Supplementary Information

Transition-Metal-Free Aerobic C-O Bond Formation via C-N Bond Cleavage

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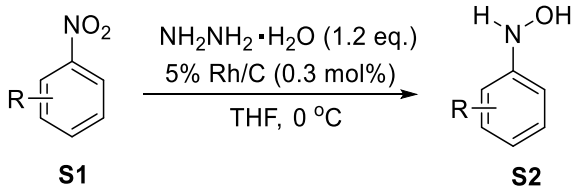
Table of Contents

General remarks

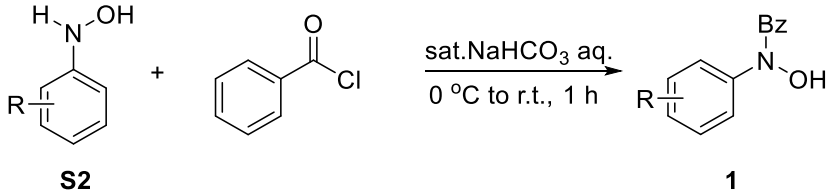
All reactions were performed in conventional Schlenk techniques under an atmosphere of nitrogen unless otherwise stated. Solvents were dried following standard procedures under argon. Syringe was used to transfer liquids and solutions. All reactions were monitored by thin-layer chromatography (TLC) with E. Merck silica gel 60 F254 pre-coated plates (0.25 mm). Silica gel (particle size 200-300 mesh) purchased from SiliCycle was used for flash chromatography. For reactions that require heating, oil bath was used.

Proton (^{1}H) and carbon (^{13}C) NMR spectra were taken on a Bruker AV-500 spectrometer operating at 500 MHz or 400 MHz for proton and 126 MHz or 101 MHz for carbon nuclei using $CDCl_3$ or DMSO- d_6 as solvent, respectively. Chemical shifts are expressed as parts per million (δ, ppm) and are referenced to 7.26 ($CDCl_3$) for ^{1}H NMR and 77.00 ($CDCl_3$) for ^{13}C NMR. Proton signal data uses the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and *J* = coupling constant. High Resolution Mass Spectrometry was obtained with a Bruker Apex II mass instrument under the conditions of electrospray ionization (ESI) in both positive and negative mode.

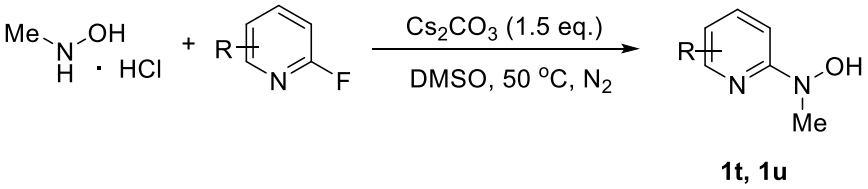
General procedure for the synthesis of protected *N*-aryl-*N*-hydroxylamines[1, 2]



Nitroarene **S1** (1.0 equiv.) was added to a solution of 5% Rh/C (0.30 mol% Rh) in THF (0.324 M) under atmosphere of nitrogen .Then hydrazine monohydrate (1.2 equiv.) was added dropwise to the above mixture at 0 ℃. Then the reaction mixture was stirred at indicated temperature for 1 hour and slowly heated to room temperature. The reaction mixture was filtered and concentrated *in vacuo*. Title compound **S2** were recrystallized from CH_2Cl_2/ Petroleum ether (PE) at –20 ℃. The crude residue was used directly for the next step without further purification.



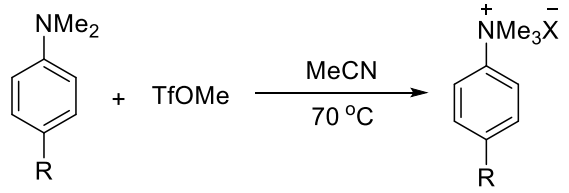
Saturated aqueous solution (1 M) of sodium bicarbonate was added to a solution of **S2** in ether (0.5 M). Benzoyl chloride was added dropwise to the mixture at 0 ℃. Then, the solution was stirred for 1 hour at room temperature. Saturated aqueous ammonium chloride was used to quench the reaction solution. After the mixture was extracted with CH_2Cl_2, the organic layer was washed by brine and dried over sodium sulfate. Solvent was then removed in vacuum and the crude product was purified by recrystallization (PE/CH_2Cl_2) to obtain the product **1**.



Under N_2 atmosphere, a suspension of *N*-methylhydroxylamine hydrochloride (3.0 equiv.), 2,6-difluoropyridine (5 mmol, 1.0 equiv.) or 2-fluoro-5-iodopyridine and Cs_2CO_3 (1.5 equiv.) in DMSO (15 mL) was heated to 50 ℃. Then, the solution was

stirred for 2 hours with cooling the solution to room temperature. The reaction was quenched by water (60 mL). The mixture was extracted with ether (3 × 25 mL) and the organic layer was washed by brine and dried over sodium sulfate. After the solvent was removed *in vacuo*, the crude product was purified by flash chromatography (PE/EtOAc = 5/1) to obtain **1t** or **1u**.

General Procedure for Preparations of Aryltrimethylammonium Salts[3]



2

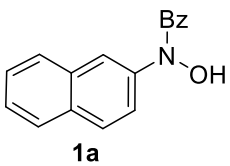
Methyl trifluoromethanesulfonate (0.62 mL, 5.5 mmol, 1.1 equiv.) was added by dropwise to a stirred solution of *N*,*N*-dimethylaniline (5 mmol) in MeCN (10 mL) at 70 ℃. The resulting solution was stirred for 12 hours at 70 ℃. Solvent was then removed in vacuum and the residue was washed with EtOAc or Et_2O, dried under vacuum to give a white solid.

For **2a′**, trimethyloxonium tetrafluoroborate (1.1 equiv.) was added instead of methyl trifluoromethanesulfonate by dropwise at 70 ℃.

For **2a″**, methyl iodide (1.1 equiv.) was added instead of methyl trifluoromethanesulfonate by dropwise at 70 ℃.

Analytical data of starting materials

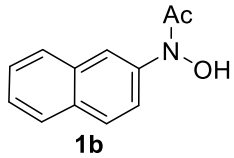
1. *N*-hydroxy-*N*-(naphthalen-2-yl)benzamide (1a)



1a

Pink solid, m.p. = 139-141 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.82 (d, *J* = 3.9 Hz, 1H), 7.95 (dd, *J* = 23.1, 8.6 Hz, 2H), 7.63 (s, 1H), 7.53-7.27 (m, 5H), 7.21 (d, J = 7.6 Hz, 1H), 7.19 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 165.7, 137.0, 133.1, 132.4, 132.3, 131.1, 129.0, 128.9, 128.3, 128.2, 127.7, 126.91, 126.87, 124.4, 123.7; HRMS (ESI) m/z calcd for $[C_{17}H_{14}NO_2]^+$ $[M+H]^+$: 264.1019, found 264.1026.

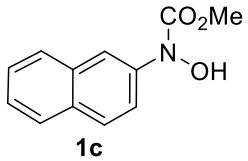
2. *N*-hydroxy-*N*-(naphthalen-2-yl)acetamide (1b)



1b

White solid, m.p. = 84-86 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (400 MHz, DMSO- *d*$_6$): δ 10.83 (s, 1H), 8.15 (s, 1H), 7.90 (dd, *J* = 15.4, 8.2 Hz, 4H), 7.67-7.36 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, DMSO- *d*$_6$): δ 139.9, 133.4, 130.8, 128.4, 128.2, 127.9, 127.0, 125.9, 120.8, 23.1; HRMS (ESI) m/z calcd for $[C_{12}H_{12}NO_2]^+$ $[M+H]^+$: 202.0863, found 202.0893.

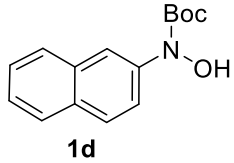
3. methyl hydroxy(naphthalen-2-yl)carbamate (1c)



1c

White solid, m.p. = 88-89 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 (s, 1H), 7.76 (d, *J* = 1.7 Hz, 1H), 7.66 (dt, *J* = 9.1, 5.8 Hz, 3H), 7.50 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.39-7.27 (m, 2H), 3.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 156.2, 138.2, 133.1, 131.4, 128.3, 128.0, 127.5, 126.4, 125.8, 121.2, 119.7, 53.8; HRMS (ESI) m/z calcd for $[C_{12}H_{12}NO_3]^+$ $[M+H]^+$: 218.0812, found 218.0817.

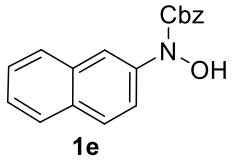
4. *tert*-butyl hydroxy(naphthalen-2-yl)carbamate (1d)



1d

White solid, m.p. = 132-134 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.94 (s, 1H), 7.81 (s, 1H), 7.76-7.68 (m, 3H), 7.56 (dd, *J* = 8.9, 1.8 Hz, 1H), 7.44-7.29 (m, 2H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 154.5, 138.4, 133.3, 131.1, 128.0, 127.9, 127.5, 126.4, 125.6, 121.2, 118.8, 83.6, 28.3; HRMS (ESI) m/z calcd for $[C_{15}H_{17}NO_3Na]^+$ $[M+Na]^+$: 282.1101, found 282.1093.

5. benzyl hydroxy(naphthalen-2-yl)carbamate (1e)

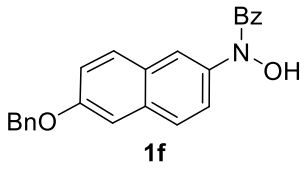


1e

White solid, m.p. = 89-91 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.77 (s, 1H), 7.67 (dd, *J* = 20.5, 10.5 Hz, 3H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.4-7.31 (m, 2H), 7.27-7.14 (m, 5H), 5.13 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.3, 138.0, 135.5, 133.2, 131.4, 128.6, 128.5, 128.4, 128.2, 128.0, 127.6, 126.5, 125.9, 121.1, 119.5, 68.7; HRMS (ESI) m/z calcd for $[C_{18}H_{16}NO_3]^+$ $[M+H]^+$:

294.1125, found 294.1131.

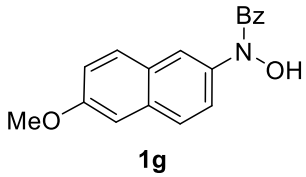
6. *N*-(7-(benzyloxy)naphthalen-2-yl)-*N*-hydroxybenzamide (1f)



1f

Yellow solid, m.p. = 162-163 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (400 MHz, DMSO- d_6): δ 10.82 (s, 1H), 8.06 -7.61 (m, 6H), 7.58-7.12 (m, 10H), 5.23 (s, 2H); ^{13}C NMR (101 MHz, DMSO- d_6): δ 168.4, 156.9, 138.3, 137.4, 136.0, 132.6, 130.71, 129.9, 128.94, 128.88, 128.6, 128.4, 128.3, 127.4, 123.0, 120.6, 119.9, 107.7, 69.8; HRMS (ESI) m/z calcd for $[C_{24}H_{20}NO_3]^+$ $[M+H]^+$: 370.1438, found 370.1440.

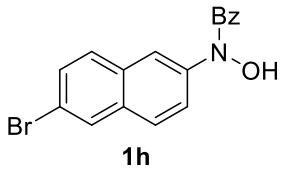
7. *N*-hydroxy-*N*-(6-methoxynaphthalen-2-yl)benzamide (1g)



1g

Yellow solid, m.p. = 167-168 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 20.2, 8.8 Hz, 3H), 7.50-7.42 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.29-7.19 (m, 3H), 7.14 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.09 (d, *J* = 2.3 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6): δ 168.4, 157.9, 138.3, 136.1, 132.8, 130.7, 129.8, 128.9, 128.5, 128.3, 128.1, 127.4, 123.0, 119.6, 106.4, 55.7; HRMS (ESI) m/z calcd for $[C_{18}H_{16}NO_3]^+$ $[M+H]^+$: 294.1125, found 294.1133.

8. *N*-(6-bromonaphthalen-2-yl)-*N*-hydroxybenzamide (1h)

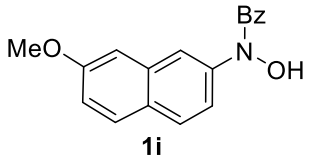


1h

White solid, m.p. = 162-164 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.92 (s, 1H), 8.20 (s, 1H), 8.10 (s, 1H), 7.90 (dt, *J* = 20.0, 8.8 Hz, 3H), 7.71 (d, *J* = 7.2 Hz, 2H), 7.63 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.53-7.41 (m, 3H); ^{13}C NMR (126 MHz, DMSO-d_6): δ 168.8, 140.7, 135.8, 132.3, 131.9, 131.0, 130.5, 130.0, 129.9, 128.9, 128.4, 127.8, 123.0, 119.3; HRMS (ESI) m/z calcd for $[C_{17}H_{13}B_rNO_2]^+$ $[M+H]^+$: 342.0124, found 342.0126.

9. *N*-hydroxy-*N*-(7-methoxynaphthalen-2-yl)benzamide (1i)

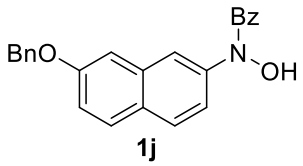
Yellow solid, m.p. = 148-149 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.86 (s, 1H), 8.00 (s, 1H), 7.82 (dd, *J* = 17.1, 8.8 Hz, 2H), 7.72 (d, *J* =



1i

7.1 Hz, 2H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.51-7.38 (m, 3H), 7.33 (s, 1H), 7.21-7.07 (m, 1H), 3.86 (s, 3H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 168.6, 158.3, 140.7, 136.1, 134.8, 130.8, 129.5, 128.9, 128.4, 128.3, 126.7, 119.7, 118.9, 118.8, 106.6; 55.7; HRMS (ESI) m/z calcd for $[C_{18}H_{16}NO_3]^+$ $[M+H]^+$: 294.1125, found 294.1119.

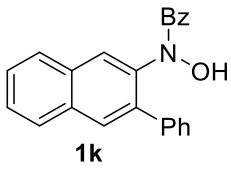
10. *N*-(7-(benzyloxy)naphthalen-2-yl)-*N*-hydroxybenzamide (1j)



1j

White solid, m.p. = 131-132 ºC; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 10.88 (s, 1H), 7.99 (s, 1H), 7.84 (s, 2H), 7.69 (d, *J* = 33.0 Hz, 3H), 7.44 (t, *J* = 39.9 Hz, 9H), 7.23 (s, 1H), 5.22 (s, 2H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 168.6, 157.3, 140.8, 137.4, 136.1, 134.7, 130.8, 129.58, 128.9, 128.4, 126.8, 119.7, 119.1, 118.8, 107.9, 69.8; HRMS (ESI) m/z calcd for $[C_{24}H_{20}NO_3]^+$ $[M+H]^+$: 370.1438, found 370.1444.

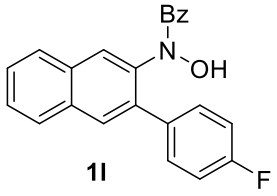
11. *N*-hydroxy-*N*-(3-phenylnaphthalen-2-yl)benzamide (1k)



1k

White solid, m.p. = 76-78 ºC; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, DMSO-*d*$_6$): δ 10.86 (s, 1H), 8.17 (s, 1H), 8.01 (d, *J* = 16.0 Hz, 3H), 7.80-6.89 (m, 12H); the benzamide has poor solubility, so we can not get its carbon (^{13}C) NMR spectra. HRMS (ESI) m/z calcd for $[C_{23}H_{18}NO_2]^+$ $[M+H]^+$: 340.1332, found 340.1337.

12. *N*-(3-(4-fluorophenyl)naphthalen-2-yl)-*N*-hydroxybenzamide (1l)

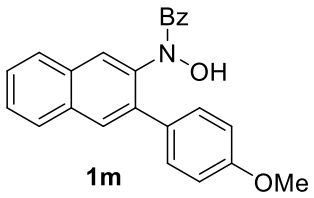


1l

White solid, m.p. = 77-79 ºC; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.14 (s, 1H), 7.93-7.84 (m, 1H), 7.83-7.71 (m, 1H), 7.64 (s, 1H), 7.51 (dd, *J* = 6.2, 3.2 Hz, 2H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.02 (s, 2H), 6.92 (dt, *J* = 22.1, 7.0 Hz, 5H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 163.6, 161.6, 137.0, 135.1, 134.0, 133.6, 132.7, 130.7, 130.5, 130.4, 130.1, 129.2, 128.4, 128.1, 127.9, 127.7, 127.0, 115.6, 115.4; ^{19}F NMR (471 MHz, $CDCl_3$): δ -114.4; HRMS (ESI) m/z calcd for $[C_{23}H_{17}FNO_2]^+$

$[M+H]^+$: 358.1238, found 358.1230.

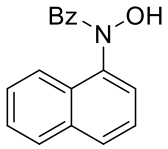
13. *N*-hydroxy-*N*-(3-(4-methoxyphenyl)naphthalen-2-yl)benzamide (1m)



1m

White solid, m.p. = 73-75 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.70-7.57 (m, 2H), 7.47-7.24 (m, 5H), 7.15 (dd, *J* = 31.5, 7.7 Hz, 5H), 6.88 (d, *J* = 8.0 Hz, 2H), 5.20 (s, 1H), 3.78 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 165.6, 159.3, 141.2, 136.4, 133.7, 132.4, 131.7, 131.1, 131.0, 130.9, 129.0, 128.6, 128.3, 126.9, 126.7, 126.1, 124.4, 123.1, 113.8, 55.4; HRMS (ESI) m/z calcd for $[C_{24}H_{20}NO_3]^+$ $[M+H]^+$: 370.1438, found 370.1430.

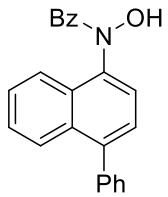
14. *N*-hydroxy-*N*-(naphthalen-1-yl)benzamide[4] (1n)



1n

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.44 (s, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 7.91 (dd, *J* = 19.6, 8.2 Hz, 2H), 7.72-7.55 (m, 2H), 7.47-7.21 (m, 5H), 7.15 (t, *J* = 7.8 Hz, 2H). Analytical data are in accordance with the literature values.

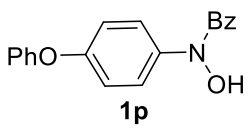
15. *N*-hydroxy-*N*-(4-phenylnaphthalen-1-yl)benzamide (1o)



1o

Yellow solid, m.p. = 70-72 °C; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.66 (s, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.55-7.39 (m, 8H), 7.31-7.12 (m, 5H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 167.4, 142.8, 139.7, 135.4, 132.7, 131.2, 130.7, 130.2, 130.0, 128.5, 128.4, 128.2, 127.8, 127.6, 127.0, 126.9, 126.8, 126.3, 123.6; HRMS (ESI) m/z calcd for $[C_{23}H_{18}NO_2]^+$ $[M+H]^+$: 340.1332, found 340.1329.

16. *N*-hydroxy-*N*-(4-phenoxyphenyl)benzamide (1p)

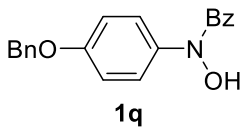


1p

White solid, m.p. = 122-124 °C; R_f = 0.4 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.36 (s, 1H), 7.43 (d, *J* = 7.3 Hz, 2H), 7.34 (ddd, *J* = 10.9, 7.2, 5.7 Hz, 3H), 7.29-7.23 (m, 2H), 7.20-7.11 (m, 3H), 6.99 (d, *J* = 7.7 Hz, 2H), 6.93-6.85 (m, 2H); ^{13}C NMR (126 MHz,

$CDCl_3$): δ 165.6, 157.4, 156.2, 134.5, 132.2, 131.0, 130.0, 128.9, 128.2, 128.0, 124.11, 120.0, 118.7; HRMS (ESI) m/z calcd for $[C_{19}H_{16}NO_3]^+$ $[M+H]^+$: 306.1125, found 306.1131.

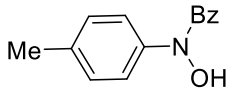
17. *N*-(4-(benzyloxy)phenyl)-*N*-hydroxybenzamide (1q)



1q

White solid, m.p. = 159-160 °C; R_f = 0.2 (PE:EA = 5:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.13 (s, 1H), 7.45-7.30 (m, 8H), 7.30-7.23 (m, 2H), 7.19-7.11 (m, 2H), 6.93-6.85 (m, 2H), 5.03 (s, 2H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 168.0, 156.8, 137.4, 136.1, 135.9, 130.5, 128.9, 128.8, 128.3, 128.3, 128.2, 128.0, 115.2, 70.0; HRMS (ESI) m/z calcd for $[C_{20}H_{18}NO_3]^+$ $[M+H]^+$: 320.1281, found 320.1288.

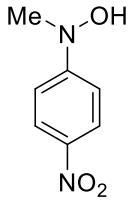
18. *N*-hydroxy-*N*-(*p*-tolyl)benzamide[5] (1r)



1r

R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.09 (s, 1H), 7.37-7.22 (m, 3H), 7.19 (t, *J* = 7.7 Hz, 2H), 7.02 (s, 4H), 2.25 (s, 3H). Analytical data are in accordance with the literature values.

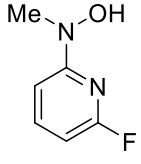
19. *N*-methyl-*N*-(4-nitrophenyl)hydroxylamine (1s)



1s

Yellow solid, m.p. = 104-106 °C; R_f = 0.3 (PE:EA = 3:1); ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 9.94 (s, 1H), 8.06 (d, *J* = 8.5 Hz, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 3.25 (s, 3H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 157.6, 138.6, 125.9, 112.3, 43.0; HRMS (ESI) m/z calcd for $[C_7H_9N_2O_3]^+$ $[M+H]^+$: 169.0608, found 169.0612.

20. *N*-(6-fluoropyridin-2-yl)-*N*-methylhydroxylamine (1t)

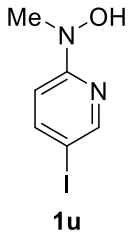


1t

White oil; R_f = 0.3 (PE:EA = 2:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (s, 1H), 7.64-7.45 (m, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.28 (d, *J* = 7.6 Hz, 1H), 3.20 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 162.15 (d, $J_{C\text{-}F}$ = 15.1 Hz), 162.04 (d, $J_{C\text{-}F}$ = 23.0 Hz), 142.20 (d, $J_{C\text{-}F}$ = 8.8 Hz), 105.38 (d, $J_{C\text{-}F}$ = 3.8 Hz), 99.1 (d, $J_{C\text{-}F}$ = 35.3 Hz), 41.8; ^{19}F NMR (471

MHz, $CDCl_3$): δ -70.3; HRMS (ESI) m/z calcd for $[C_6H_8FN_2O]^+$ $[M+H]^+$: 143.0615, found 143.0616.

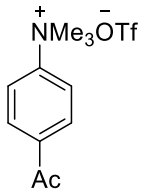
21. *N*-(5-iodopyridin-2-yl)-*N*-methylhydroxylamine (1u)



1u

White oil; R_f = 0.4 (PE:EA = 3:1); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.35 (d, *J* = 1.0 Hz, 1H), 7.77 (dd, *J* = 8.8, 1.7 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 1H), 3.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 162.2, 152.6, 145.5, 111.6, 81.1, 42.3; HRMS (ESI) m/z calcd for $[C_6H_8IN_2O]^+$ $[M+H]^+$: 250.9676, found 250.9674.

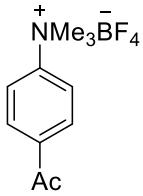
22. 4-acetyl-*N*,*N*,*N*-trimethylbenzenaminium trifluoromethanesulfonate (2a)[3]



2a

White solid; ^{1}H NMR (500 MHz, DMSO- *d*$_6$): 8.14 (dd, J = 20.3, 8.9 Hz, 4H), 3.65 (s, 9H), 2.65 (s, 3H). Analytical data are in accordance with the literature values.

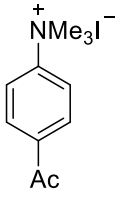
23. 4-acetyl-*N*,*N*,*N*-trimethylbenzenaminium tetrafluoroborate(2a′)[3]



2a'

White solid; ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 8.14 (dd, *J* = 21.6, 9.0 Hz, 4H), 3.65 (s, 9H), 2.64 (s, 3H). Analytical data are in accordance with the literature values.

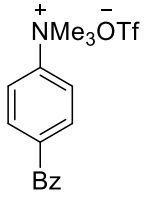
24. 4-acetyl-*N*,*N*,*N*-trimethylbenzenaminium iodide (2a′′)[3]



2a"

White solid; ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 8.15 (d, *J* = 4.3 Hz, 4H), 3.67 (s, 9H), 2.66 (s, 3H). Analytical data are in accordance with the literature values.

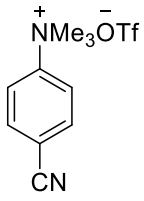
25. 4-benzoyl-*N*,*N*,*N*-trimethylbenzenaminium trifluoromethanesulfonate (2b)[3]



2b

White solid; ^{1}H NMR (500 MHz, DMSO- *d*$_6$): 8.18 (d, J = 9.0 Hz, 2H), 7.95 (d, J = 8.9 Hz, 2H), 7.85-7.69 (m, 3H), 7.60 (t, J = 7.7 Hz, 2H), 3.69 (s, 9H). Analytical data are in accordance with the literature values.

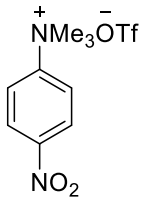
26. 4-cyano-*N*,*N*,*N*-trimethylbenzenaminium trifluoromethanesulfonate (2c)[3]



2c

White solid; ^{1}H NMR (500 MHz, DMSO- d_6): 8.27-8.08 (m, 4H), 3.65 (s, 9H). Analytical data are in accordance with the literature values.

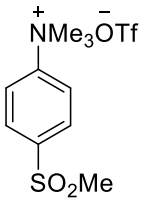
27. *N*,*N*,*N*-trimethyl-4-nitrobenzenaminium trifluoromethanesulfonate (2d)[3]



2d

White solid; ^{1}H NMR (500 MHz, DMSO- d_6): 8.47 (d, J = 9.1 Hz, 2H), 8.28 (d, J = 9.2 Hz, 2H), 3.69 (s, 9H). Analytical data are in accordance with the literature values.

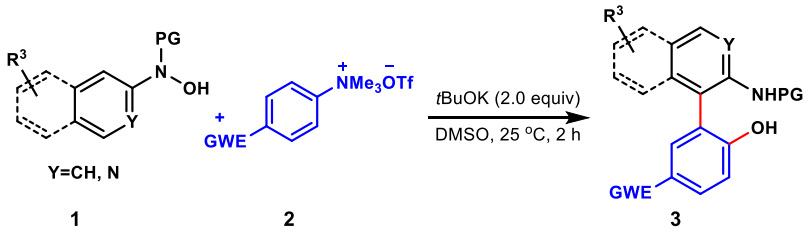
28. *N*,*N*,*N*-trimethyl-4-(methylsulfonyl)benzenaminium-trifluoromethanesulfonate (2e)[3]



2e

White solid; ^{1}H NMR (500 MHz, DMSO- d_6): 8.32-8.25 (m, 2H), 8.23-8.14 (m, 2H), 3.68 (s, 9H), 3.33 (s, 3H). Analytical data are in accordance with the literature values.

General procedure for the synthesis of biaryls

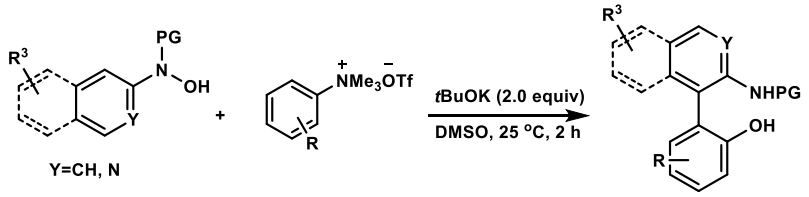


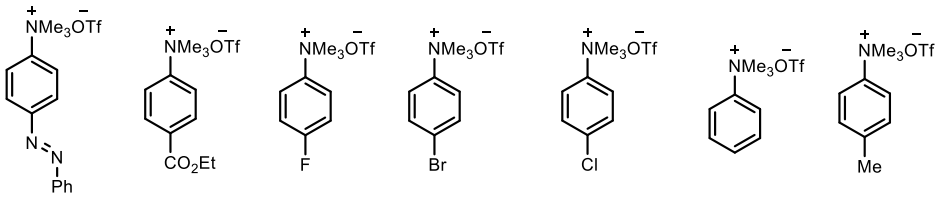
1 **2** **3**

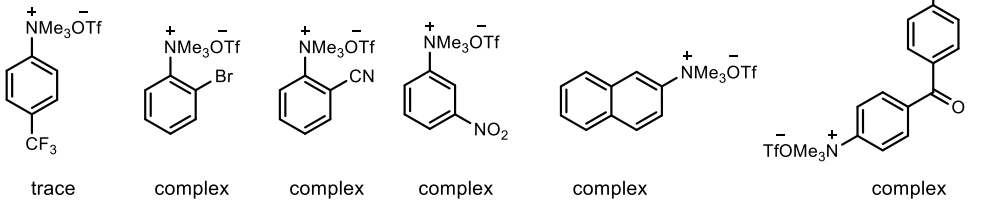
A solution of *t*BuOK (0.6 mmol, 2.0 equiv.), **1** (0.3 mmol, 1.0 equiv.) and **2** (0.45 mmol, 1.5 equiv.) in anhydrous DMSO (3 mL) under air was stirred at 25 °C until the complete consumption of **1** detected by TLC analysis. Then water (30 mL) was added and the aqueous layer was extracted with ethyl acetate (3 x 10 mL). The combined organic layer was dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography to give the desired product **3**.

Screening of ammonium salts with various electron-withdrawing groups

A number of ammonium salts bearing various electron-withdrawing groups rather than nitro group were tried. For the details, see the following scheme. All the reactions were carried out following the general procedure.

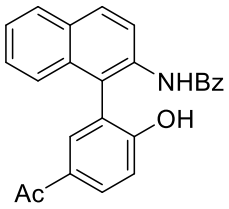






Analytical data of biaryl products

1. *N*-(1-(5-acetyl-2-hydroxyphenyl)naphthalen-2-yl)benzamide (3a)

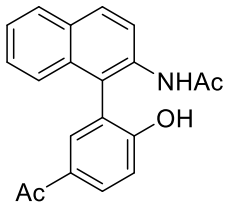


3a

91 mg, 80% yield; Yellow solid, m.p. = 229-230 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.27 (d, *J* = 6.9 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.86 (s, 1H), 7.83-7.71 (m, 3H), 7.41 (d, *J* = 5.9 Hz, 2H), 7.35 (dd, *J* = 16.4, 7.9 Hz, 3H), 7.28 (d, *J* = 7.1 Hz, 1H), 7.23 (d, *J* = 6.7 Hz, 2H), 7.14-7.08 (m, 1H), 6.67 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 196.5, 166.1, 160.4, 135.1, 134.3, 134.0, 132.7, 131.9, 130.6, 130.3, 128.9, 128.43, 128.35, 127.7, 126.8, 126.2, 125.9, 125.8, 123.0, 116.2, 26.7; HRMS (ESI) m/z calcd for

$[C_{25}H_{20}NO_3]^+$ $[M+H]^+$: 382.1438, found 382.1443.

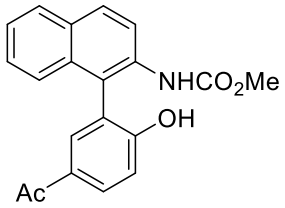
2. *N*-(1-(5-acetyl-2-hydroxyphenyl)naphthalen-2-yl)acetamide (3b)



3b

40 mg, 42% yield; White solid, m.p. = 141-143 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.38 (s, 1H), 8.96 (s, 1H), 8.05-7.90 (m, 3H), 7.75 (dd, *J* = 33.0, 5.3 Hz, 2H), 7.44 (dt, *J* = 14.9, 7.0 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.6 Hz, 1H), 2.51 (d, *J* = 3.2 Hz, 3H), 1.89 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 196.6, 169.2, 160.6, 134.5, 133.7, 132.7, 131.4, 130.7, 129.1, 129.1, 128.6, 128.3, 128.0, 126.6, 126.1, 125.5, 123.0, 116.2, 26.8, 23.7; HRMS (ESI) m/z calcd for $[C_{20}H_{18}NO_3]^+$ $[M+H]^+$: 320.1281, found 320.1301.

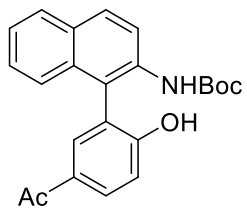
3. methyl (1-(5-acetyl-2-hydroxyphenyl)naphthalen-2-yl)carbamate (3c)



3c

76 mg, 76% yield; Yellow solid, m.p. = 103-105 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.46 (s, 1H), 8.21 (s, 1H), 8.05-7.92 (m, 3H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.75 (d, *J* = 2.2 Hz, 1H), 7.53-7.36 (m, 2H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 1H), 3.58 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 196.6, 160.5, 155.2, 134.1, 133.9, 132.8, 131.2, 130.7, 129.2, 128.5, 128.3, 126.8, 125.9, 125.4, 124.1, 122.8, 116.3, 52.2, 26.8; HRMS (ESI) m/z calcd for $[C_{20}H_{18}NO_4]^+$ $[M+H]^+$: 336.1230, found 336.1226.

4. *tert*-butyl (1-(5-acetyl-2-hydroxyphenyl)naphthalen-2-yl)carbamate (3d)

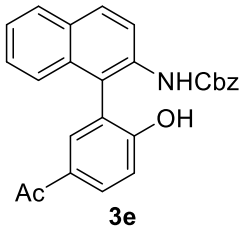


3d

88 mg, 78% yield; White Oil; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.9 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 9.1 Hz, 1H), 7.70 (dd, *J* = 17.8, 5.0 Hz, 2H), 7.36-7.22 (m, 2H), 7.17 (d, *J* =

8.0 Hz, 1H), 7.00 (d, *J* = 8.3 Hz, 1H), 6.69 (d, *J* = 8.6 Hz, 1H), 6.33 (s, 1H), 2.38 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 197.1, 158.8, 153.5, 134.8, 133.3, 132.7, 131.2, 130.8, 130.5, 129.8, 128.2, 127.1, 125.1, 124.9, 121.7, 121.0, 116.7, 81.3, 28.3, 26.3; HRMS (ESI) m/z calcd for $[C_{23}H_{23}NO_4Na]^+$ $[M+Na]^+$: 400.1519, found 400.1512.

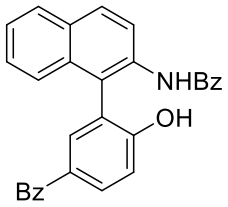
5. benzyl (1-(5-acetyl-2-hydroxyphenyl)naphthalen-2-yl)carbamate (3e)



3e

78 mg, 63% yield; Yellow solid, m.p. = 155-157 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (4:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.15 (s, 1H), 7.95 -7.59 (m, 4H), 7.43-7.13 (m, 8H), 7.03 (d, *J* = 8.6 Hz, 1H), 6.53 (s, 1H), 6.39 (s, 1H), 4.95 (q, *J* = 11.9 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 196.9, 158.7, 153.8, 135.7, 134.5, 133.1, 132.6, 131.5, 130.8, 130.8, 130.1, 128.6, 128.5, 128.4, 128.3, 127.3, 125.3, 124.9, 121.3, 116.8, 67.3, 26.3; HRMS (ESI) m/z calcd for $[C_{26}H_{22}NO_4]^+$ $[M+H]^+$: 412.1543, found 412.1546.

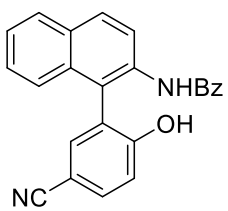
6. *N*-(1-(5-benzoyl-2-hydroxyphenyl)naphthalen-2-yl)benzamide (3f)



3f

71 mg, 53% yield; White solid, m.p. = 216-218 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.65 (s, 1H), 9.68 (s, 1H), 8.00 (t, *J* = 8.5 Hz, 2H), 7.86-7.78 (m, 2H), 7.75 (d, *J* = 7.2 Hz, 2H), 7.66-7.63 (m, 2H), 7.58 (dd, *J* = 14.8, 4.8 Hz, 2H), 7.52-7.42 (m, 8H), 7.21 (d, *J* = 8.6 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 194.8, 166.0, 160.5, 138.4, 135.9, 135.1, 134.4, 132.7, 132.3, 132.2, 132.0, 130.3, 129.6, 128.82, 128.75, 128.44, 128.36, 128.3, 127.8, 126.8, 126.1, 126.08, 125.9, 123.0, 116.5; HRMS (ESI) m/z calcd for $[C_{30}H_{22}NO_3]^+$ $[M+H]^+$: 444.1594, found 444.1602.

7. *N*-(1-(5-cyano-2-hydroxyphenyl)naphthalen-2-yl)benzamide (3g)

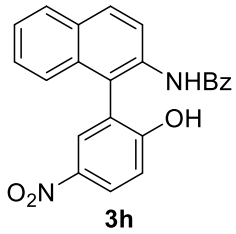


3g

58 mg, 53% yield; Brown solid, m.p. = 259-261 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica

gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.74 (s, 1H), 9.65 (s, 1H), 8.05-7.97 (m, 2H), 7.80-7.73 (m, 2H), 7.70 (d, *J* = 7.4 Hz, 2H), 7.61 (d, *J* = 1.7 Hz, 1H), 7.53 (dd, *J* = 11.6, 7.1 Hz, 2H), 7.46 (q, *J* = 7.3 Hz, 3H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.2, 160.2, 137.0, 135.2, 134.4, 134.2, 132.5, 132.0, 131.9, 129.6, 128.8, 128.7, 128.5, 127.8, 126.9, 126.2, 126.0, 124.7, 120.0, 117.2, 101.5; HRMS (ESI) m/z calcd for $[C_{24}H_{17}N_2O_2]^+$ $[M+H]^+$: 365.1285, found 365.1285.

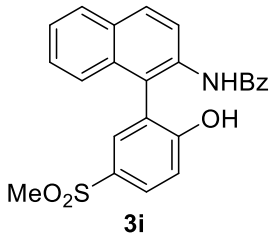
8. *N*-(1-(2-hydroxy-5-nitrophenyl)naphthalen-2-yl)benzamide (3h)



3h

90 mg, 78% yield; Yellow solid, m.p. = 262-263 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.19 (s, 1H), 9.81 (s, 1H), 8.24 (dd, *J* = 9.0, 2.7 Hz, 1H), 8.13 (d, *J* = 2.7 Hz, 1H), 8.03 (dd, *J* = 16.7, 8.4 Hz, 2H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.59-7.47 (m, 4H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.19 (d, *J* = 9.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.4, 162.6, 139.8, 135.2, 134.6, 132.5, 132.0, 131.9, 129.6, 129.1, 128.9, 128.8, 128.6, 127.9, 127.1, 126.5, 126.09, 126.07, 125.9, 124.2, 116.6; HRMS (ESI) m/z calcd for $[C_{23}H_{17}N_2O_4]^+$ $[M+H]^+$: 385.1183, found 385.1176.

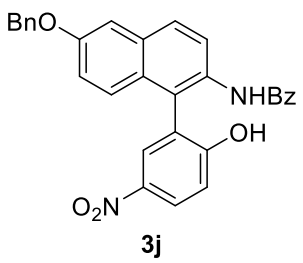
9. *N*-(1-(2-hydroxy-5-(methylsulfonyl)phenyl)naphthalen-2-yl)benzamide (3i)



3i

62 mg, 50% yield; white solid, m.p. = 229-231 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:2, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.70 (s, 1H), 9.71 (s, 1H), 8.02 (dd, *J* = 12.9, 8.4 Hz, 2H), 7.83 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.75-7.66 (m, 3H), 7.58-7.39 (m, 6H), 7.21 (d, *J* = 8.6 Hz, 1H), 3.00 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.2, 160.4, 135.0, 134.4, 132.4, 132.1, 132.0, 131.9, 131.1, 130.3, 129.2, 128.8, 128.7, 128.5, 127.8, 126.9, 126.3, 126.1, 126.0, 124.0, 116.6, 44.6; HRMS (ESI) m/z calcd for $[C_{24}H_{20}NO_4S]^+$ $[M+H]^+$: 418.1108, found 418.1105.

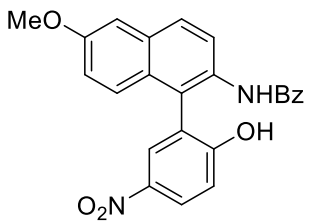
10. *N*-(6-(benzyloxy)-1-(2-hydroxy-5-nitrophenyl)naphthalen-2-yl)benzamide (3j)



3j

130 mg, 89% yield; Brown solid, m.p. = 224-226 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.16 (s, 1H), 9.75 (s, 1H), 8.24-8.18 (m, 1H), 8.09 (s, 1H), 7.92 (d, J = 8.7 Hz, 1H), 7.68 (t, J = 8.4 Hz, 3H), 7.58-7.48 (m, 4H), 7.45-7.33 (m, 6H), 7.22 (d, J = 8.8 Hz, 1H), 7.16 (d, J = 9.0 Hz, 1H), 5.27 (s, 2H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.4, 162.5, 156.6, 139.7, 137.4, 135.2, 133.4, 132.5, 131.8, 130.0, 129.0, 128.7, 128.4, 128.3, 127.81, 127.77, 127.7, 127.6, 127.2, 126.0, 124.3, 119.7, 116.5, 108.2, 69.9; HRMS (ESI) m/z calcd for $[C_{30}H_{23}N_2O_5]^+$ $[M+H]^+$: 491.1601, found 491.1594.

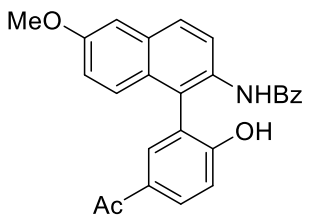
11. *N*-(1-(2-hydroxy-5-nitrophenyl)-6-methoxynaphthalen-2-yl)benzamide (3k)



3k

98 mg, 79% yield; Green solid, m.p. = 256-258 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (5:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.15 (s, 1H), 9.74 (s, 1H), 8.22 (dd, J = 9.0, 2.6 Hz, 1H), 8.11 (d, J = 2.5 Hz, 1H), 7.95 (d, J = 8.7 Hz, 1H), 7.69 (t, J = 8.5 Hz, 3H), 7.50 (t, J = 7.2 Hz, 1H), 7.46-7.34 (m, 4H), 7.24-7.04 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.4, 162.5, 157.6, 139.8, 135.2, 133.5, 132.5, 131.8, 130.0, 128.9, 128.7, 127.8, 127.72, 127.71, 127.5, 127.1, 126.0, 124.4, 119.4, 116.5, 106.9, 55.8; HRMS (ESI) m/z calcd for $[C_{24}H_{19}N_2O_5]^+$ $[M+H]^+$: 415.1288, found 415.1283.

12. *N*-(1-(5-acetyl-2-hydroxyphenyl)-6-methoxynaphthalen-2-yl)benzamide (3l)

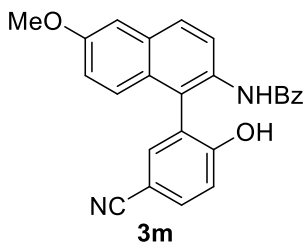


3l

57 mg, 46% yield; Yellow solid, m.p. = 139-141 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (5:2, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.54 (s, 1H),

9.50 (s, 1H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.83 (d, *J* = 2.0 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.69 (d, *J* = 7.4 Hz, 2H), 7.50 (d, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 3H), 7.36 (d, *J* = 9.2 Hz, 1H), 7.18-7.04 (m, 2H), 3.90 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 196.5, 166.2, 160.3, 157.4, 135.2, 133.91, 133.4, 132.2, 131.9, 130.9, 130.5, 128.9, 128.8, 127.94, 127.92, 127.7, 127.2, 126.7, 123.2, 119.1, 116.1, 106.8, 55.7, 26.7; HRMS (ESI) m/z calcd for $[C_{26}H_{22}NO_4]^+$ $[M+H]^+$: 412.1543, found 412.1543.

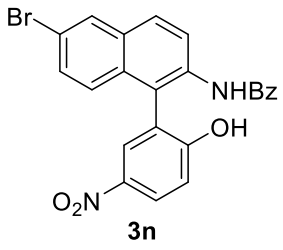
13. *N*-(1-(5-cyano-2-hydroxyphenyl)-6-methoxynaphthalen-2-yl)benzamide (3m)



3m

49 mg, 42% yield; Yellow solid, m.p. = 242-243 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (5:2, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.70 (s, 1H), 9.59 (s, 1H), 8.04-7.85 (m, 1H), 7.77-7.64 (m, 4H), 7.58 (d, *J* = 2.1 Hz, 1H), 7.52 (ddd, *J* = 7.4, 4.2, 1.2 Hz, 1H), 7.47-7.39 (m, 3H), 7.30 (d, *J* = 9.2 Hz, 1H), 7.18-7.03 (m, 2H), 3.89 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.3, 160.1, 157.5, 136.9, 135.2, 134.1, 133.4, 132.3, 131.8, 130.0, 129.0, 128.8, 127.9, 127.8, 127.7, 127.6, 127.5, 127.0, 124.9, 119.9, 119.3, 117.2, 106.8, 101.4, 55.8; HRMS (ESI) m/z calcd for $[C_{25}H_{19}N_2O_3]^+$ $[M+H]^+$: 395.1390, found 395.1383.

14. *N*-(6-bromo-1-(2-hydroxy-5-nitrophenyl)naphthalen-2-yl)benzamide (3n)

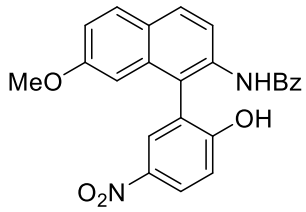


3n

65 mg, 47% yield; Yellow solid, m.p. = 303-305 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.23 (s, 1H), 9.84 (s, 1H), 8.31 (d, *J* = 1.9 Hz, 1H), 8.23 (dd, *J* = 9.1, 2.9 Hz, 1H), 8.09 (d, *J* = 2.9 Hz, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.60 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.48-7.34 (m, 3H), 7.17 (d, *J* = 9.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.4, 162.5, 139.8, 135.2, 135.0, 133.2, 132.0, 131.1, 130.3, 130.0, 129.7, 129.0, 128.8, 128.3, 128.1, 127.9, 127.7, 126.3,

123.6, 119.4, 116.6； HRMS (ESI) m/z calcd for $[C_{23}H_{16}BrN_2O_4]^+$ $[M+H]^+$: 463.0288, found 463.0280.

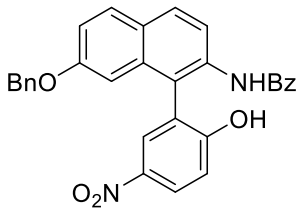
15. *N*-(1-(2-hydroxy-5-nitrophenyl)-7-methoxynaphthalen-2-yl)benzamide (3o)



3o

95 mg, 77% yield; Brown solid, m.p. = 225-227 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 11.18 (s, 1H), 9.75 (s, 1H), 8.22 (dd, *J* = 9.1, 2.9 Hz, 1H), 8.13 (d, *J* = 2.9 Hz, 1H), 7.95 (t, *J* = 9.0 Hz, 2H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.27-7.17 (m, 2H), 6.77 (d, *J* = 2.2 Hz, 1H), 3.68 (s, 3H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 166.3, 162.5, 158.1, 139.9, 135.23, 135.19, 133.8, 131.9, 130.3, 129.1, 128.8, 128.7, 128.5, 128.0, 127.9, 127.5, 126.1, 124.3, 124.0, 117.8, 116.6, 105.1, 55.5; HRMS (ESI) m/z calcd for $[C_{24}H_{19}N_2O_5]^+$ $[M+H]^+$: 415.1288, found 415.1287.

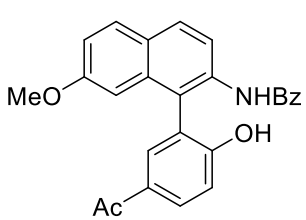
16. *N*-(7-(benzyloxy)-1-(2-hydroxy-5-nitrophenyl)naphthalen-2-yl)benzamide(3p)



3p

91 mg, 62% yield; White solid, m.p. = 235-236 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- *d*$_6$): δ 11.14 (s, 1H), 9.73 (s, 1H), 8.26 (dd, *J* = 9.1, 2.8 Hz, 1H), 8.05 (d, *J* = 2.8 Hz, 1H), 7.95 (dd, *J* = 8.8, 4.9 Hz, 2H), 7.70 (d, *J* = 7.3 Hz, 2H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.34-7.25 (m, 6H), 7.20 (d, *J* = 9.1 Hz, 1H), 6.83 (d, *J* = 2.1 Hz, 1H), 5.08-4.99 (m, 2H); ^{13}C NMR (126 MHz, DMSO- *d*$_6$): δ 166.3, 162.5, 157.2, 139.9, 137.2, 135.23, 135.18, 133.8, 131.9, 130.3, 129.1, 128.82, 128.79, 128.6, 128.4, 128.3, 128.2, 127.9, 127.5, 126.1, 124.2, 124.0, 118.3, 116.6, 106.7, 70.0; HRMS (ESI) m/z calcd for $[C_{30}H_{23}N_2O_5]^+$ $[M+H]^+$: 491.1601, found 491.1599.

17. *N*-(1-(5-acetyl-2-hydroxyphenyl)-7-methoxynaphthalen-2-yl)benzamide (3q)

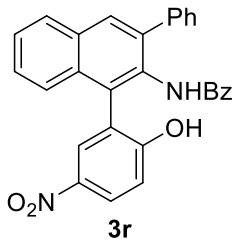


3q

65 mg, 53% yield; Yellow solid, m.p. = 148-150 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash

chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.8 Hz, 1H), 8.04 (s, 1H), 7.97 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.84 (d, *J* = 2.2 Hz, 1H), 7.68 (dd, *J* = 21.1, 8.9 Hz, 2H), 7.46 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.43-7.37 (m, 1H), 7.29-7.22 (m, 2H), 7.17 (d, *J* = 8.6 Hz, 1H), 7.08 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 3.65 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.9, 166.1, 158.9, 158.6, 134.7, 134.1, 134.0, 133.2, 132.0, 131.3, 130.6, 129.9, 129.6, 128.8, 127.0, 126.9, 121.99, 121.95, 119.4, 117.9, 117.0, 104.0, 55.2, 26.3; HRMS (ESI) m/z calcd for $[C_{26}H_{22}NO_4]^+$ $[M+H]^+$: 412.1543, found 412.1544.

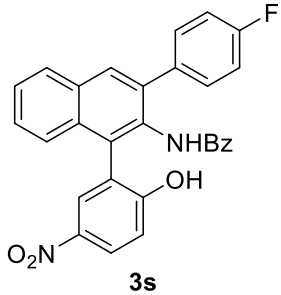
18. *N*-(1-(2-hydroxy-5-nitrophenyl)-3-phenylnaphthalen-2-yl)benzamide (3r)



3r

76 mg, 55% yield; Yellow solid, m.p. = 188-190 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 (d, *J* = 6.6 Hz, 1H), 7.97 (dd, *J* = 27.3, 7.8 Hz, 3H), 7.60 (d, *J* = 24.5 Hz, 3H), 7.50-7.16 (m, 12H), 7.10 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 169.0, 161.1, 141.2, 138.6, 138.2, 133.1, 132.9, 132.1, 132.0, 131.3, 131.0, 129.1, 128.6, 128.6, 128.4, 127.9, 127.4, 127.3, 127.0, 125.7, 125.6, 118.2；HRMS (ESI) m/z calcd for $[C_{29}H_{21}N_2O_4]^+$ $[M+H]^+$: 461.1496, found 461.1489.

19. *N*-(3-(4-fluorophenyl)-1-(2-hydroxy-5-nitrophenyl)naphthalen-2-yl)benzamid e (3s)

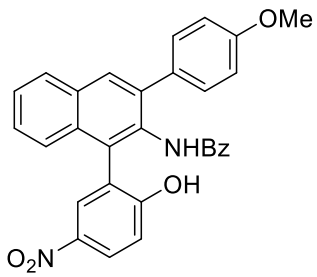


3s

90 mg, 63% yield; Yellow solid, m.p. = 250-252 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.15 (s, 1H), 9.92 (s, 1H), 8.27-8.14 (m, 2H), 8.09 (d, *J* = 4.9 Hz, 2H), 7.65 (dd, *J* = 8.5, 5.6 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.48-7.40 (m, 4H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.26 (t, *J* = 8.8 Hz, 2H), 7.16 (d, *J* = 8.9 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 163.1, 162.5, 161.1, 139.6, 138.6, 136.4, 135.2, 134.4, 132.7, 132.7, 131.9, 131.6, 131.5, 131.4, 130.0, 128.7, 128.6, 128.2, 127.5, 127.1,

126.9, 126.2, 126.0, 124.9, 116.3, 115.4, 115.2；^{19}F NMR (471 MHz, DMSO- d_6): δ -115.4; HRMS (ESI) m/z calcd for $[C_{29}H_{20}FN_2O_4]^+$ $[M+H]^+$: 479.1402, found 479.1410.

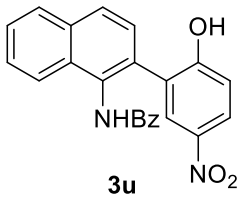
20. *N*-(1-(2-hydroxy-5-nitrophenyl)-3-(4-methoxyphenyl)naphthalen-2-yl)benzamide (3t)



3t

68 mg, 69% yield; Yellow solid, m.p. = 101-103 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ11.22 (s, 1H), 9.84 (s, 1H), 8.24 (dd, *J* = 9.0, 2.7 Hz, 1H), 8.14 (d, *J* = 2.7 Hz, 1H), 7.93 (d, *J* = 7.4 Hz, 1H), 7.68 (d, *J* = 9.9 Hz, 3H), 7.52 (dd, *J* = 14.2, 8.3 Hz, 6H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.18 (dd, *J* = 15.6, 8.8 Hz, 3H), 3.87 (s, 3H)；^{13}C NMR (126 MHz, DMSO- d_6): δ 166.4, 162.7, 159.4, 140.2, 139.9, 135.2, 134.1, 133.0, 132.1, 131.9, 131.4, 130.1, 129.2, 128.8, 128.7, 127.9, 127.0, 126.9, 126.4, 126.3, 126.2, 126.1, 124.1, 116.6, 114.6, 55.7; HRMS (ESI) m/z calcd for $[C_{30}H_{23}N_2O_5]^+$ $[M+H]^+$: 491.1601, found 491.1593.

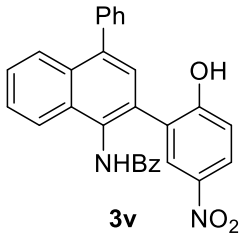
21. *N*-(2-(2-hydroxy-5-nitrophenyl)naphthalen-1-yl)benzamide (3u)



3u

54 mg, 47% yield; Brown solid, m.p. = 208-210 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (2:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.27 (s, 1H), 10.19 (s, 1H), 8.21 (d, *J* = 2.6 Hz, 1H), 8.09 (dd, *J* = 9.0, 2.9 Hz, 1H), 8.04 (dd, *J* = 5.2, 4.1 Hz, 1H), 7.99 (dd, *J* = 9.9, 5.7 Hz, 2H), 7.83 (d, *J* = 7.3 Hz, 2H), 7.60 (td, *J* = 5.3, 2.5 Hz, 3H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 167.1, 161.8, 139.6, 135.0, 133.8, 133.0, 132.5, 131.9, 131.4, 128.82, 128.79, 128.4, 127.9, 127.5, 127.3, 127.2, 127.1, 126.9, 125.5, 124.4, 116.5; HRMS (ESI) m/z calcd for $[C_{23}H_{17}N_2O_4]^+$ $[M+H]^+$: 385.1183, found 385.1184.

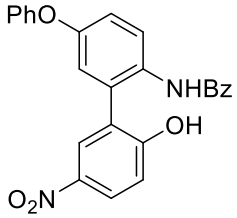
22. *N*-(2-(2-hydroxy-5-nitrophenyl)-4-phenylnaphthalen-1-yl)benzamide (3v)



3v

45 mg, 33% yield; Yellow solid, m.p. = 189-191 ℃; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (5:2, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.74 (s, 1H), 8.05 (d, *J* = 2.7 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.40-7.08 (m, 11H), 6.64 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ168.3, 159.3, 141.1, 140.7, 139.3, 132.76, 132.60, 132.09, 131.13, 130.4, 130.1, 129.9, 128.9, 128.8, 128.4, 127.7, 127.3, 127.1, 126.8, 126.7, 125.2, 123.9, 116.6； HRMS (ESI) m/z calcd for $[C_{29}H_{21}N_2O_4]^+$ $[M+H]^+$: 461.1496, found 461.1494.

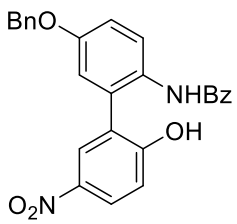
23. *N*-(2'-hydroxy-5'-nitro-5-phenoxy-[1,1'-biphenyl]-2-yl)benzamide (3w)



3w

58 mg, 46% yield; Yellow solid, m.p. = 145-146 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 9.77 (s, 1H), 8.10 -8.04 (m, 2H), 7.71 (d, *J* = 7.4 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.41 (ddd, *J* = 7.6, 6.0, 2.7 Hz, 4H), 7.16 (d, *J* = 7.4 Hz, 1H), 7.13-7.06 (m, 6H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.0, 161.9, 157.1, 154.7, 139.6, 135.1, 134.9, 131.9, 130.6, 129.2, 129.0, 128.8, 128.2, 127.8, 126.4, 125.7, 124.1, 121.1, 119.2, 118.7, 116.7; HRMS (ESI) m/z calcd for $[C_{25}H_{19}N_2O_5]^+$ $[M+H]^+$: 427.1288, found 427.1283.

24. *N*-(5-(benzyloxy)-2'-hydroxy-5'-nitro-[1,1'-biphenyl]-2-yl)benzamide(3x)

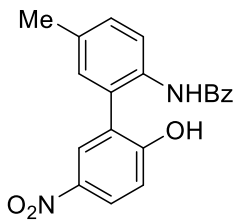


3x

66mg, 50% yield; Yellow solid, m.p. = 198-200 °C; R_f = 0.2 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (4:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.36 (s, 1H), 9.58 (s, 1H), 8.18-8.00 (m, 2H), 7.70 (d, *J* = 7.5 Hz, 2H), 7.58-7.46 (m, 4H), 7.43-7.37 (m, 4H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.10 (dt, *J* = 14.4, 6.2 Hz, 3H), 5.17 (s, 2H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 166.0, 161.5, 156.6, 139.8, 137.5, 135.3, 134.7, 131.8,

129.5, 128.9, 128.8, 128.3, 128.2, 127.9, 127.7, 127.0, 125.6, 117.2, 116.4, 115.2, 70.0; HRMS (ESI) m/z calcd for $[C_{26}H_{21}N_2O_5]^+$ $[M+H]^+$: 441.1445, found 441.1439.

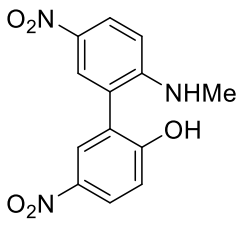
25. *N*-(2'-hydroxy-5-methyl-5'-nitro-[1,1'-biphenyl]-2-yl)benzamide (3y)



3y

55 mg, 53% yield; Yellow solid, m.p. = 181-182 ℃; R_f = 0.2 (PE:EA = 3:1); Purified directly by flash chromatography on silica gel (4:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.32 (s, 1H), 9.59 (s, 1H), 8.17-7.98 (m, 2H), 7.69 (d, *J* = 7.4 Hz, 2H), 7.53-7.45 (m, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.26 (d, *J* = 8.1 Hz, 1H), 7.22 (s, 1H), 7.07 (d, *J* = 9.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 165.8, 161.8, 139.7, 135.5, 135.3, 133.9, 133.1, 131.8, 131.7, 129.3, 128.8, 127.9, 127.7, 127.4, 127.1, 125.5, 116.4, 21.0; HRMS (ESI) m/z calcd for $[C_{20}H_{17}N_2O_4]^+$ $[M+H]^+$: 349.1183, found 349.1179.

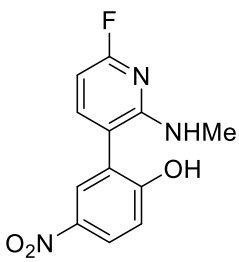
26. 2'-(methylamino)-5,5'-dinitro-[1,1'-biphenyl]-2-ol (3z)



3z

31 mg, 36% yield; Yellow solid, m.p. = 166-168 ℃; R_f = 0.2 (PE:EA = 3:1); Purified directly by flash chromatography on silica gel (3:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.45 (s, 1H), 8.16 (dd, *J* = 8.2, 2.2 Hz, 2H), 8.04 (d, *J* = 9.5 Hz, 2H), 7.19 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.65 (d, *J* = 9.2 Hz, 2H), 3.32 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 160.8, 154.0, 140.5, 137.8, 132.8, 126.09, 126.05, 125.4, 117.9, 112.6; HRMS (ESI) m/z calcd for $[C_{13}H_{12}N_3O_5]^+$ $[M+H]^+$: 290.0771, found 290.0774.

27. 2-(6-fluoro-2-(methylamino)pyridin-3-yl)-4-nitrophenol (3aa)

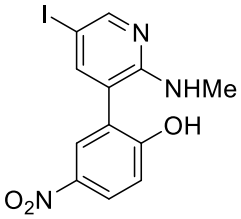


3aa

40 mg, 51% yield; Yellow solid, m.p. = 107-109 ℃; R_f = 0.2 (PE:EA = 5:1); Purified directly by flash chromatography on silica gel (6:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.16 (s, 1H), 8.16 (dd, *J* = 9.0, 2.9 Hz, 1H), 7.96 (d, *J* = 2.9 Hz, 1H), 7.38 (t, *J* = 8.1 Hz, 1H), 7.10 (d, *J* = 9.0

Hz, 1H), 6.19 (dd, *J* = 7.7, 2.6 Hz, 1H), 6.04 (s, 1H), 2.72 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 163.9, 162.5, 162.1, 156.5, 156.3, 142.9, 142.8, 140.2, 128.1, 125.9, 124.6, 116.8, 113.89, 113.85, 93.5, 93.1, 28.7; ^{19}F NMR (471 MHz, DMSO- d_6): δ -71.2. HRMS (ESI) m/z calcd for $[C_{12}H_{11}FN_3O_3]^+$ $[M+H]^+$: 264.0779, found 264.0773.

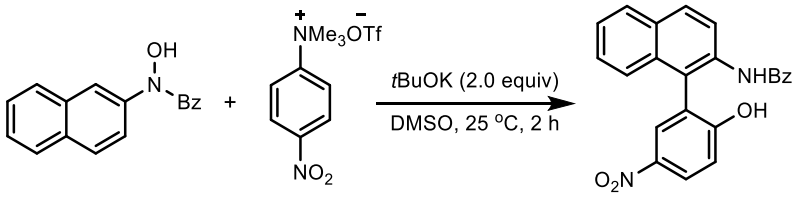
28. 2-(5-iodo-2-(methylamino)pyridin-3-yl)-4-nitrophenol (3ab)



3ab

40 mg, 36% yield; Yellow solid, m.p. = 204-206 ℃; R_f = 0.3 (PE:EA = 3:1); Purified directly by flash chromatography on silica gel (5:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.28 (s, 1H), 8.27 (d, *J* = 1.9 Hz, 1H), 8.10 (dd, *J* = 8.3, 2.2 Hz, 2H), 7.69 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.13 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.25 (d, *J* = 8.9 Hz, 1H), 3.27 (s, 3H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 161.0, 157.4, 153.1, 144.9, 140.3, 133.0, 126.0, 124.8, 117.5, 110.8, 78.7,37.8; HRMS (ESI) m/z calcd for $[C_{12}H_{11}IN_3O_3]^+$ $[M+H]^+$: 371.9840, found 371.9866.

Experimental procedure for large scale reaction

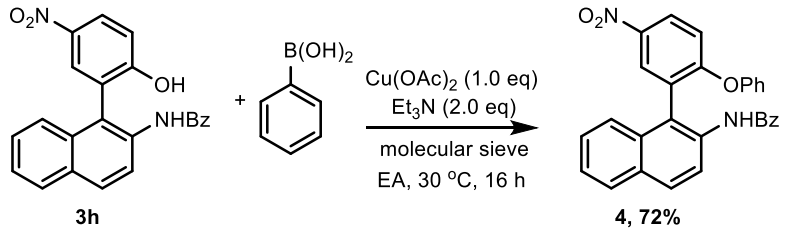


6 mmol **3h, 1.82 g, 79%**

N-hydroxy-*N*-(naphthalen-2-yl)benzamide (1.58 g, 6 mmol, 1.0 equiv.) and aryltrimethylammonium triflates (9 mmol, 1.5 equiv.) were dissolved in anhydrous DMSO (60 mL) under air atmosphere and *t*BuOK (12 mmol, 2.0 equiv.) was added. The resulting mixture was stirred at 25 ℃ for 2 hours. The mixture was quenched by water (600 mL) and was extracted with ethyl acetate (3 × 100 mL), the organic layer was washed by brine and dried over sodium sulfate. After the solvent was removed *in vacuum*, the crude product was purified by flash chromatography (PE/EtOAc = 2/1) to obtain **3h** (1.82 g, 79 %) as a yellow solid.

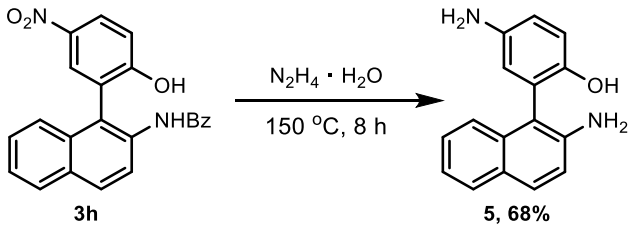
Synthetic applications of the biaryl products

General Procedure for the Synthesis of biaryl 4[6]



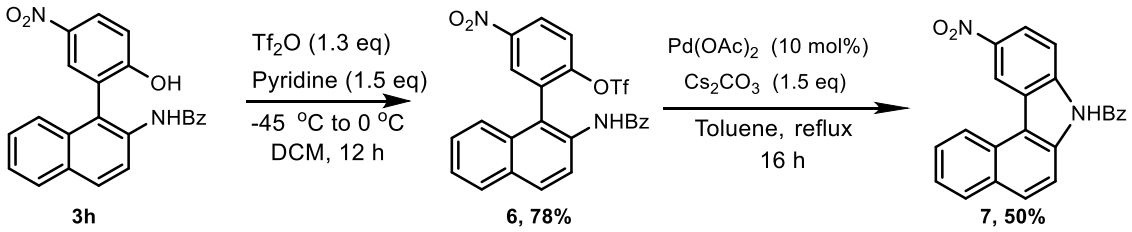
Biaryl **3h** (0.3 mmol, 1.00 equiv.), $Cu(OAc)_2$ (56.2 mg, 0.3 mmol, 1.0 equiv.), phenylboronic acid (75 mg, 0.6 mmol, 2.0 equiv.), and activated 4Å molecular sieves were added to ethyl acetate (3.0 mL) under an atmosphere of nitrogen, triethylamine (85 μL, 0.61 mmol., 2.0 equiv.) was added to the mixture via microsyringe, and the mixture was stirred at 30 ℃ for 16 hours. The reaction mixture was separated by silica gel chromatography (PE/EtOAc = 6/1) to obtain biaryl product **4** (99 mg, 72%).

General Procedure for the Synthesis of biaryl 5[7].



Biaryl 3h (0.2 mmol, 1.0 equiv.) was dissolved in $NH_2NH_2.H_2O$ (2.0 mL) in a sealed-tube. The tube was heated at 150 ℃ for 8 hours. After the reaction mixture was cooled to 30 ℃ and neutralized to pH = 7 by concentrated HCl (2 M). Then the mixture was diluted with EtOAc (45 mL), the organic layer was washed with brine and dried over sodium sulfate. Finally, the residue was purified by silica gel column chromatography (PE/EtOAc = 1/1) to obtain the desired product **5** (34 mg, 68%).

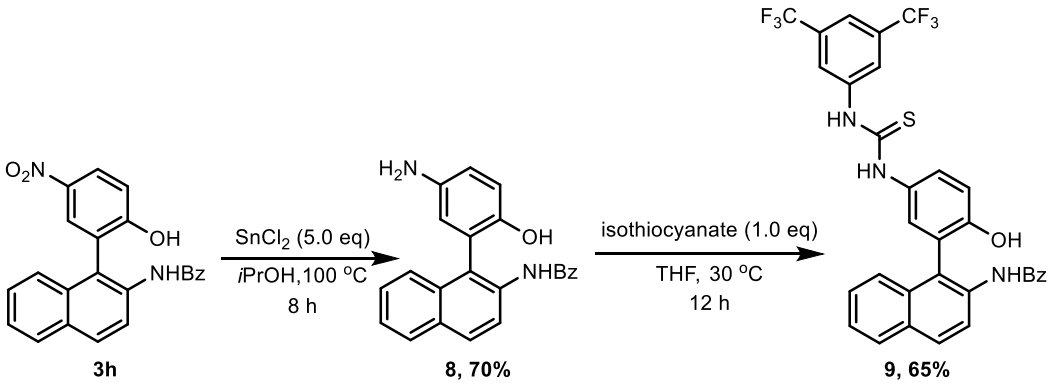
General Procedure for the Synthesis of carbazole 7[8,9]



Pyridine (1.5 mmol, 1.5 equiv.) was added to a solution of **3h** (0.1 mmol, 1.0 equiv.) in anhydrous CH_2Cl_2 (2 mL) at -45 ℃ under nitrogen atmosphere, and then triflic anhydride (1.3 mmol, 1.3 equiv.) was slowly added to the mixture. The mixture was stirred at 0 ℃ for 12 hours. 1M HCl (aq.) was slowly added to the reaction mixture. Then the mixture was extracted with brine, and dried over $MgSO_4$. The residue was purified by silica gel column chromatography (PE/EtOAc = 6/1) to obtain product **6** (40 mg, 78%) as a yellow solid.

