Supporting Information

For

Palladium-Catalyzed Regiospecific Synthesis of Indoles from Aroyloxycarbamates with Alkynes via Decarboxylation/Cyclization

Nuannuan Ma, Peihe Li, Zheng Wang, Qipu Dai,* and Changwen Hu*

Key Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory of Photoelectronic/Electrophotonic, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing 100081, People's Republic of China

E-mail: daiqipu@bit.edu.cn, cwhu@bit.edu.cn.

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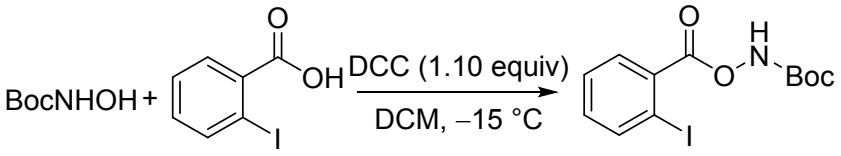
General Information

Unless stated otherwise, all reactions were carried out in oven-dried Schlenk Tube under an inert atmosphere of dry argon or nitrogen atmosphere. All commercially available reagents were used without further purification. All solvents were purified and dried according to standard methods prior to use. For product purification by flash column chromatography, silica gel (200-300 mesh) was used. ^{1}H NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. Chemical shifts were reported in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, dd = doublet of doublet, td = triplet of doublet, br = broad, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR spectra were recorded on a 101 MHz NMR spectrometer. Chemical shifts were reported in ppm referenced to the center of a triplet at 77.0 ppm of chloroform-*d*. IR spectra were obtained on a FT-IR spectrometer using KBr plates (thin film). Melting points were determined using an X-4 apparatus and are uncorrected. GC-MS data were performed on Agilent 7890A. GC analyses were performed on a Shimadzu GC-2014 equipped with a capillary column (HP-5 30 m × 0.25 μm) using a flame ionization detector. HRMS was performed on TOF LC-MS in ESI mode.

Procedures for the preparation of starting materials

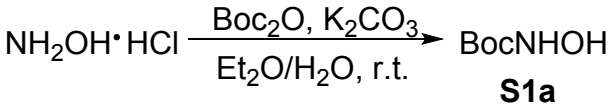


S1a 1.05 equiv **1a**

To a 250 mL flame-dried round bottom flask equipped with a stir bar, N-hydroxyl tert-butyl carbamate **S1a** (2.66 g, 20 mmol), 2-iodobenzoic acid (5.11 g, 21 mmol) and anhydrous CH_2Cl_2 (80 mL) were added. The flask was cooled to −15 °C. DCC (4.53 g, 22 mmol, dissolved in 20 mL anhydrous CH_2Cl_2) solution was then added dropwise. The reaction mixture was stirred at the same temperature for additional 30 mins until the N-hydroxyl carbamate was fully consumed (monitored by TLC). The white precipitate (N, N'-dicyclohexylurea) was removed by filtration and the filtrate was concentrated in vacuo and

dissolved again in Et_2O (30 mL). The solution was cooled to −20 °C for 2 h and filtered again to remove additional precipitate. The organic layer was then concentrated in vacuo and the residue was recrystallized from hexanes and EtOAc to afford corresponding product **1a** in 78% yield as a white solid.

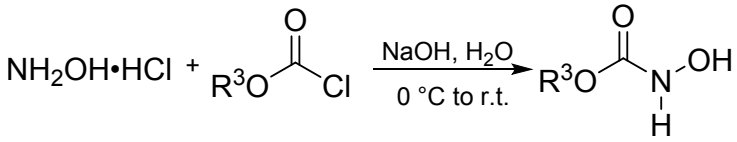
D.-F. Lu, C.-L. Zhu, Z.-X. Jia, H. Xu, *J. Am. Chem. Soc.*, 2014, **136**, 13186.



S1a

N-hydroxyl tert-butyl carbamate **S1a** was prepared from hydroxylamine hydrochloride with $(Boc)_2O$, according to a known procedure. A suspension of $NH_2OH{\cdot}HCl$ (9.6 g, 140 mmol) and K_2CO_3 (7.2 g, 70 mmol) in Et_2O (60 mL) and H_2O (2 mL) was stirred for about 1 h at room temperature with evolution of CO_2 gas. A solution of Boc_2O (20 g, 92 mmol) in Et_2O (40 mL) was then added dropwise at 0 °C and the suspension was stirred at room temperature for 12 h. The organic phase was decanted and the solid was washed with Et_2O (30 mL × 2) and the organic layers were combined and concentrated. Recrystallization with a cyclohexane/toluene mixture afforded the desired product **S1a**.

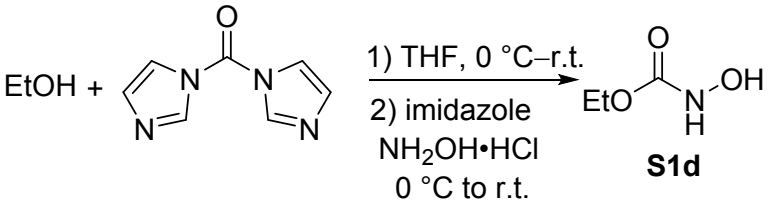
D.-F. Lu, C.-L. Zhu, Z.-X. Jia, H. Xu, *J. Am. Chem. Soc.*, 2014, **136**, 13186.



S1b: R = Me **S1c**: R = Bn

N-hydroxyl carbamates were prepared from hydroxylamine with the corresponding chloroformates according to a known procedure. Hydroxylamine hydrochloride (13.9 g, 200 mmol) was added to aqueous solution of NaOH (1.5 M, 160 mL, 240 mmol). The solution was cooled to 0 °C and chloroformate (38 mmol) was added dropwise. Upon the completion of addition, the mixture was warmed up to room temperature and stirred for additional 2 h. The reaction was then acidified with aqueous HCl (6 M) till pH was around 4.5. Then the mixture was extracted with Et_2O (200 mL × 3) and the combined organic layers were washed with brine and dried over anhydrous Na_2SO_4. After removal of the solvent in vacuo, the N-hydroxyl carbamate was used directly without further purification.

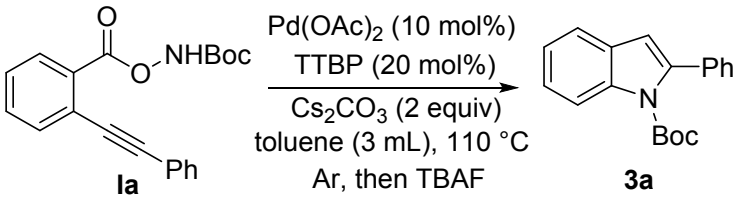
D.-F. Lu, C.-L. Zhu, Z.-X. Jia, H. Xu, *J. Am. Chem. Soc.*, 2014, **136**, 13186.



To a flame-dried 100 mL round bottom flask equipped with a stir bar was added CDI (1.78 g, 11 mmol) in anhydrous THF (30 mL). The flask was cooled to 0 °C and ethylalcohol (0.46 g, 10 mmol) was added dropwise. The mixture was stirred for additional 1 h at room temperature and then $NH_2OH{\cdot}HCl$ (1.04 g, 15 mmol) and imidazole (0.82 g, 12 mmol) were added in one portion. The reaction was monitored by TLC, until the starting material disappeared (about 1 h). Then the mixture was filtered and concentrated in vacuo. The residue was dissolved in EtOAc (40 mL) and washed with aqueous HCl (1 M, 20 mL × 3). The organic layer was dried over anhydrous Na_2SO_4 and concentrated to afford the crude product **S1d** in 85% yield, which can be used directly for next step.

D.-F. Lu, C.-L. Zhu, Z.-X. Jia, H. Xu, *J. Am. Chem. Soc.*, 2014, **136**, 13186.

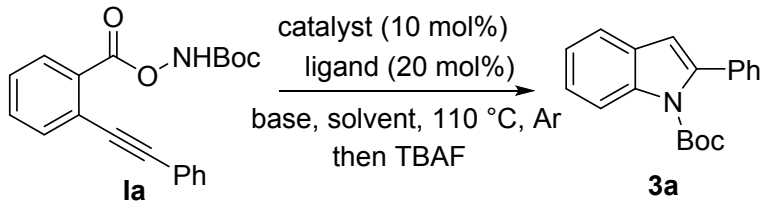
Synthesis of 3a via path a



To a solution of **Ia** (101.2 mg, 0.30 mmol), $Pd(OAc)_2$ (6.7 mg, 10 mol%), TTBP (17.4 mg, 20 mol%) and Cs_2CO_3 (195.5 mg, 0.60 mmol) in toluene (3 mL) in a Schlenk Pressure Tube (10 mL) under a dry argon atmosphere. The reaction mixture was vigorously stirred at 110 °C for 1.5 h, then we added TBAF (156.9 mg, 2 equiv) to the reaction system. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 100 / 1) to afford the product **3a** (57.2 mg, 65%).

A. Yasuhara, Y. Knamori, M. Kaneko, A. Numata, Y. Kondo, T. Sakamoto, *J. Chem. Soc., Perkin Trans. 1* **1999**, 529.

Table S1. Optimization of the reaction conditions of path a.[a]

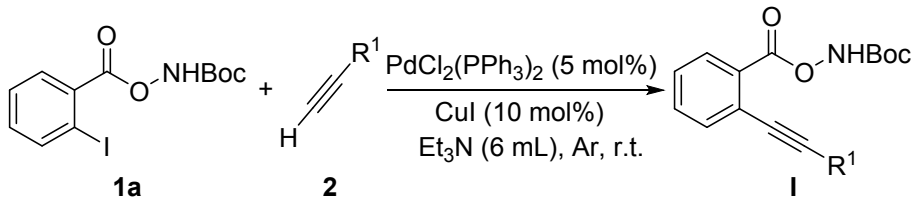


Ia **3a**

Entry	Catalyst	Ligand	Time (h)	Solvent	Yield[b] (%)
1	$PdCl_2$	PPh_3	Cs_2CO_3	Toluene	30
2	$Pd(OAc)_2$	PPh_3	Cs_2CO_3	Toluene	34
3	$PdCl_2(PPh_3)_2$	No	Cs_2CO_3	Toluene	28
4	$Pd(TFA)_2$	PPh_3	Cs_2CO_3	Toluene	26
5	$Pd(OAc)_2$	No	No	Toluene	Trace
6	$Pd(OAc)_2$	PPh_3	No	Toluene	Trace
7	No	No	Cs_2CO_3	Toluene	18
8	$Pd(OAc)_2$	BINAP	Cs_2CO_3	Toluene	47
9	$Pd(OAc)_2$	Xantphos	Cs_2CO_3	Toluene	50
10	$Pd(OAc)_2$	TTBP	Cs_2CO_3	Toluene	56
11	$Pd(OAc)_2$	$P(o\text{-}tol)_3$	Cs_2CO_3	Toluene	48
12	$Pd(OAc)_2$	2,2'-Bipyridine	Cs_2CO_3	Toluene	42
13	$Pd(OAc)_2$	TTBP	K_2CO_3	Toluene	20
14	$Pd(OAc)_2$	TTBP	*t*-BuOK	Toluene	17
15	$Pd(OAc)_2$	TTBP	*t*-BuONa	Toluene	18
16	$Pd(OAc)_2$	TTBP	Et_3N	Toluene	6
17	$Pd(OAc)_2$	TTBP	Cs_2CO_3	$CHCl_3$	29
18	$Pd(OAc)_2$	TTBP	Cs_2CO_3	DMF	0
19	$Pd(OAc)_2$	TTBP	Cs_2CO_3	Xylene	50
20	**$Pd(OAc)_2$ (10 mol%)**	**TTBP (20 mol%)**	**Cs_2CO_3**	**Toluene**	**69 (65)[c]**
21	$Pd(OAc)_2$ (20 mol%)	TTBP (40 mol%)	Cs_2CO_3	Toluene	63

[a] Reaction conditions: **Ia** (0.2 mmol), catalyst (5 mol%), ligand (10 mol%), base (0.4 mmol, 2 equiv), TBAF (2 equiv) in solvent (1 mL) under argon atmosphere at 110 °C. [b] The yields were determinded by GC analysis using biphenyl as internal standard. [c] Yield of the isolated product.

Table S2. **Synthesis of starting materials I via Sonogashira cross-coupling reaction.**[a]



1a **2** **I**

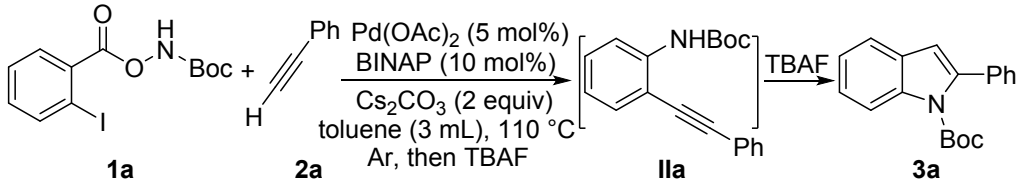
Entry	R^1	**I**	Time (h)	Yield[b] (%)
1	C_6H_5	**Ia**	1.5	78
2	4-FC_6H_4	**Ib**	1	71
3	4-ClC_6H_4	**Ic**	2	69
4	4-BrC_6H_4	**Id**	2.5	46
5	3-ClC_6H_4	**Ie**	3	48
6	4-MeC_6H_4	**If**	2	85
7	4-EtC_6H_4	**Ig**	4	86
8	4-$MeOC_6H_4$	**Ih**	2	83

[a] Reaction conditions: **1a** (2.0 mmol), **2** (3.2 mmol), $PdCl_2(PPh_3)_2$ (5 mol%), CuI (10 mol%) in Et_3N (6 mL) at room temperature under argon atmosphere. [b] Yield of the isolated product.

To a Et_3N (6 mL) solution of **1a** (726.3 mg, 2 mmol) and **2a** (326.8 mg, 3.2 mmol) were added $PdCl_2(PPh_3)_2$ (70.2 mg, 0.1 mmol) and CuI (38.1 mg, 0.2 mmol) in a Schlenk Pressure Tube (25 mL) under a dry argon atmosphere at room temperature. The resulting mixture was monitored by TLC until **1a** was consumed about 1.5 h. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 50 / 1) to afford the product **Ia** (526.3 mg, 78%). We used the similar method to afford **Ib**-**Ih** (Table S2).

A. Yasuhara, Y. Knamori, M. Kaneko, A. Numata, Y. Kondo, T. Sakamoto, *J. Chem. Soc.,Perkin Trans. 1* 1999, 529.

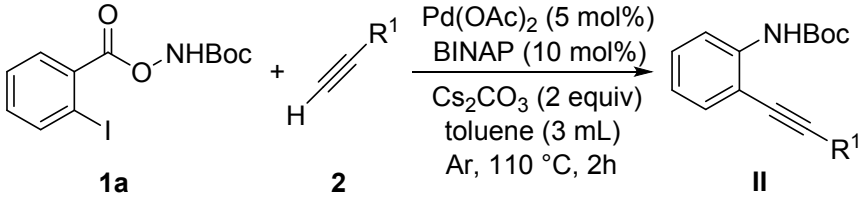
Synthesis of 3a via path b



1a **2a** **IIa** **3a**

To a toluene (3 mL) solution of *t*-buty[((2-iodinebenzoyl)oxy)]carbamate **1a** (108.9 mg, 0.30 mmol), $Pd(OAc)_2$ (3.4 mg, 5 mol%), BINAP (18.6 mg, 10 mol%), Cs_2CO_3 (195.5 mg, 0.6 mmol) were added phenylaccetylene **2a** (49.0 mg, 0.48 mmol) in a Schlenk Pressure Tube (10 mL) under a dry argon atmosphere. The resulting mixture was vigorously stirred at 110 °C and monitored by TLC until the starting material **1a** was transformed into **IIa** about 2 hours. Then we added the TBAF (156.9 mg, 2 equiv) to the reaction system. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 100 / 1) to afford the product **3a** (52.8 mg, 60%).

Table S3. **Synthesis of II.**[a]



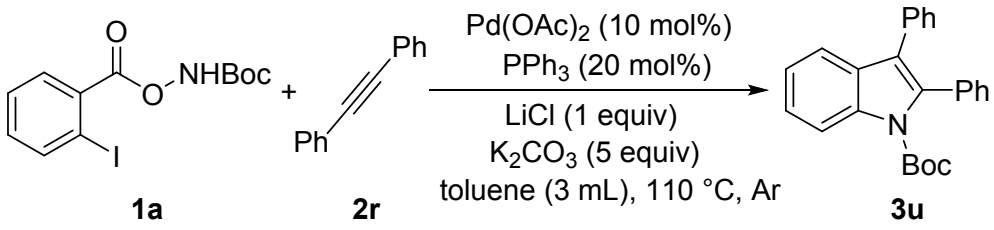
1a **2** **II**

Entry	R^1	**II**	Yield[b] (%)
1	C_6H_4	**IIa**	71
2	2-FC_6H_4	**IIb**	88
3	3-FC_6H_4	**IIc**	87
4	4-FC_6H_4	**IId**	71
5	4-ClC_6H_4	**IIe**	73
6	4-BrC_6H_4	**IIf**	61
7	4-MeC_6H_4	**IIg**	85
8	4-$MeOC_6H_4$	**IIh**	83
9	thiophene	**IIi**	67
10	cyclopropane	**IIj**	59
11	$(CH_2)_5CH_3$	**IIk**	65
12	TMS	**III**	63

[a] Reaction conditions: **1a** (0.30 mmol), **2** (0.48 mmol, 1.6 equiv), $Pd(OAc)_2$ (5 mol%), BINAP (10 mol%) Cs_2CO_3 (0.6 mmol, 2 equiv) in toluene (3 mL) at 110 °C under argon atmosphere. [b] Yield of the isolated product.

To a toluene (3 mL) solution of *t*-buty [((2-iodinebenzoyl)oxy)]carbamate **1a** (108.9 mg, 0.30 mmol), $Pd(OAc)_2$ (3.4 mg, 5 mol%), BINAP (18.6 mg, 10 mol%), Cs_2CO_3 (195.5 mg, 0.60 mmol) were added phenylaccetylene **2a** (49.0 mg, 0.48 mmol) in a Schlenk Pressure Tube (10 mL) under a dry argon atmosphere. The resulting mixture was vigorously stirred at 110 °C and monitored by TLC until the starting material **1a** was consumed about 2 hours. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 40 / 1) to afford the product **IIa** (62.5 mg, 71%). We used this same method to afford **IIb-III** (Table S3).

Synthesis of 2, 3-disubstituted indole 3u

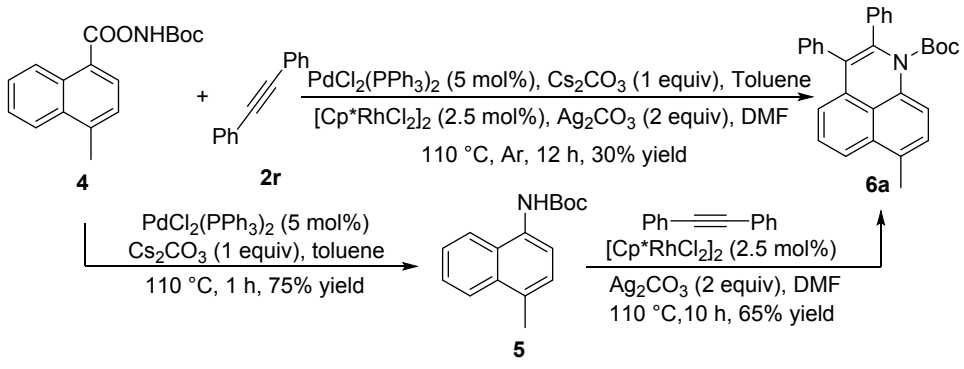


1a **2r** **3u**

To a toluene (3 mL) solutin of **1a** (108.9 mg, 0.30 mmol), **2r** (85.6 mg, 0.48 mmol), $Pd(OAc)_2$ (6.7 mg, 10 mol%), PPh_3 (15.7 mg, 20 mol%) and K_2CO_3 (207.3 mg, 1.50 mmol), LiCl (12.7 mg, 0.30 mmol) in a Schlenk Pressure Tube (10 mL) under a dry argon atmosphere. The reaction mixture was vigorously stirred at 110 °C for overnight. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 50 / 1) to afford the product **3u** (72 mg, 65%).

