171.0, 162.4, 141.1, 135.8, 134.0, 130.7, 129.8, 128.5, 125.9, 124.0, 99.6, 21.5; HRMS calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$ 280.0968;

found: 280.0971.



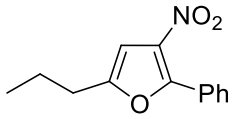
5-(4-(*tert*-butyl)phenyl)-3-nitro-2-phenylfuran (3o)

Yellow oil (24.4 mg, 38% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.36-8.34 (d, *J* = 8.0 Hz, 2 H), 7.80-7.78 (d, *J* = 8.0 Hz, 2 H), 7.67-7.64 (m, 1 H), 7.56-7.52 (m, 4 H), 7.01 (s, 1 H), 1.36 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.9, 170.9, 162.4, 154.2, 135.8, 134.0, 130.7, 128.5, 126.1, 125.8, 124.0, 99.7, 35.0, 31.1; HRMS calcd for $C_{20}H_{20}NO_3$ $[M+H]^+$ 322.1438; found: 322.1435.



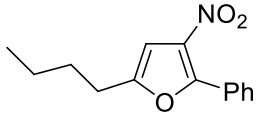
5-(3-methoxyphenyl)-3-nitro-2-phenylfuran (3p)

Yellow solid (28.3 mg, 48% yield), melting point: 102-104 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.35-8.34 (d, *J* = 4.0 Hz, 2 H), 7.67-7.64 (m, 1 H), 7.42-7.37 (m, 3 H), 7.04-7.01 (m, 2 H), 3.88 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.7, 170.6, 162.3, 159.9, 135.6, 134.0, 130.6, 130.3, 128.5, 127.7, 118.4, 116.6, 111.0, 100.4, 55.4; HRMS calcd for $C_{17}H_{14}NO_4$ $[M+H]^+$ 296.0918; found: 296.0923.



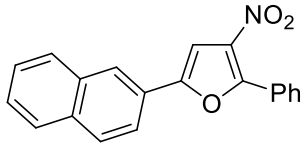
3-nitro-2-phenyl-5-propylfuran (3r)

Yellow oil (27.9 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.31-8.29 (d, *J* = 8.0 Hz, 2 H), 7.65-7.61 (m, 1 H), 7.53-7.49 (m, 2 H), 6.53 (s, 1 H), 2.84-2.80 (m, 2 H), 1.84-1.75 (m, 2 H), 1.05-1.01 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 186.1, 174.5, 161.8, 135.8, 133.8, 130.6, 128.5, 101.6, 28.5, 20.8, 13.6; HRMS calcd for $C_{13}H_{14}NO_3$ $[M+H]^+$ 232.0968; found: 232.0973.



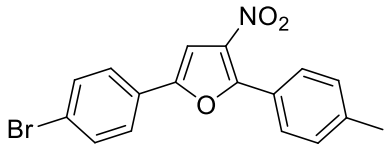
5-butyl-3-nitro-2-phenylfuran (3s)

Yellow oil (28.5 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.30-8.29 (d, *J* = 4.0 Hz, 2 H), 7.65-7.61 (m, 1 H), 7.53-7.49 (m, 2 H), 6.52 (s, 1 H), 2.86-2.82 (m, 2 H), 1.78-1.70 (m, 2 H), 1.48-1.39 (m, 2 H), 0.98-0.94 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 186.1, 174.7, 161.8, 135.8, 133.8, 130.6, 128.5, 101.4, 29.4, 26.2, 22.1, 13.6; HRMS calcd for $C_{14}H_{16}NO_3$ $[M+H]^+$ 246.1125; found: 246.1130.



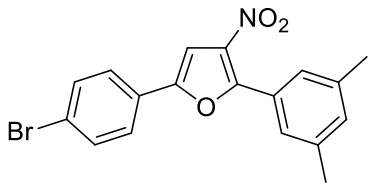
5-(naphthalen-2-yl)-3-nitro-2-phenylfuran (3t)

Yellow solid (22.1 mg, 35% yield), melting point: 101-103 ºC. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.43-8.40 (m, 2 H), 8.35-8.32 (d, *J* = 9.0 Hz, 1 H), 8.02-7.99 (d, *J* = 9.0 Hz, 1 H), 7.96-7.88 (m, 2 H), 7.70-7.54 (m, 6 H), 7.17 (s, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 185.8, 170.8, 162.2, 135.8, 134.1, 133.8, 131.4, 130.7, 130.2, 128.8, 128.6, 128.0, 127.7, 126.6, 125.1, 124.7, 124.3, 104.3; HRMS calcd for $C_{20}H_{14}NO_3$ $[M+H]^+$ 316.0968; found: 316.0974.



5-(4-bromophenyl)-3-nitro-2-(*p*-tolyl)furan (3u)

Yellow solid (31.7 mg, 46% yield), melting point: 182-184 ºC. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.24 (d, *J* = 8.0 Hz, 2 H), 7.73-7.71 (d, *J* = 8.0 Hz, 2 H), 7.66-7.64 (d, *J* = 8.0 Hz, 2 H), 7.35-7.33 (d, *J* = 8.0 Hz, 2 H), 7.04 (s, 1 H), 2.46 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.1, 169.5, 162.6, 145.3, 133.1, 132.4, 130.8, 129.4, 127.4, 125.6, 125.1, 100.7, 21.8; HRMS calcd for $C_{17}H_{13}BrNO_3$ $[M+H]^+$ 358.0074; found: 358.0080.



5-(4-bromophenyl)-2-(3,5-dimethylphenyl)-3-nitrofuran (3v)

Yellow solid (33.5 mg, 45% yield), melting point: 150-152 ºC. ^{1}H NMR (400 MHz,

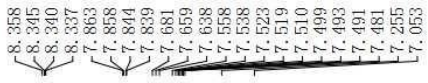
$CDCl_3$, ppm): δ = 7.91 (s, 2 H), 7.72-7.69 (m, 2 H), 7.64-7.62 (m, 2 H), 7.29 (s, 1 H), 2.41 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 185.9, 169.5, 162.5, 138.3, 135.9, 135.6, 132.4, 128.3, 127.3, 125.6, 125.1, 100.6, 21.2; HRMS calcd for $C_{18}H_{15}BrNO_3$ $[M+H]^+$ 372.0230; found: 372.0235.

Refrence:

[1] P. Gao, Y. -W. Shen, R. Fang, X.-H. Hao, Z.-H. Qiu, F. Yang, X.-B. Yan, Q. Wang, X.-J. Gong, X.-Y. Liu and Y. -M. Liang, *Angew. Chem., Int. Ed.*, 2014, **53**, 7629.

[2] D.-Q. Chen, P. Gao, P.-X. Zhou, X.-R. Song, Y.-F. Qiu, X.-Y. Liu and Y.-M. Liang, *Chem. Commun.*, 2015, **51**, 6637.

[3]. J. A. Cabezas, *Tetrahedron Lett.* **2001**, *42*,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7.510
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7.491
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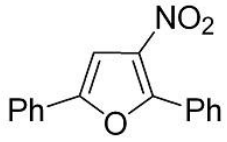
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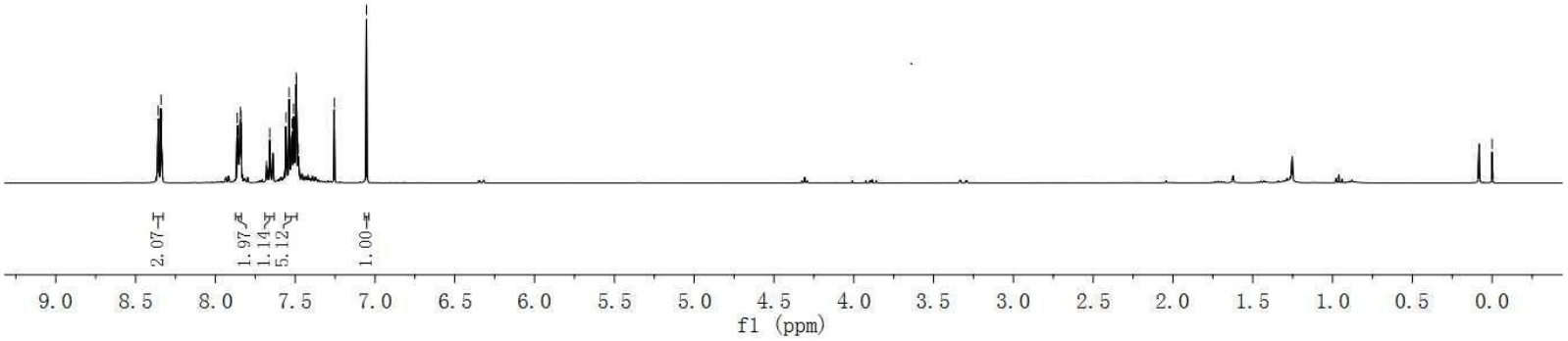
Ph
O
Ph

3a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6.0
5.5
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4.0
3.5
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2.5
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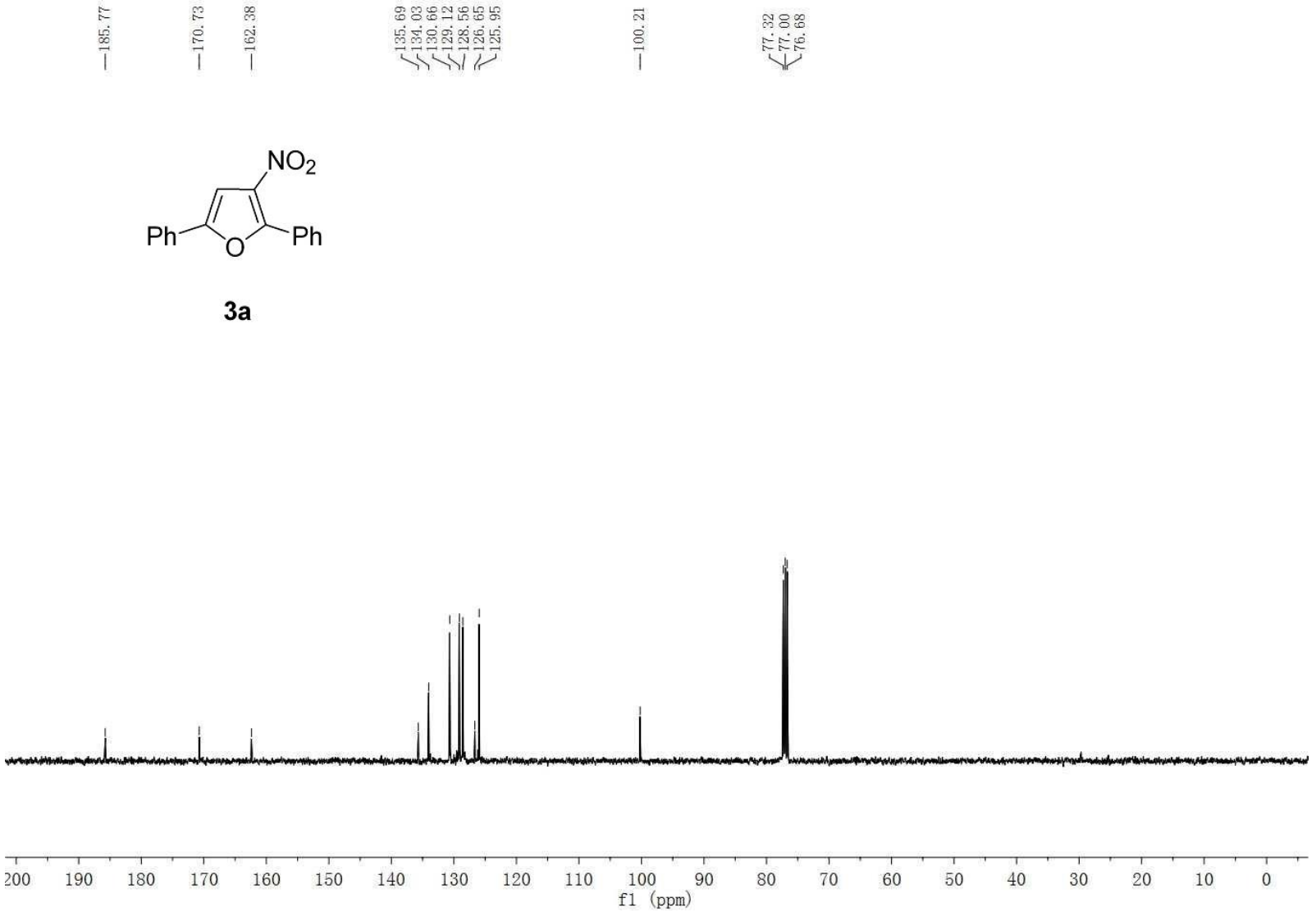
f1 (ppm)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77.00
76.68
NO2
Ph
Ph
O
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190
180
170
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110
100
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80
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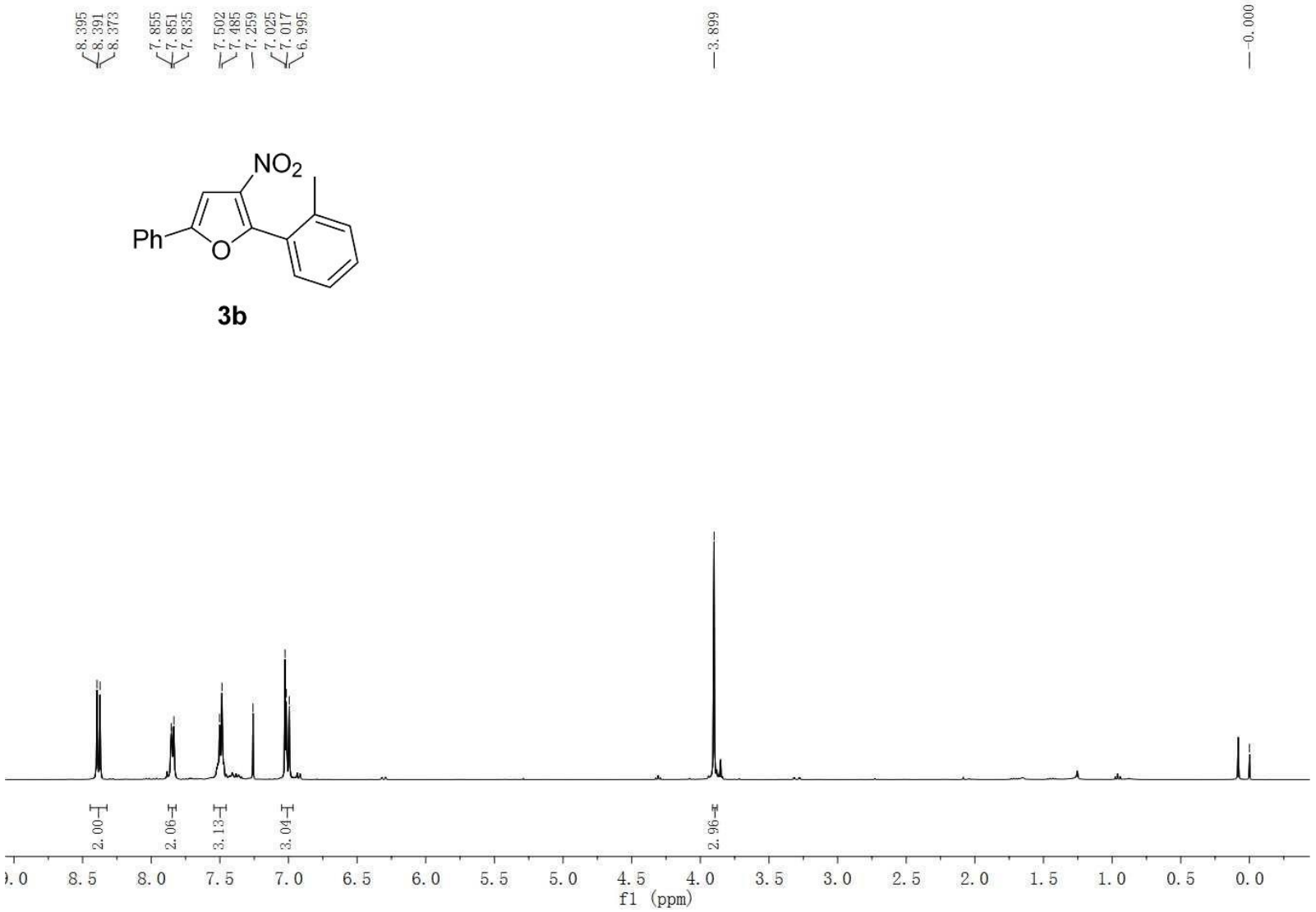
40
30
20
10
0
f1 (ppm)