Biaryl **6** (0.1 mmol, 1.0 equiv.), $Pd(OAc)_2$ (3 mg, 10 mol%), and Cs_2CO_3 (0.15 mmol, 1.5 equiv.) was dissolved in toluene (0.4 mL) under nitrogen atmosphere. The mixture was refluxed at 120 ℃ for 16 hours. After the reaction mixture was cooled to room temperature, the residue was purified by flash chromatography (PE/EtOAc = 12/1) to obtain the carbazole **7** (19 mg, 50%) as a yellow oil.

General Procedure for the Synthesis of biaryl 9[10,11]



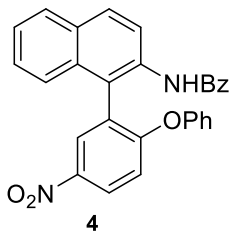
3h **8, 70%** **9, 65%**

Biaryl **3h** (0.2 mmol, 1.0 equiv.) was dissolved in *i*PrOH (0.5 mL) and stannous chloride (235 mg, 5.0 equiv.) was added slowly to the mixture at 100 ℃ under air, then the mixture was stirred at 100 ℃ for 8 hour. The mixture was quenched by water (3 mL) and it was extracted with ethyl acetate (3 × 25 mL), the organic layer was washed with brine and dried over sodium sulfate. After the solvent was removed *in vacuum*, the crude product was purified by flash chromatography (PE/EtOAc = 1/1) to obtain desired product **8** (50mg, 70%) as a black solid.

To a solution of **8** (0.1 mmol, 35.4 mg) in THF (3.0 mL) was added 3,5-bis(trifluoromethyl)phenyl isothiocyanate (27.1 mg, 0.1 mmol). After being stirred at room temperature for 12 h, the mixture was concentrated in vacuo. The residue was purified by recrystallization (n-hexane/AcOEt) to afford **9** as white solid (41 mg, 65%).

Analytical data of starting materials and synthetic applications

29. *N*-(1-(5-nitro-2-phenoxyphenyl)naphthalen-2-yl)benzamide (4)

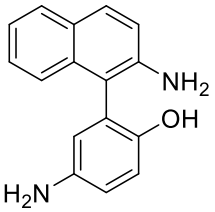


4

99 mg, 72% yield; White solid, m.p. = 68-70 ℃; R_f = 0.3 (PE:EA = 4:1); Purified directly by flash chromatography on silica gel (6:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23 (t, *J* = 5.5 Hz, 2H), 8.17 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.94-7.82 (m, 2H), 7.78 (dd, *J* = 5.5, 2.7 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.45-7.27 (m, 6H), 7.13 (dd, *J* = 12.7, 4.9 Hz, 2H), 7.05-6.92 (m,

2H), 6.72 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 165.6, 161.4, 154.5, 142.9, 134.7, 133.9, 132.3, 132.1, 131.4, 130.2, 129.8, 129.2, 128.9, 128.4, 126.99, 126.96, 126.8, 125.9, 125.5, 124.9, 123.1, 122.1, 120.3, 116.9; HRMS (ESI) m/z calcd for $[C_{29}H_{21}N_2O_4]^+$ $[M+H]^+$: 461.1496, found 461.1494.

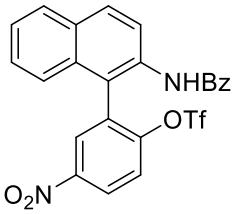
30. 4-amino-2-(2-aminonaphthalen-1-yl)phenol (5)



5

47 mg, Yield = 68%; Black solid, m.p. = 104-106 ℃; R_f = 0.2 (PE:EA = 1:1); Purified directly by flash chromatography on silica gel (1:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- *d_6*): δ 8.11 (s, 1H), 7.63 (dd, *J* = 29.8, 7.8 Hz, 2H), 7.37-6.99 (m, 4H), 6.75 (d, *J* = 8.0 Hz, 1H), 6.53 (d, *J* = 6.8 Hz, 1H), 6.32 (s, 1H), 4.60 (s, 4H); ^{13}C NMR (126 MHz, DMSO- *d_6*): δ 146.8, 143.3, 141.7, 134.1, 128.02, 127.95, 127.3, 125.9, 124.5, 123.7, 121.2, 118.9, 118.3, 117.2, 116.1, 115.5; HRMS (ESI) m/z calcd for $[C_{16}H_{15}N_2O]^+$ $[M+H]^+$: 251.1179, found 251.1173.

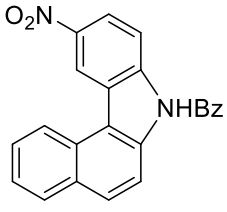
31. 2-(2-benzamidonaphthalen-1-yl)-4-nitrophenyl trifluoromethanesulfonate (6)



6

48 mg, Yield = 78%; Yellow solid, m.p. = 113-115 ℃; R_f = 0.3 (PE:EA = 2:1); Purified directly by flash chromatography on silica gel (6:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.35 (dt, *J* = 4.1, 2.7 Hz, 2H), 8.05 (d, *J* = 8.9 Hz, 1H), 7.97 (d, *J* = 8.9 Hz, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.60 (dd, *J* = 19.2, 10.7 Hz, 4H), 7.51-7.25 (m, 5H), 7.08 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 166.0, 151.4, 147.6, 134.3, 134.0, 132.9, 132.2, 131.6, 131.52, 131.1, 129.2, 128.9, 128.6, 127.6, 127.1, 126.1, 125.9, 124.1, 123.6, 123.5, 122.4; ^{19}F NMR (471 MHz, $CDCl_3$): δ -73.6; HRMS (ESI) m/z calcd for $[C_{24}H_{16}F_3N_2O_6S]^+$ $[M+H]^+$: 517.0676, found 517.0680.

32. (10-nitro-7H-7l4-benzo[c]carbazol-7-yl)(phenyl)methanone (7)

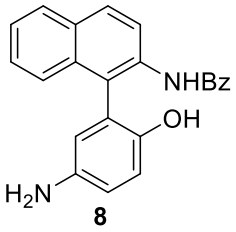


7

55 mg, Yield = 50%; Black solid, m.p. = 230-232 ℃; R_f = 0.3 (PE:EA = 5:1); Purified directly by flash chromatography on

silica gel (12:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 9.32 (d, J = 2.1 Hz, 1H), 8.79 (d, J = 8.4 Hz, 1H), 8.27 (dd, J = 9.2, 2.2 Hz, 1H), 8.06 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.94 (s, 1H), 7.82 (t, J = 7.6 Hz, 1H), 7.79-7.70 (m, 4H), 7.65-7.56 (m, 3H), 7.42 (d, J = 9.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 167.4, 142.0, 140.0, 136.9, 132.5, 132.5, 128.7, 128.3, 127.9, 127.8, 127.0, 126.3, 124.0, 123.7, 121.8, 119.4, 116.0, 115.5, 113.3; the product has poor solubility, so we can not get its perfect NMR spectra; HRMS (ESI) m/z calcd for $[C_{23}H_{15}N_2O_3]^+$ $[M]^+$: 367.1083, found 367.1083.

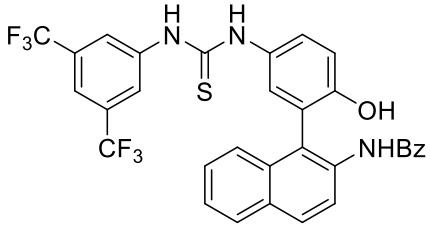
33. *N*-(1-(5-amino-2-hydroxyphenyl)naphthalen-2-yl)benzamide (8)



8

74 mg, 70% yield; Black solid, m.p. = 132-134 ℃; R_f = 0.2 (PE:EA = 1:1); Purified directly by flash chromatography on silica gel (1:1, petroleum ether: ethyl acetate); ^{1}H NMR (500 MHz, DMSO- d_6): δ 9.04 (d, J = 24.4 Hz, 2H), 8.19 (d, J = 8.8 Hz, 1H), 7.97 (t, J = 7.9 Hz, 2H), 7.71 (d, J = 7.5 Hz, 2H), 7.59 (dd, J = 18.2, 7.8 Hz, 2H), 7.47 (dt, J = 15.3, 7.2 Hz, 4H), 6.91 (d, J = 8.6 Hz, 1H), 6.65 (dd, J = 8.5, 2.3 Hz, 1H), 6.46 (d, J = 2.2 Hz, 1H), 4.75 (s, 2H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 165.0, 145.9, 141.8, 135.0, 133.5, 132.9, 132.3, 131.5, 129.3, 128.4, 128.3, 127.8, 127.3, 126.6, 126.5, 125.4, 123.0, 122.6, 118.1, 117.4, 116.5; HRMS (ESI) m/z calcd for $[C_{23}H_{19}N_2O_2]^+$ $[M+H]^+$: 355.1441, found 355.1435.

34. *N*-(1-(5-(3-(3,5-bis(trifluoromethyl)phenyl)thioureido)-2-hydroxyphenyl)naphthalen-2-yl)benzamide (9)



9

41 mg, 65% yield; White solid, m.p. = 280-282 ℃; R_f = 0.2 (PE:EA = 2:1); Purified by recrystallization (n-hexane/AcOEt); ^{1}H NMR (500 MHz, DMSO- d_6): δ 10.52-9.72 (m, 3H), 9.28 (s, 1H), 8.26 (s, 2H), 7.99 (s, 3H), 7.84-7.59 (m, 4H), 7.59 -7.18 (m, 7H), 7.10 (d, J = 7.3 Hz, 1H); ^{13}C NMR (126 MHz, DMSO- d_6): δ 180.4, 165.5, 153.4, 142.4, 135.0, 134.0, 132.8, 132.1, 131.7, 130.5, 130.2, 129.8, 129.0, 128.5, 128.3, 128.3, 127.6, 126.9, 126.6, 126.4, 125.6, 124.8, 124.3, 123.9,

122.9, 122.6, 117.2, 116.6; ^{19}F NMR (471 MHz, DMSO- d_6) δ -61.53; HRMS (ESI) m/z calcd for $[C_{32}H_{22}F_6N_3O_2S]^+$ $[M+H]^+$: 626.1331, found 626.1331.

References

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X-Ray Crystal Structure Data for Compound 3q

Single crystal was chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) to prevent decomposition. Intensity data and cell parameters were recorded at 173 K on a Bruker Apex II single crystal diffractometer, employing a Mo K_α radiation (λ = 0.71073 Å) and a CCD area detector. The raw frame data were processed using SAINT and SADABS to yield the reflection data file.[1] The structure was solved using the charge-flipping algorithm, as implemented in the program *SUPERFLIP*[2] and refined by full-matrix least-squares techniques against F_o^2 using the SHELXL program[3] through the OLEX2 interface.[4] Hydrogen atoms at carbon were placed in calculated positions and refined isotropically by using a riding model. Appropriate restraints or constraints were applied to the geometry and the atomic displacement parameters of the atoms in the cluster. All structures were examined using the Addsym subroutine of PLATON[5] to ensure that no additional symmetry could be applied to the models. CCDC **1961871** (**3q**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

References

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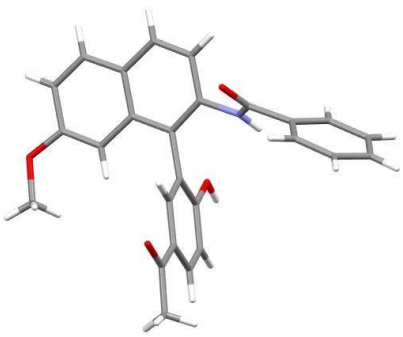

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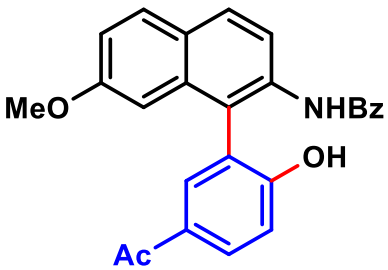
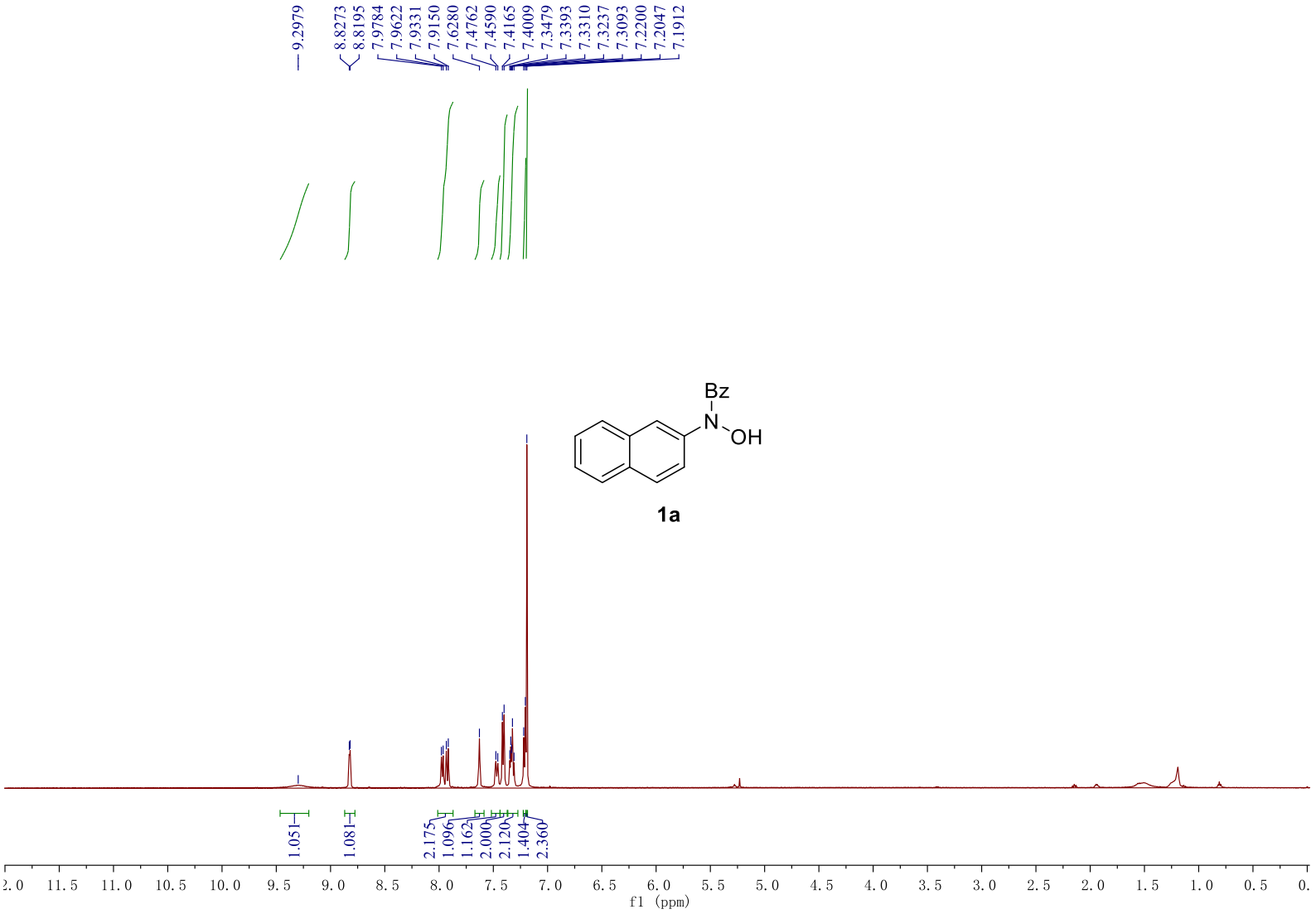


3q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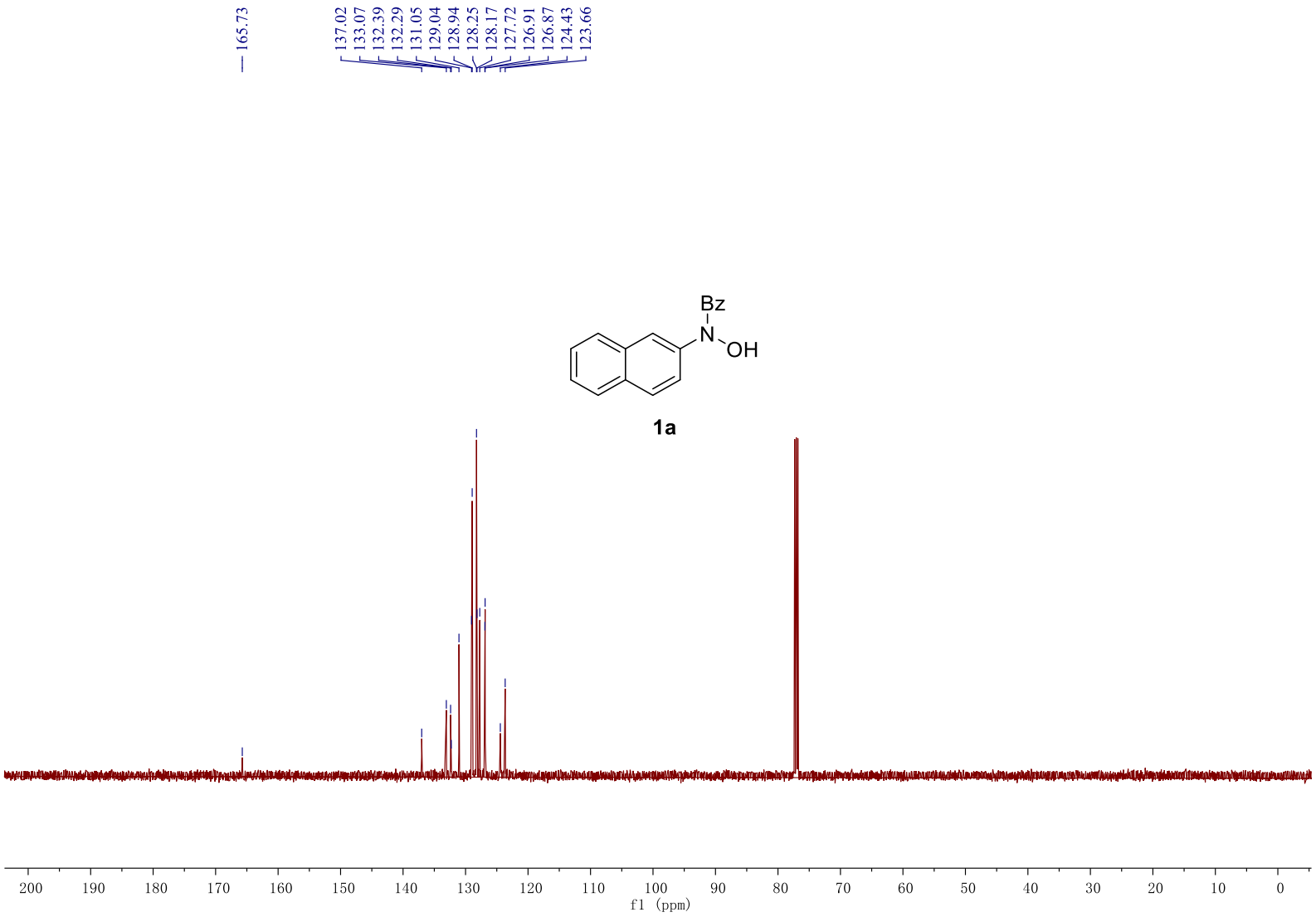
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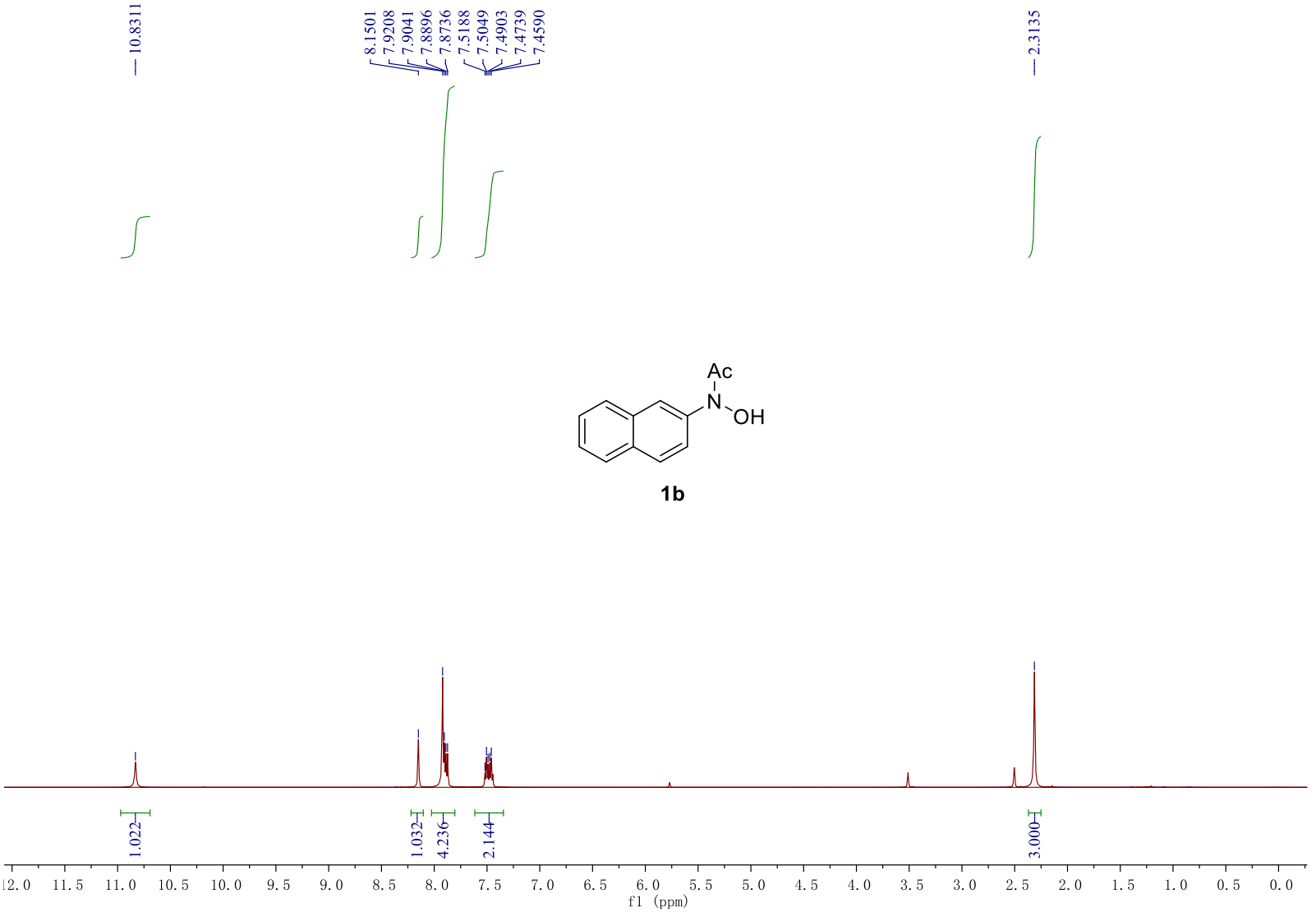
f1 (ppm)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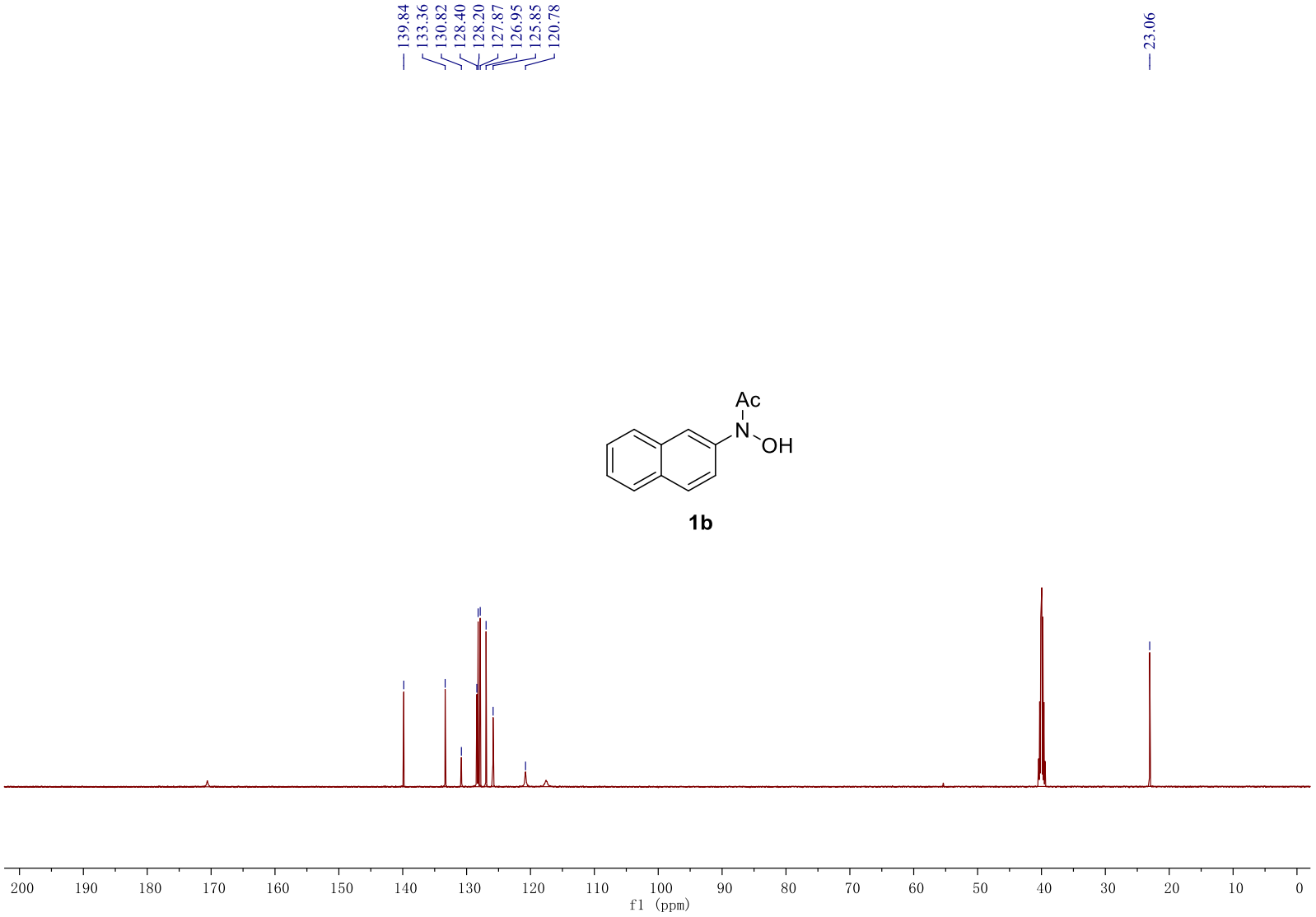
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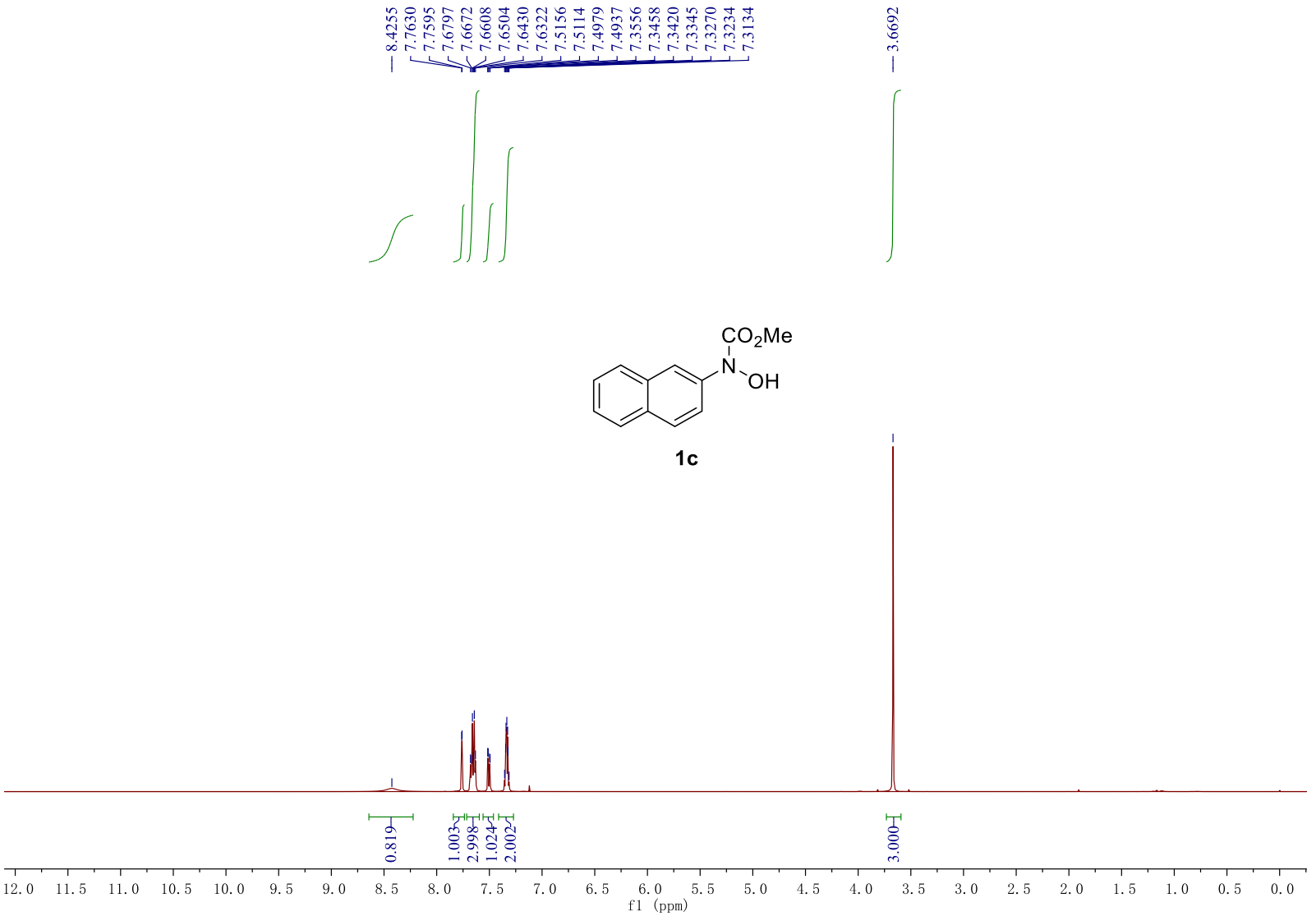
f1 (ppm)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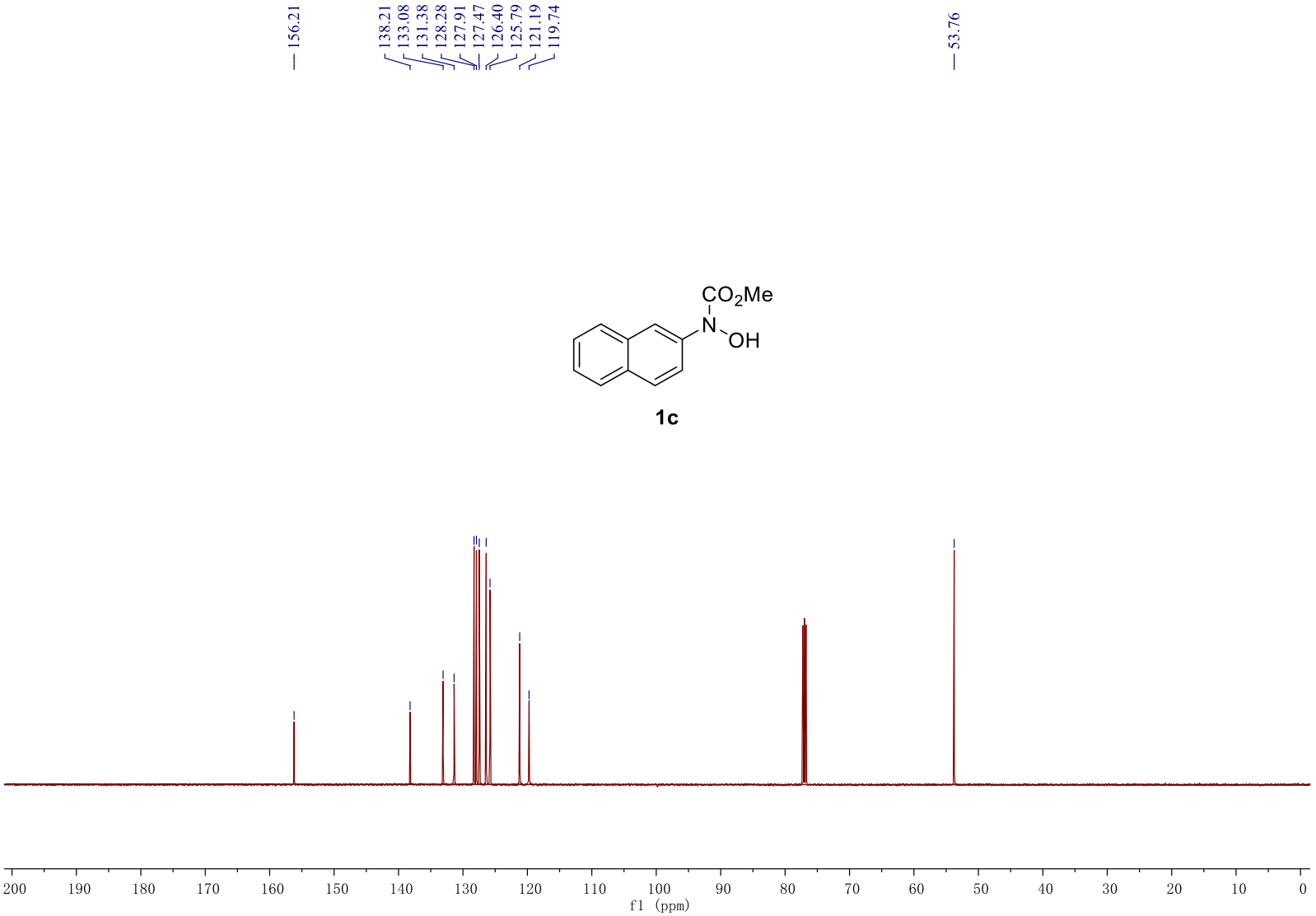
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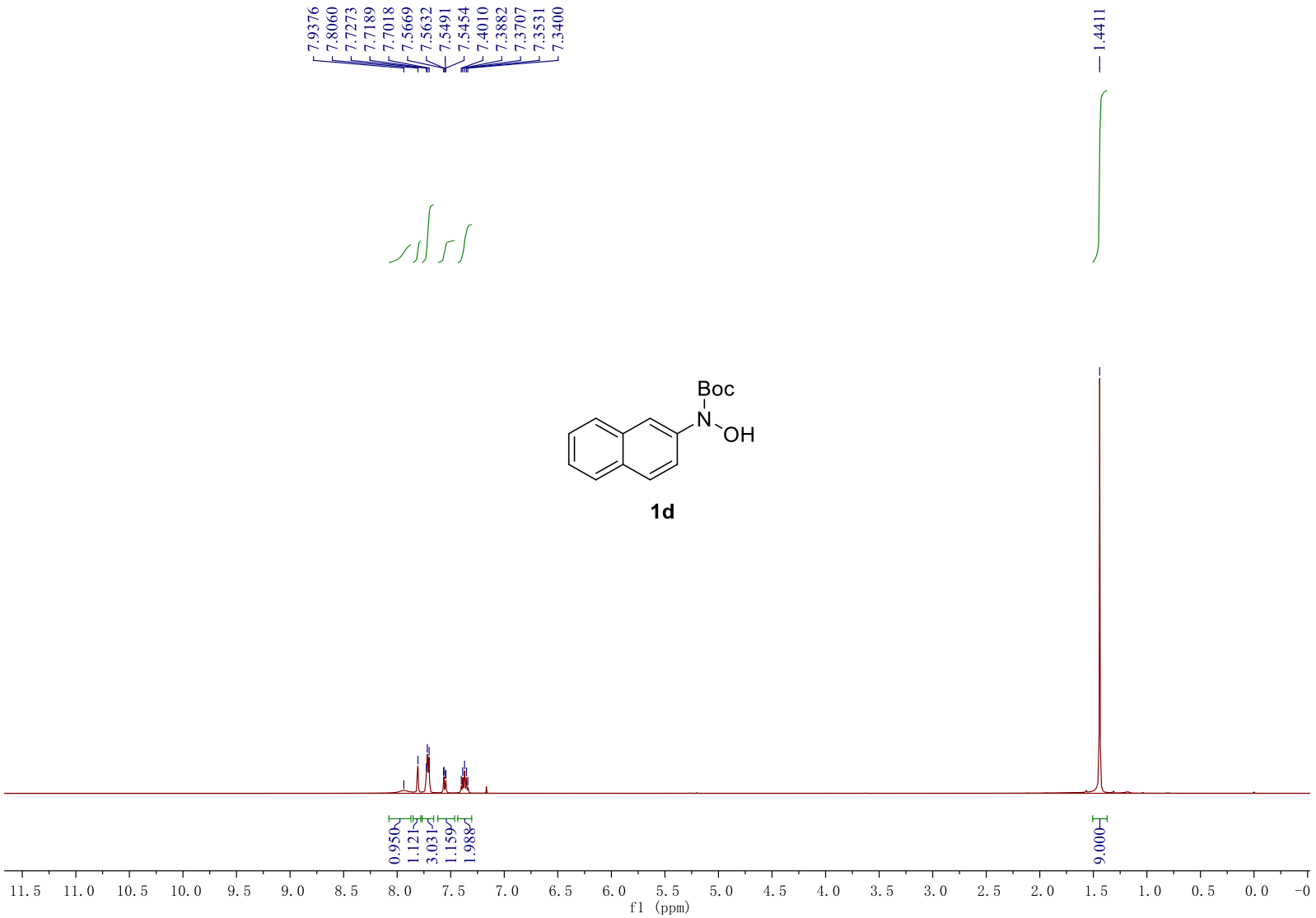
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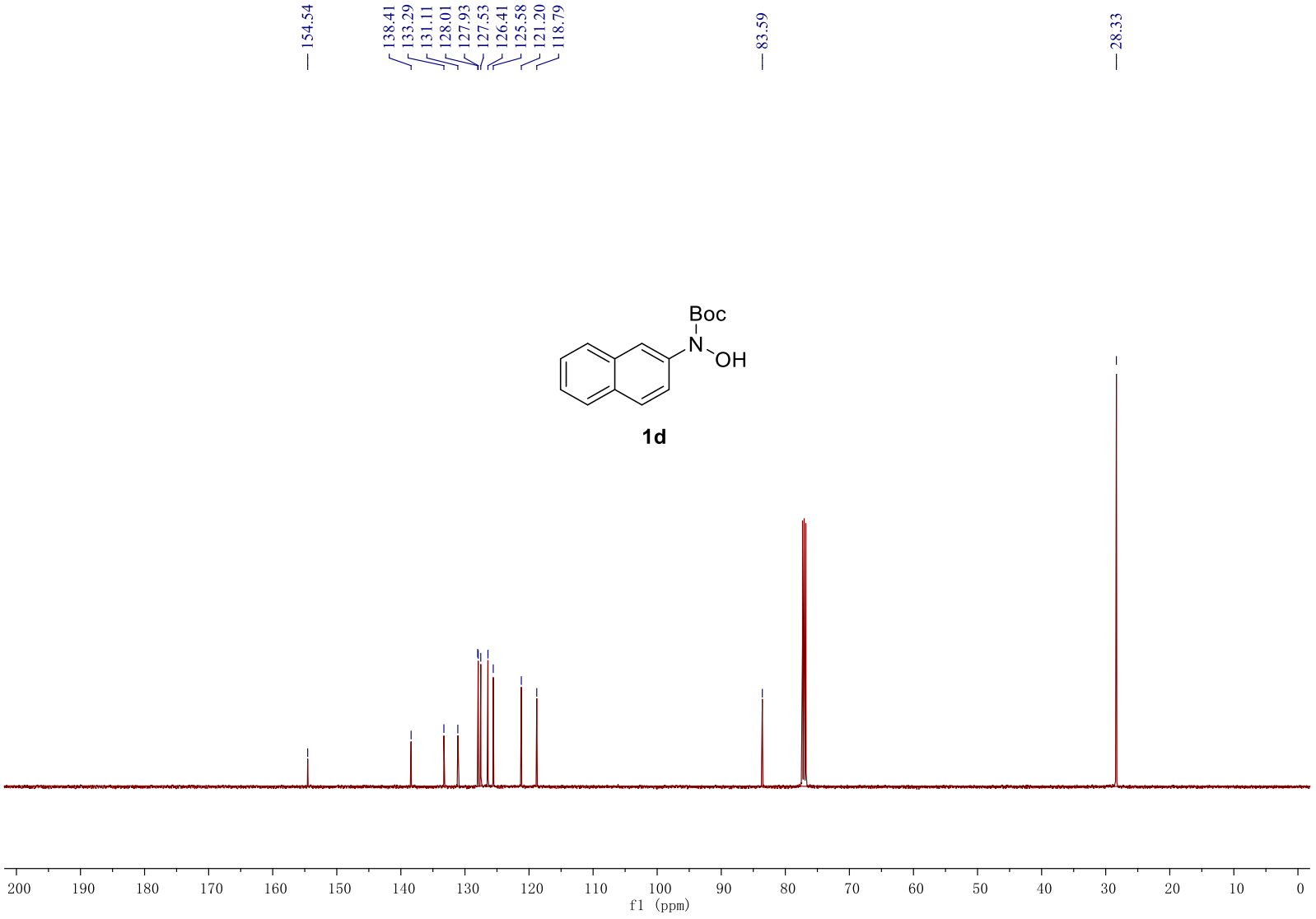
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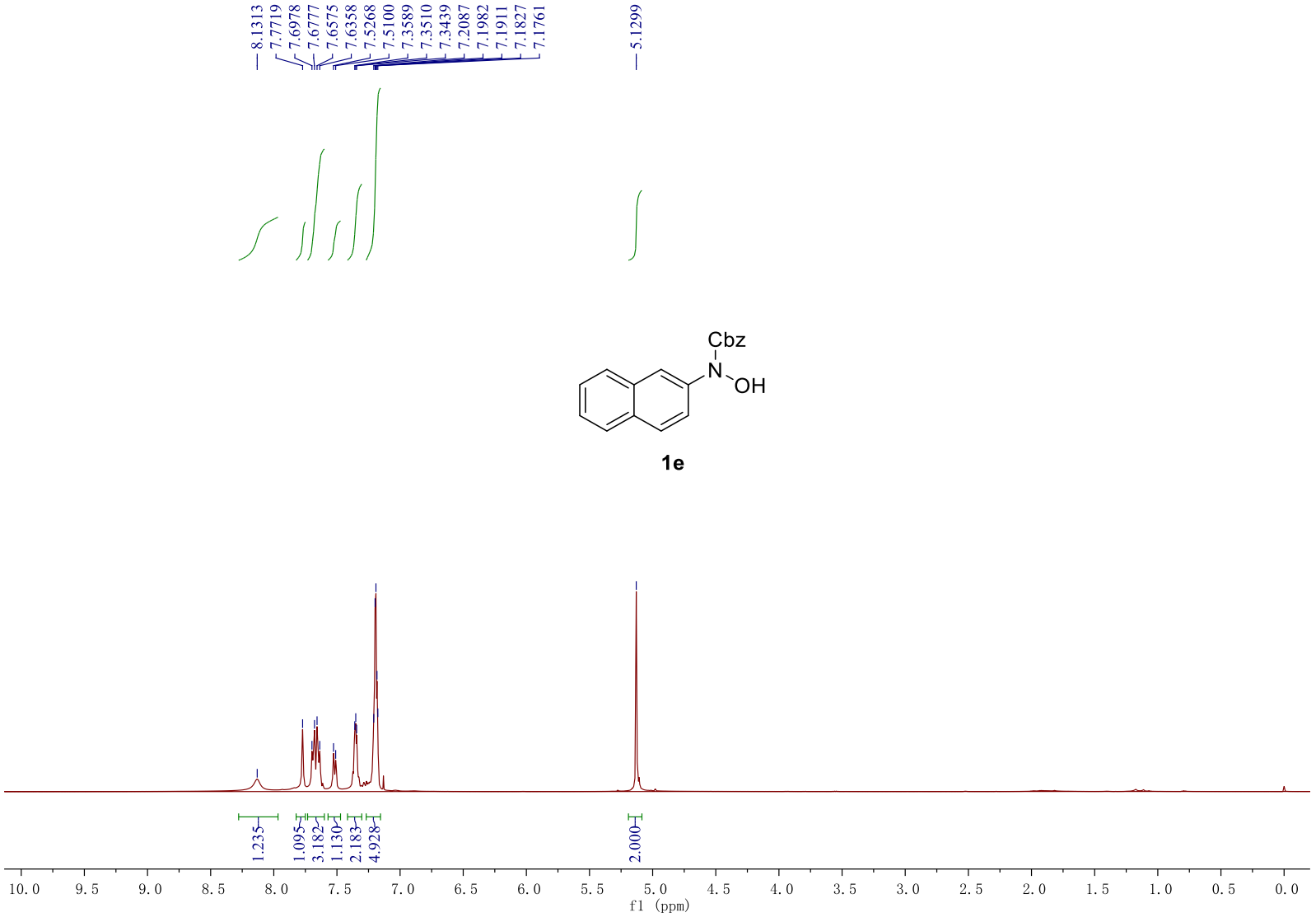
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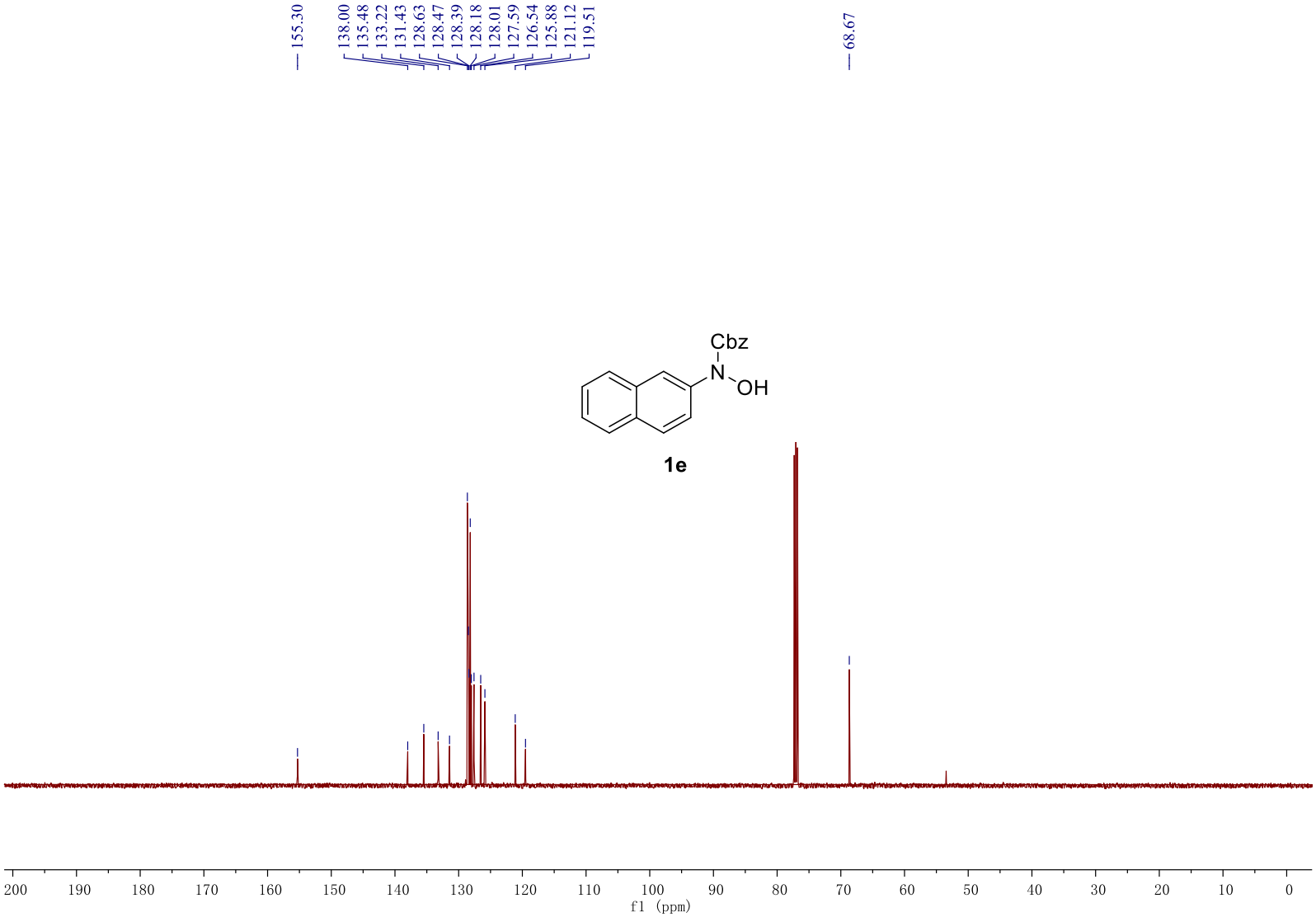
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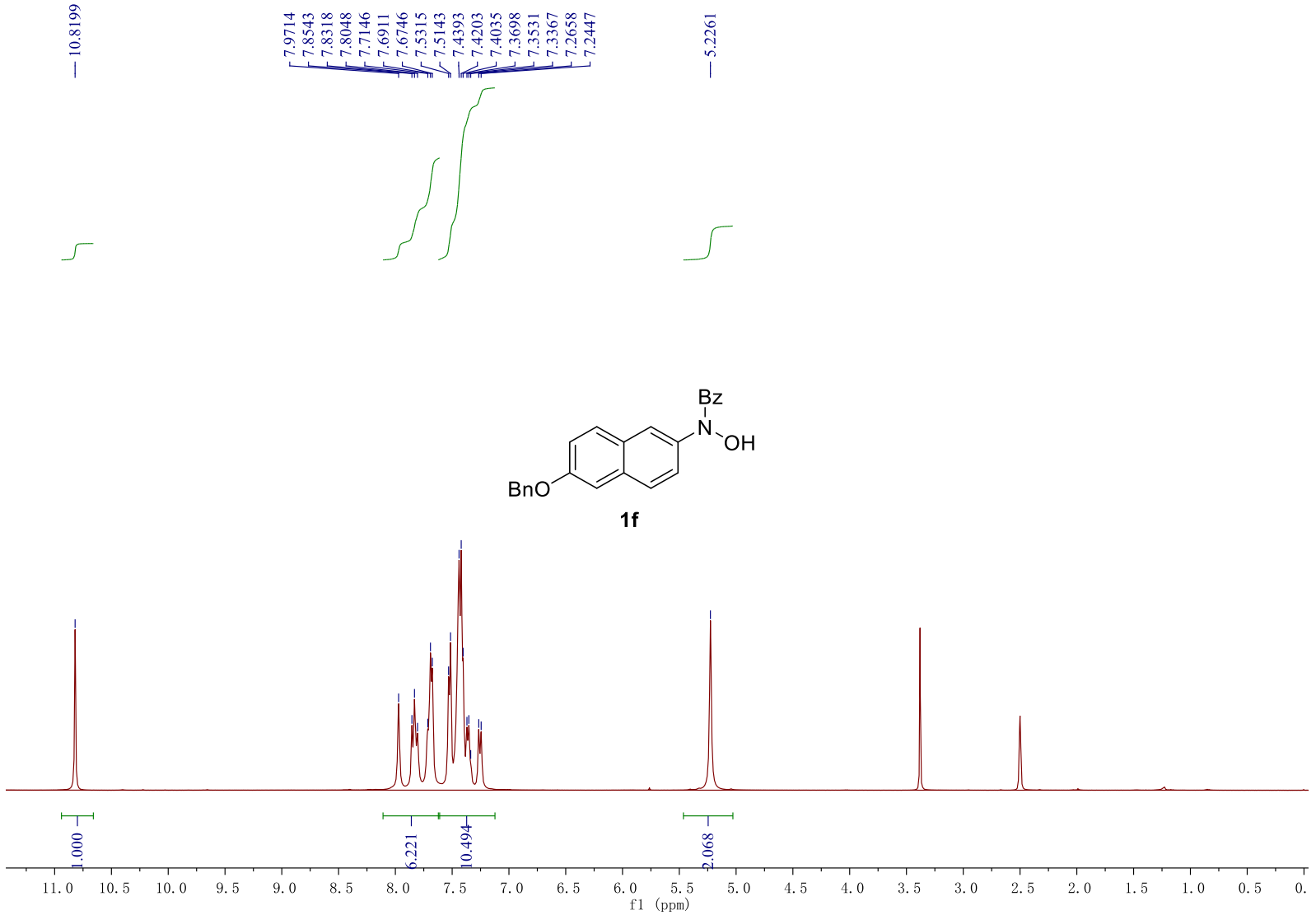
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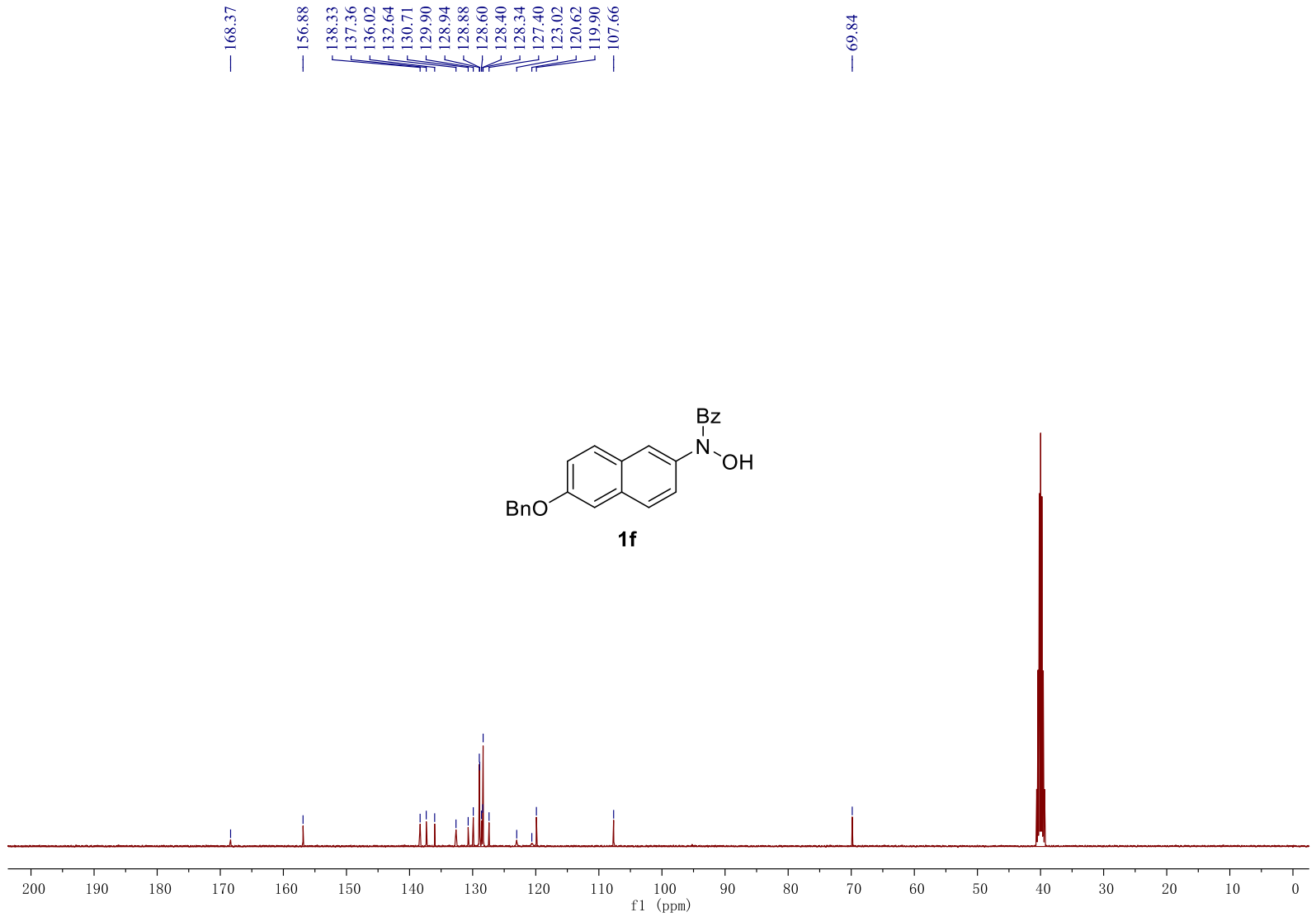
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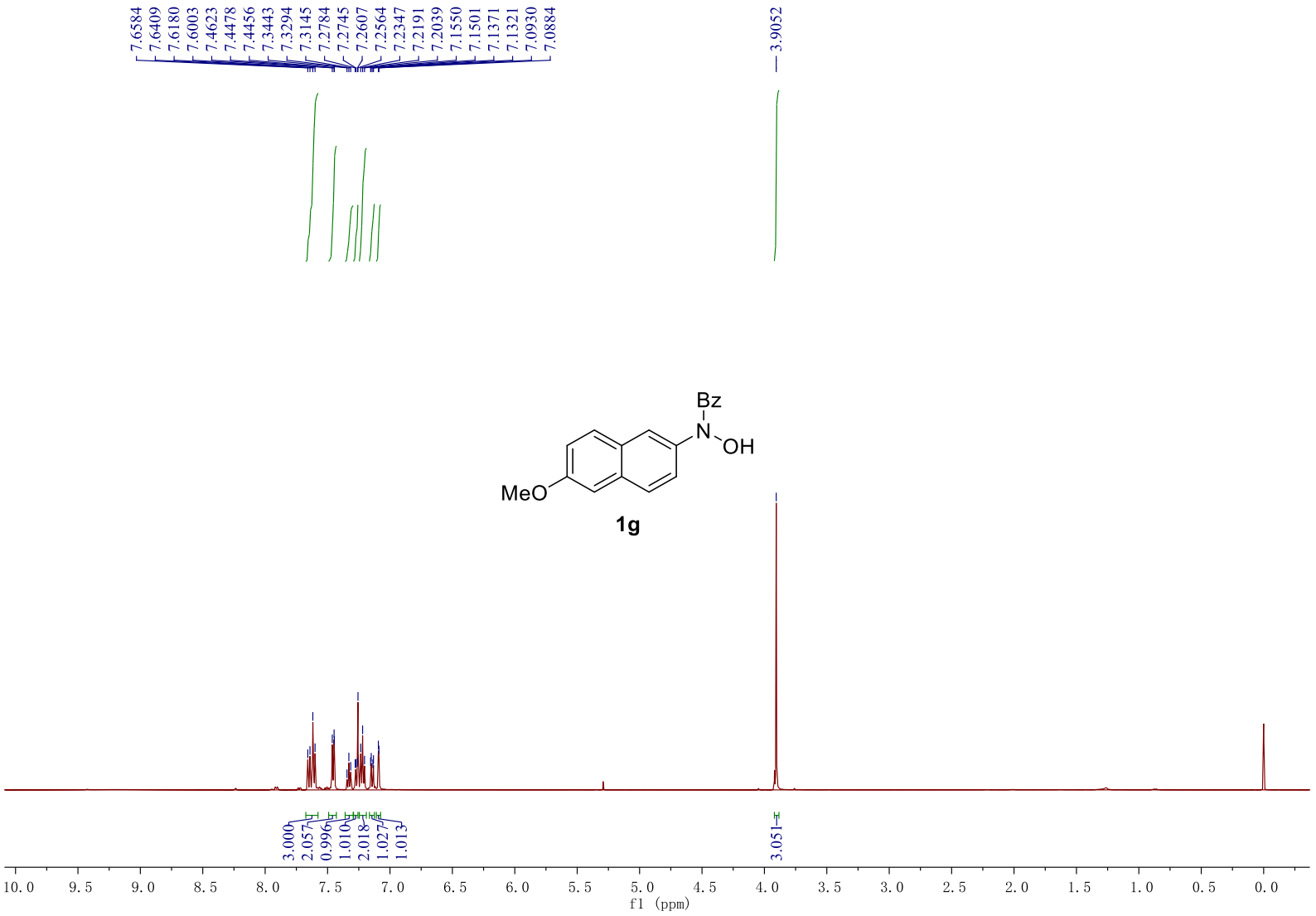
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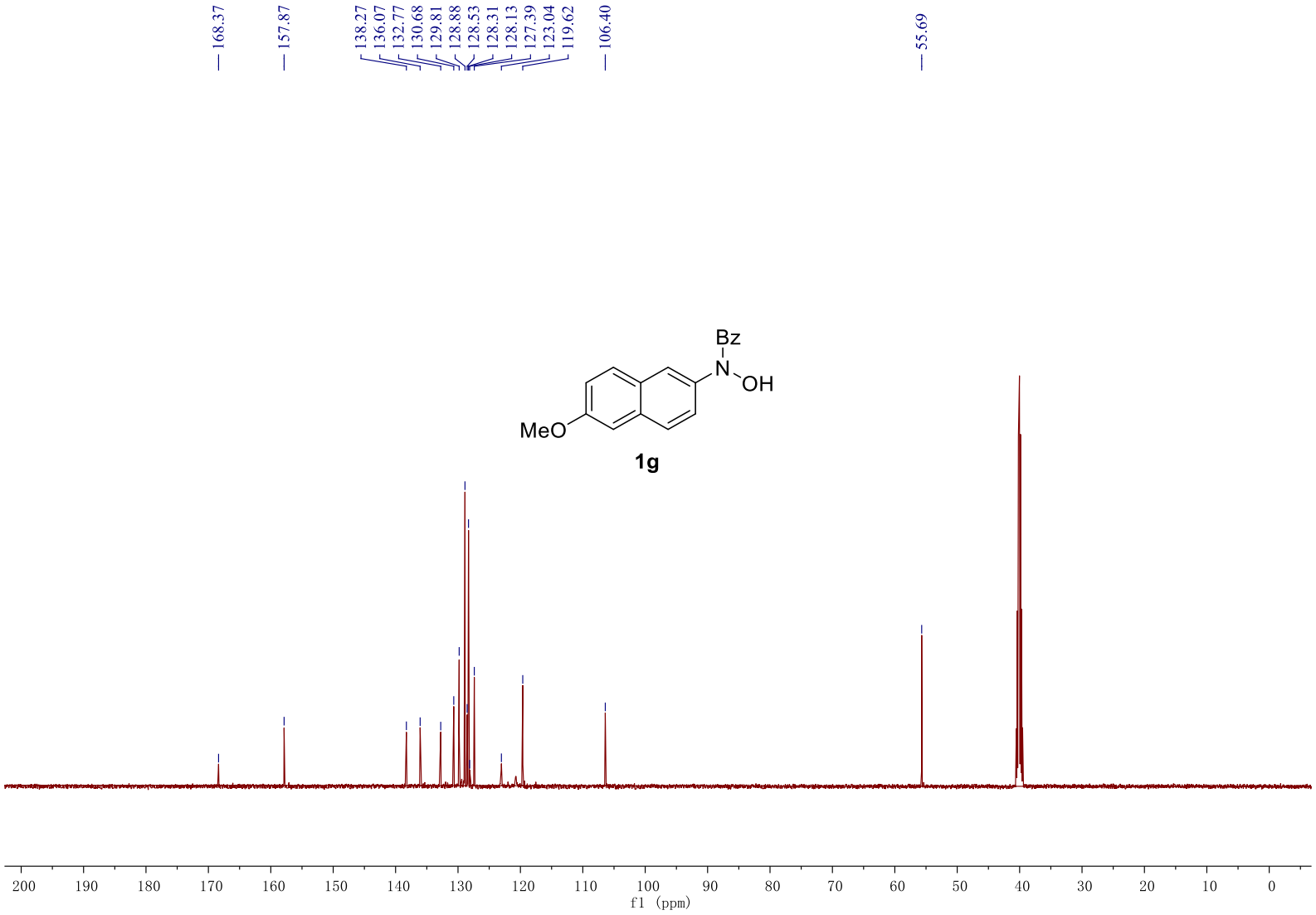
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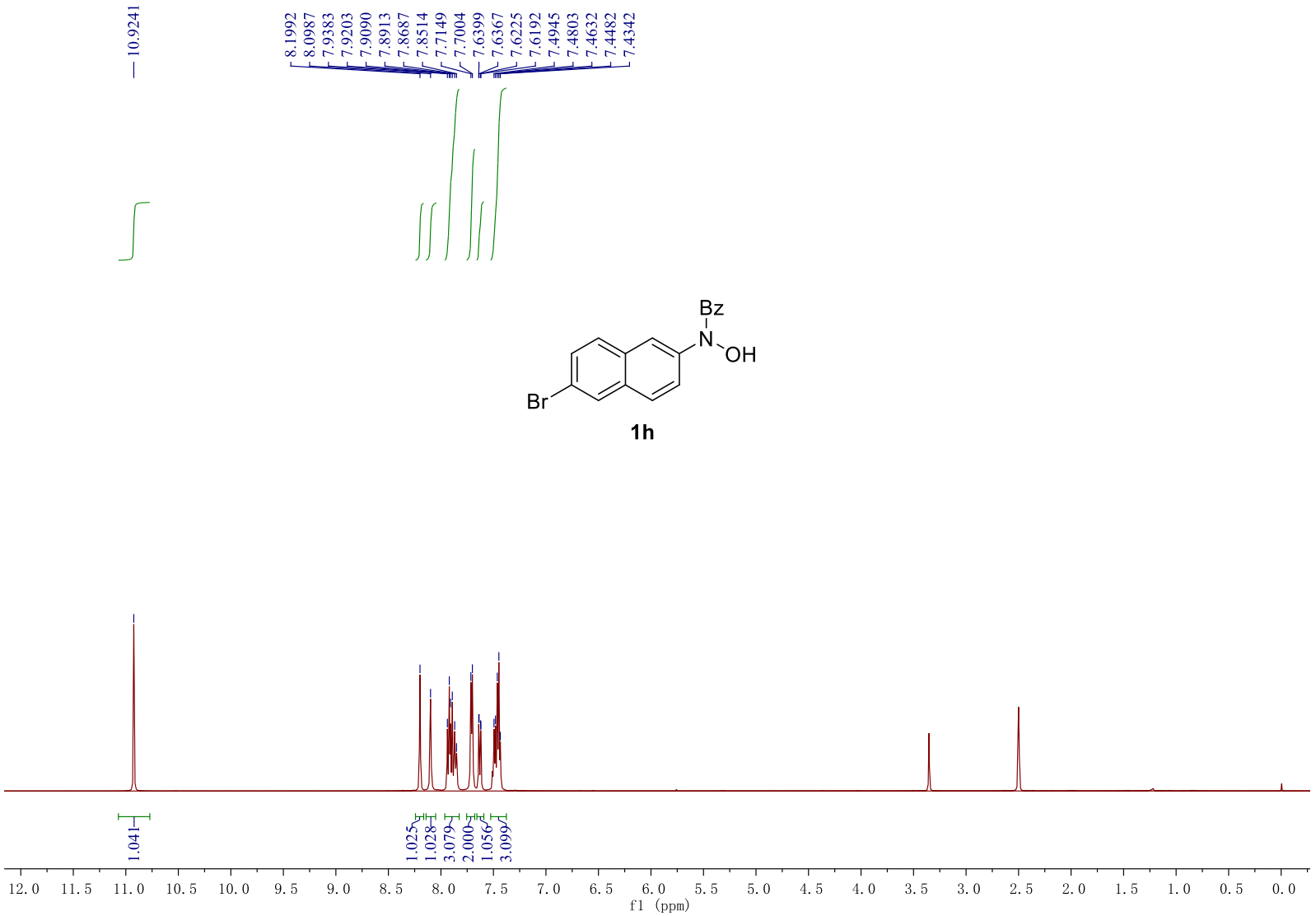
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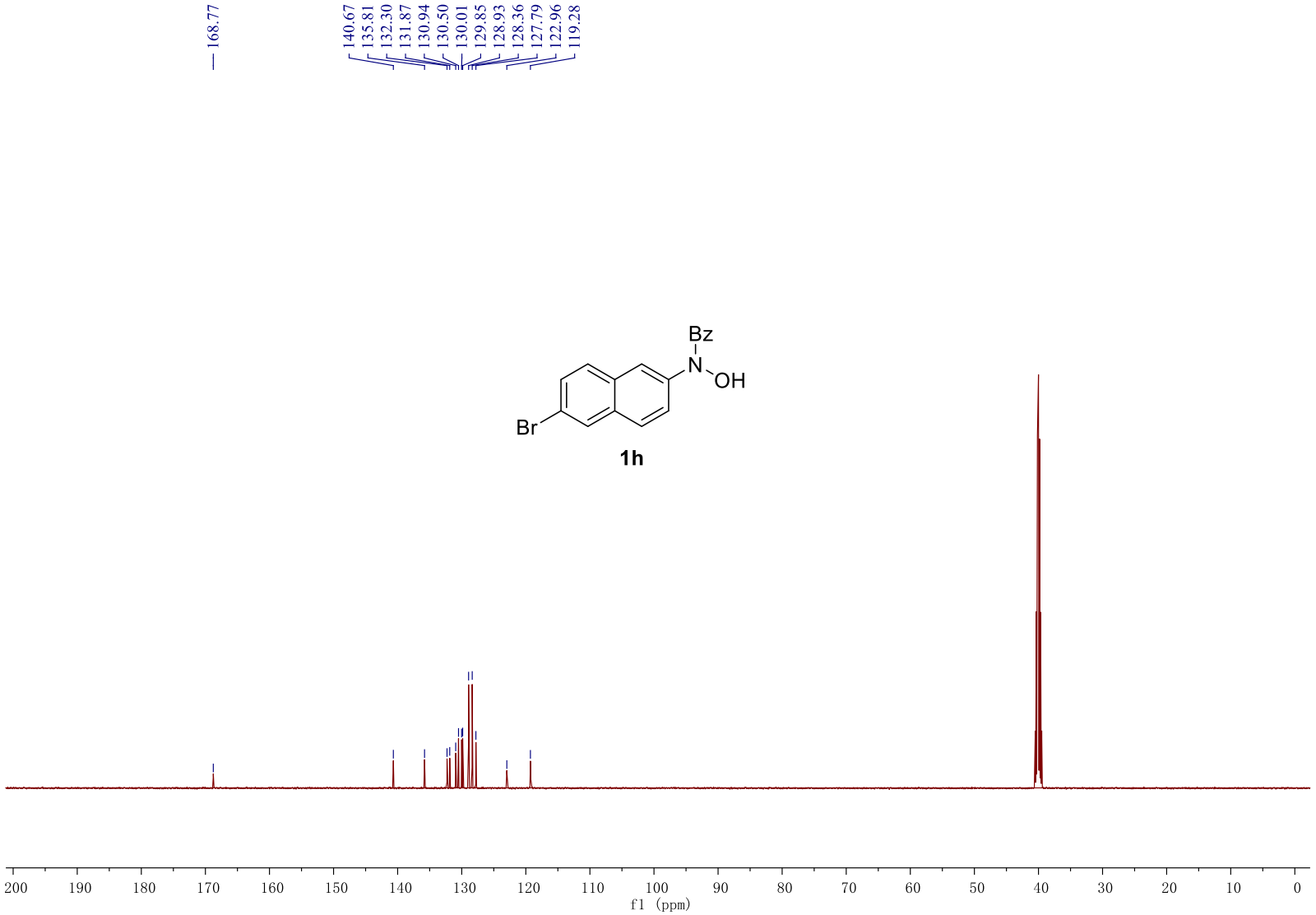
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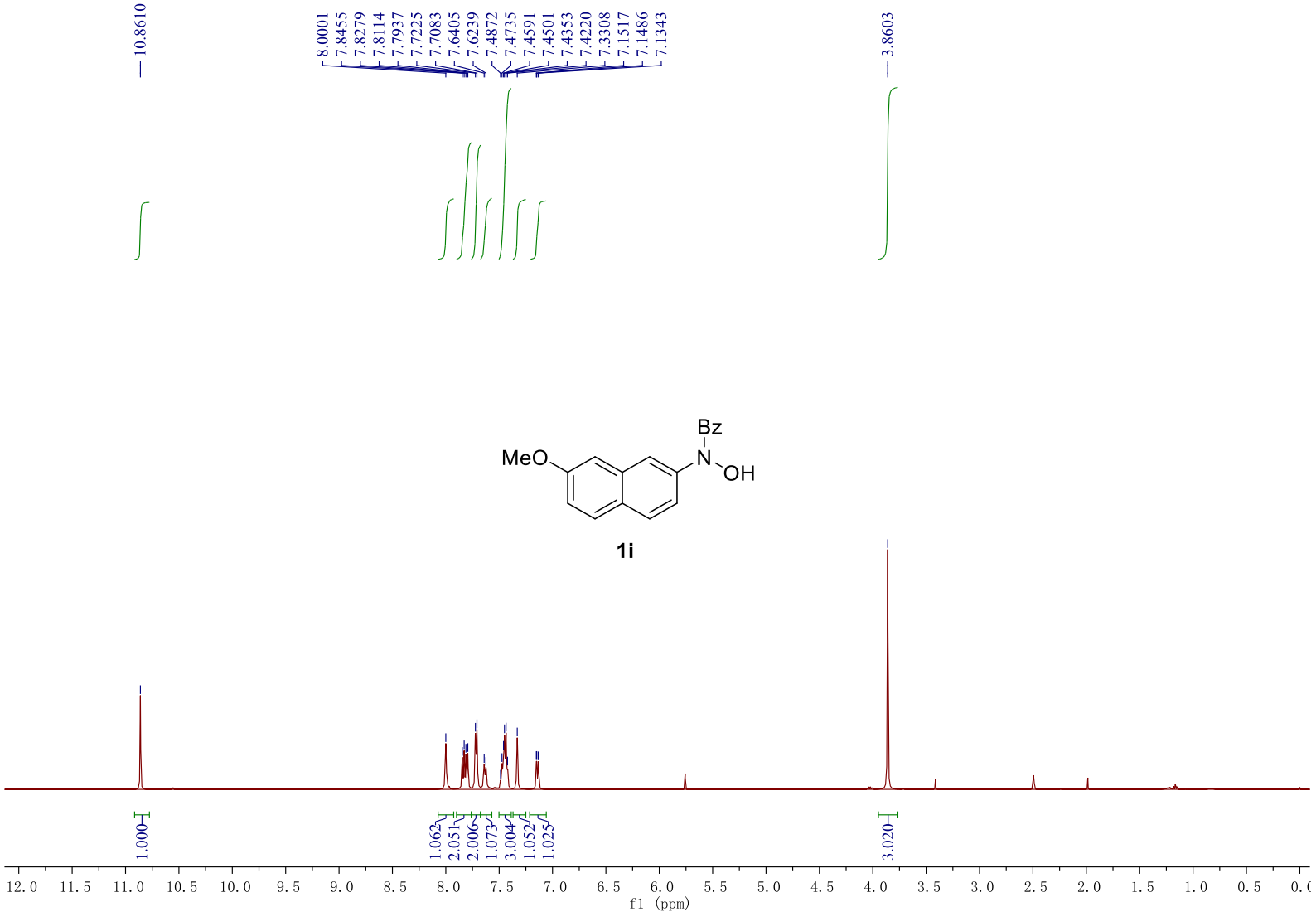
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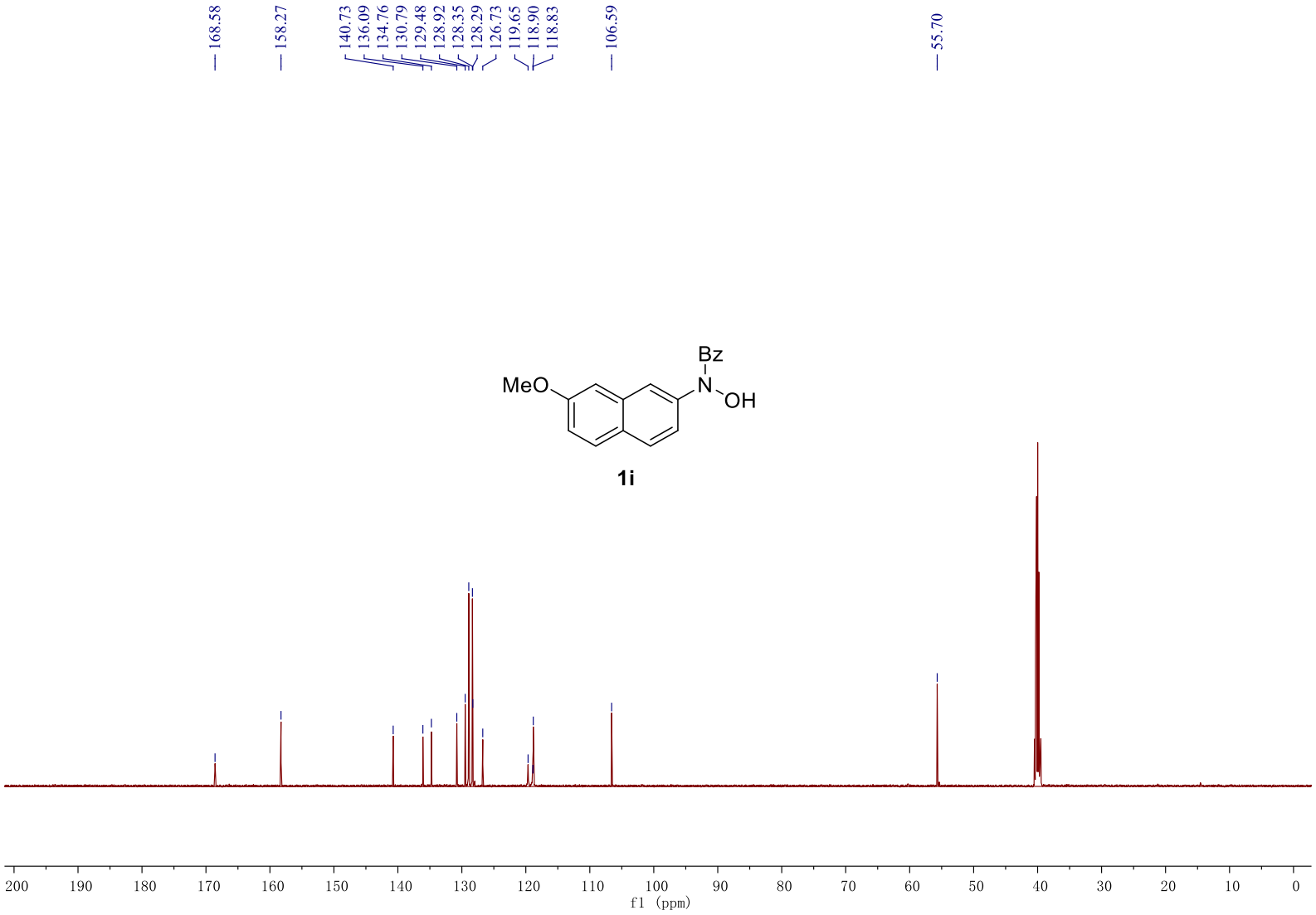
1.025
3.020
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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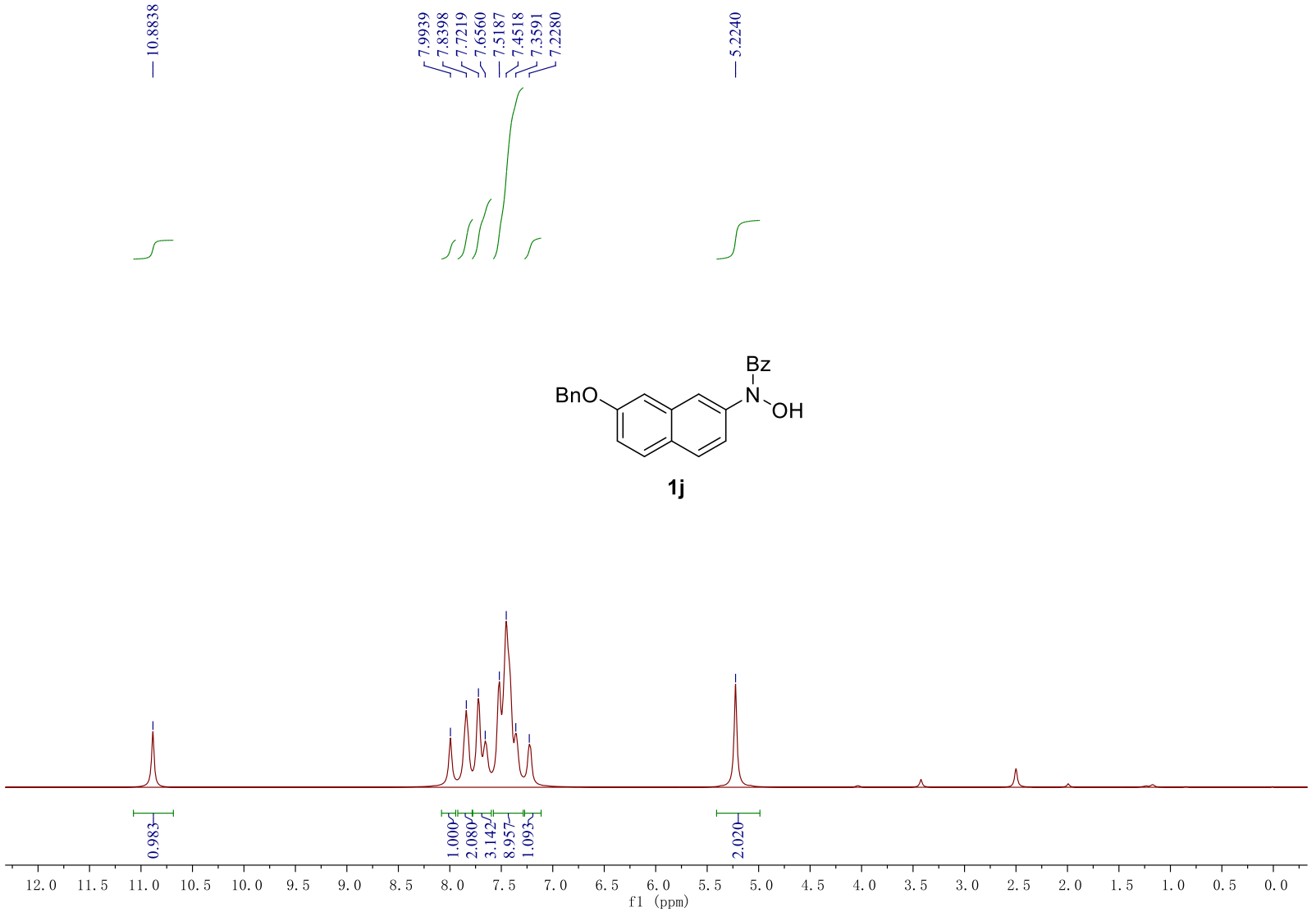
140.73
136.09
134.76
130.79
129.48
128.92
128.35
128.29
126.73
119.65
118.90
118.83
106.59
55.70
MeO
Bz
N
OH
1i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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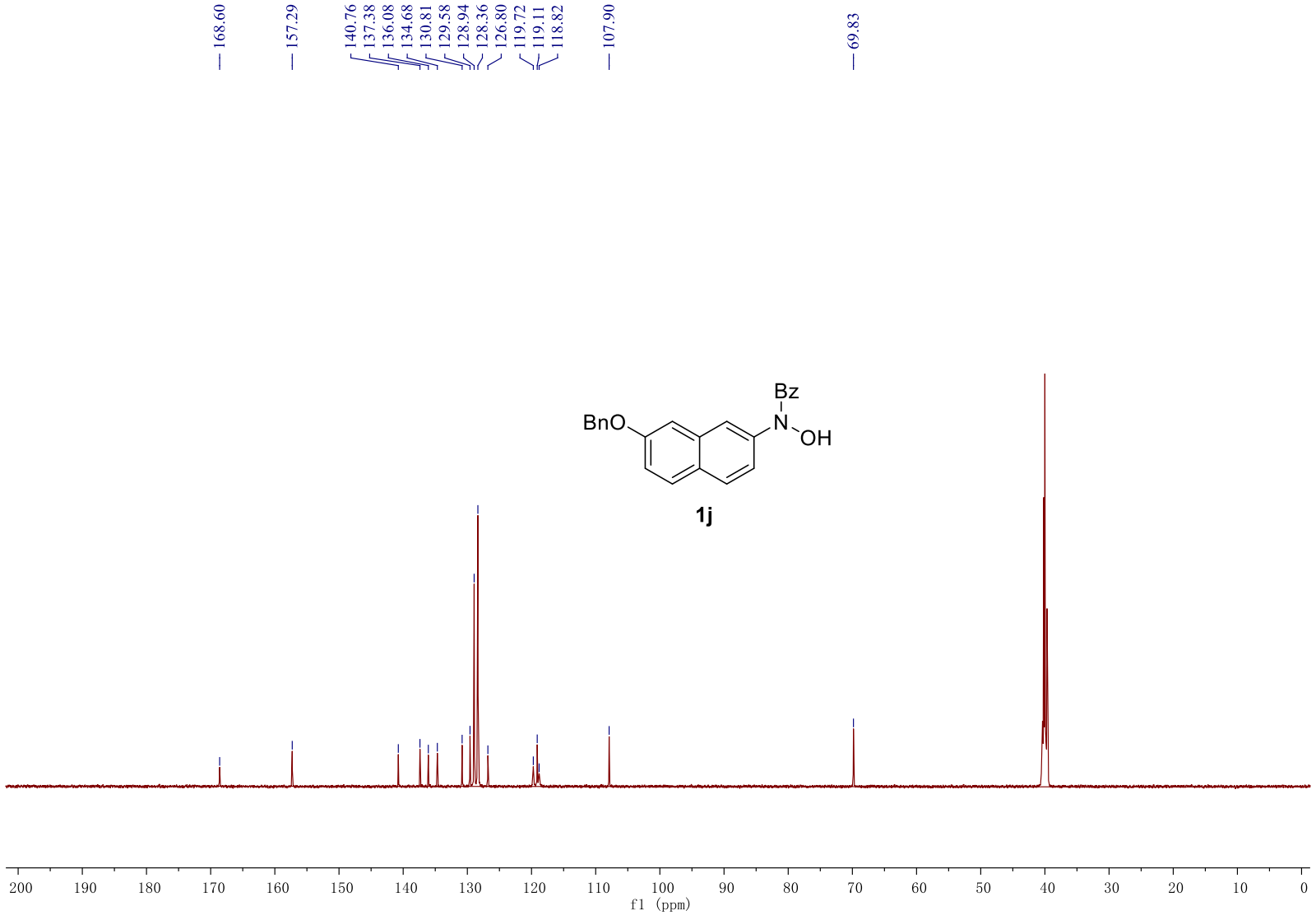
7.9939
7.8398
7.7219
7.6560
7.5187
7.4518
7.3591
7.2280
5.2240
BnO
Bz
N
OH
1j
0.983
1.000
2.080
3.142
8.957
1.093
2.020
f1 (ppm)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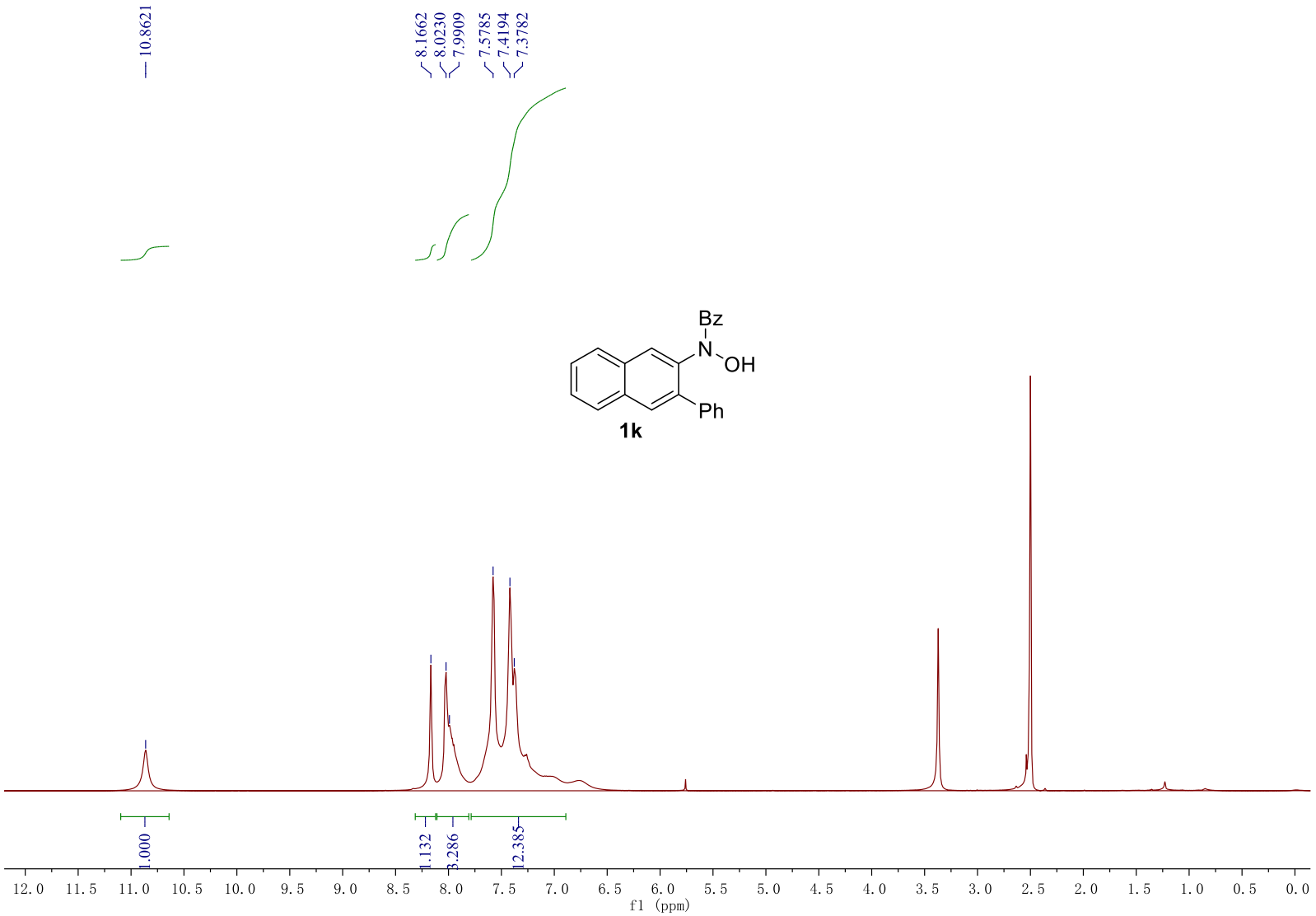
157.29
140.76
137.38
136.08
134.68
130.81
129.58
128.94
128.36
126.80
119.72
119.11
118.82
107.90
69.83
BnO
Bz
N
OH
1j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.1662
8.0230
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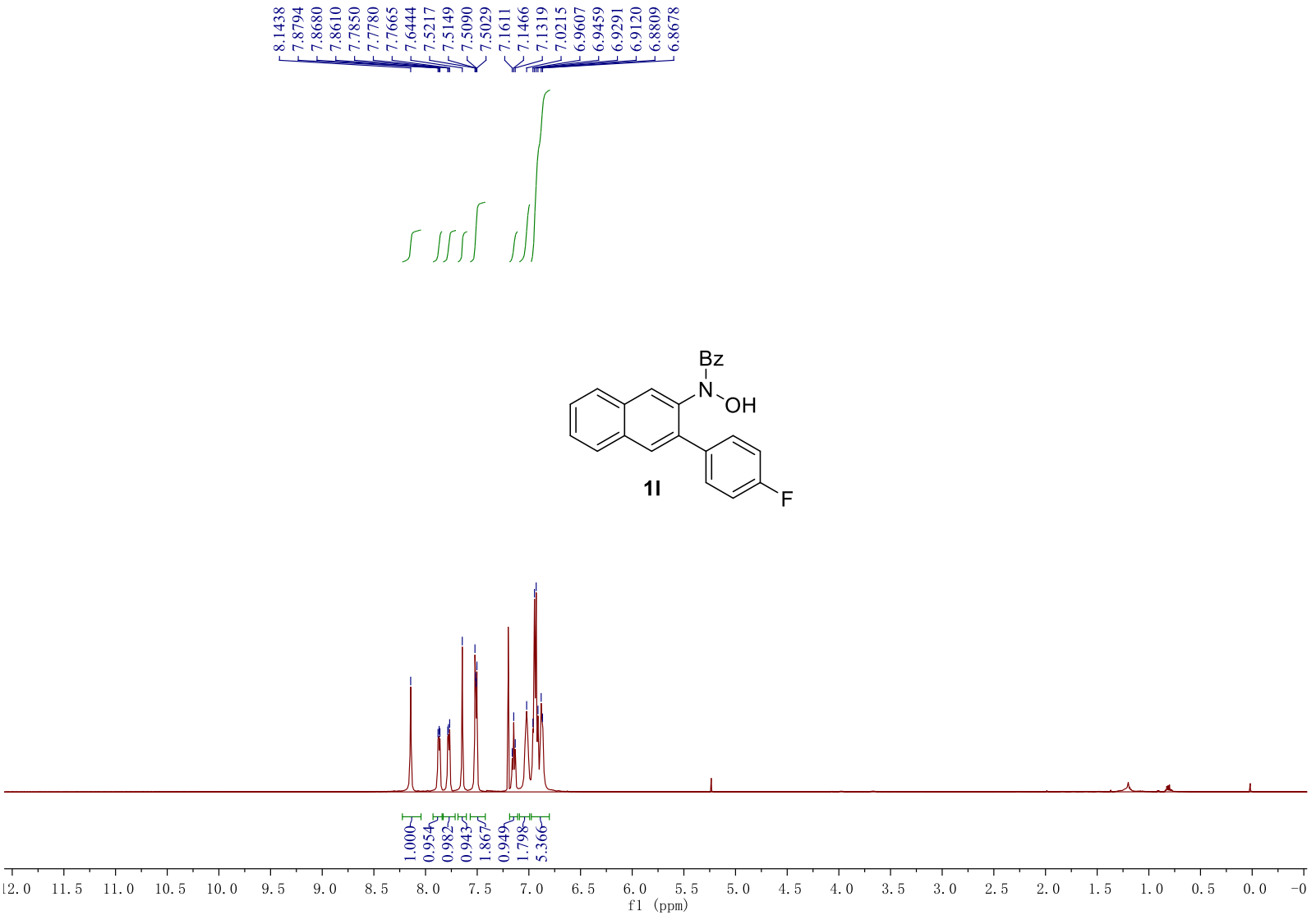
7.5785
7.4194
7.3782
Bz
N
OH
Ph
1k
1.000
1.132
3.286
12.385
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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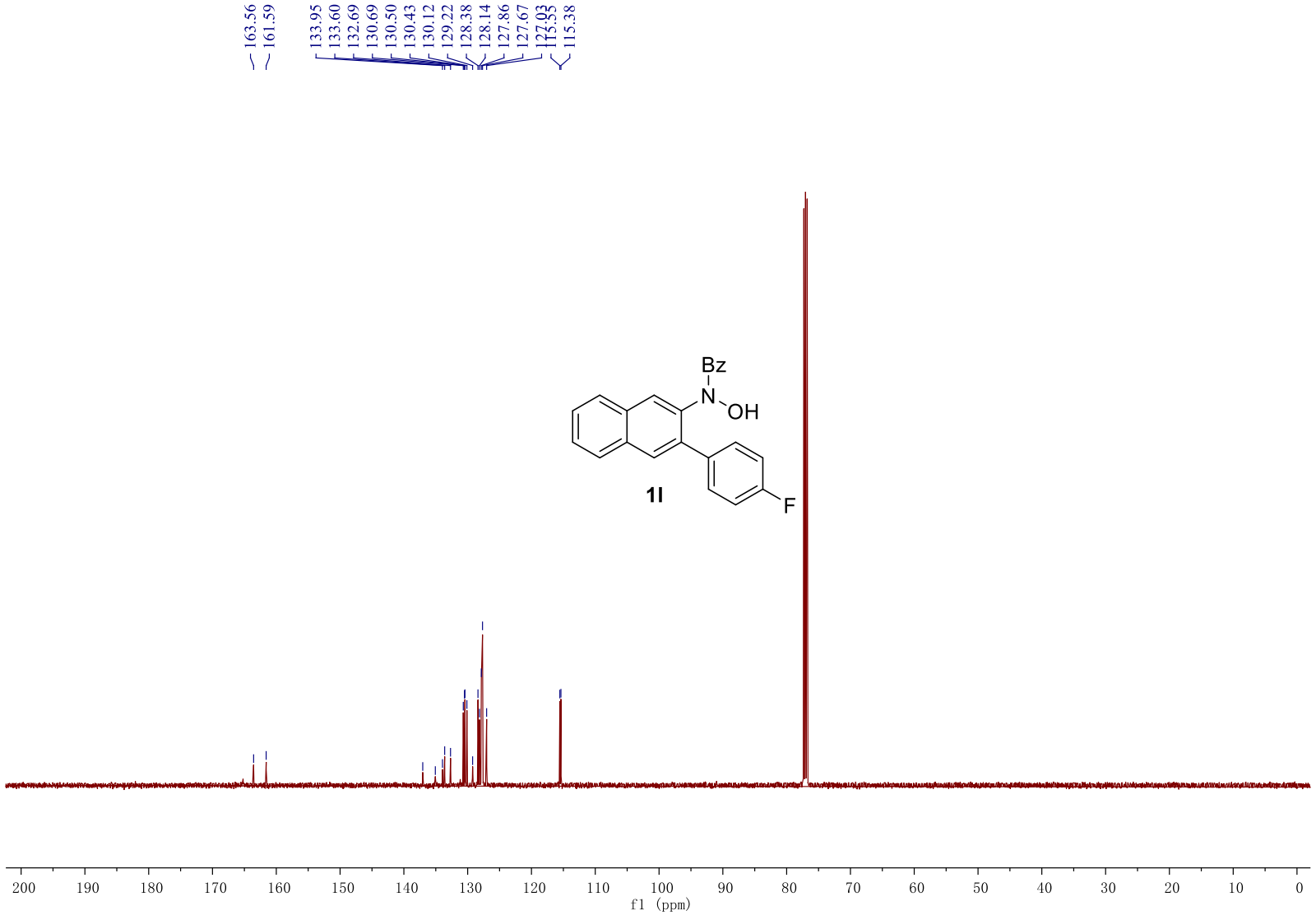
7.8794
7.8680
7.8610
7.7850
7.7780
7.7665
7.6444
7.5217
7.5149
7.5090
7.5029
7.1611
7.1466
7.1319
7.0215
6.9607
6.9459
6.9291
6.9120
6.8809
6.8678
Bz
N
OH
F
1l
1.000
0.954
0.982
0.943
1.867
0.949
1.798
5.366
f1 (ppm)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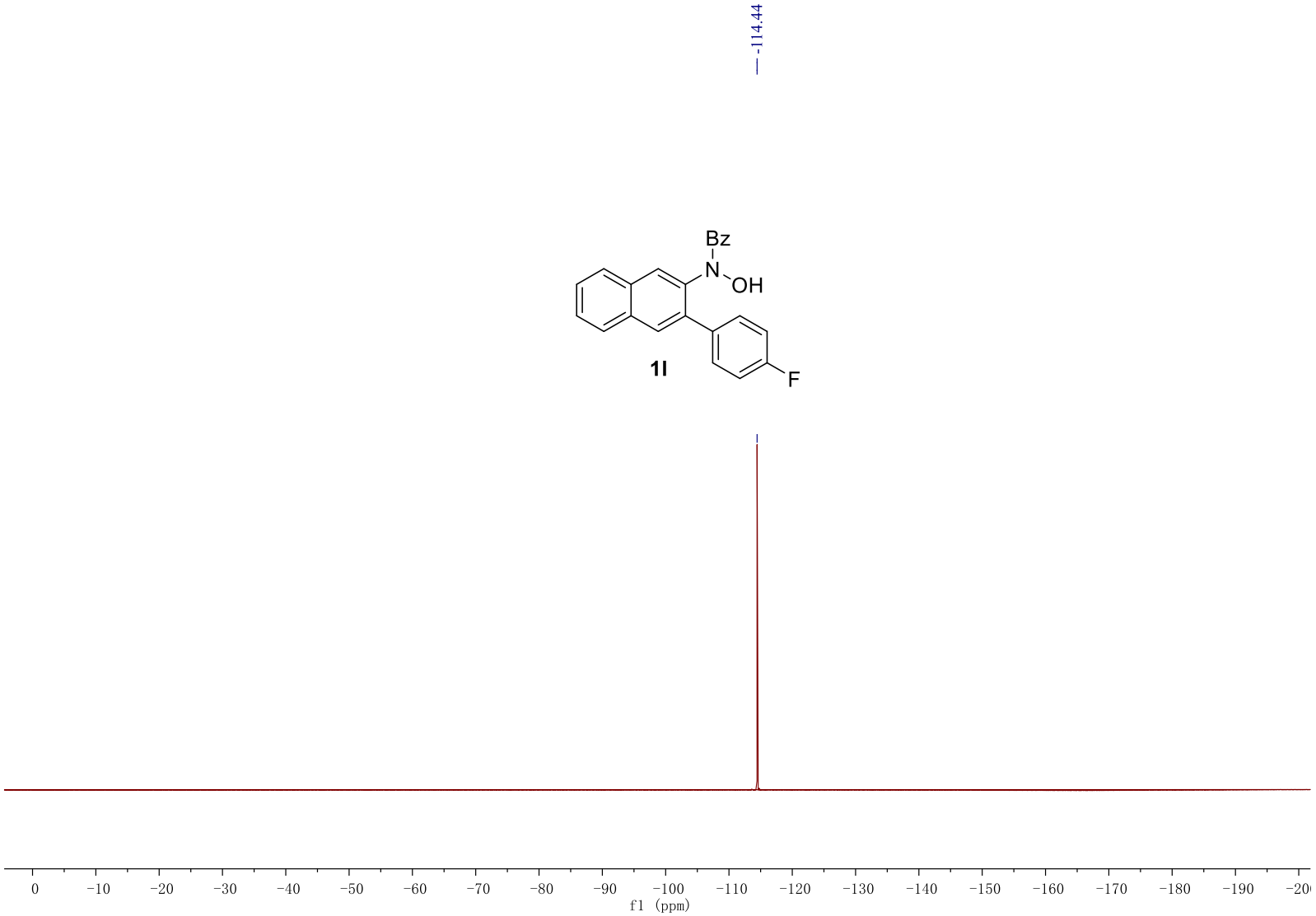
161.59
133.95
133.60
132.69
130.69
130.50
130.43
130.12
129.22
128.38
128.14
127.86
127.67
115.55
115.38
Bz
N
OH
F
1l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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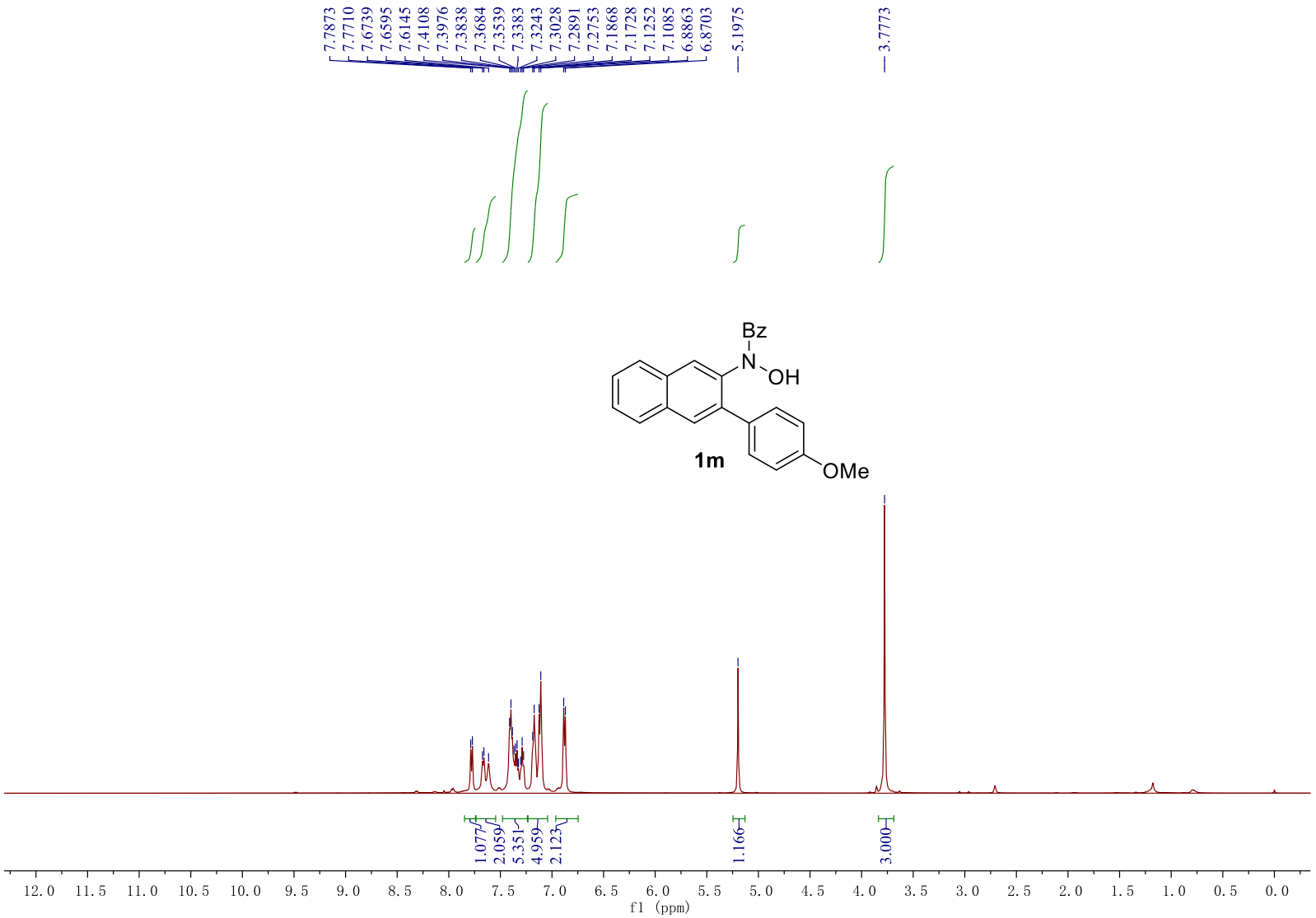
Bz
N
OH
F
1l
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)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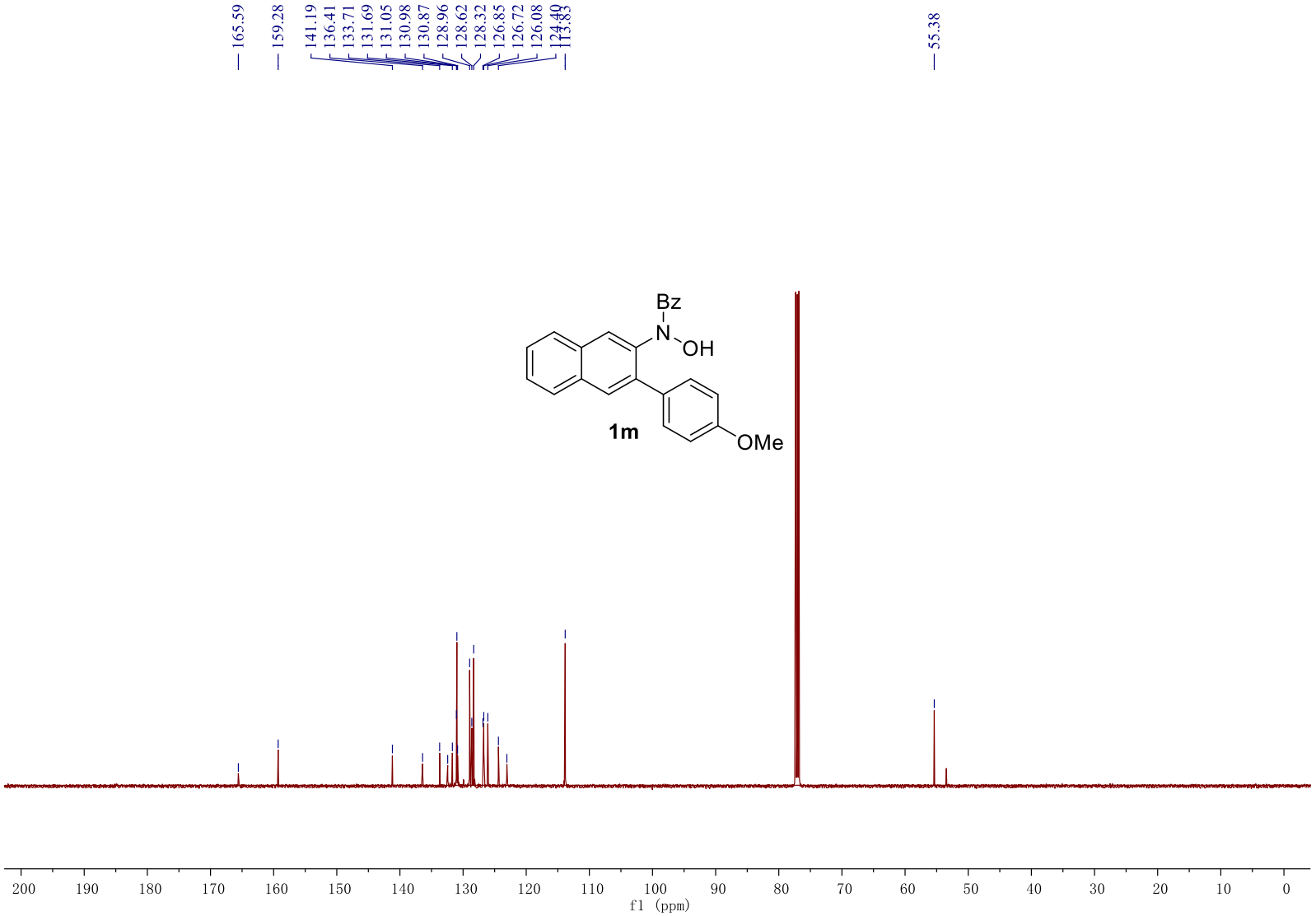
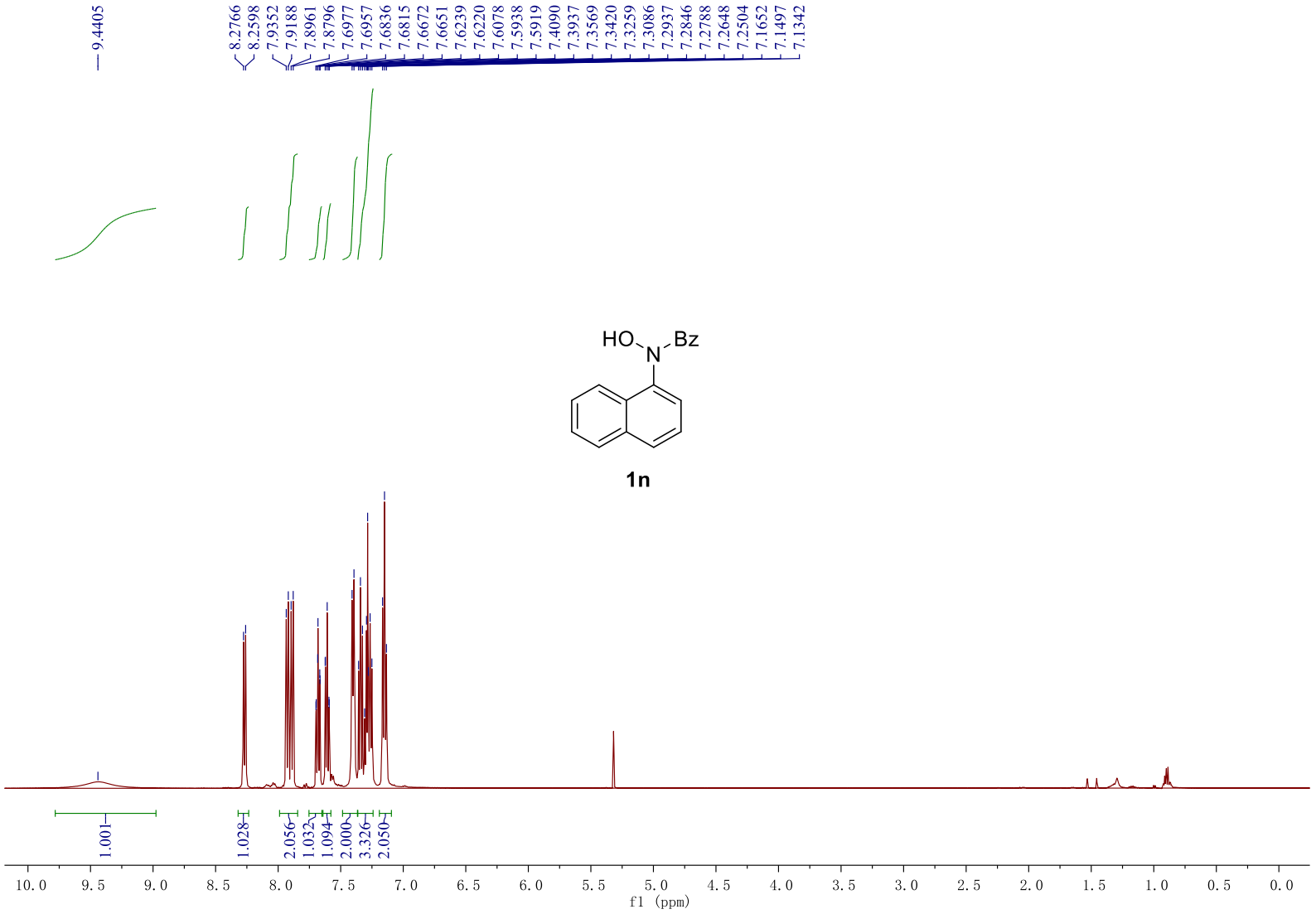
7.6595
7.6145
7.4108
7.3976
7.3838
7.3684
7.3539
7.3383
7.3243
7.3028
7.2891
7.2753
7.1868
7.1728
7.1252
7.1085
6.8863
6.8703
5.1975
3.7773
Bz
N
OH
1m
OMe
1.077
2.059
5.351
4.959
2.123
1.166
3.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