M. Somei and F. Yamada, *Nat*. *Prod*. *Rep*., 2004, **21**, 278.

Synthesis of compound 6a



4 **2r** **6a**

5

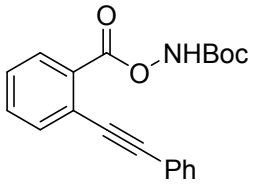
To a solution of **4** (90.4 mg, 0.3 mmol), $Pd(PPh_3)_2Cl_2$ (10.5 mg, 0.015 mmol) and Cs_2CO_3 (97.7 mg, 0.3 mmol) in toluene (3 mL) in a Schlenk Pressure Tube (10 mL) under a dry argon atmosphere. The reaction mixture was vigorously stirred at 110 °C and monitored by TLC until the starting material **5** was consumed about 1 h. After removing the solvent by reduced pressure distillation, we added the diphenylacetylene (85.6 mg, 0.48 mmol), $[Cp^*RhCl_2]_2$ (4.6 mg, 0.015 mmol), Ag_2CO_3 (165.5 mg, 0.6 mmol) and DMF (3 mL) to the reaction system. After completion of the reaction, the solvent was removed under pressure and the crude product was subjected to silica gel column chromatography (eluent: petroleum ether / ethyl acetate = 50 / 1) to afford the product **6** (39.0 mg, 30%).

(1) X. Zhang, W. Si, M. Bao, N. Asao, Y. Yamamoto and T. Jin, *Org. Lett*., 2014, **16**, 4830.

(2) Q. Dai, P. Li, N. Ma and C. Hu, *Org. Lett.*, 2016, **18**, 5560.

Characterization data

Table S2, entry 1

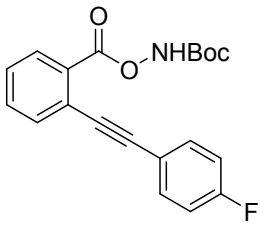


***tert*-butyl ((2-(phenylethynyl)benzoyl)oxy)carbamate Ia**

Yellow solid (526.3 mg, 78%). mp: 84-85 °C. IR (film) 2943, 2834, 1451, 1012, 756 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.61-7.53 (m, 3H), 7.41 (t, J = 8.0 Hz, 1H), 7.36-7.33 (m, 3H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 155.6, 133.9, 132.8, 131.8, 130.7, 128.7, 128.5, 128.3, 127.9, 124.5, 123.0, 95.3, 87.3, 83.3, 28.0. HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}ClNO_4$ 355.1652; Found 355.1663.

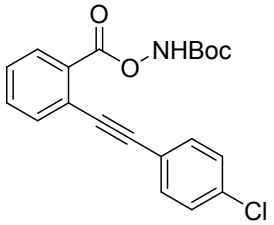
Table S2, entry 2



***tert*-butyl ((2-((4-fluorophenyl)ethynyl)benzoyl)oxy)carbamatecarbamate Ib**

Oil (503.0 mg, 71%). IR (film) 2976, 1733, 1227, 1012, 756 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.28 (s, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.58-7.52 (m, 3H), 7.40 (t, J = 7.6 Hz, 1H), 7.06-7.02 (m, 2H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 162.7 (d, J = 251.2 Hz), 155.5, 133.8 (d, J = 1.6 Hz), 133.7, 132.8, 130.7, 128.4, 128.0, 124.3, 119.1 (d, J = 3.4 Hz), 115.6 (d, J = 222.2 Hz), 94.2, 87.0, 83.3, 28.0. HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}FNO_4$ 373.1558; Found 373.1563.

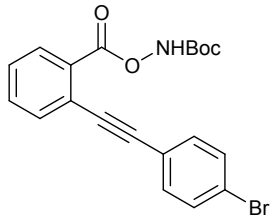
Table S2, entry 3



***tert*-butyl ((2-((4-chlorophenyl)ethynyl)benzoyl)oxy)carbamate Ic**

White solid (513.1 mg, 69%). mp: 59-60 °C. IR (film) 2952, 1660, 1451, 1053, 1012 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.42 (t, J = 7.6 Hz, 1H), 7.32 (d, J = 8.4 Hz, 2H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 155.5, 134.7, 133.9, 133.1, 132.8, 130.8, 128.7, 128.5, 128.2, 124.1, 121.5, 94.0, 88.2, 83.4, 28.0. HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}ClNO_4$ 389.1263; Found 389.1263.

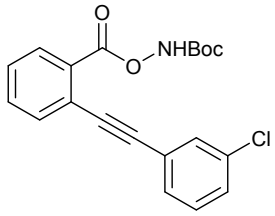
Table S2, entry 4



***tert*-butyl ((2-((4-bromophenyl)ethynyl)benzoyl)oxy)carbamate Id**

Oil (383.0 mg, 46%). IR (film) 2979, 1733, 1224, 1006, 750 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.26 (s, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.49-7.40 (m, 5H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.4, 155.5, 133.9, 133.2, 132.8, 131.6, 130.8, 128.5, 128.2, 124.1, 123.0, 121.9, 94.1, 88.4, 83.4, 28.0. HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}BrNO_4$ 435.0740; Found 435.0745.

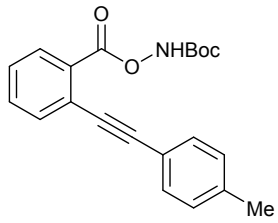
Table S2, entry 5



***tert*-butyl ((2-((3-chlorophenyl)ethynyl)benzoyl)oxy)carbamate Ie**

White solid (357.0 mg, 48%). mp: 93-95 ^{o}C. IR (film) 2973, 1739, 1050, 1006, 750 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (s, 1H), 8.09-8.07 (m, 1H), 7.68-7.66 (m, 1H), 7.59-7.55 (m, 2H), 7.47-7.41 (m, 2H), 7.34-7.28 (m, 2H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 155.5, 134.2, 134.1, 132.9, 131.7, 130.8, 130.0, 129.6, 129.0, 128.6, 128.4, 124.7, 124.0, 93.7, 88.4, 83.5, 28.1. HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}ClNO_4$ 389.1263; Found 389.1263.

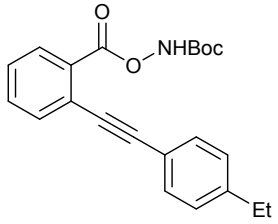
Table S2, entry 6



***tert*-butyl ((2-(p-tolylethynyl)benzoyl)oxy)carbamate If**

Oil (597.4 mg, 85%). IR (film) 2949, 2522, 1457, 1033, 756 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s 1H), 8.06 (d, J = 7.6 Hz, 1H), 7.66 (d, J = 7.6 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 8.0 Hz, 2H), 7.39 (t, J = 7.6 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.6, 155.6, 138.9, 133.9, 132.7, 131.8, 130.7, 129.1, 128.4, 127.7, 124.7, 119.9, 95.6, 86.7, 83.3, 28.0, 21.5. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{21}NO_4$ 352.1543; Found 352.1551.

Table S2, entry 7

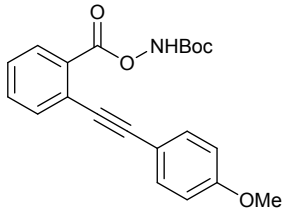


***tert*-butyl ((2-((4-ethylphenyl)ethynyl)benzoyl)oxy)carbamate Ig**

Oil (628.1 mg, 86%). IR (film) 2967, 1739, 1224, 1018, 750 cm^{-1}. ^{1}H NMR (400 MHz,

$CDCl_3$): δ 8.21 (s, 1H), 8.06 (dd, J = 7.6 Hz, 0.8 Hz, 1H), 7.66 (dd, J = 7.6 Hz, 0.8 Hz, 1H), 7.55 (td, J = 7.2 Hz, 1.2 Hz, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.39 (td, J = 8.0 Hz, 1.2 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 2.66 (q, J = 7.6 Hz, 2H), 1.51 (s, 9H), 1.24 (t, J = 8.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.6, 155.6, 145.2, 133.9, 132.7, 131.9, 130.7, 128.4, 127.9, 127.7, 124.8, 120.1, 95.6, 86.7, 83.3, 28.9, 28.0, 15.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{23}NO_4$ 366.1700; Found 366.1702.

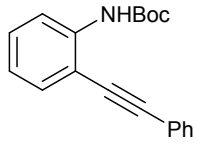
Table S2, entry 8



***tert*-butyl ((2-((4-methoxyphenyl)ethynyl)benzoyl)oxy)carbamate Ih**

Oil (609.9 mg, 83%). IR (film) 2976, 1742, 1249, 1059, 759 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 1H), 8.06 (dd, J = 8.0, 1.2 Hz, 1H), 7.65 (dd, J = 7.6, 0.8 Hz, 1H), 7.56-7.51 (m, 3H), 7.38 (td, J = 7.8, 1.2 Hz, 1H), 6.90-6.86 (m, 2H), 3.83 (s, 3H), 1.51 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.6, 160.0, 155.6, 133.7, 133.4, 132.7, 130.7, 128.2, 127.6, 124.9, 115.1, 114.0, 95.6, 86.2, 83.3, 55.3, 28.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{21}NO_5$ 368.1492; Found 368.1503.

Table S3, entry 1

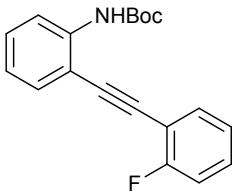


***tert*-butyl (2-(phenylethynyl)phenyl)carbamate IIa**

White solid (62.5 mg, 71%). mp: 62-65 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, J = 8.4 Hz, 1H), 7.57-7.54 (m, 2H), 7.46 (dd, J = 7.6, 1.6 Hz, 1H), 7.41-7.37 (m, 3H), 7.35-7.30 (m, 2H), 6.99 (td, J = 7.6, 0.8 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.3, 139.4, 131.6, 131.4, 129.6, 128.6, 128.4, 122.5, 122.0, 117.5, 111.1, 96.0, 84.5, 80.7, 28.2.

T. Ishida, S. Kikuch, T. Tsubo and T. Yamada, *Org. Lett.*, 2013, **15**, 848.

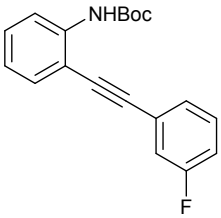
Table S3, entry 2



***tert*-butyl (2-((2-fluorophenyl)ethynyl)phenyl)carbamate IIb**

Yellow solid (82.2 mg, 88%). mp: 68-70 °C. IR (film) 3408, 2967, 1733, 1056, 756 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.4 Hz, 1H), 7.54-7.51 (m, 2H), 7.47 (d, J = 7.6 Hz, 1H), 7.38-7.32 (m, 2H), 7.18-7.12 (m, 2H), 7.00 (t, J = 7.6 Hz, 1H), 1.56 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.6 (d, J = 252.5 Hz), 152.5, 139.9, 132.8, 131.4, 130.3 (d, J = 8.1 Hz), 130.0, 124.1 (d, J = 3.7 Hz), 122.0, 117.5, 115.6 (d, J = 209.1 Hz), 111.4 (d, J = 15.6 Hz), 110.7, 90.0, 89.5, 80.7, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}NO_2$ 312.1394; Found 312.1412.

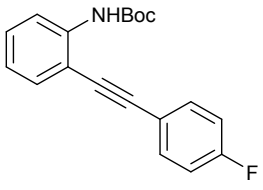
Table S3, entry 3



***tert*-butyl (2-((3-fluorophenyl)ethynyl)phenyl)carbamate IIc**

Yellow solid (81.3 mg, 87%). mp: 57-61 °C. IR (film) 3408, 2967, 1731, 1074, 873 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, J = 8.4 Hz, 1H), 7.46 (dd, J = 7.8, 1.0 Hz, 1H), 7.38-7.32 (m, 3H), 7.26-7.23 (m, 2H), 7.11-7.06 (m, 1H), 7.00 (t, J = 7.6 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.4 (d, J = 248.1 Hz), 152.4, 139.6, 131.8, 130.1 (d, J = 8.7 Hz), 130.0, 127.4 (d, J = 2.1 Hz), 124.4 (d, J = 9.6 Hz), 122.2, 118.3 (d, J = 23 Hz), 117.7, 116.0 (d, J = 21.2 Hz), 110.7, 94.7, 85.5, 81.0, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}NO_2$ 312.1394; Found 312.1412.

Table S3, entry 4

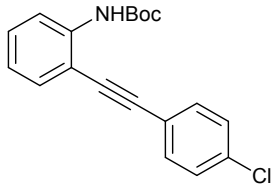


***tert*-butyl (2-((4-fluorophenyl)ethynyl)phenyl)carbamate IId**

Yellow solid (66.3 mg, 71%). mp: 69-71 °C. IR (film) 3405, 2973, 1383, 1048, 880 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, J = 8.4 Hz, 1H), 7.55-7.51 (m, 2H), 7.45 (d, J = 8.0 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 7.28 (br, 1H), 7.09 (t, J = 8.4 Hz, 2H), 6.99 (t, J = 7.2 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.7 (d, J = 251.4 Hz), 152.4, 139.5, 133.5 (d, J = 8.5 Hz), 131.7, 129.7, 122.2, 118.7 (d, J = 3.5 Hz), 117.7, 115.9 (d, J = 22.2 Hz), 111.0, 94.9, 84.3, 80.9, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}FNO_2$ 312.1394; Found 312.1412.

Table S3, entry 5

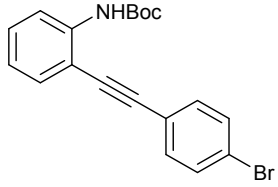


***tert*-butyl (2-((4-chlorophenyl)ethynyl)phenyl)carbamate IIe**

White solid (81.6 mg, 83%). mp: 87-90 ^{o}C. IR (film) 3405, 2976, 1380, 1056, 880 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, J = 8.4 Hz, 1H), 7.49-7.44 (m, 3H), 7.37-7.31 (m, 3H), 7.26 (s, 1H), 7.00 (t, J = 7.6 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.4, 139.5, 134.8, 132.7, 131.8, 129.9, 128.9, 122.1, 121.1, 117.7, 110.8, 94.8, 85.5, 80.9, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}ClNO_2$ 328.1099; Found 328.1105.

Table S3, entry 6

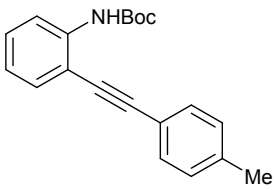


***tert*-butyl (2-((4-bromophenyl)ethynyl)phenyl)carbamate IIf**

Yellow solid(68.1 mg, 71%). mp: 92-95 ^{o}C. IR (film) 3402, 2973, 1386, 1051, 880 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, J = 8.4 Hz, 1H), 7.52 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 6.8 Hz, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 8.4 Hz, 1H), 7.26 (s, 1H), 7.00 (t, J = 7.6 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.4, 139.5, 132.9, 131.8, 131.7, 129.9, 123.0, 122.2, 121.6, 117.7, 110.8, 94.9, 85.7, 80.9, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}BrNO_2$ 372.0594; Found 372.0586.

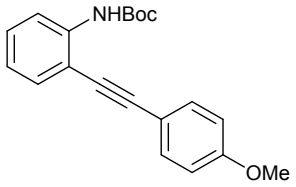
Table S3, entry 7



***tert*-butyl (2-(p-tolylethynyl)phenyl)carbamate IIg**

Yellow solid (78.4 mg, 85%). mp: 47-52 ^{o}C. IR (film) 3411, 2979, 1739, 1518, 815 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 8.4 Hz, 3H), 7.34 (s, 1H), 7.31 (t, J = 8.8 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 6.99 (t, J = 7.6 Hz, 1H), 2.39 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.4, 139.4, 139.0, 131.6, 131.4, 129.5, 129.3, 122.1, 119.5, 117.5, 111.3, 96.2, 83.9, 80.8, 28.3, 21.5. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{21}NO_2$ 308.1645; Found 308.1648.

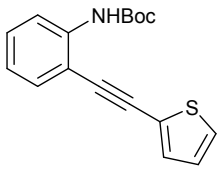
Table S3, entry 8



***tert*-butyl (2-((4-methoxyphenyl)ethynyl)phenyl)carbamate IIh**

Yellow solid (79.6 mg, 82%). mp: 92-95 ^{o}C. IR (film) 3411, 2973, 1731, 1383, 1045 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 7.6 Hz, 1H), 7.34-7.28 (m, 2H), 6.98 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 8.4 Hz, 2H), 3.85 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.0, 152.4, 139.3, 133.0, 131.5, 129.3, 122.1, 117.5, 114.7, 114.1, 111.5, 96.1, 83.2, 80.7, 55.3, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{21}NO_3$ 324.1594; Found 308.1590.

Table S3, entry 9

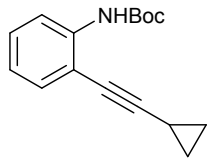


***tert*-butyl (2-(thiophen-3-ylethynyl)phenyl)carbamate IIi**

Brown solid (60.2 mg, 67%). mp: 111-113 ^{o}C. IR (film) 3414, 1733, 1513, 1383, 1157 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 8.4 Hz, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.35-7.31 (m, 3H), 7.24 (br, 1H), 7.06-7.04 (m, 1H), 6.99 (t, J = 7.6 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR

(101 MHz, $CDCl_3$): δ 152.4, 139.4, 132.3, 131.7, 129.9, 127.8, 127.2, 122.5, 122.1, 117.7, 110.8, 89.0, 88.2, 80.9, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{17}H_{17}NO_2S$ 300.1053; Found 300.1059.

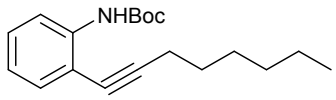
Table S3, entry 10



***tert*-butyl (2-(cyclopropylethynyl)phenyl)carbamate IIj**

Oil (45.5 mg, 59%). IR (film) 3400, 2973, 1733, 1515, 1053 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, J = 8.4 Hz, 1H), 7.29 (d, J = 7.2 Hz, 1H), 7.26-7.22 (m, 2H), 6.91 (t, J = 7.6 Hz, 1H), 1.54 (s, 9H), 1.53-1.50 (m, 1H), 0.96-0.92 (m, 2H), 0.87-0.83 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.5, 139.6, 131.6, 128.7, 121.9, 117.2, 111.7, 100.5, 80.6, 70.9, 28.3, 9.0, 6.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{19}NO_2$ 258.1489; Found 258.1488.

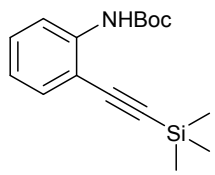
Table S3, entry 11



***tert*-butyl (2-(oct-1-yn-1-yl)phenyl)carbamate IIk**

Oil (58.8 mg, 65%). IR (film) 3402, 2979, 1733, 1051, 756 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, J = 8.4 Hz, 1H), 7.32 (d, J = 8 Hz, 1H), 7.30 (br, 1H), 7.27-7.23 (m, 1H), 6.92 (t, J = 7.6 Hz, 1H), 2.50 (t, J = 6.8 Hz, 2H), 1.69-1.61 (m, 2H), 1.54 (s, 9H), 1.51-1.47 (m, 2H), 1.38-1.31 (m, 4H), 0.91 (t, J = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.5, 139.4, 131.5, 128.7, 121.9, 117.2, 111.9, 97.5, 80.5, 76.0, 31.3, 28.6, 28.5, 28.3, 22.5, 19.6, 14.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{27}NO_2$ 302.2115; Found 302.2116.

Table S3, entry 12



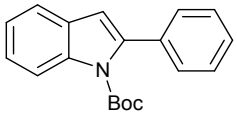
***tert*-butyl (2-((trimethylsilyl)ethynyl)phenyl)carbamate IIl**

Oil (54.7 mg, 63%). ^1H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, J = 8.4 Hz, 1H), 7.36 (d, J = 7.2

Hz, 2H), 7.30 (t, J = 8.0 Hz, 1H), 6.93 (t, J = 7.6 Hz, 1H), 1.53 (s, 9H), 0.29 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.4, 140.3, 131.3, 129.9, 121.8, 117.2, 110.9, 102.0, 100.5, 80.6, 28.3, 0.1.