3a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Ph
O
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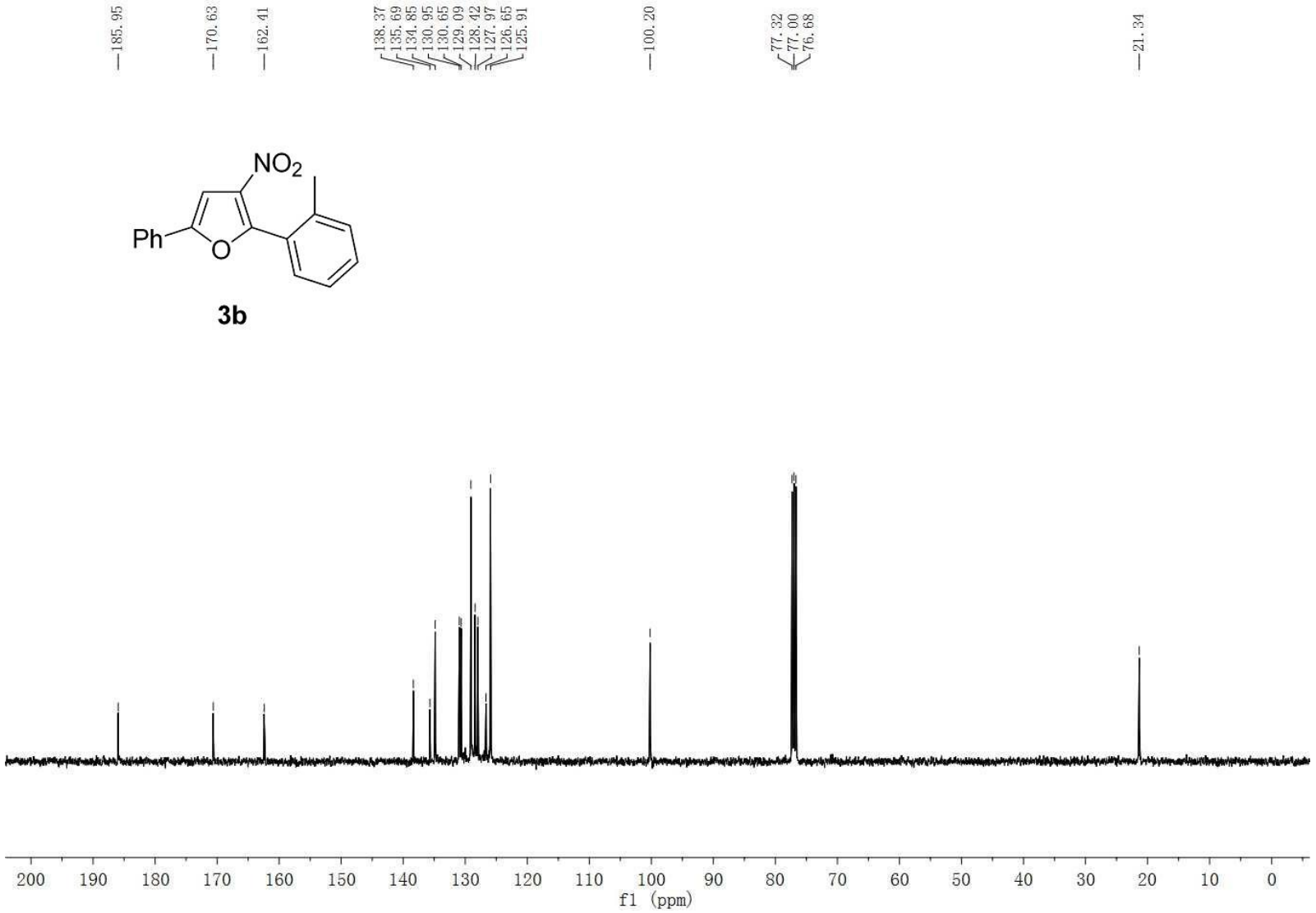
f1 (ppm)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77.00
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NO2
Ph
O
3b
200
190
180
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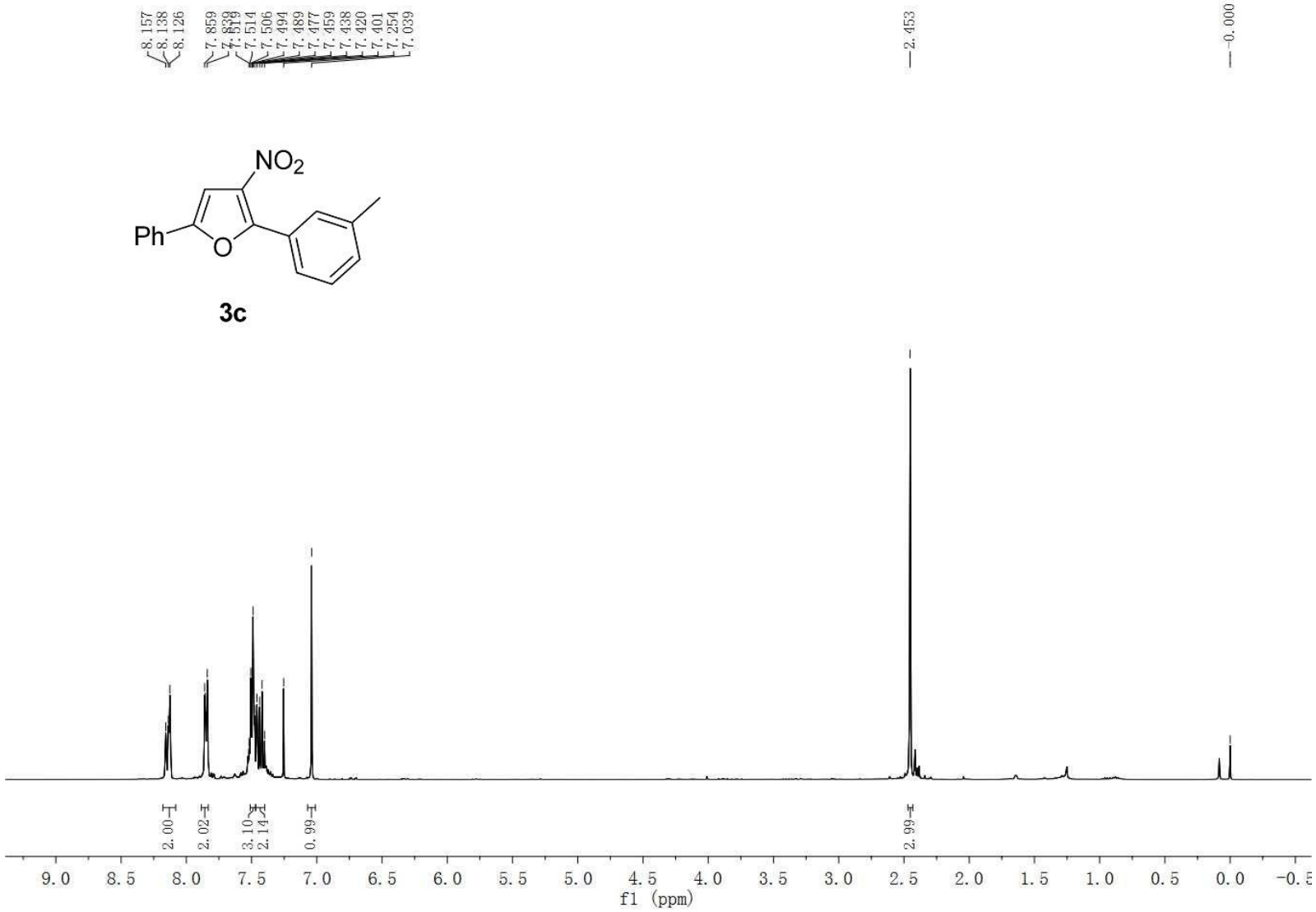
f1 (ppm)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7.401
7.254
7.039
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Ph
O
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2.02
3.10
2.14
0.99
2.99
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8.0
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7.0
6.5
6.0
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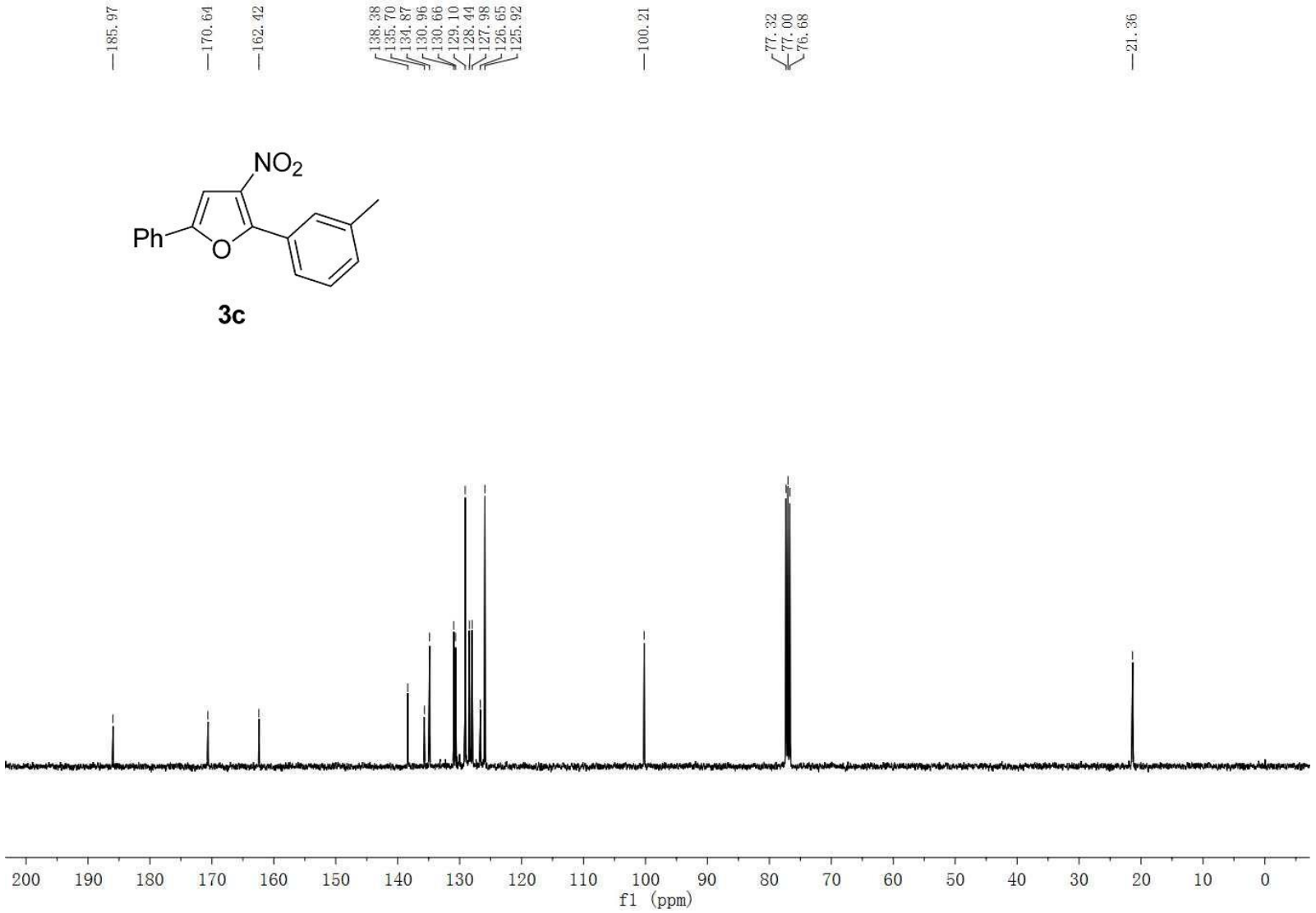
0.0
f1 (ppm)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180
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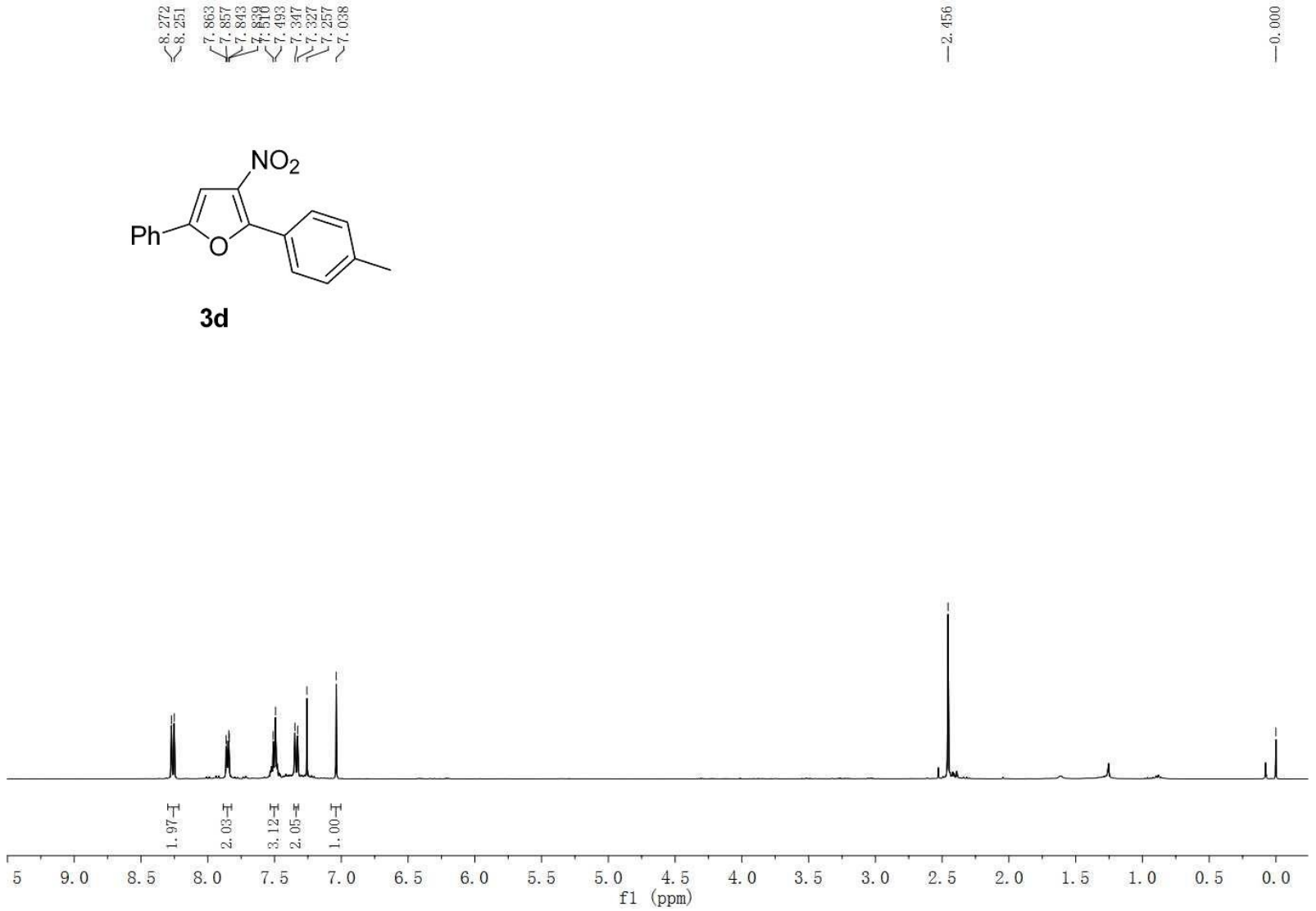
f1 (ppm)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Ph
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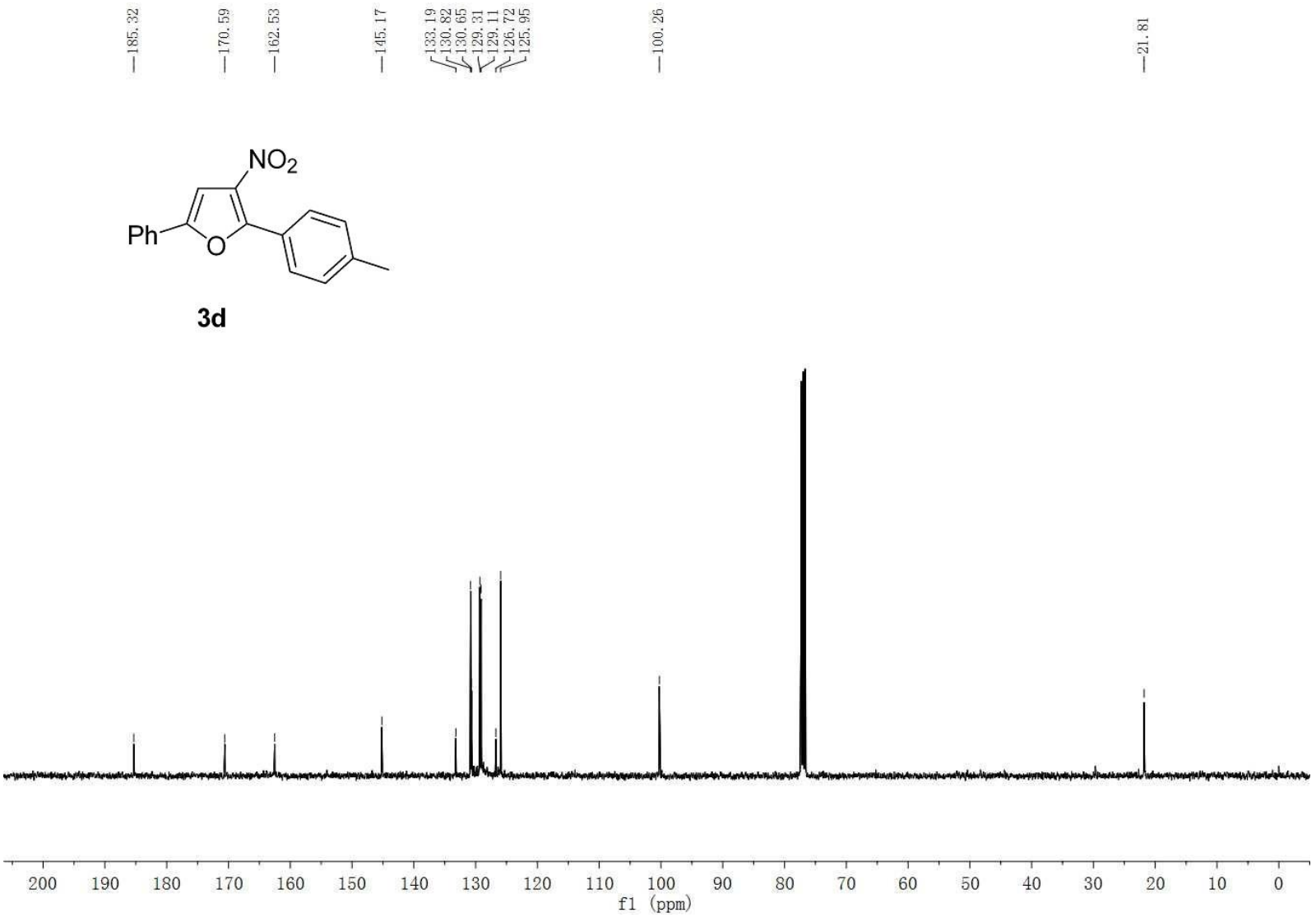
f1 (ppm)