165.59
159.28
141.19
136.41
133.71
131.69
131.05
130.98
130.87
128.96
128.62
128.32
126.85
126.72
126.08
124.40
113.83
55.38
Bz
N
OH
1m
OMe
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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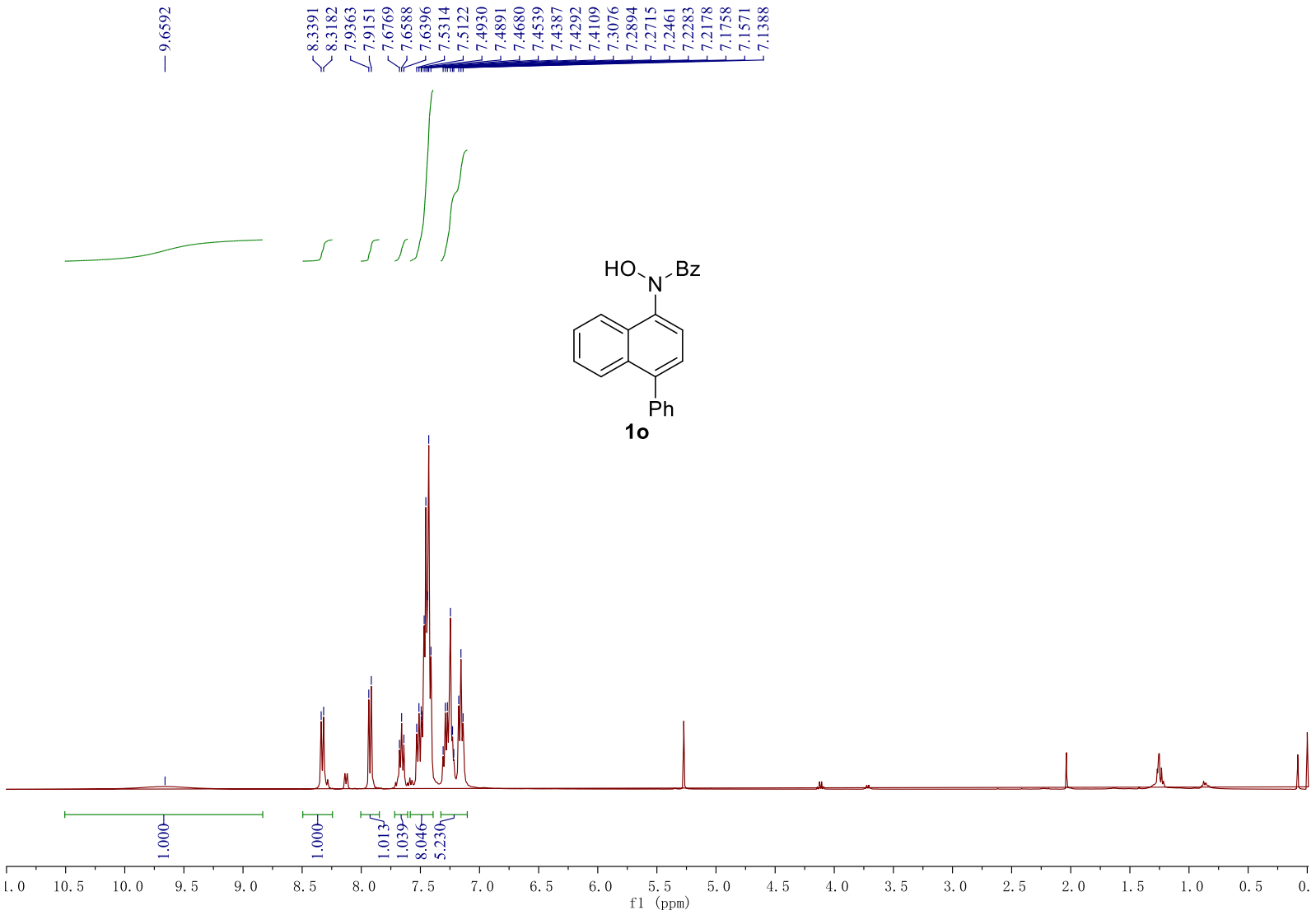
8.2766
8.2598
7.9352
7.9188
7.8961
7.8796
7.6977
7.6957
7.6836
7.6815
7.6672
7.6651
7.6239
7.6220
7.6078
7.5938
7.5919
7.4090
7.3937
7.3569
7.3420
7.3259
7.3086
7.2937
7.2846
7.2788
7.2648
7.2504
7.1652
7.1497
7.1342
HO
N
Bz
1n
1.001
1.028
2.056
1.032
1.094
2.000
3.326
2.050
10.0
9.5
9.0
8.5
8.0
7.5
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)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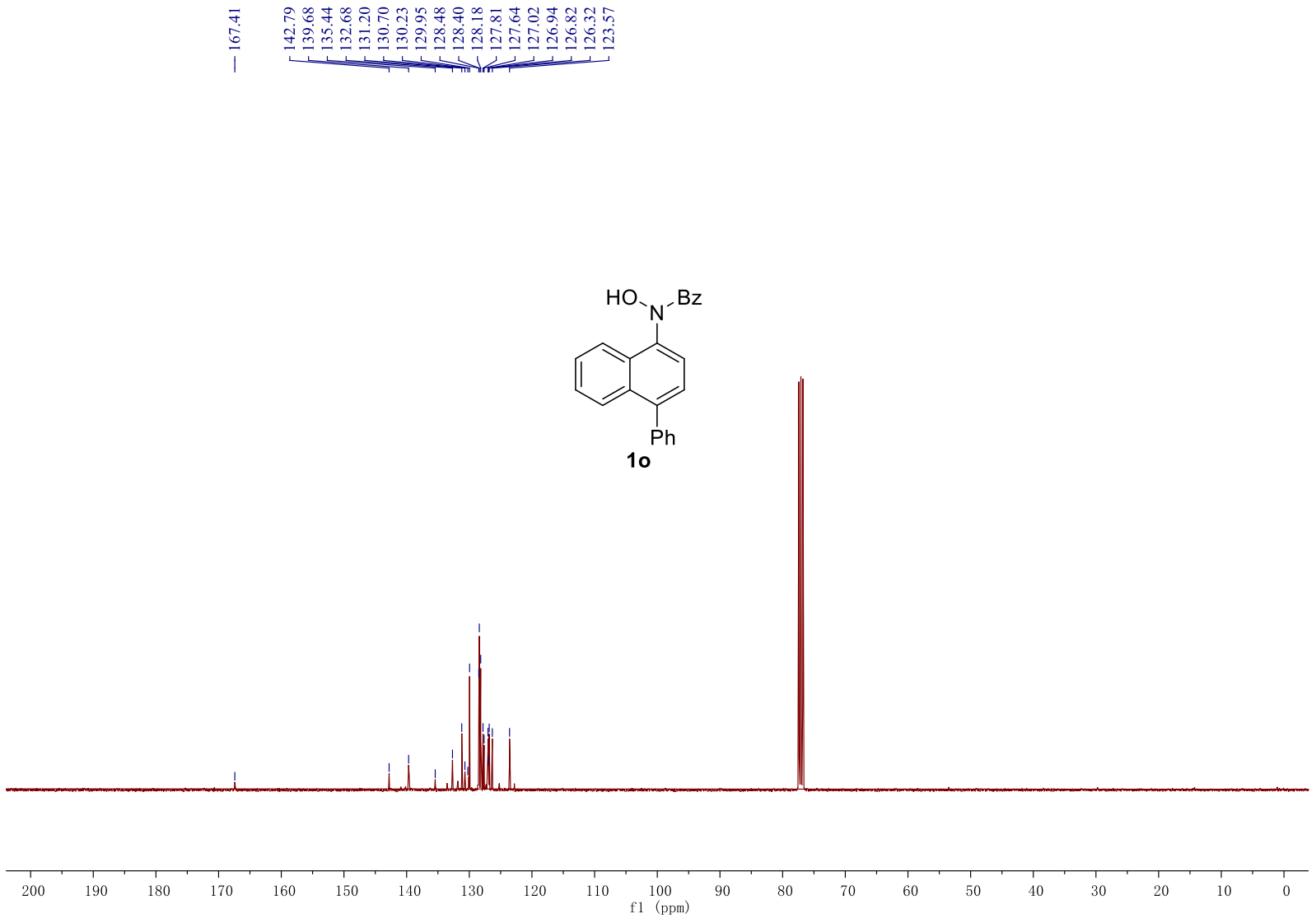
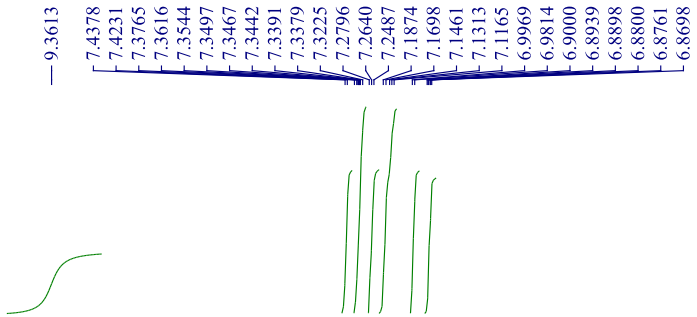
8.3391
8.3182
7.9363
7.9151
7.6769
7.6588
7.6396
7.5314
7.5122
7.4930
7.4891
7.4680
7.4539
7.4387
7.4292
7.4109
7.3076
7.2894
7.2715
7.2461
7.2283
7.2178
7.1758
7.1571
7.1388
HO
N
Bz
Ph
1o
1.000
1.000
1.013
1.039
8.046
5.230
f1 (ppm)


167.41
142.79
139.68
135.44
132.68
131.20
130.70
130.23
129.95
128.48
128.40
128.18
127.81
127.64
127.02
126.94
126.82
126.32
123.57
HO
N
Bz
Ph
1o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4231
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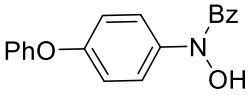
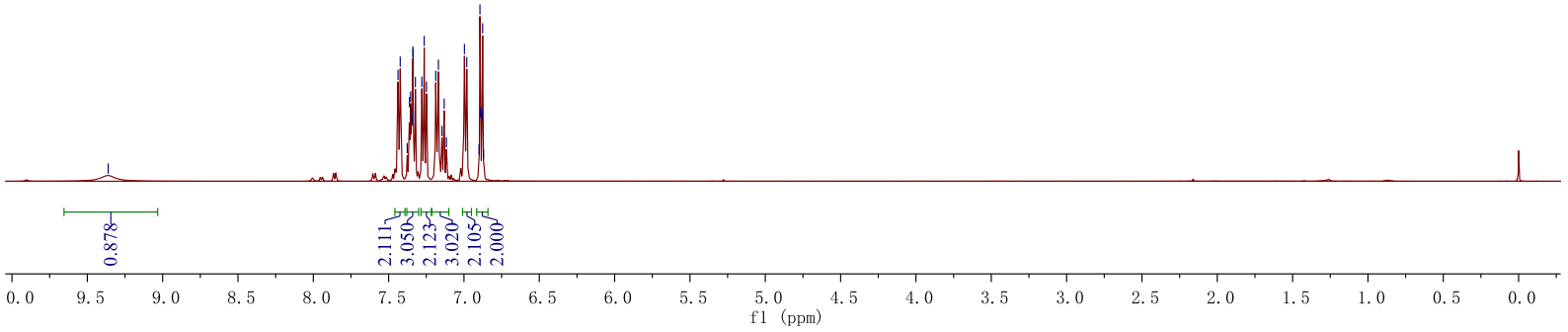
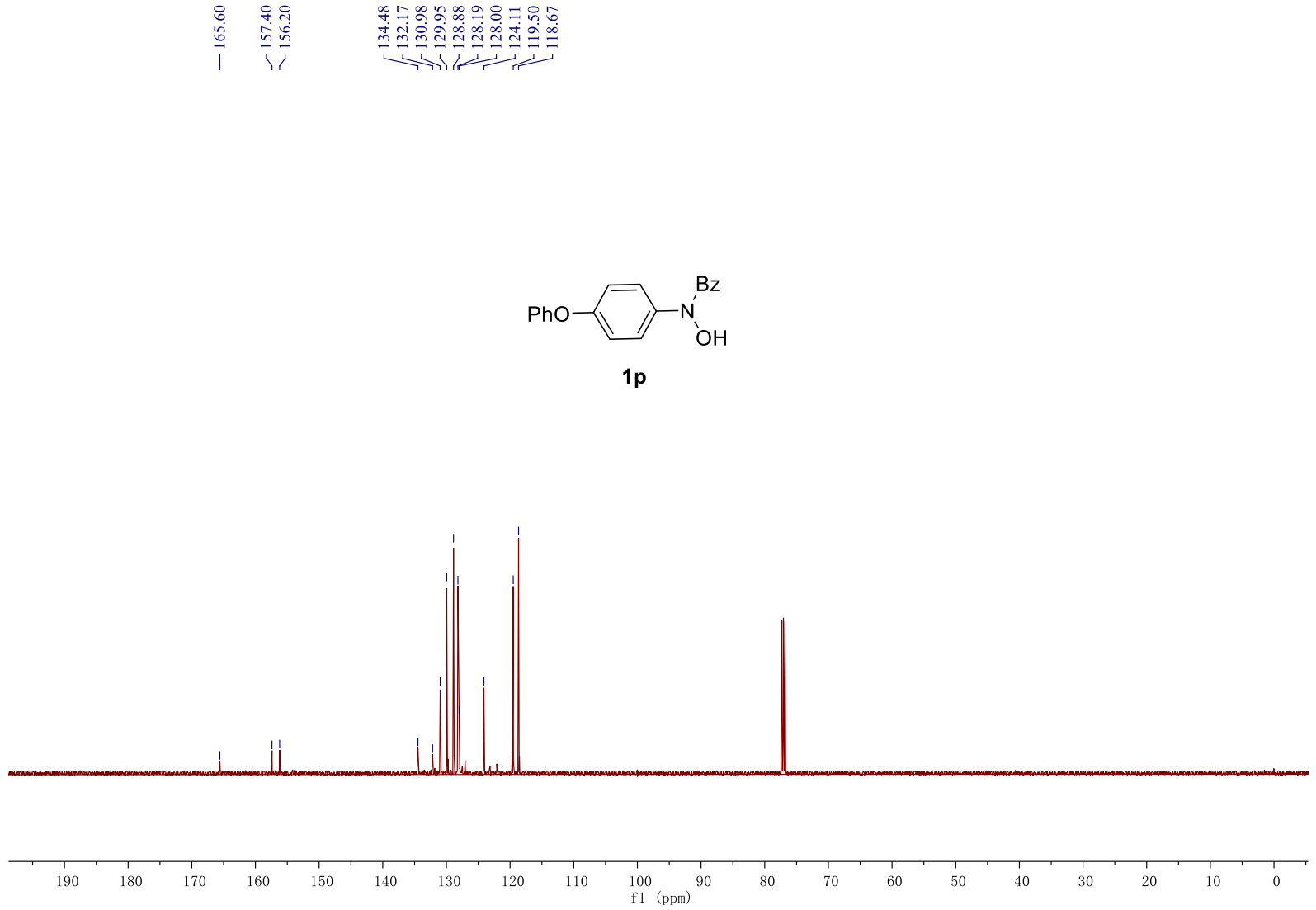
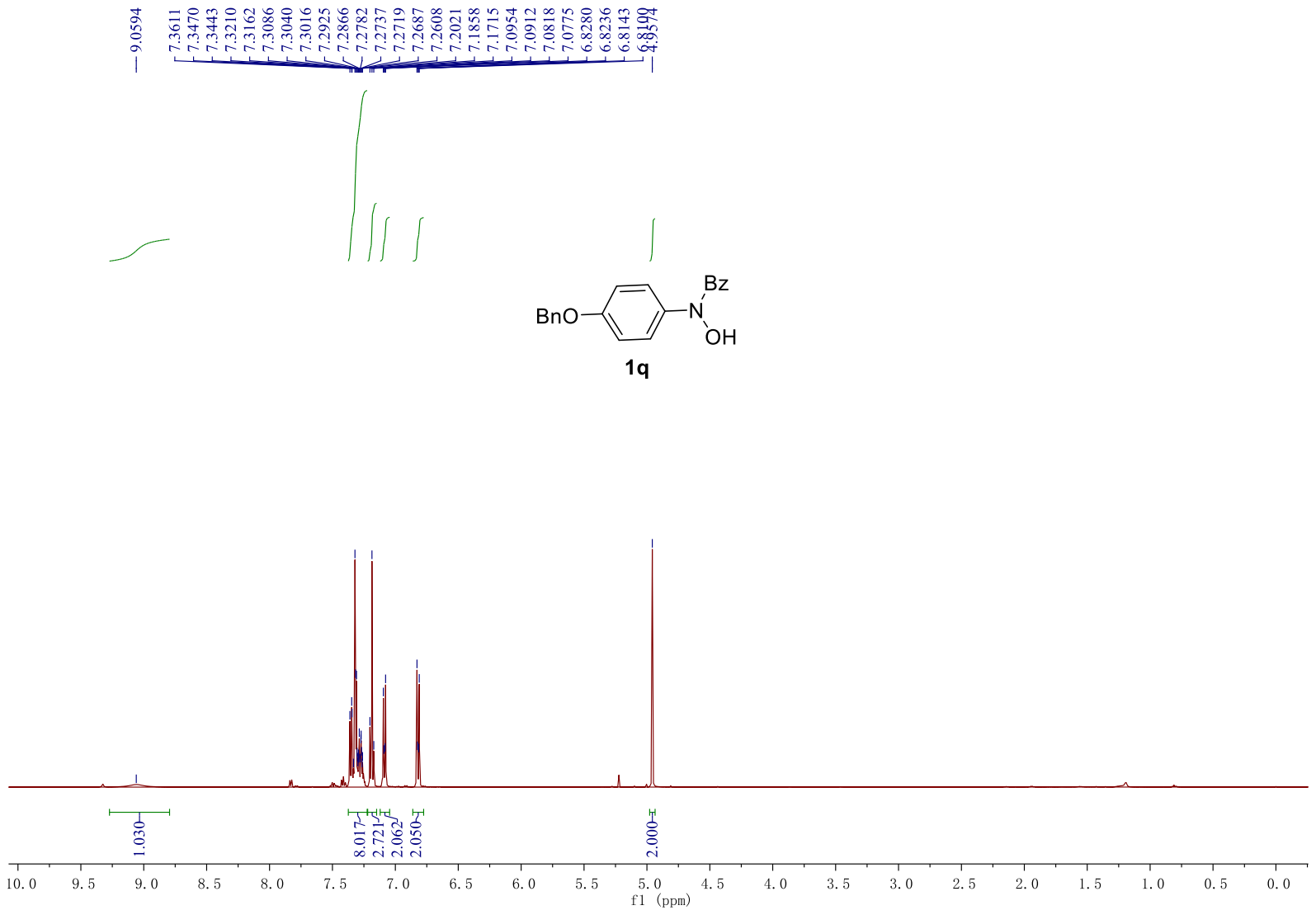
7.3616
7.3544
7.3497
7.3467
7.3442
7.3391
7.3379
7.3225
7.2796
7.2640
7.2487
7.1874
7.1698
7.1461
7.1313
7.1165
6.9969
6.9814
6.9000
6.8939
6.8898
6.8800
6.8761
6.8698


PhO
Bz
N
OH

1p


0.878
2.111
3.050
2.123
3.020
2.105
2.000
0.0
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)