J. Neuhaus, S. Morrow, M. Brunavs and M. C. Willis, *Org. Lett*., 2016, **18**, 1562.

Table 2, entry 1

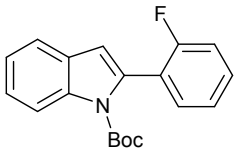


***tert*-butyl 2-phenyl-1H-indene-1-carboxylate 3a**

White solid (52.8 mg, 60%). mp: 76-78 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.45-7.33 (m, 6H), 7.29-7.25 (m, 1H), 6.57 (s, 1H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.2, 140.5, 137.4, 135.0, 129.2, 128.7, 127.8, 127.5, 124.3, 122.9, 120.4, 115.2, 109.9, 83.3, 27.5.

R. Kuwano and M. Kashiwabara, *Org. Lett.,* 2006, **8**, 2653.

Table 2, entry 2

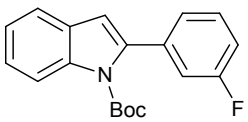


***tert*-butyl 2-(2-fluorophenyl)-1H-indene-1-carboxylate 3b**

White solid (60.7 mg, 65%). mp: 85-86 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.36-7.32 (m, 2H), 7.27-7.24 (m, 1H), 7.20 (d, J = 7.6 Hz, 1H), 7.13 (d, J = 9.6 Hz, 1H), 7.08-7.03 (m, 1H), 6.57 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.3 (d, J = 8.0 Hz), 150.0, 139.0 (d, J = 2.3 Hz), 137.5, 137.0 (d, J = 8.5 Hz), 129.2 (d, J = 8.5 Hz), 129.0, 124.6, 124.5 (d, J = 2.9 Hz), 123.0, 120.6, 115.8 (d, J = 22.4 Hz), 115.3, 114.3 (d, J = 21.3 Hz), 110.5, 83.6, 27.6.

P. Kassis, V. Bénéteau, J. Y. Mérour and S. Routier, *Synthesis*, 2009, **14**, 2447.

Table 2, entry 3

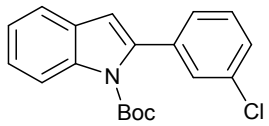


***tert*-butyl 2-(3-fluorophenyl)-1H-indene-1-carboxylate 3c**

White solid (57.0 mg, 61%). mp: 89-91 ^{o}C. IR (film) 2979, 1733, 1327, 1021, 744 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.45 (td, J = 7.6, 1.6 Hz, 1H), 7.41-7.35 (m, 2H), 7.29-7.25 (m, 1H), 7.21 (t, J = 9.2 Hz, 1H), 7.14-7.10 (m, 1H), 6.61 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.0 (d, J = 248.5 Hz), 149.9, 137.3, 134.1, 130.4 (d, J = 3.2 Hz), 129.6 (d, J = 8.1 Hz), 128.9, 124.6, 123.8 (d, J = 3.5 Hz), 123.4, (d, J = 15.5 Hz), 122.8, 120.5, 115.3, 115.0 (d, J = 21.6 Hz), 110.7, 83.4, 27.5. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}FNO_2$ 312.1394; Found 312.1395.

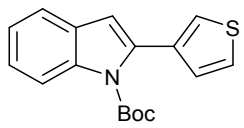
Table 2, entry 4



***tert*-butyl 2-(3-chlorophenyl)-1H-indole-1-carboxylate 3d**

Oil (47.2 mg, 48%). IR (film) 2979, 1736, 1321, 1030, 741 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 7.6 Hz, 1H), 7.42 (s, 1H), 7.37-7.31 (m, 4H), 7.28-7.24 (m, 1H), 6.58 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 138.8, 137.5, 136.7, 133.6, 129.1, 129.0, 128.9, 127.5, 126.8, 124.7, 123.1, 120.6, 115.3, 110.5, 83.7, 27.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{19}H_{18}ClNO_2$ 328.1099; Found 328.1104.

Table 2, entry 5

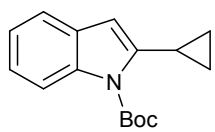


***tert*-butyl 2-(thiophen-3-yl)-1H-indole-1-carboxylate 3e**

White solid (49.4 mg, 55%). mp: 61-62 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (dd, J = 8.4, 0.8 Hz, 1H), 7.56-7.54 (m, 1H), 7.38-7.32 (m, 2H), 7.27-7.23 (m, 1H), 7.12-7.11 (s, 1H), 7.08-7.06 (m, 1H), 6.68 (s, 1H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 137.4, 135.5, 132.6, 128.7, 127.5, 126.5, 125.9, 124.7, 123.0, 120.5, 115.3, 111.9, 83.6, 27.7.

P. Kassis, V. Bénéteau, J. Y. Mérour and S. Routier, *Synthesis*, 2009, **14**, 2447.

Table 2, entry 6

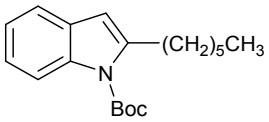


***tert*-butyl 2-cyclopropyl-1H-indole-1-carboxylate 3f**

Oil (40.1 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, J = 8.4 Hz, 1H), 7.42-7.40 (m, 1H), 7.26-7.22 (m, 1H), 7.18 (td, J = 7.6, 1.2 Hz, 1H), 6.24 (s, 1H), 2.41-2.34 (m, 1H), 1.70 (s, 9H), 0.99-0.94 (m, 2H), 0.77-0.73 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.7, 144.0, 136.9, 129.1, 123.4, 122.6, 119.8, 115.4, 105.6, 83.4, 28.3, 11.2, 7.5.

Y. Wang, L. Liu, L. Zhang, *Chem. Sci.*, 2013, **4**, 739.

Table 2, entry 7

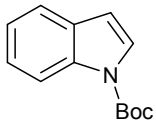


***tert*-butyl 2-hexyl-1H-indole-1-carboxylate 3g**

White solid (52.4 mg, 58%). mp: 39-40 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 7.6 Hz, 1H), 7.24-7.16 (m, 2H), 6.34 (s, 1H), 2.99 (t, J = 7.2 Hz, 2H), 1.68 (s, 9H), 1.42-1.23 (m, 8H), 0.92-0.90 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.6, 142.6, 136.6, 129.4, 123.1, 122.5, 119.6, 115.4, 106.9, 83.5, 31.8, 30.2, 29.1, 28.9, 28.2, 22.6, 14.1.

C. Mukai and Y. Takahashi, *Org. Lett.*, 2005, **7**, 5793.

Table 2, entry 8

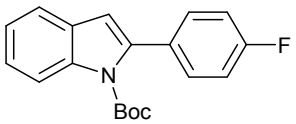


***tert*-butyl 1H-indole-1-carboxylate 3h**

Oil (35.8 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 7.6 Hz, 1H), 7.62-7.57 (m, 2H), 7.33 (t, J = 7.6 Hz, 1H), 7.26-7.22 (m, 1H), 6.59-6.58 (m, 1H), 1.69 (s, 9H),; ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.8, 135.1, 130.5, 125.8, 124.1, 122.6, 120.9, 115.1, 107.2, 83.6, 28.2.

J. Malmgren, A. Nagendiran, C. W. Tai, J. E. Bäckvall and B. Olofsson, *Chem. Eur. J.*, 2014, **20**, 13531.

Table 2, entry 9

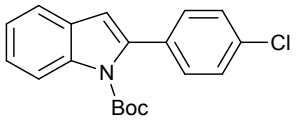


***tert*-butyl 2-(4-fluorophenyl)-1H-indene-1-carboxylate 3i**

White solid (57.0 mg, 61%). mp: 113-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (dd, J = 8.0, 0.4 Hz, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.43-7.38 (m, 2H), 7.38-7.33 (m, 1H), 7.29-7.25 (m, 1H), 7.14-7.09 (m, 2H), 6.55 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.4 (d, J = 248.1 Hz), 150.1, 139.3, 137.3, 131.0 (d, J = 3.5 Hz), 130.4 (d, J = 8.2 Hz), 129.1, 124.4, 123.0, 120.4, 115.3, 114.7 (d, J = 21.7 Hz), 110.1, 83.6, 27.6.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed.*, 2006, **53**, 9603.

Table 2, entry 10

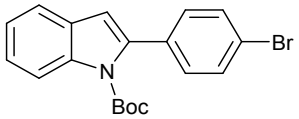


***tert*-butyl 2-(4-chlorophenyl)-1H-indole-1-carboxylate 3j**

White solid (55.9 mg, 57%). mp: 86-88 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, J = 8.4 Hz, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.41-7.33 (m, 5H), 7.29-7.25 (m, 1H), 6.56 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 139.1, 137.4, 133.6, 133.4, 130.0, 129.1, 128.0, 124.5, 123.0, 120.5, 115.3, 110.4, 83.7, 27.6.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed.*, 2006, **53**, 9603.

Table 2, entry 11

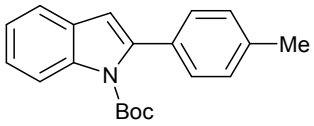


***tert*-butyl 2-(4-bromophenyl)-1H-indole-1-carboxylate 3k**

White solid (48.0 mg, 43%). mp: 89-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 8.4 Hz, 1H), 7.53-7.49 (m, 3H), 7.34-7.30 (m, 1H), 7.28-7.21 (m, 3H), 6.53 (s, 1H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 139.2, 137.4, 133.9, 130.9, 130.3, 129.1, 124.6, 123.0, 121.7, 120.5, 115.3, 110.4, 83.8, 27.6.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed.*, 2006, **53**, 9603.

Table 2, entry 12

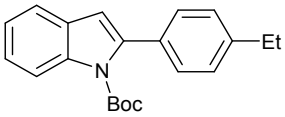


***tert*-butyl 2-(p-tolyl)-1H-indole-1-carboxylate 3l**

White solid; mp: 120-122 ^{o}C; 61.8 g, 67% yield; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.26-7.23 (m, 3H), 7.18-7.12 (m, 3H), 6.45 (s, 1H), 2.33 (s, 3H), 1.27 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.3, 140.7, 137.4, 132.0, 129.3, 128.6, 128.4, 124.1, 122.8, 120.3, 115.1, 109.6, 83.3, 27.6, 21.3, 1.0.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed.*, 2006, **53**, 9603.

Table 2, entry 13

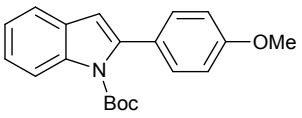


***tert*-butyl 2-(4-ethylphenyl)-1H-indole-1-carboxylate 3m**

White solid (46.3 mg, 48%). mp: 64-66 ^{o}C. IR (film) 2964, 1654, 1324, 1029, 744 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.6 Hz, 1H), 7.33-7.29 (m, 3H), 7.25-7.21 (m, 3H), 6.52 (s, 1H), 2.69 (q, J = 7.6 Hz, 2H), 1.30 (s, 9H), 1.26 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.2, 143.8, 140.6, 137.4, 132.2, 129.2, 128.7, 127.2, 124.1, 122.8, 120.3, 115.1, 109.5, 83.2, 28.7, 27.5, 15.7. HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $C_{21}H_{23}NO_2$ 322.1802; Found 322.1820.

Table 2, entry 14

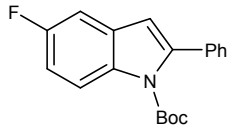


***tert*-butyl 2-(4-methoxyphenyl)-1H-indole-1-carboxylate 3n**

White solid (63.1 mg, 65%). mp: 94-95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, J = 8.4 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.38-7.31 (m, 3H), 7.28-7.24 (m, 1H), 6.97-6.95 (m, 2H), 6.52 (s, 1H), 3.87 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.2, 150.3, 140.4, 137.3, 129.9, 129.3, 127.4, 124.0, 122.8, 120.2, 115.2, 113.2, 109.5, 83.3, 55.3, 27.7.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed.*, 2006, **53**, 9603.

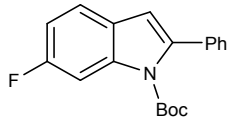
Table 2, entry 15



***tert*-butyl 5-fluoro-2-phenyl-1H-indole-1-carboxylate 3o**

Oil (49.50 mg, 53%). IR (film) 2923, 1727, 1463, 1321, 1156, 735 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 (dd, J = 8.8, 4.4 Hz, 1H), 7.40 (s, 5H), 7.20 (d, J = 8.8 Hz, 1H), 7.05 (t, J = 8.8 Hz, 1H), 6.51 (s, 1H), 1.29 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.5, 158.2, 150.0, 142.0, 134.7, 133.7, 130.0, 129.9, 128.7, 127.8, 116.3, 116.2, 112.1, 111.8, 109.5, 105.9, 105.6, 83.6, 29.7, 27.5.

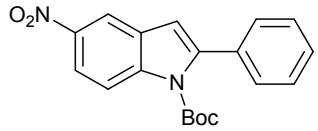
Table 2, entry 16



***tert*-butyl 6-fluoro-2-phenyl-1H-indole-1-carboxylate 3p**

Oil (64.44 mg, 69%). IR (film) 2920, 1733, 1327, 1157, 862, 694 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 10.8 Hz, 1H), 7.48-7.44 (m, 1H), 7.40-7.36 (m, 5H), 7.01 (t, J = 8.8 Hz, 1H), 6.51 (s, 1H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 134.7, 128.7, 127.7, 125.5, 121.0, 111.3, 111.0, 109.4, 102.8, 102.6, 83.8, 29.7, 27.5.

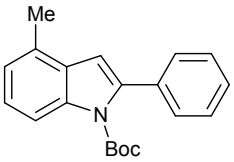
Table 2, entry 17



***tert*-butyl 5-nitro-2-phenyl-1H-indole-1-carboxylate 3q**

Oil (51.31 mg, 69%). IR (film) 2920, 1740, 1521, 1322, 1154, 748 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.48 (d, J = 2.0 Hz, 1H), 8.32 (d, J = 9.2 Hz, 1H), 8.22 (dd, J = 9.2 Hz, 1H), 7.43 (s, 5H), 6.68 (s, 1H), 1.30 (s, 9H), ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.4, 143.9, 143.5, 140.5, 133.8, 128.9, 128.7, 128.3, 128.0, 119.4, 116.7, 115.3, 109.9, 84.8, 27.4; HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}ClNO_4$ 339.1339; Found 339.1333.

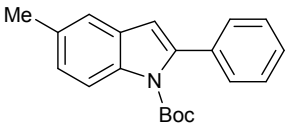
Table 2, entry 18



***tert*-butyl 4-methyl-2-phenyl-1H-indole-1-carboxylate 3r**

Oil (37.8 mg, 41%). IR (film) 2923, 1731, 1328, 1140, 758, 697 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.05 (d, J = 8.4 Hz, 1H), 7.38-7.35 (m, 5H), 7.23 (d, J = 8 Hz, 1H), 7.06 (d, J = 7.6 Hz, 1H), 6.60 (s, 1H), 2.53 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.3, 139.9, 137.2, 135.1, 129.9, 128.8, 128.7, 127.8, 127.5, 124.4, 123.3, 112.7, 108.4, 83.3, 27.5, 18.4; HRMS (ESI-TOF) m/z: $[M + NH_4]^+$ Calcd for $C_{20}H_{18}ClNO_4$ 308.1645; Found 308.1633.

Table 2, entry 19



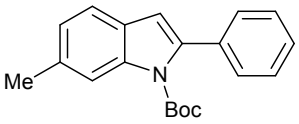
***tert*-butyl 5-methyl-2-phenyl-1H-indole-1-carboxylate 3s**

Oil (43.4 mg, 47%). mp: 59-60 ^oC. IR (film) 3422, 2918, 1732, 1384, 1132, 767 cm^{-1}.

^1H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, J = 8.4 Hz, 1H), 7.38-7.26 (m, 6H), 7.15 (d, J = 8.4 Hz, 1H), 6.48 (s, 1H) 2.45 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.2, 140.5, 135.7, 135.1, 132.3, 129.4, 128.7, 127.7, 127.5, 125.6, 120.3, 114.8, 109.7, 83.2, 27.6, 21.3.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed*., 2006, **53**, 9603.

Table 2, entry 20

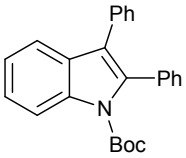


***tert*-butyl 6-methyl-2-phenyl-1H-indole-1-carboxylate 3t**

Oil (48.9 mg, 53%). mp: 59-60 ^oC. IR (film) 2977, 1732, 1328, 1157, 753 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.07 (s, 1H), 7.42 (dd, J = 13.2 Hz, 6H), 7.09 (d, J = 8.0 Hz, 1H), 6.51 (s, 1H), 2.51 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.3, 139.9, 137.9, 135.2, 134.3, 128.7, 127.7, 127.4 126.9, 124.3, 120.0, 115.4, 109.8, 83.2, 27.5, 22.0.

M. T. Hovey, C. T. Check, A. F. Sipher and K. A. Scheidt, *Angew. Chem. Int. Ed*., 2006, **53**, 9603.

Table 3, entry 1

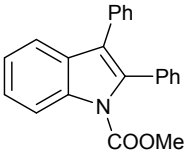


***tert*-butyl 2,3-diphenyl-1H-indole-1-carboxylate 3u**

White solid (72.0 mg, 65%). mp: 115-117 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (d, J = 8.4 Hz, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.2 Hz, 1H), 7.26-7.19 (m, 11H), 1.24 (s, 9H),; ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.3, 136.6, 135.7, 133.9, 133.4, 130.3, 130.1, 129.3, 128.1, 127.7, 127.4, 126.6, 124.7, 123.0, 121.9, 119.6, 115.2, 83.3, 27.5.

Y. Hoshino, Y. Shibata and K. Tanaka. *Adv. Synth. Catal*., 2014, **356**, 1577.

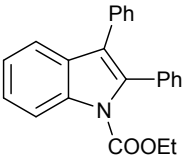
Table 3, entry 2



methyl 2,3-diphenyl-1H-indole-1-carboxylate 3v

White solid (52.1 mg, 53%). mp: 171-174 °C. IR (film) 2946, 1645, 1321, 1050, 1015 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.42-7.38 (m, 1H), 7.31-7.21 (m, 11H), 3.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.3, 136.1, 135.9, 133.1, 133.0, 130.3, 130.1, 129.6, 128.2, 127.7, 127.6, 126.8, 124.9, 123.4, 122.7, 119.8, 115.5, 53.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{17}NO_2$ 328.1332; Found 328.1335.

Table 3, entry 3



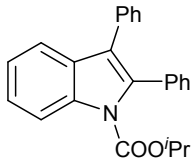
ethyl 2,3-diphenyl-1H-indole-1-carboxylate 3w

Oil (56.3 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.42-7.38 (m, 1H), 7.31-7.21 (m, 11H), 4.20 (q, J = 7.2 Hz, 2H), 1.03 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.8, 136.3, 135.8, 133.4, 133.2, 130.4, 130.1, 129.5, 128.1, 127.6, 127.5, 126.7, 124.9, 123.3, 122.5, 119.7, 115.4, 62.8, 13.6.

H. Minami, T. Kanayama, R. Tanaka, N. Okamoto and T. Sueda, *Eur. J. Org. Chem*., 2016,

5990.

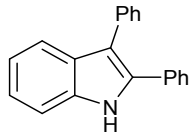
Table 3, entry 4



isopropyl 2,3-diphenyl-1H-indole-1-carboxylate 3x

White solid (54.4 mg, 51%). mp: 160-162 ^oC. IR (film) 2973, 1648, 1324, 1053, 1006 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 8.31 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.42-7.38 (m, 1H), 7.31-7.22 (m, 11H), 5.04-4.98 (m, 1H), 1.05 (d, J = 6.4 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.1, 136.4, 135.8, 133.6, 130.5, 130.1, 129.4, 128.1, 127.6, 126.7, 124.8, 123.2, 122.3, 119.7, 115.4, 71.1, 21.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{21}NO_2$ 356.1645; Found 356.1648.

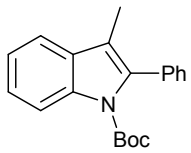
Table 3, entry 5



2,3-diphenyl-1H-indole 3y

White solid (49.3 mg, 61%). mp: 121-123 ^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.41-7.31 (m, 7H), 7.28-7.18 (m, 5H), 7.11 (t, J = 7.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.9, 135.0, 134.1, 132.7, 130.1, 128.7, 128.6, 128.5, 128.1, 127.7, 126.2, 122.7, 120.4, 119.7, 115.0, 110.9.