3d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O
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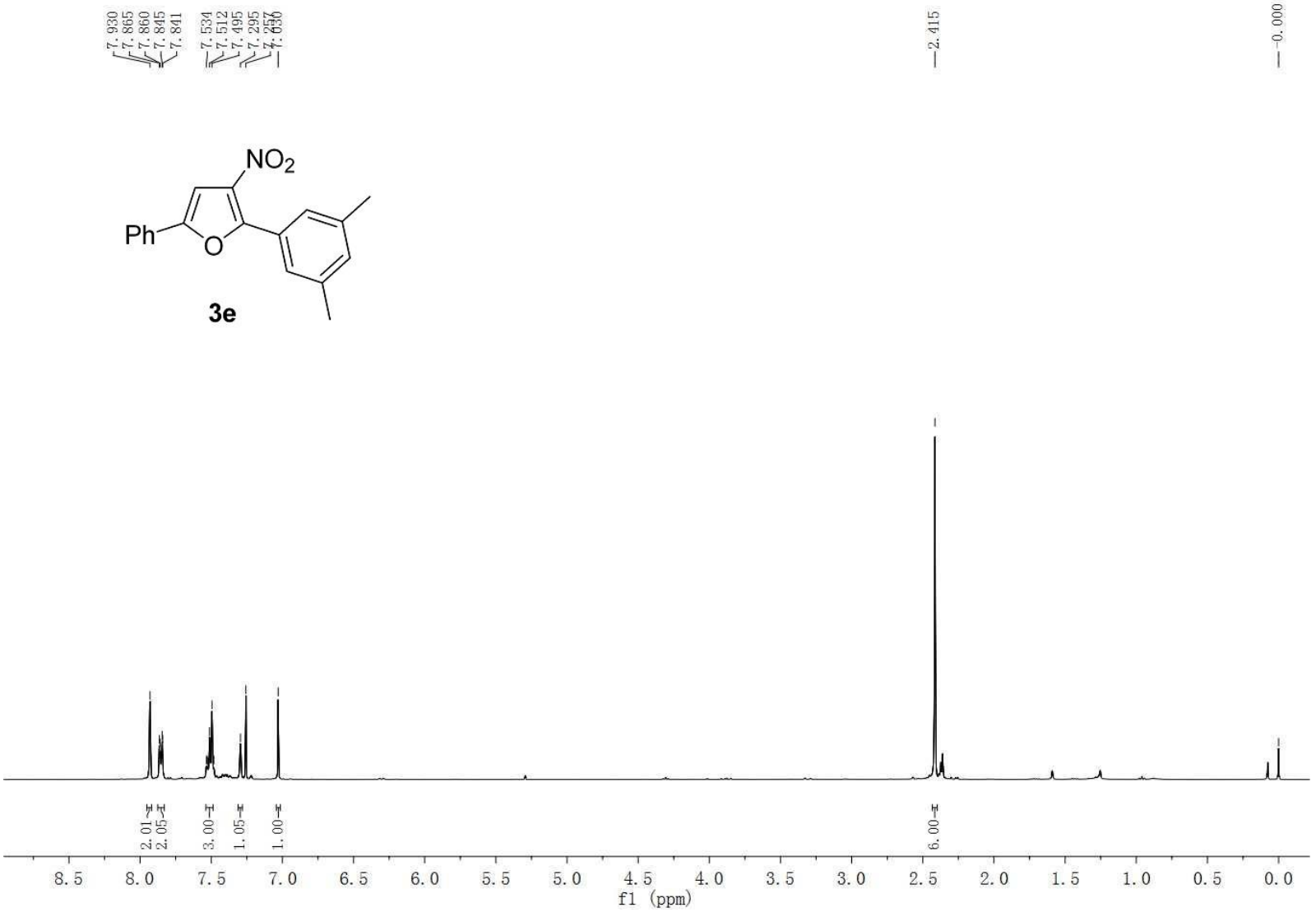
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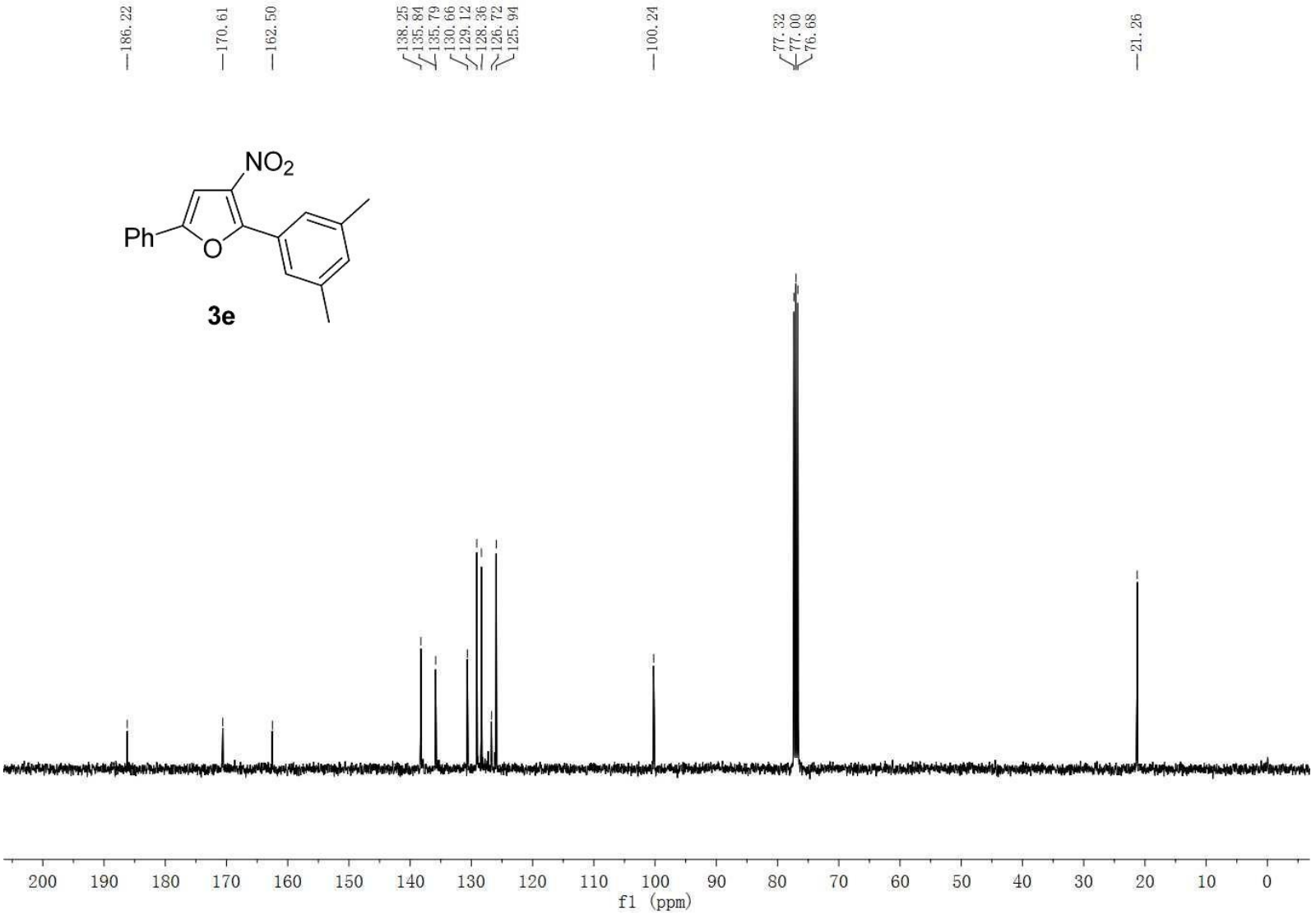
f1 (ppm)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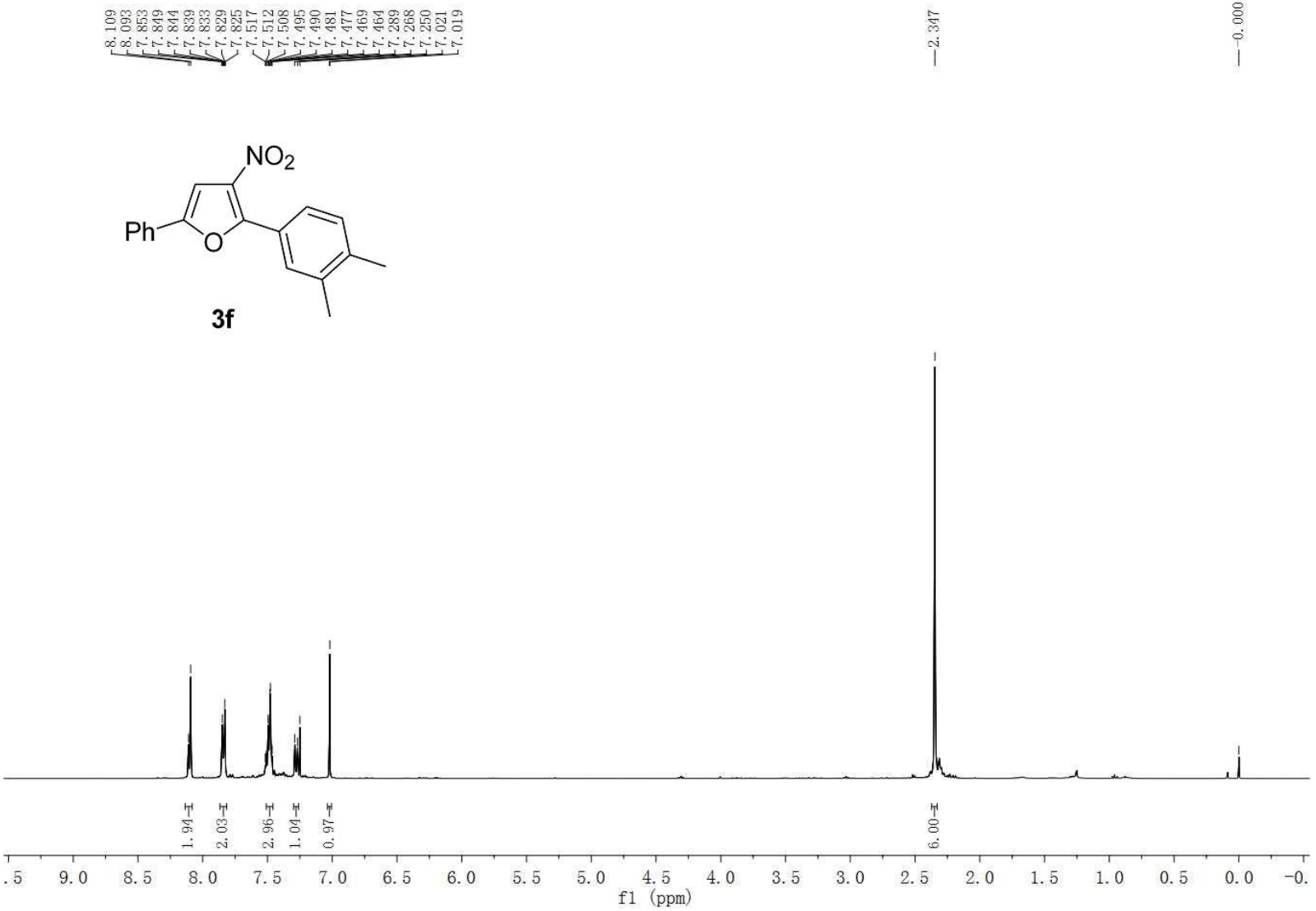
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Ph
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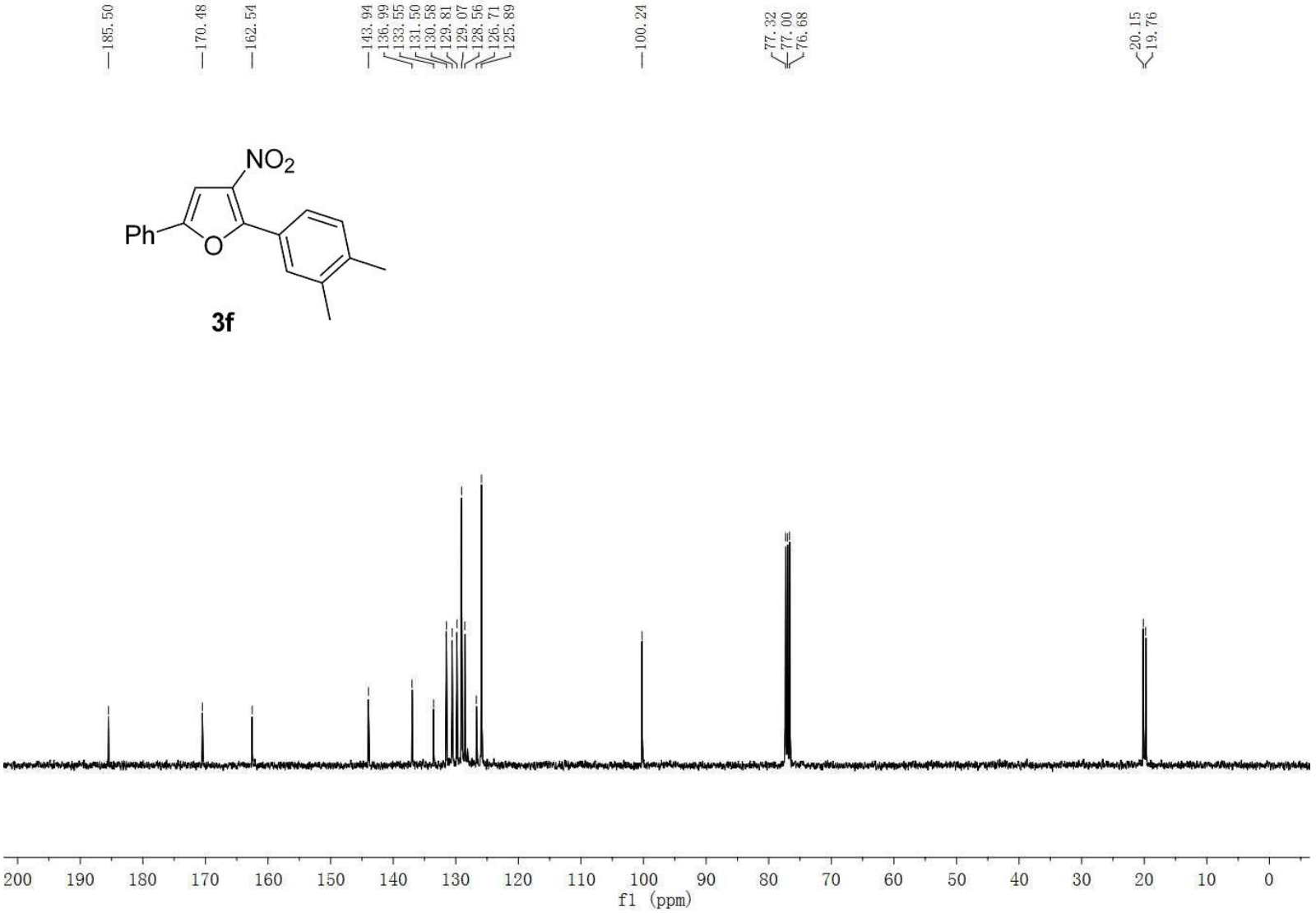
f1 (ppm)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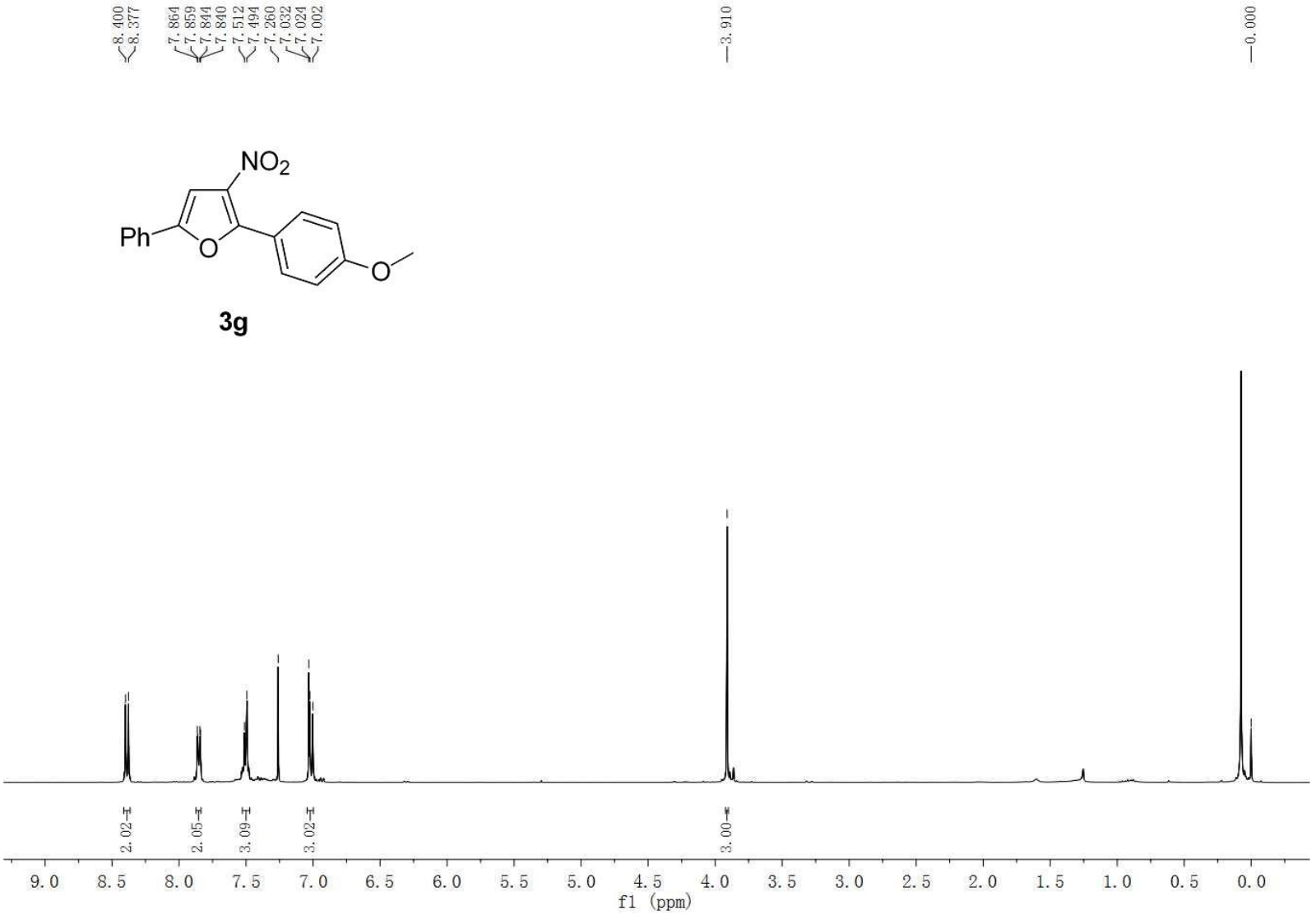
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2.05
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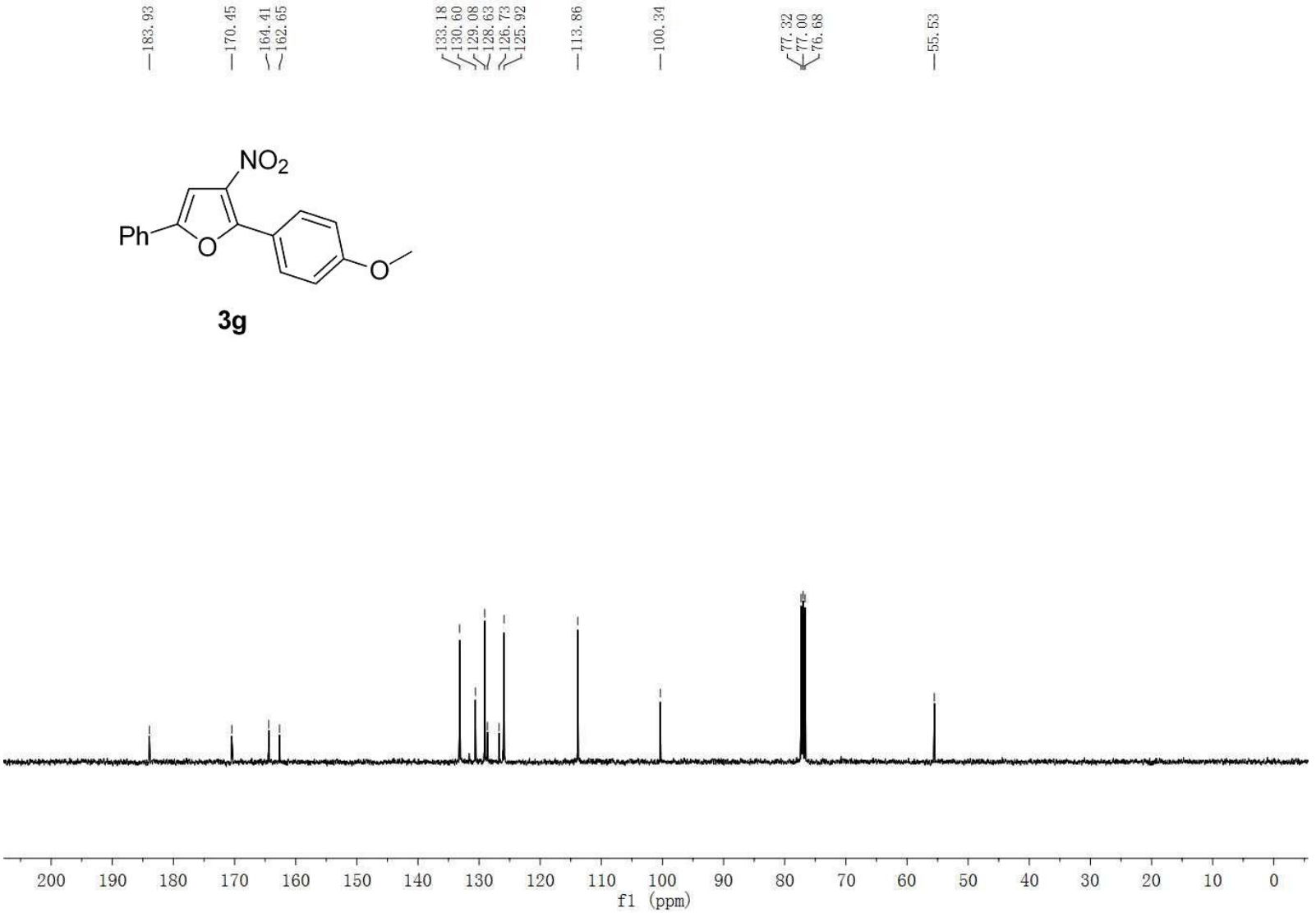
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O
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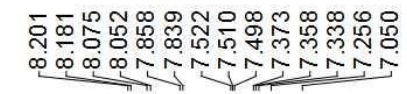
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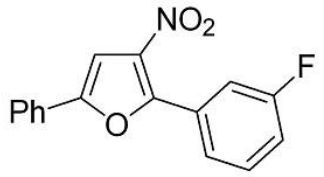
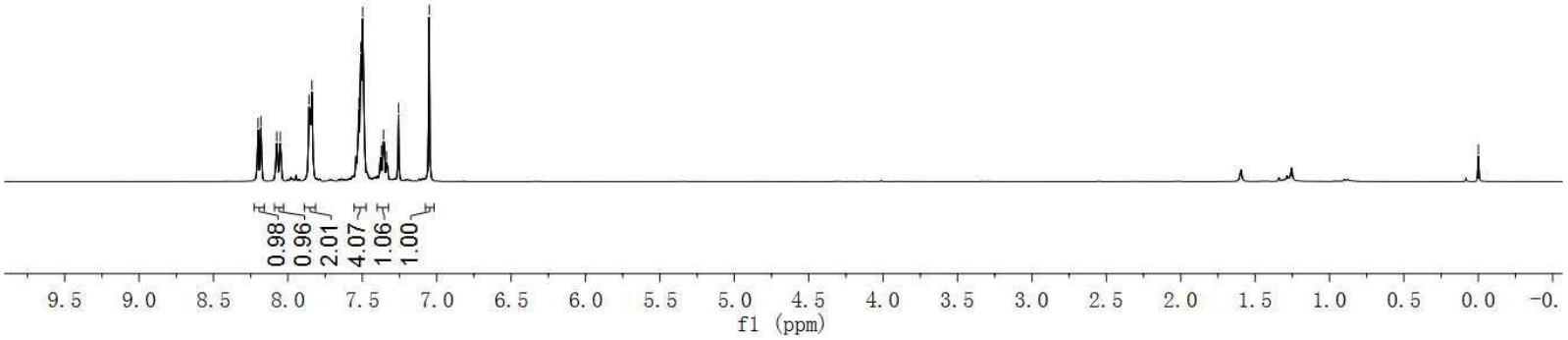
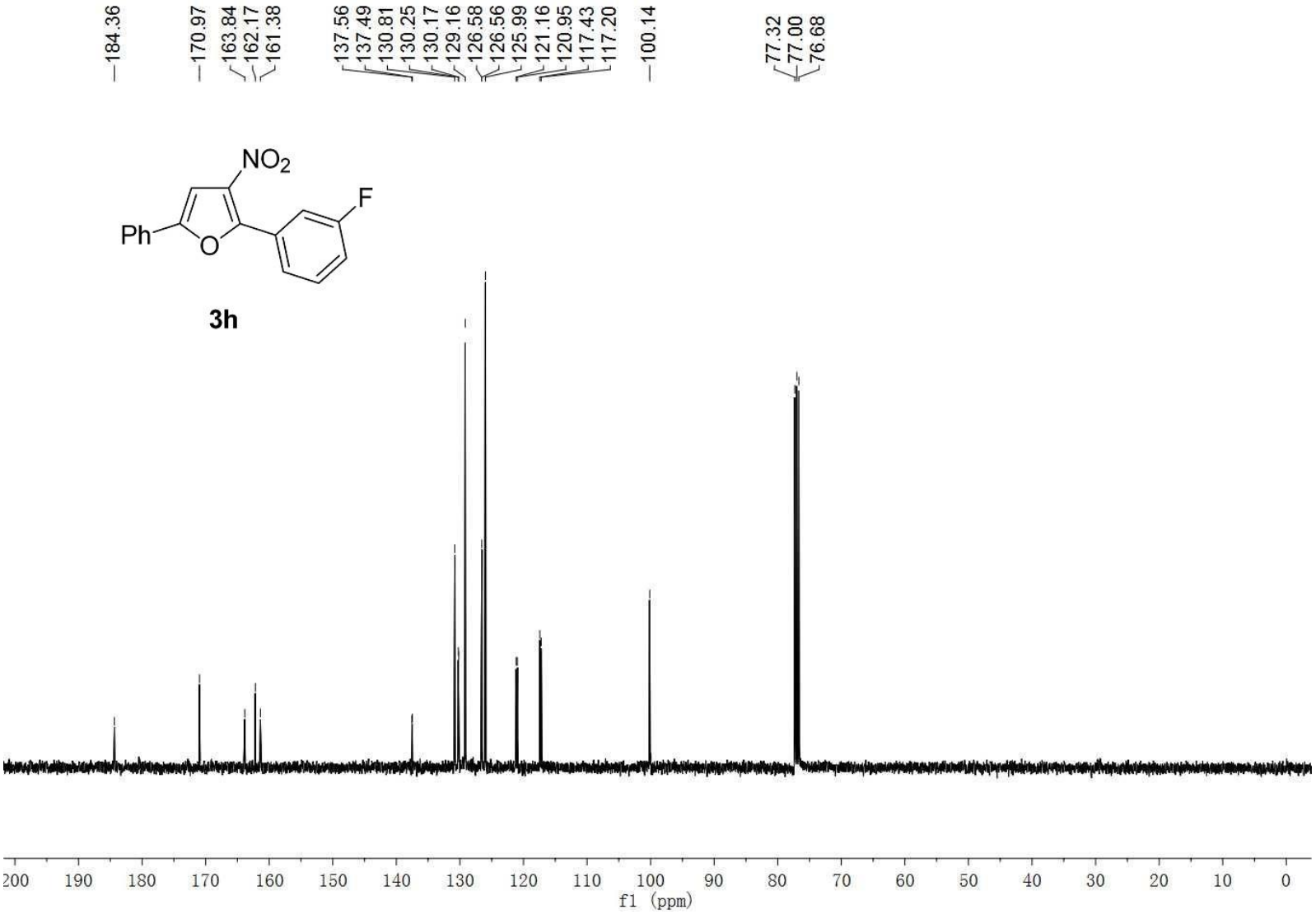
7.050