165.60
157.40
156.20
134.48
132.17
130.98
129.95
128.88
128.19
128.00
124.11
119.50
118.67
PhO
N
Bz
OH
1p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3443
7.3210
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7.3086
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7.3016
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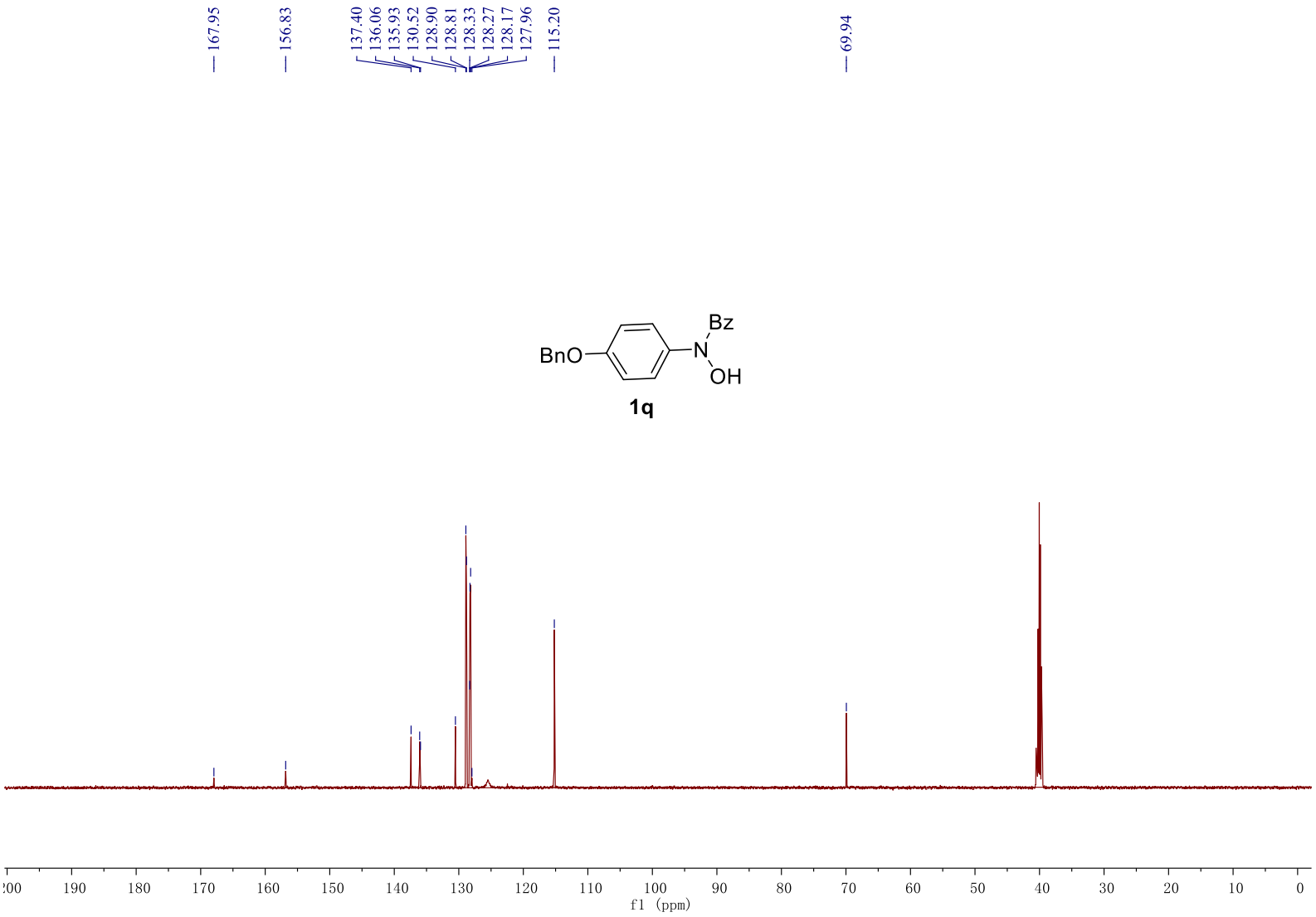
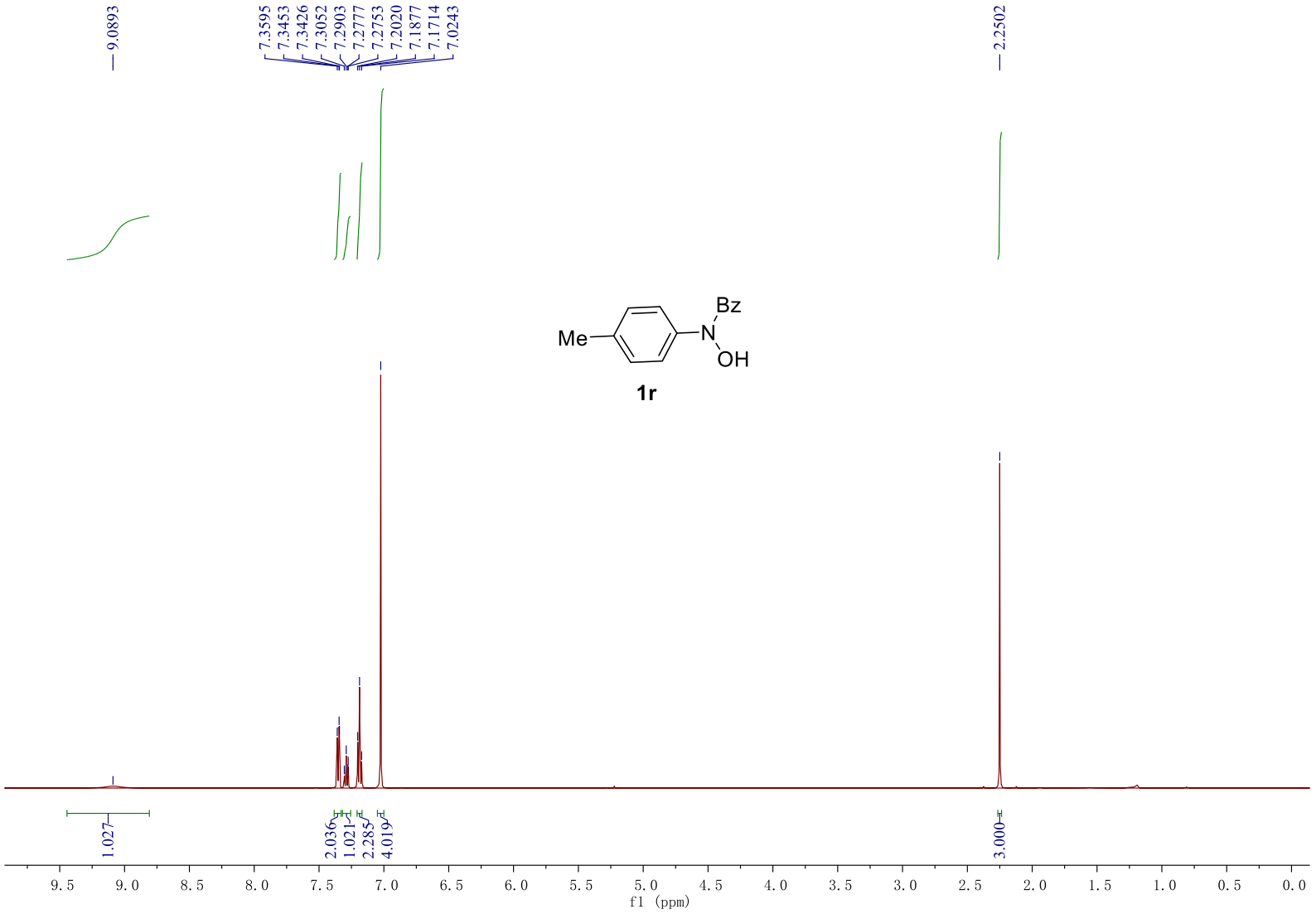
7.2866
7.2782
7.2737
7.2719
7.2687
7.2608
7.2021
7.1858
7.1715
7.0954
7.0912
7.0818
7.0775
6.8280
6.8236
6.8143
6.8100
4.9574
BnO
N
Bz
OH
1q
1.030
8.017
2.721
2.062
2.050
2.000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.95
156.83
137.40
136.06
135.93
130.52
128.90
128.81
128.33
128.27
128.17
127.96
115.20
69.94
BnO
N
Bz
OH
1q
f1 (ppm)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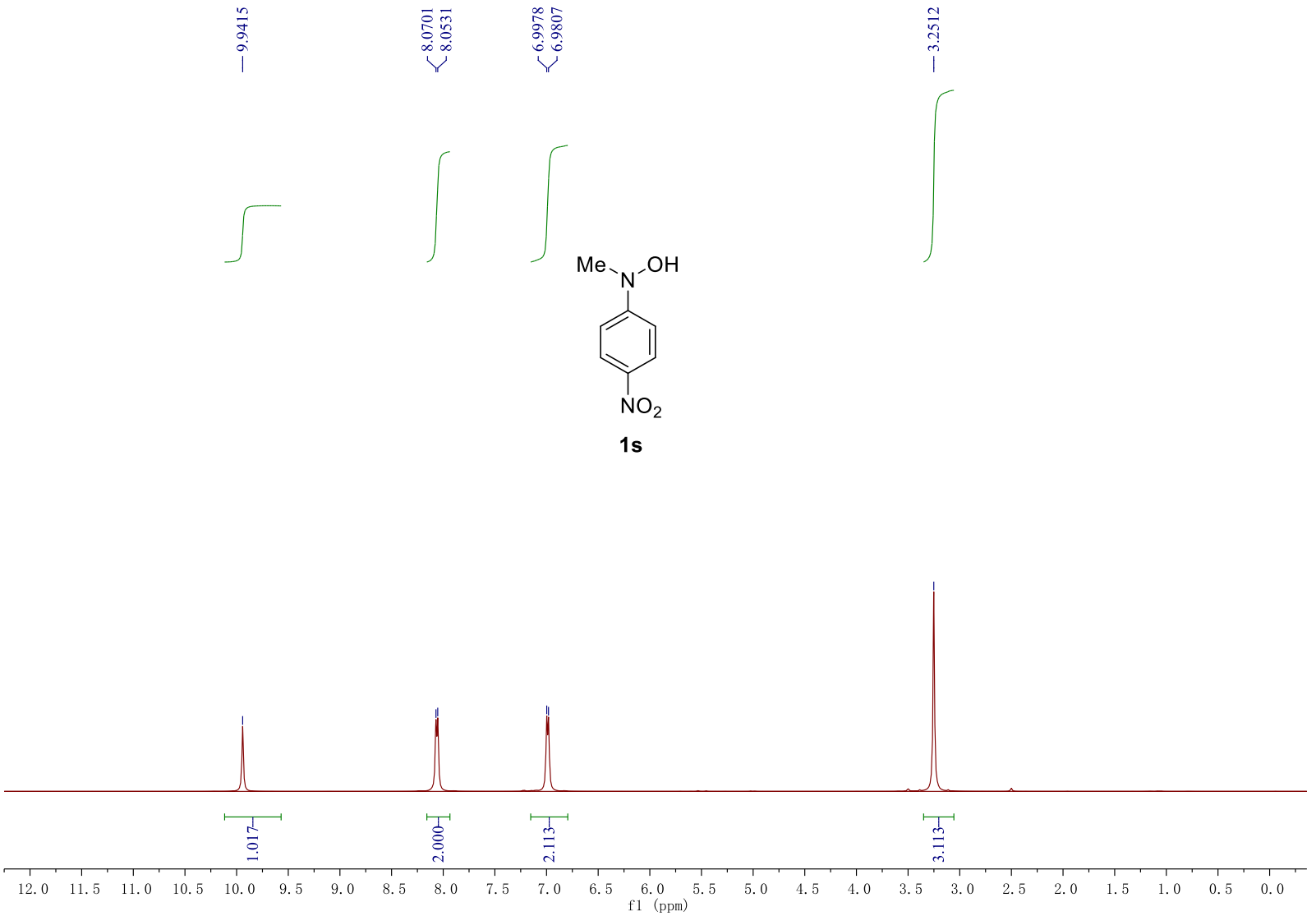
7.3595
7.3453
7.3426
7.3052
7.2903
7.2777
7.2753
7.2020
7.1877
7.1714
7.0243
2.2502
Me
Bz
N
OH
1r
1.027
2.036
1.021
2.285
4.019
3.000
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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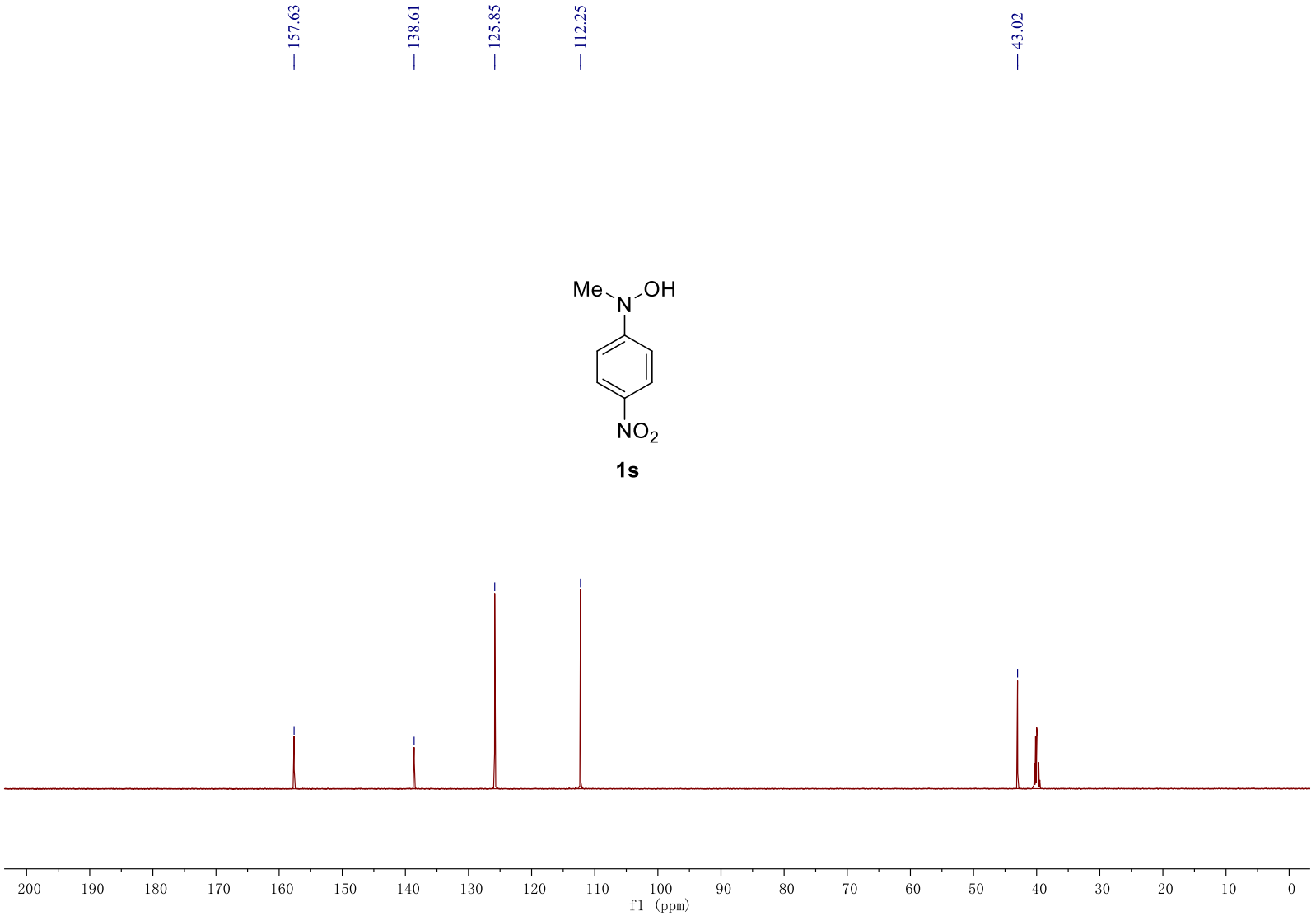
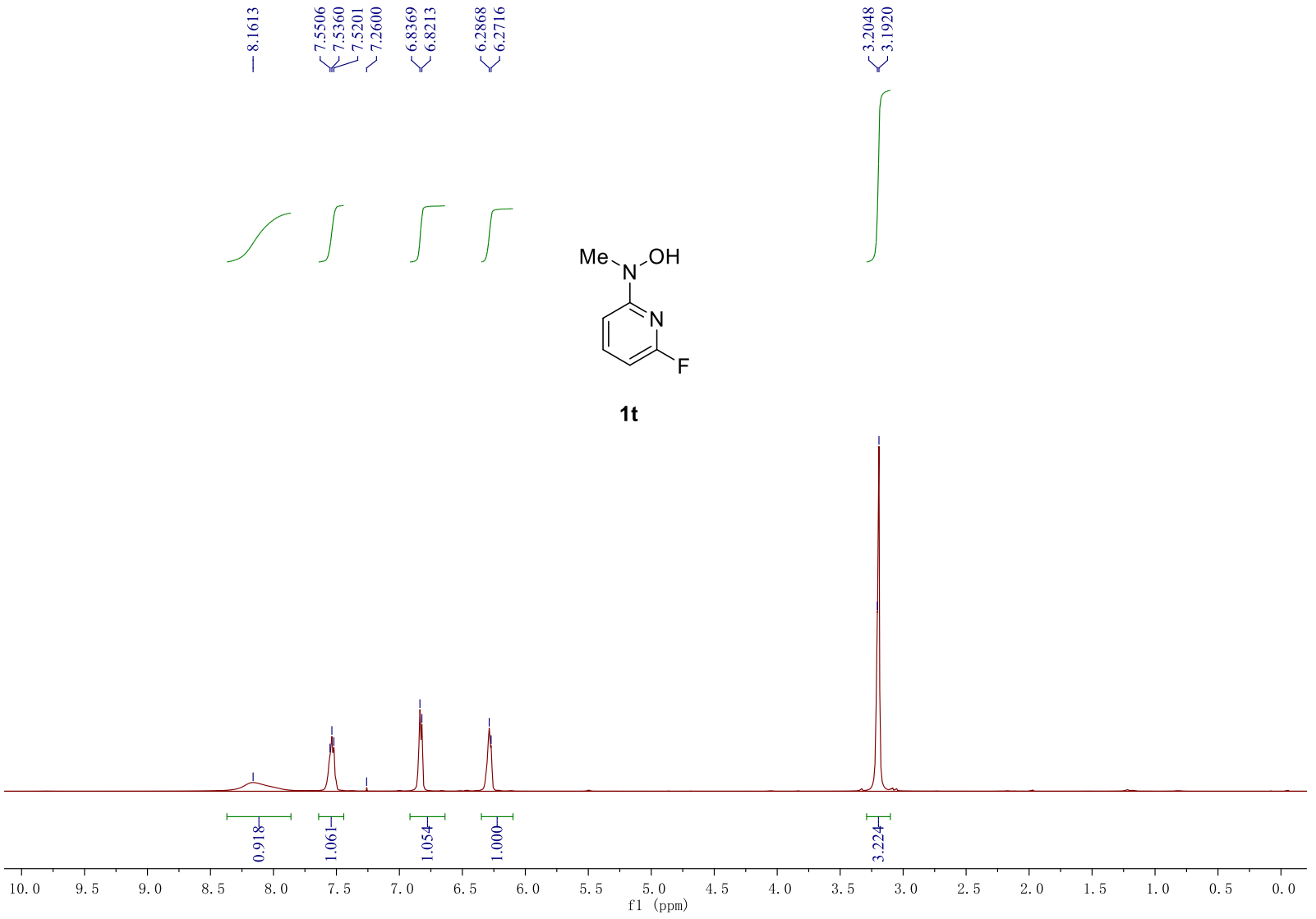
8.0531
6.9978
6.9807
3.2512
Me
N
OH
NO2
1s
1.017
2.000
2.113
3.113
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.63
138.61
125.85
112.25
43.02
Me
N
OH
NO2
1s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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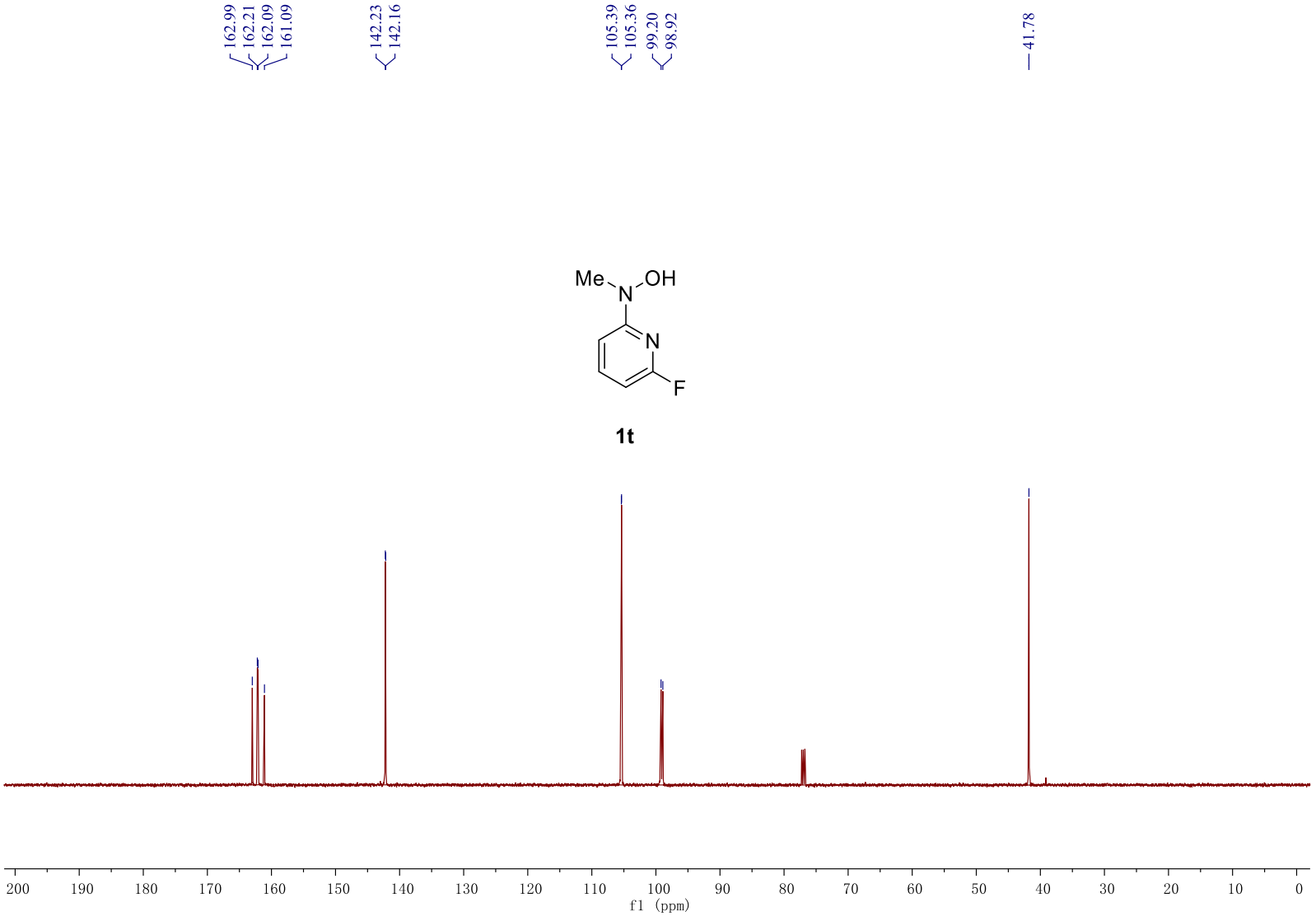
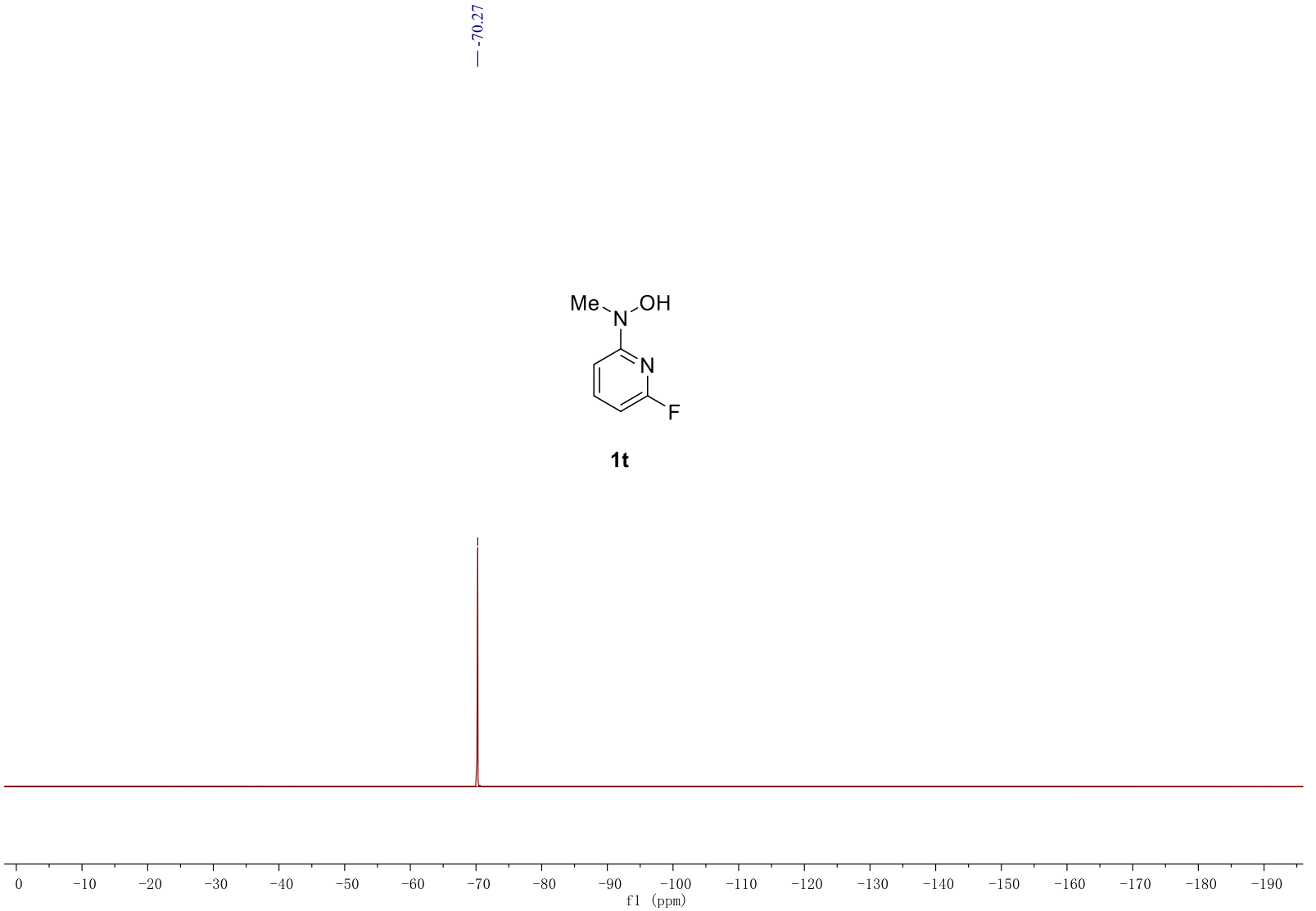
7.5360
7.5201
7.2600
6.8369
6.8213
6.2868
6.2716
3.2048
3.1920
Me
N
OH
N
F
1t
0.918
1.061
1.054
1.000
3.224
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.99
162.21
162.09
161.09
142.23
142.16
105.39
105.36
99.20
98.92
41.78
Me
N
OH
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1t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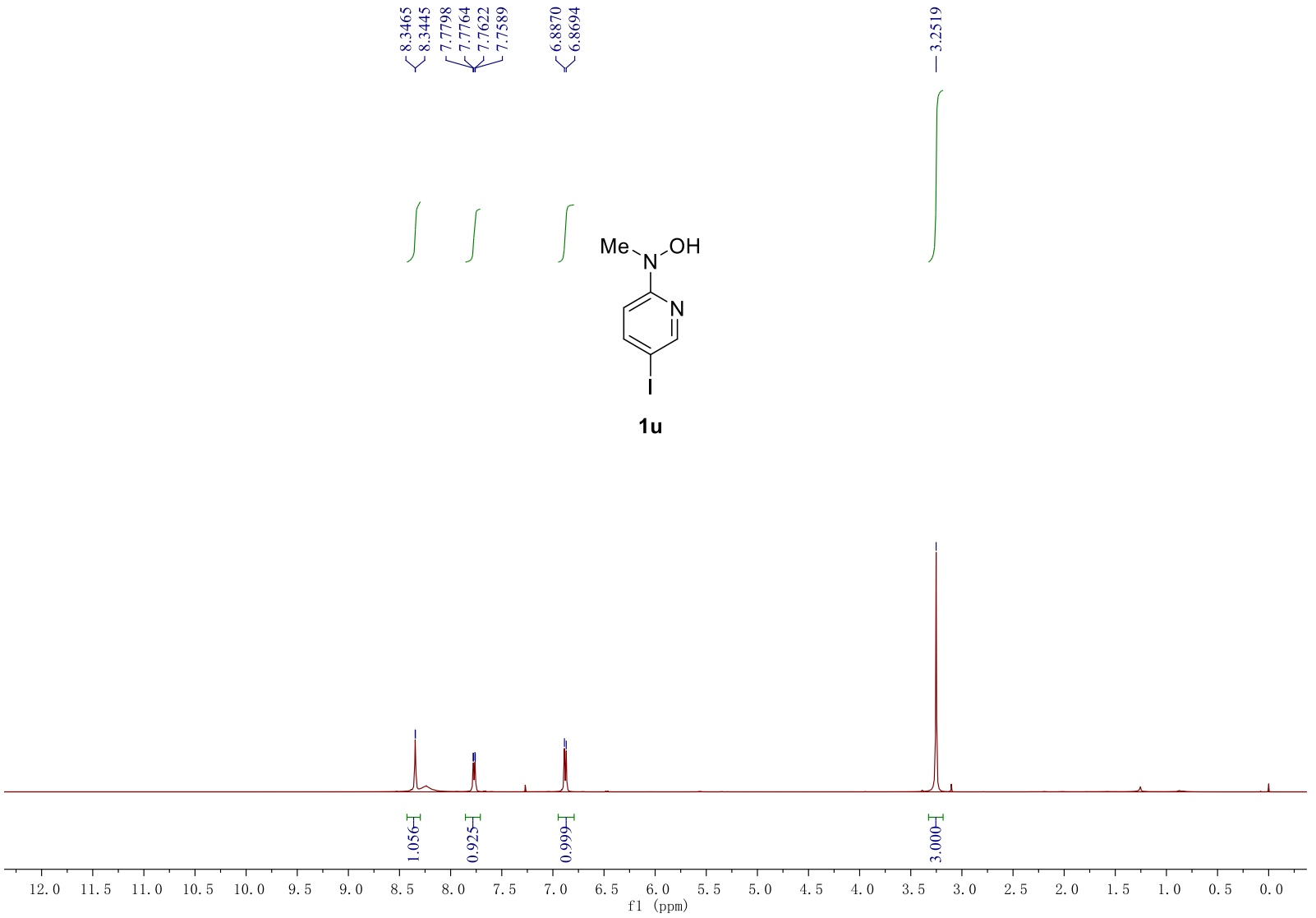
Me
N
OH
N
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

1t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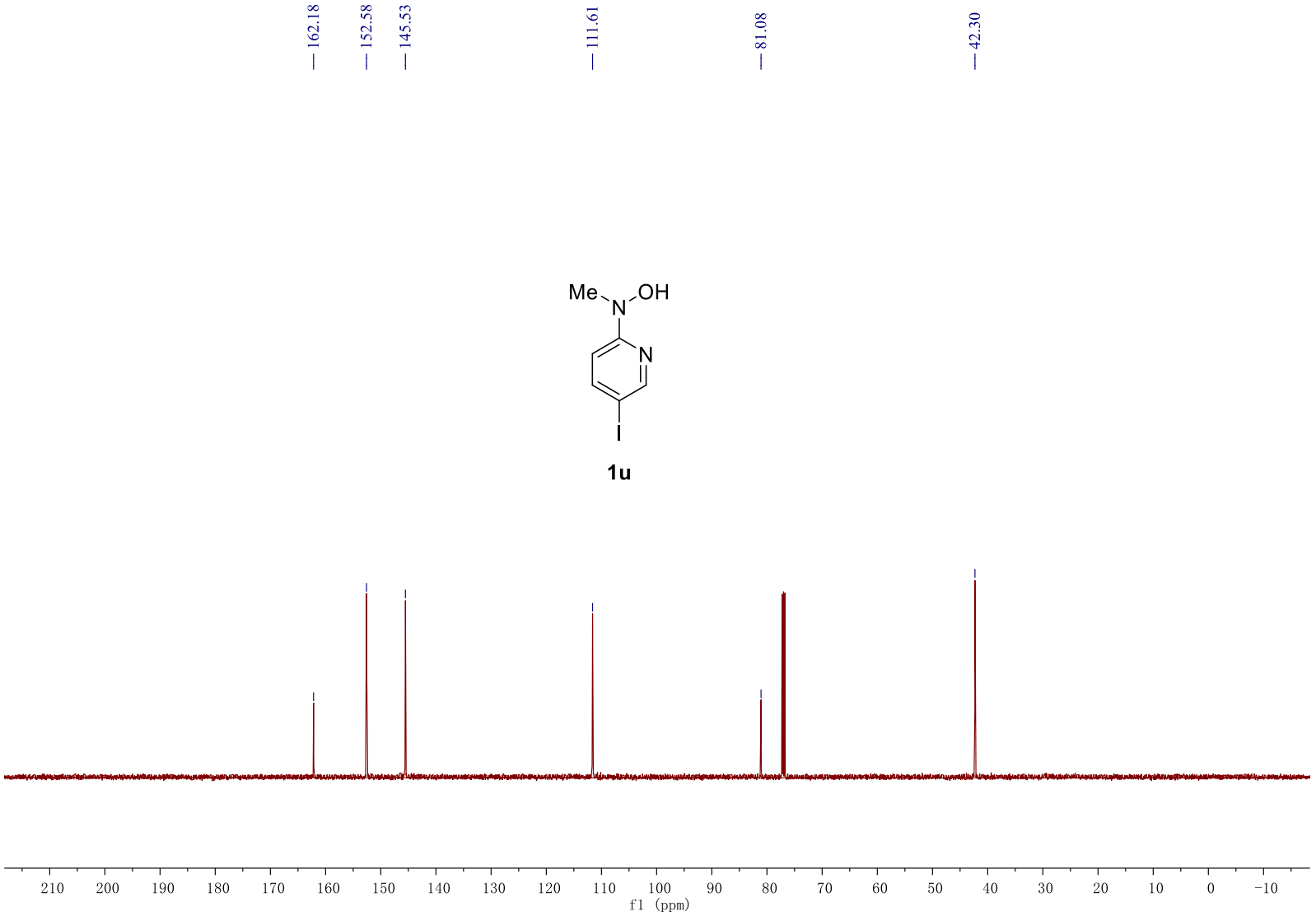
7.7622
7.7589
6.8870
6.8694
3.2519
Me
N
OH
N
I
1u
1.056
0.925
0.999
3.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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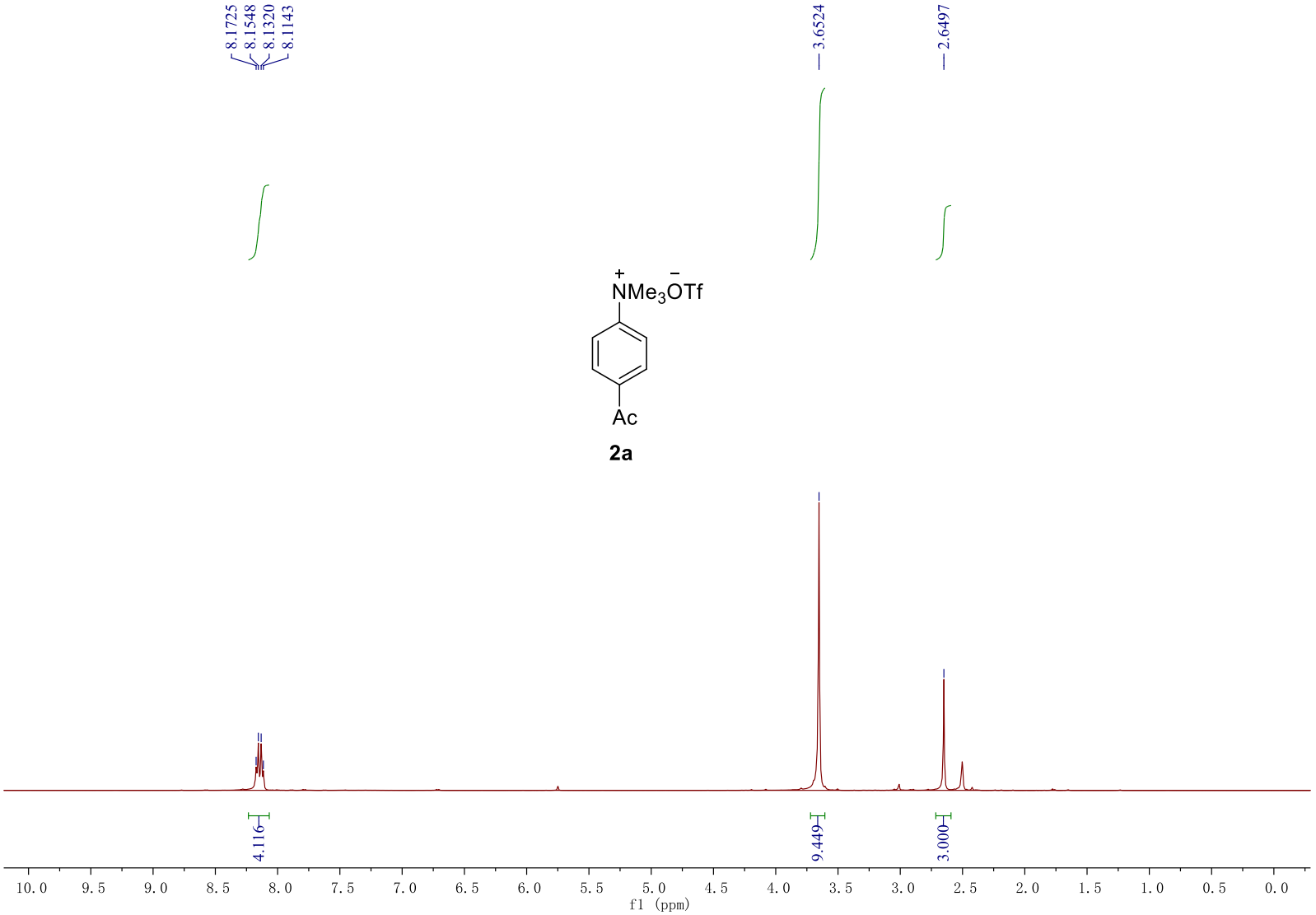
152.58
145.53
111.61
81.08
42.30
Me
N
OH
N
I
1u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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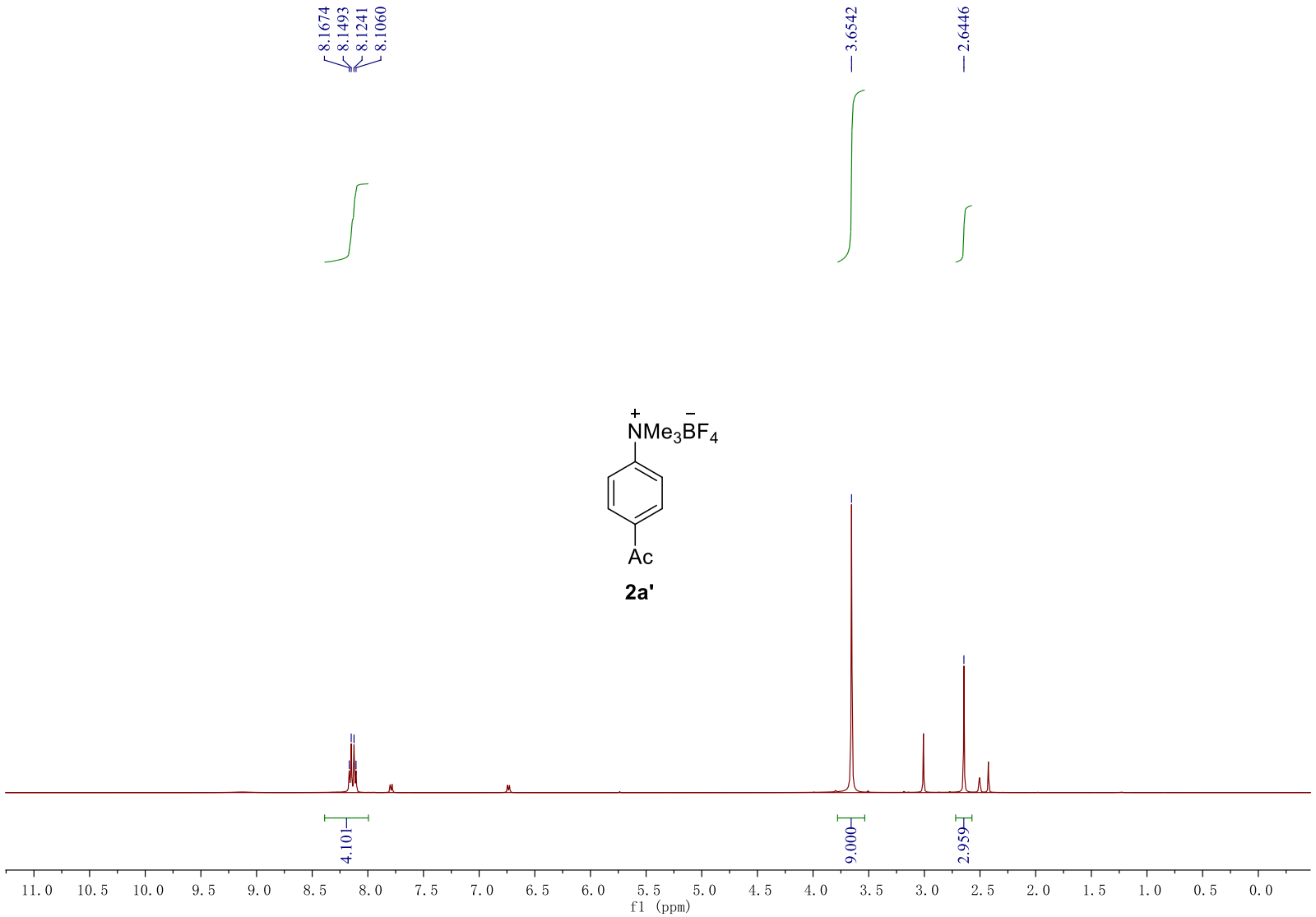
8.1548
8.1320
8.1143
3.6524
2.6497
NMe3OTf
Ac
2a
4.116
9.449
3.000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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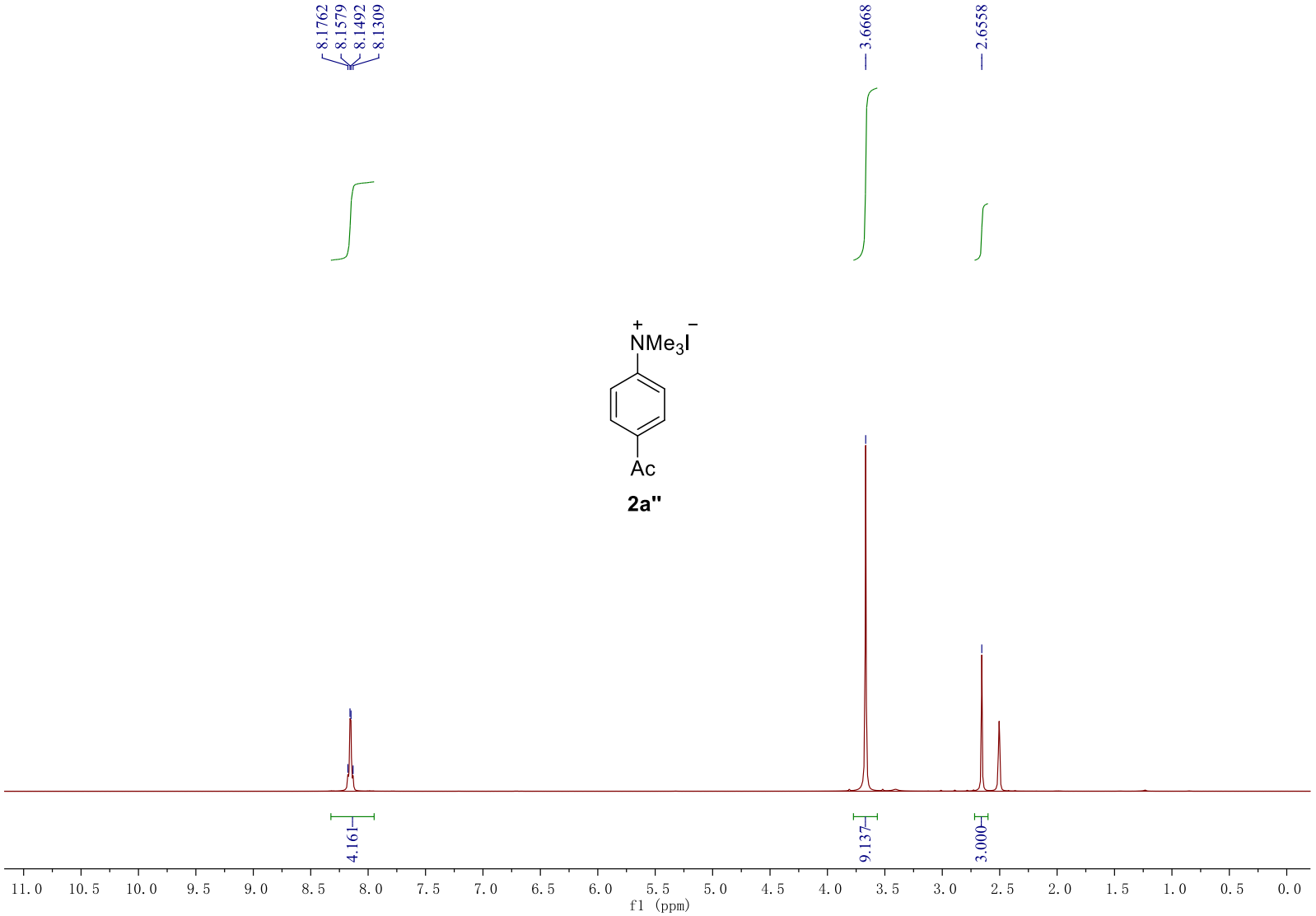
8.1493
8.1241
8.1060
3.6542
2.6446
NMe3BF4
Ac
2a'
4.101
9.000
2.959
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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8.1579
8.1492
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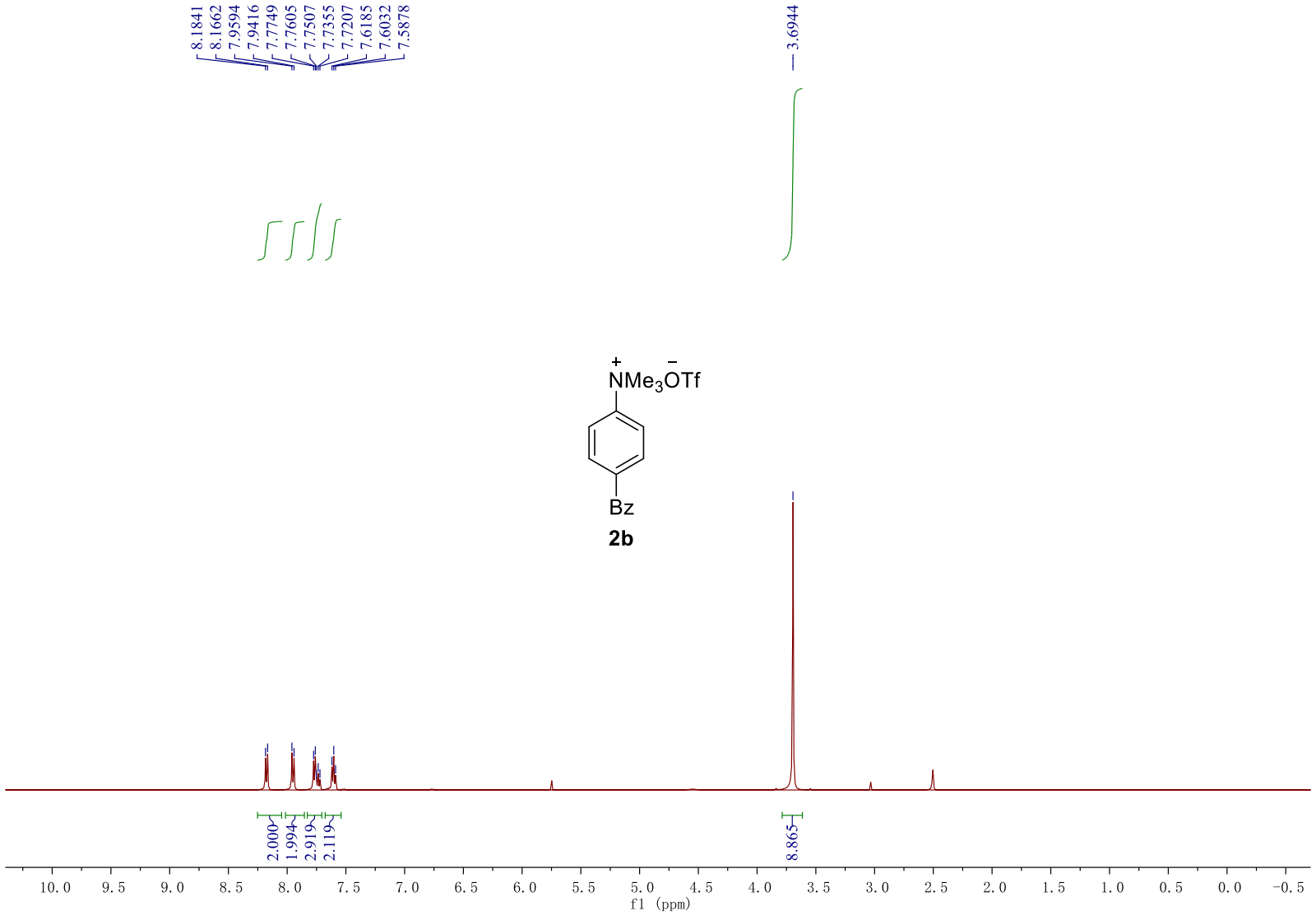
3.6668
2.6558
NMe3I
Ac
2a''
4.161
9.137
3.000
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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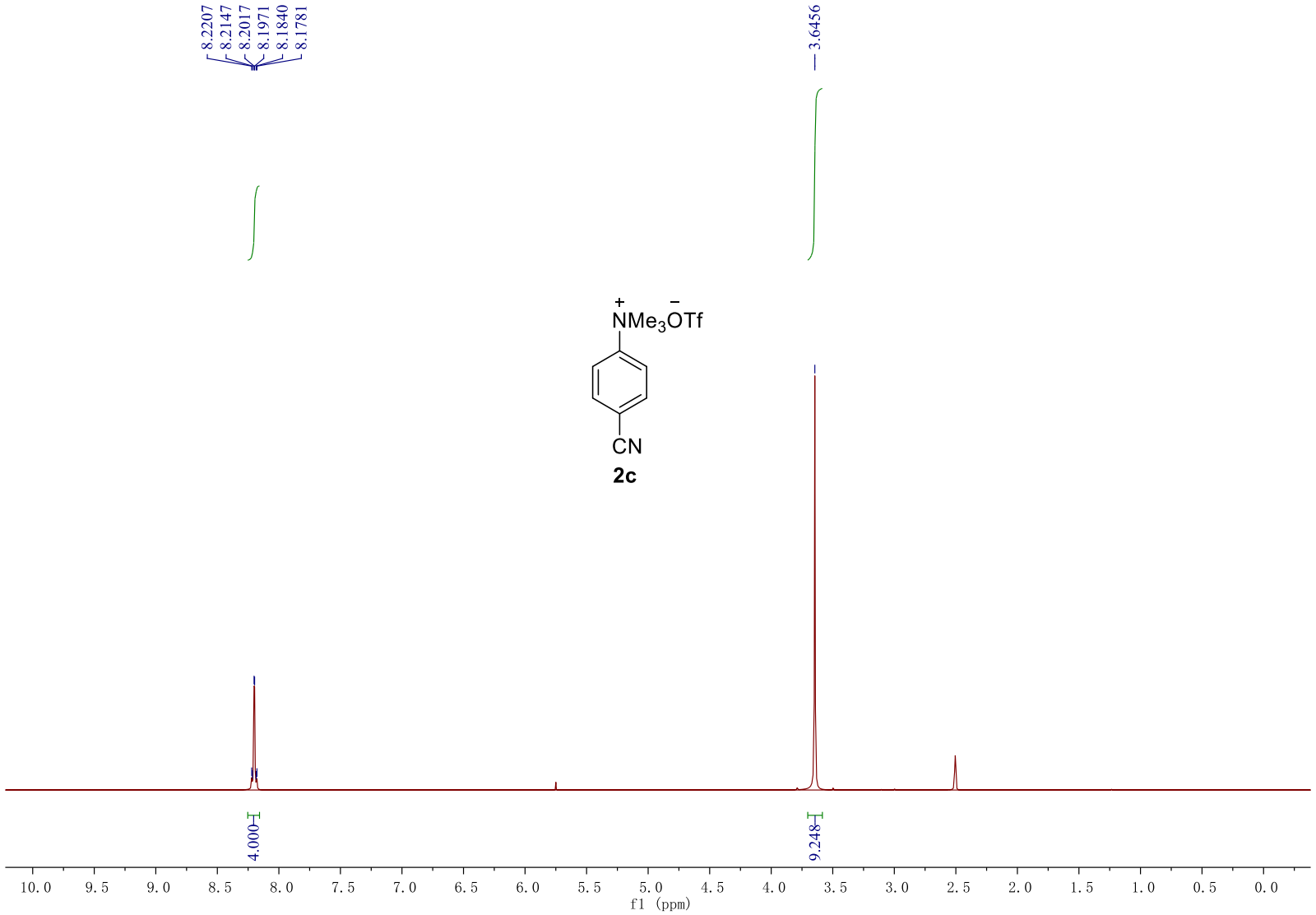
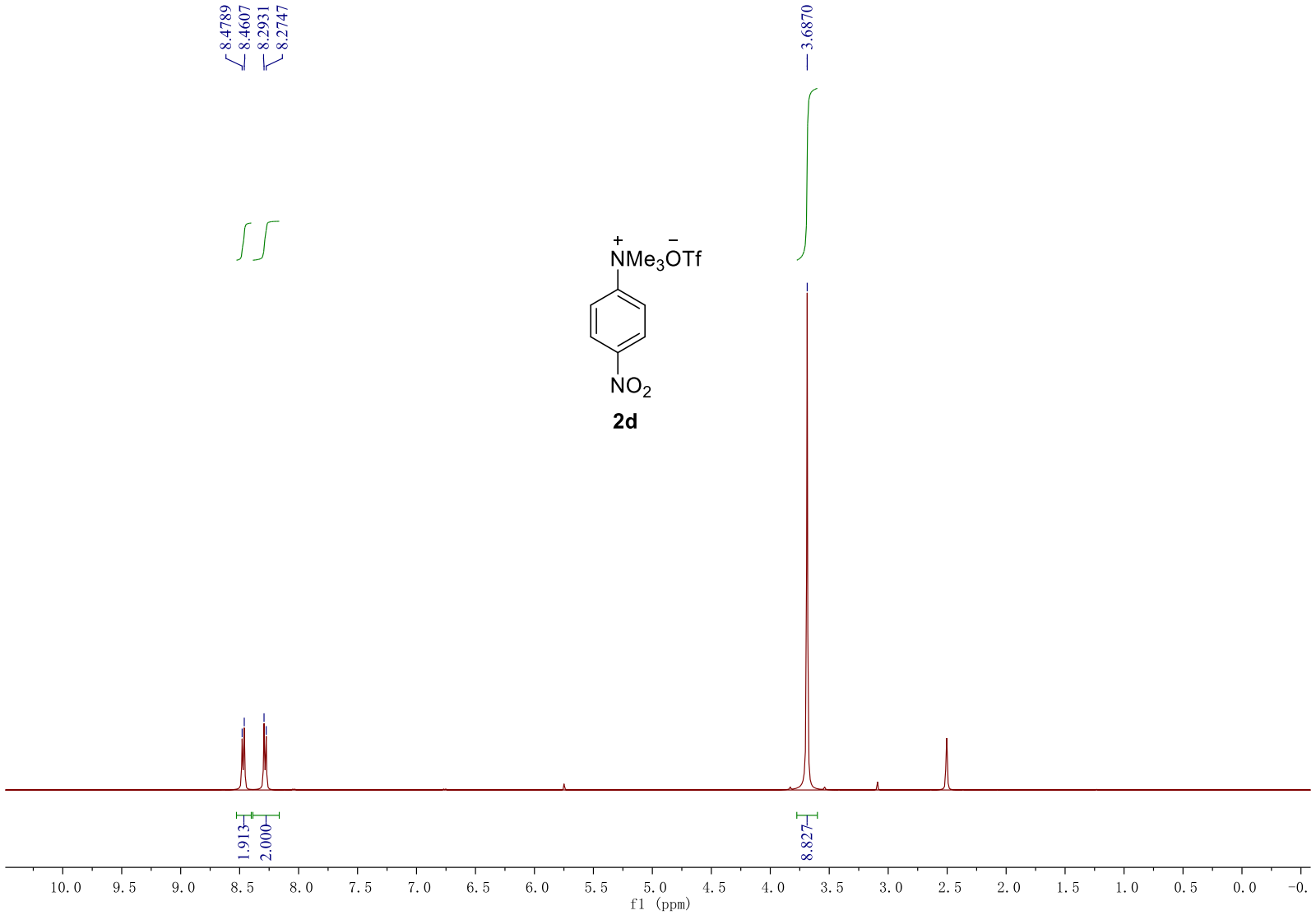
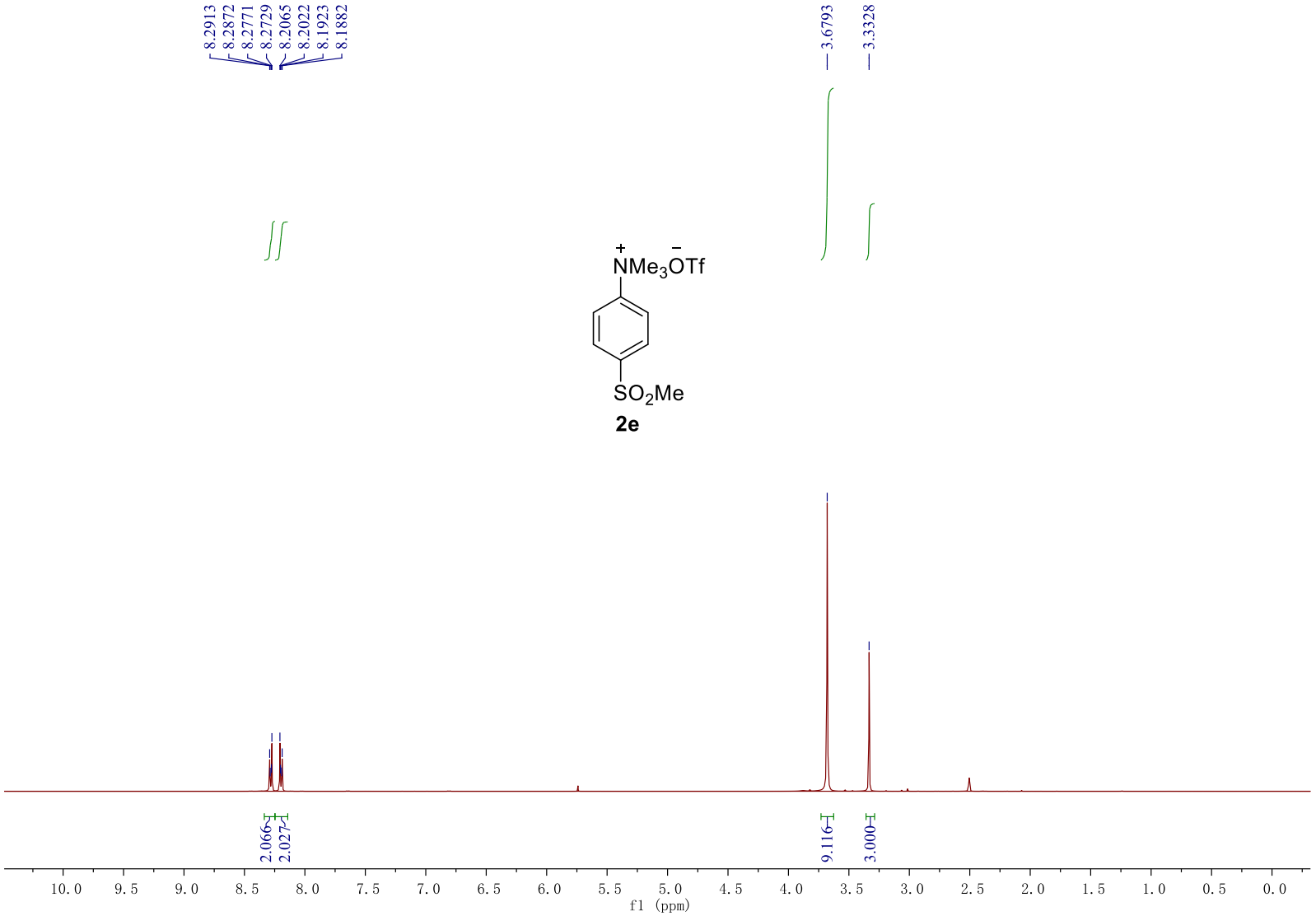
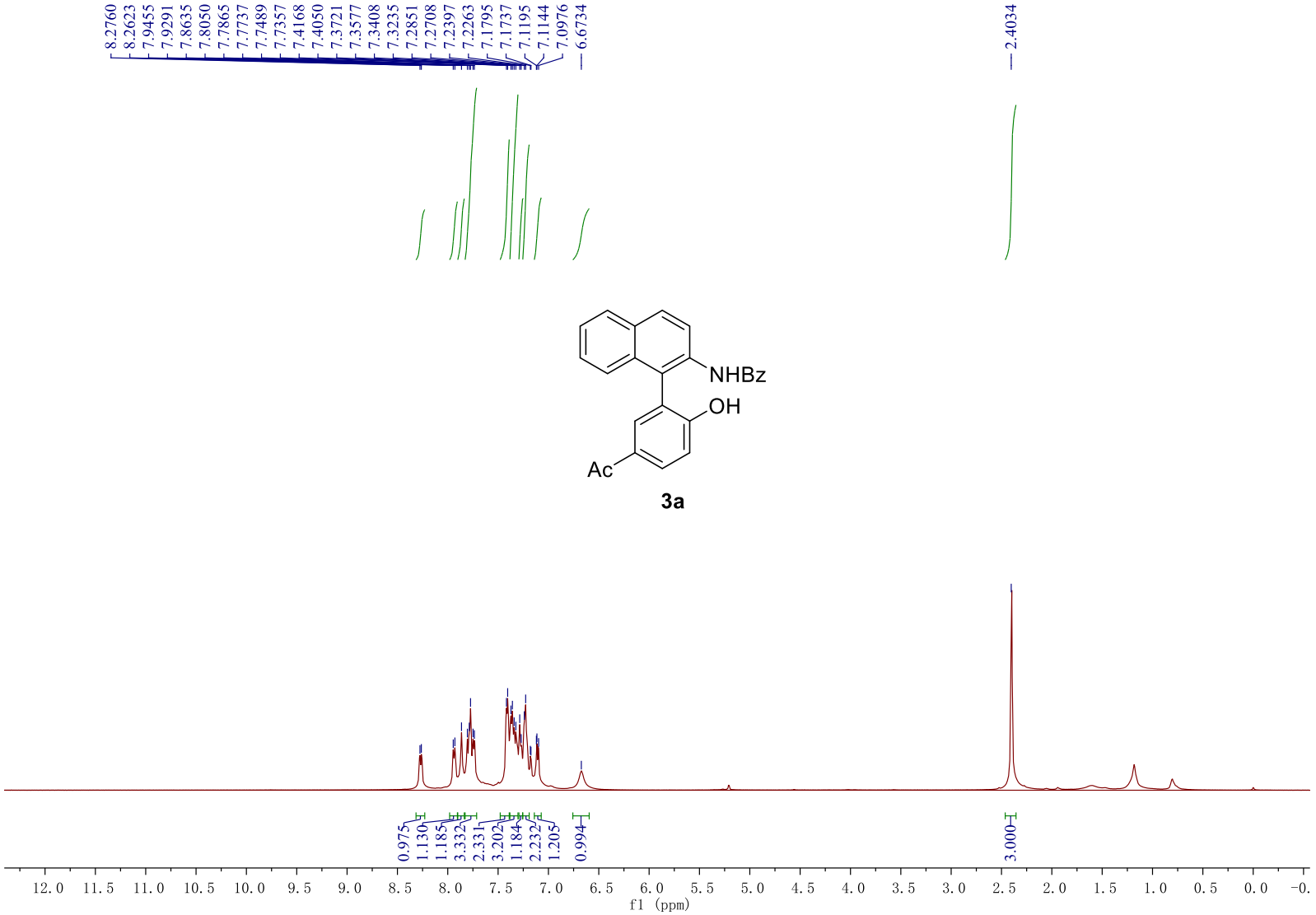
8.1662
7.9594
7.9416
7.7749
7.7605
7.7507
7.7355
7.7207
7.6185
7.6032
7.5878
3.6944
+
NMe3OTf
−
Bz
2b
2.000
1.994
2.919
2.119
8.865
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


8.2207
8.2147
8.2017
8.1971
8.1840
8.1781
3.6456
NMe3OTf
CN
2c
4.000
9.248
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)


8.4789
8.4607
8.2931
8.2747
3.6870
NMe3OTf
NO2
2d
1.913
2.000
8.827
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.
f1 (ppm)


8.2913
8.2872
8.2771
8.2729
8.2065
8.2022
8.1923
8.1882
3.6793
3.3328
NMe3OTf
SO2Me
2e
2.066
2.027
9.116
3.000
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)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7.8635
7.8050
7.7865
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7.7489
7.7357
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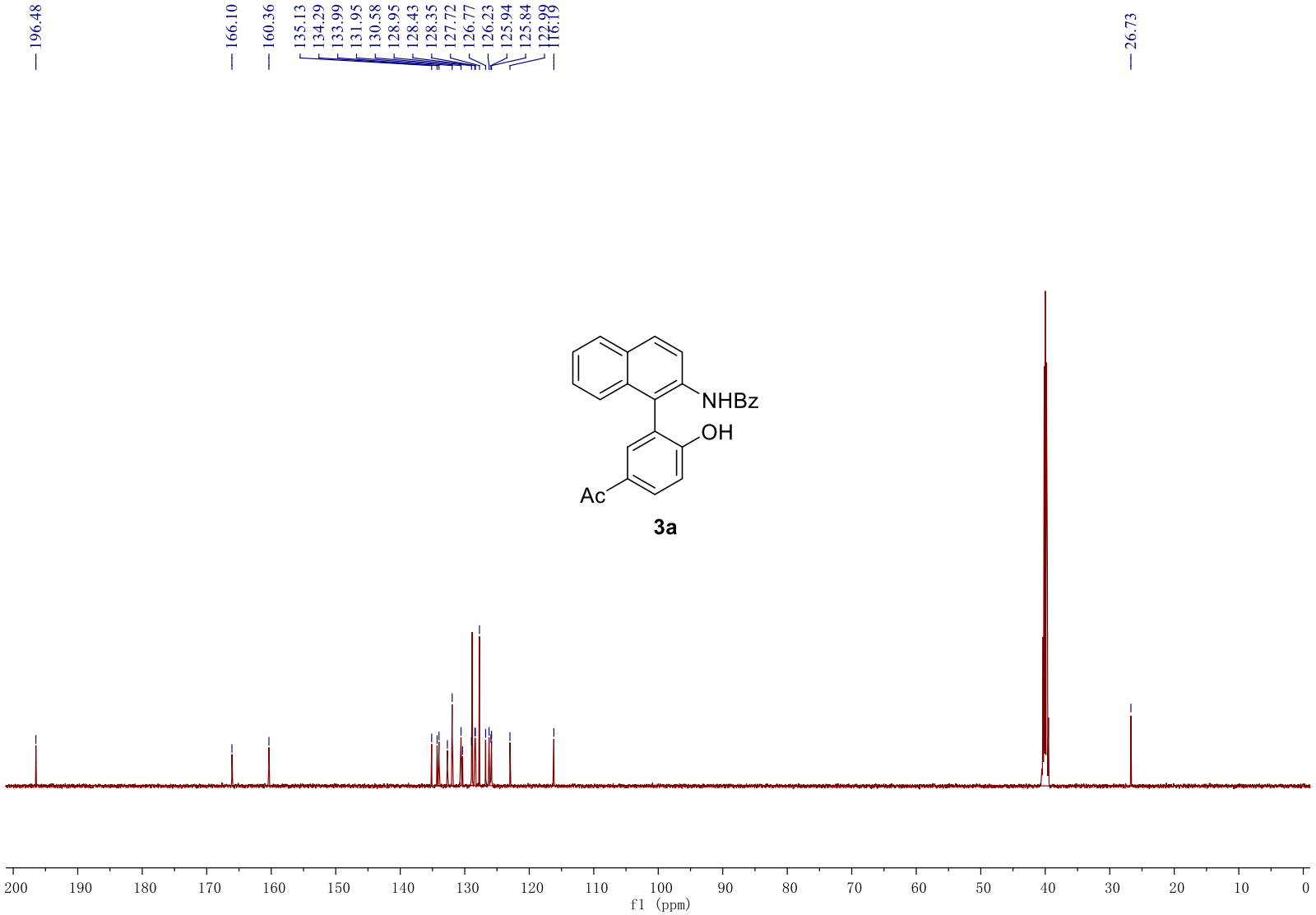
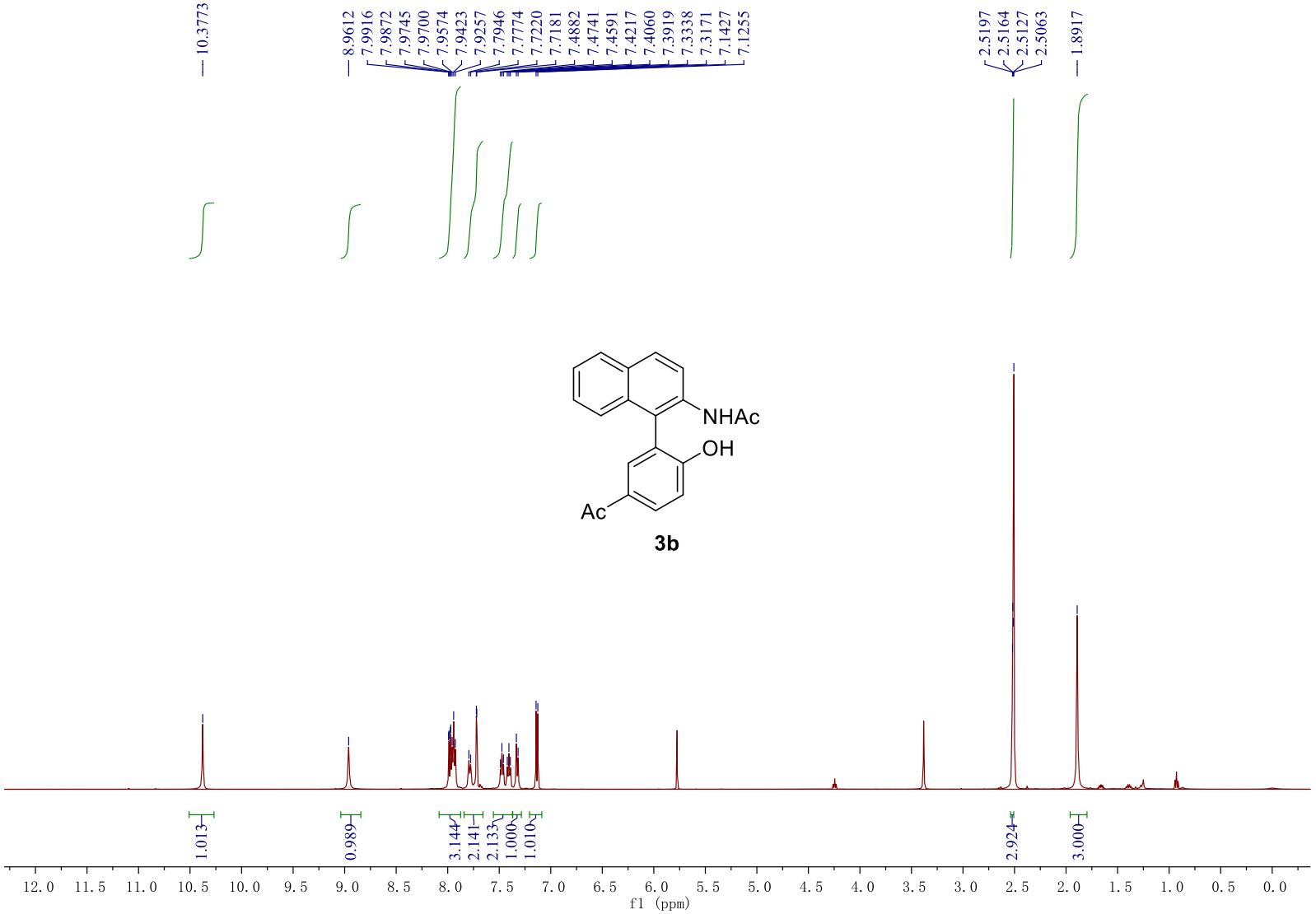
7.4050
7.3721
7.3577
7.3408
7.3235
7.2851
7.2708
7.2397
7.2263
7.1795
7.1737
7.1195
7.1144
7.0976
6.6734
2.4034
NHBz
OH
Ac
3a
0.975
1.130
1.185
3.332
2.331
3.202
1.184
2.232
1.205
0.994
3.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