Table 3, entry 6



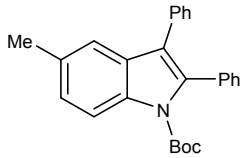
***tert*-butyl 3-methyl-2-phenyl-1H-indole-1-carboxylate 3z**

White solid (44.3 mg, 48%). mp: 97-100 ^oC.^1H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.6 Hz, 1H), 7.45-7.41 (m, 3H), 7.39-7.32 (m, 4H), 2.14 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.3, 136.5, 135.6, 134.5, 130.4, 130.2, 129.8, 127.8, 127.3, 124.5, 122.6, 118.6, 116.3, 115.1, 82.7, 27.5, 9.1.

(1) K. Sun, S. Liu, P. B. Bec and T. G. Driver, *Angew. Chem. Int. Ed.*, 2011, **50**, 1702.

(2) M. Todd Hovey, Christopher T. Check, Alexandra F. Sipher and Karl A. Scheidt, *Angew. Chem. Int. Ed.*, 2014, **53**, 9603.

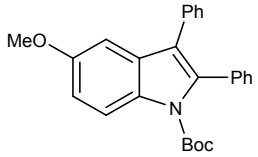
Table 3, entry 7



***tert*-butyl 5-methyl-2-phenyl-1H-indole-1-carboxylate 3aa**

Oil (57.5 mg, 50%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (s, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.25-7.19 (m, 9H), 7.09 (d, J = 8.0 Hz, 1H), 6.83 (s, 1H), 2.52 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.4, 137.0, 135.0, 134.8, 134.1, 133.6, 130.3, 130.1, 128.1, 127.7, 127.3, 126.5, 124.4, 121.8, 119.2, 115.3, 83.1, 27.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{25}NO_2$ 384.1958; Found 384.1951.

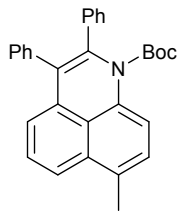
Table 3, entry 8



***tert*-butyl 5-methoxy-2-phenyl-1H-indole-1-carboxylate 3ab**

Oil (55.1 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.57-7.53 (m, 1H), 7.35 (d, J = 8.0 Hz, 2H), 7.24-7.20 (m, 3H), 7.07-6.95 (m, 2H), 6.84 (s, 3H), 6.49 (d, J = 8.8 Hz, 1H), 3.80 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7, 152.3, 137.0, 132.3, 131.6, 131.5, 131.3, 131.2, 128.7, 128.3, 128.2, 127.6, 127.5, 126.5, 126.4, 110.5, 104.9, 81.1, 55.5, 28.3. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{25}NO_3$ 400.1907; Found 400.1894.

Scheme 3

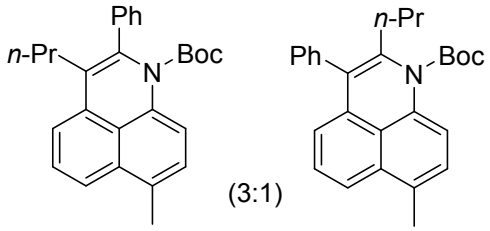


***tert*-butyl 7-methyl-2,3-diphenyl-1H-benzo[de]quinoline-1-carboxylate 6a**

White solid (39.0 mg, 30%). mp: 176-177 °C. IR (film) 2926, 2357, 1654, 1036, 1018 cm^{-1}.

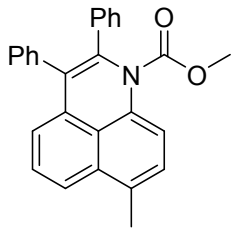
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.35-7.32 (m, 1H), 7.30-7.23 (m, 4H), 7.20-7.14 (m, 4H), 7.12-7.09 (m, 3H), 6.77 (d, J = 7.6 Hz, 1H), 2.57 (s, 3H), 1.06 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.9, 139.5, 137.1, 136.8, 135.2, 132.6, 131.2, 129.3, 128.4, 127.9, 127.3, 127.0, 126.9, 126.8, 126.3, 121.4, 119.5, 114.1, 82.6, 27.3, 26.9, 19.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{29}H_{25}NO_2$ 433.2036; Found 433.2033.

X. Zhang, W. Si, M. Bao. N. Asao, Y. Yamamoto and T. Jin, *Org. Lett*., 2014, **16**, 4830.



6b **6b'**

Yellow oil; 43mg, isolated yield 38%; ^{1}H NMR (400MHz, $CDCl_3$) δ 7.77 (d, J = 8 Hz, 1H), 7.62-7.55 (m, 2H), 7.46-7.37 (m, 6H), 7.33 (d, J = 6.8 Hz, 1H), 7.29-7.21 (m, 3H), 6.50 (d, J = 6.8 Hz, 0.33 H), 2.55 (s, 4H), 2.51-2.47 (m, 2.66H), 1.57-1.52 (m, 5.6H), 1.06 (s, 9H), 0.82-0.74 (m, 4.2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 152.9, 139.7, 138.5, 138.0, 136.1, 135.0, 134.9, 133.0, 132.6, 132.1, 131.6, 130.9, 130.0, 129.6, 128.8, 128.2, 127.9, 127.6, 127.4, 127.4, 126.8, 126.6, 126.4, 126.2, 122.9, 121.3, 121.1, 119.7, 118.5, 117.4, 116.2, 113.5, 82.6, 82.5, 34.9, 30.8, 28.1, 27.4, 22.7, 21.4, 19.1, 19.0, 14.2, 13.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{27}H_{29}NO_2$ 400.2271; Found 400.2265.

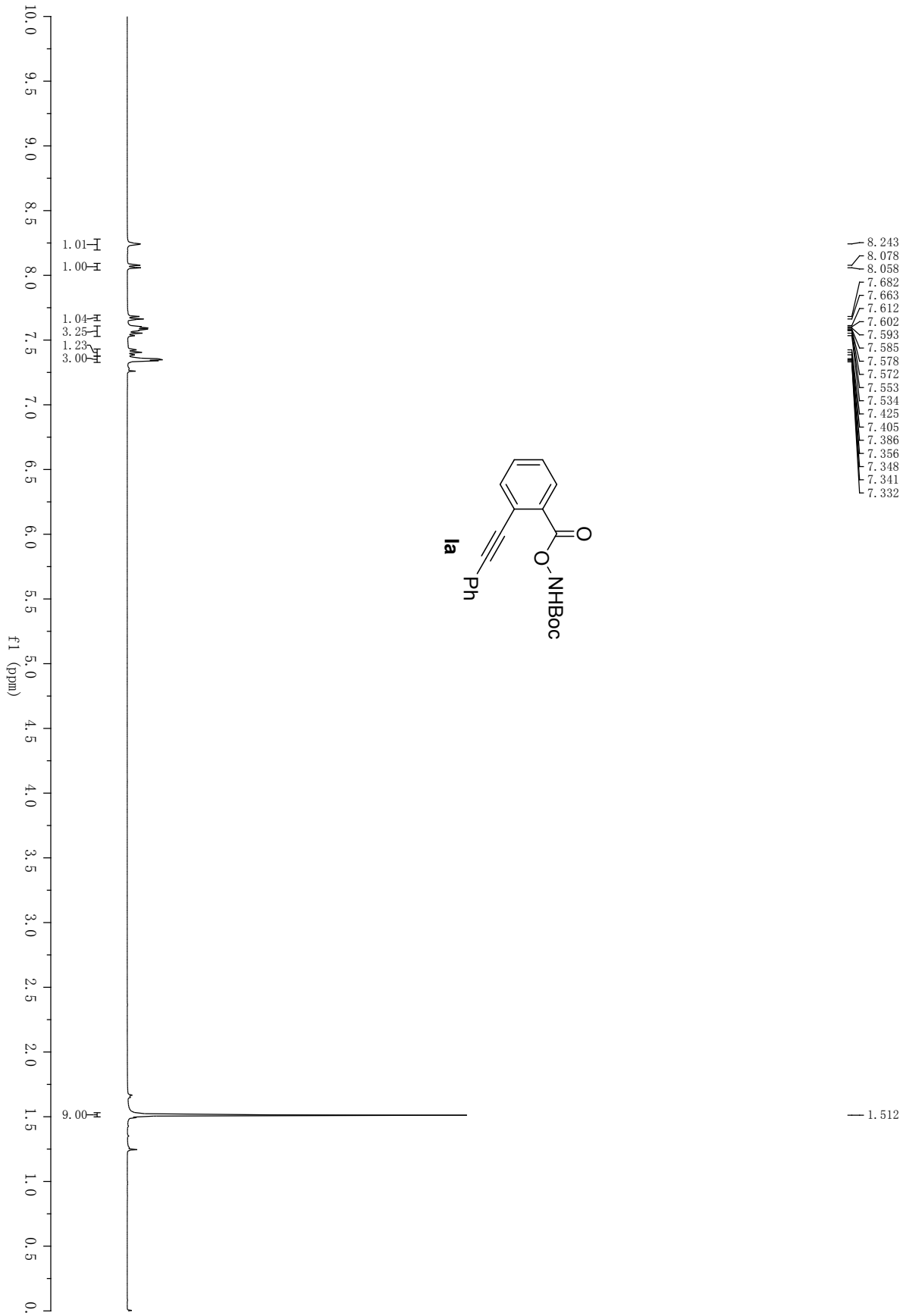


methyl 7-methyl-2,3-diphenyl-1H-benzo[de]quinoline-1-carboxylate 6c

Yellow solid; 56mg, isolated yield 48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 7.9 Hz, 1H), 7.61 (d, J = 8.5 Hz, 1H), 7.34 (d, J = 7.9 Hz, 1H), 7.29-7.24 (m, 4H), 7.17-7.08 (m, 7H), 6.80 (d, J = 7.2 Hz, 1H), 3.35 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.9,

139.1, 136.8, 136.5, 134.6, 132.5, 132.2, 131.1, 128.7, 128.7, 128.4, 127.7, 127.4, 127.0, 126.9, 126.8, 126.7, 126.4, 121.9, 120.3, 115.4, 53.1, 19.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{27}H_{21}NO_2$ 392.1645; Found 392.1654.

NMR spectra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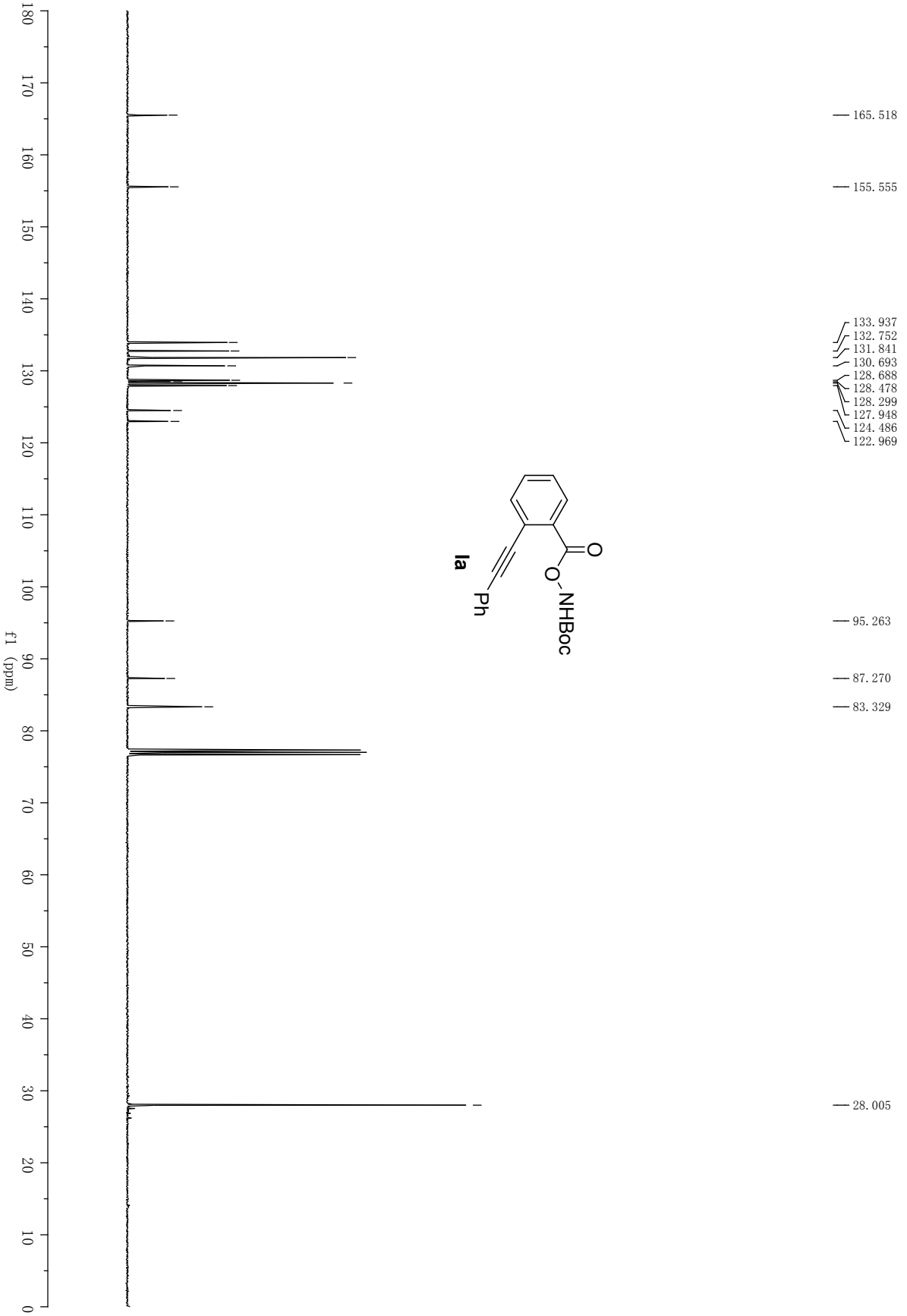
8.058
7.682
7.663
7.612
7.602
7.593
7.585
7.578
7.572
7.553
7.534
7.425
7.405
7.386
7.356
7.348
7.341
7.332
1.512
1.01
1.00
1.04
3.25
1.23
3.00
9.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
O
NHBoc
Ph
Ia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155.555
133.937
132.752
131.841
130.693
128.688
128.478
128.299
127.948
124.486
122.969
95.263
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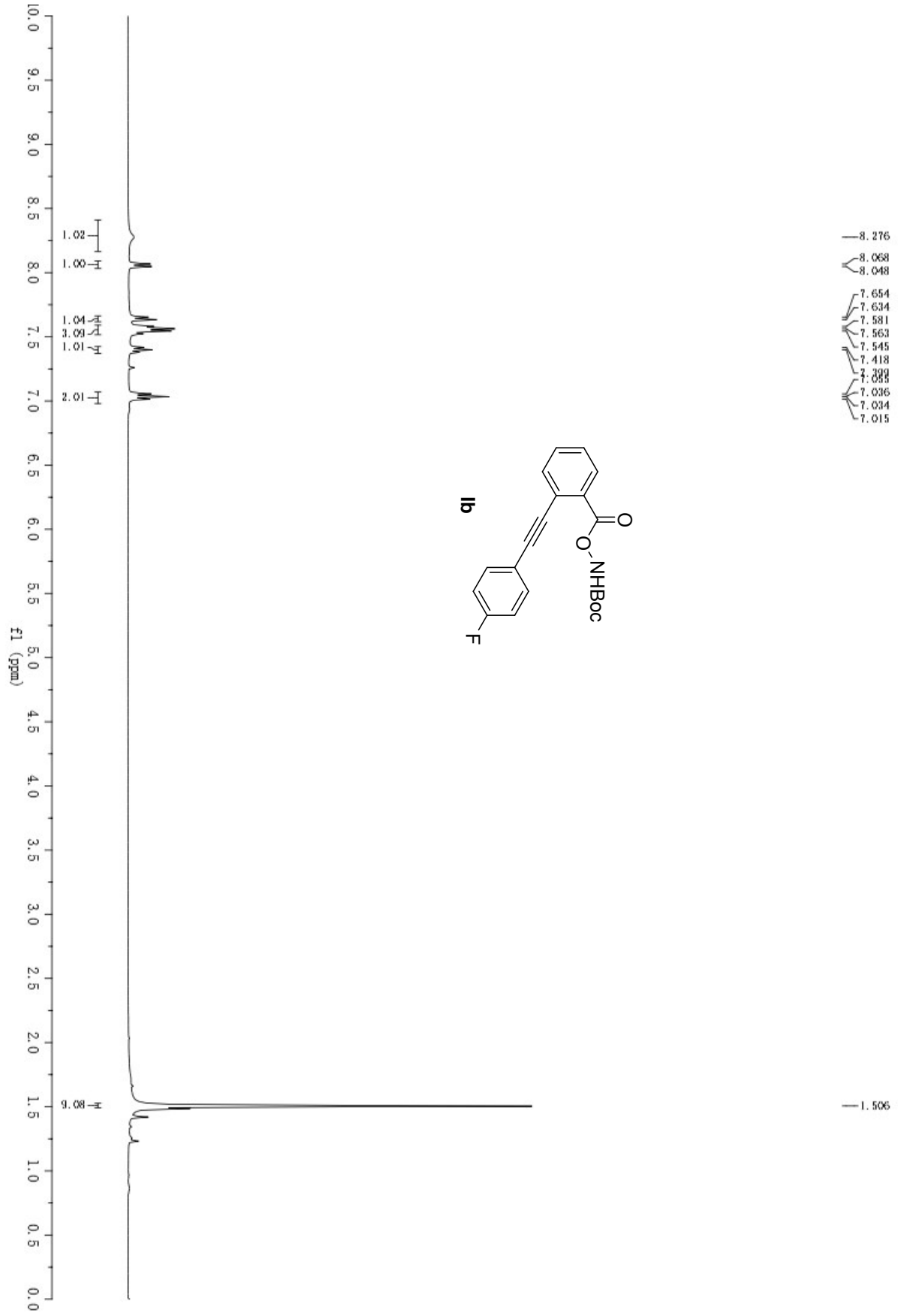
83.329
28.005
f1 (ppm)
Ph
O
O
NHBoc

Ia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7.634
7.581
7.563
7.545
7.418
7.399
7.055
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7.034
7.015
1.506
1.02
1.00
1.04
3.09
1.01
2.01
9.08
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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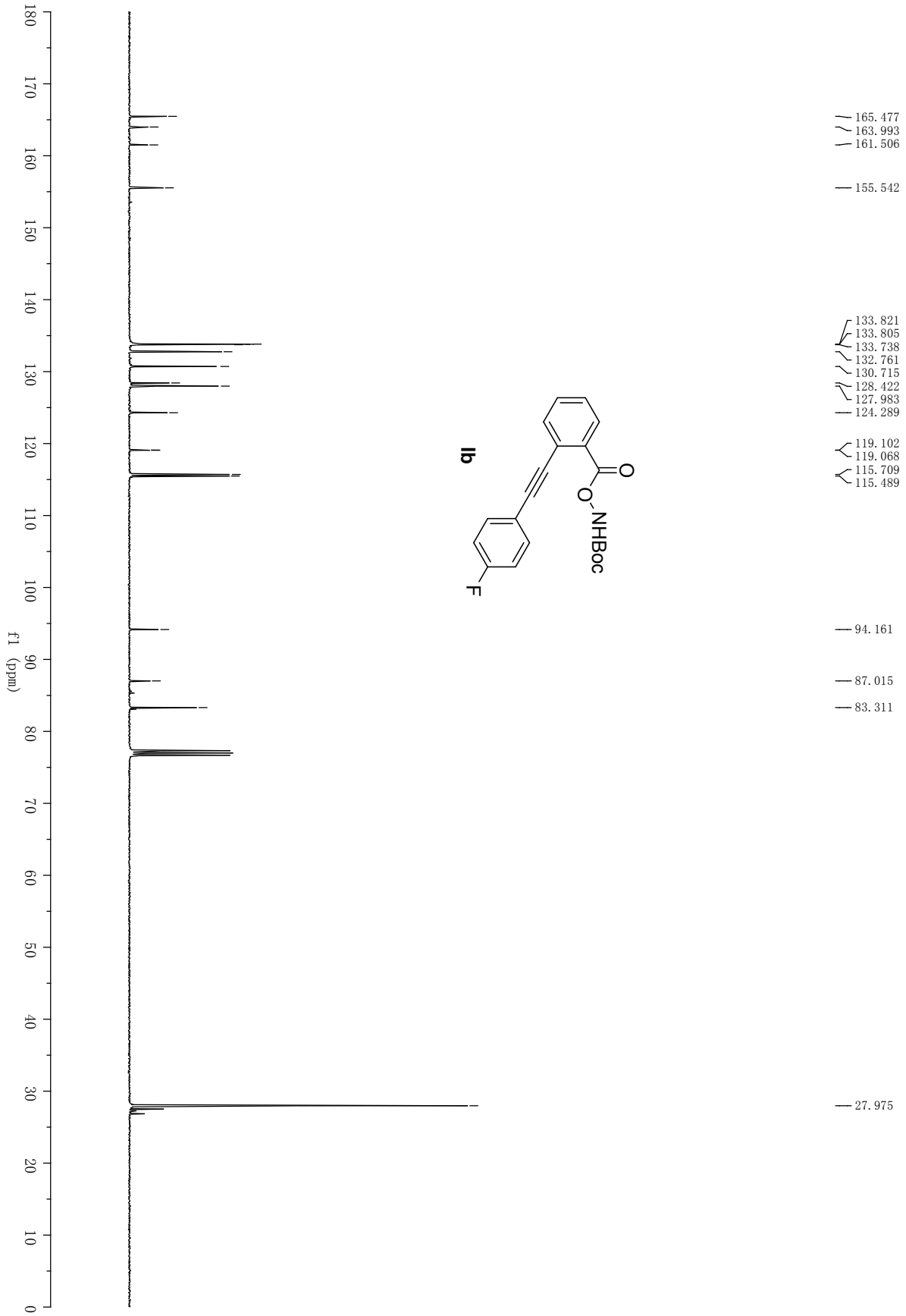
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