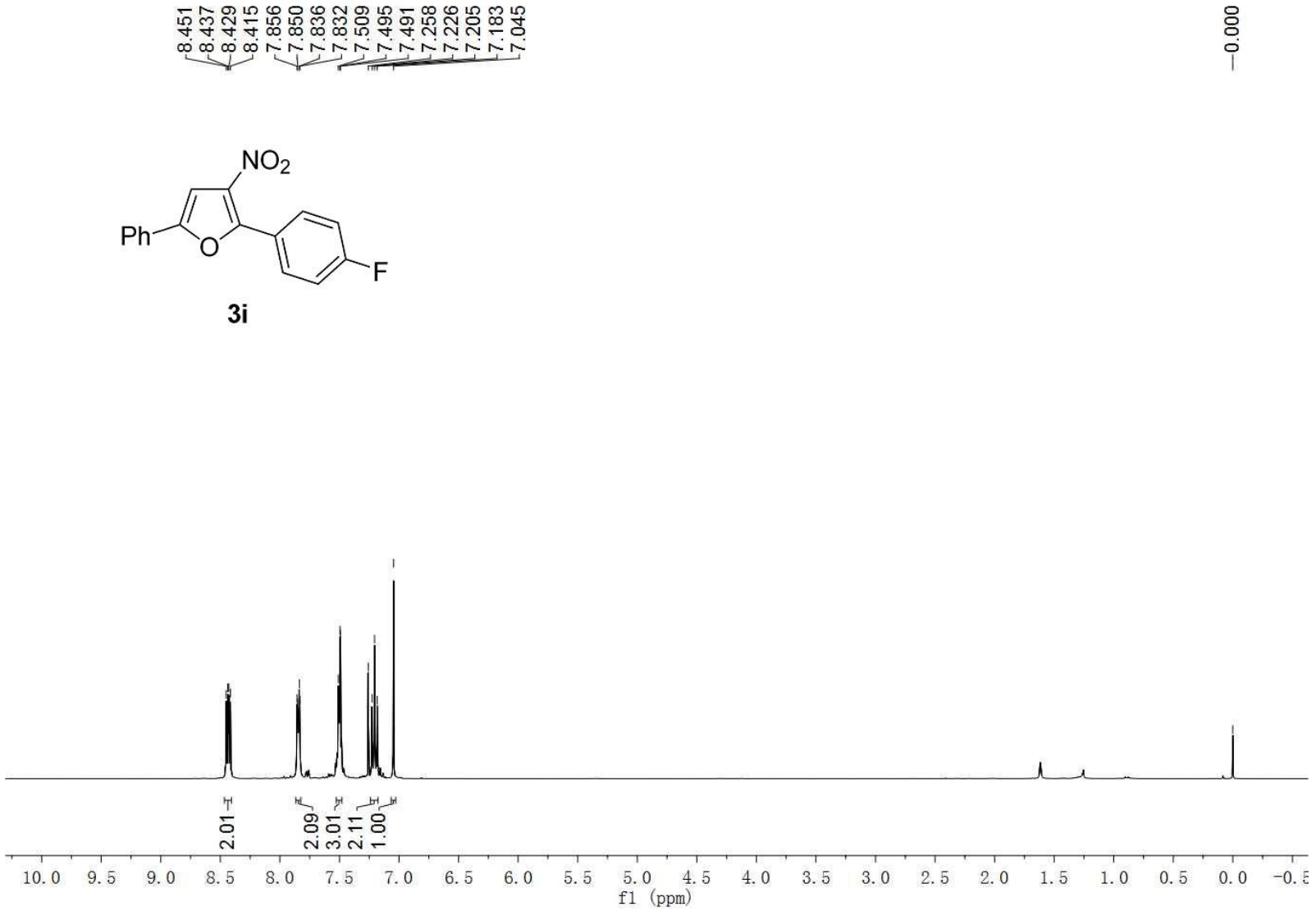

0.000

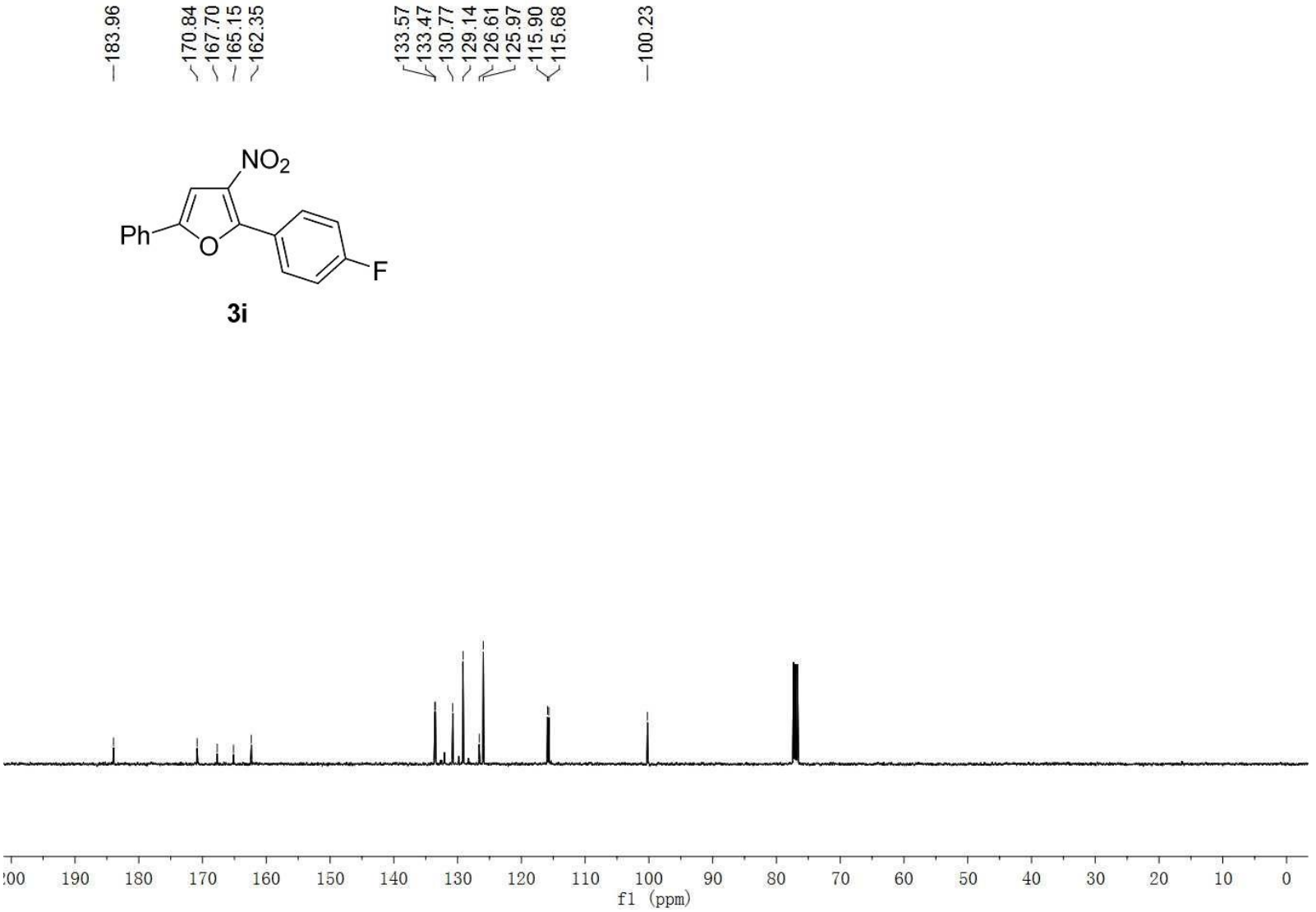

NO2
F
Ph
O

3h

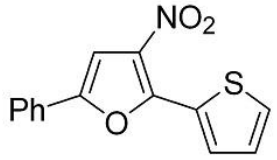

0.98
0.96
2.01
4.07
1.06
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


184.36
170.97
163.84
162.17
161.38
137.56
137.49
130.81
130.25
130.17
129.16
126.58
126.56
125.99
121.16
120.95
117.43
117.20
100.14
77.32
77.00
76.68
NO2
F
Ph
O
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

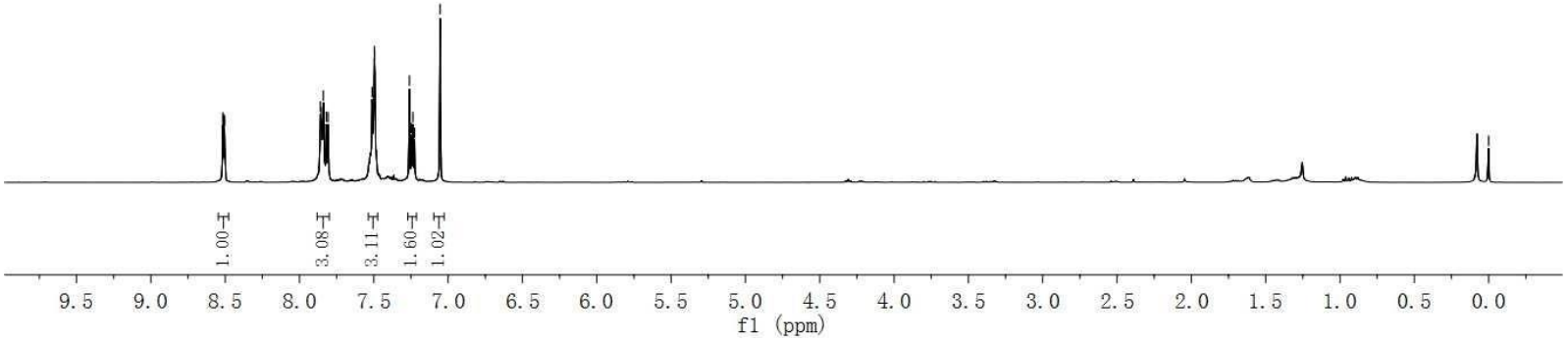

8.451
8.437
8.429
8.415
7.856
7.850
7.836
7.832
7.509
7.495
7.491
7.258
7.226
7.205
7.183
7.045
0.000
NO2
Ph
O
F
3i
2.01
2.09
3.01
2.11
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

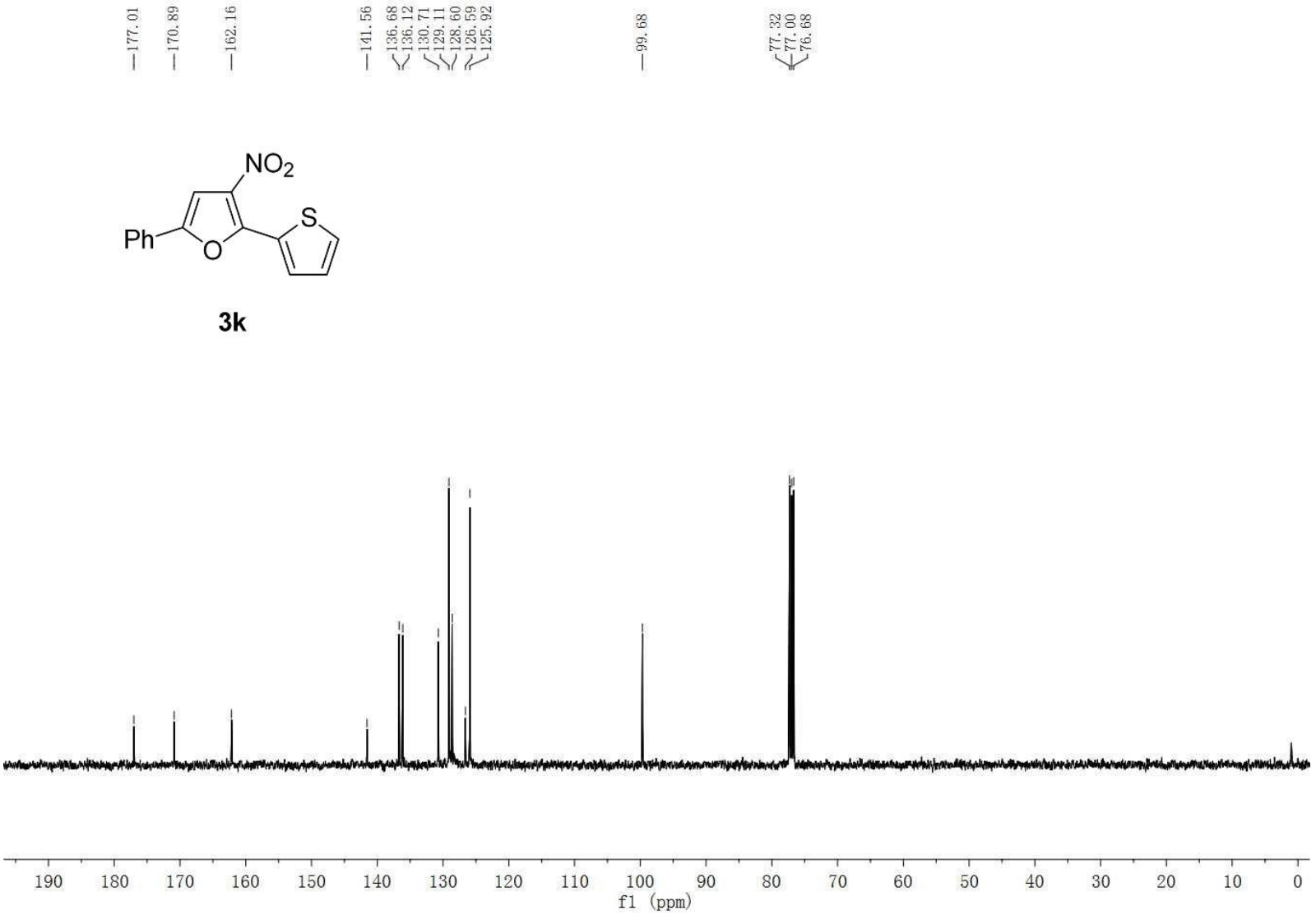

183.96
170.84
167.70
165.15
162.35
133.57
133.47
130.77
129.14
126.61
125.97
115.90
115.68
100.23
NO2
Ph
O
F
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