196.48
166.10
160.36
135.13
134.29
133.99
131.95
130.58
128.95
128.43
128.35
127.72
126.77
126.23
125.94
125.84
122.99
116.19
26.73
NHBz
OH
Ac
3a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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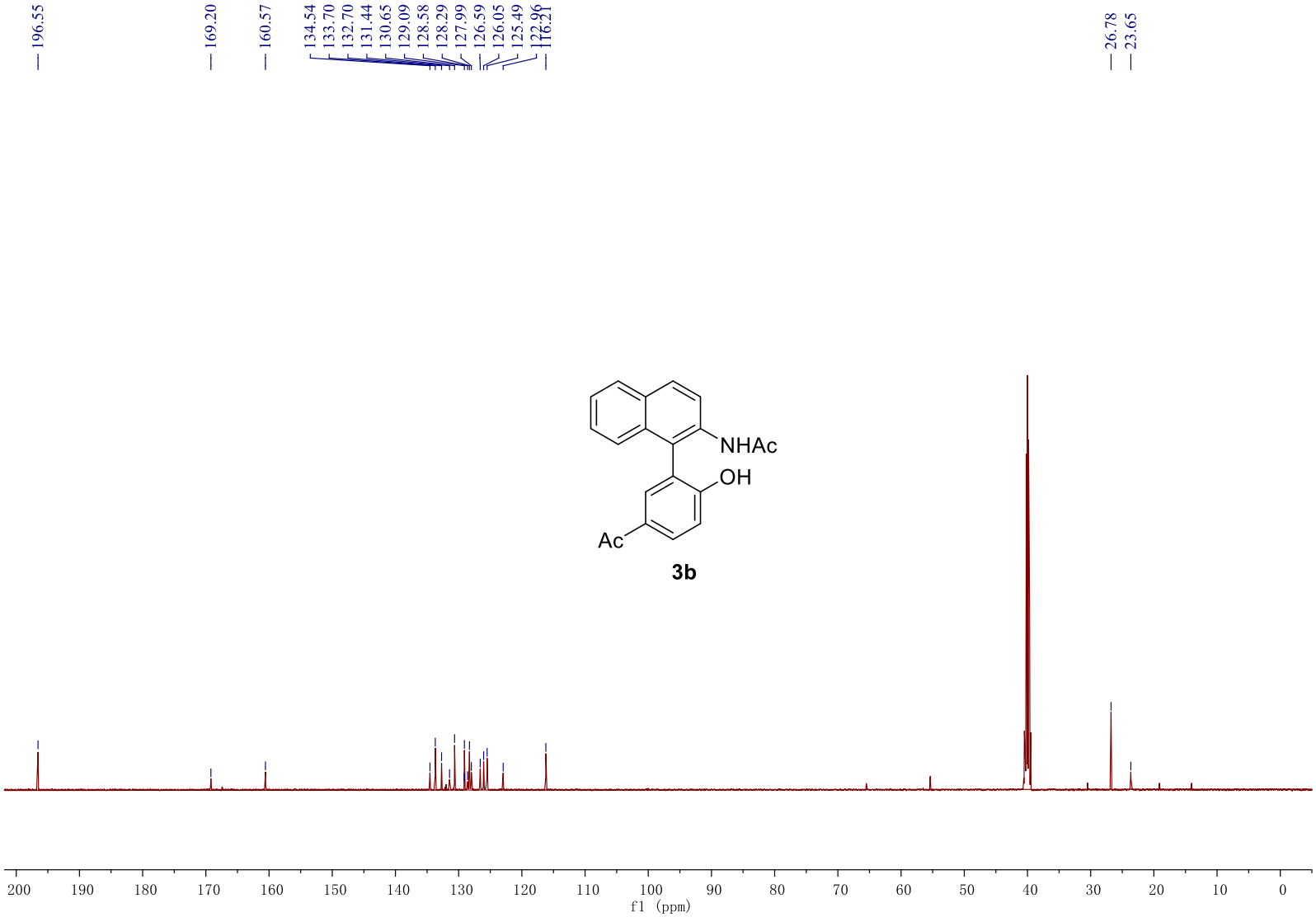
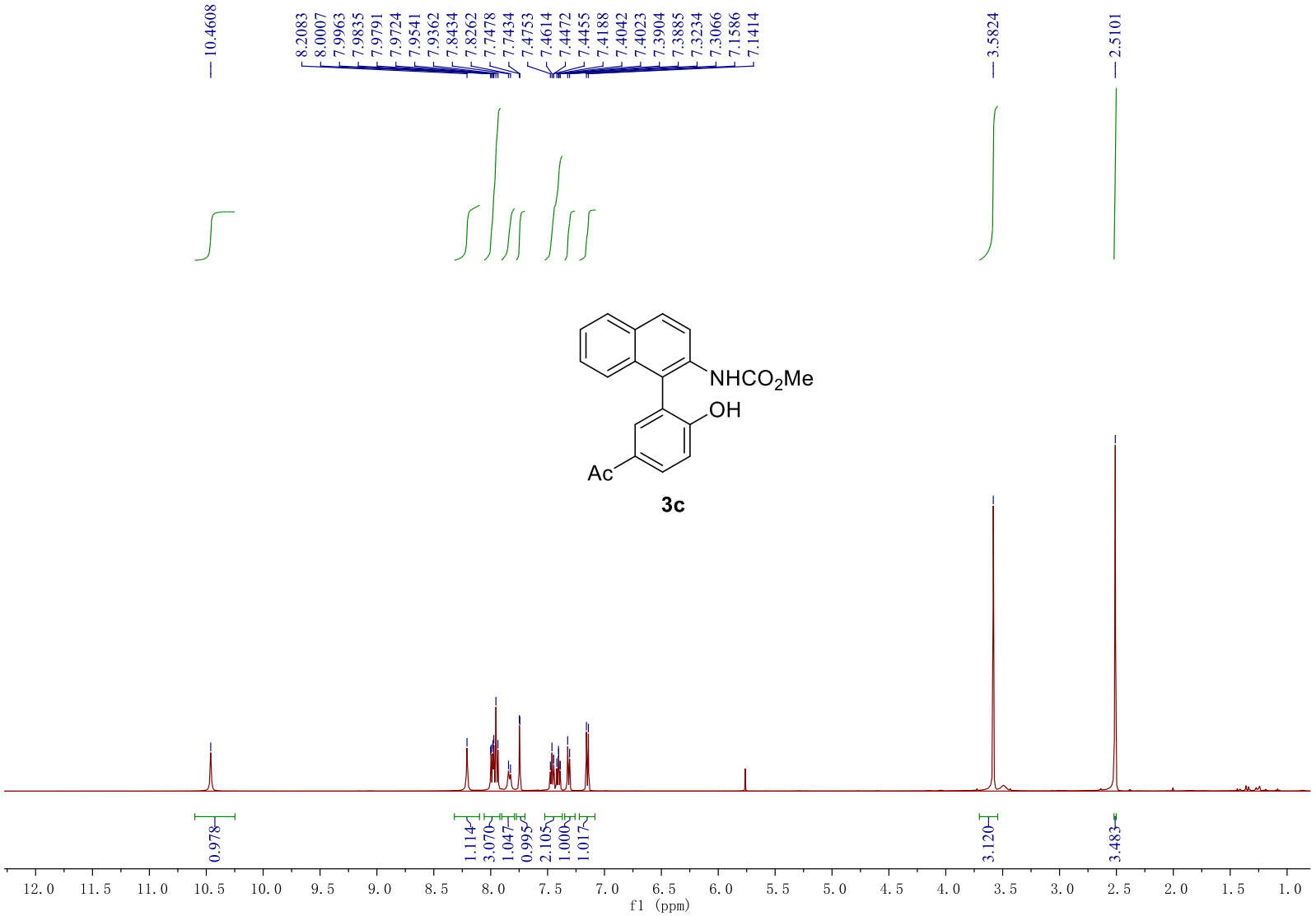
7.9916
7.9872
7.9745
7.9700
7.9574
7.9423
7.9257
7.7946
7.7774
7.7220
7.7181
7.4882
7.4741
7.4591
7.4217
7.4060
7.3919
7.3338
7.3171
7.1427
7.1255
2.5197
2.5164
2.5127
2.5063
1.8917
NHAc
OH
Ac
1.013
0.989
3.144
2.141
2.133
1.000
1.010
2.924
3.000
f1 (ppm)

3b


196.55
169.20
160.57
134.54
133.70
132.70
131.44
130.65
129.09
128.58
128.29
127.99
126.59
126.05
125.49
122.96
116.21
26.78
23.65
NHAc
OH
Ac
3b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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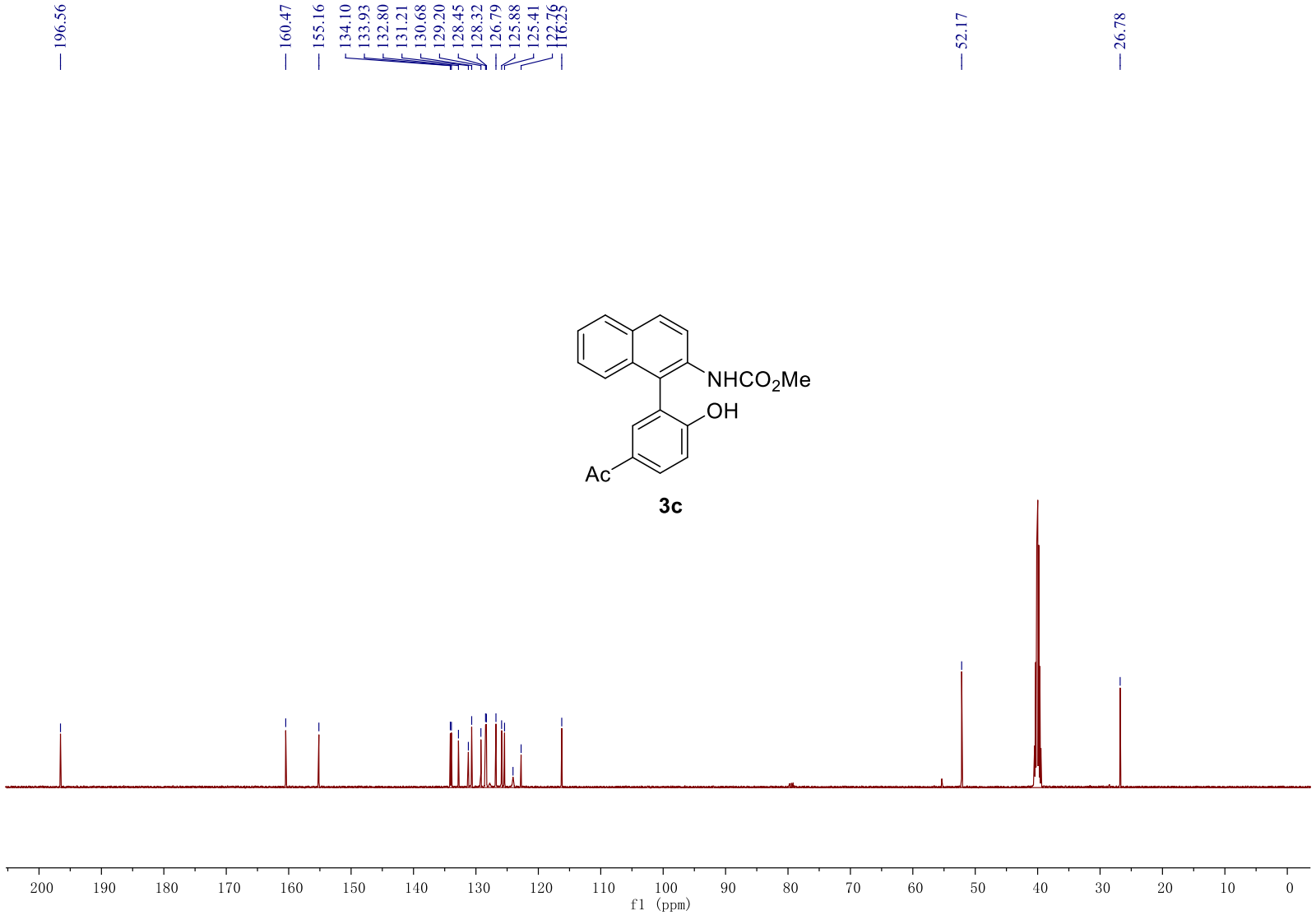
8.2083
8.0007
7.9963
7.9835
7.9791
7.9724
7.9541
7.9362
7.8434
7.8262
7.7478
7.7434
7.4753
7.4614
7.4472
7.4455
7.4188
7.4042
7.4023
7.3904
7.3885
7.3234
7.3066
7.1586
7.1414
3.5824
2.5101
NHCO2Me
OH
Ac
3c
0.978
1.114
3.070
1.047
0.995
2.105
1.000
1.017
3.120
3.483
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 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
f1 (ppm)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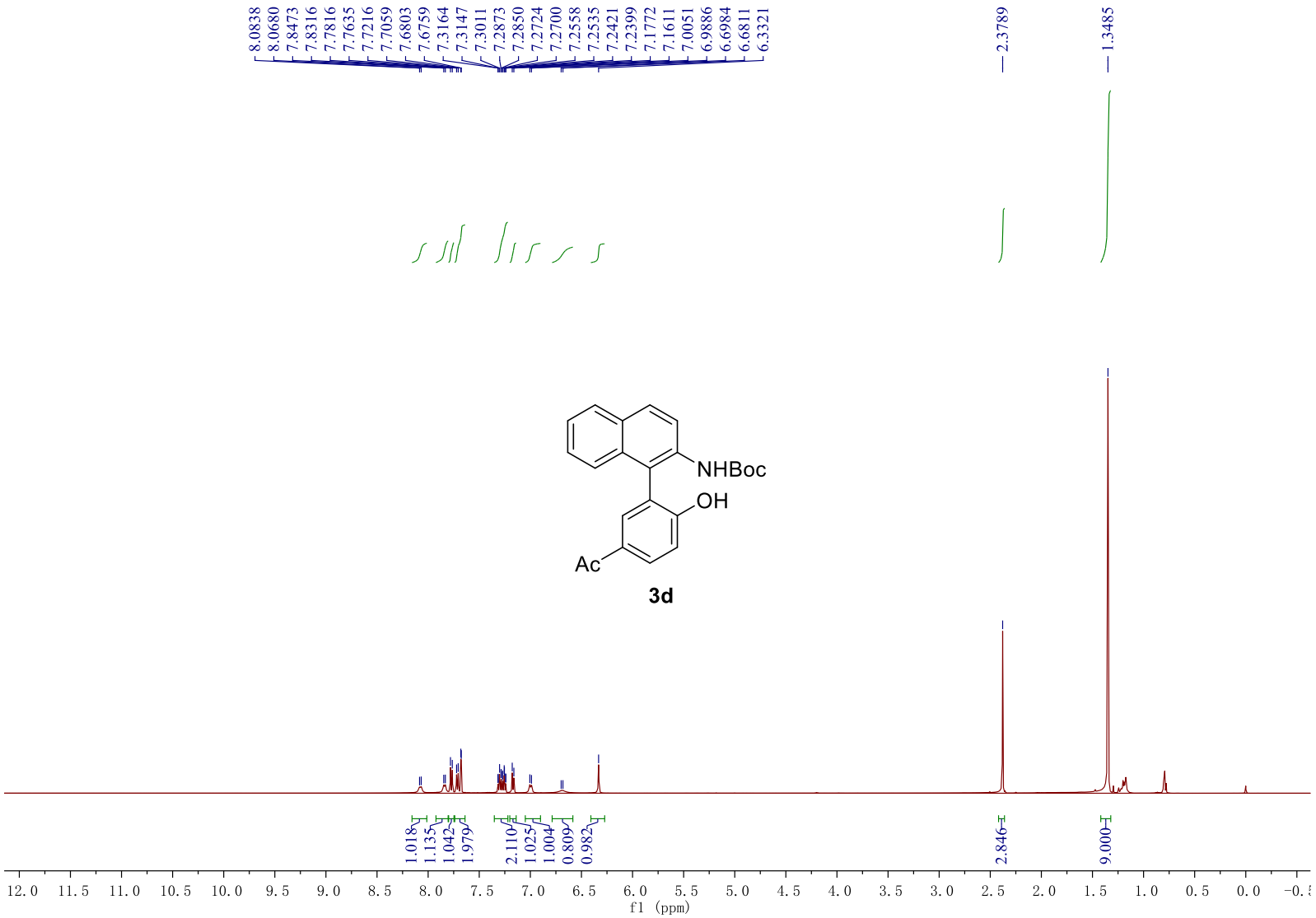
160.47
155.16
134.10
133.93
132.80
131.21
130.68
129.20
128.45
128.32
126.79
125.88
125.41
122.76
116.25
52.17
26.78
NHCO2Me
OH
Ac
3c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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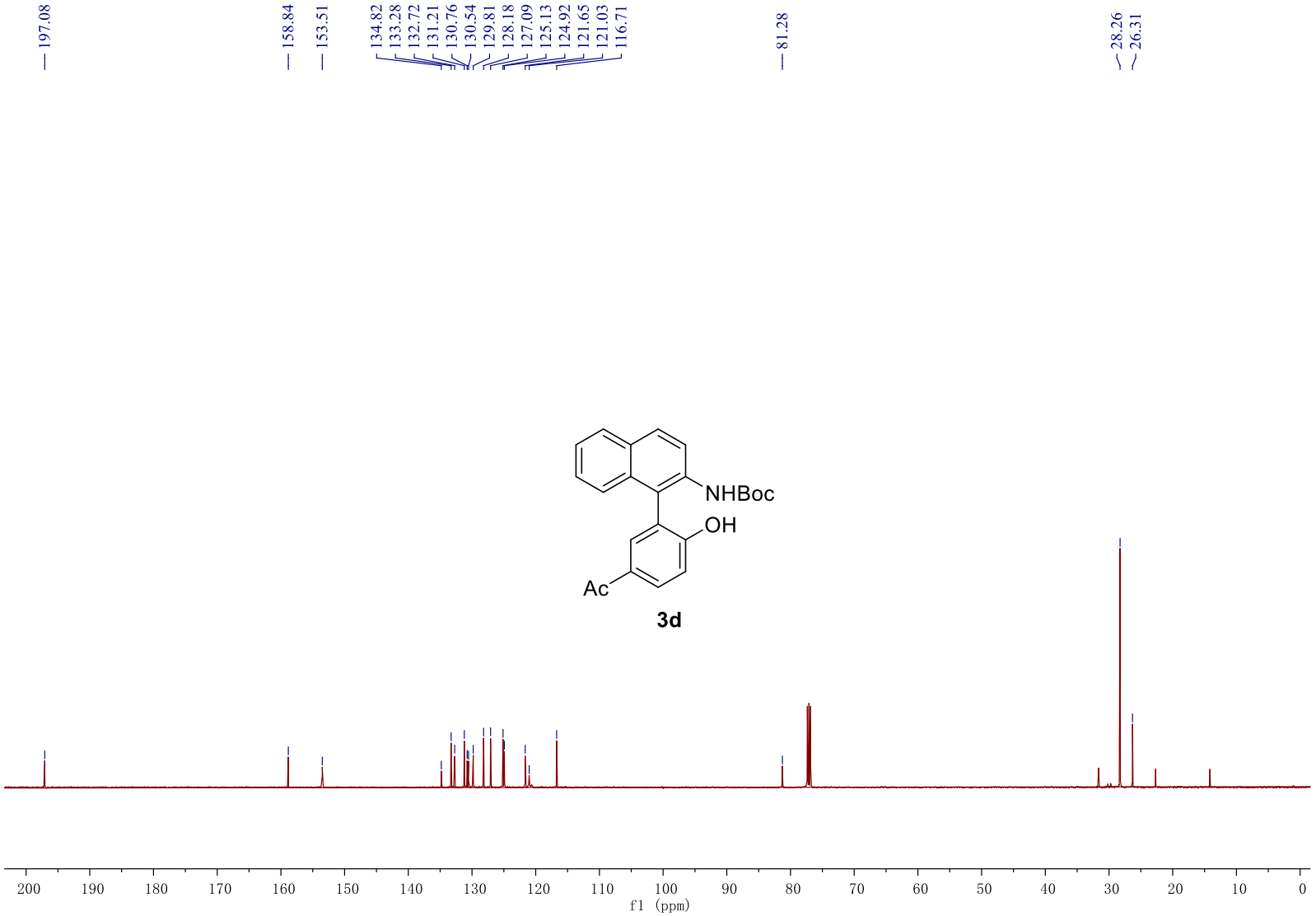
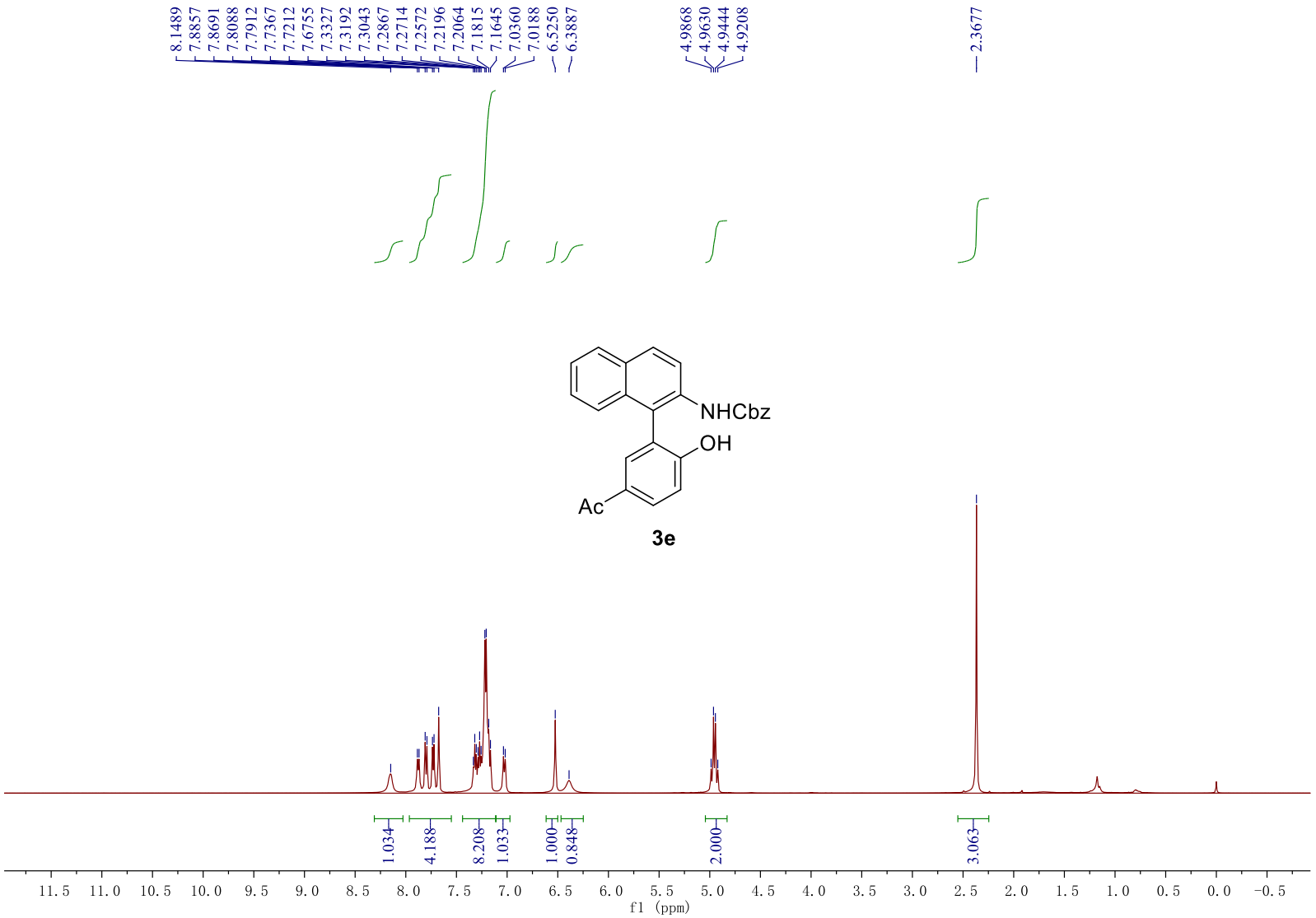
8.0680
7.8473
7.8316
7.7816
7.7635
7.7216
7.7059
7.6803
7.6759
7.3164
7.3147
7.3011
7.2873
7.2850
7.2724
7.2700
7.2558
7.2535
7.2421
7.2399
7.1772
7.1611
7.0051
6.9886
6.6984
6.6811
6.3321
2.3789
1.3485
NHBoc
OH
Ac
3d
1.018
1.135
1.042
1.979
2.110
1.025
1.004
0.809
0.982
2.846
9.000
f1 (ppm)


197.08
158.84
153.51
134.82
133.28
132.72
131.21
130.76
130.54
129.81
128.18
127.09
125.13
124.92
121.65
121.03
116.71
81.28
28.26
26.31
NHBoc
OH
Ac
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.8691
7.8088
7.7912
7.7367
7.7212
7.6755
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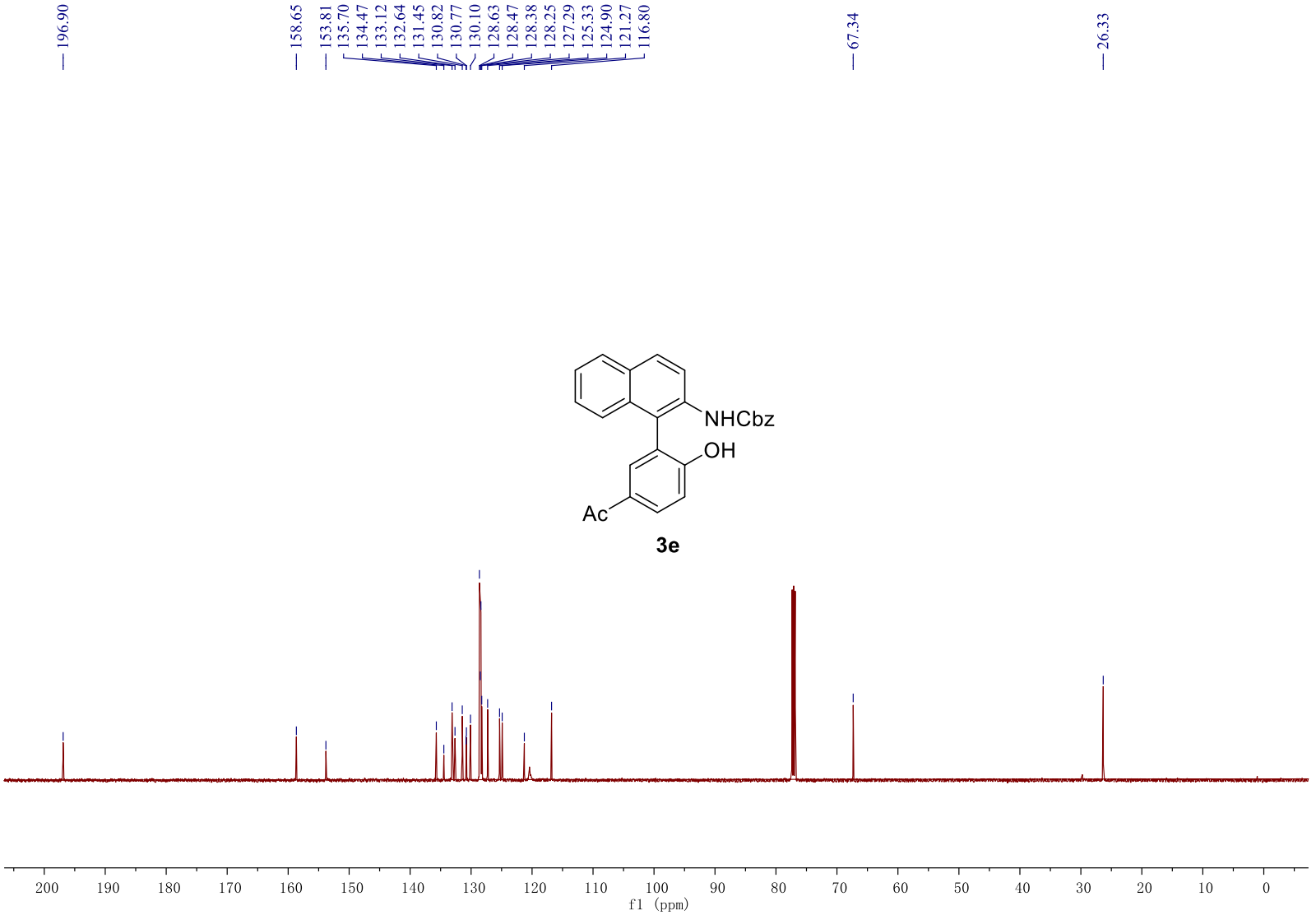
7.3192
7.3043
7.2867
7.2714
7.2572
7.2196
7.2064
7.1815
7.1645
7.0360
7.0188
6.5250
6.3887
4.9868
4.9630
4.9444
4.9208
2.3677
NHCbz
OH
Ac
3e
1.034
4.188
8.208
1.033
1.000
0.848
2.000
3.063
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.90
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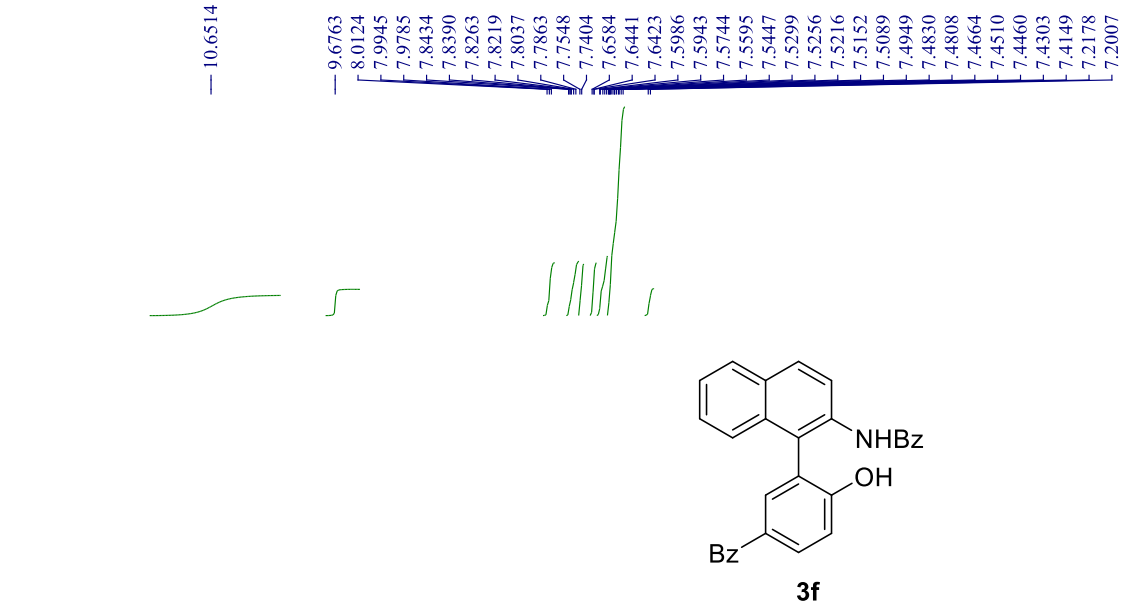
153.81
135.70
134.47
133.12
132.64
131.45
130.82
130.77
130.10
128.63
128.47
128.38
128.25
127.29
125.33
124.90
121.27
116.80
67.34
26.33
NHCbz
OH
Ac
3e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.0124
7.9945
7.9785
7.8434
7.8390
7.8263
7.8219
7.8037
7.7863
7.7548
7.7404
7.6584
7.6441
7.6423
7.5986
7.5943
7.5744
7.5595
7.5447
7.5299
7.5256
7.5216
7.5152
7.5089
7.4949
7.4830
7.4808
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7.4460
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7.4149
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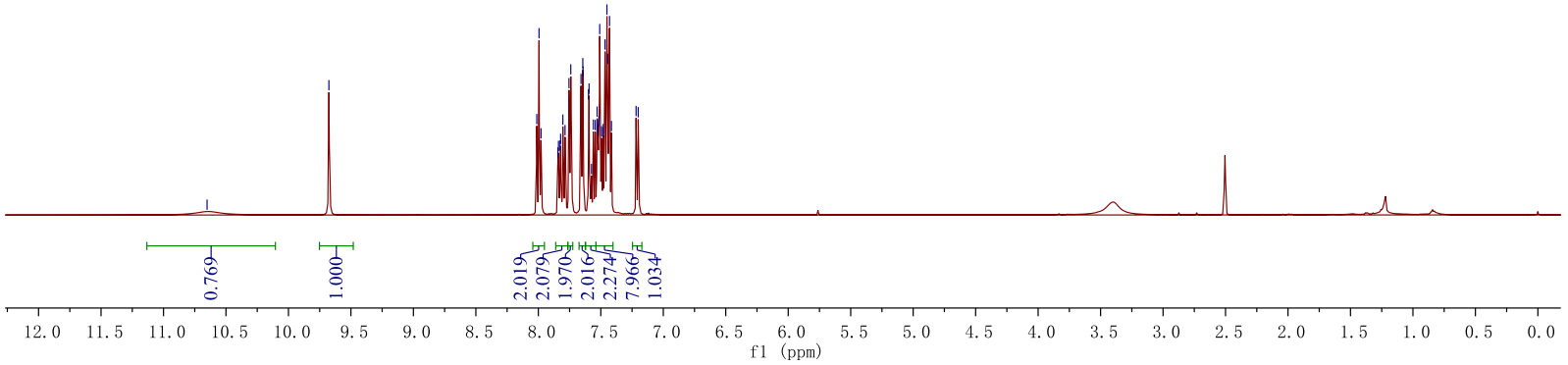
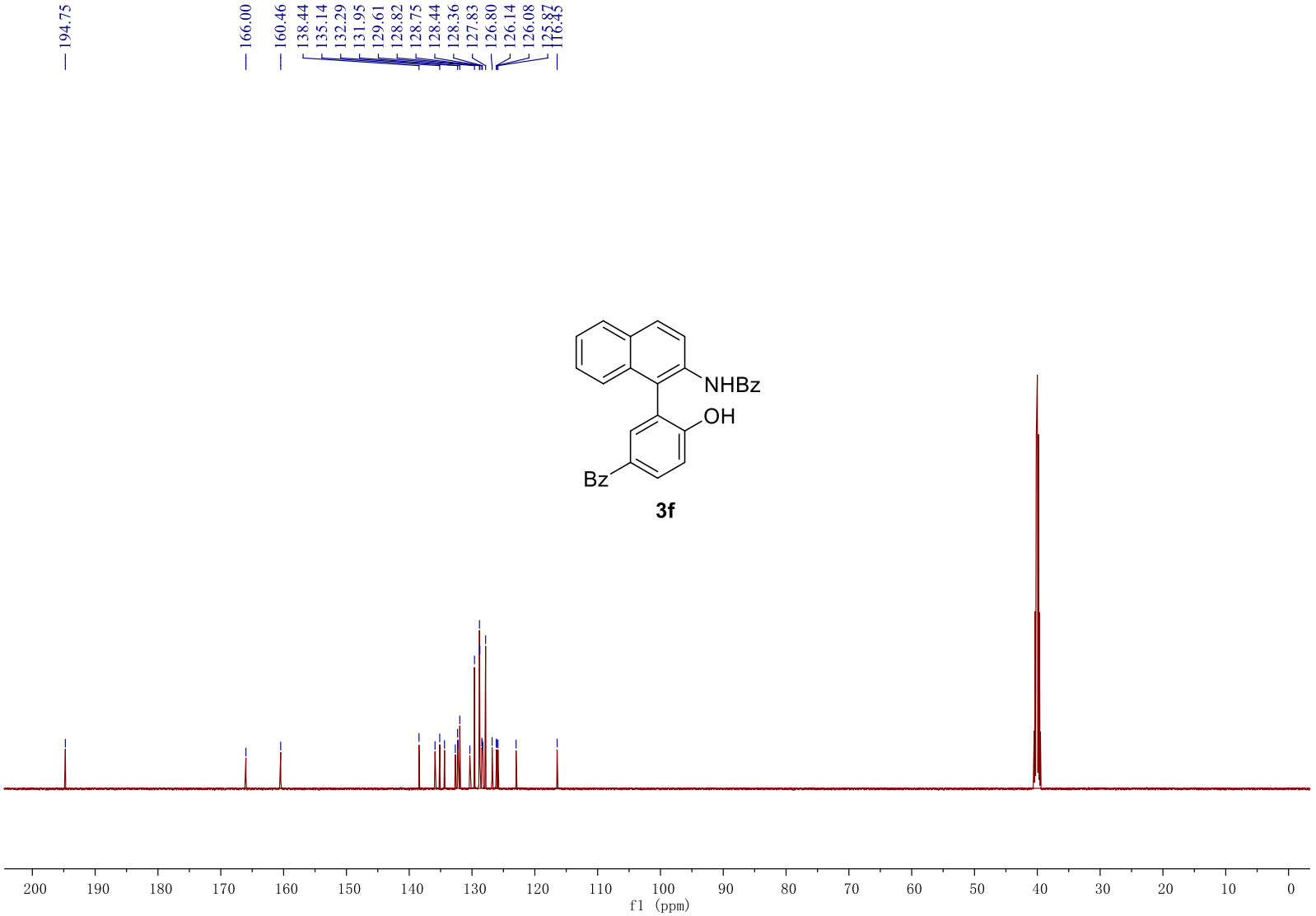
7.2007

NHBz
OH
Bz

3f


0.769
1.000
2.019
2.079
1.970
2.016
2.274
7.966
1.034
12.0 11.5 11.0 10.5 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)


194.75
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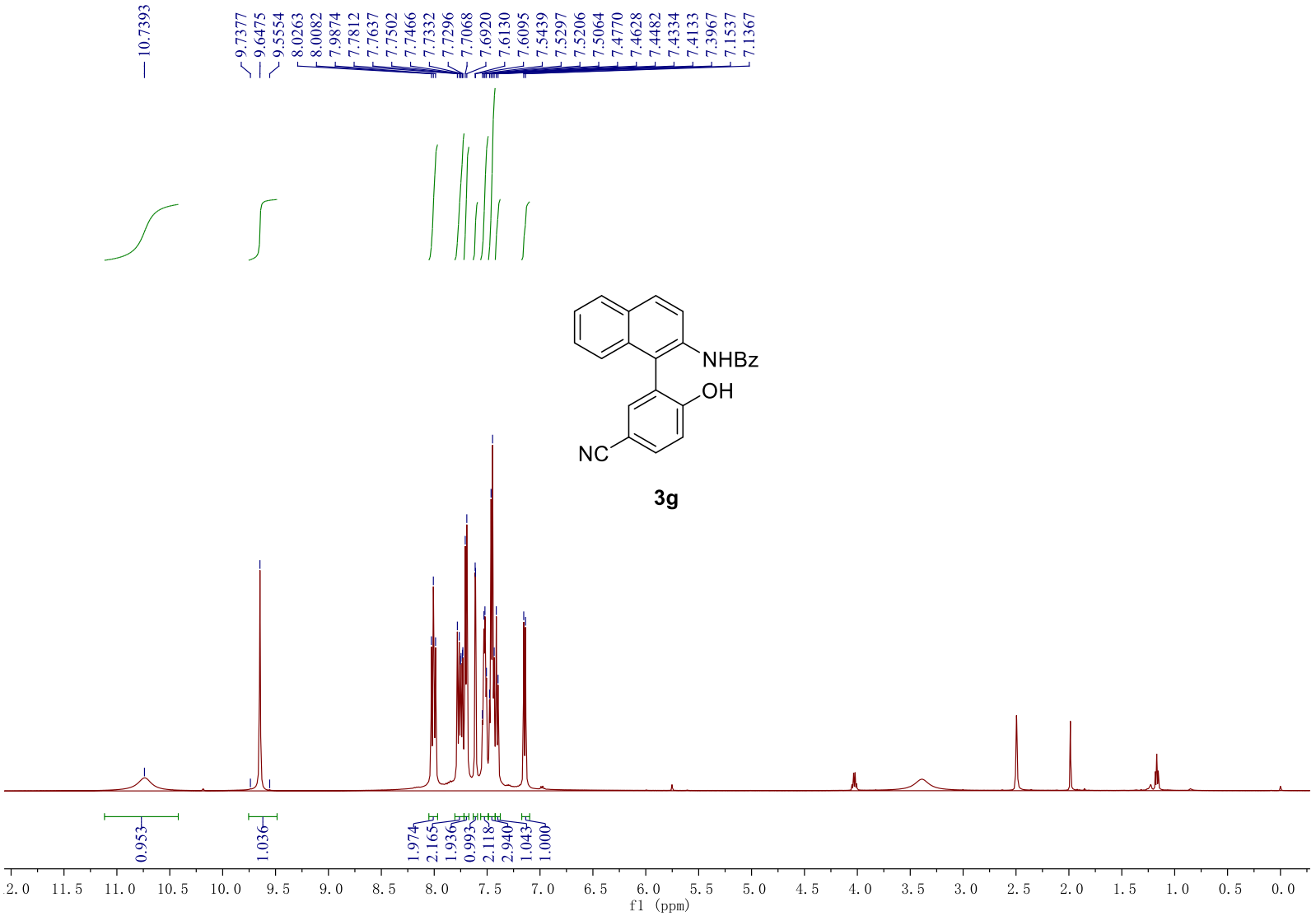
160.46
138.44
135.14
132.29
131.95
129.61
128.82
128.75
128.44
128.36
127.83
126.80
126.14
126.08
125.87
116.45
NHBz
OH
Bz
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.9874
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7.7637
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7.7466
7.7332
7.7296
7.7068
7.6920
7.6130
7.6095
7.5439
7.5297
7.5206
7.5064
7.4770
7.4628
7.4482
7.4334
7.4133
7.3967
7.1537
7.1367
NHBz
OH
NC
3g
0.953
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1.974
2.165
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2.118
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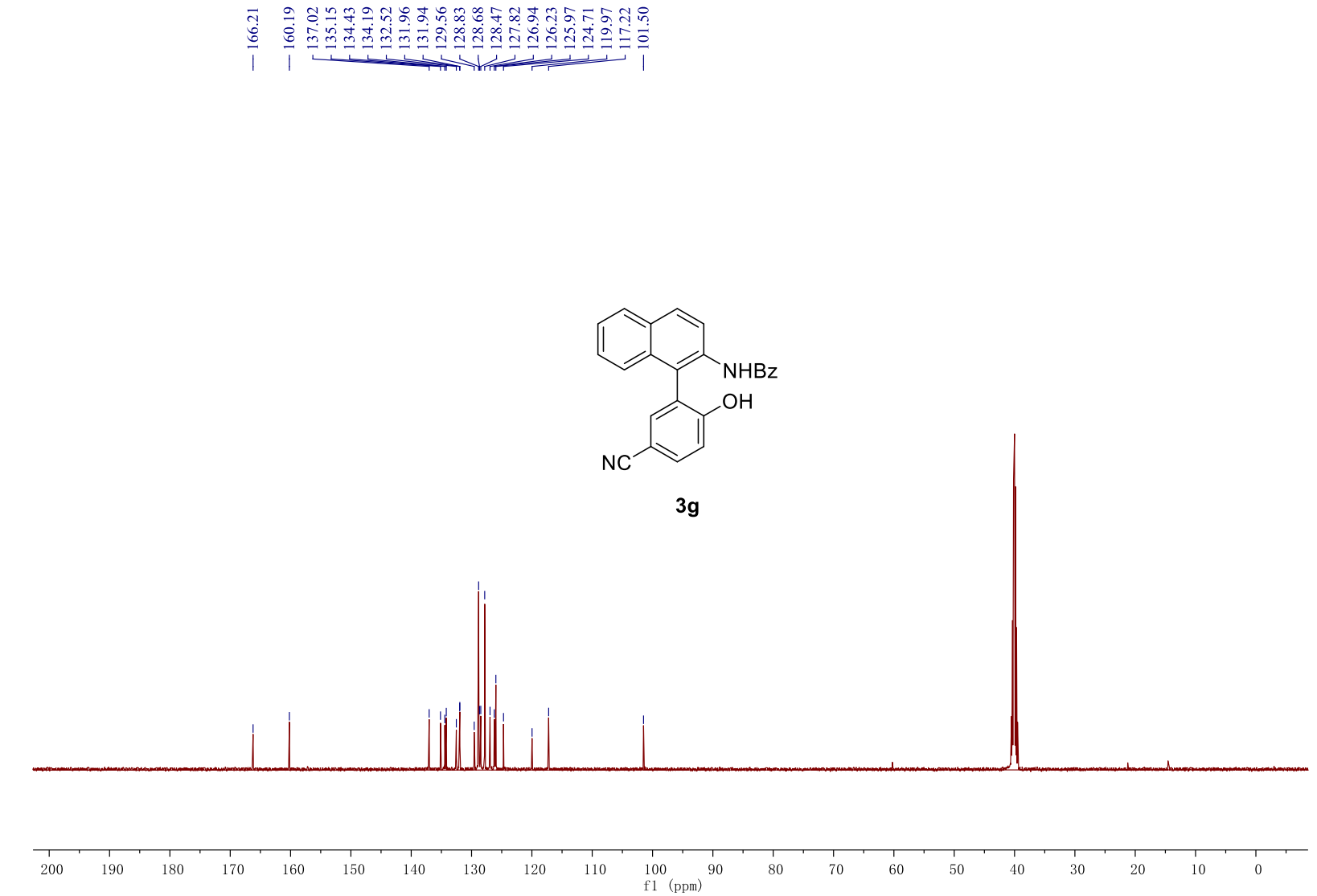
1.043
1.000
f1 (ppm)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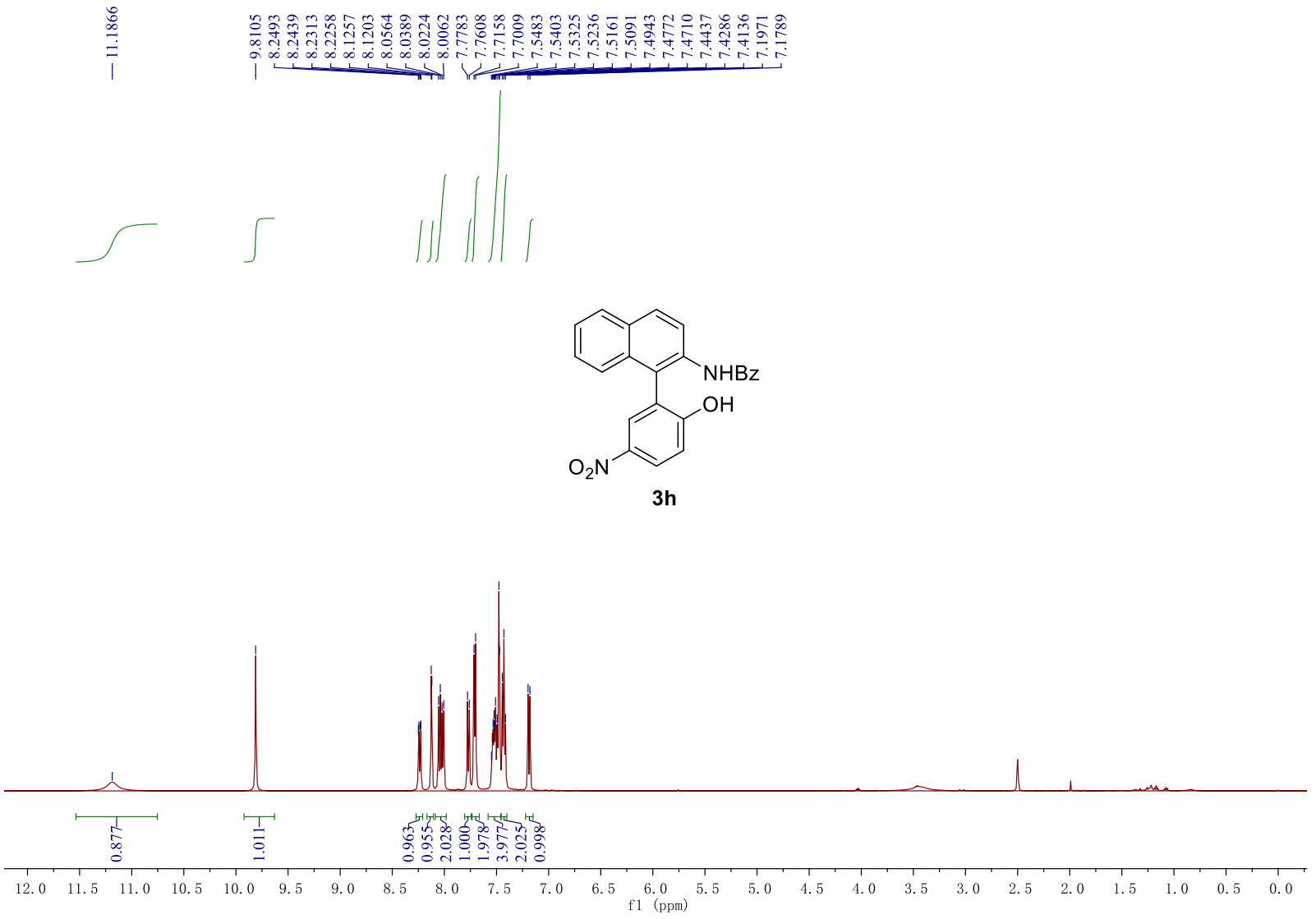
137.02
135.15
134.43
134.19
132.52
131.96
131.94
129.56
128.83
128.68
128.47
127.82
126.94
126.23
125.97
124.71
119.97
117.22
101.50
NHBz
OH
NC
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.2439
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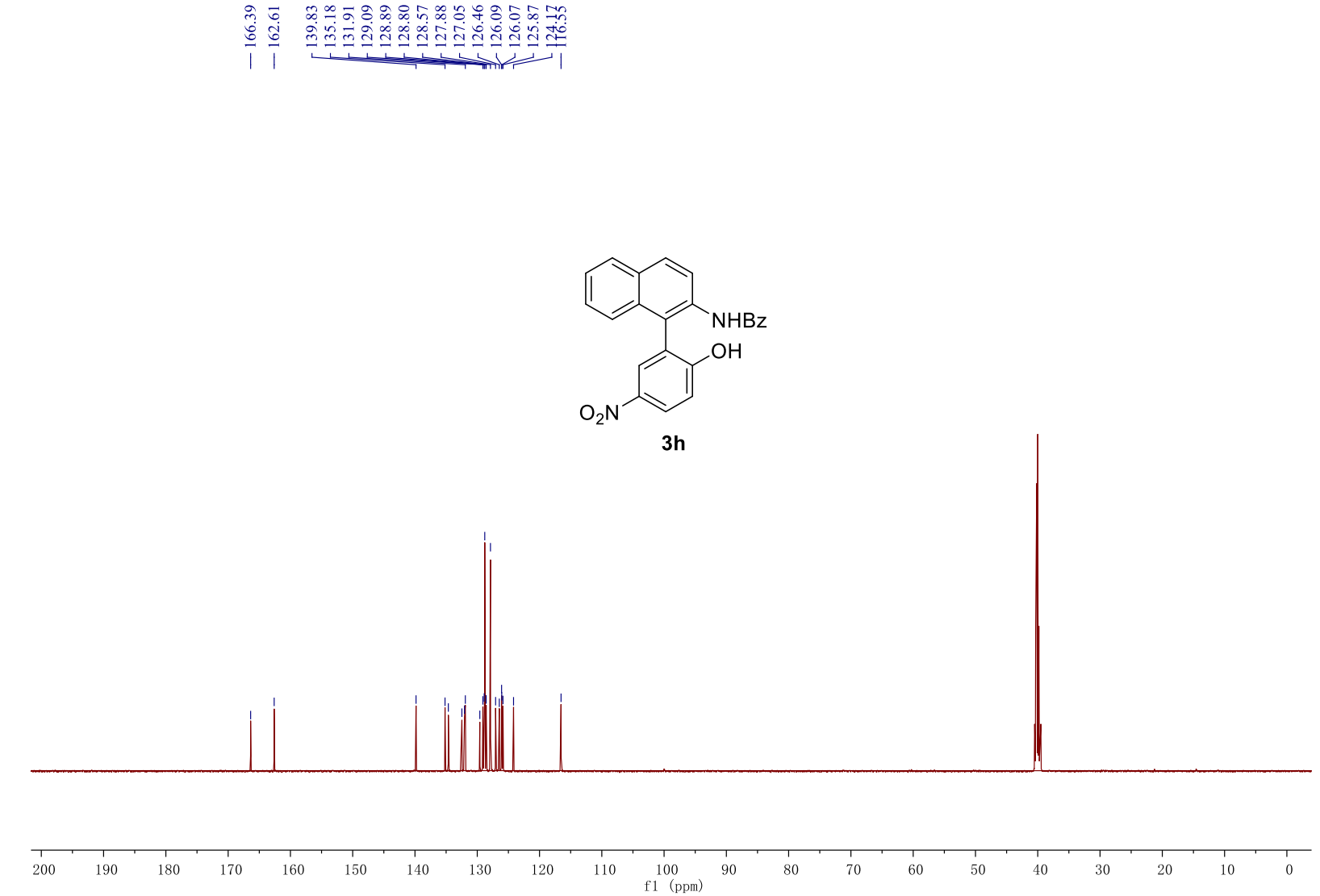
8.1257
8.1203
8.0564
8.0389
8.0224
8.0062
7.7783
7.7608
7.7158
7.7009
7.5483
7.5403
7.5325
7.5236
7.5161
7.5091
7.4943
7.4772
7.4710
7.4437
7.4286
7.4136
7.1971
7.1789
NHBz
OH
O2N
3h
0.877
1.011
0.963
0.955
2.028
1.000
1.978
3.977
2.025
0.998
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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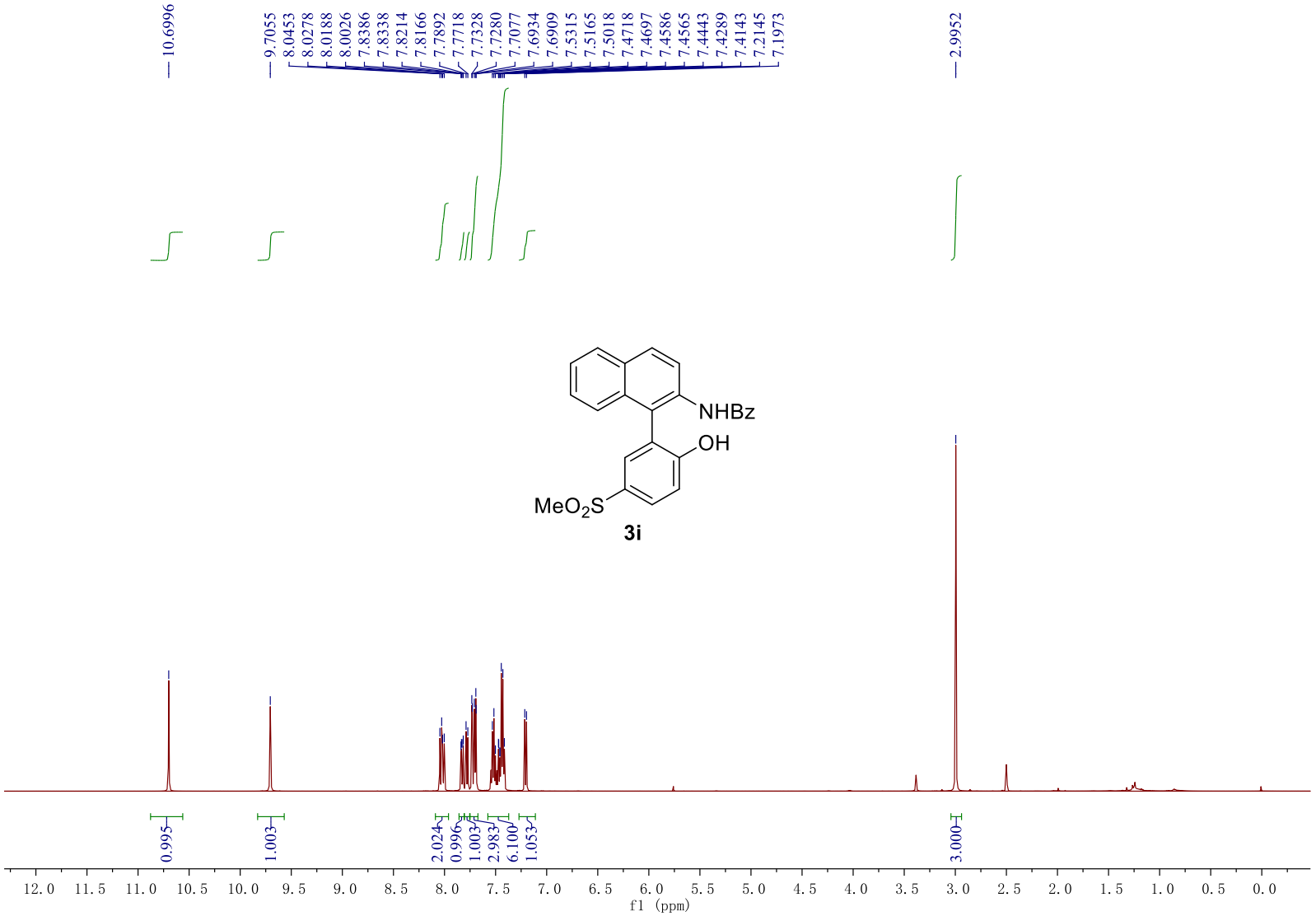
162.61
139.83
135.18
131.91
129.09
128.89
128.80
128.57
127.88
127.05
126.46
126.09
126.07
125.87
124.17
116.55
NHBz
OH
O2N
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.0026
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7.7718
7.7328
7.7280
7.7077
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7.6909
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7.5018
7.4718
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7.4586
7.4565
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7.4289
7.4143
7.2145
7.1973
2.9952
NHBz
OH
MeO2S
3i
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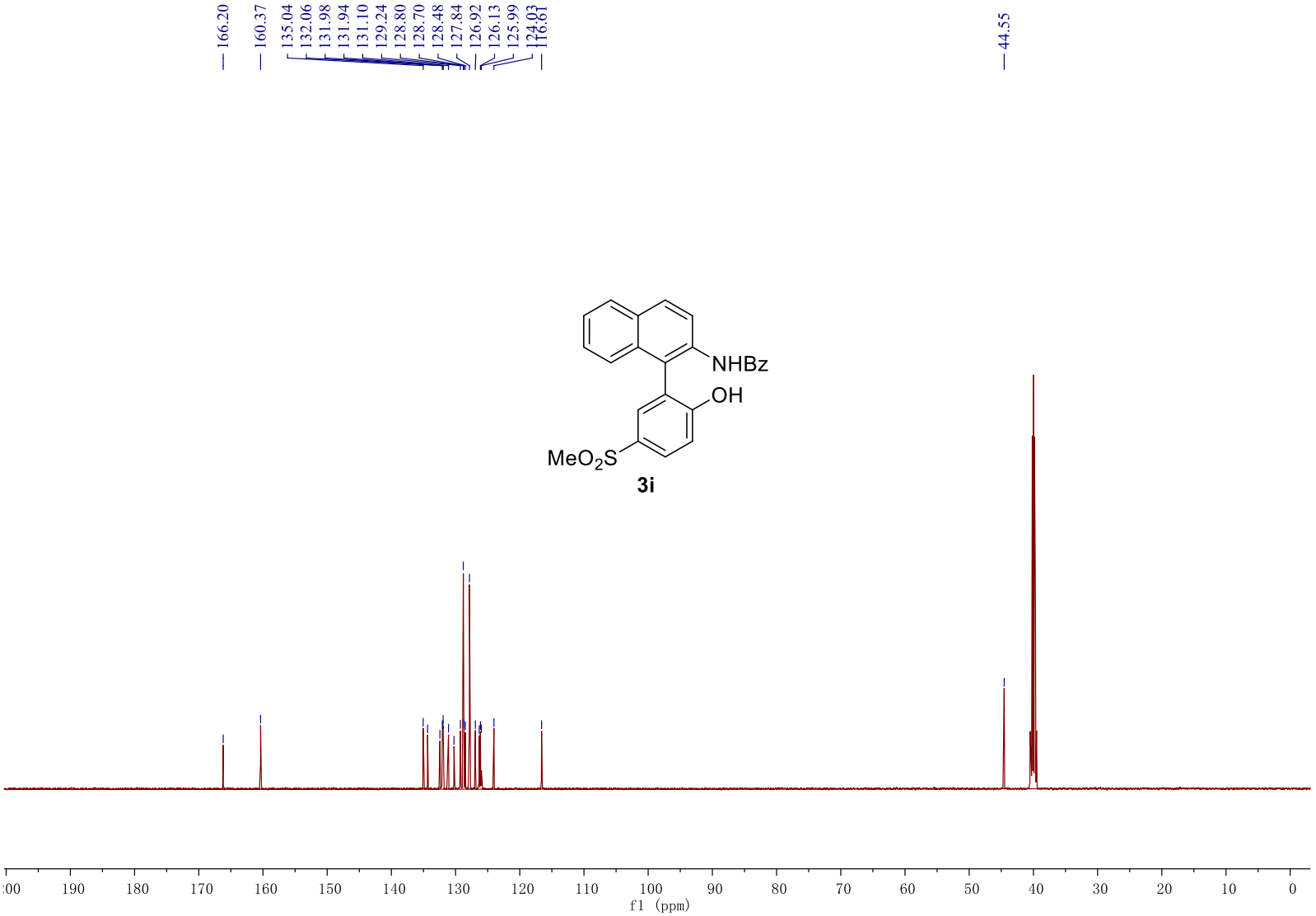
1.003
2.024
0.996
1.003
2.983
6.100
1.053
3.000
f1 (ppm)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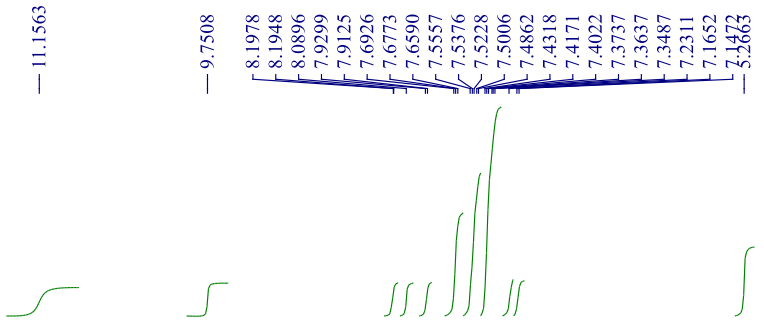
160.37
135.04
132.06
131.98
131.94
131.10
129.24
128.80
128.70
128.48
127.84
126.92
126.13
125.99
124.03
116.61
44.55
NHBz
OH
MeO2S
3i
f1 (ppm)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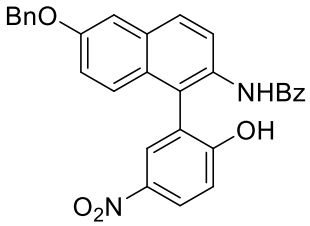
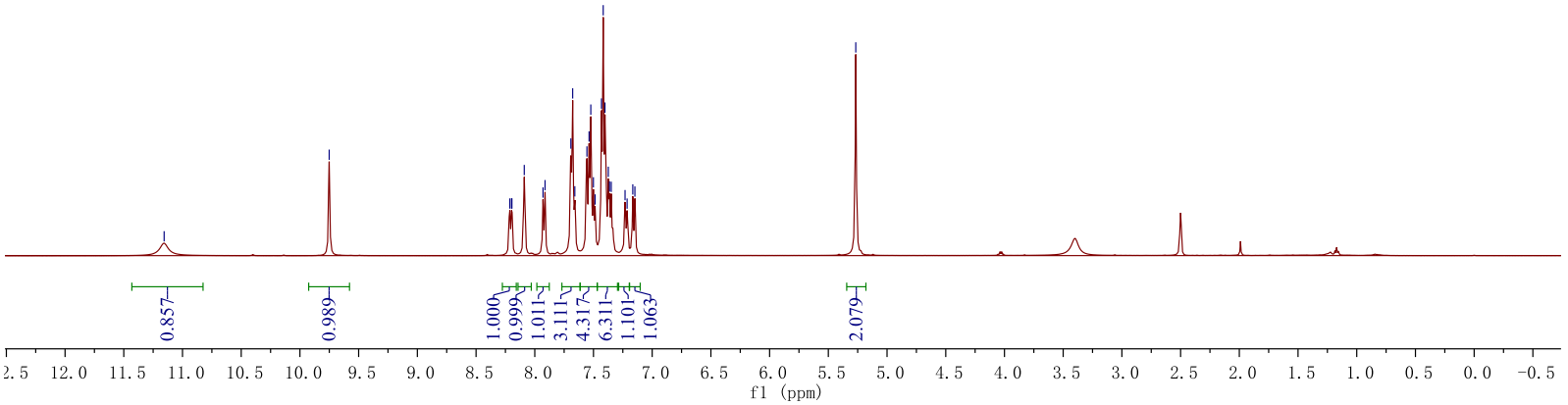
8.1978
8.1948
8.0896
7.9299
7.9125
7.6926
7.6773
7.6590
7.5557
7.5376
7.5228
7.5006
7.4862
7.4318
7.4171
7.4022
7.3737
7.3637
7.3487
7.2311
7.1652
7.1472
5.2663