Ib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163.993
161.506
155.542
133.821
133.805
133.738
132.761
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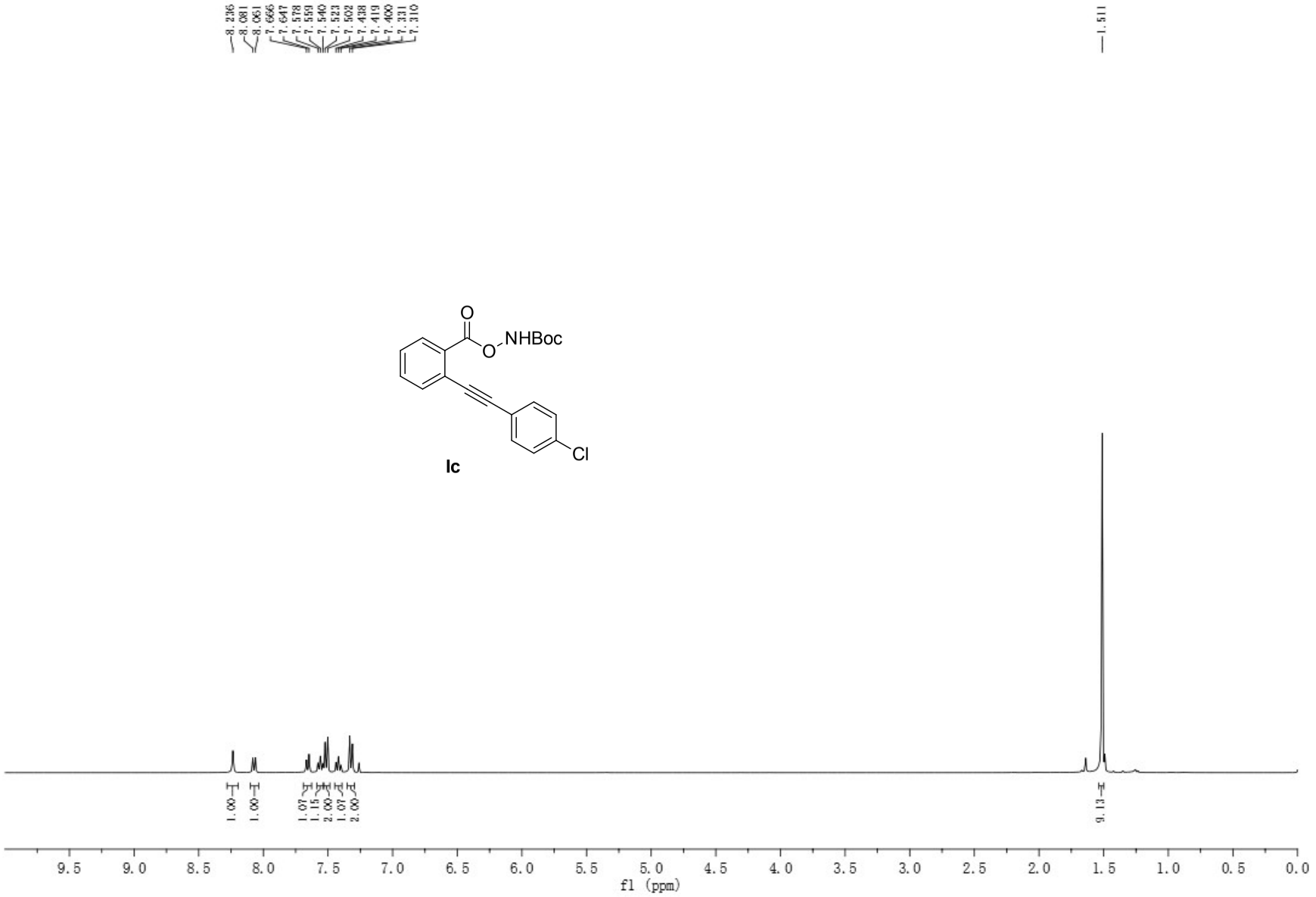
128.422
127.983
124.289
119.102
119.068
115.709
115.489
94.161
87.015
83.311
27.975
Ib
O
O
NHBoc
F
f1 (ppm)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8.061
7.666
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7.578
7.559
7.540
7.523
7.502
7.438
7.419
7.400
7.331
7.310
1.511
O
O
NHBoc
Cl
1.00
1.00
1.07
1.15
2.00
1.07
2.00
9.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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2.0
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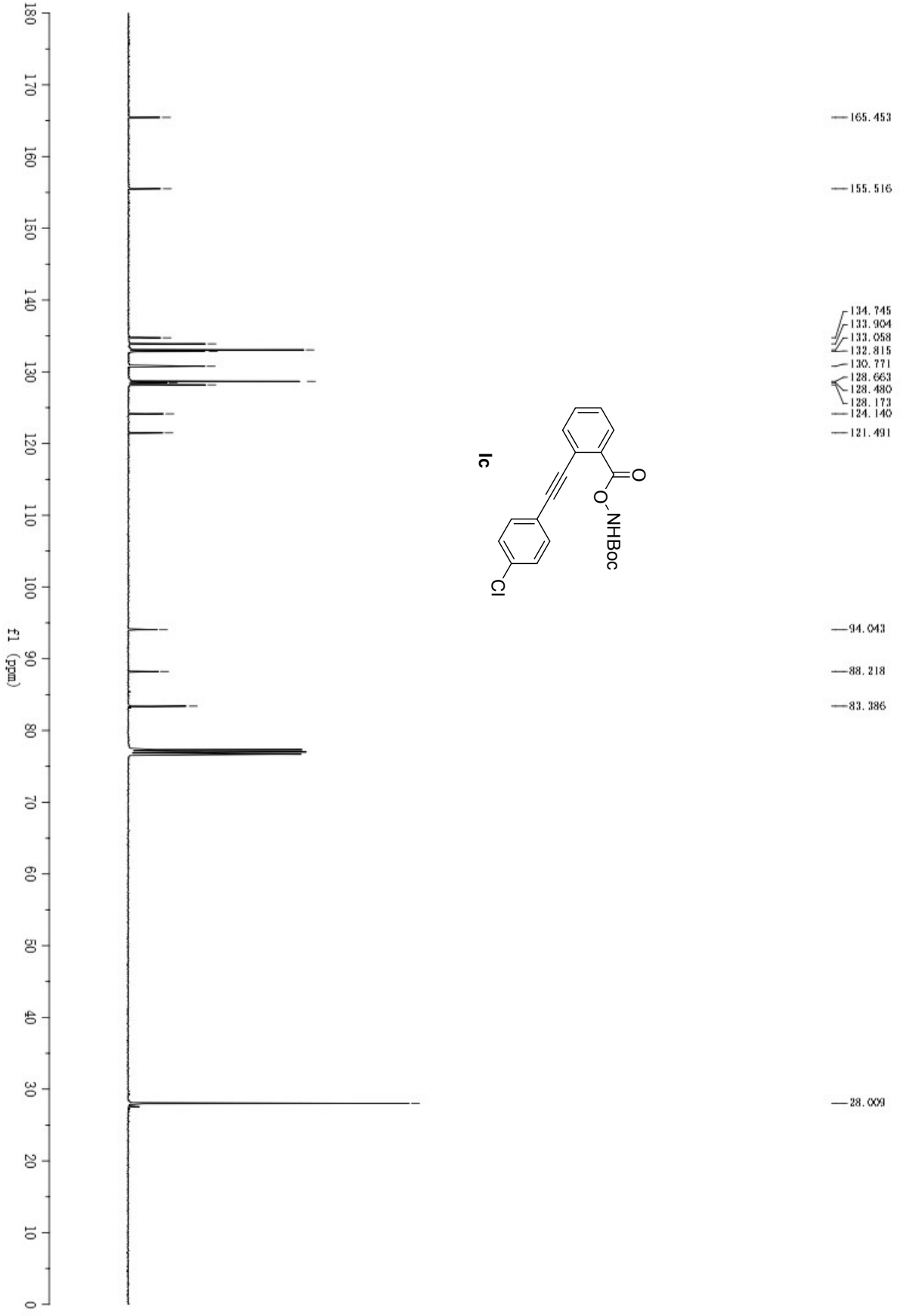
0.0
f1 (ppm)

Ic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134.745
133.904
133.058
132.815
130.771
128.663
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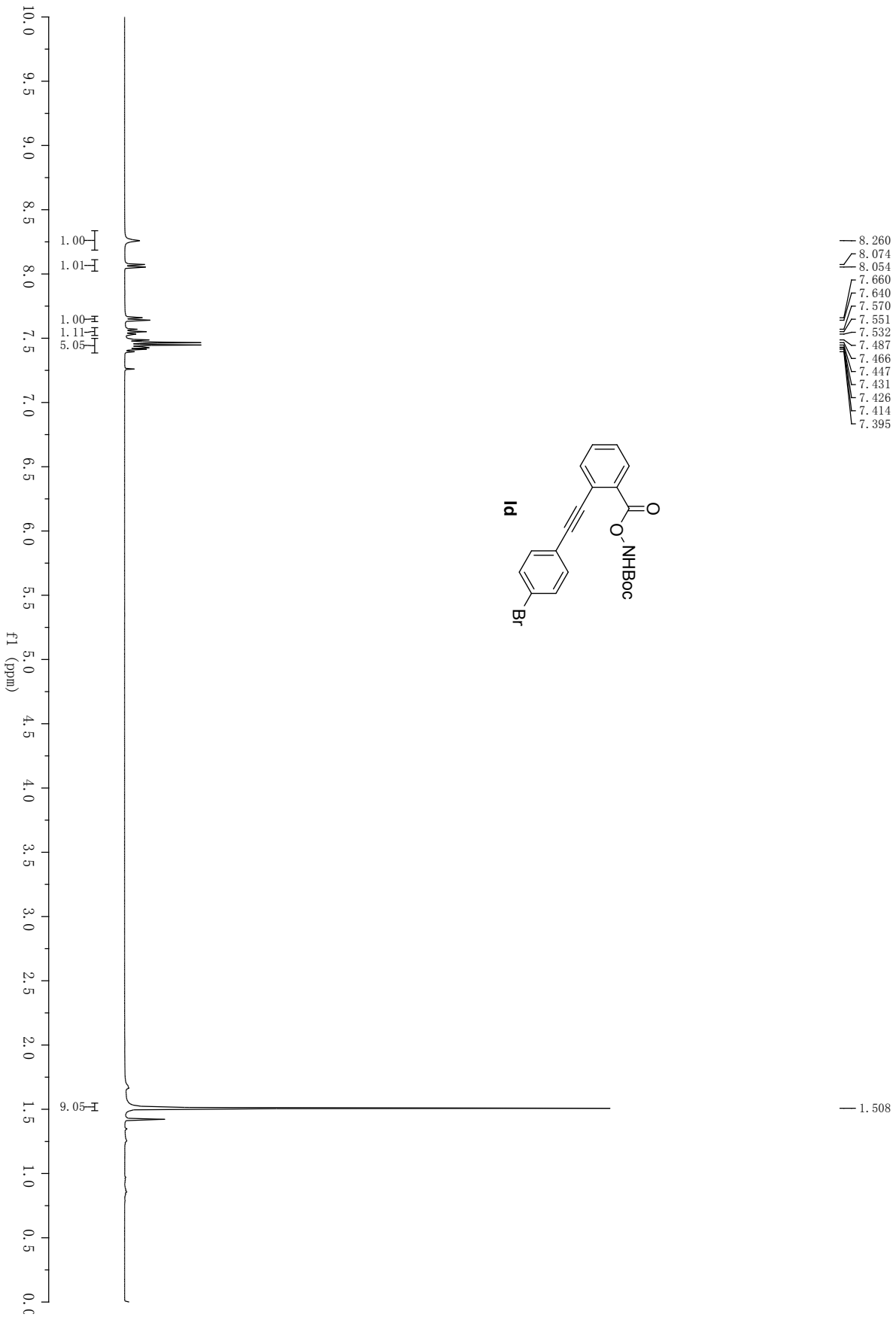
121.491
94.043
88.218
83.386
28.009
f1 (ppm)
Ic
O
O
NHBoc
Cl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7.640
7.570
7.551
7.532
7.487
7.466
7.447
7.431
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7.414
7.395
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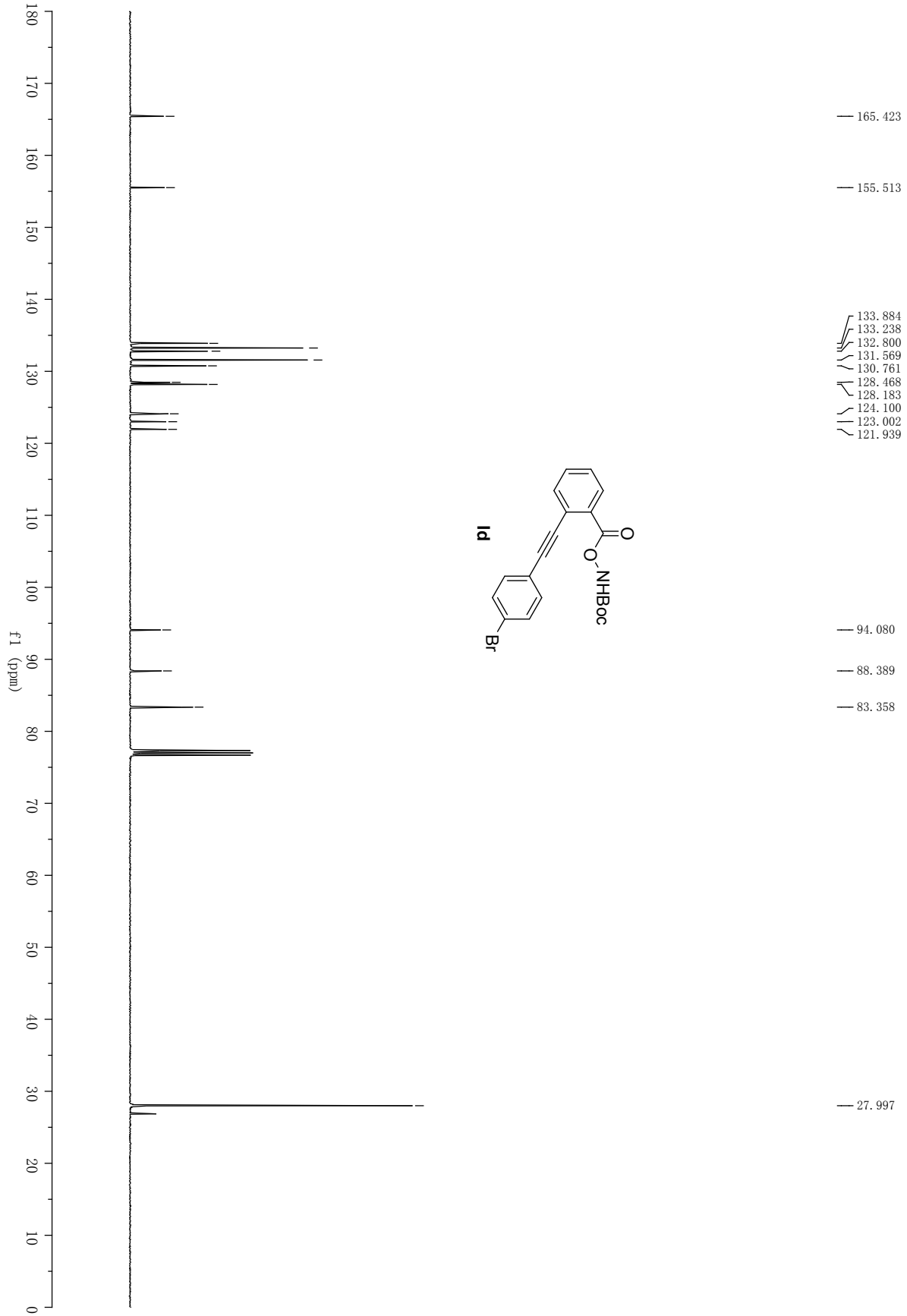
1.01
1.00
1.11
5.05
9.05
f1 (ppm)
1d
O
O
NHBoc
Br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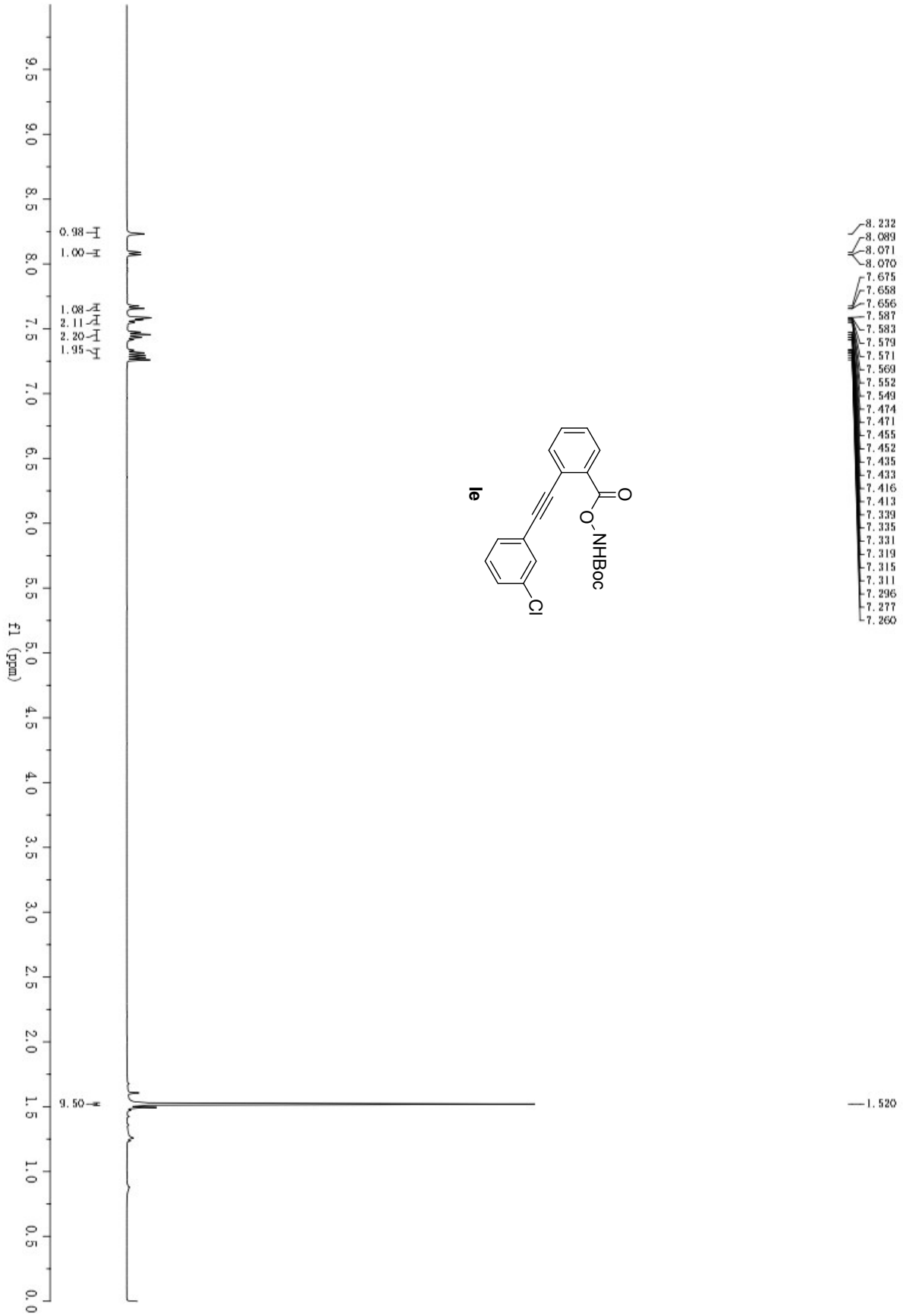
27.997
f1 (ppm)
Id
Br
NHBoc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8.070
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7.587
7.583
7.579
7.571
7.569
7.552
7.549
7.474
7.471
7.455
7.452
7.435
7.433
7.416
7.413
7.339
7.335
7.331
7.319
7.315
7.311
7.296
7.277
7.260
O
O
NHBoc
Cl
Ie
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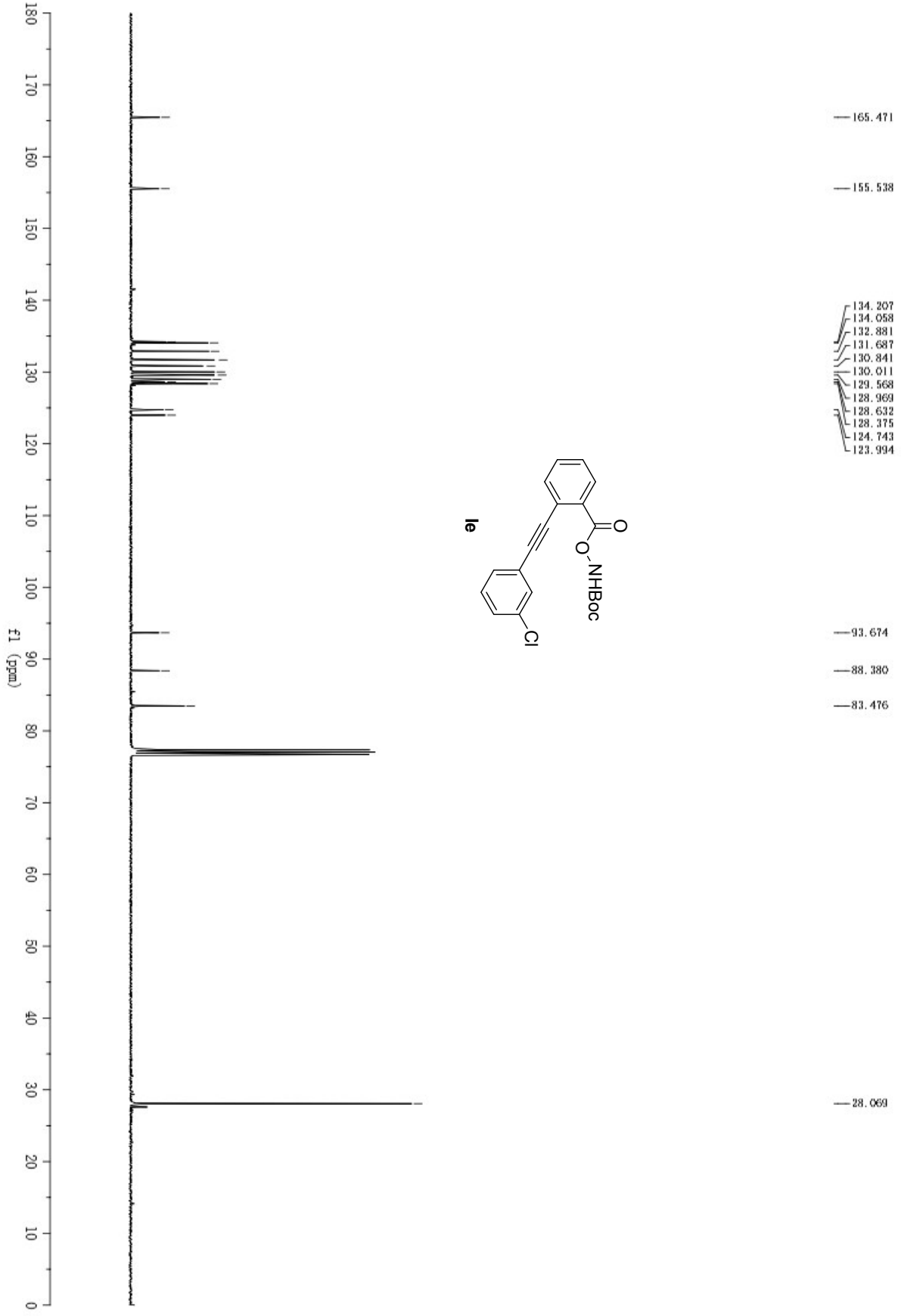
2.11
2.20
1.95
9.50
1.520
f1 (ppm)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93.674
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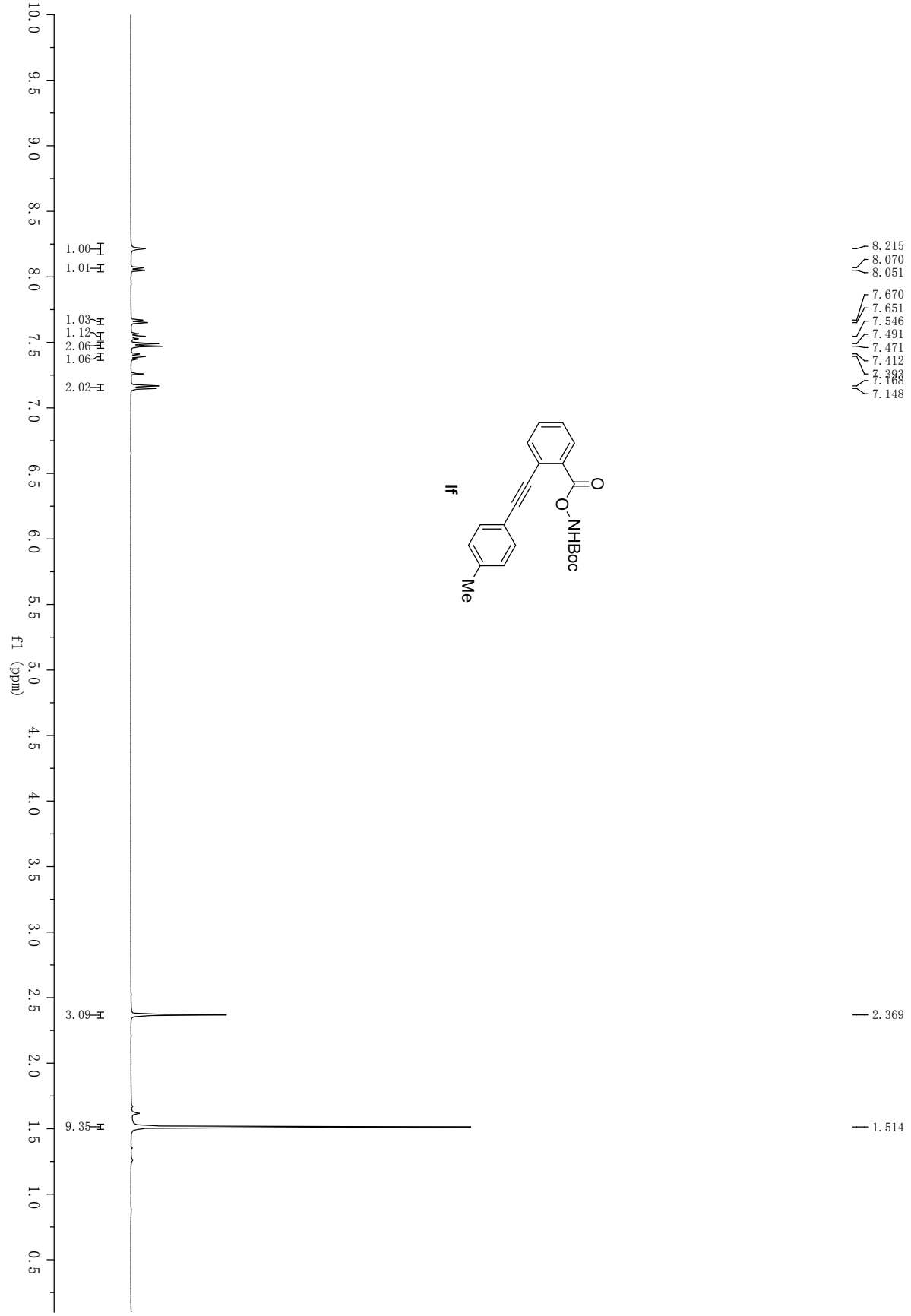
28.069
f1 (ppm)
Ie
O
O
NHBoc
Cl