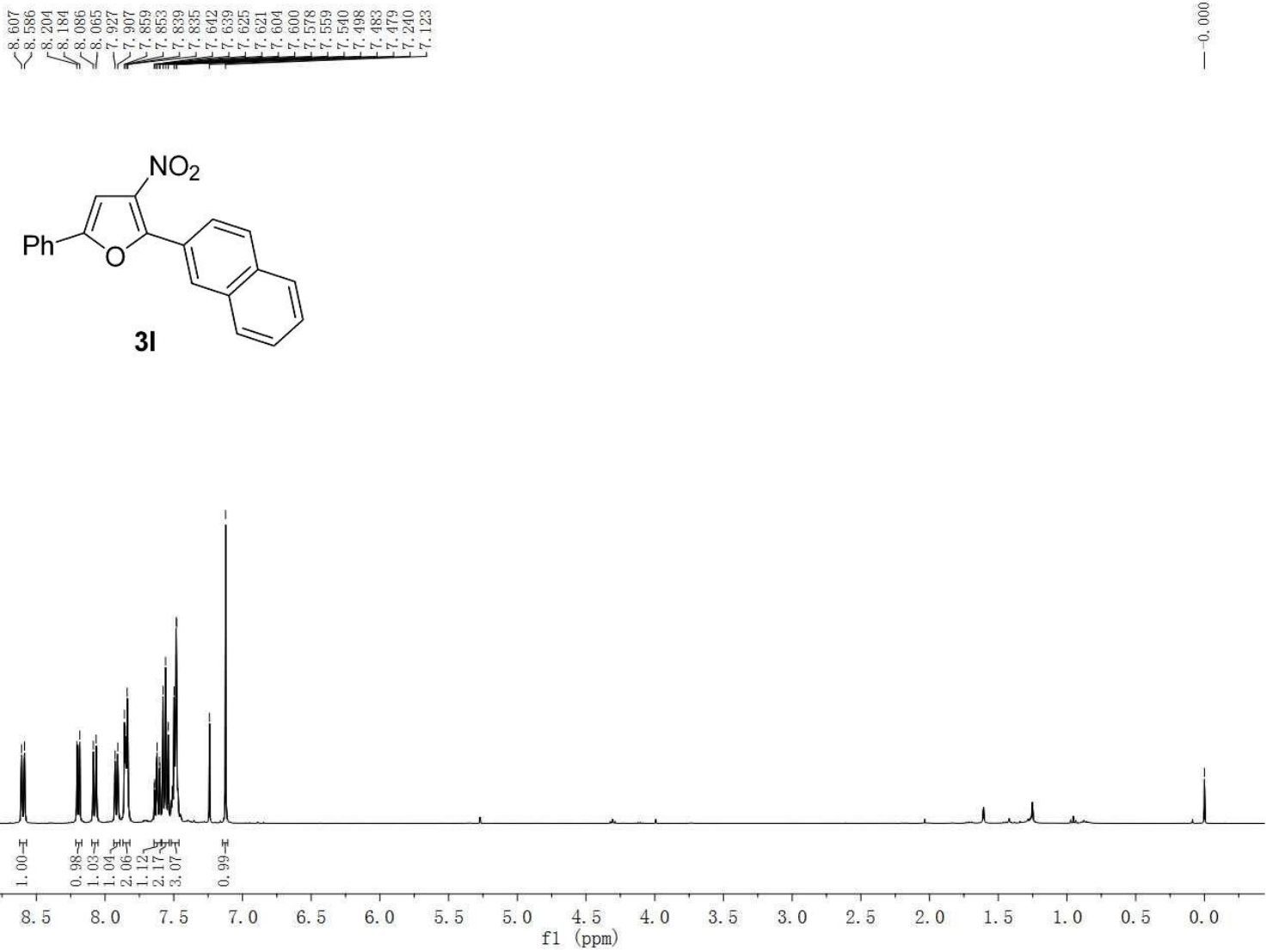

8.515
8.513
8.506
8.503
7.860
7.854
7.840
7.496
7.494
7.260
7.247
7.237
7.226
7.054
0.000

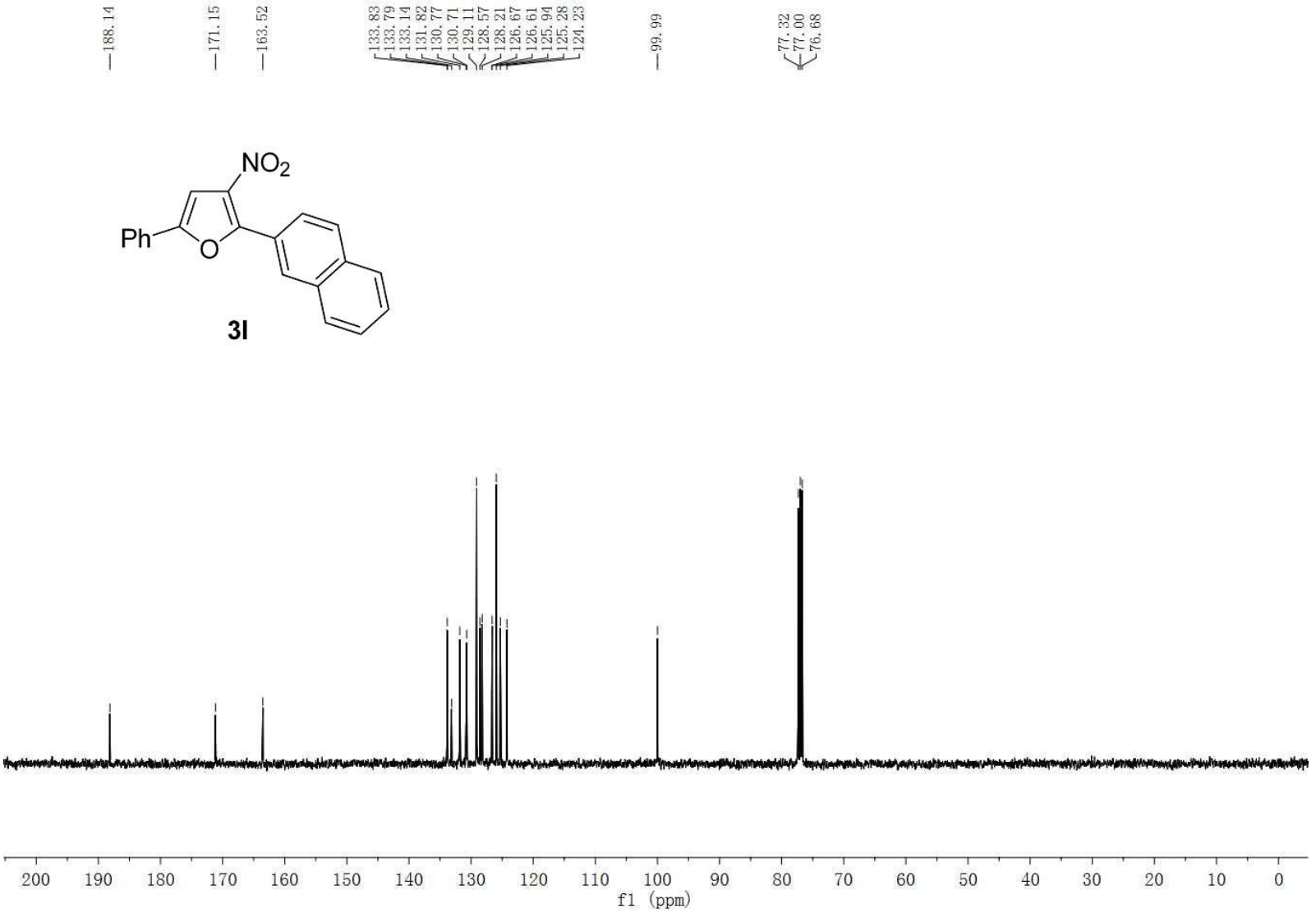

NO2
Ph
O
S

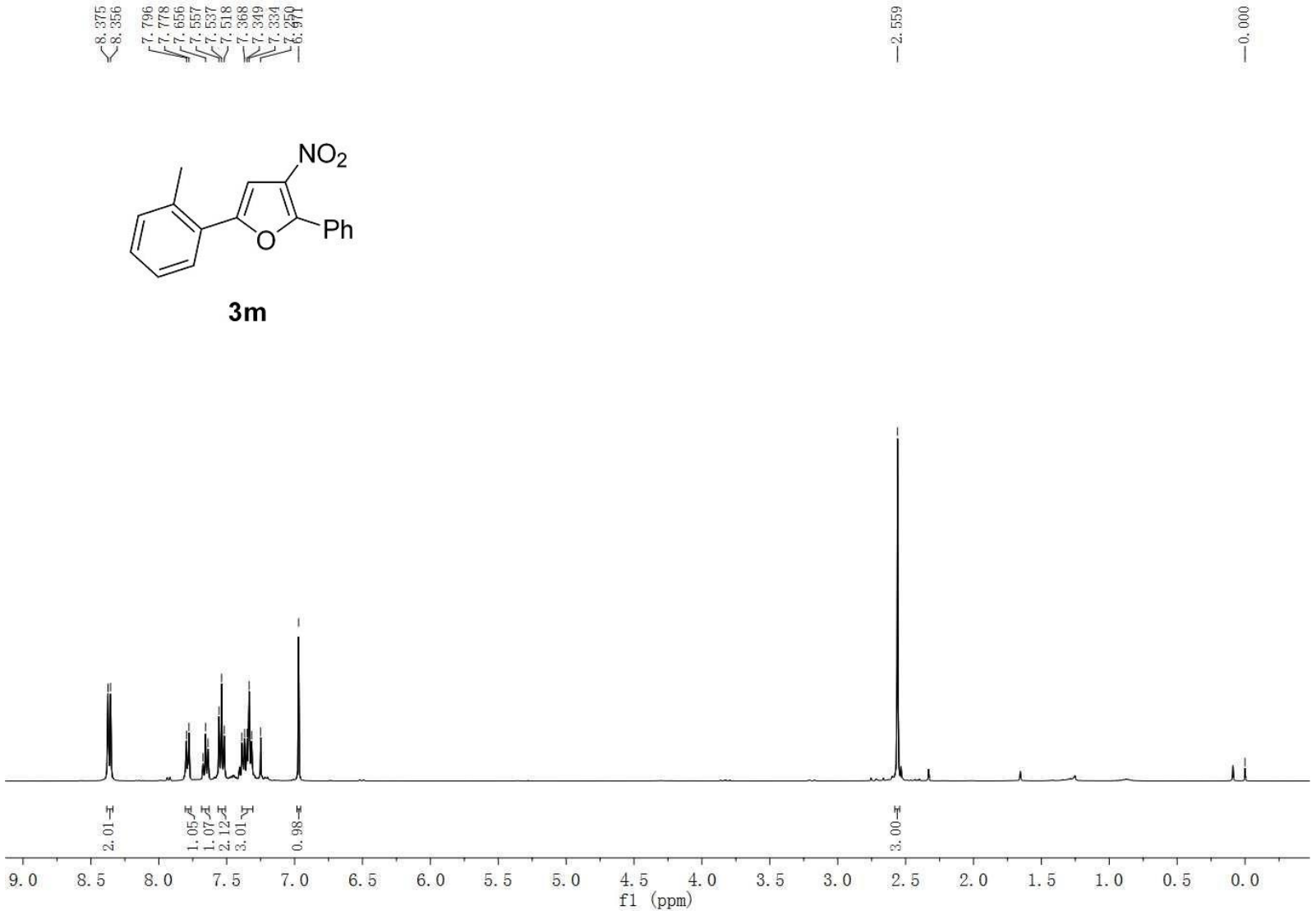
3k

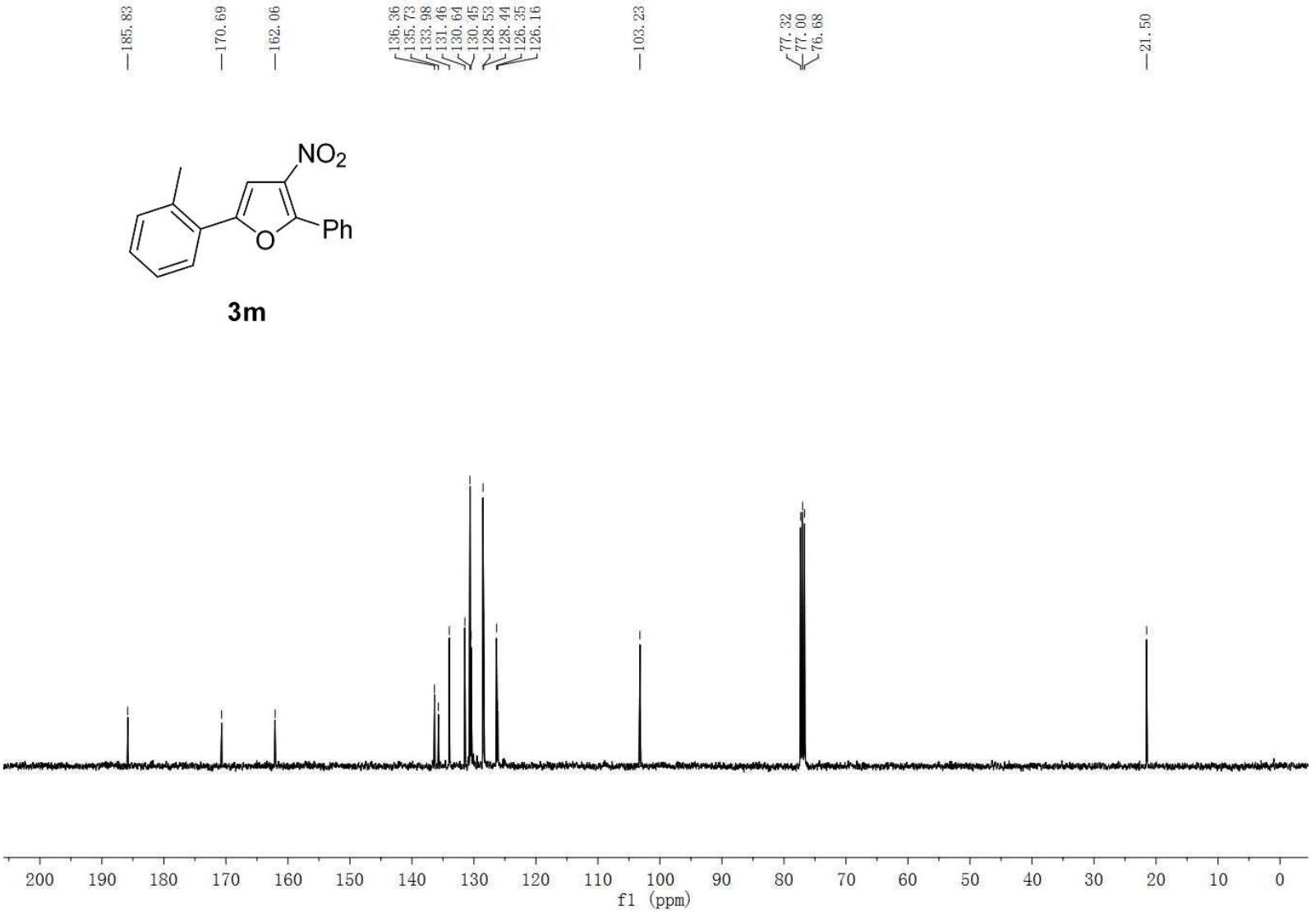

1.00
3.08
3.11
1.60
1.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

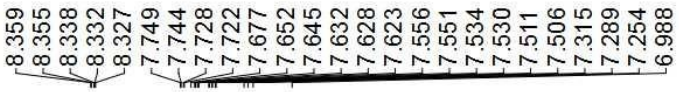

177.01
170.89
162.16
141.56
136.68
136.12
130.71
129.11
128.60
126.59
125.92
99.68
77.32
77.00
76.68
NO2
Ph
O
S
3k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

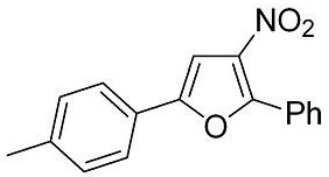

8.607
8.586
8.204
8.184
8.086
8.065
7.927
7.907
7.859
7.853
7.839
7.835
7.642
7.639
7.625
7.621
7.604
7.600
7.578
7.559
7.540
7.498
7.483
7.479
7.240
7.123
0.000
NO2
Ph
O
3l
1.00
0.98
1.03
1.04
2.06
1.12
2.17
3.07
0.99
f1 (ppm)


188.14
171.15
163.52
133.83
133.79
133.14
131.82
130.77
130.71
129.11
128.57
128.21
126.67
126.61
125.94
125.28
124.23
99.99
77.32
77.00
76.68
NO2
Ph
O
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

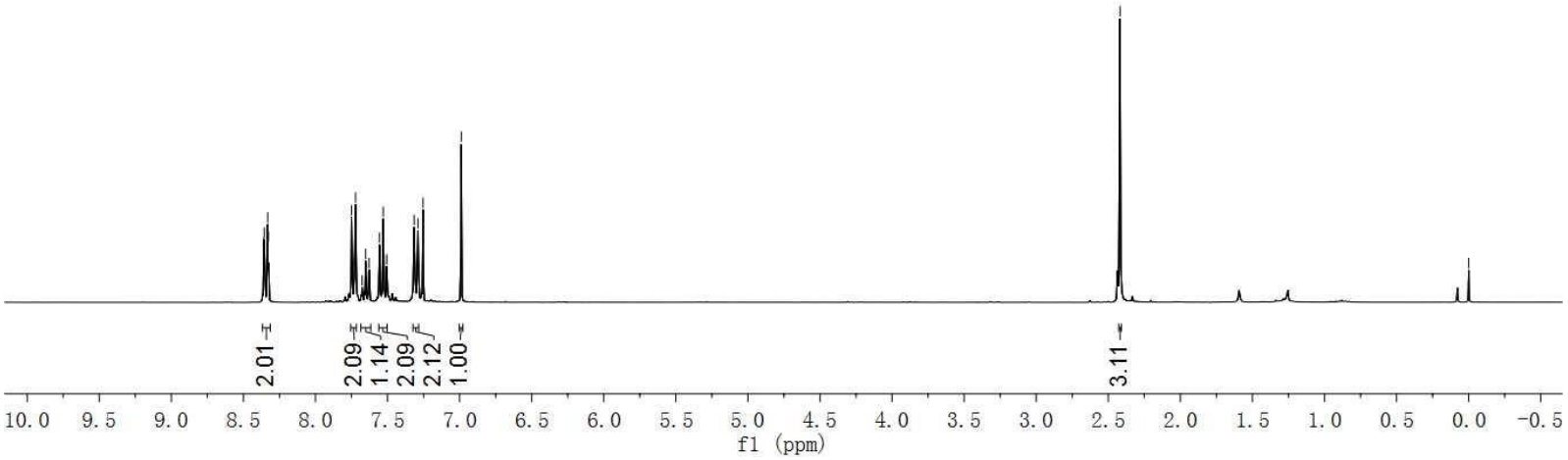

8.375
8.356
7.796
7.778
7.656
7.557
7.537
7.518
7.368
7.349
7.334
7.250
6.971
2.559
0.000
NO2
Ph
O
3m
2.01
1.05
1.07
2.12
3.01
0.98
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