BnO
NHBz
OH
O2N

3j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0.989
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0.999
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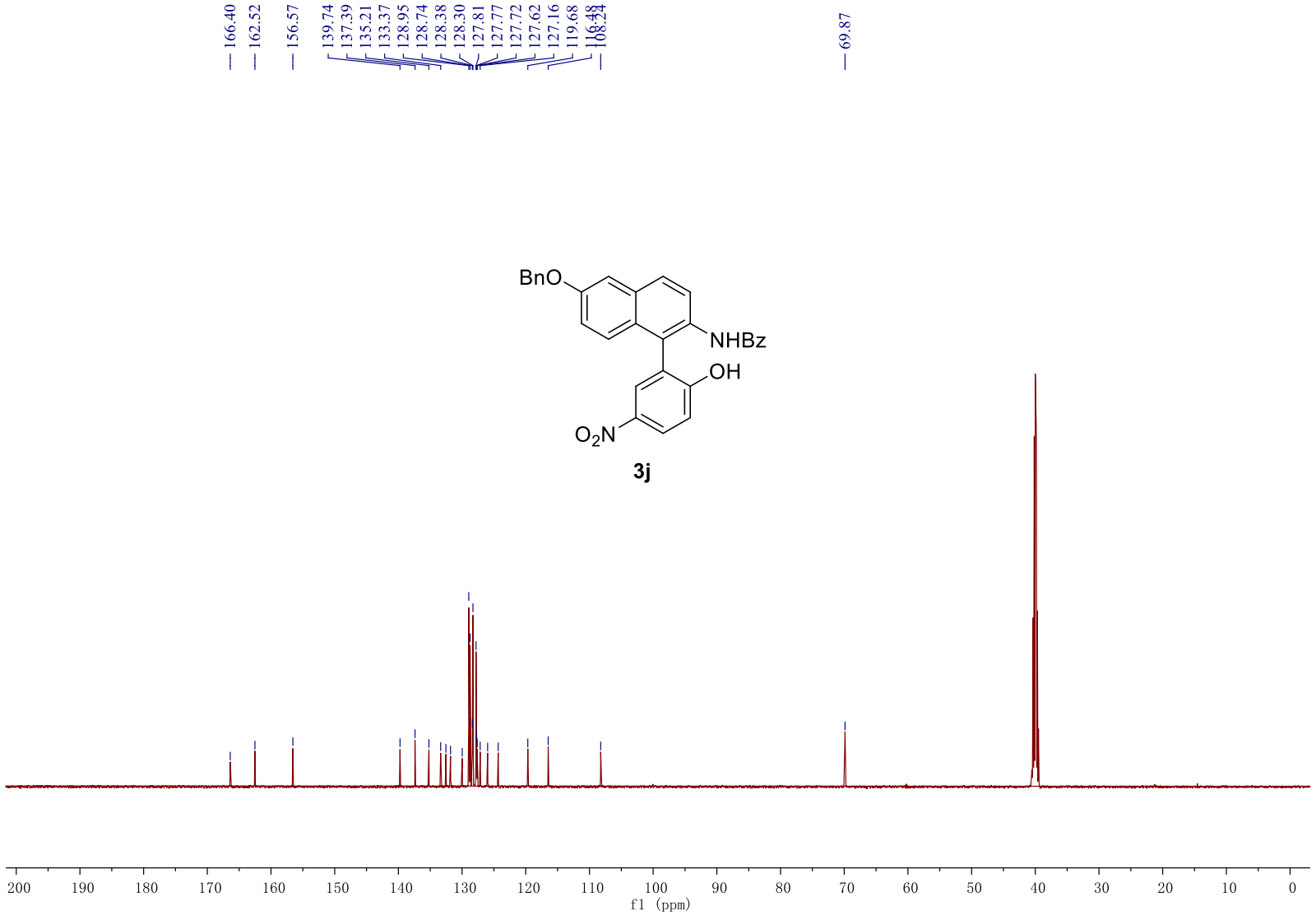
3.111
4.317
6.311
1.101
1.063
2.079
f1 (ppm)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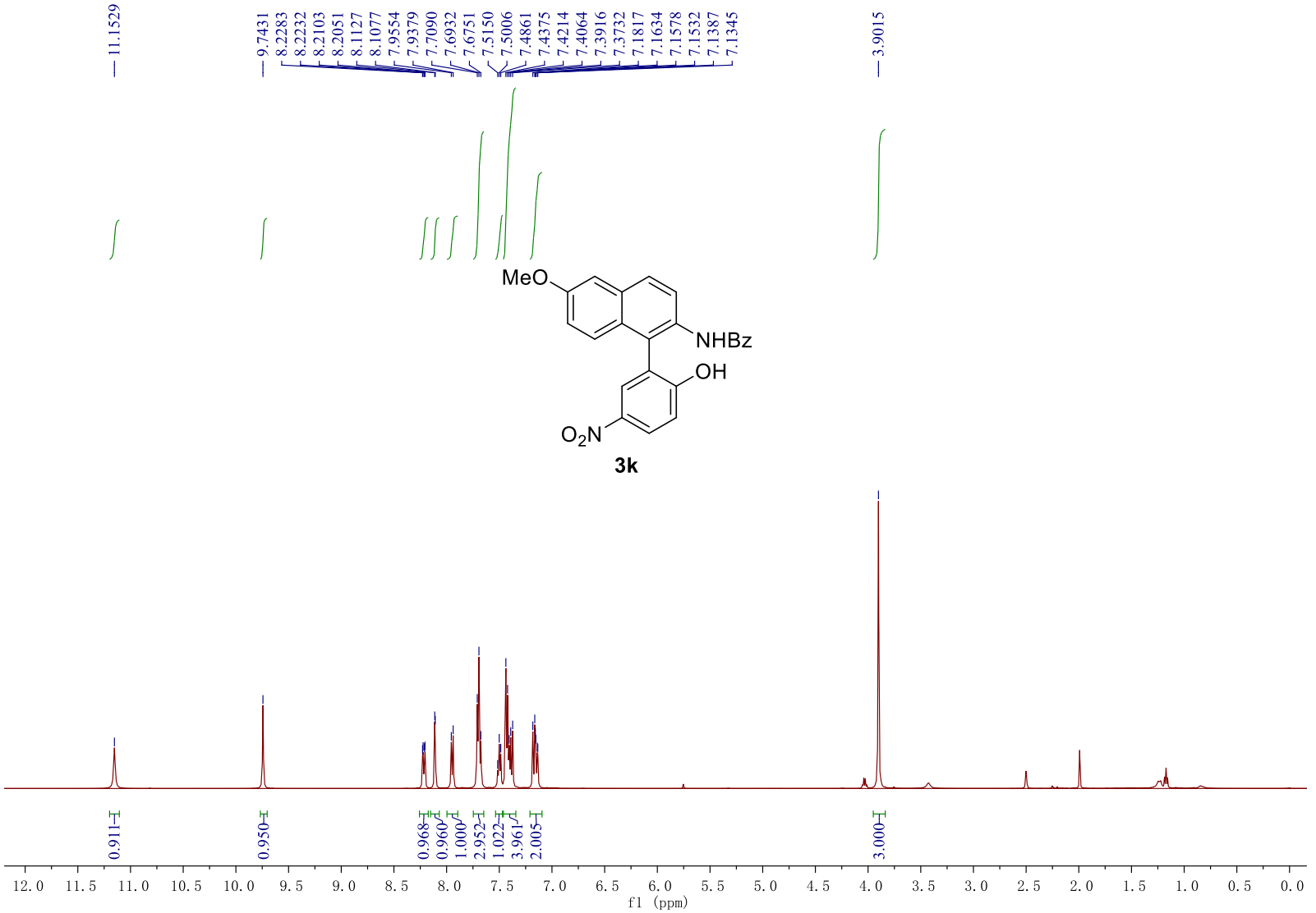
162.52
156.57
139.74
137.39
135.21
133.37
128.95
128.74
128.38
128.30
127.81
127.77
127.72
127.62
127.16
119.68
69.87
BnO
NHBz
OH
O2N
3j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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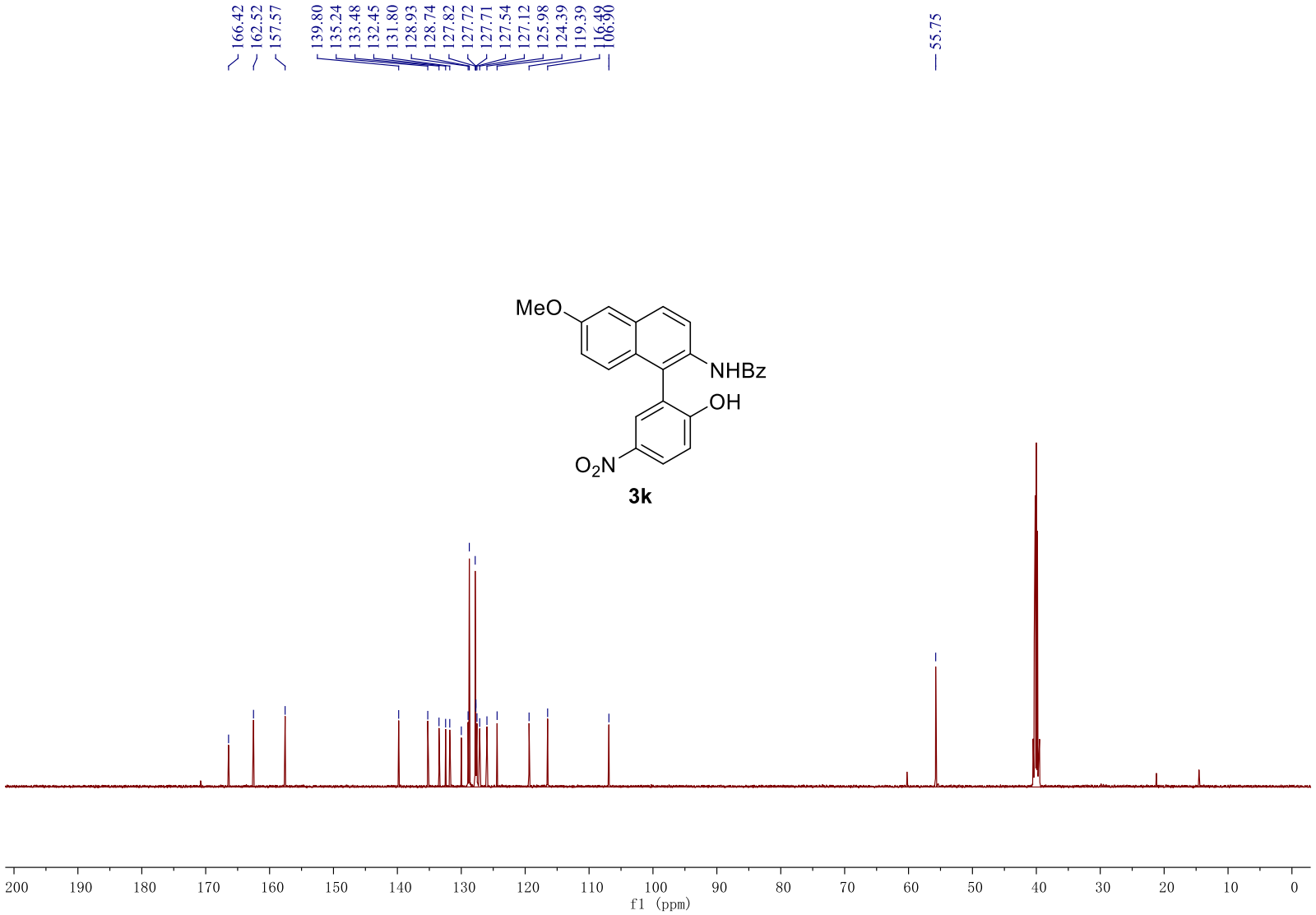
9.7431
8.2283
8.2232
8.2103
8.2051
8.1127
8.1077
7.9554
7.9379
7.7090
7.6932
7.6751
7.5150
7.5006
7.4861
7.4375
7.4214
7.4064
7.3916
7.3732
7.1817
7.1634
7.1578
7.1532
7.1387
7.1345
3.9015
MeO
NHBz
OH
O2N
3k
0.911
0.950
0.968
0.960
1.000
2.952
1.022
3.961
2.005
3.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 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)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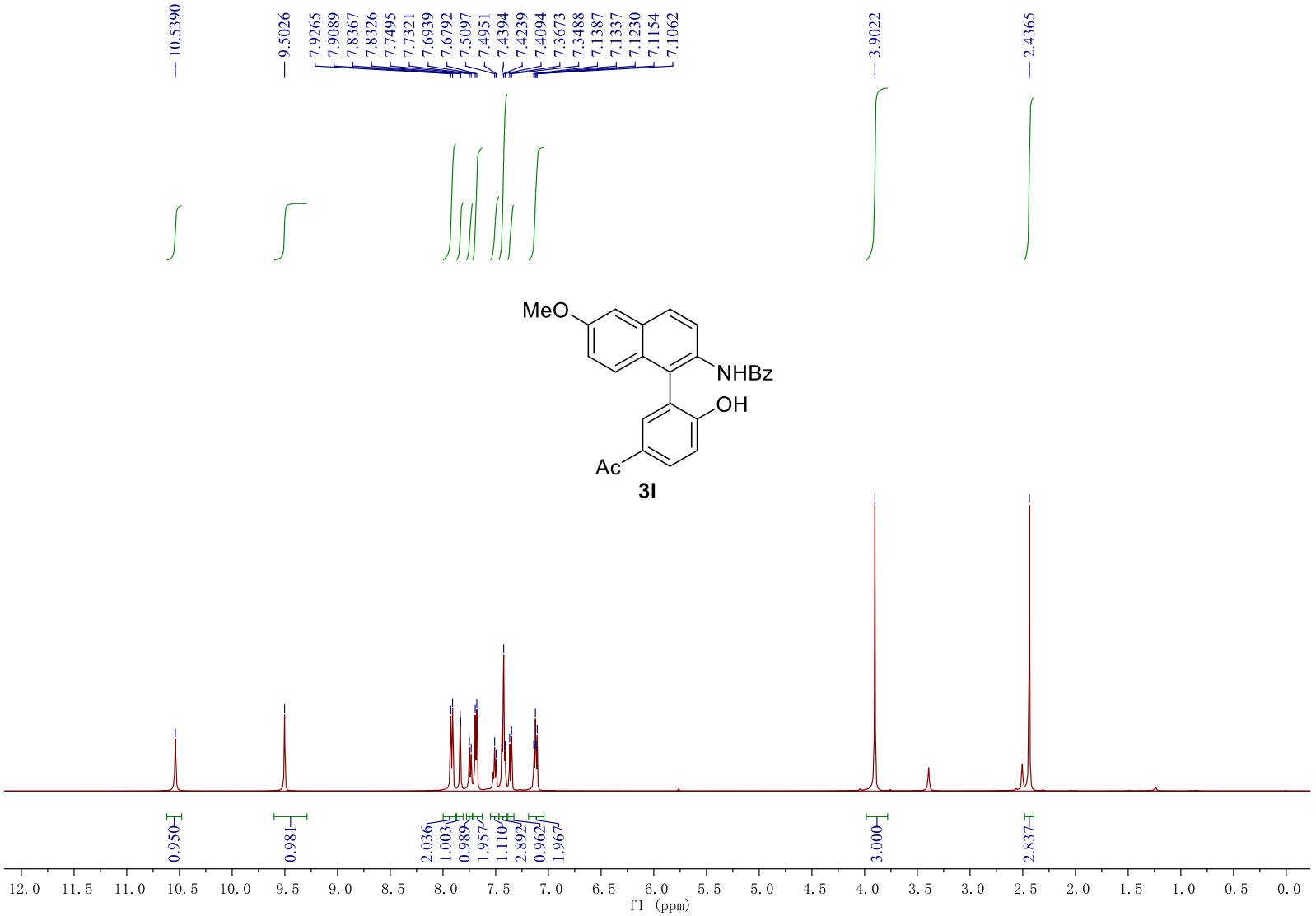
139.80
135.24
133.48
132.45
131.80
128.93
128.74
127.82
127.72
127.71
127.54
127.12
125.98
124.39
119.39
116.49
106.90
55.75
MeO
NHBz
OH
O2N
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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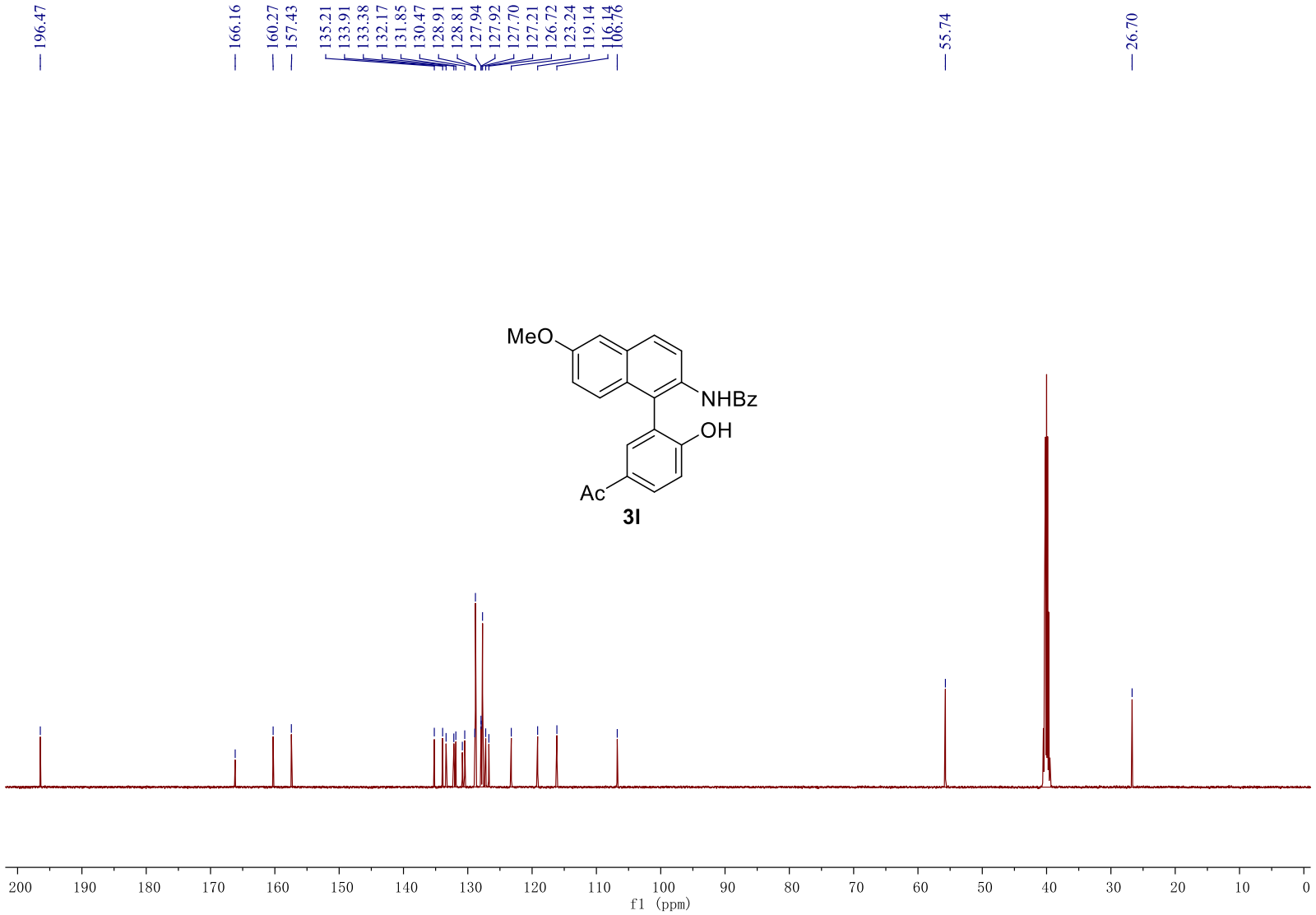
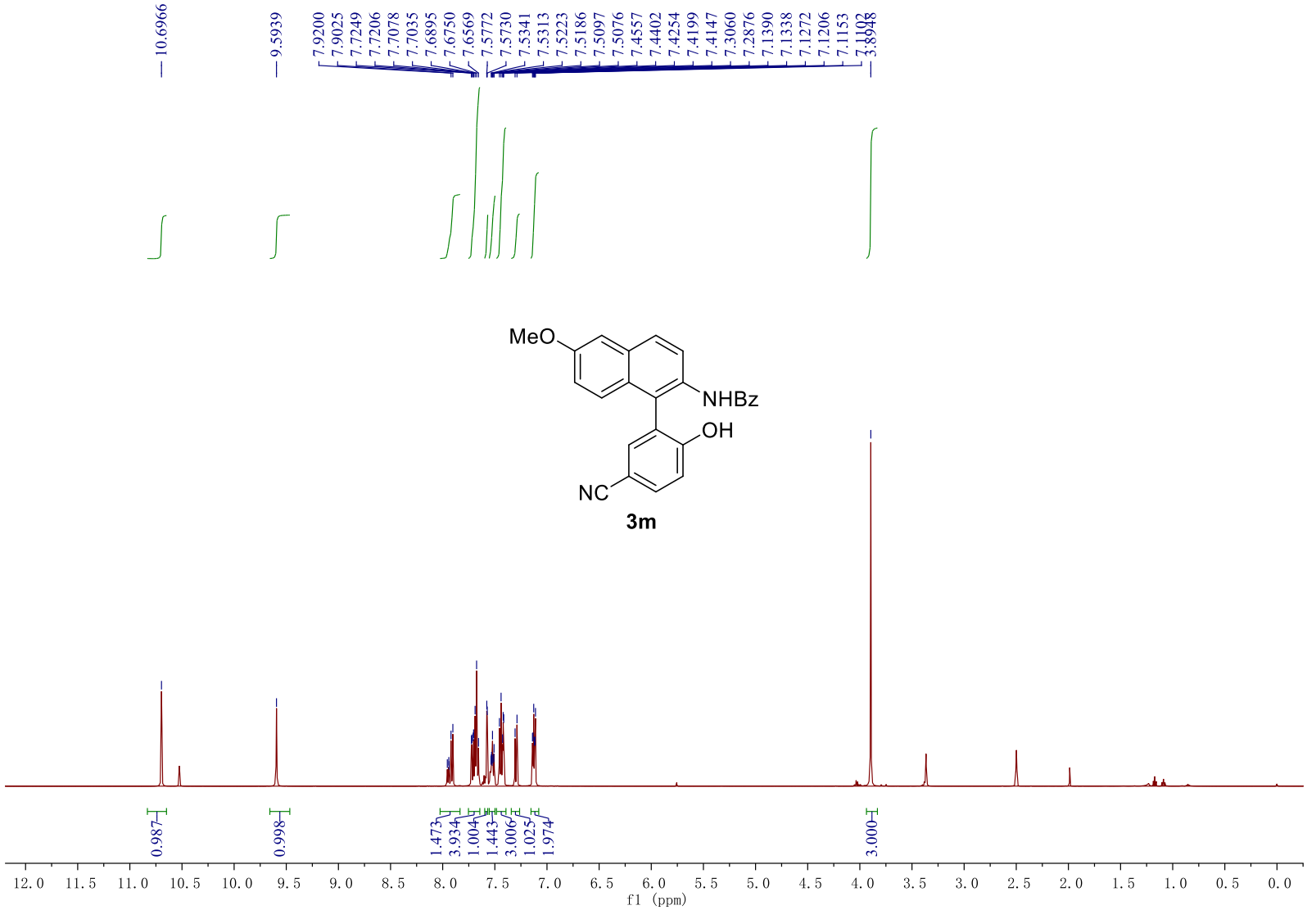
9.5026
7.9265
7.9089
7.8367
7.8326
7.7495
7.7321
7.6939
7.6792
7.5097
7.4951
7.4394
7.4239
7.4094
7.3673
7.3488
7.1387
7.1337
7.1230
7.1154
7.1062
3.9022
2.4365
MeO
NHBz
OH
Ac
3l
0.950
0.981
2.036
1.003
0.989
1.957
1.110
2.892
0.962
1.967
3.000
2.837
f1 (ppm)


196.47
166.16
160.27
157.43
135.21
133.91
133.38
132.17
131.85
130.47
128.91
128.81
127.94
127.92
127.70
127.21
126.72
123.24
119.14
116.14
106.76
55.74
26.70
MeO
NHBz
OH
Ac
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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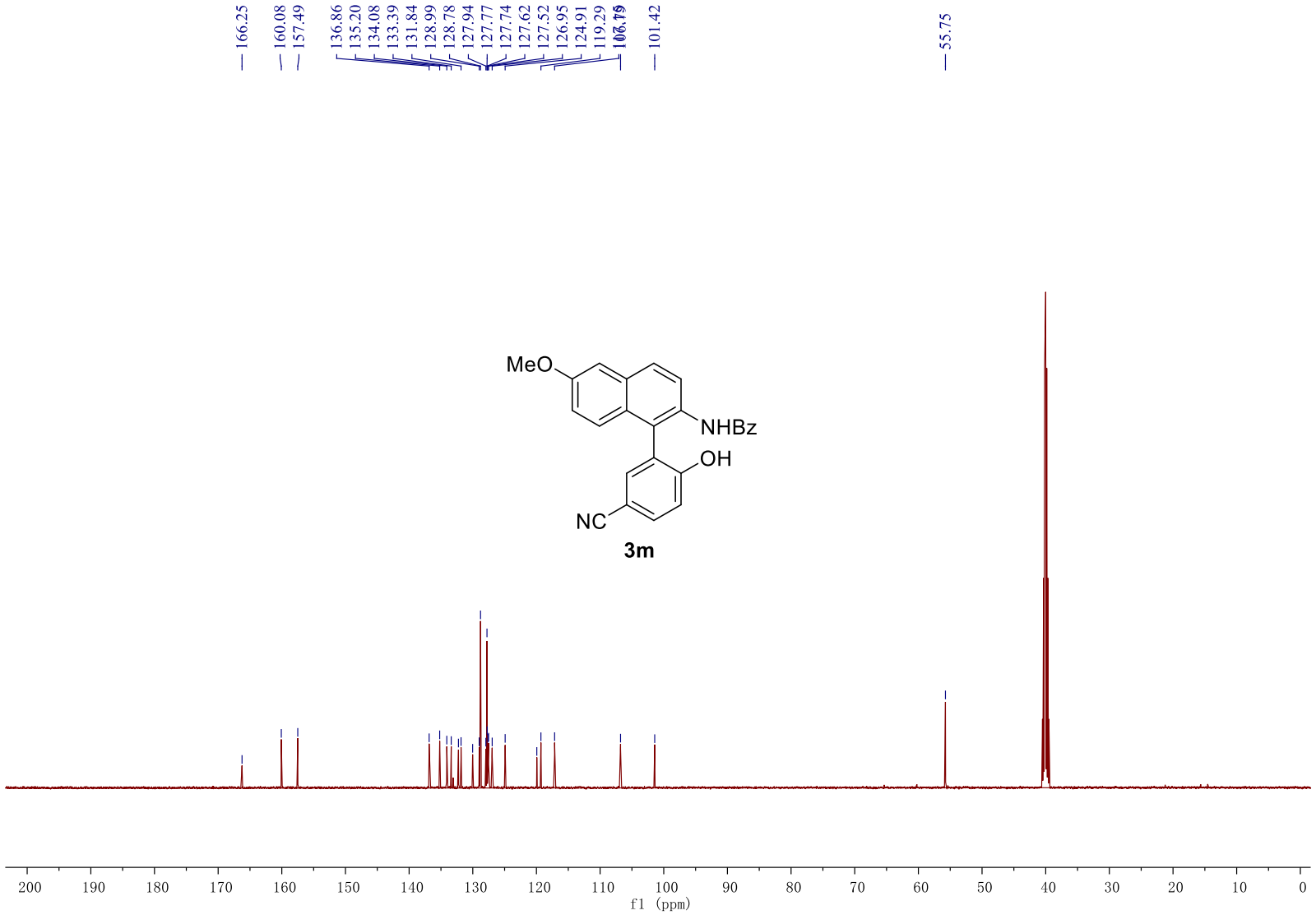
7.9025
7.7249
7.7206
7.7078
7.7035
7.6895
7.6750
7.6569
7.5772
7.5730
7.5341
7.5313
7.5223
7.5186
7.5097
7.5076
7.4557
7.4402
7.4254
7.4199
7.4147
7.3060
7.2876
7.1390
7.1338
7.1272
7.1206
7.1153
3.8948
MeO
NHBz
OH
NC
3m
0.987
0.998
1.473
3.934
1.004
1.443
3.006
1.025
1.974
3.000
12.0 11.5 11.0 10.5 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)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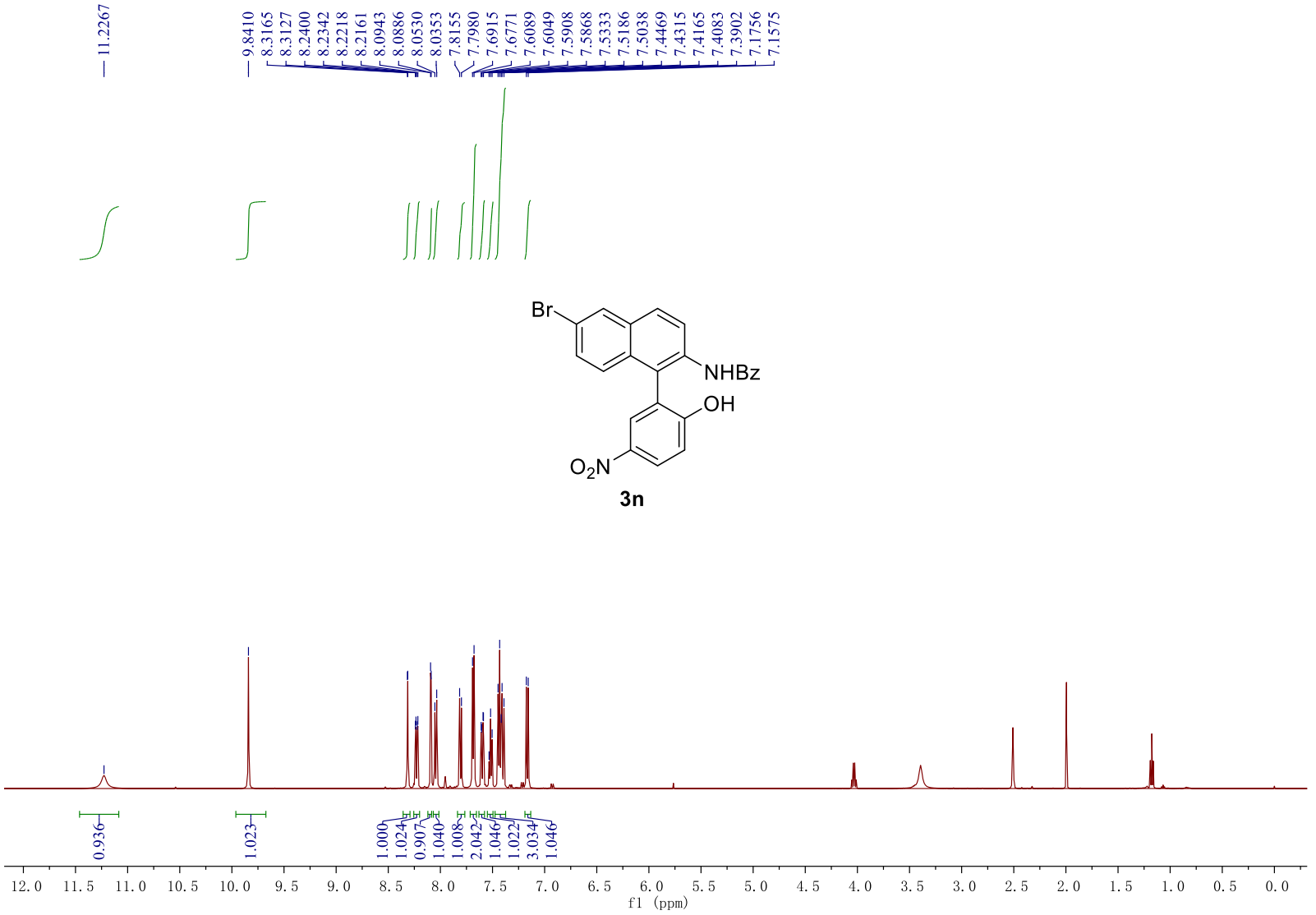
160.08
157.49
136.86
135.20
134.08
133.39
131.84
128.99
128.78
127.94
127.77
127.74
127.62
127.52
126.95
124.91
119.29
101.42
55.75
MeO
NHBz
OH
NC
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.8410
8.3165
8.3127
8.2400
8.2342
8.2218
8.2161
8.0943
8.0886
8.0530
8.0353
7.8155
7.7980
7.6915
7.6771
7.6089
7.6049
7.5908
7.5868
7.5333
7.5186
7.5038
7.4469
7.4315
7.4165
7.4083
7.3902
7.1756
7.1575
Br
NHBz
OH
O2N
3n
0.936
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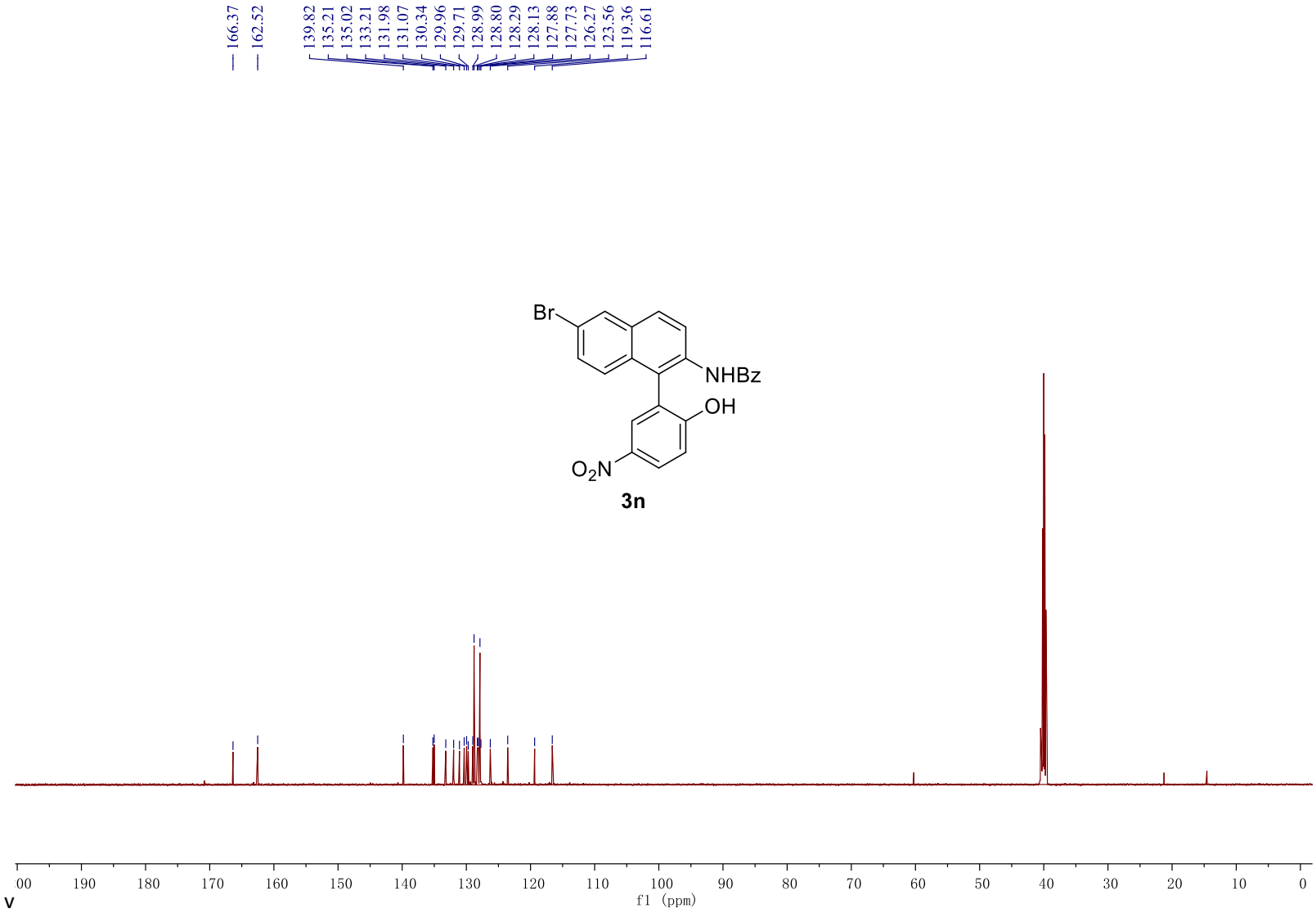
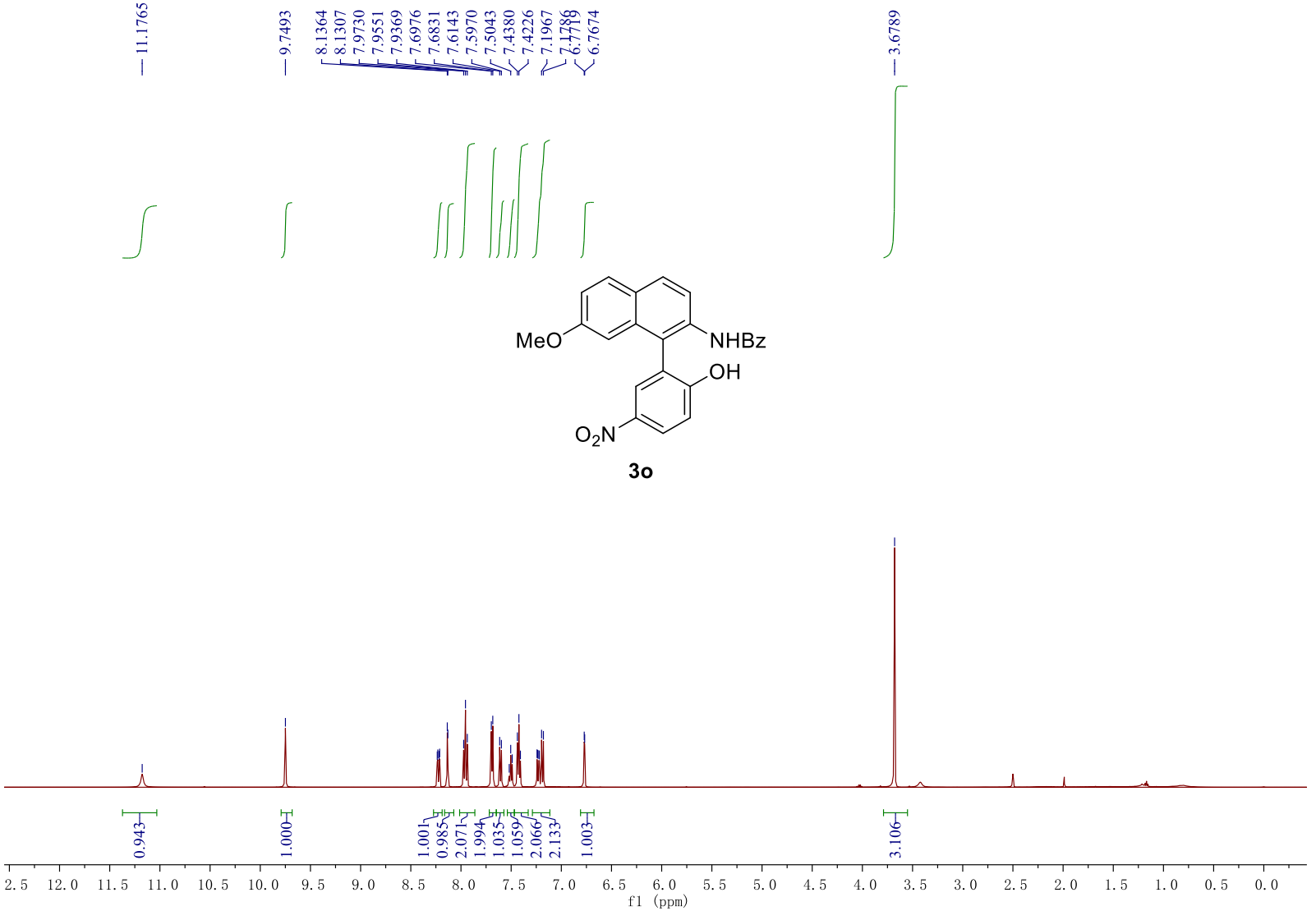
1.000
1.024
0.907
1.040
1.008
2.042
1.046
1.022
3.034
1.046
f1 (ppm)


166.37
162.52
139.82
135.21
135.02
133.21
131.98
131.07
130.34
129.96
129.71
128.99
128.80
128.29
128.13
127.88
127.73
126.27
123.56
119.36
116.61
Br
NHBz
OH
O2N
3n
f1 (ppm)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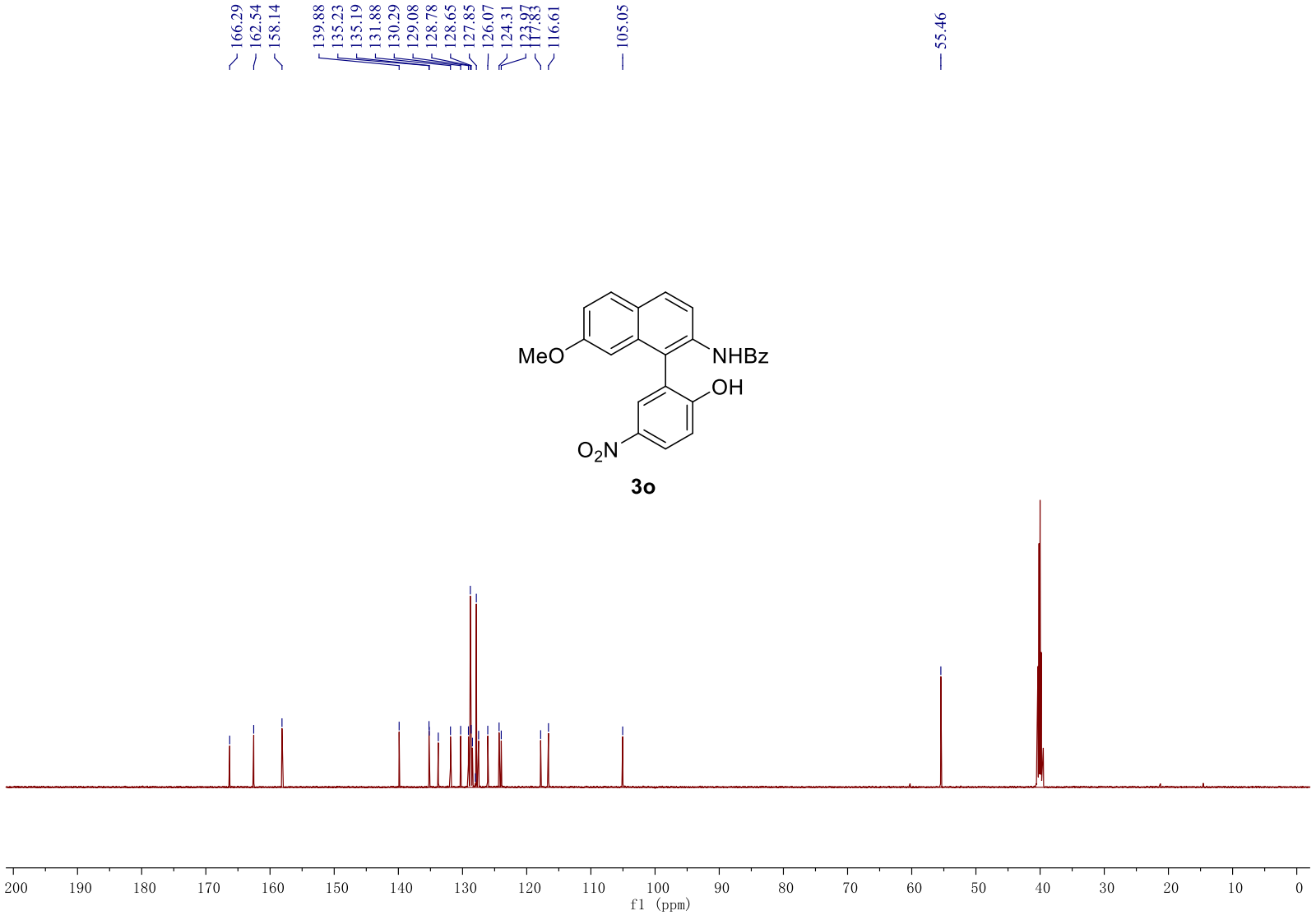
8.1364
8.1307
7.9730
7.9551
7.9369
7.6976
7.6831
7.6143
7.5970
7.5043
7.4380
7.4226
7.1967
6.7719
6.7674
3.6789
MeO
NHBz
OH
O2N
3o
0.943
1.000
1.001
0.985
2.071
1.994
1.035
1.059
2.066
2.133
1.003
3.106
f1 (ppm)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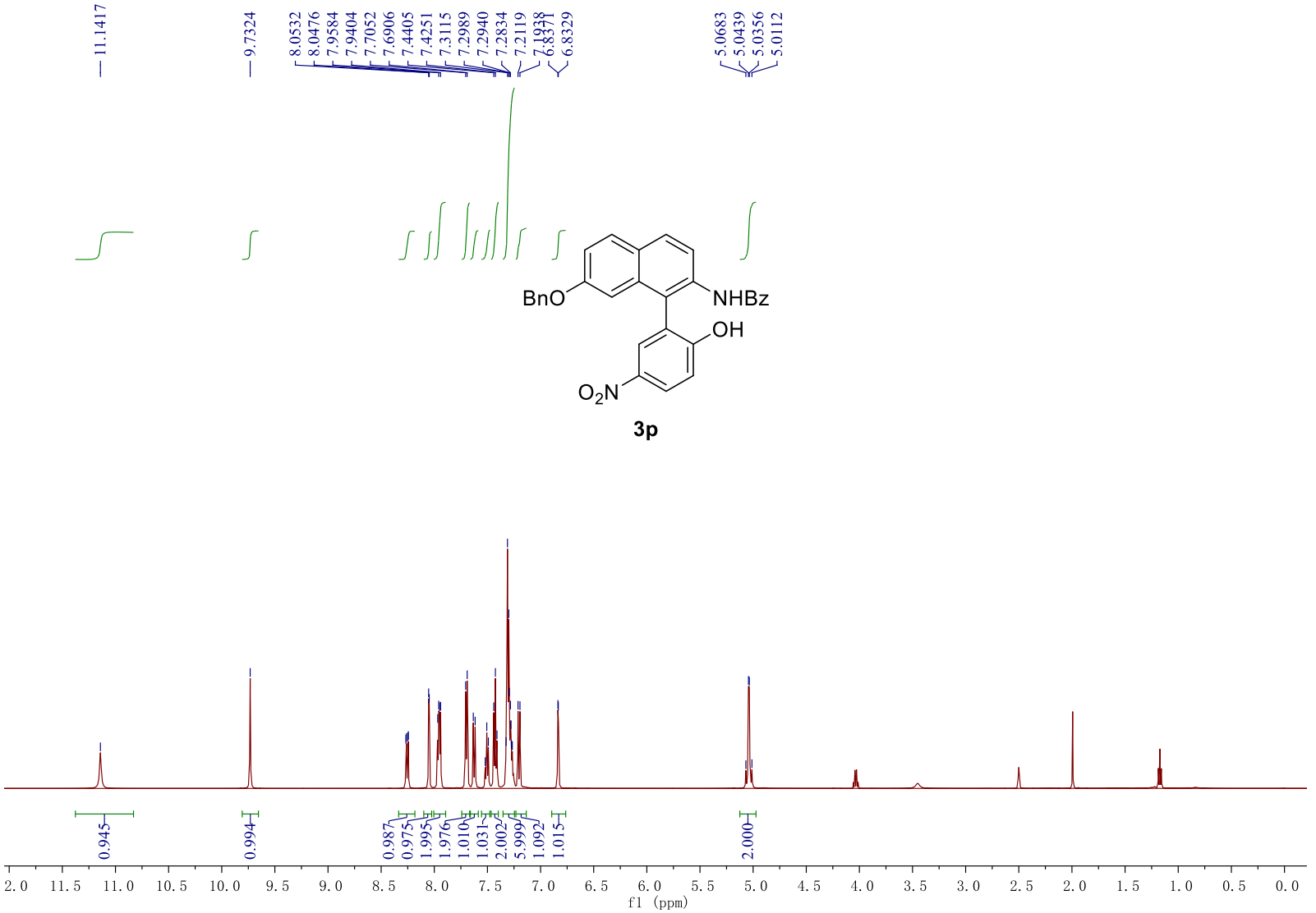
158.14
139.88
135.23
135.19
131.88
130.29
129.08
128.78
128.65
127.85
126.07
124.31
123.97
117.83
116.61
105.05
55.46
MeO
NHBz
OH
O2N
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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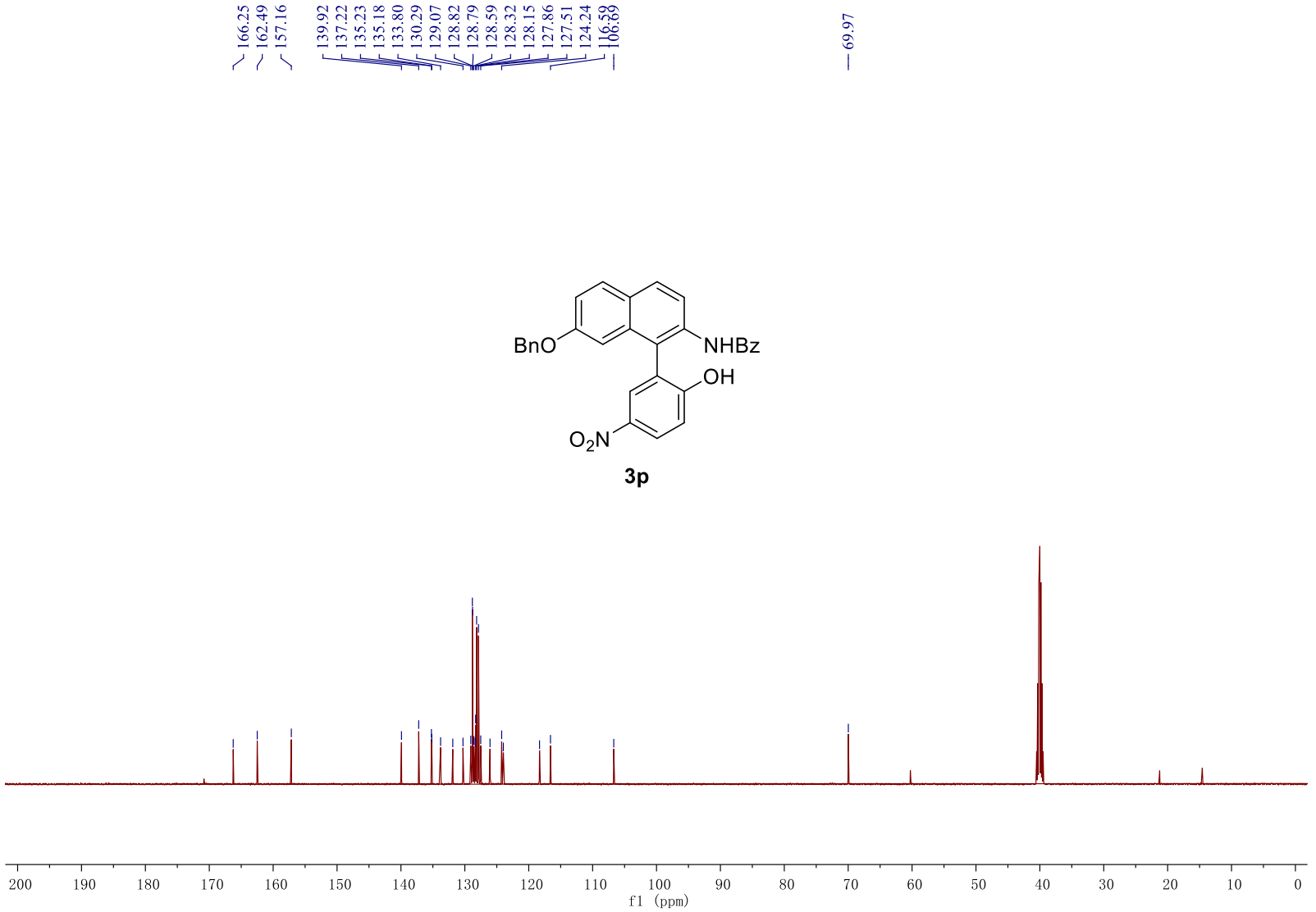
7.9584
7.9404
7.7052
7.6906
7.4405
7.4251
7.3115
7.2989
7.2940
7.2834
7.2119
7.1938
6.8371
6.8329
5.0683
5.0439
5.0356
5.0112
BnO
NHBz
OH
O2N
3p
0.945
0.994
0.987
0.975
1.995
1.976
1.010
1.031
2.002
5.999
1.092
1.015
2.000
f1 (ppm)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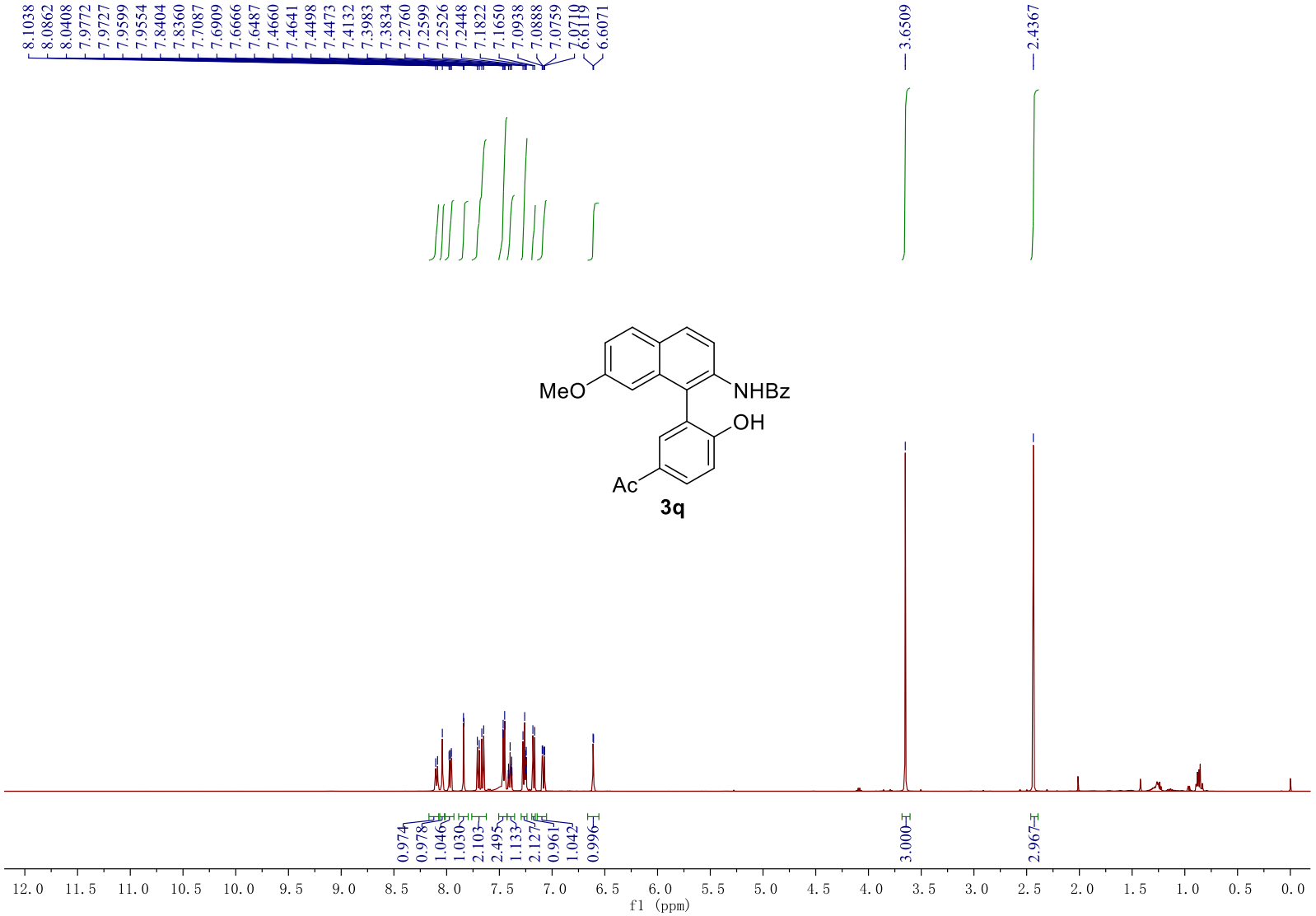
137.22
135.23
135.18
133.80
130.29
129.07
128.82
128.79
128.59
128.32
128.15
127.86
127.51
124.24
116.59
106.69
69.97
BnO
NHBz
OH
O2N
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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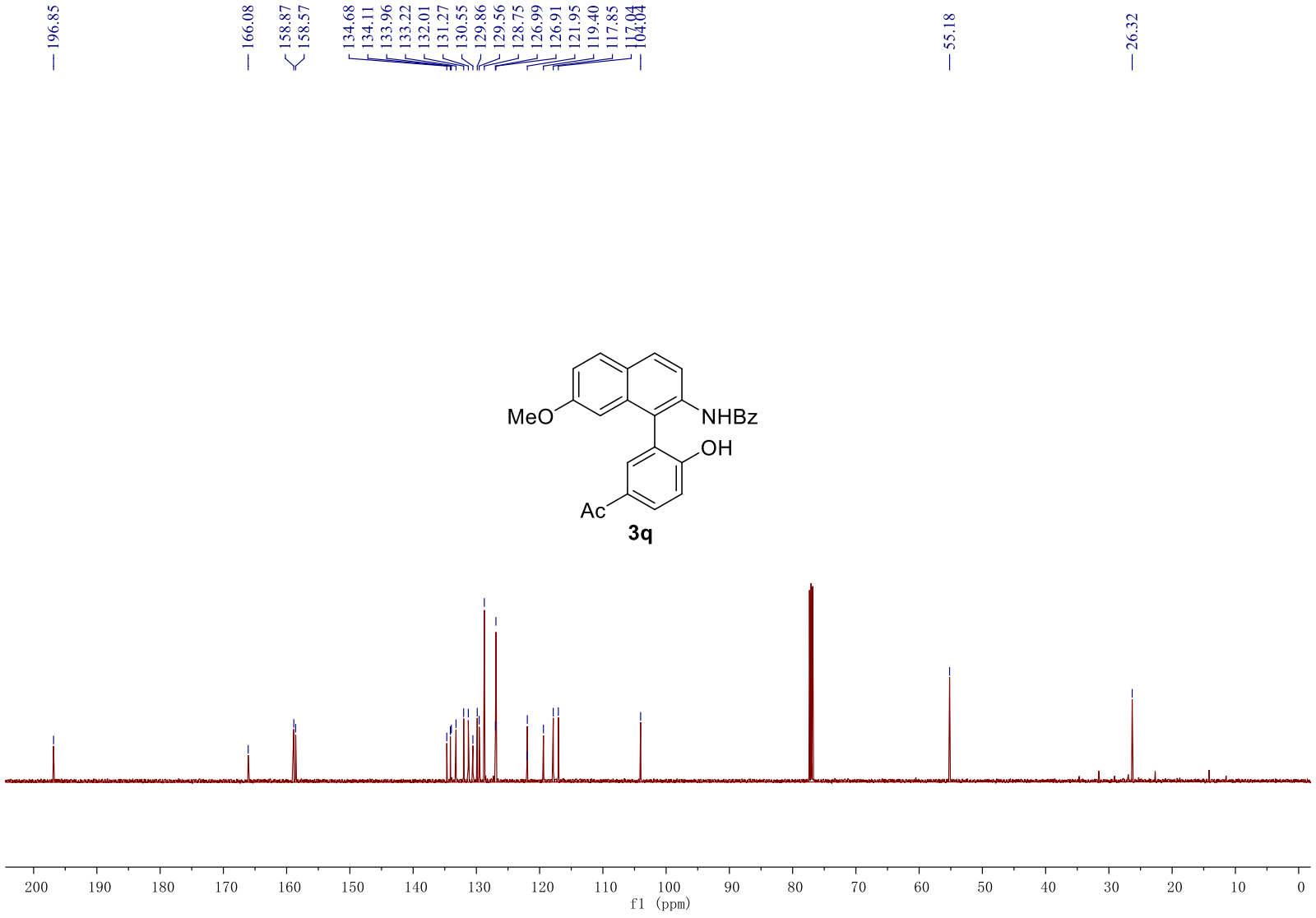
7.7087
7.6909
7.6666
7.6487
7.4660
7.4641
7.4498
7.4473
7.4132
7.3983
7.3834
7.2760
7.2599
7.2526
7.2448
7.1822
7.1650
7.0938
7.0888
7.0759
7.0710
6.8119
6.6071
3.6509
2.4367
MeO
NHBz
OH
Ac
3q
0.974
0.978
1.046
1.030
2.103
2.495
1.133
2.127
0.961
1.042
0.996
3.000
2.967
12.0 11.5 11.0 10.5 10.0 9.5 9.0 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)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134.11
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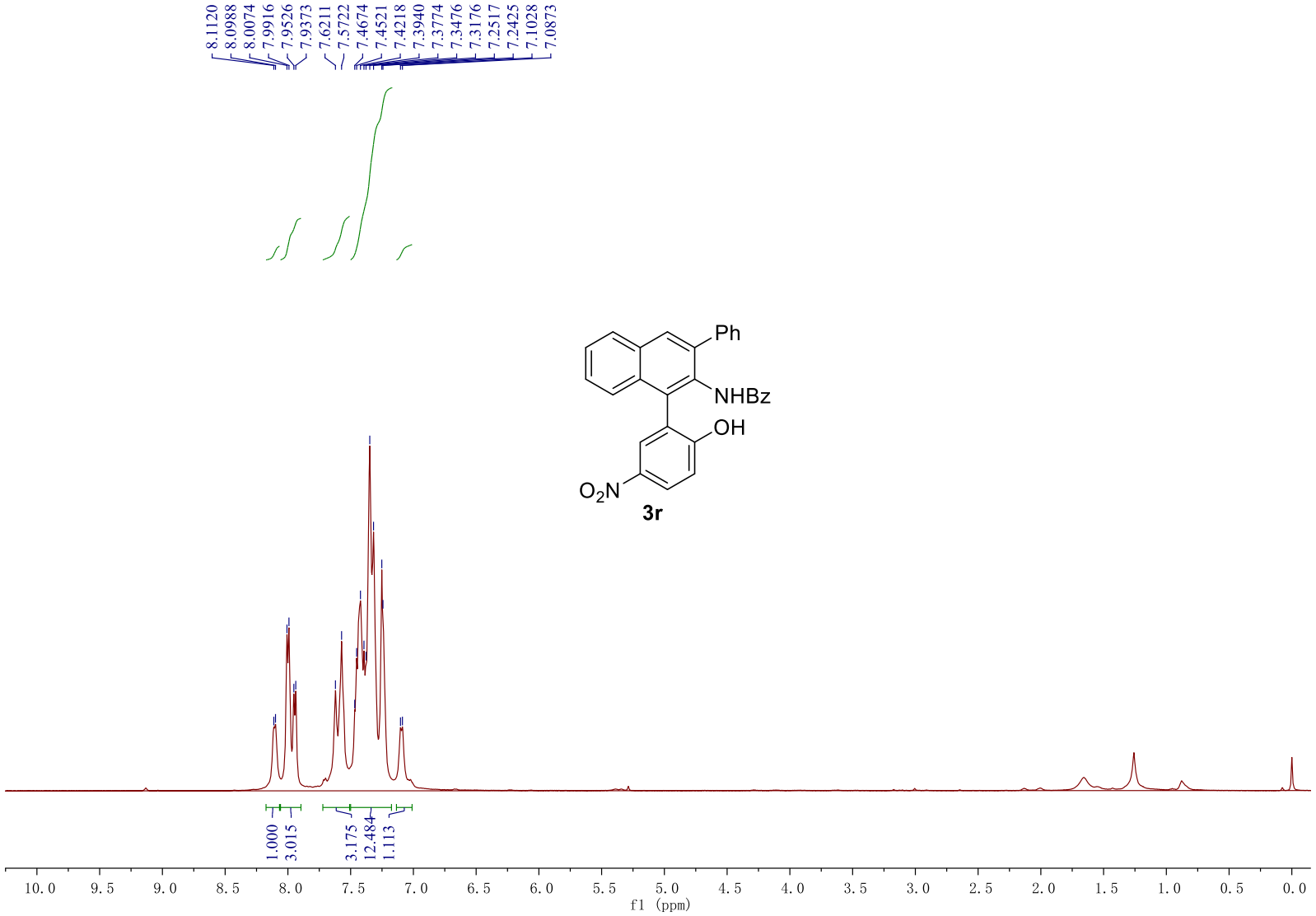
133.22
132.01
131.27
130.55
129.86
129.56
128.75
126.99
126.91
121.95
119.40
117.85
117.04
104.04
55.18
26.32
MeO
NHBz
OH
Ac
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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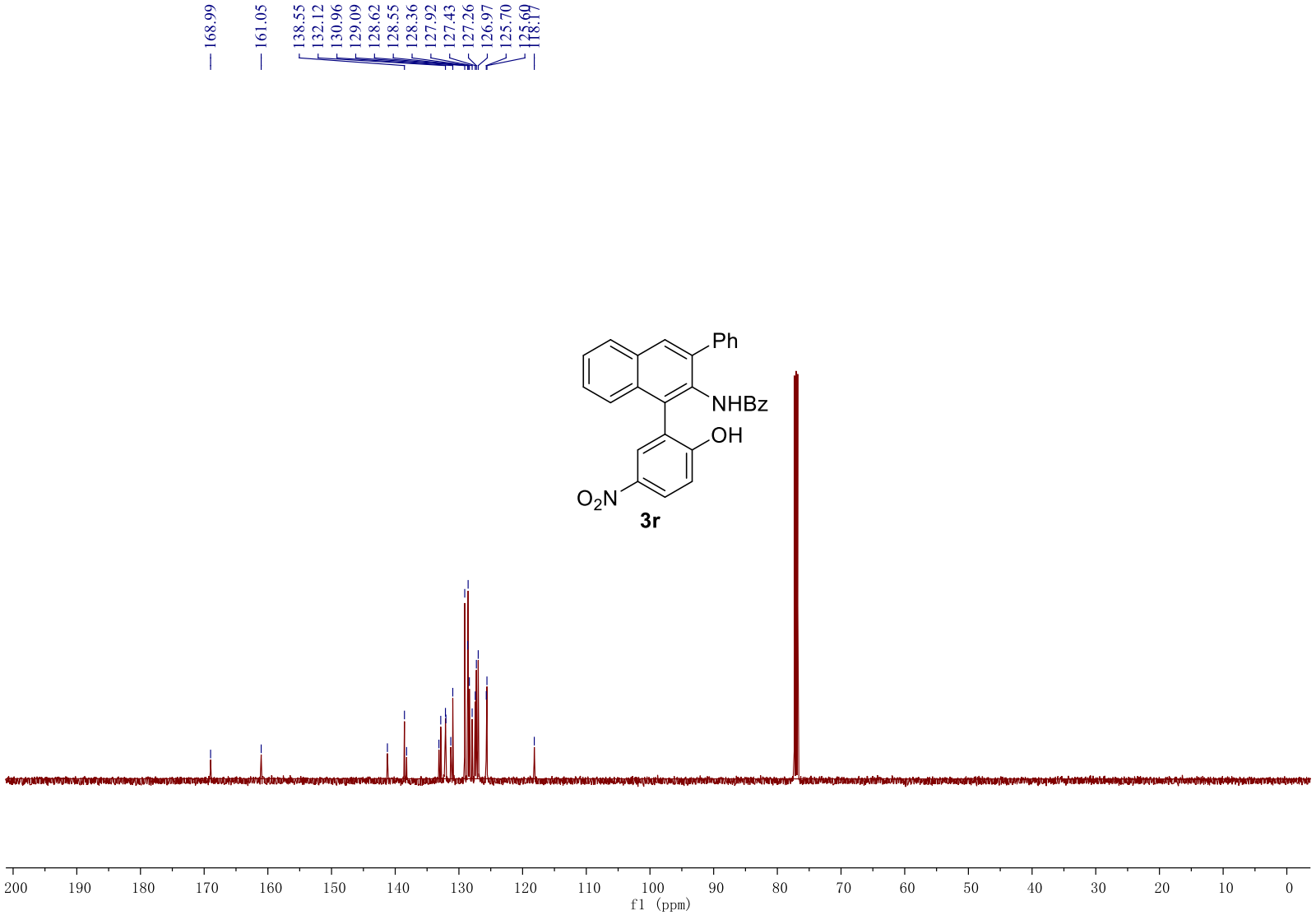
7.6211
7.5722
7.4674
7.4521
7.4218
7.3940
7.3774
7.3476
7.3176
7.2517
7.2425
7.1028
7.0873
Ph
NHBz
OH
O2N
3r
1.000
3.015
3.175
12.484
1.113
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.99
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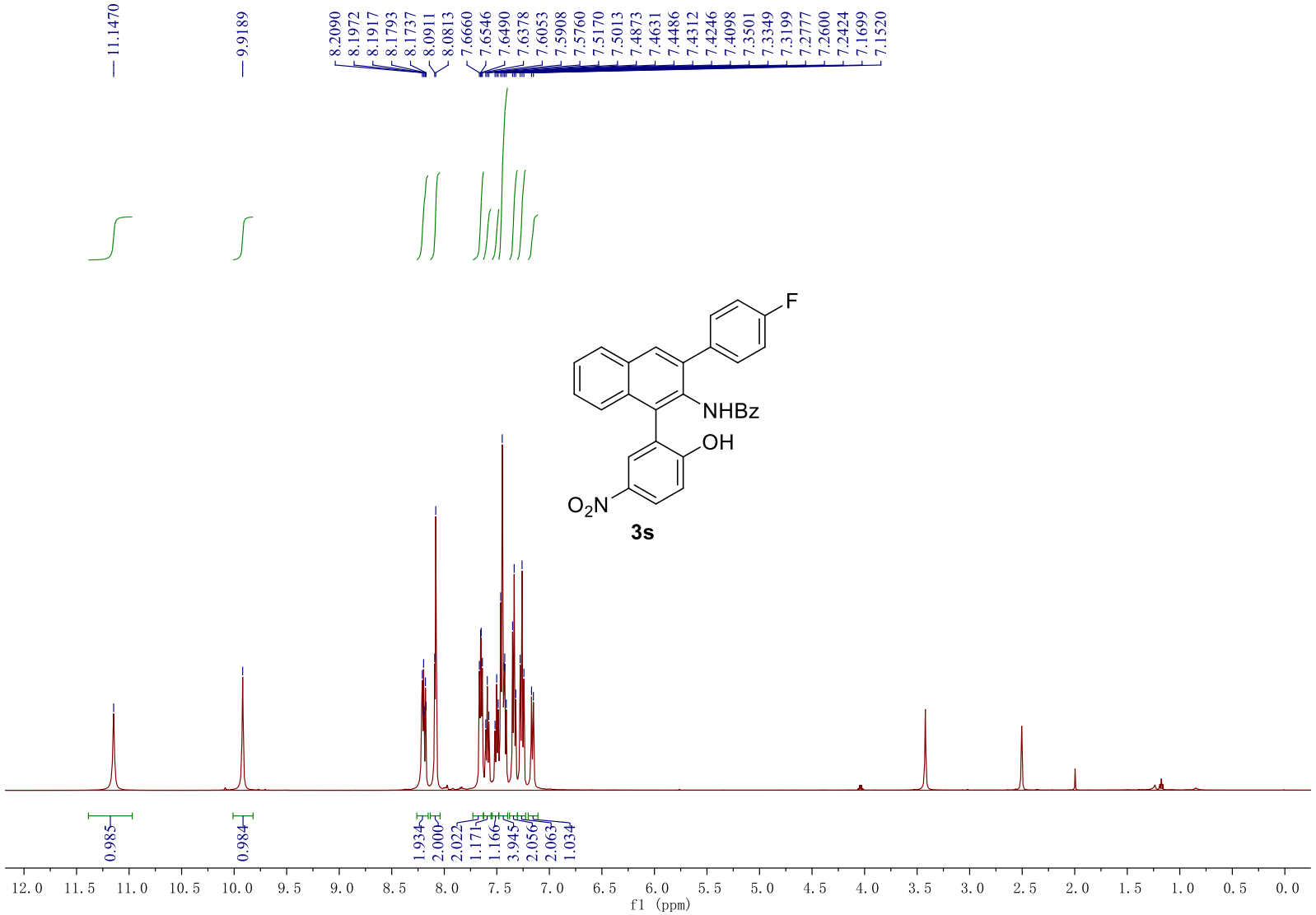
132.12
130.96
129.09
128.62
128.55
128.36
127.92
127.43
127.26
126.97
125.70
125.69
118.17
Ph
NHBz
OH
O2N
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.1737
8.0911
8.0813
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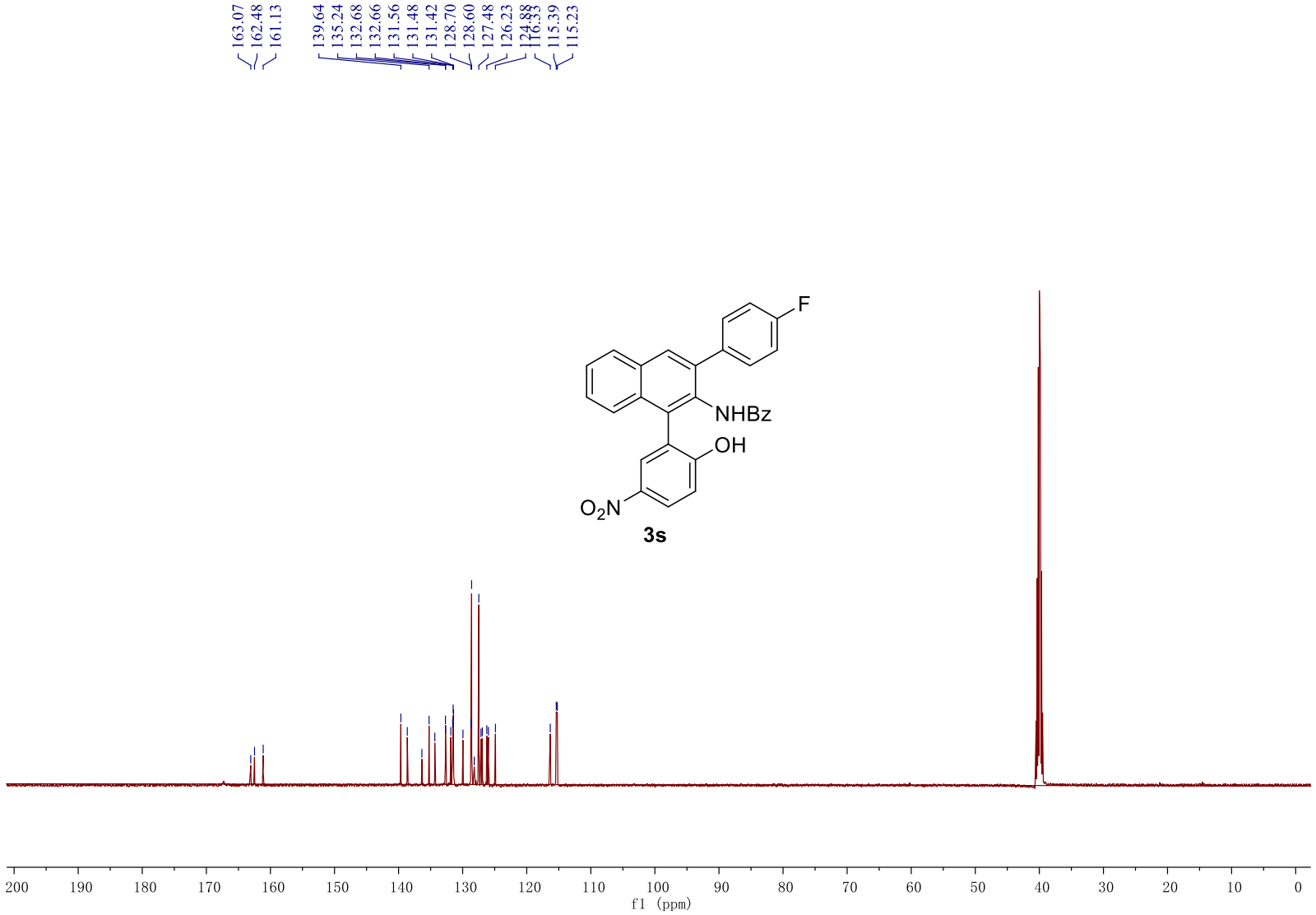
7.6546
7.6490
7.6378
7.6053
7.5908
7.5760
7.5170
7.5013
7.4873
7.4631
7.4486
7.4312
7.4246
7.4098
7.3501
7.3349
7.3199
7.2777
7.2600
7.2424
7.1699
7.1520
F
NHBz
OH
O2N
3s
0.985
0.984
1.934
2.000
2.022
1.171
1.166
3.945
2.056
2.063
1.034
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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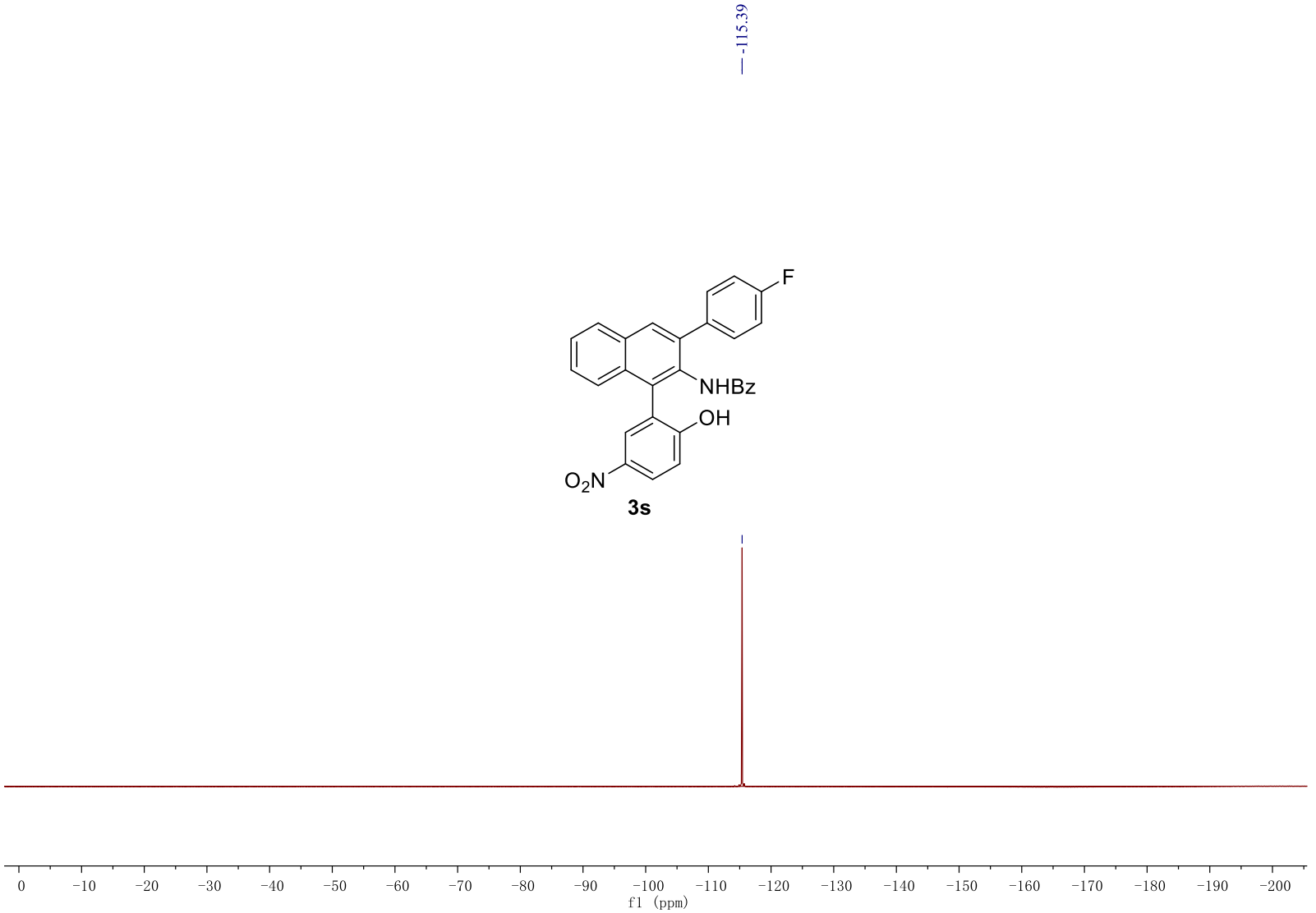
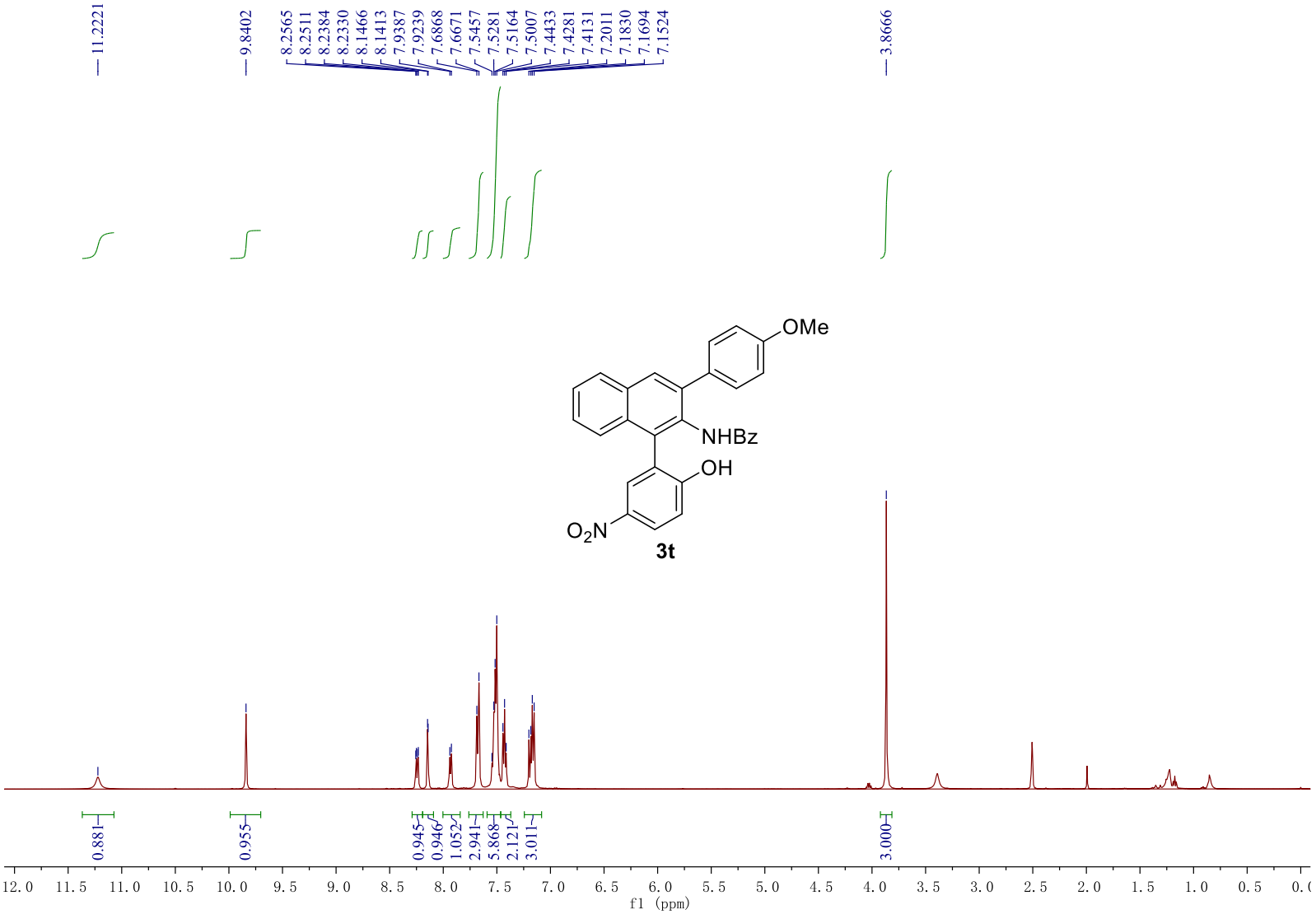
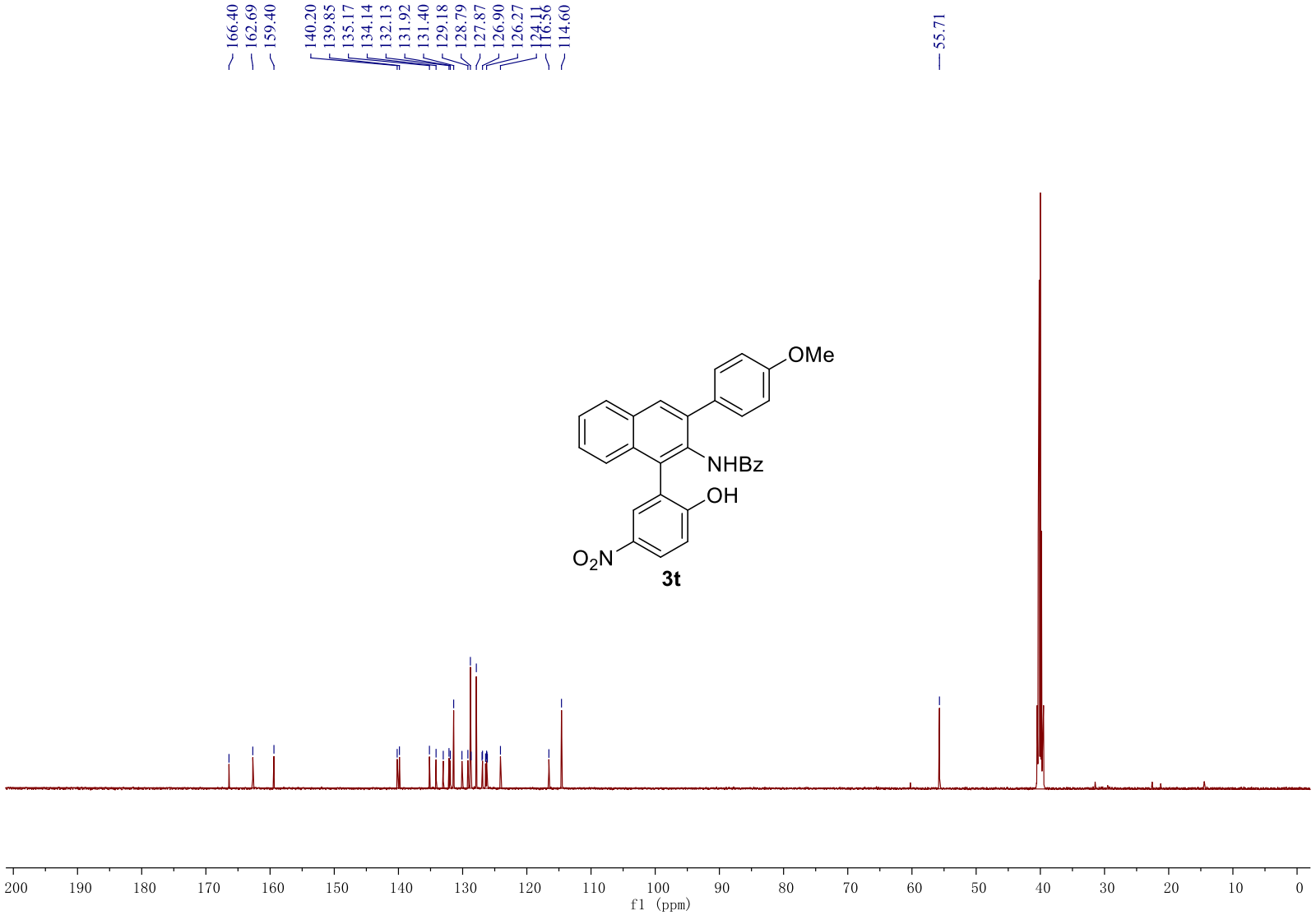
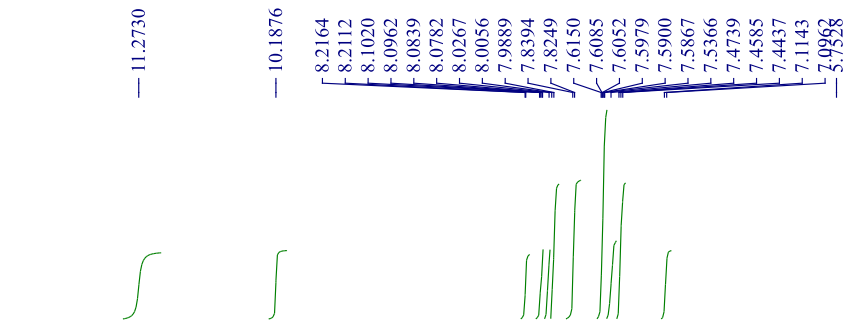
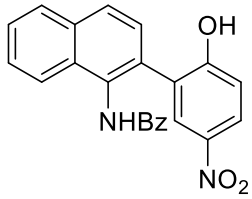
161.13
139.64
135.24
132.68
132.66
131.56
131.48
131.42
128.70
128.60
127.48
126.23
124.88
116.33
115.39
115.23
F
NHBz
OH
O2N
3s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-115.39
F
NHBz
OH
O_2N
3s
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