10.0
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9.0
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8.0
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6.5
6.0
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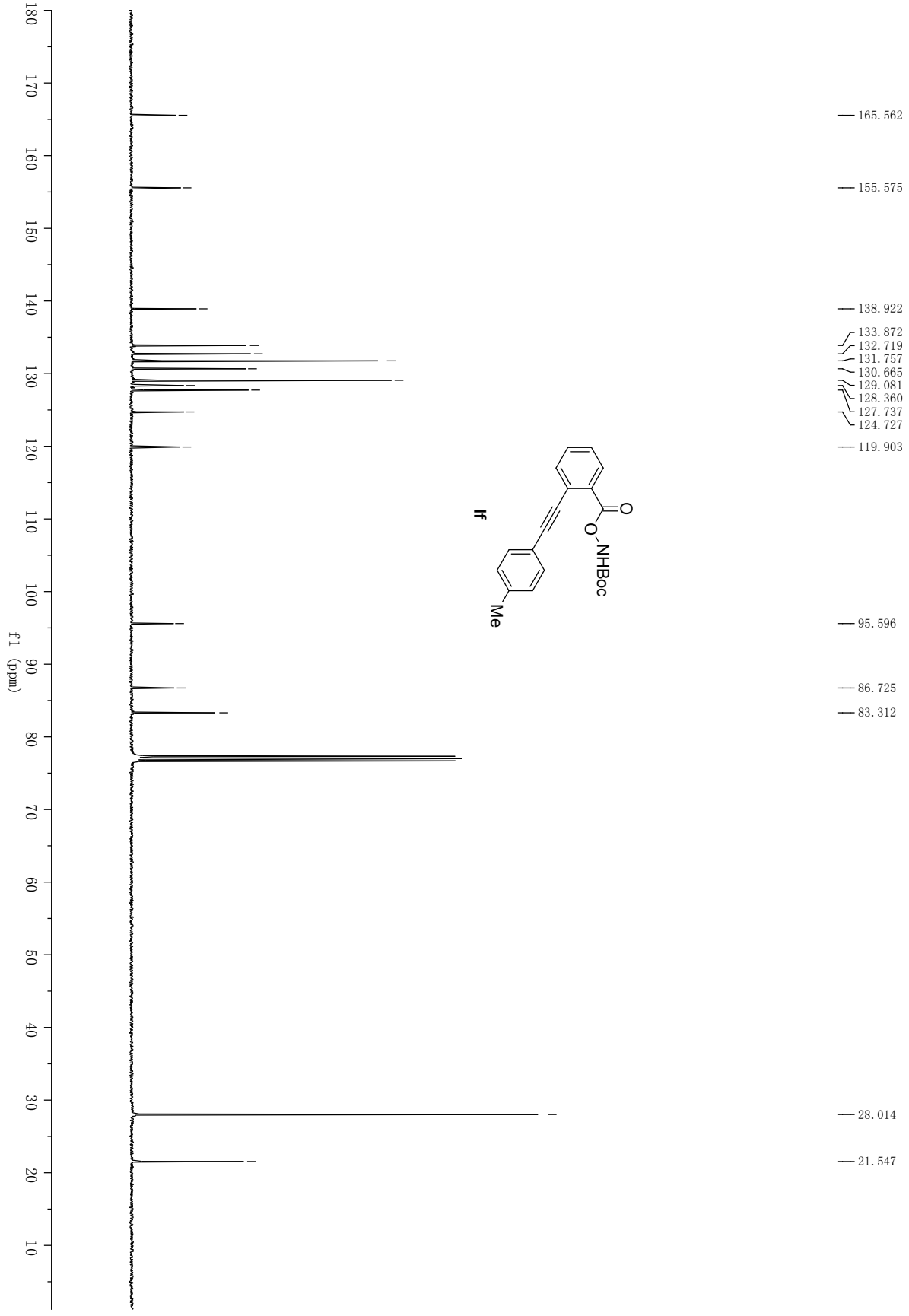
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
1.00
1.01
1.03
1.12
2.06
1.06
2.02
3.09
9.35
8.215
8.070
8.051
7.670
7.651
7.546
7.491
7.471
7.412
7.148
2.369
1.514
O
O
NHBoc
Me