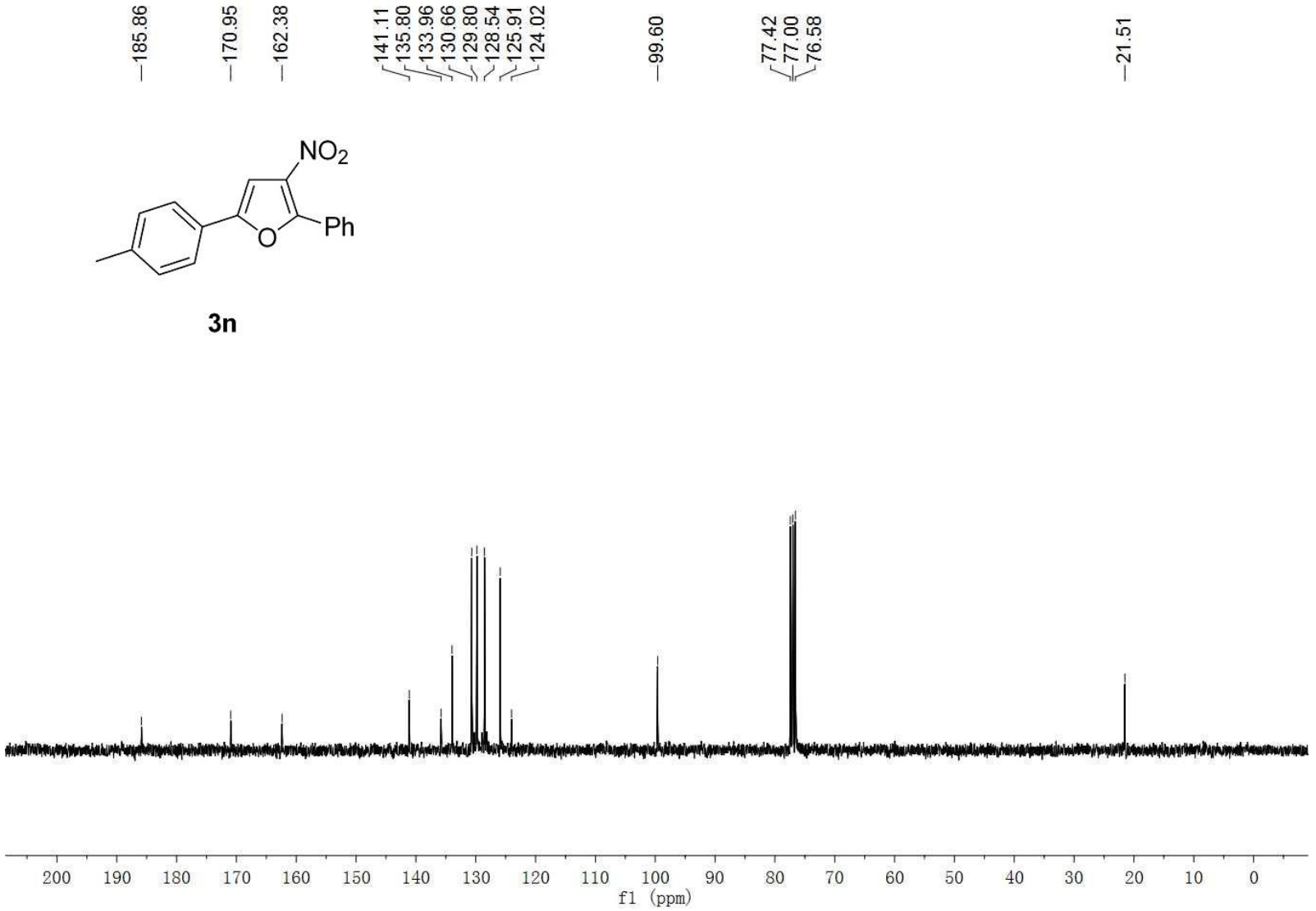

185.83
170.69
162.06
136.36
135.73
133.98
131.46
130.64
130.45
128.53
128.44
126.35
126.16
103.23
77.32
77.00
76.68
21.50
NO2
Ph
O
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

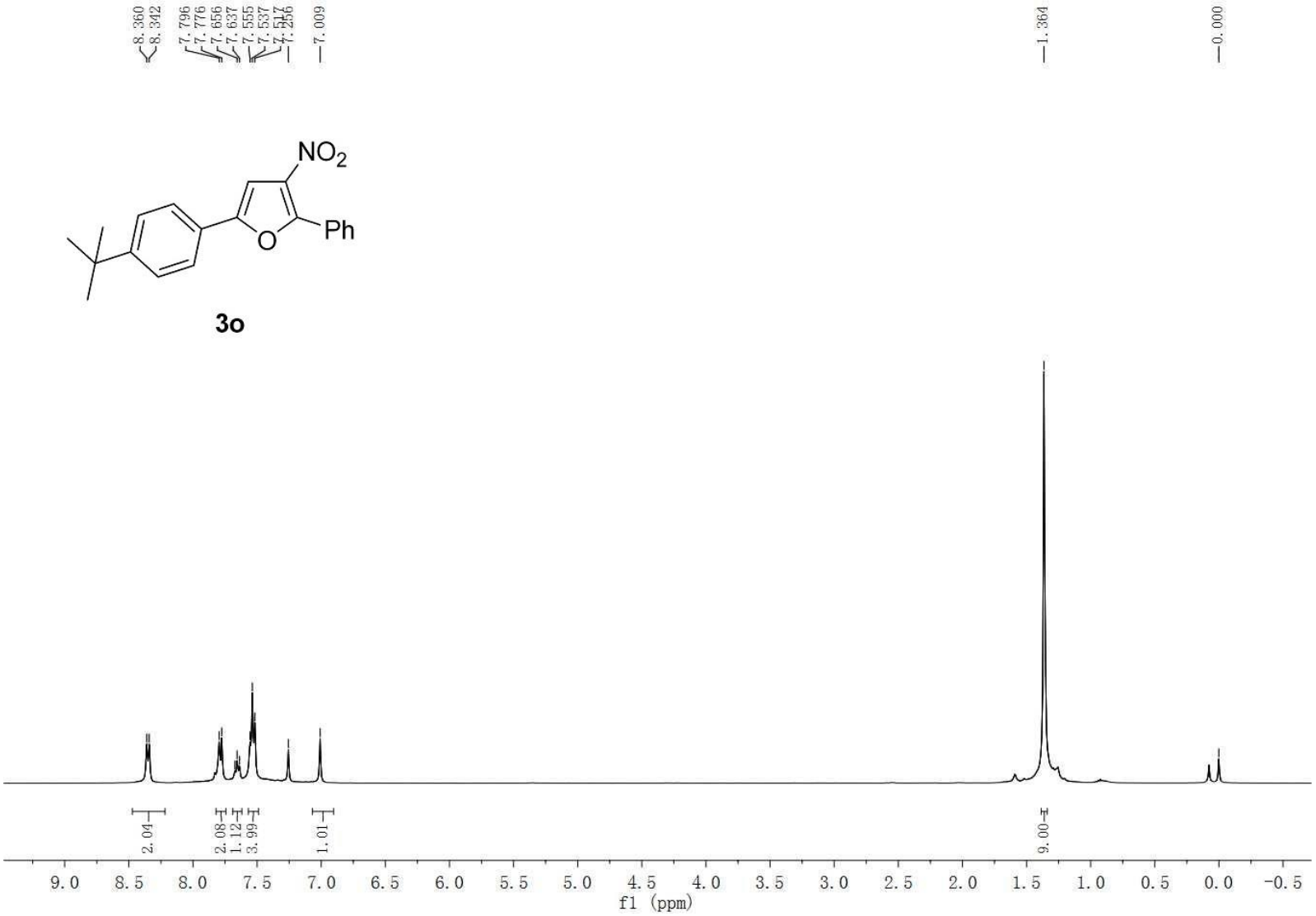

8.359
8.355
8.338
8.332
8.327
7.749
7.744
7.728
7.722
7.677
7.652
7.645
7.632
7.628
7.623
7.556
7.551
7.534
7.530
7.511
7.506
7.315
7.289
7.254
6.988
2.418
0.000

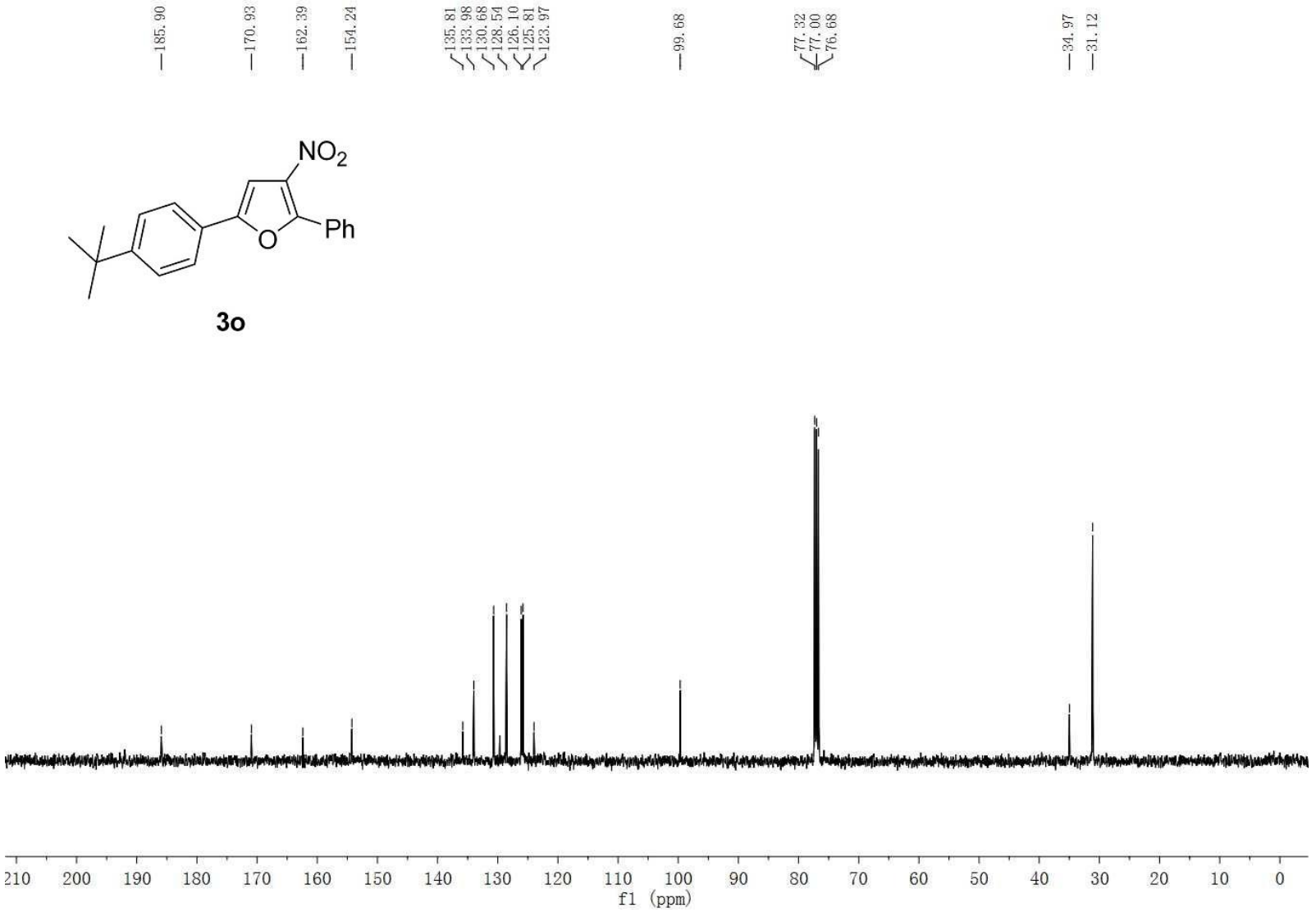

NO2
Ph
O

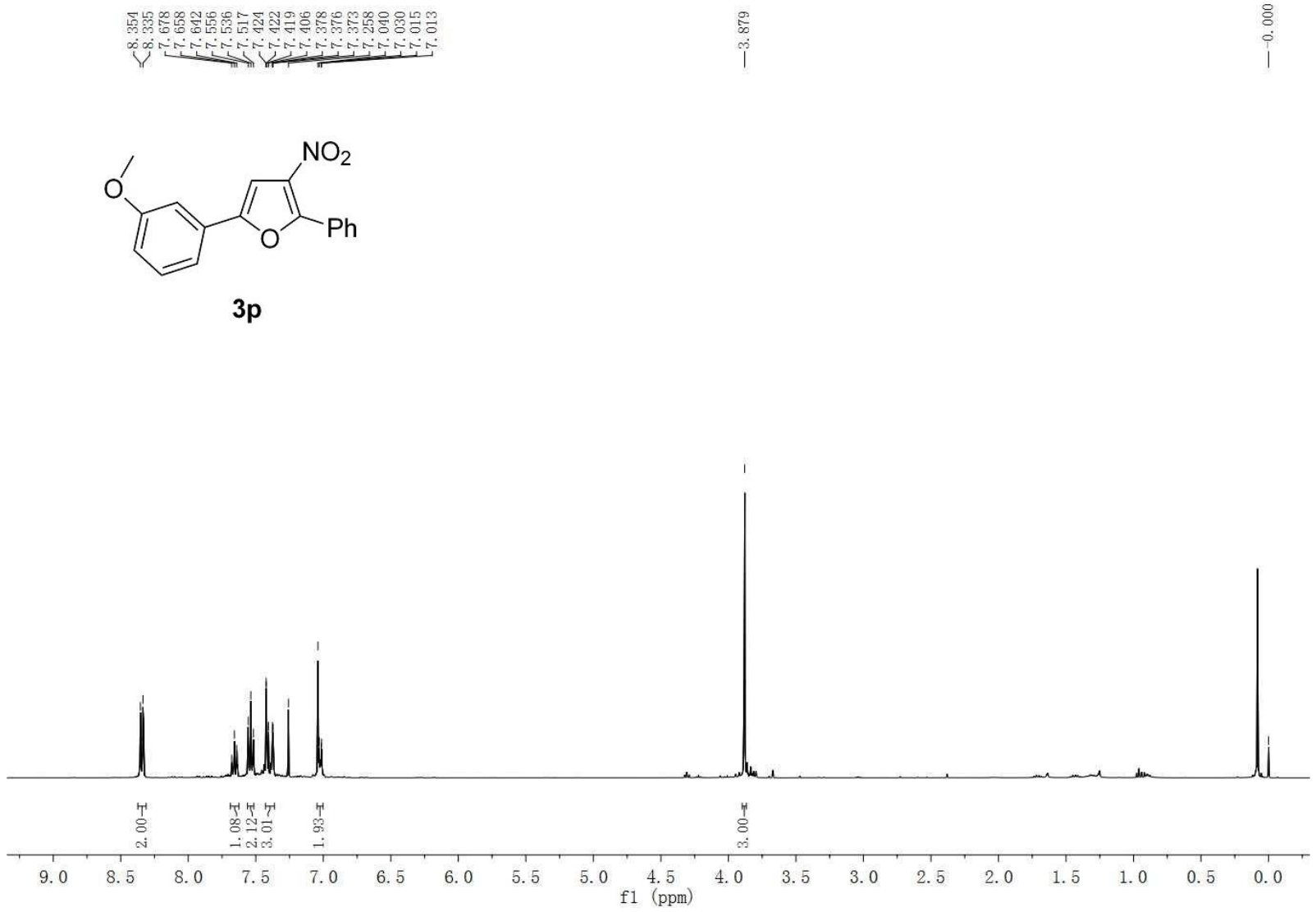
3n

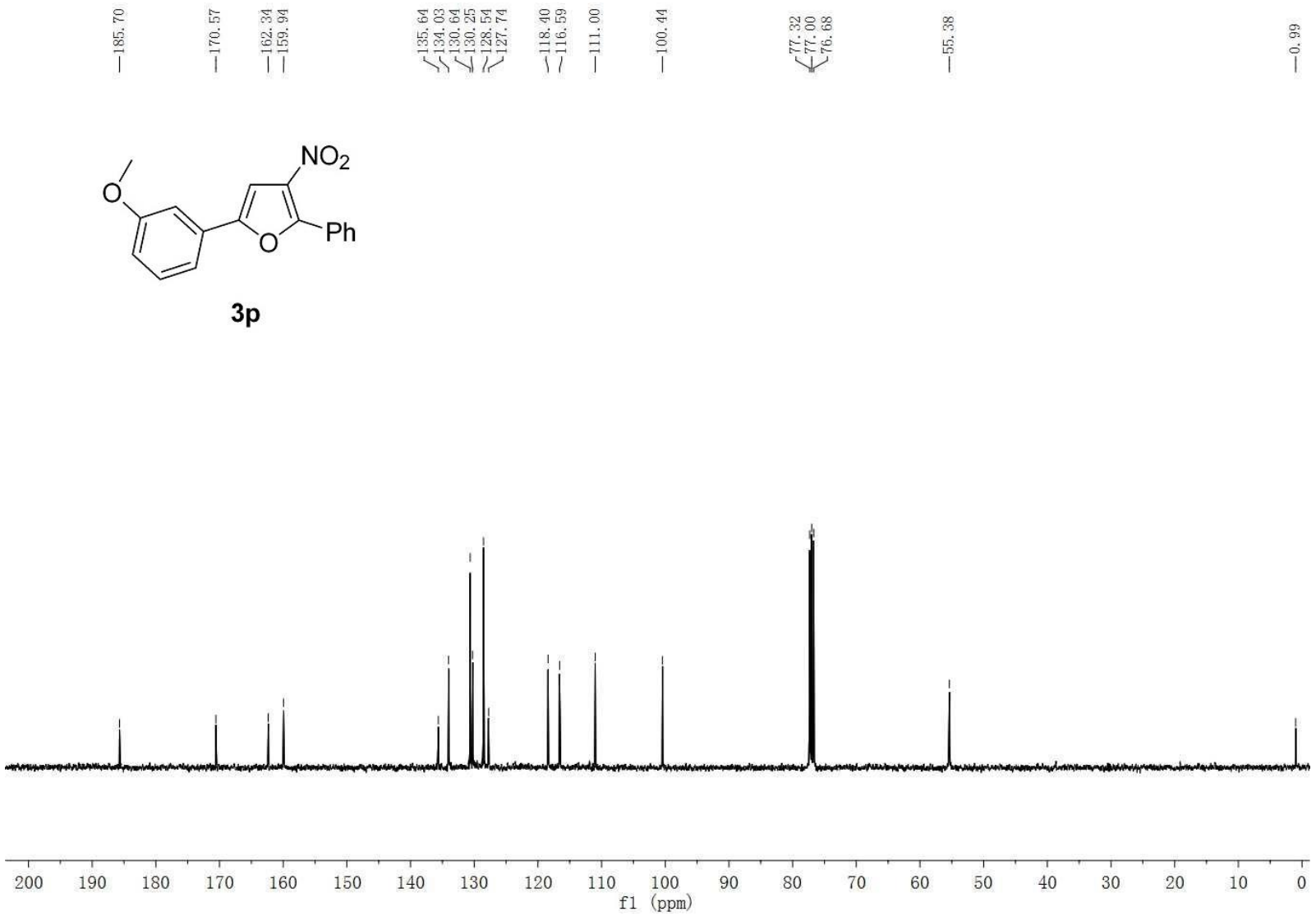

2.01
2.09
1.14
2.09
2.12
1.00
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