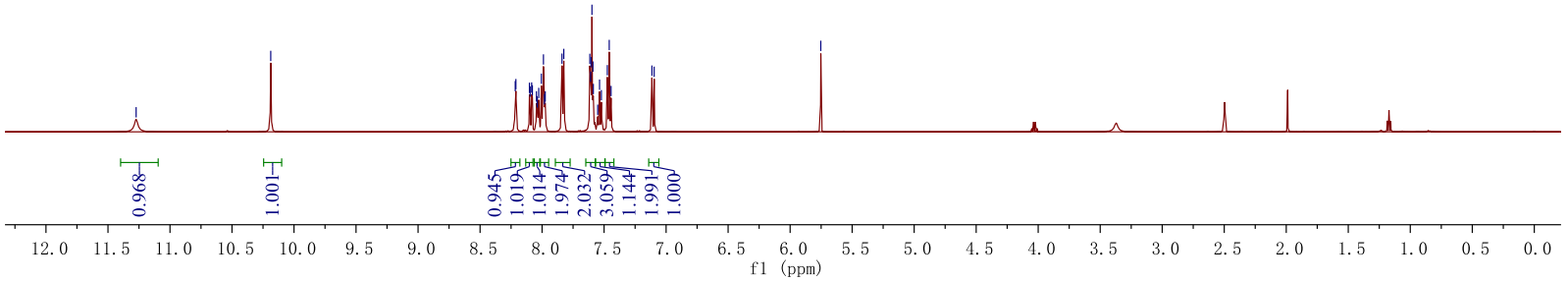

11.2221
9.8402
8.2565
8.2511
8.2384
8.2330
8.1466
8.1413
7.9387
7.9239
7.6868
7.6671
7.5457
7.5281
7.5164
7.5007
7.4433
7.4281
7.4131
7.2011
7.1830
7.1694
7.1524
3.8666
OMe
NHBz
OH
O2N
3t
0.881
0.955
0.945
0.946
1.052
2.941
5.868
2.121
3.011
3.000
f1 (ppm)

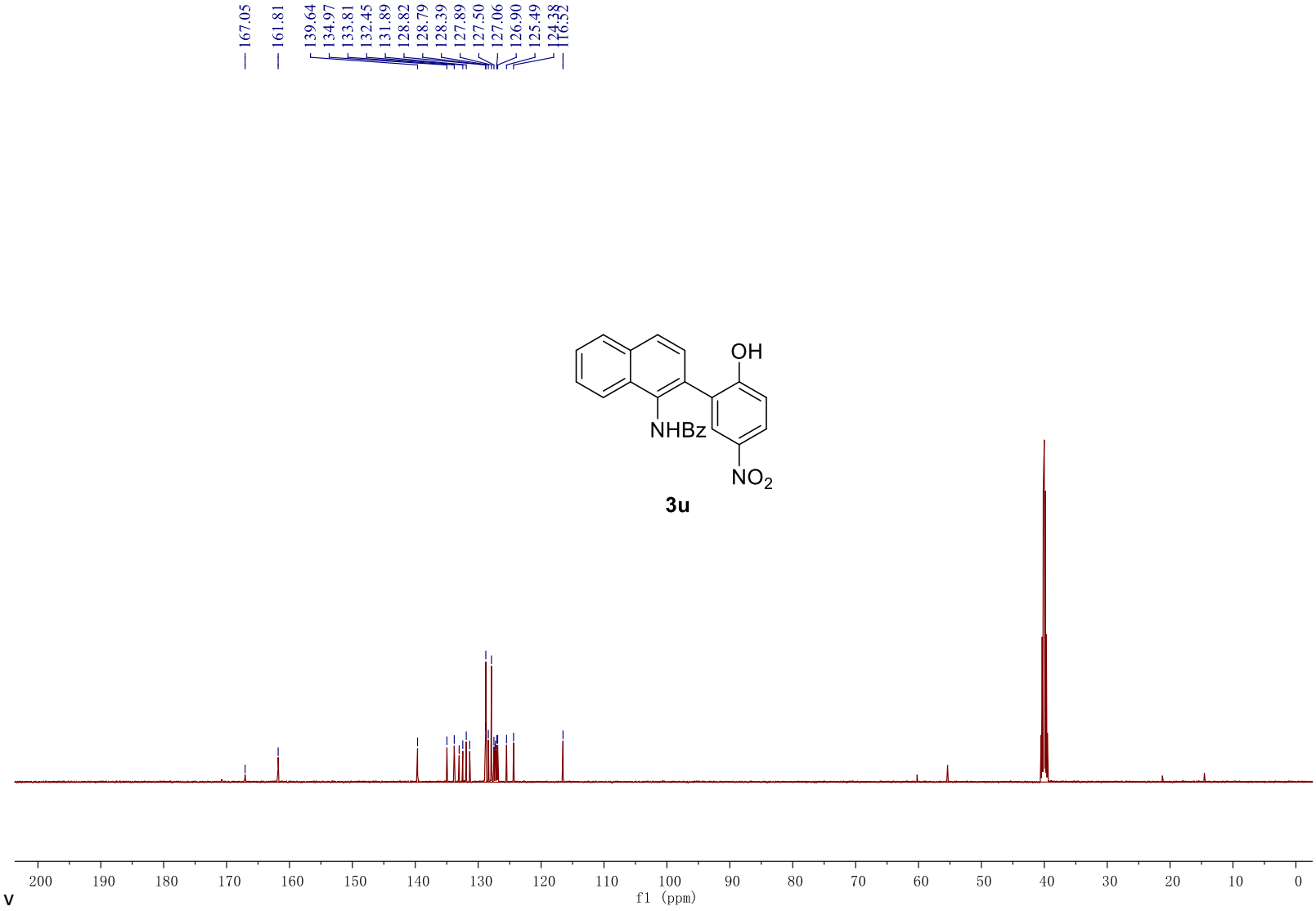

166.40
162.69
159.40
140.20
139.85
135.17
134.14
132.13
131.92
131.40
129.18
128.79
127.87
126.90
126.27
124.11
116.56
114.60
55.71
OMe
NHBz
OH
O2N
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

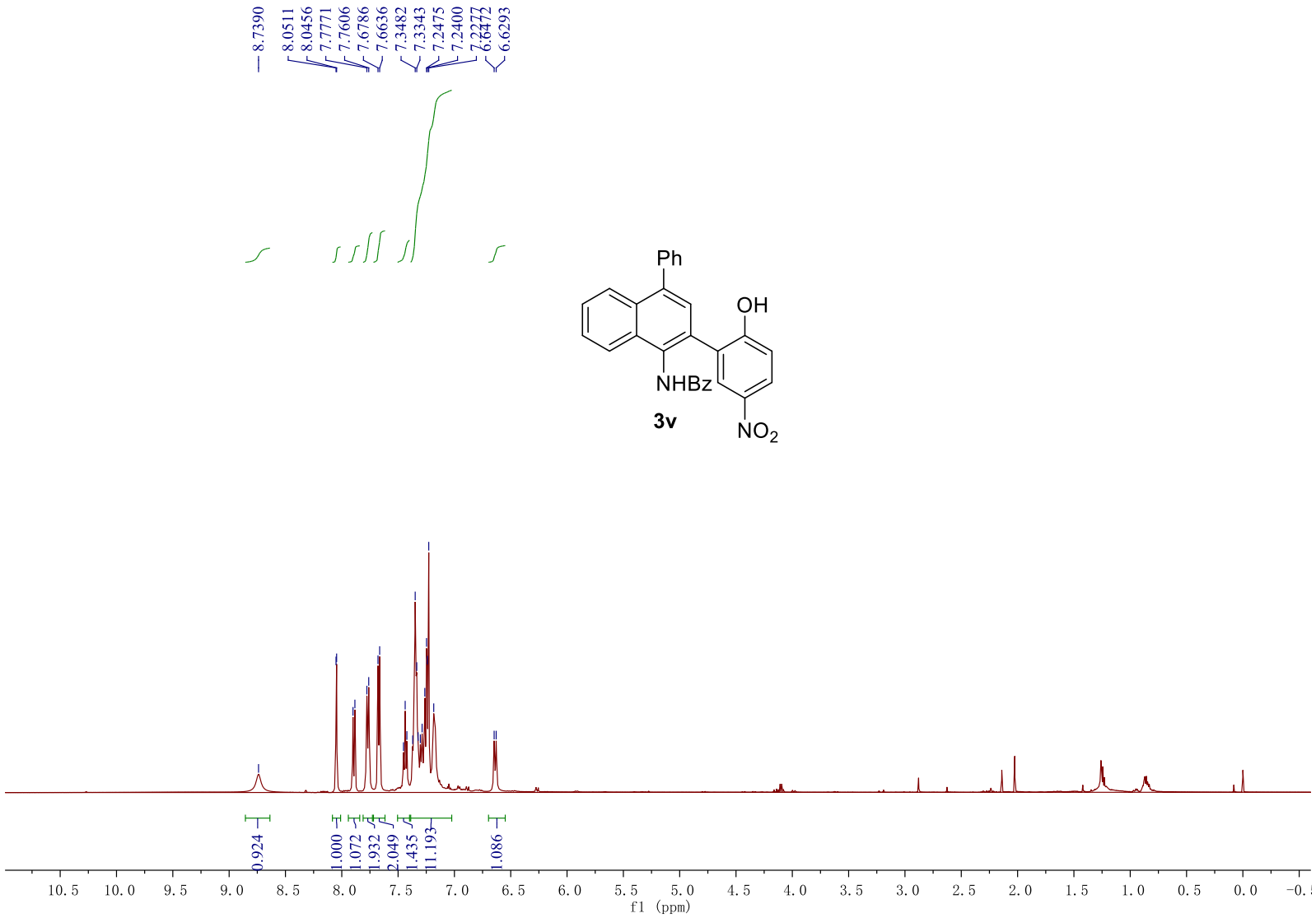

11.2730
10.1876
8.2164
8.2112
8.1020
8.0962
8.0839
8.0782
8.0267
8.0056
7.9889
7.8394
7.8249
7.6150
7.6085
7.6052
7.5979
7.5900
7.5867
7.5366
7.4739
7.4585
7.4437
7.1143
5.7528

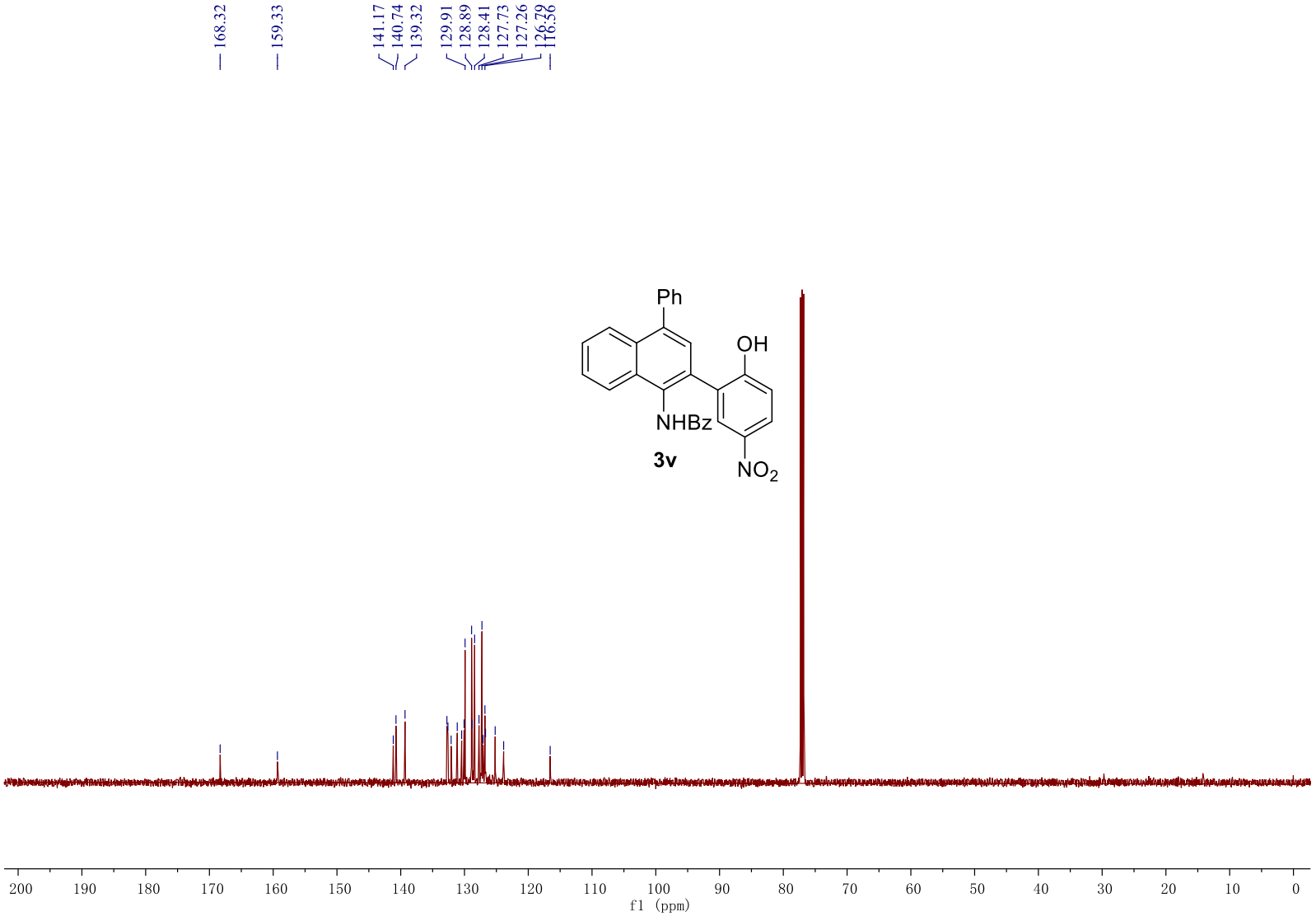

OH
NHBz
NO2

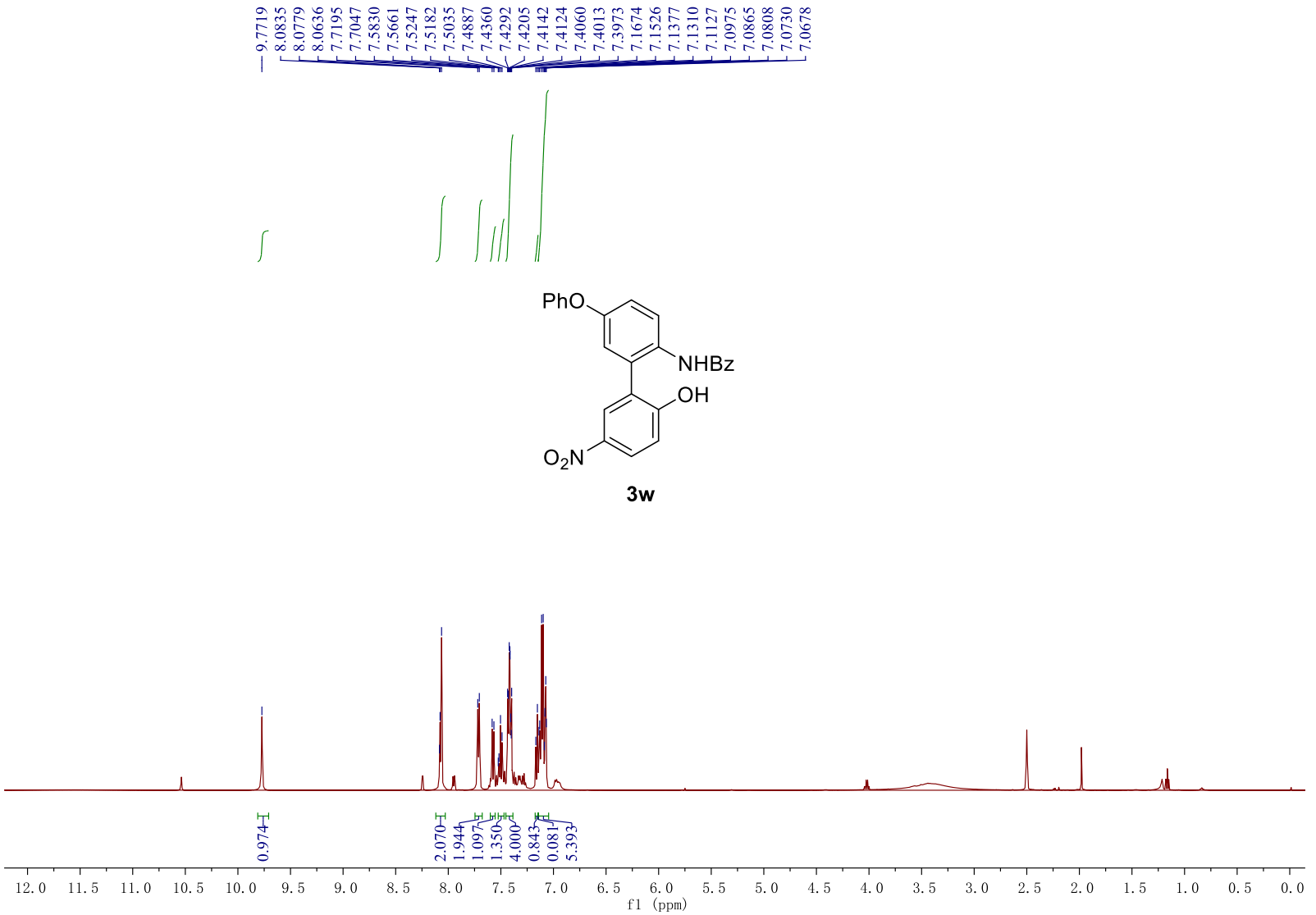
3u

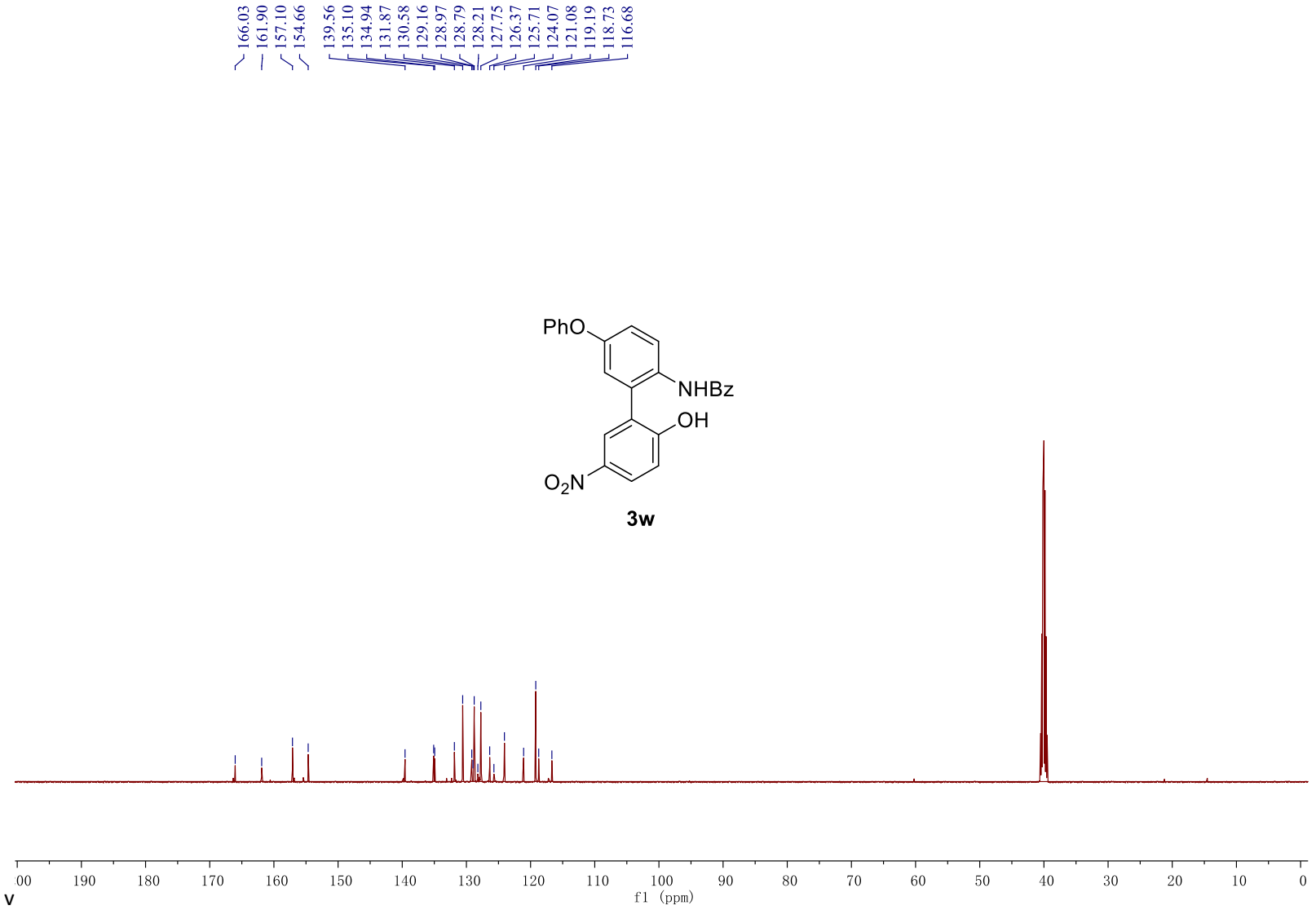

0.968
1.001
0.945
1.019
1.014
1.974
2.032
3.059
1.144
1.991
1.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

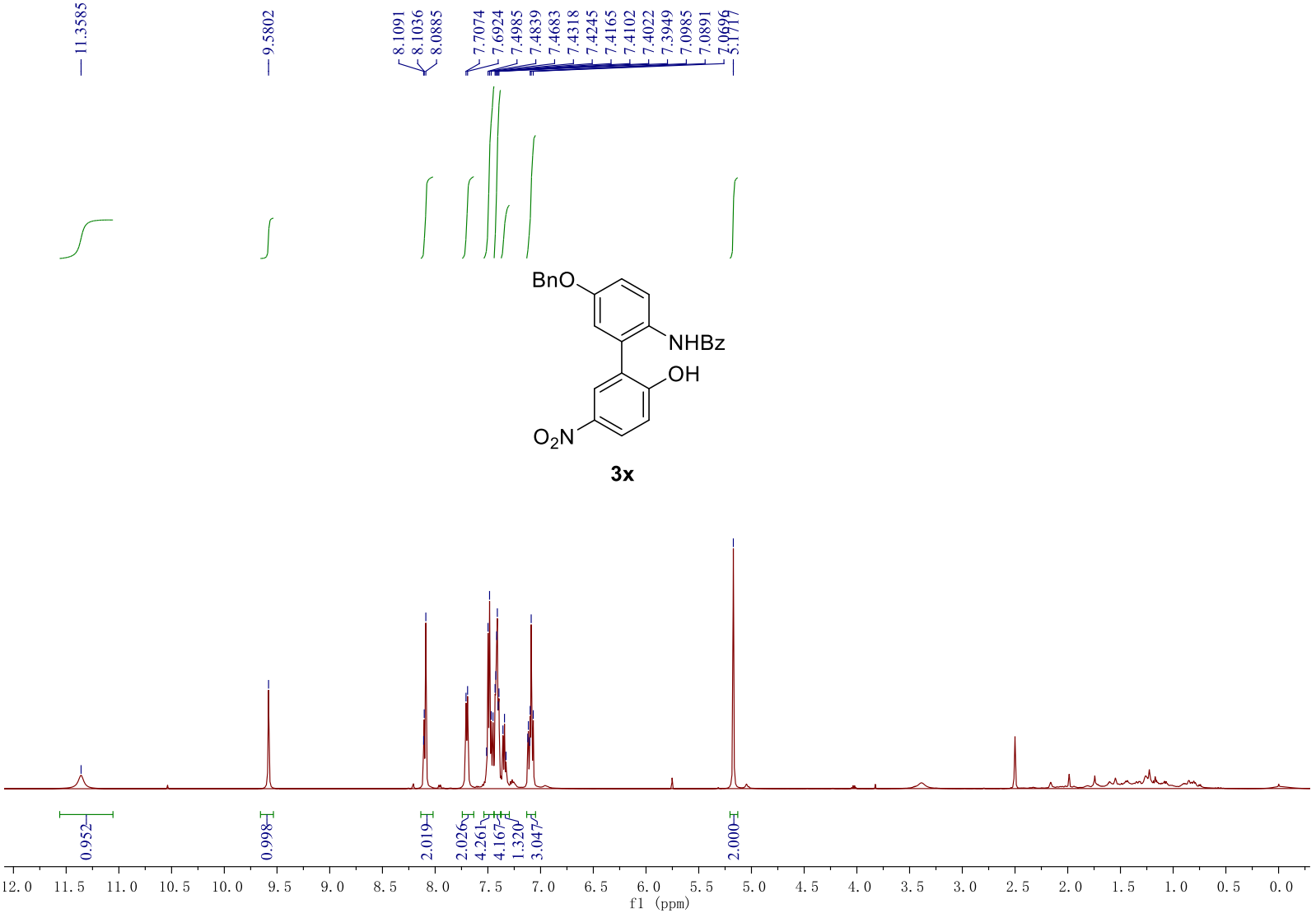

167.05
161.81
139.64
134.97
133.81
132.45
131.89
128.82
128.79
128.39
127.89
127.50
127.06
126.90
125.49
124.38
116.32
OH
NHBz
NO2
3u
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

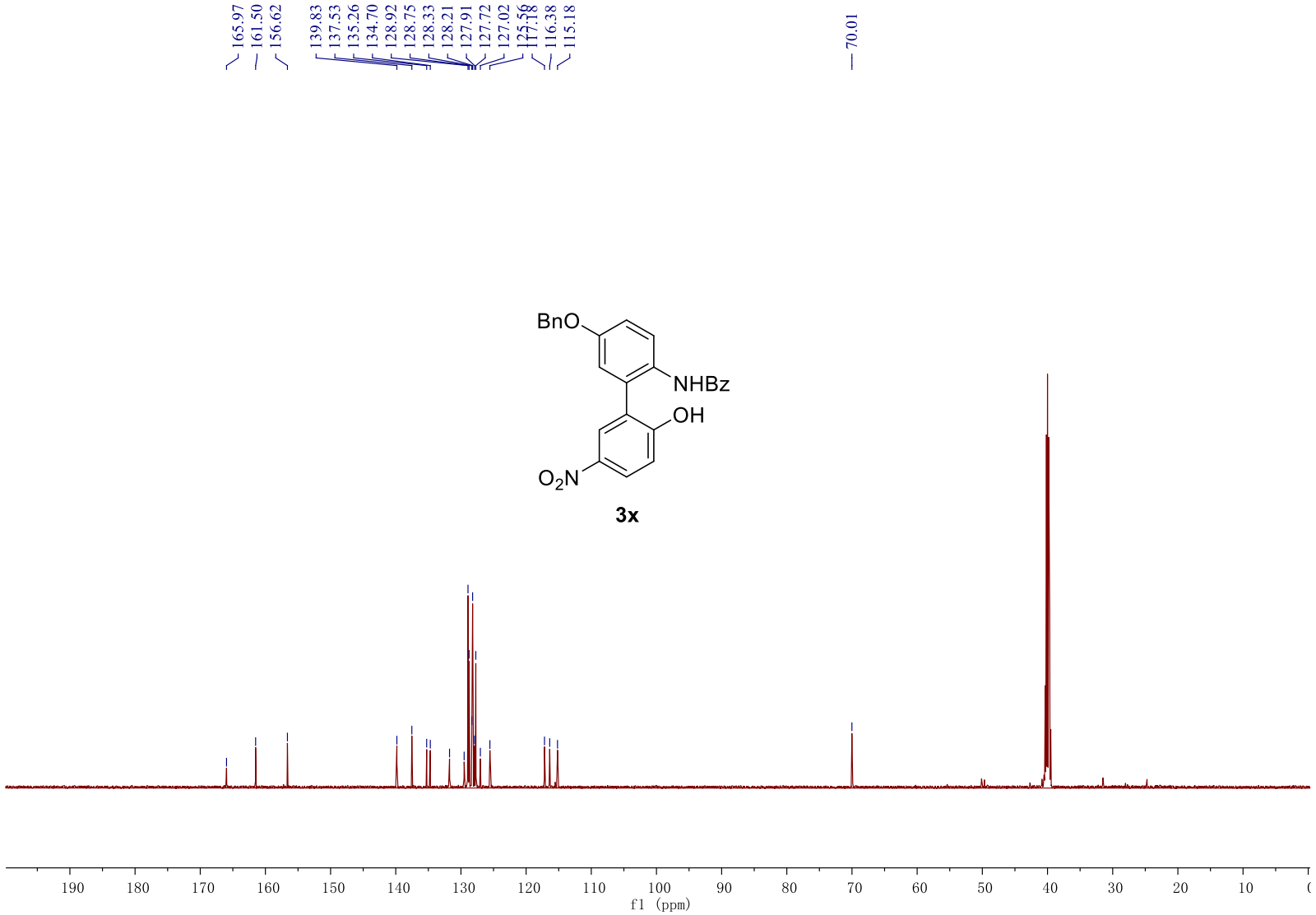

8.7390
8.0511
8.0456
7.7771
7.7606
7.6786
7.6636
7.3482
7.3343
7.2475
7.2400
7.2377
6.6472
6.6293
Ph
OH
NHBz
NO2
3v
0.924
1.000
1.072
1.932
2.049
1.435
11.193
1.086
f1 (ppm)

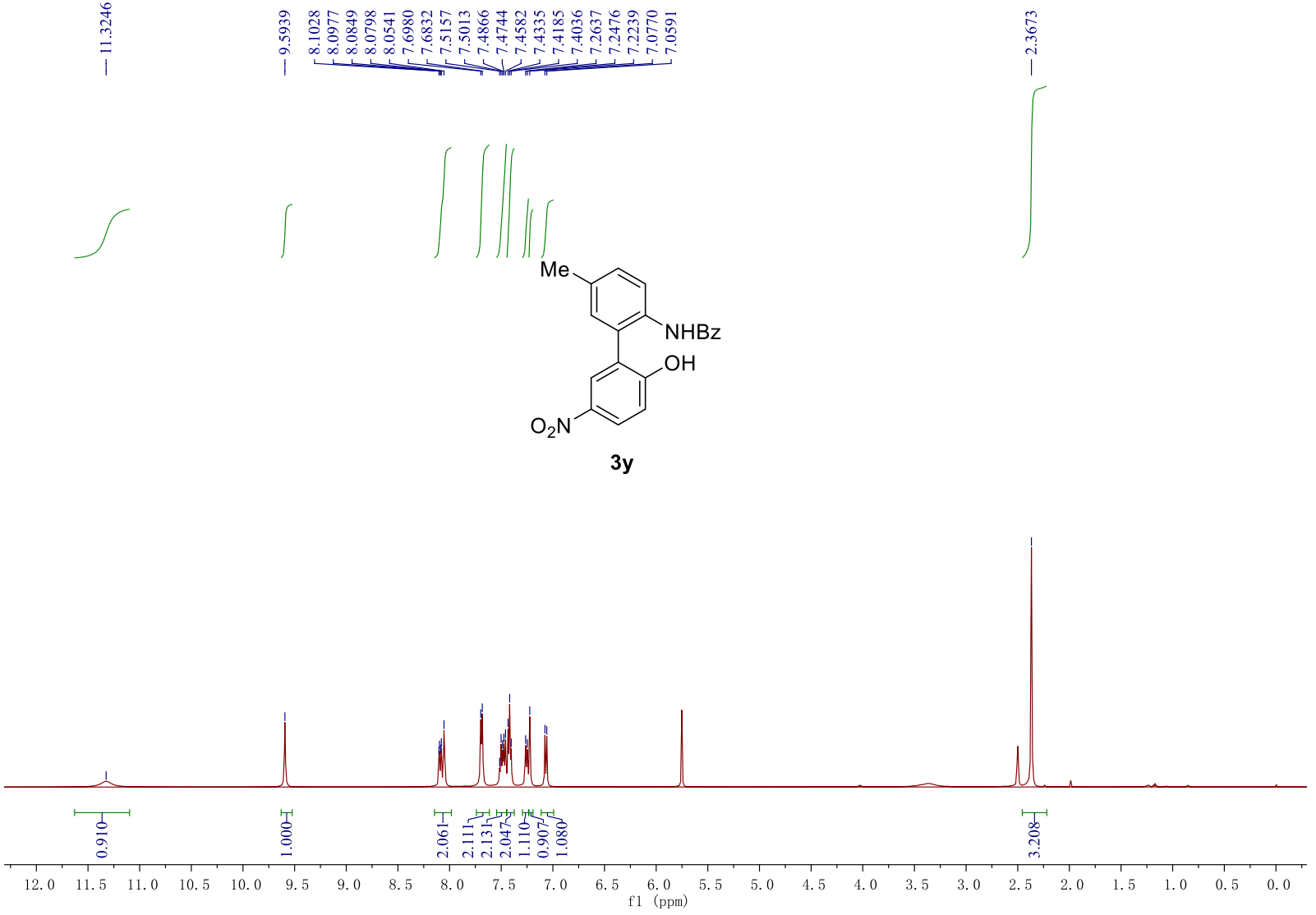

168.32
159.33
141.17
140.74
139.32
129.91
128.89
128.41
127.73
127.26
126.79
116.56
Ph
OH
NHBz
NO2
3v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

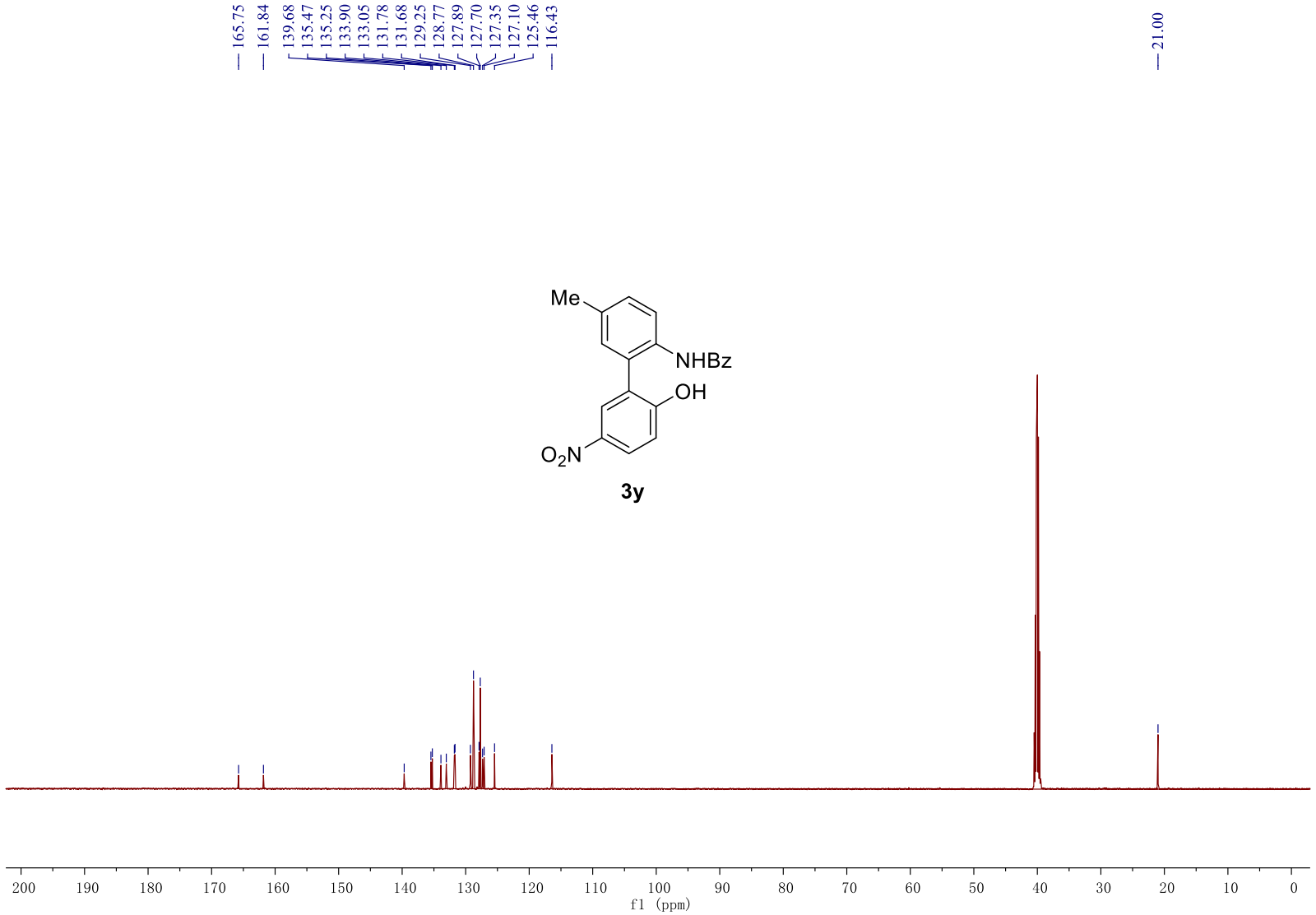

9.7719
8.0835
8.0779
8.0636
7.7195
7.7047
7.5830
7.5661
7.5247
7.5182
7.5035
7.4887
7.4360
7.4292
7.4205
7.4142
7.4124
7.4060
7.4013
7.3973
7.1674
7.1526
7.1377
7.1310
7.1127
7.0975
7.0865
7.0808
7.0730
7.0678
PhO
NHBz
OH
O2N
3w
0.974
2.070
1.944
1.097
1.350
4.000
0.843
0.081
5.393
12.0 11.5 11.0 10.5 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)

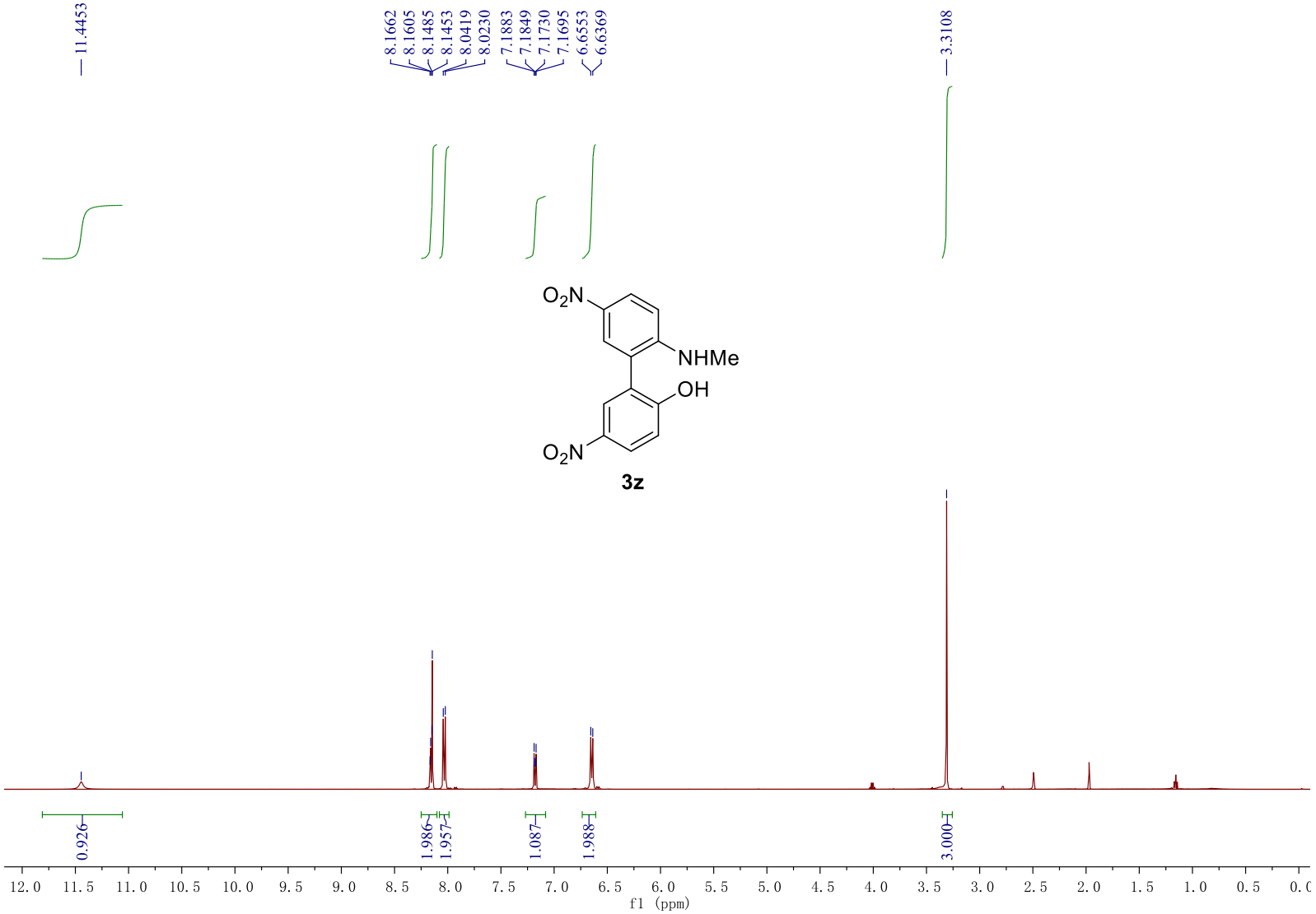

166.03
161.90
157.10
154.66
139.56
135.10
134.94
131.87
130.58
129.16
128.97
128.79
128.21
127.75
126.37
125.71
124.07
121.08
119.19
118.73
116.68
PhO
NHBz
OH
O2N
3w
f1 (ppm)

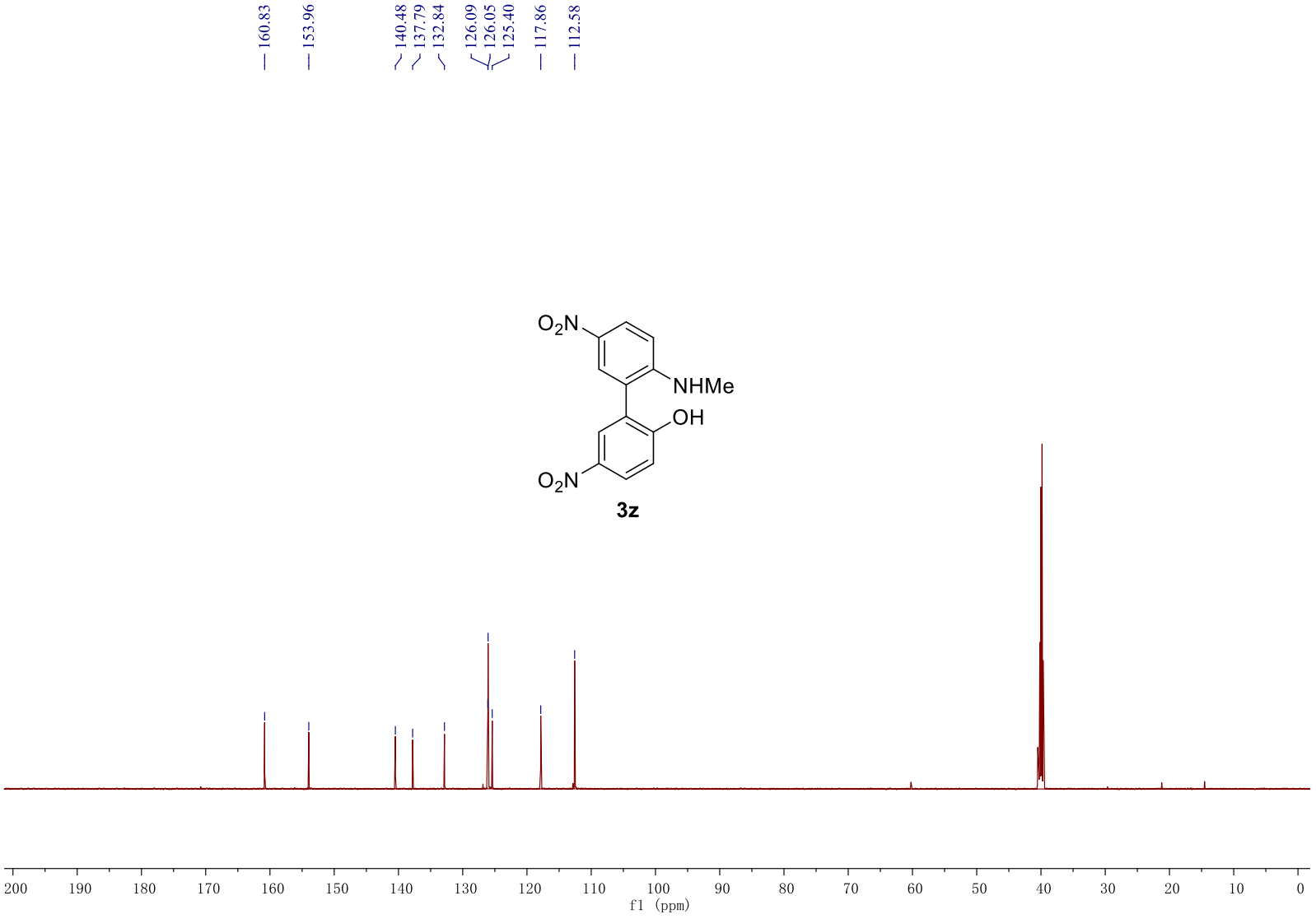

11.3585
9.5802
8.1091
8.1036
8.0885
7.7074
7.6924
7.4985
7.4839
7.4683
7.4318
7.4245
7.4165
7.4102
7.4022
7.3949
7.0985
7.0891
7.0696
5.1717
BnO
NHBz
OH
O2N
3x
0.952
0.998
2.019
2.026
4.261
4.167
1.320
3.047
2.000
f1 (ppm)

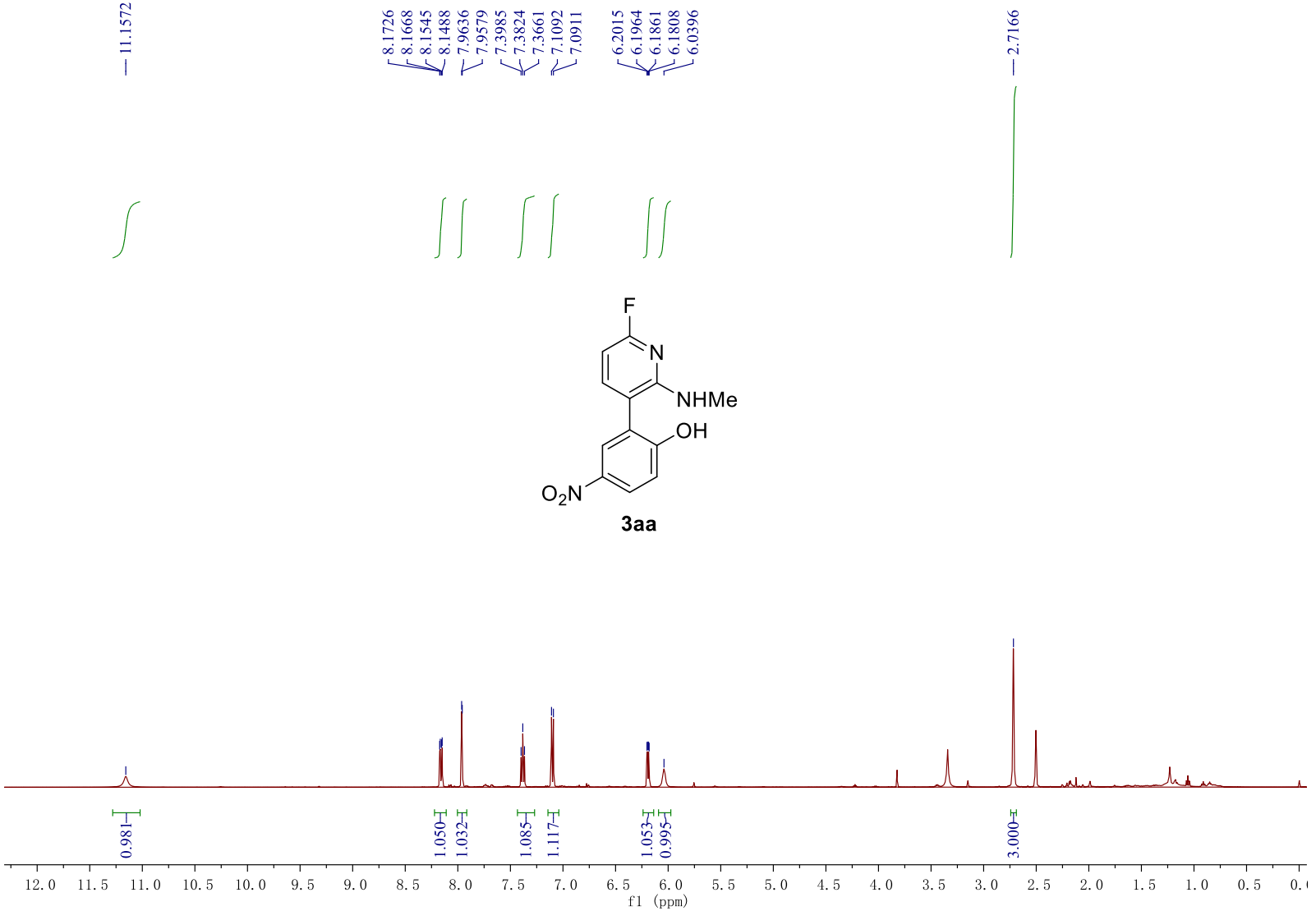

165.97
161.50
156.62
139.83
137.53
135.26
134.70
128.92
128.75
128.33
128.21
127.91
127.72
127.02
125.56
117.18
116.38
115.18
70.01
BnO
NHBz
OH
O2N
3x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

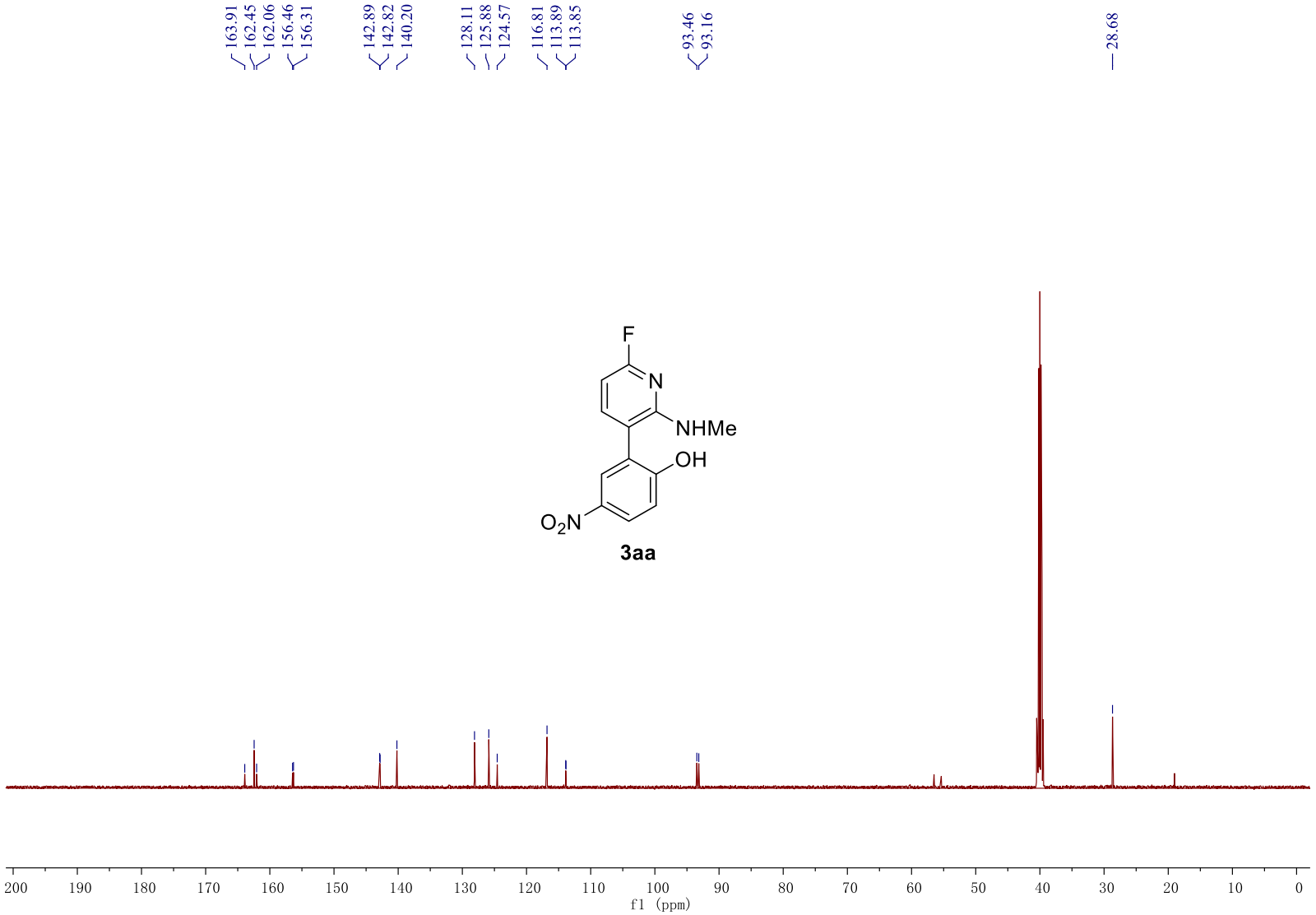

11.3246
9.5939
8.1028
8.0977
8.0849
8.0798
8.0541
7.6980
7.6832
7.5157
7.5013
7.4866
7.4744
7.4582
7.4335
7.4185
7.4036
7.2637
7.2476
7.2239
7.0770
7.0591
2.3673
Me
NHBz
OH
O2N
3y
0.910
1.000
2.061
2.111
2.131
2.047
1.110
0.907
1.080
3.208
f1 (ppm)