1f


165.562
155.575
138.922
133.872
132.719
131.757
130.665
129.081
128.360
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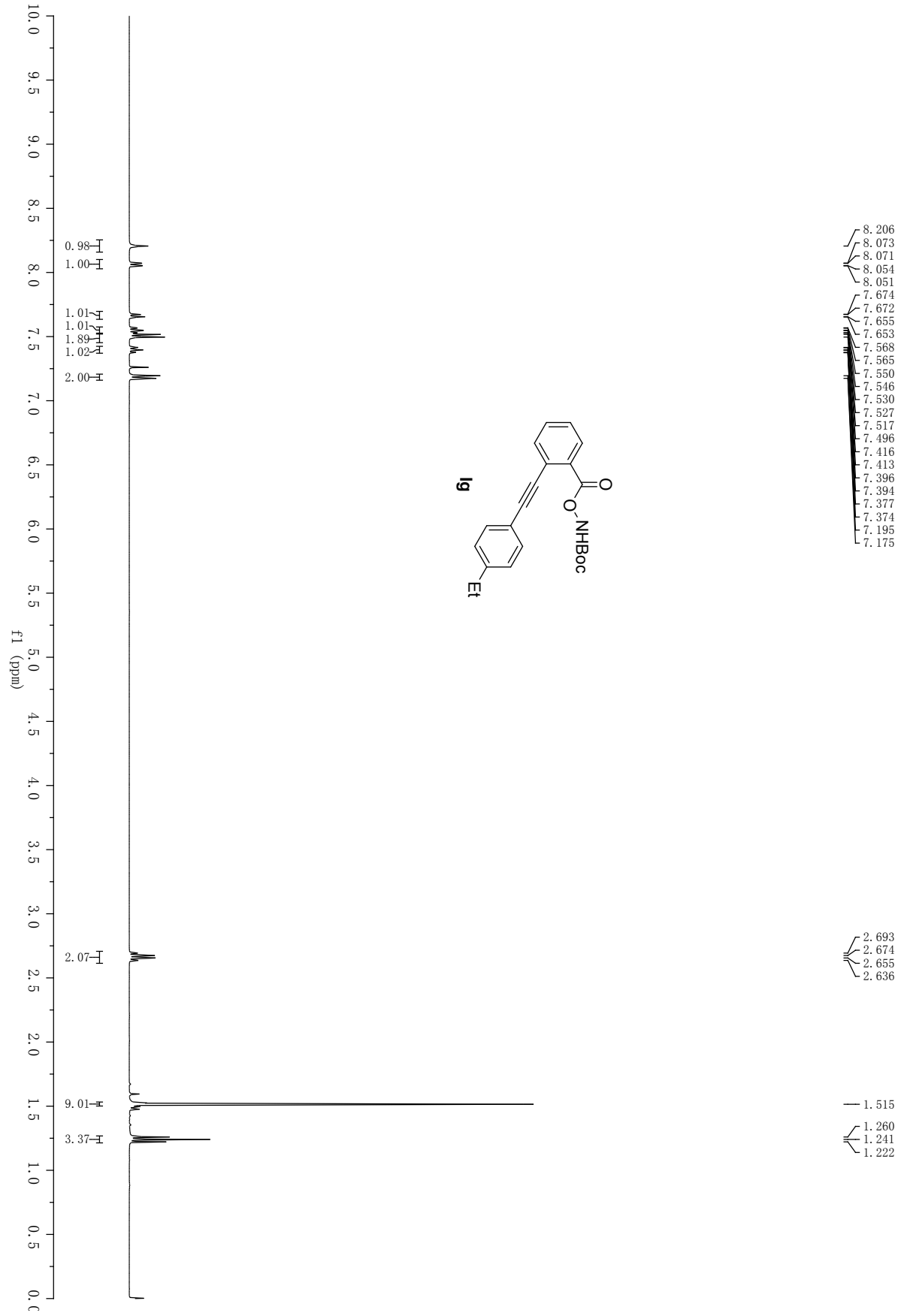
124.727
119.903
95.596
86.725
83.312
28.014
21.547
f1 (ppm)
If
NHBoc
Me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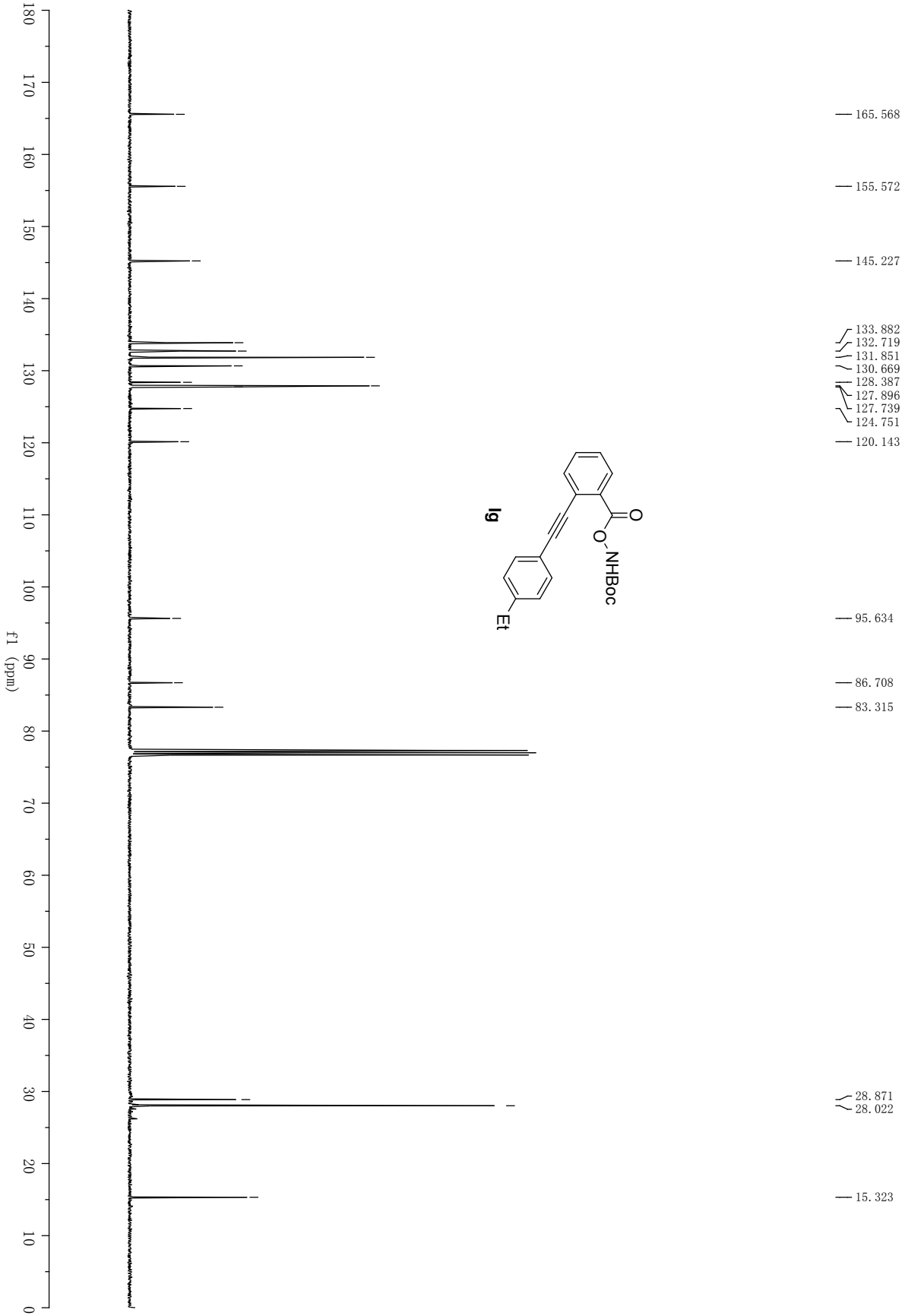
8.073
8.071
8.054
8.051
7.674
7.672
7.655
7.653
7.568
7.565
7.550
7.546
7.530
7.527
7.517
7.496
7.416
7.413
7.396
7.394
7.377
7.374
7.195
7.175
2.693
2.674
2.655
2.636
1.515
1.260
1.241
1.222
0.98
1.00
1.01
1.01
1.89
1.02
2.00
2.07
9.01
3.37
1g
O
O
NHBoc
Et
f1 (ppm)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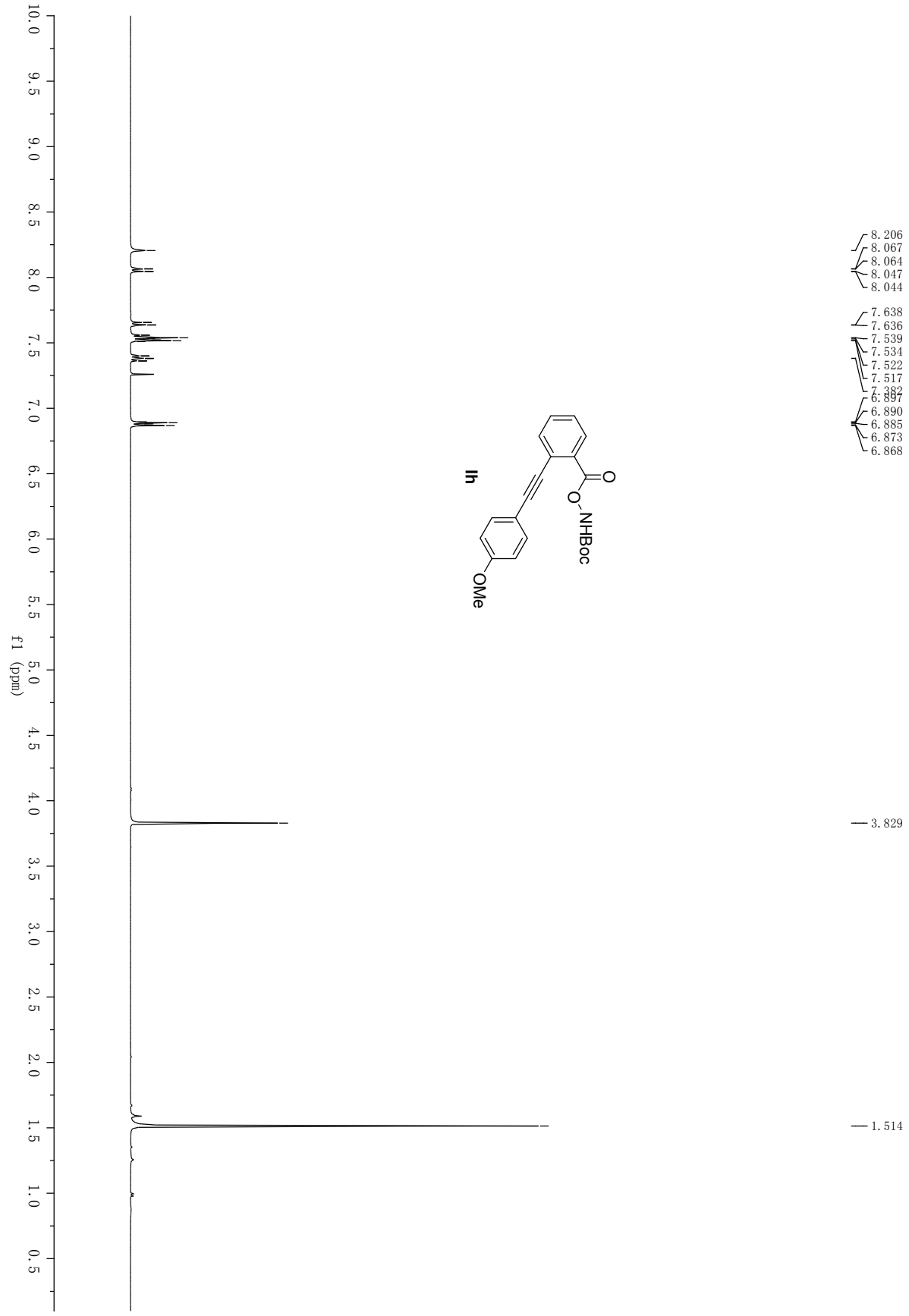
155.572
145.227
133.882
132.719
131.851
130.669
128.387
127.896
127.739
124.751
120.143
95.634
86.708
83.315
28.871
28.022
15.323
1g
O
O
NHBoc
Et
f1 (ppm)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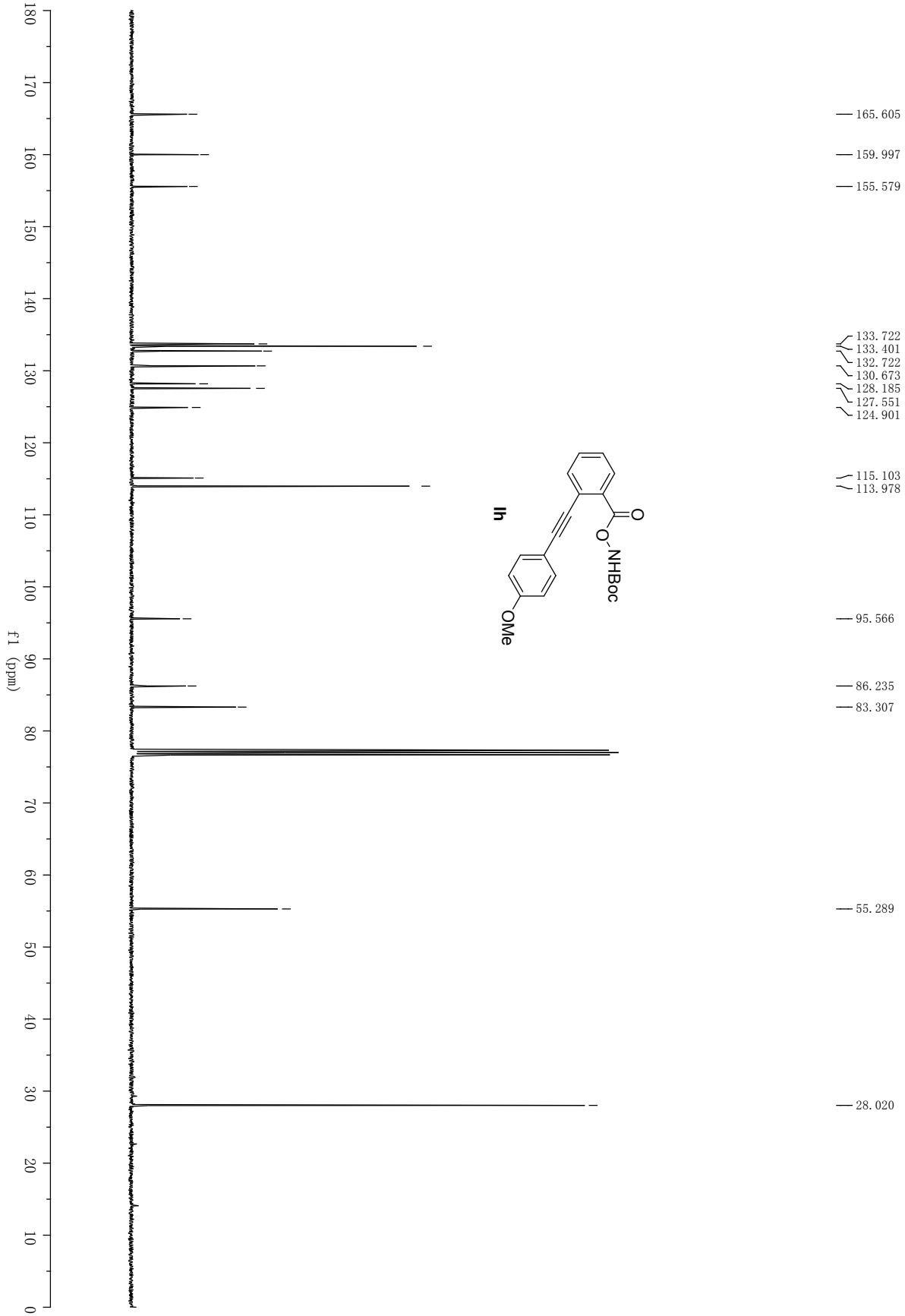
8.067
8.064
8.047
8.044
7.638
7.636
7.539
7.534
7.522
7.517
7.382
6.897
6.890
6.885
6.873
6.868
3.829
1.514
1h
O
O
NHBoc
OMe
f1 (ppm)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133.401
132.722
130.673
128.185
127.551
124.901
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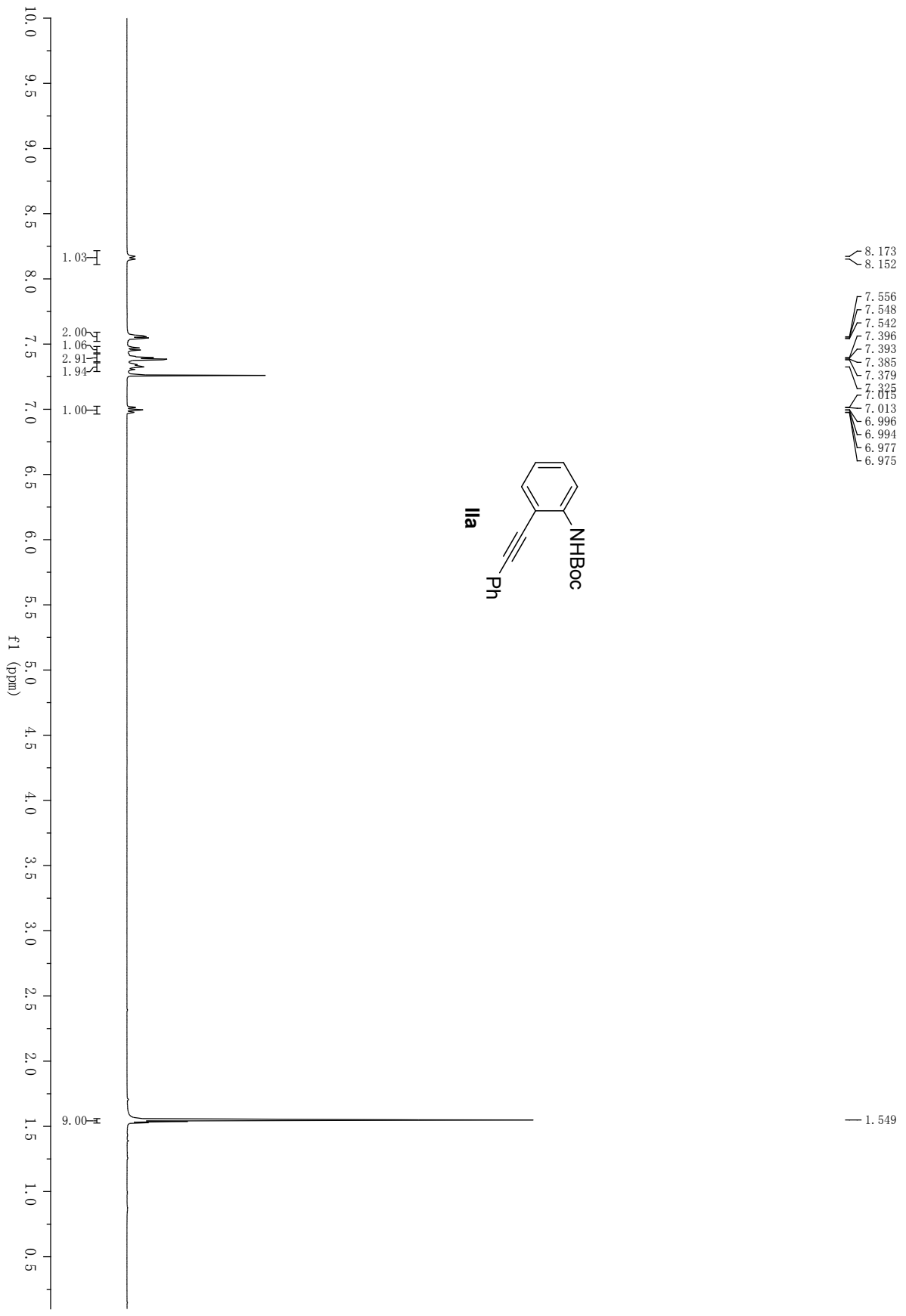
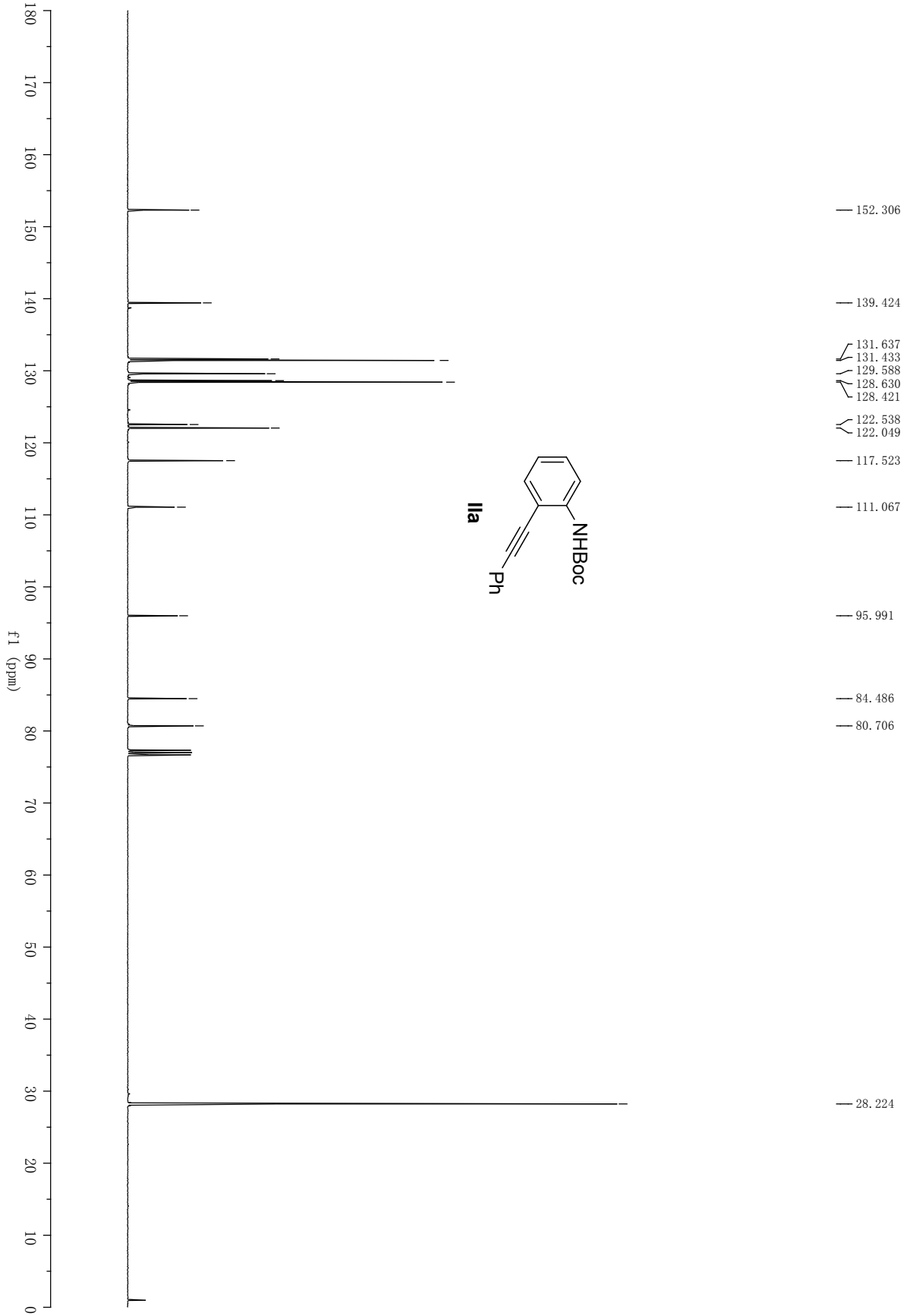
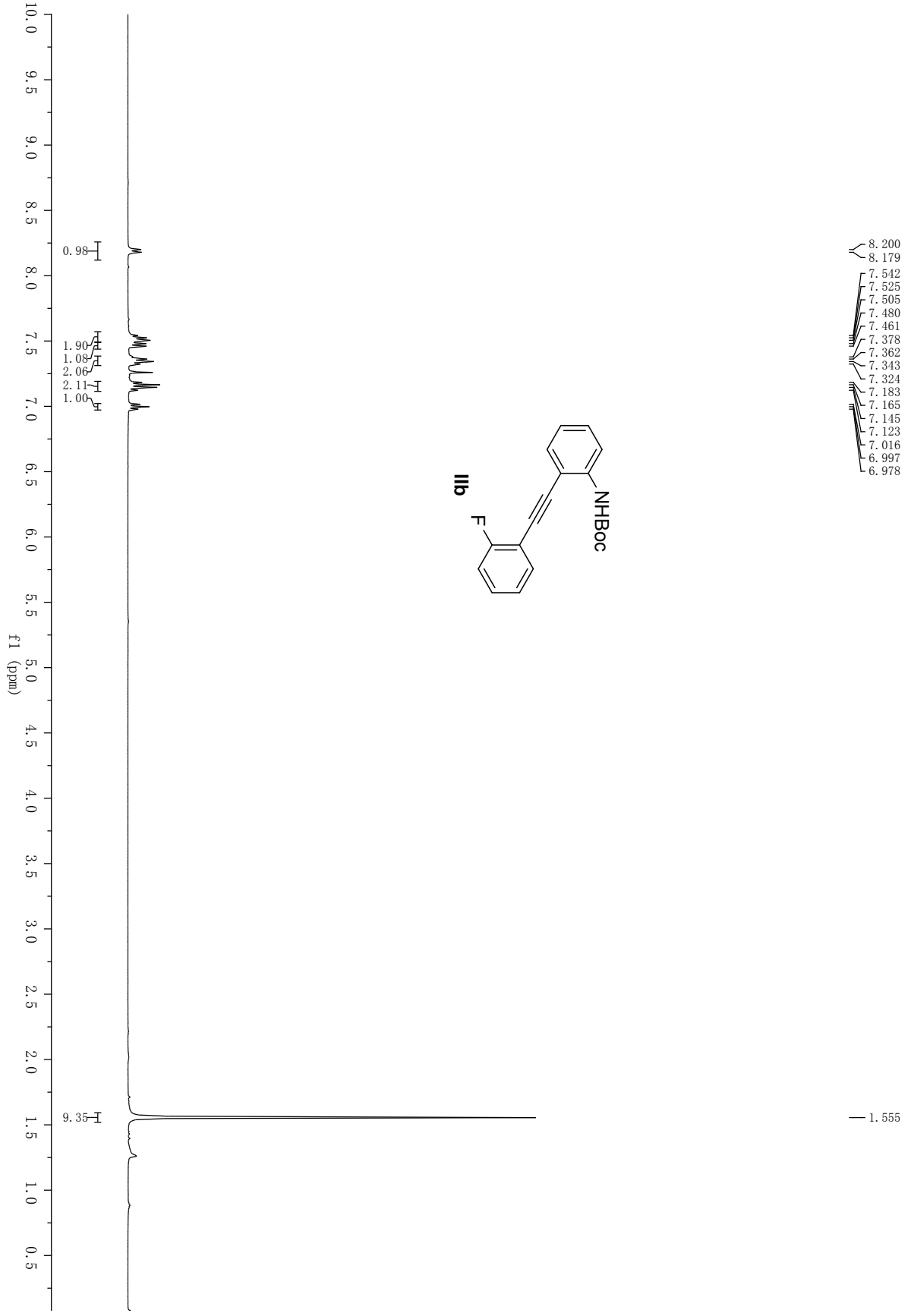
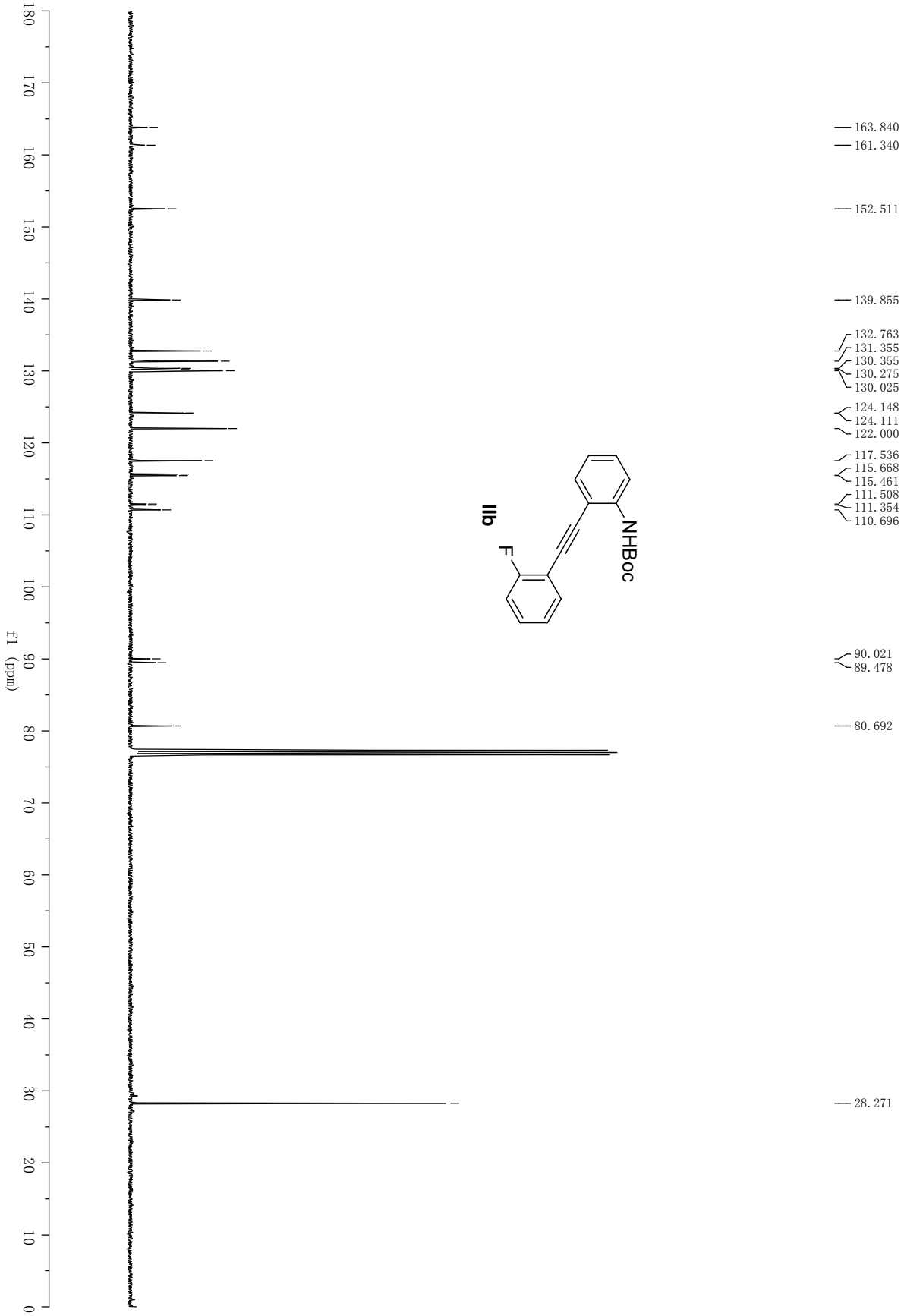
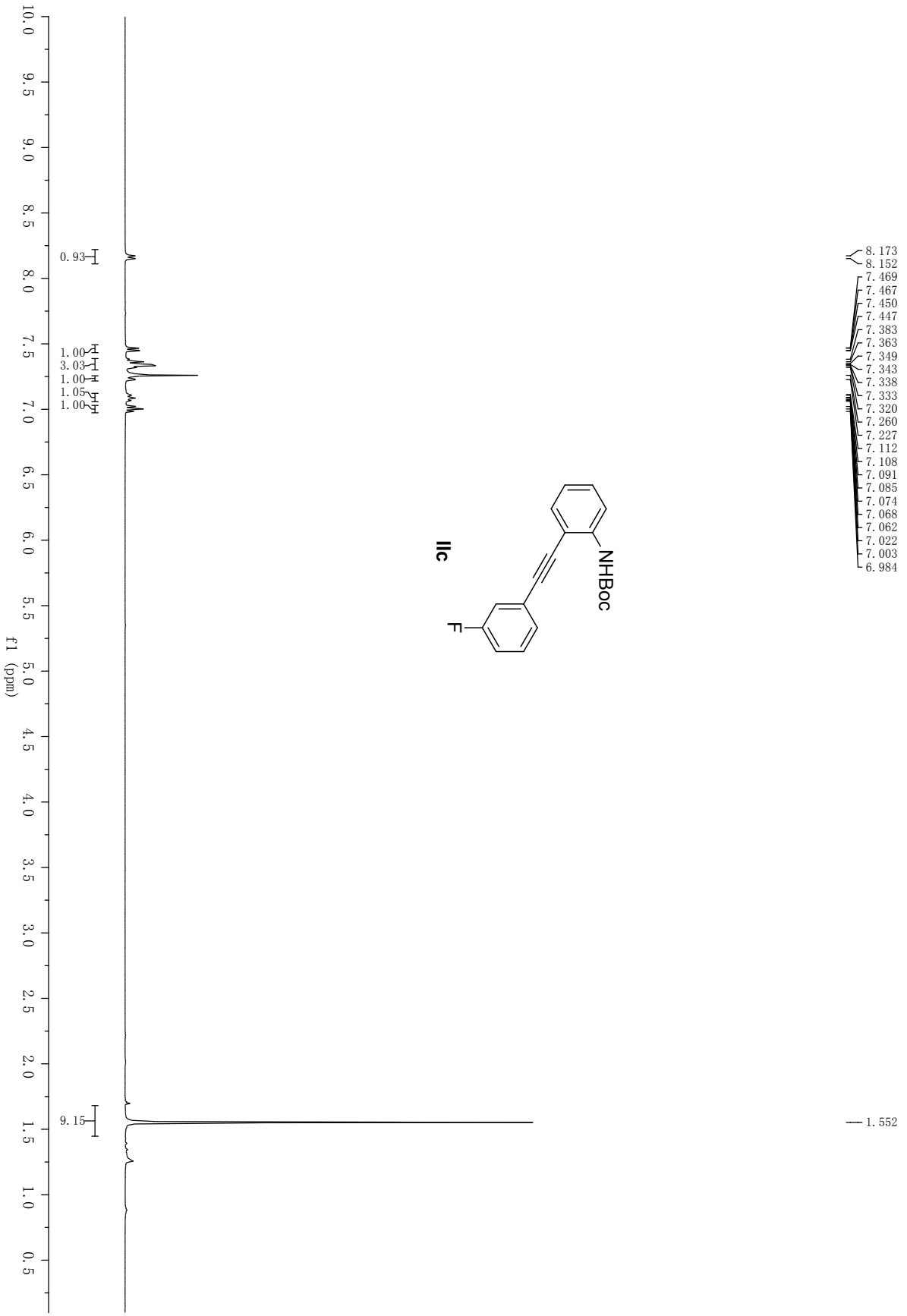
113.978
95.566
86.235
83.307
55.289
28.020
1h
O
O
NHBoc
OMe
f1 (ppm)