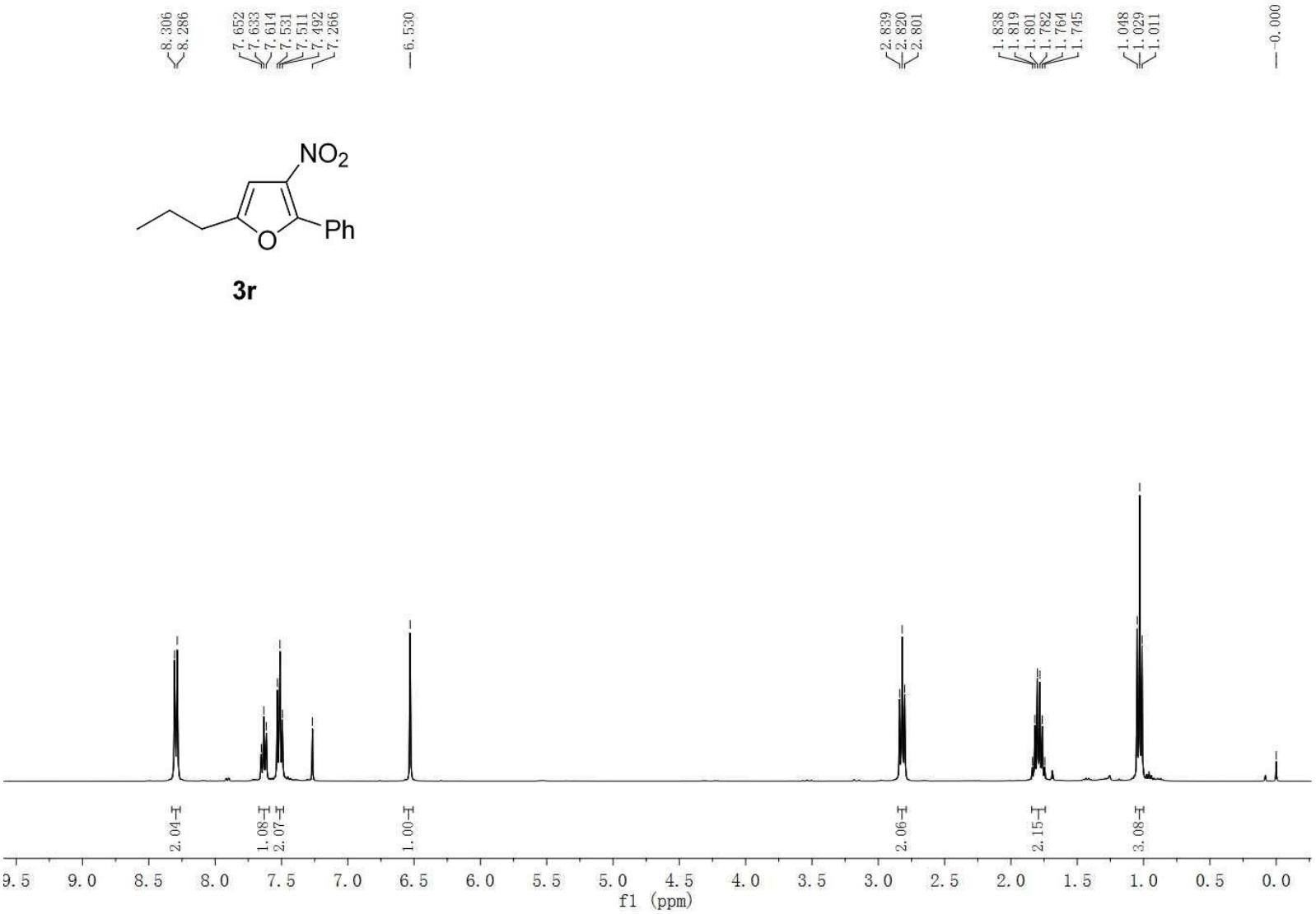

185.86
170.95
162.38
141.11
135.80
133.96
130.66
129.80
128.54
125.91
124.02
99.60
77.42
77.00
76.58
21.51
NO2
Ph
O
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

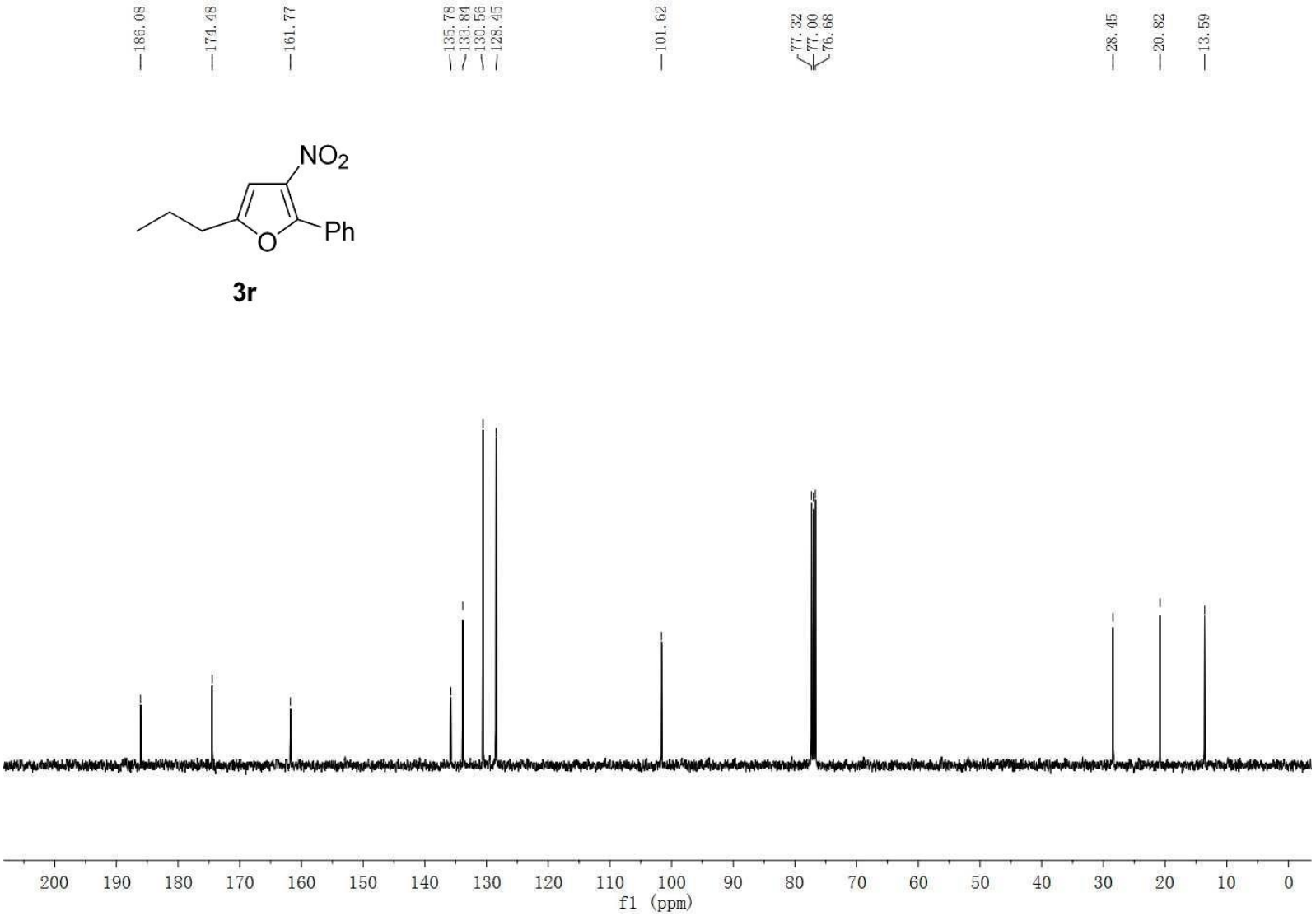

8.360
8.342
7.796
7.776
7.656
7.637
7.555
7.537
7.517
7.255
7.009
1.364
0.000
NO2
Ph
O
3o
2.04
2.08
1.12
3.99
1.01
9.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

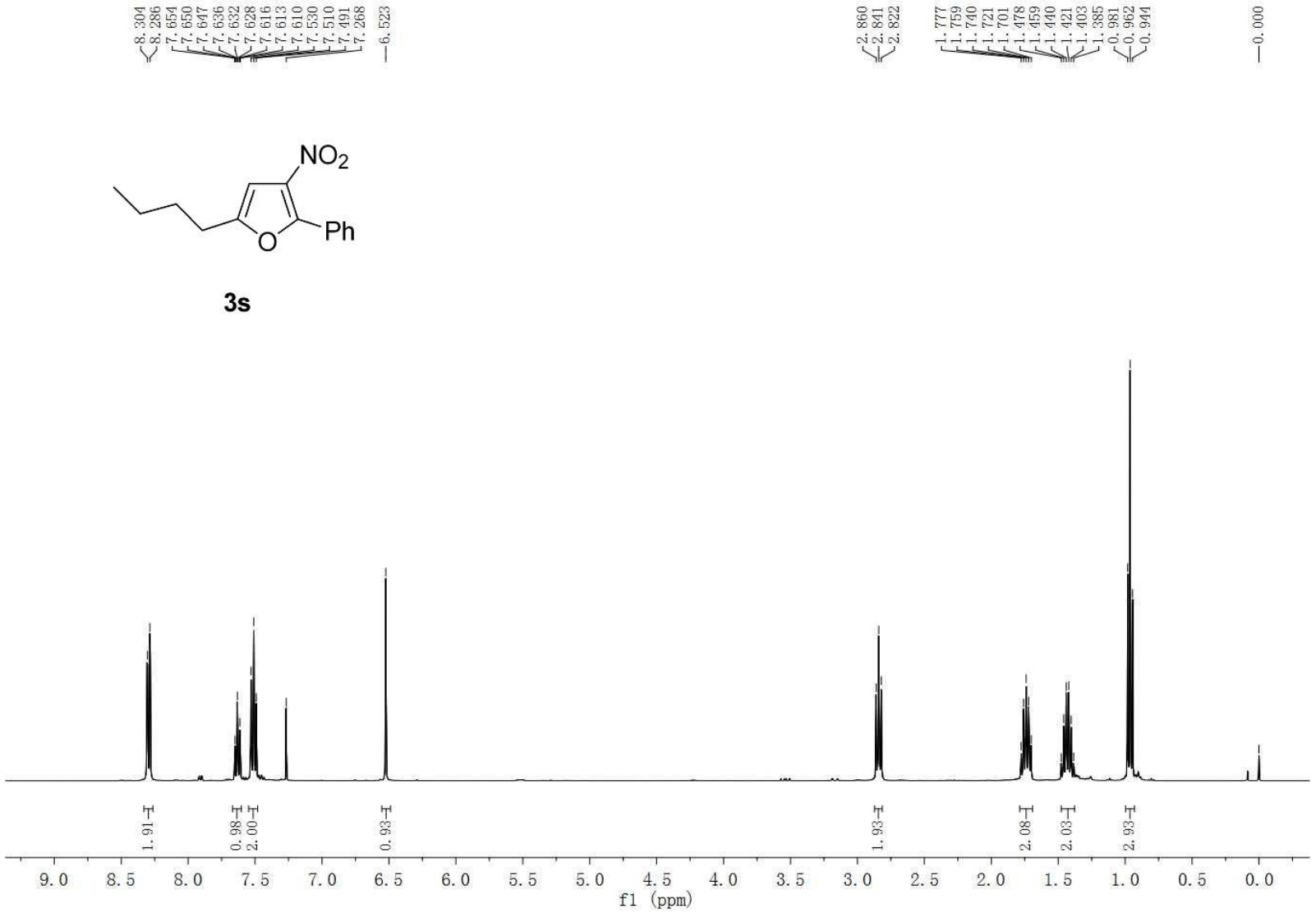

185.90
170.93
162.39
154.24
135.81
133.98
130.68
128.54
126.10
125.81
123.97
99.68
77.32
77.00
76.68
34.97
31.12
NO2
Ph
O
3o
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

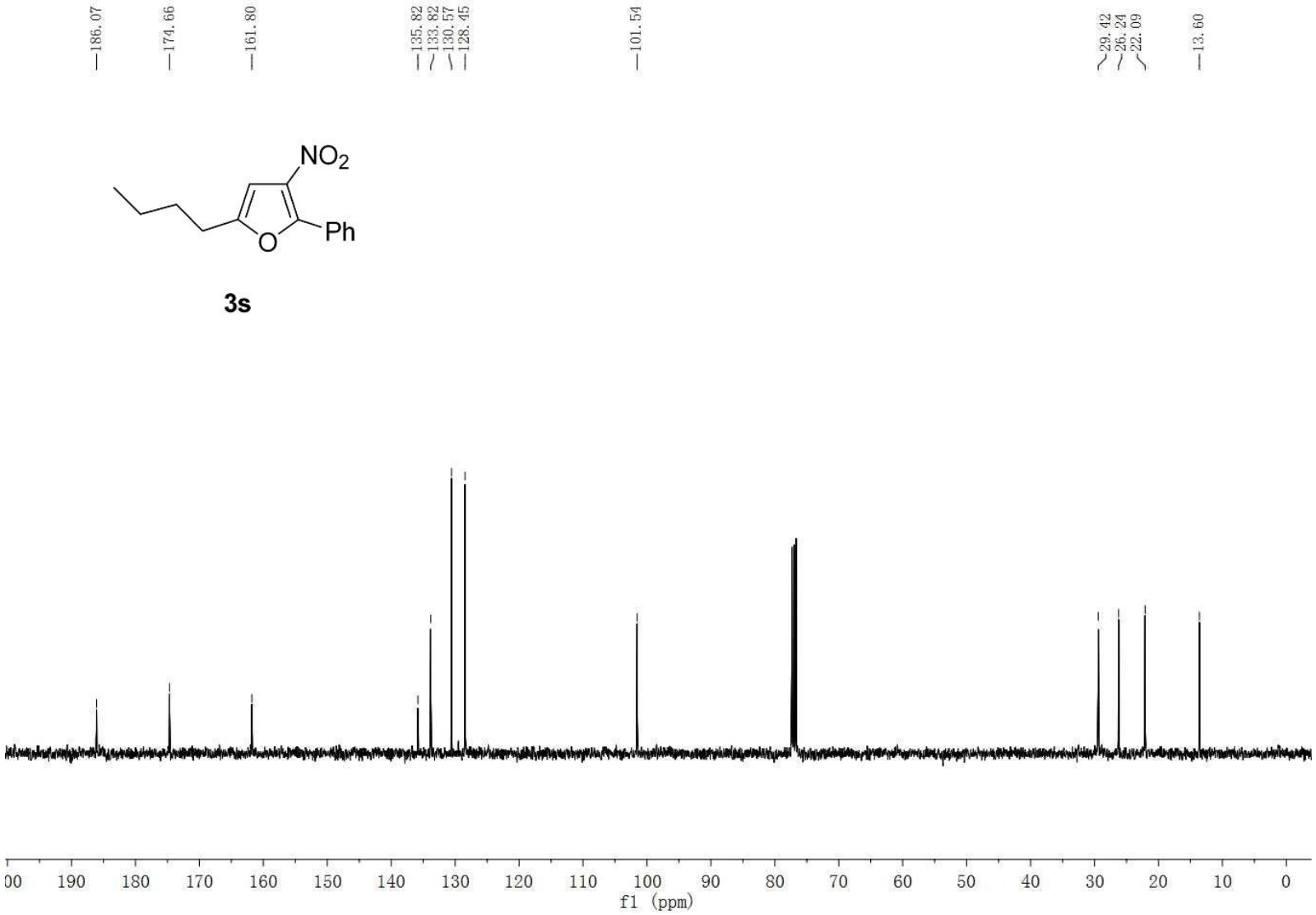

8.354
8.335
7.678
7.658
7.642
7.556
7.536
7.517
7.424
7.422
7.419
7.406
7.378
7.376
7.373
7.258
7.040
7.030
7.015
7.013
3.879
0.000
NO2
O
O
Ph
3p
2.00
1.08
2.12
3.01
1.93
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

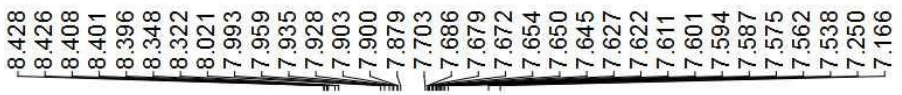

185.70
170.57
162.34
159.94
135.64
134.03
130.64
130.25
128.54
127.74
118.40
116.59
111.00
100.44
77.32
77.00
76.68
55.38
0.99
NO2
O
O
Ph
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

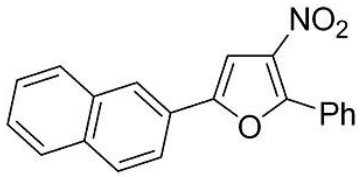

8.306
8.286
7.652
7.633
7.614
7.531
7.511
7.492
7.266
6.530
2.839
2.820
2.801
1.838
1.819
1.801
1.782
1.764
1.745
1.048
1.029
1.011
0.000
NO2
Ph
O
3r
2.04
1.08
2.07
1.00
2.06
2.15
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


186.08
174.48
161.77
135.78
133.84
130.56
128.45
101.62
77.32
77.00
76.68
28.45
20.82
13.59
NO2
Ph
O
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

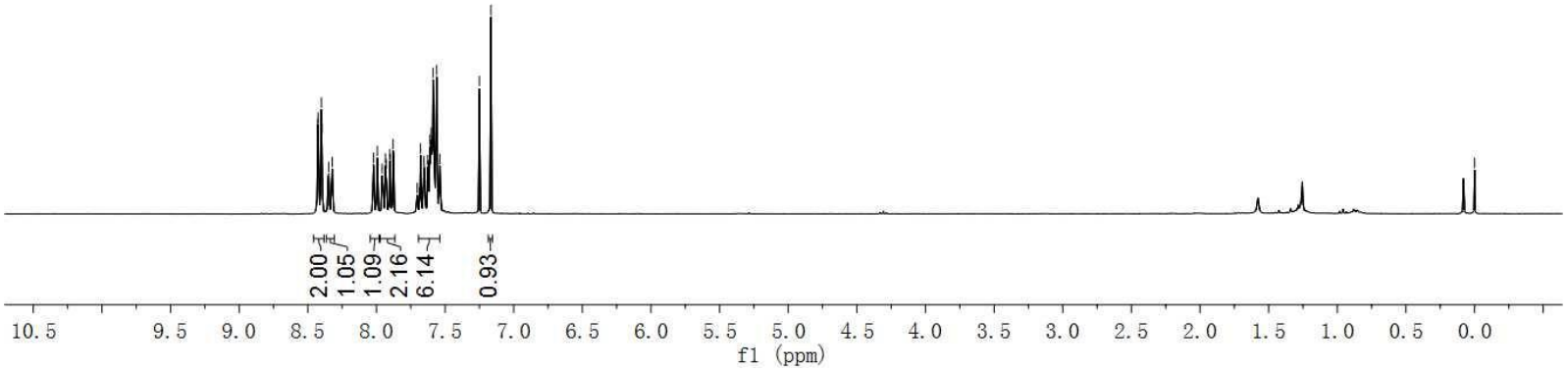

8.304
8.286
7.654
7.650
7.647
7.636
7.632
7.628
7.616
7.613
7.610
7.530
7.510
7.491
7.268
6.523
2.860
2.841
2.822
1.777
1.759
1.740
1.721
1.701
1.478
1.459
1.440
1.421
1.403
1.385
0.981
0.962
0.944
0.000
NO2
Ph
O
3s
1.91
0.98
2.00
0.93
1.93
2.08
2.03
2.93
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