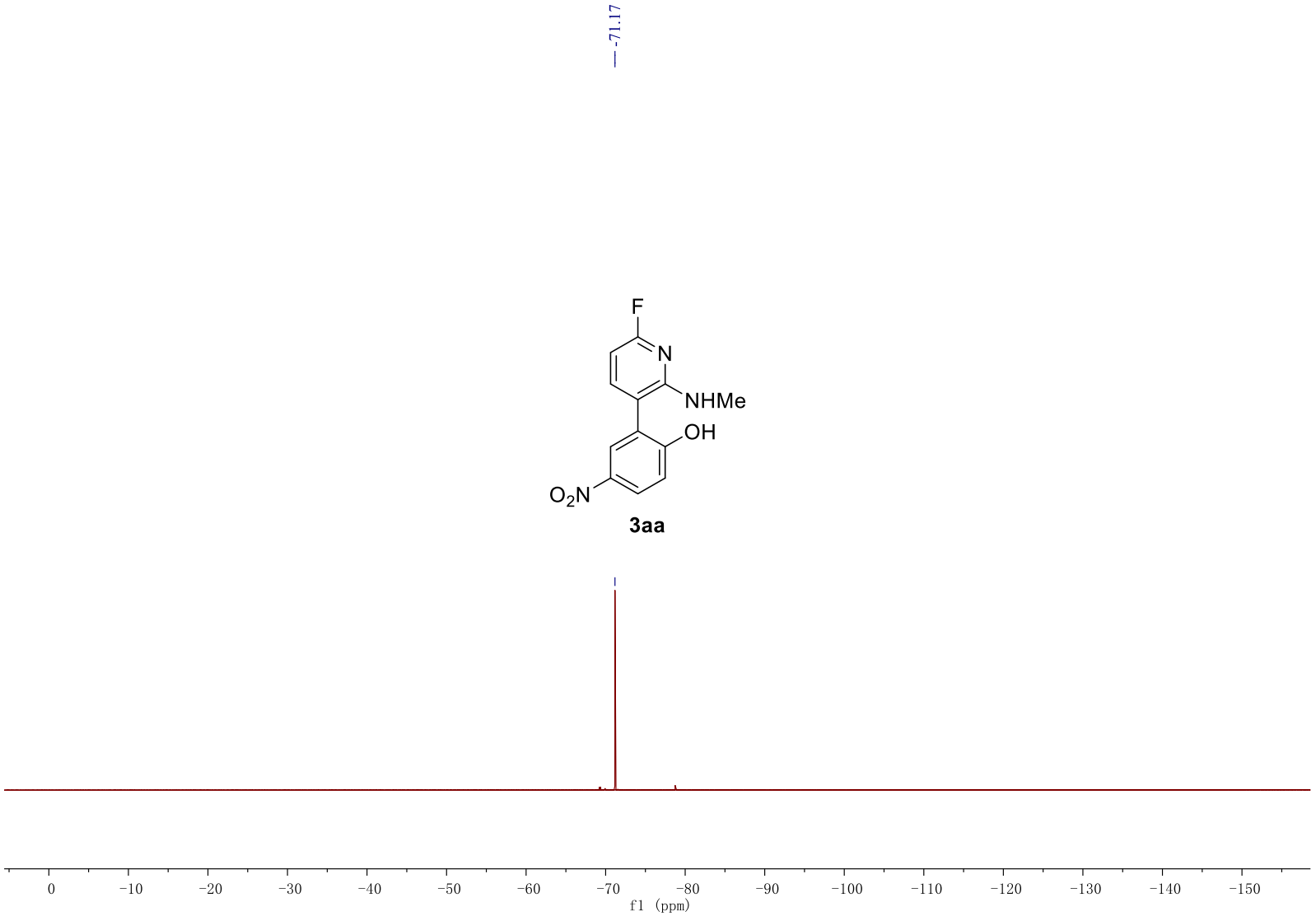

165.75
161.84
139.68
135.47
135.25
133.90
133.05
131.78
131.68
129.25
128.77
127.89
127.70
127.35
127.10
125.46
116.43
21.00
Me
NHBz
OH
O2N
3y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

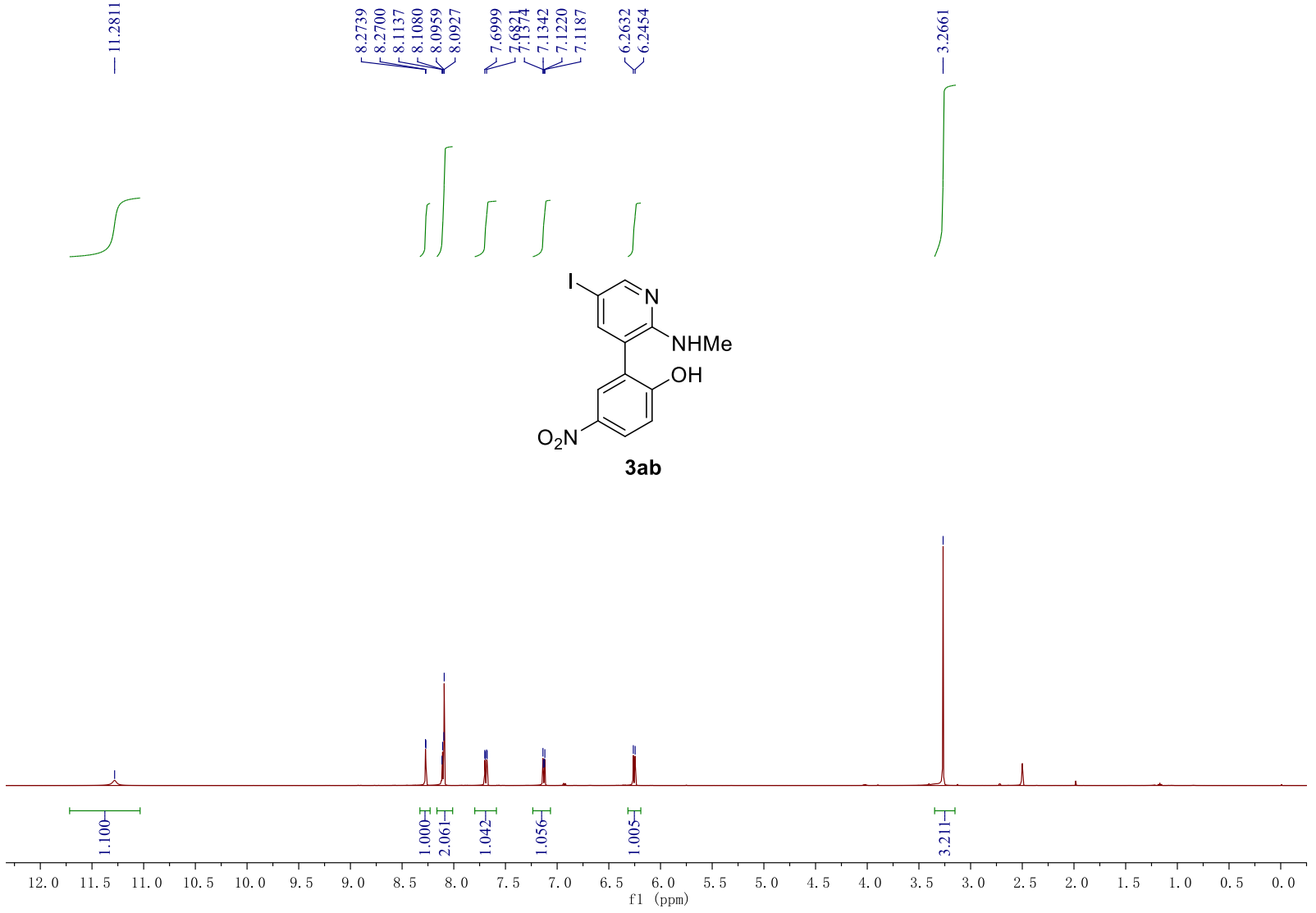

11.4453
8.1662
8.1605
8.1485
8.1453
8.0419
8.0230
7.1883
7.1849
7.1730
7.1695
6.6553
6.6369
3.3108
O2N
NHMe
OH
O2N
3z
0.926
1.986
1.957
1.087
1.988
3.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.83
153.96
140.48
137.79
132.84
126.09
126.05
125.40
117.86
112.58
O2N
NHMe
OH
O2N
3z
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.1572
8.1726
8.1668
8.1545
8.1488
7.9636
7.9579
7.3985
7.3824
7.3661
7.1092
7.0911
6.2015
6.1964
6.1861
6.1808
6.0396
2.7166
F
N
NHMe
OH
O2N
3aa
0.981
1.050
1.032
1.085
1.117
1.053
0.995
3.000
f1 (ppm)


163.91
162.45
162.06
156.46
156.31
142.89
142.82
140.20
128.11
125.88
124.57
116.81
113.89
113.85
93.46
93.16
28.68
F
N
NHMe
OH
O2N
3aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-71.17
F
N
NHMe
OH
O2N
3aa
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)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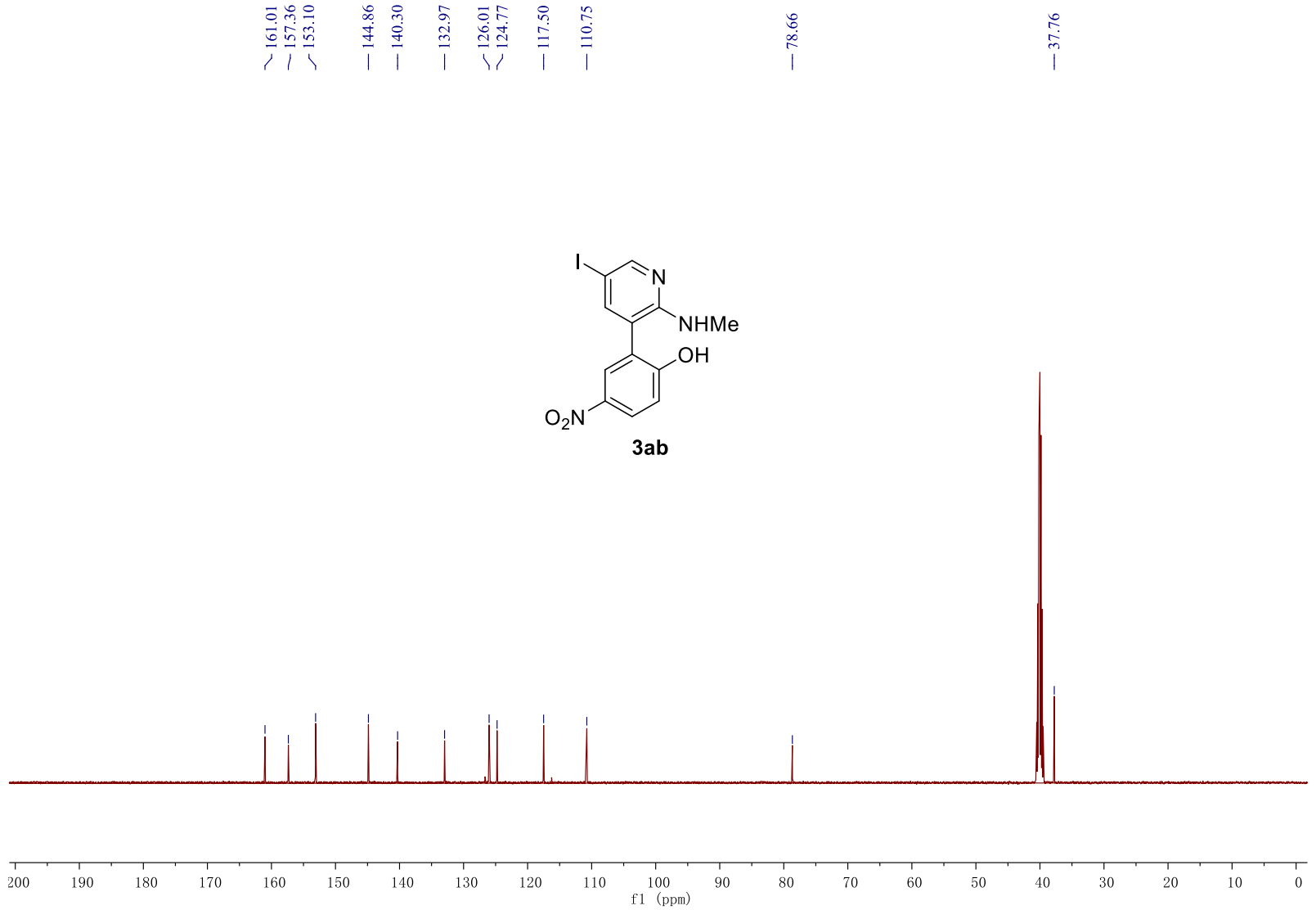
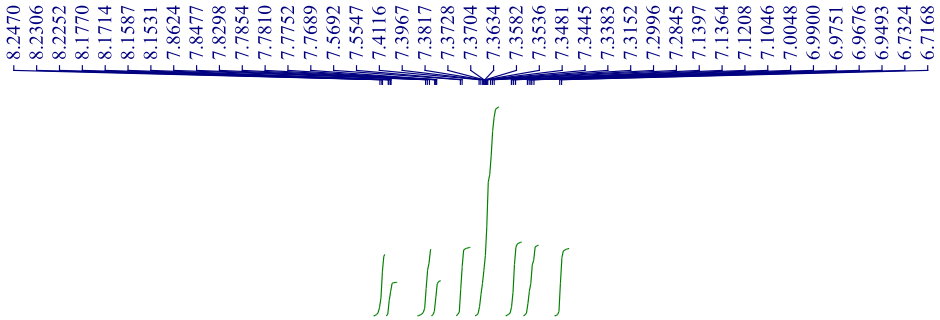
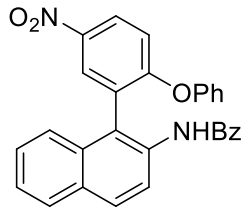
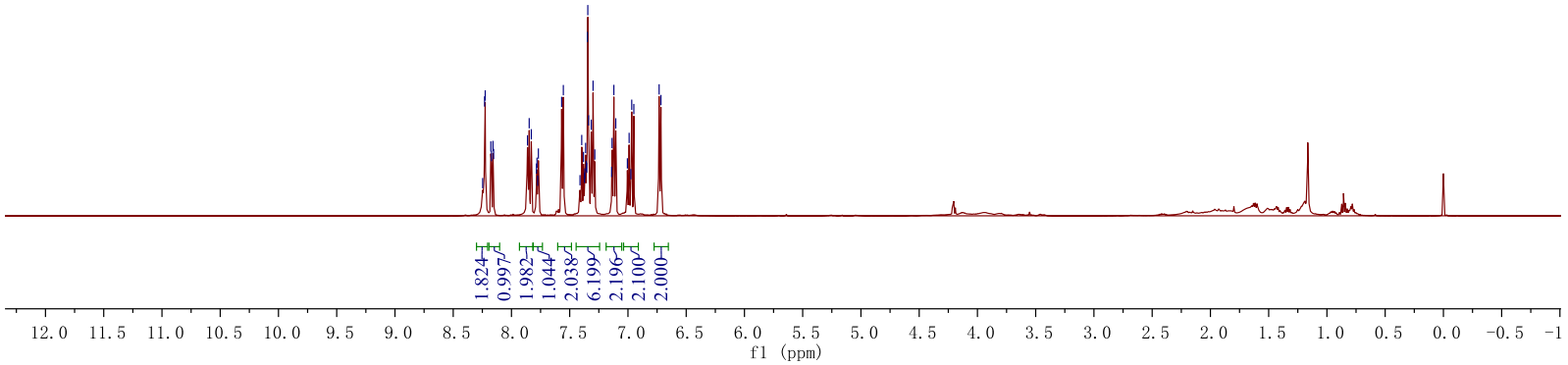
8.2739
8.2700
8.1137
8.1080
8.0959
8.0927
7.6999
7.6821
7.1374
7.1342
7.1220
7.1187
6.2632
6.2454
3.2661
I
N
NHMe
OH
O2N
3ab
1.100
1.000
2.061
1.042
1.056
1.005
3.211
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.01
157.36
153.10
144.86
140.30
132.97
126.01
124.77
117.50
110.75
78.66
37.76
I
N
NHMe
OH
O2N
3ab
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

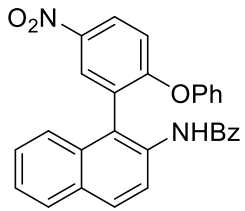

8.2470
8.2306
8.2252
8.1770
8.1714
8.1587
8.1531
7.8624
7.8477
7.8298
7.7854
7.7810
7.7752
7.7689
7.5692
7.5547
7.4116
7.3967
7.3817
7.3728
7.3704
7.3634
7.3582
7.3536
7.3481
7.3445
7.3383
7.3152
7.2996
7.2845
7.1397
7.1364
7.1208
7.1046
7.0048
6.9900
6.9751
6.9676
6.9493
6.7324
6.7168


O2N
OPh
NHBz

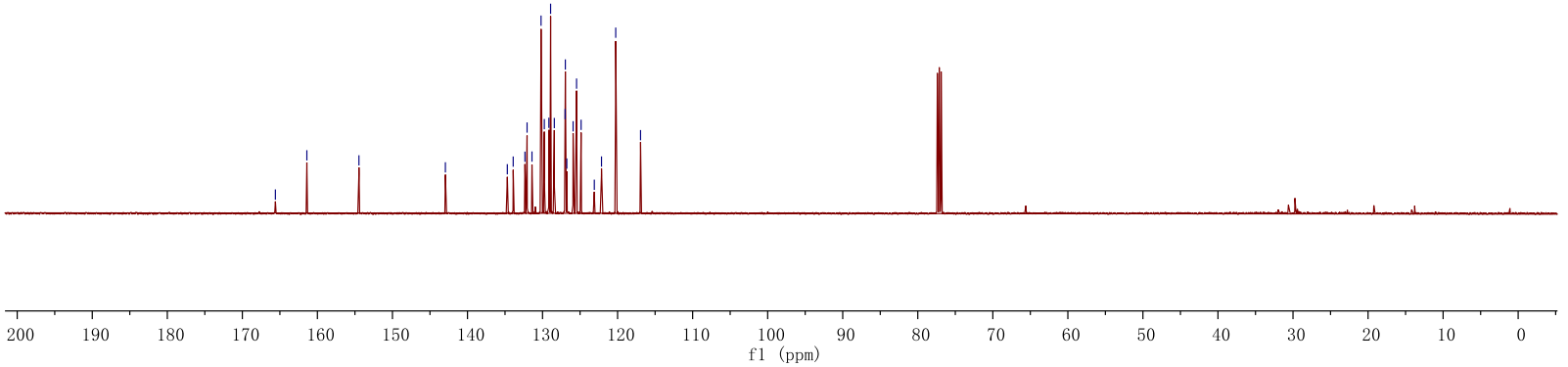
4

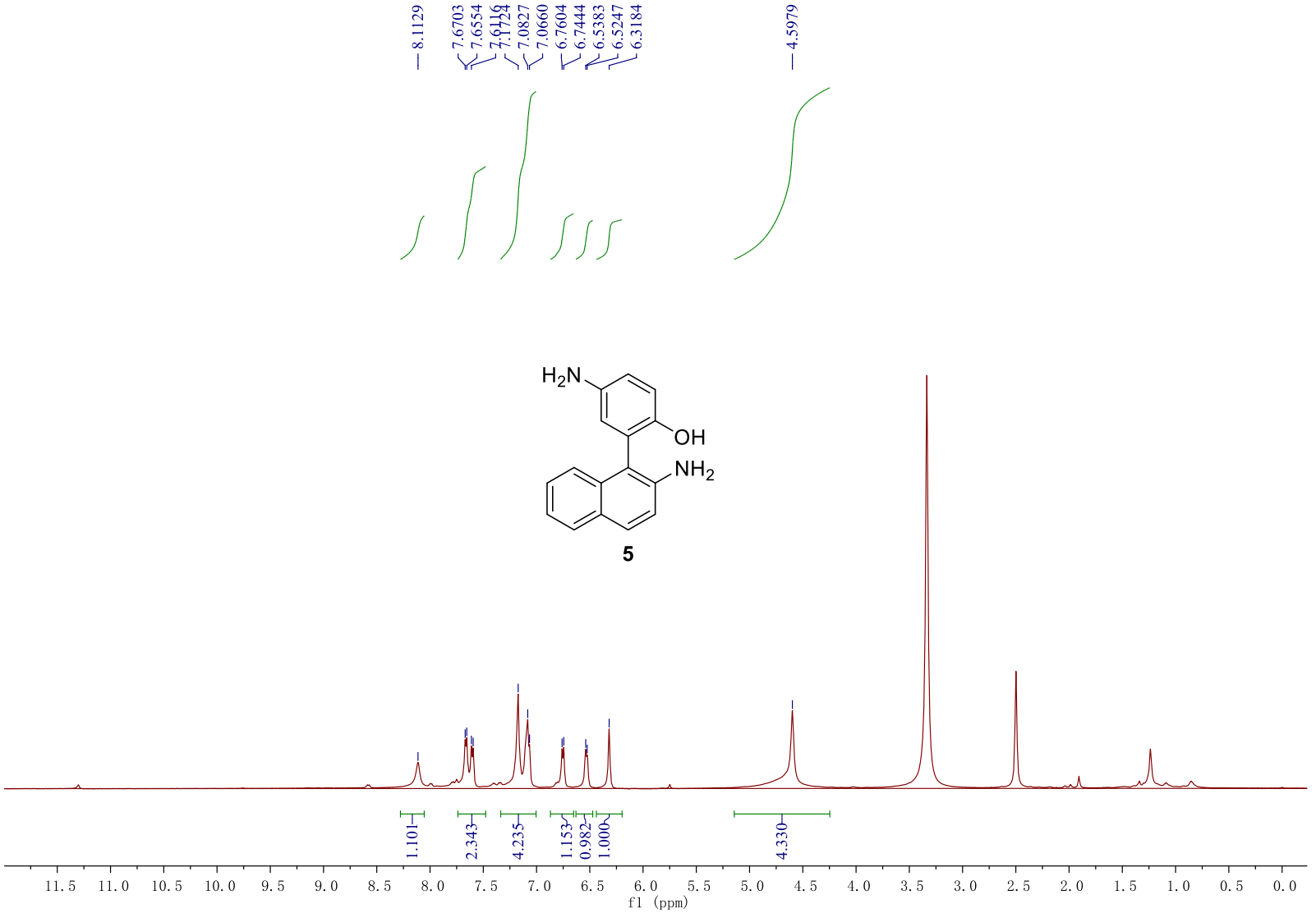

1.824
0.997
1.982
1.044
2.038
6.199
2.196
2.100
2.000
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

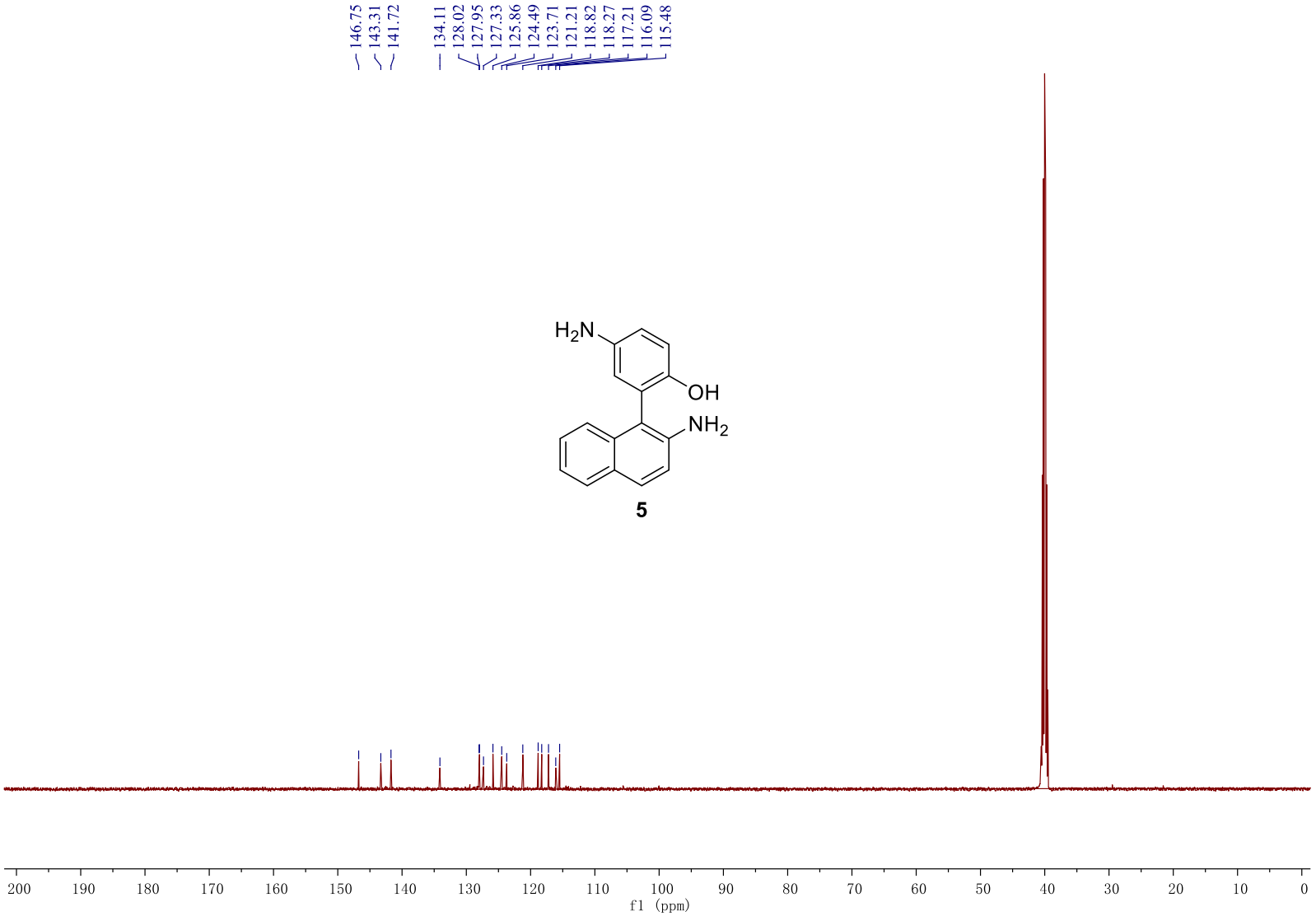

165.60
161.40
154.46
142.94
134.69
133.91
132.34
132.06
131.41
130.20
129.76
129.16
128.92
128.43
126.99
126.96
126.77
125.93
125.47
124.86
123.10
122.14
120.25
116.94


O2N
OPh
NHBz

4


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.1129
7.6703
7.6554
7.6116
7.1724
7.0827
7.0660
6.7604
6.7444
6.5383
6.5247
6.3184
4.5979
H2N
OH
NH2
5
1.101
2.343
4.235
1.153
0.982
1.000
4.330
11.5 11.0 10.5 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)


146.75
143.31
141.72
134.11
128.02
127.95
127.33
125.86
124.49
123.71
121.21
118.82
118.27
117.21
116.09
115.48
H2N
OH
NH2
5
200
190
180
170
160
150
140
130
120
110
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90
80
70
60
50
40
30
20
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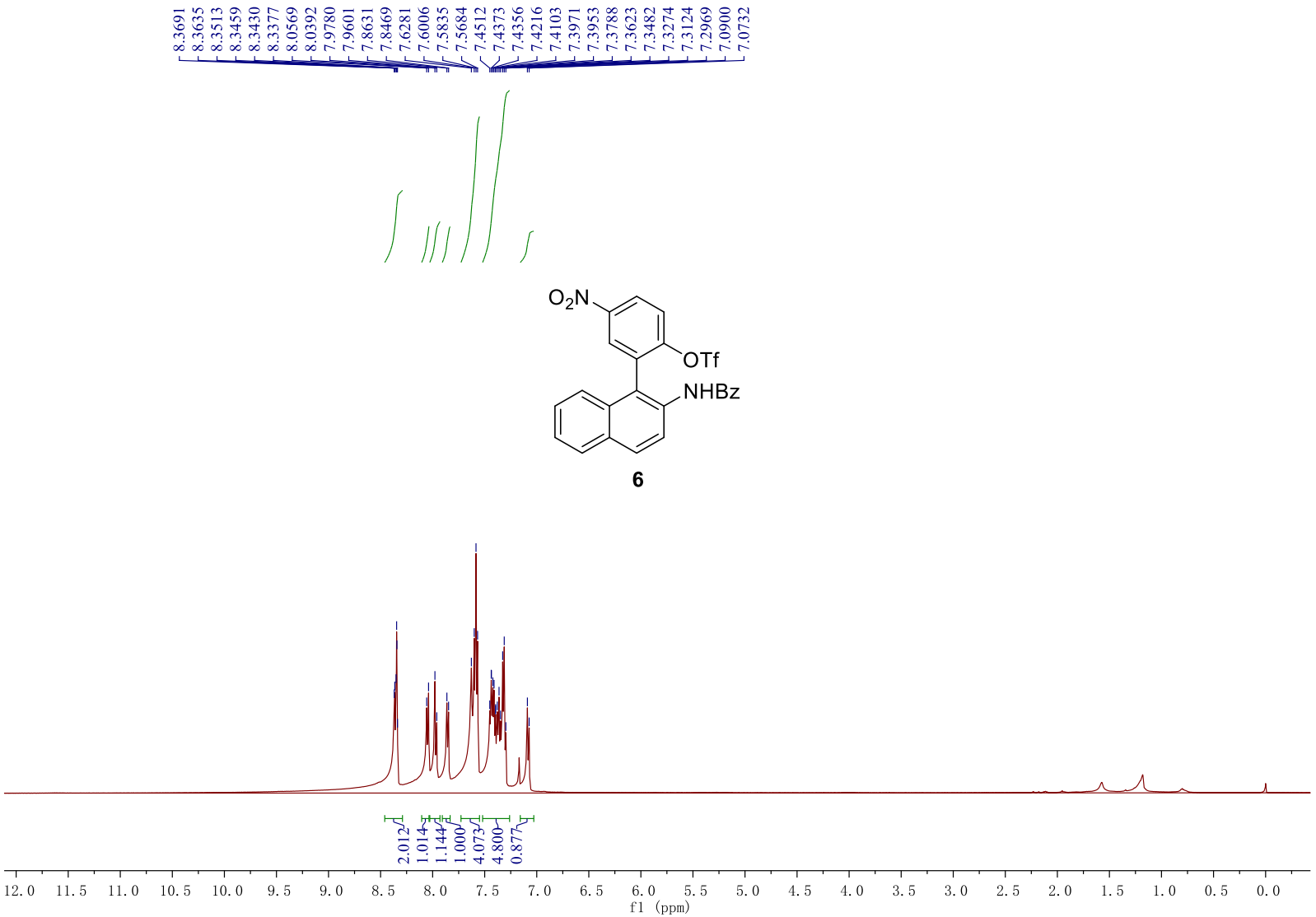
0
f1 (ppm)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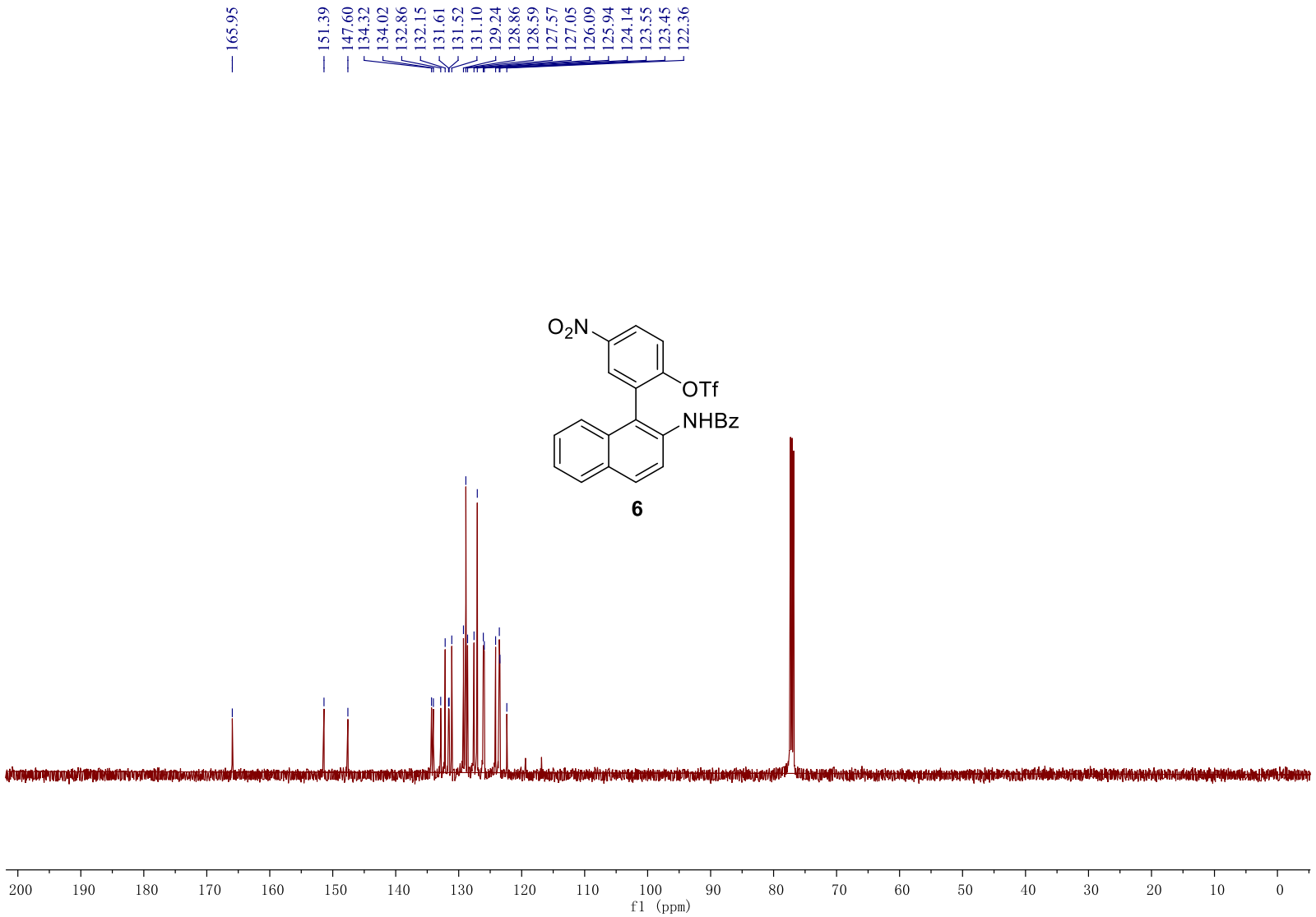
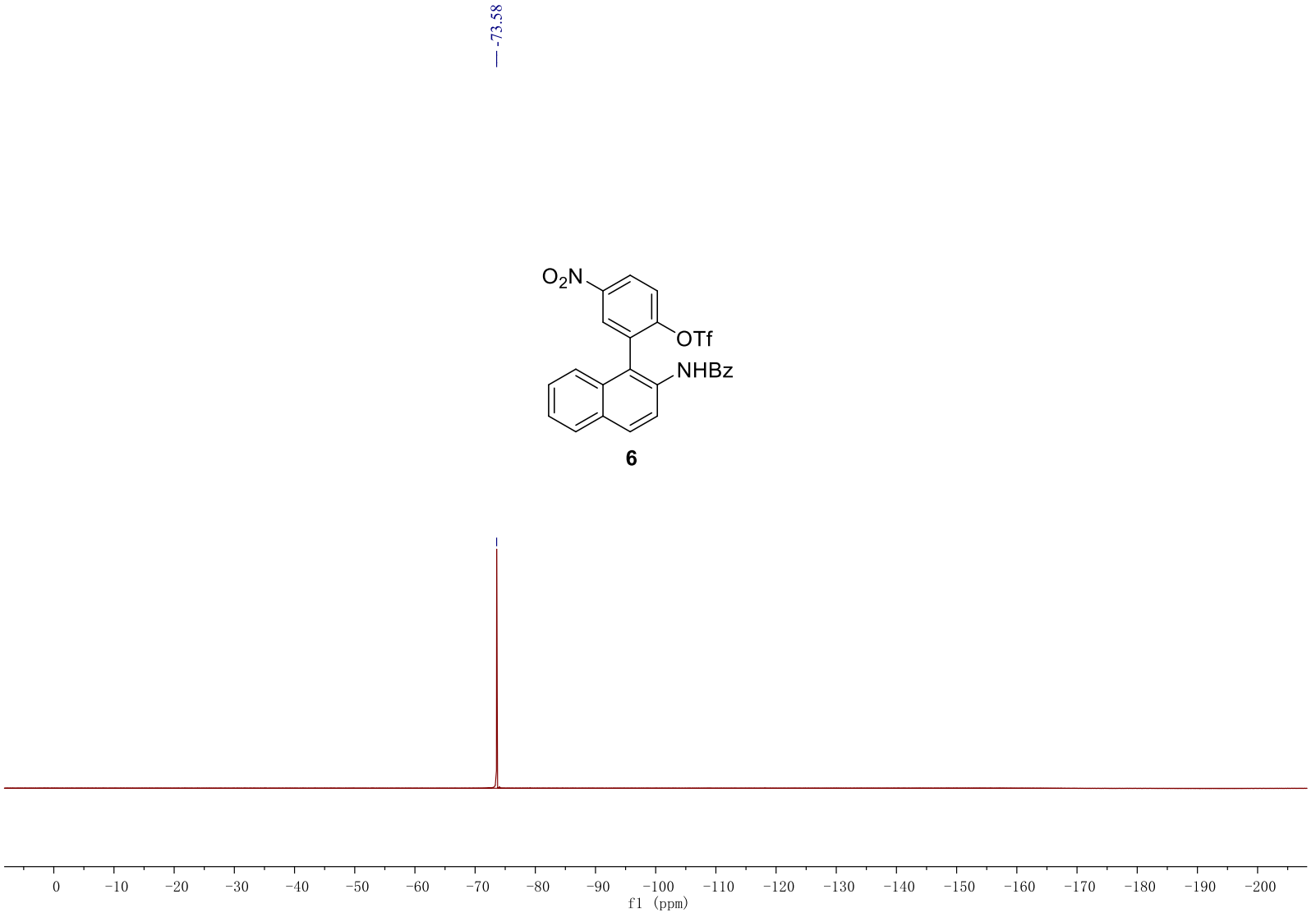
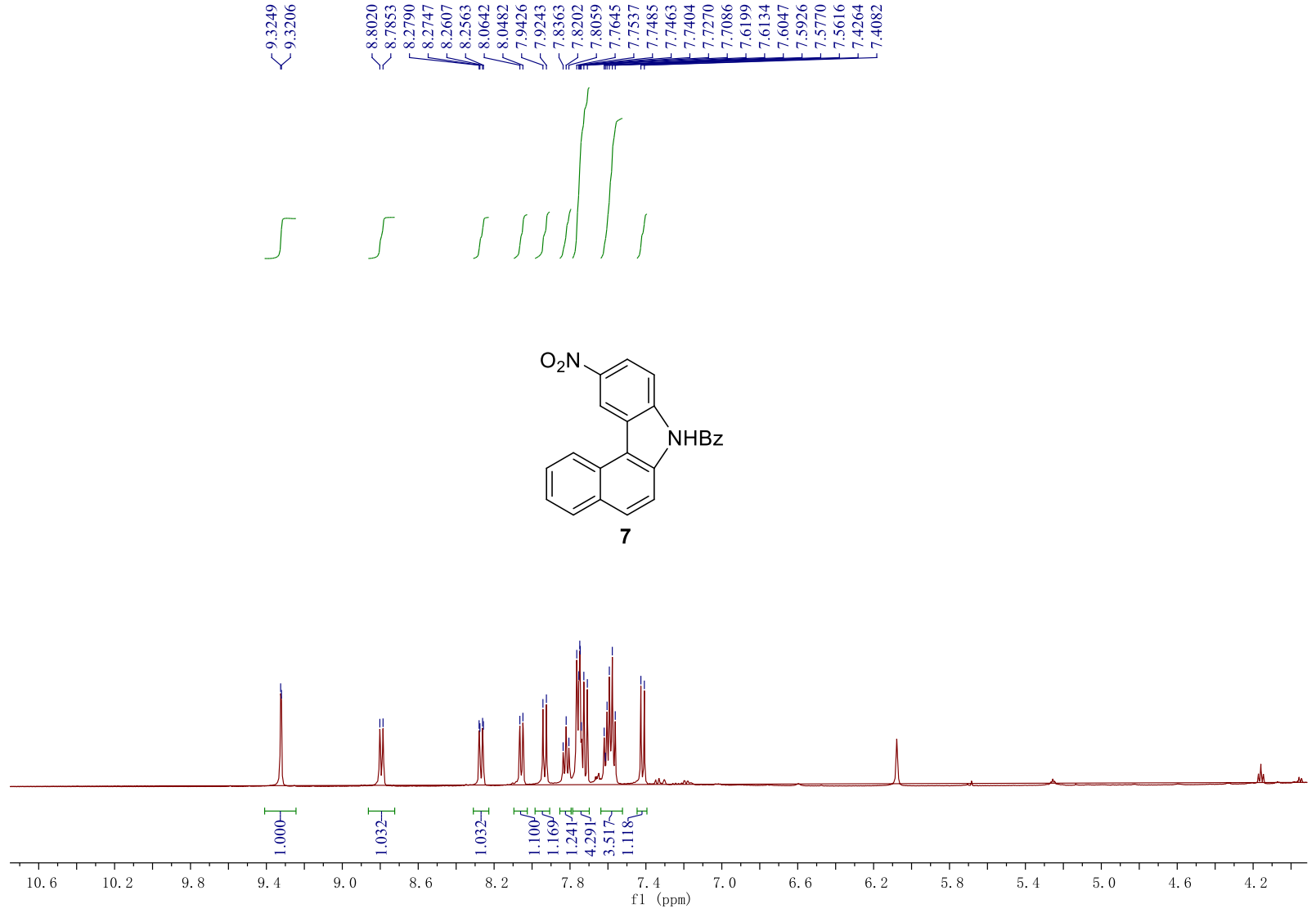
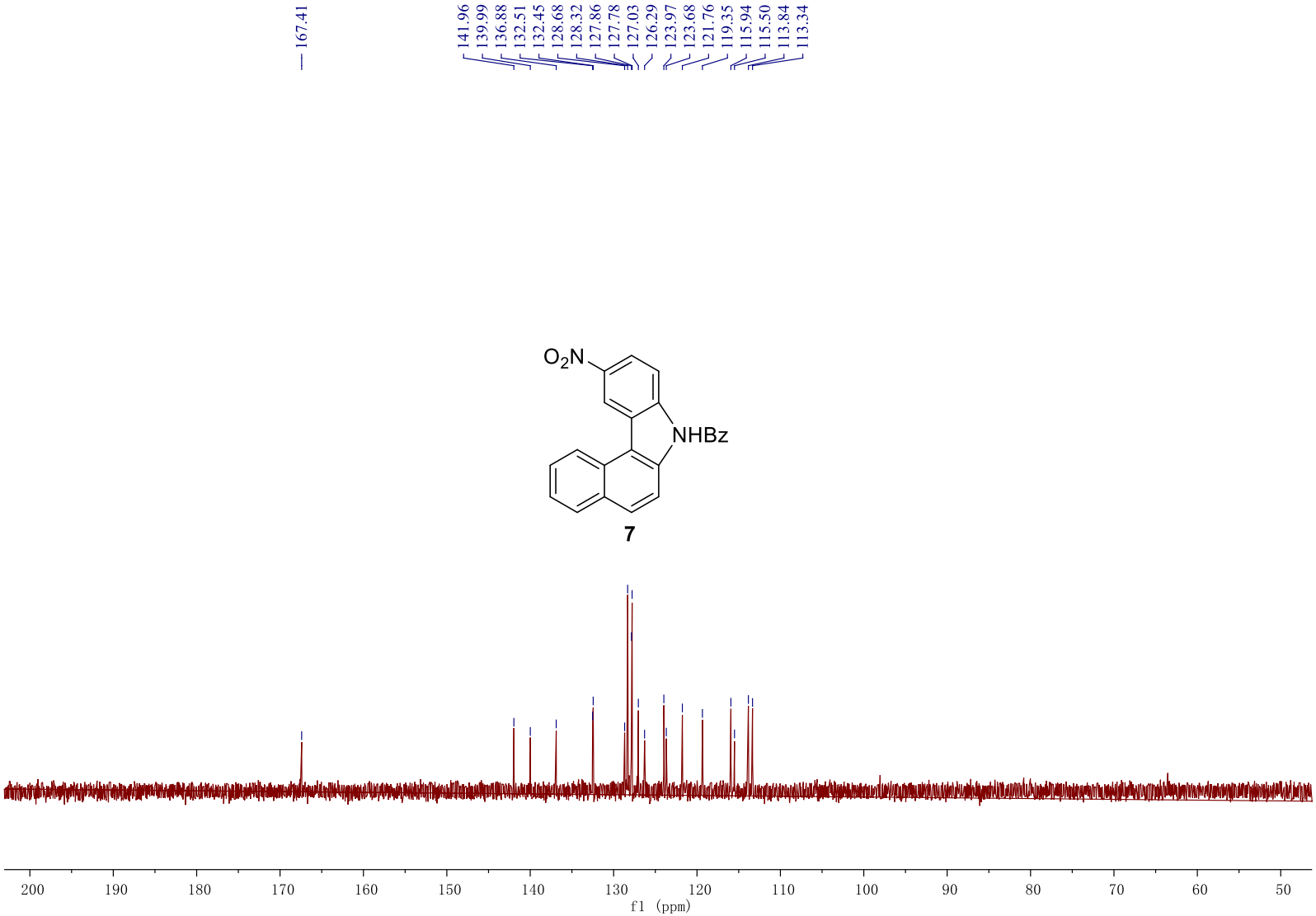
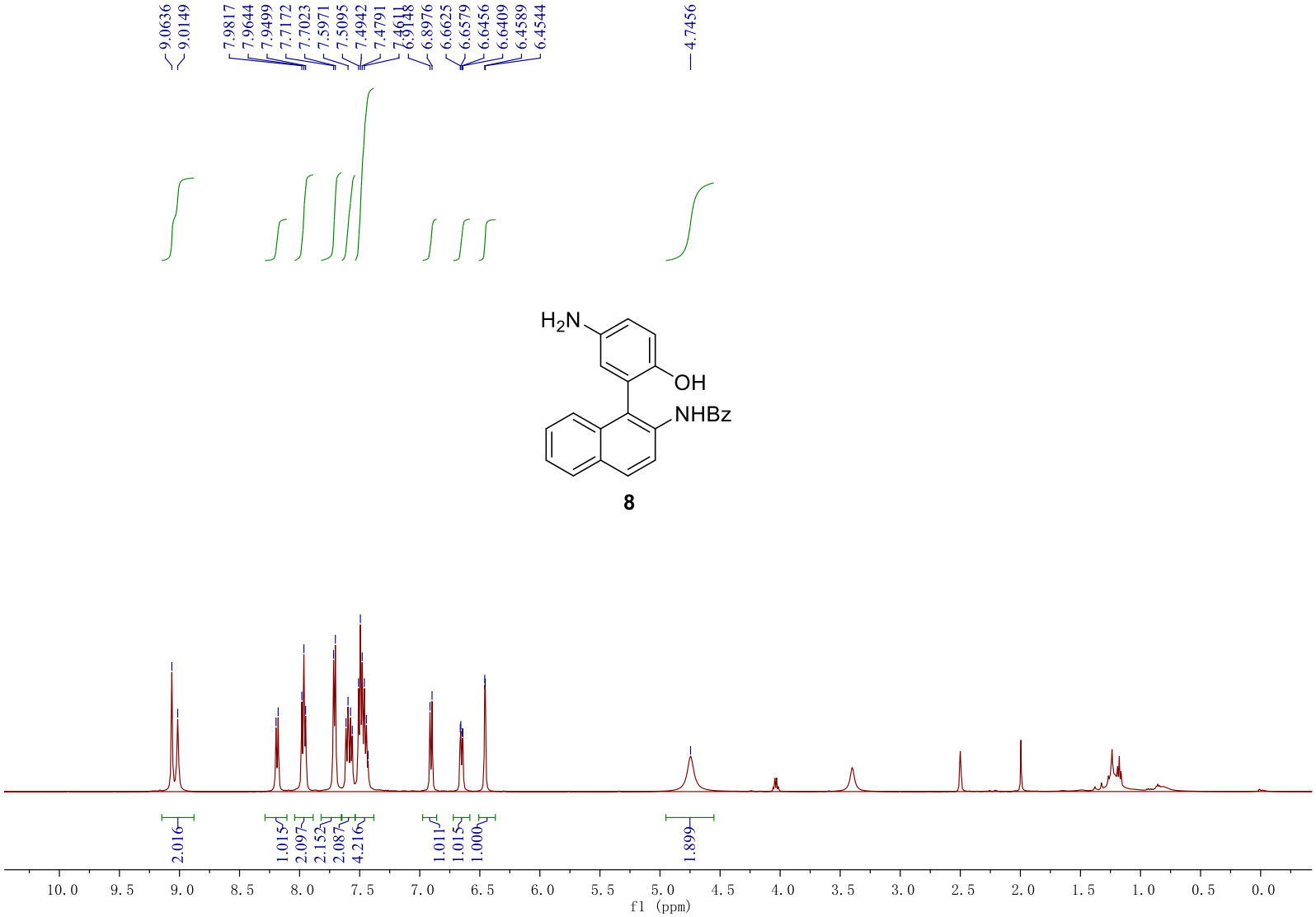
8.3635
8.3513
8.3459
8.3430
8.3377
8.0569
8.0392
7.9780
7.9601
7.8631
7.8469
7.6281
7.6006
7.5835
7.5684
7.4512
7.4373
7.4356
7.4216
7.4103
7.3971
7.3953
7.3788
7.3623
7.3482
7.3274
7.3124
7.2969
7.0900
7.0732
O2N
OTf
NHBz
6
2.012
1.014
1.144
1.000
4.073
4.800
0.877
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 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)

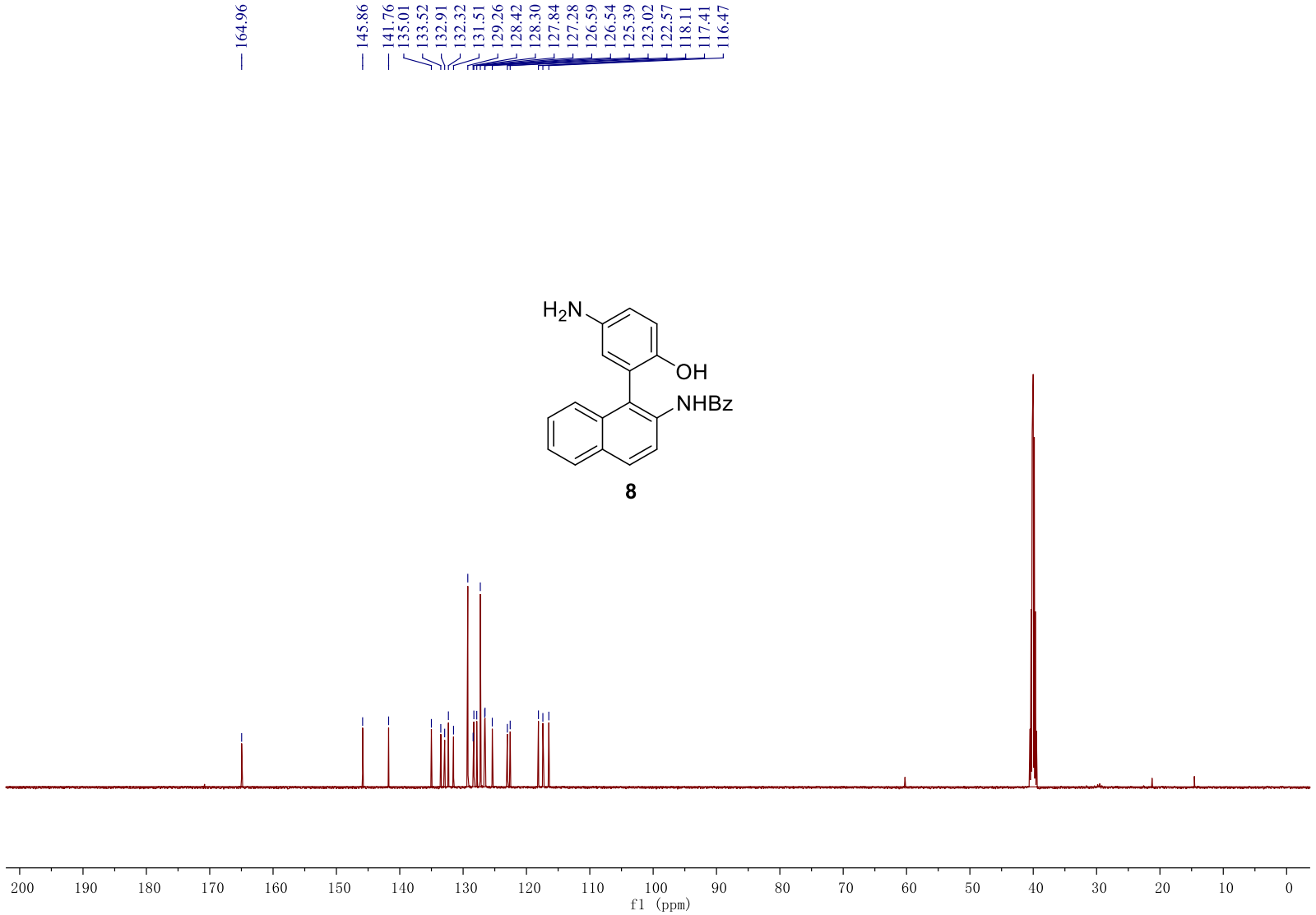

165.95
151.39
147.60
134.32
134.02
132.86
132.15
131.61
131.52
131.10
129.24
128.86
128.59
127.57
127.05
126.09
125.94
124.14
123.55
123.45
122.36
O2N
OTf
NHBz
6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

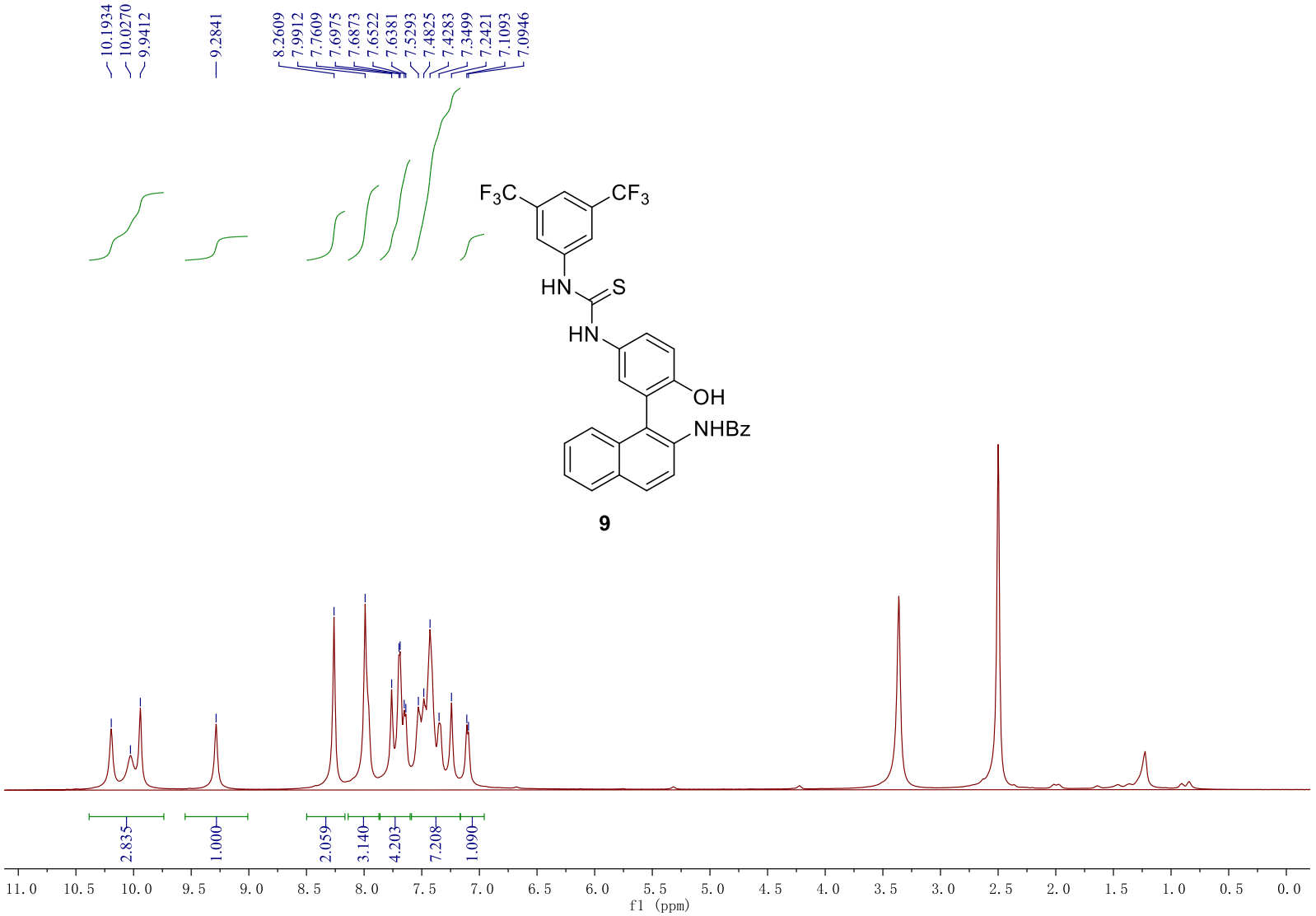

-73.58
O2N
OTf
NHBz
6
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

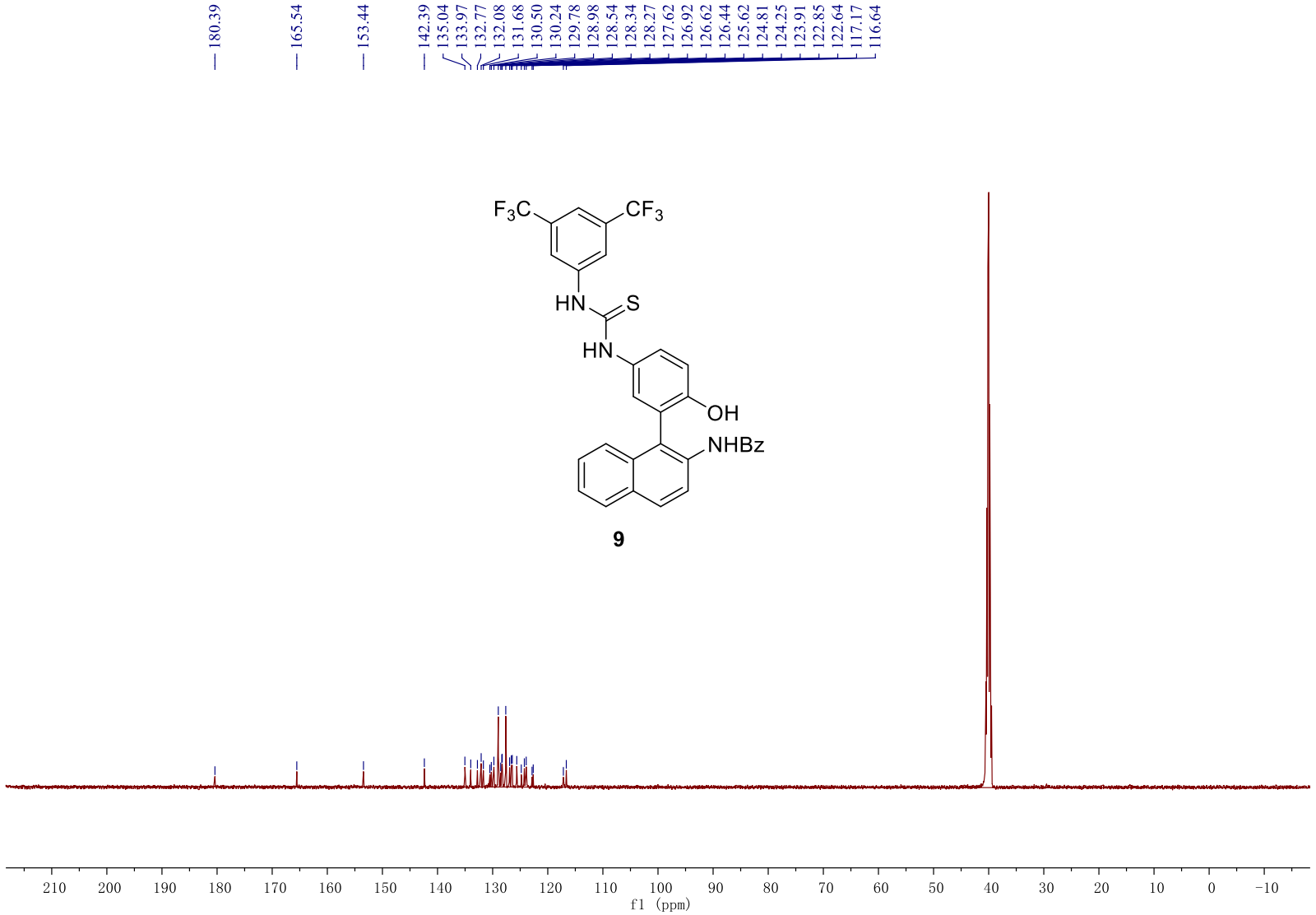

9.3249
9.3206
8.8020
8.7853
8.2790
8.2747
8.2607
8.2563
8.0642
8.0482
7.9426
7.9243
7.8363
7.8202
7.8059
7.7645
7.7537
7.7485
7.7463
7.7404
7.7270
7.7086
7.6199
7.6134
7.6047
7.5926
7.5770
7.5616
7.4264
7.4082
O2N
NHBz
7
1.000
1.032
1.032
1.100
1.169
1.241
4.291
3.517
1.118
10.6
10.2
9.8
9.4
9.0
8.6
8.2
7.8
7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
f1 (ppm)

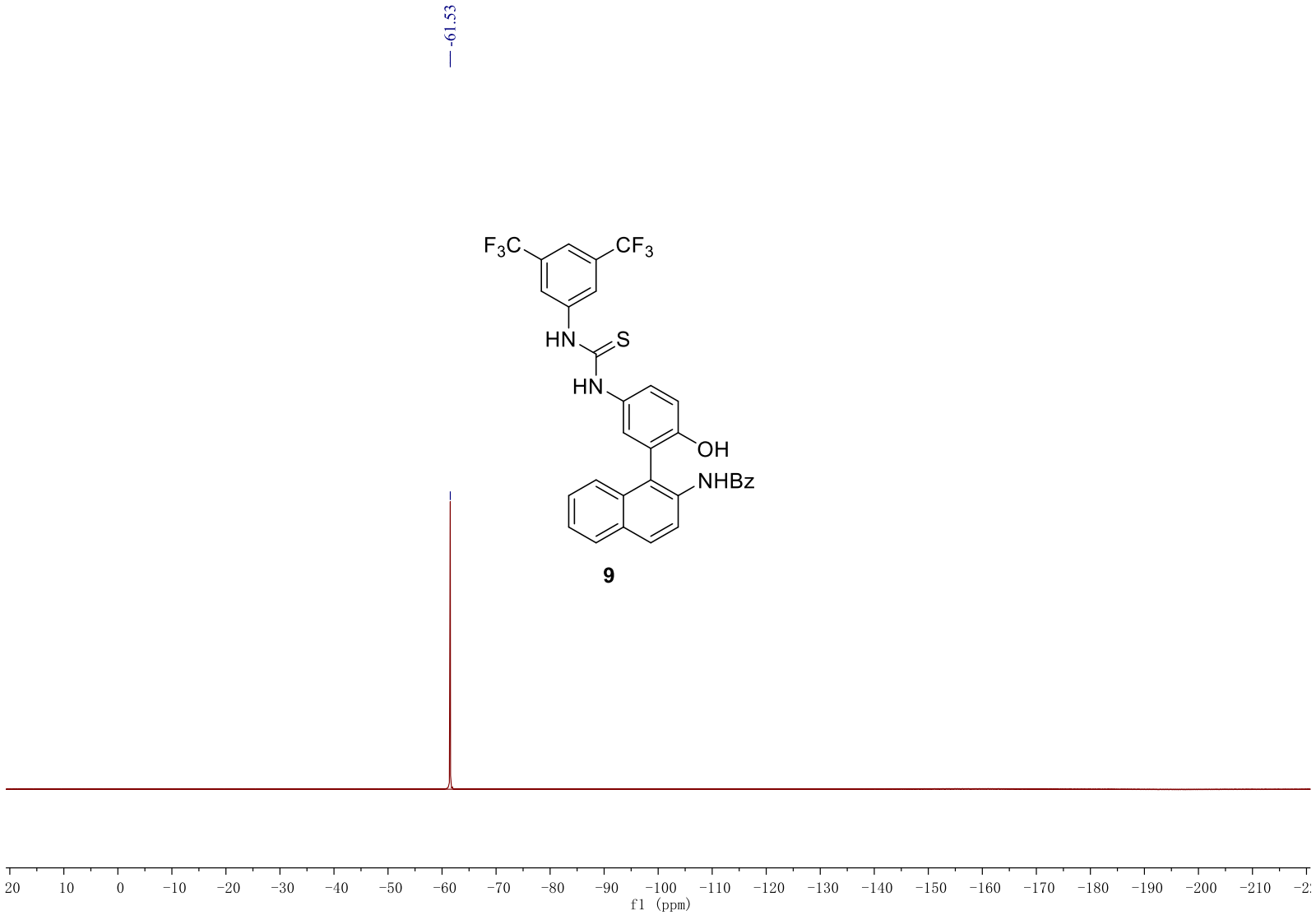

167.41
141.96
139.99
136.88
132.51
132.45
128.68
128.32
127.86
127.78
127.03
126.29
123.97
123.68
121.76
119.35
115.94
115.50
113.84
113.34
O2N
NHBz
7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)


9.0636
9.0149
7.9817
7.9644
7.9499
7.7172
7.7023
7.5971
7.5095
7.4942
7.4791
7.4611
7.3148
6.8976
6.6625
6.6579
6.6456
6.6409
6.4589
6.4544
4.7456
H2N
OH
NHBz
8
2.016
1.015
2.097
2.152
2.087
4.216
1.011
1.015
1.000
1.899
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)


164.96
145.86
141.76
135.01
133.52
132.91
132.32
131.51
129.26
128.42
128.30
127.84
127.28
126.59
126.54
125.39
123.02
122.57
118.11
117.41
116.47
H2N
OH
NHBz
8
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.1934
10.0270
9.9412
9.2841
8.2609
7.9912
7.7609
7.6975
7.6873
7.6522
7.6381
7.5293
7.4825
7.4283
7.3499
7.2421
7.1093
7.0946
F3C
CF3
HN
S
HN
OH
NHBz
9
2.835
1.000
2.059
3.140
4.203
7.208
1.090
f1 (ppm)


180.39
165.54
153.44
142.39
135.04
133.97
132.77
132.08
131.68
130.50
130.24
129.78
128.98
128.54
128.34
128.27
127.62
126.92
126.62
126.44
125.62
124.81
124.25
123.91
122.85
122.64
117.17
116.64
F3C
CF3
HN
S
HN
OH
NHBz
9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


-61.53
F3C
CF3
HN
S
HN
OH
NHBz
9
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)