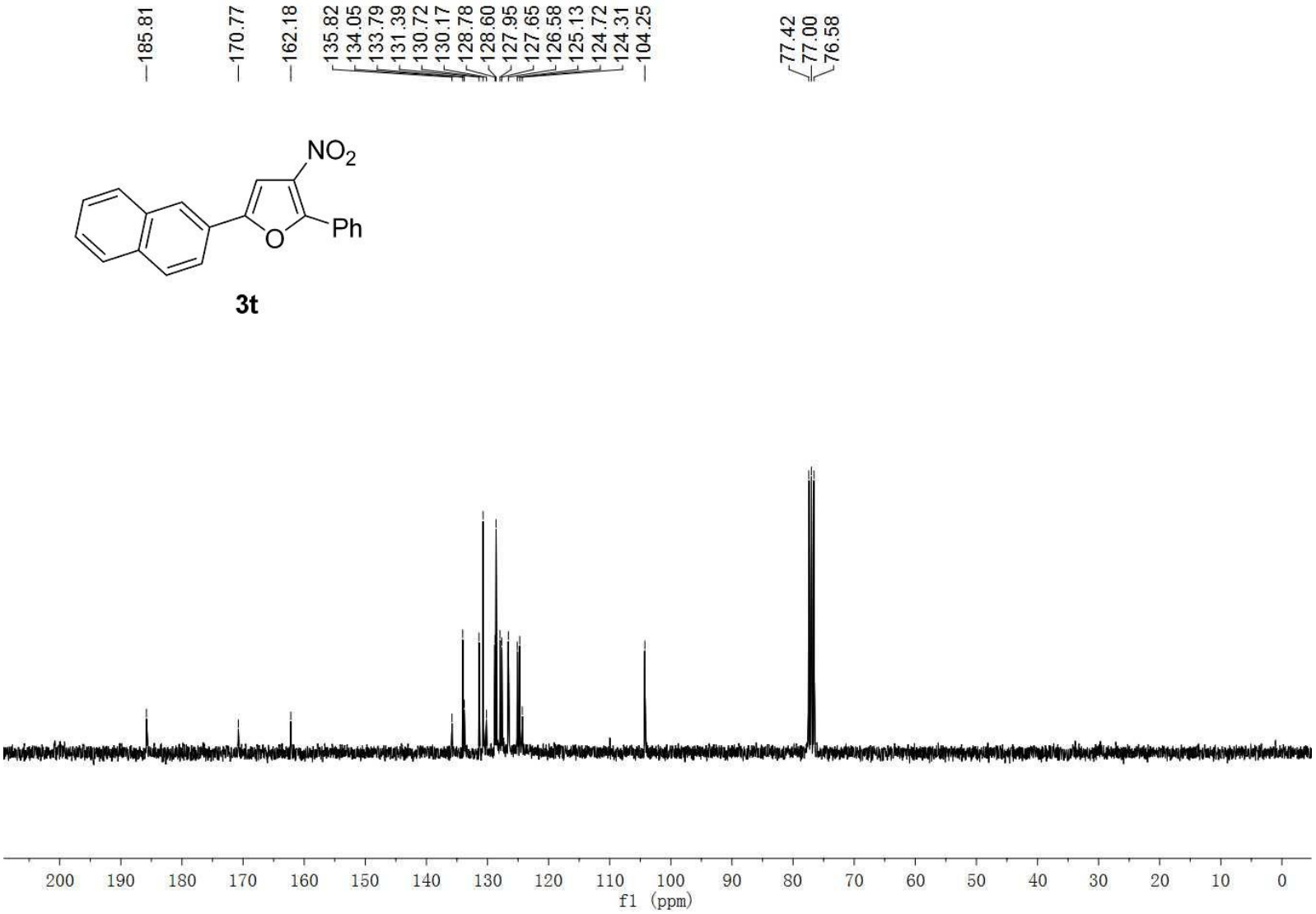

186.07
174.66
161.80
135.82
133.82
130.57
128.45
101.54
29.42
26.24
22.09
13.60
NO2
Ph
O
3s
f1 (ppm)

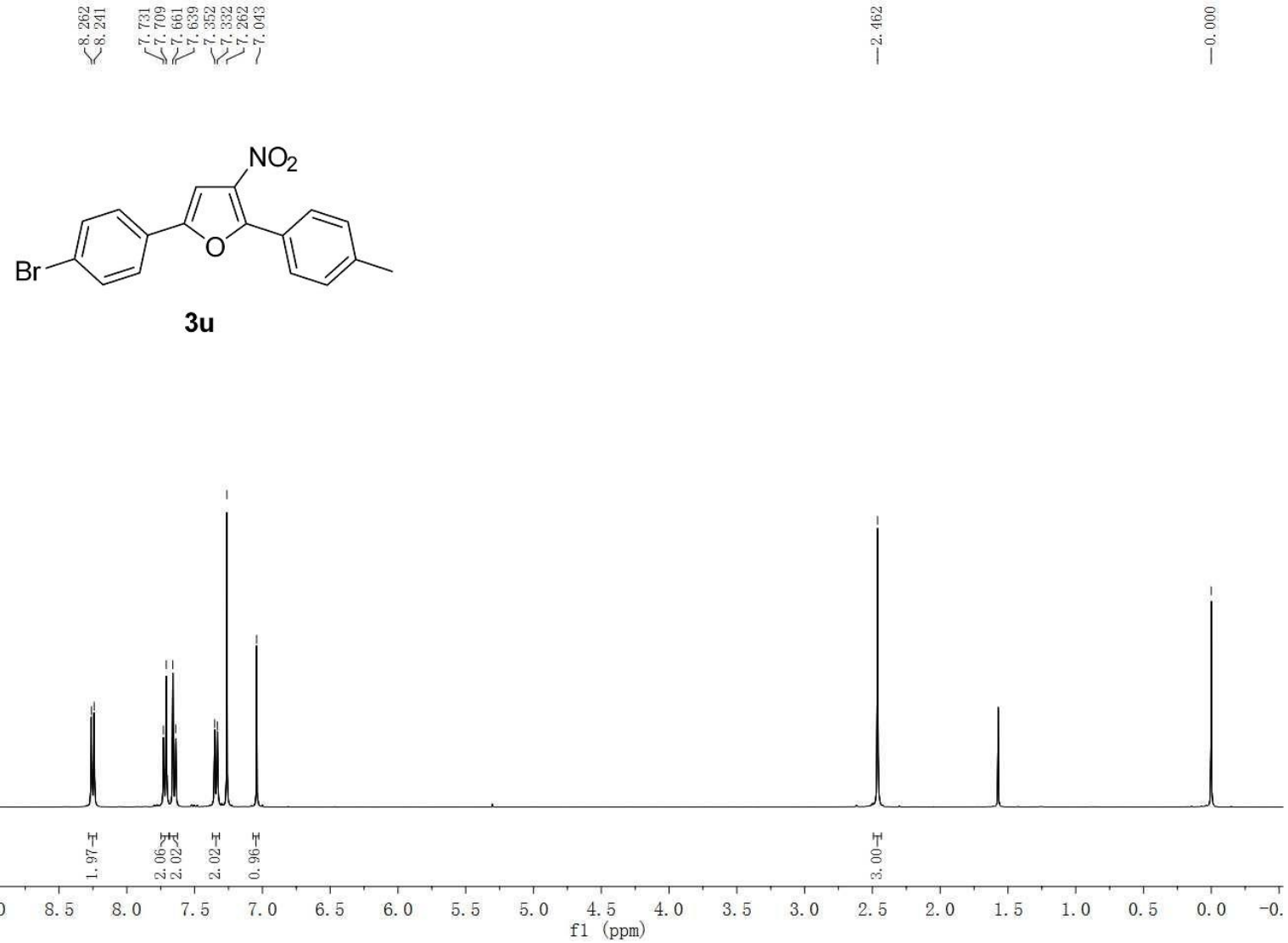

8.428
8.426
8.408
8.401
8.396
8.348
8.322
8.021
7.993
7.959
7.935
7.928
7.903
7.900
7.879
7.703
7.686
7.679
7.672
7.654
7.650
7.645
7.627
7.622
7.611
7.601
7.594
7.587
7.575
7.562
7.538
7.250
7.166
0.000

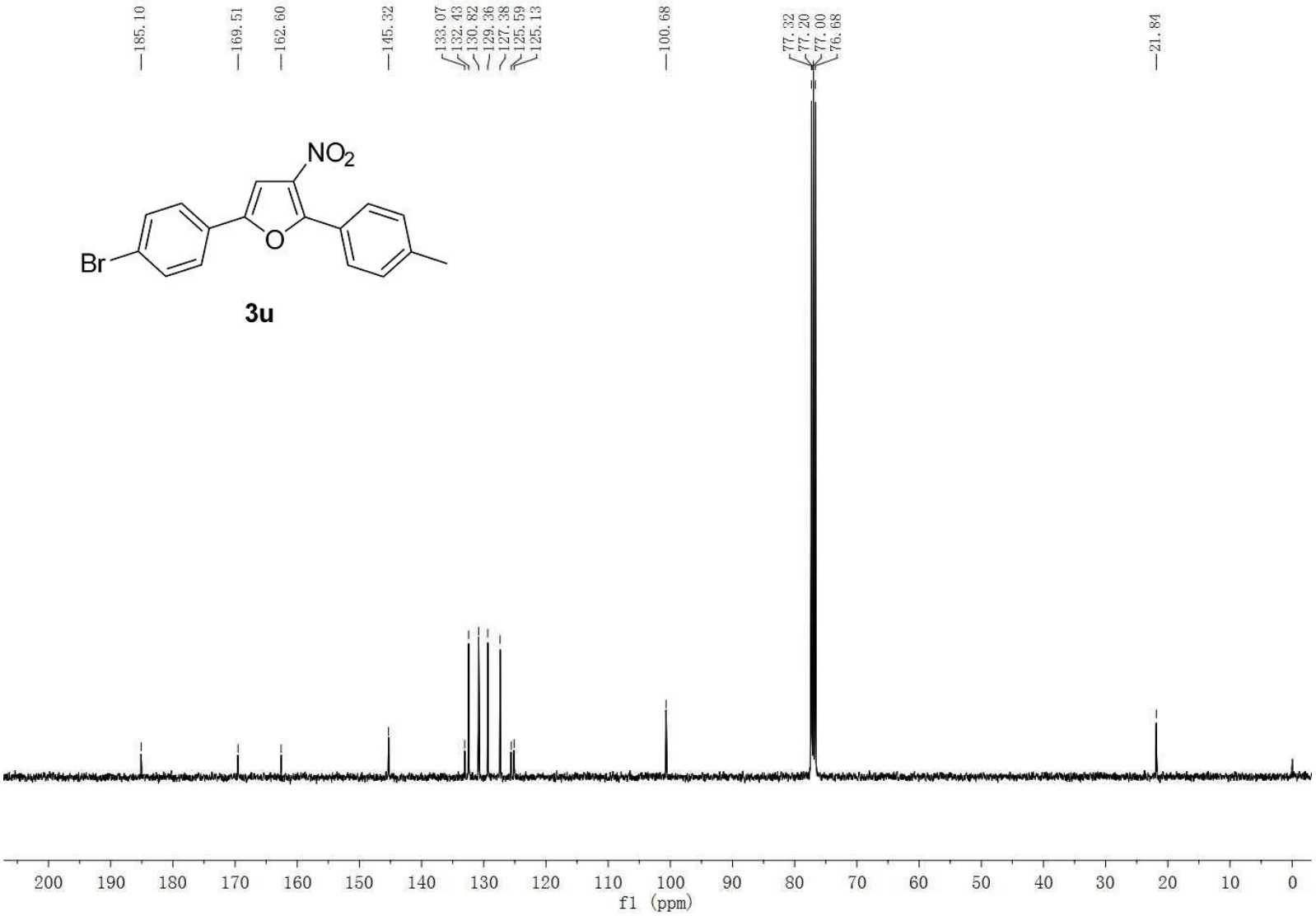

NO2
Ph
O

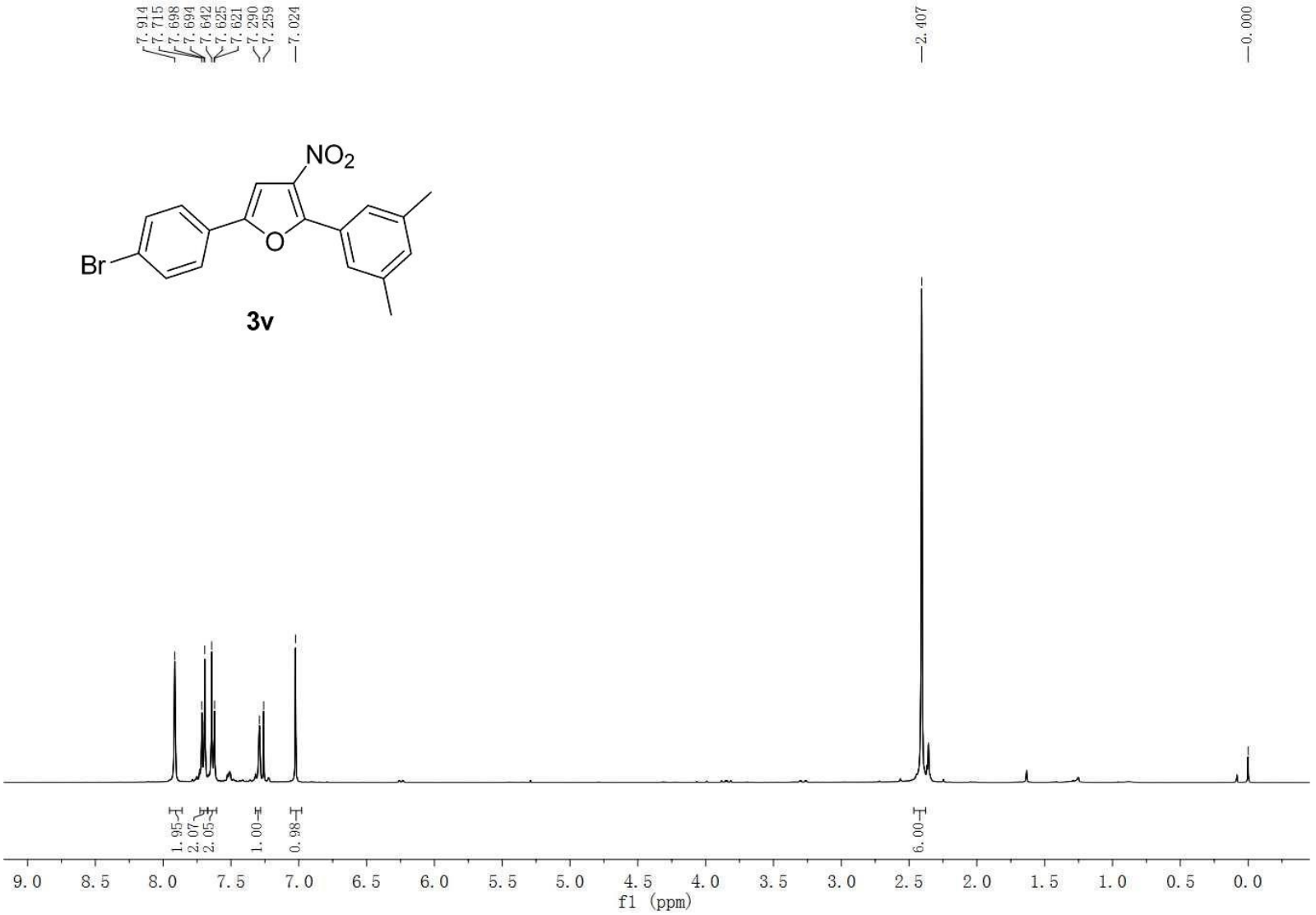
3t

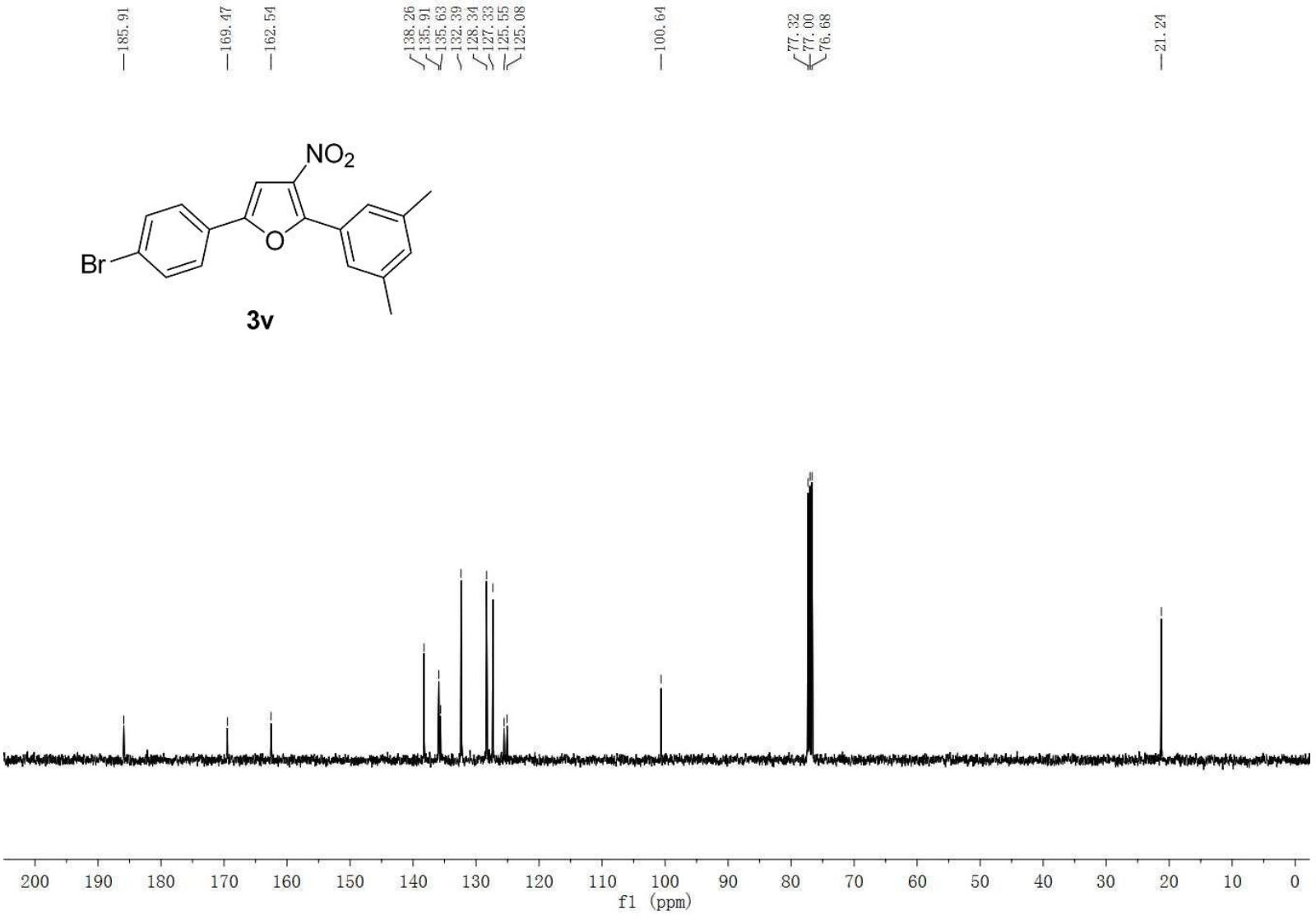

2.00
1.05
1.09
2.16
6.14
0.93
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


185.81
170.77
162.18
135.82
134.05
133.79
131.39
130.72
130.17
128.78
128.60
127.95
127.65
126.58
125.13
124.72
124.31
104.25
77.42
77.00
76.58
NO2
O
Ph
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.262
8.241
7.731
7.709
7.661
7.639
7.352
7.332
7.262
7.043
2.462
0.000
NO2
Br
O
3u
1.97
2.06
2.02
2.02
0.96
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


185.10
169.51
162.60
145.32
133.07
132.43
130.82
129.36
127.38
125.59
125.13
100.68
77.32
77.20
77.00
76.68
21.84
NO2
Br
O
3u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.914
7.715
7.698
7.694
7.642
7.625
7.621
7.290
7.259
7.024
2.407
0.000
NO2
Br
O
3v
1.95
2.07
2.05
1.00
0.98
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


185.91
169.47
162.54
138.26
135.91
135.63
132.39
128.34
127.33
125.55
125.08
100.64
77.32
77.00
76.68
21.24
NO2
Br
O
3v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)