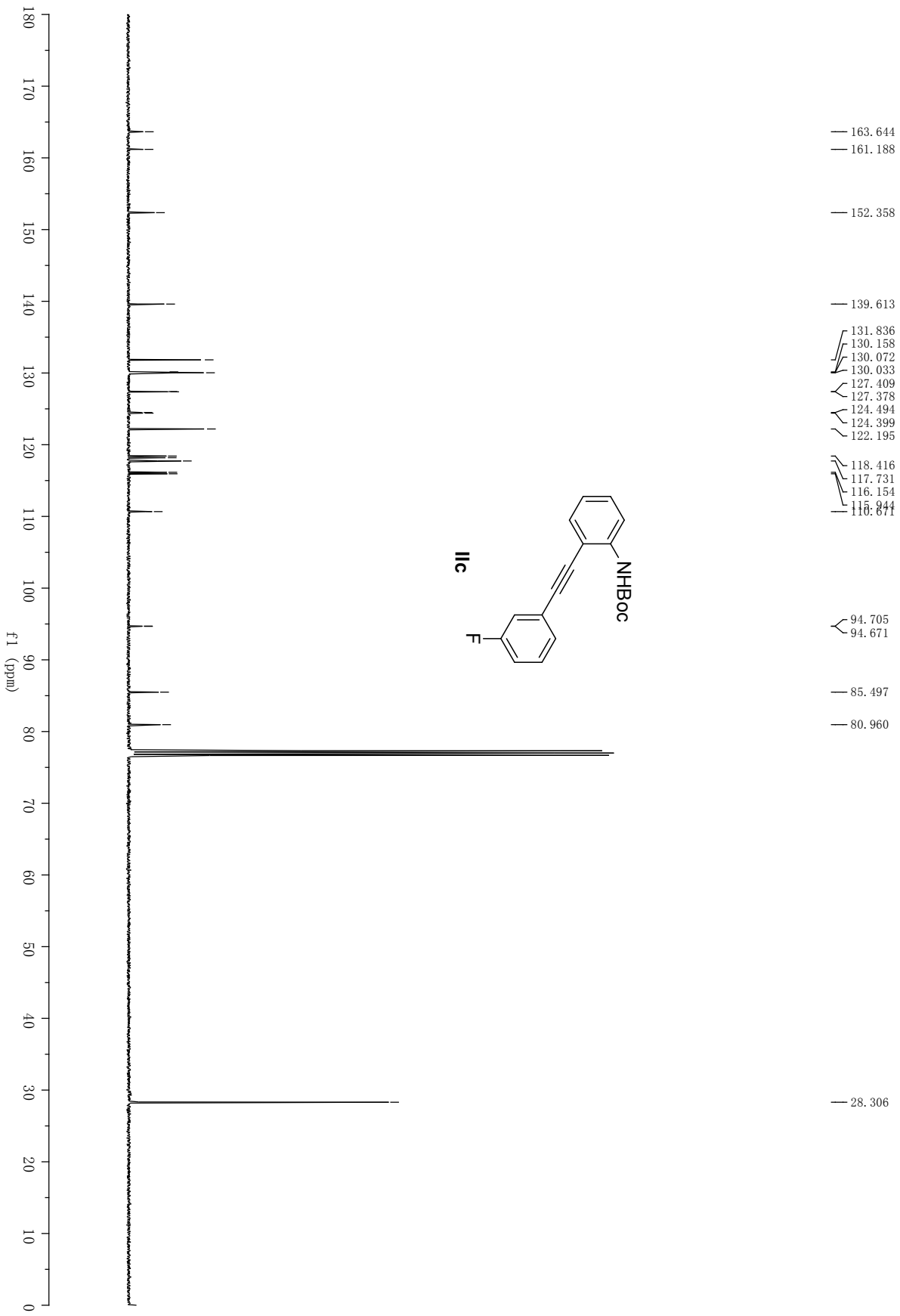

8.173
8.152
7.556
7.548
7.542
7.396
7.393
7.385
7.379
7.325
7.015
7.013
6.996
6.994
6.977
6.975
1.549
1.03
2.00
1.06
2.91
1.94
1.00
9.00
IIa
NHBoc
Ph
f1 (ppm)


152.306
139.424
131.637
131.433
129.588
128.630
128.421
122.538
122.049
117.523
111.067
95.991
84.486
80.706
28.224
IIa
NHBoc
Ph
f1 (ppm)


8.200
8.179
7.542
7.525
7.505
7.480
7.461
7.378
7.362
7.343
7.324
7.183
7.165
7.145
7.123
7.016
6.997
6.978
1.555
0.98
1.90
1.08
2.06
2.11
1.00
9.35
f1 (ppm)
IIb
F
NHBoc


163.840
161.340
152.511
139.855
132.763
131.355
130.355
130.275
130.025
124.148
124.111
122.000
117.536
115.668
115.461
111.508
111.354
110.696
90.021
89.478
80.692
28.271
IIb
F
NHBoc
f1 (ppm)


8.173
8.152
7.469
7.467
7.450
7.447
7.383
7.363
7.349
7.343
7.338
7.333
7.320
7.260
7.227
7.112
7.108
7.091
7.085
7.074
7.068
7.062
7.022
7.003
6.984
1.552
0.93
1.00
3.03
1.00
1.05
1.00
9.15
IIc
NHBoc
F
f1 (ppm)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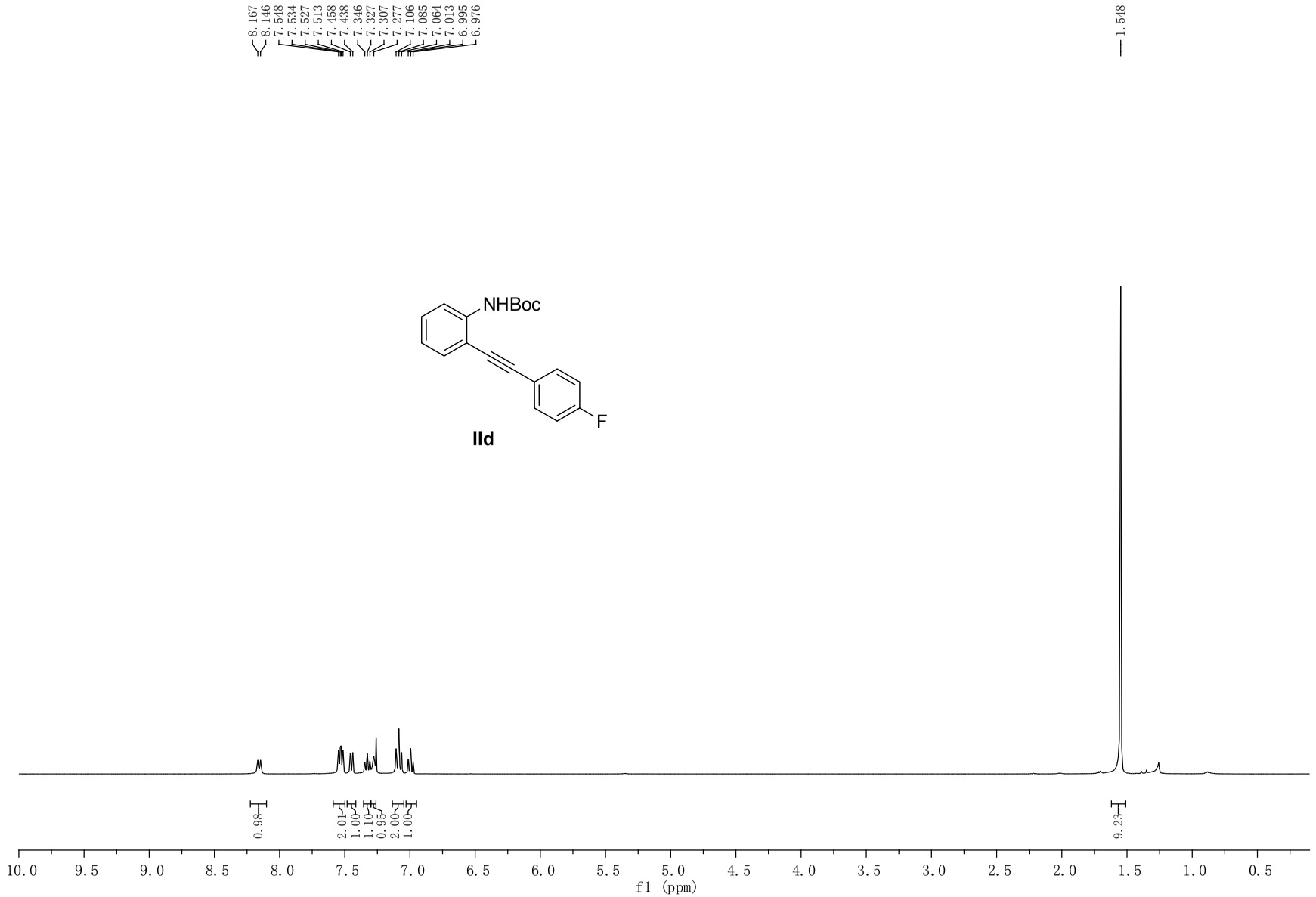
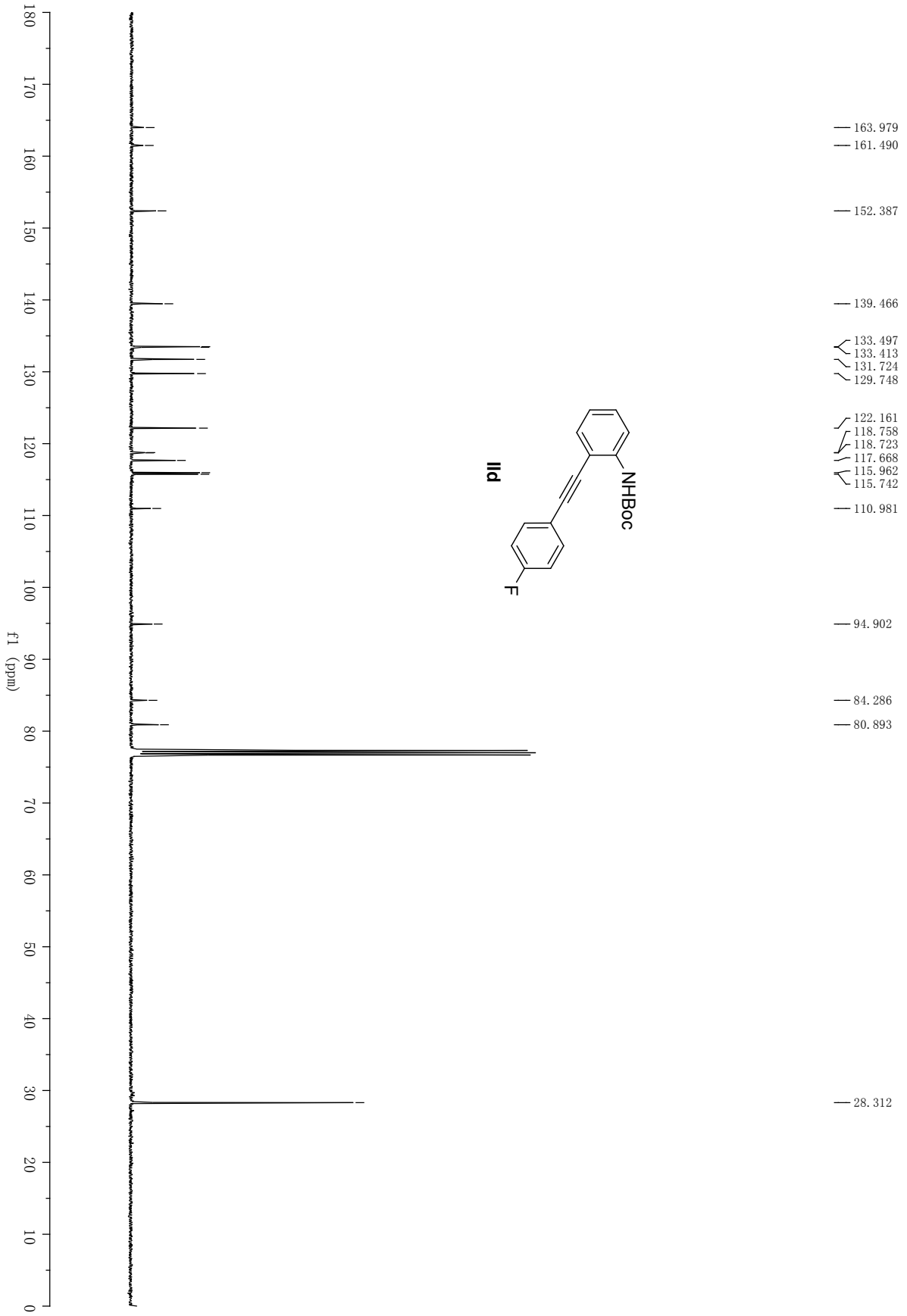
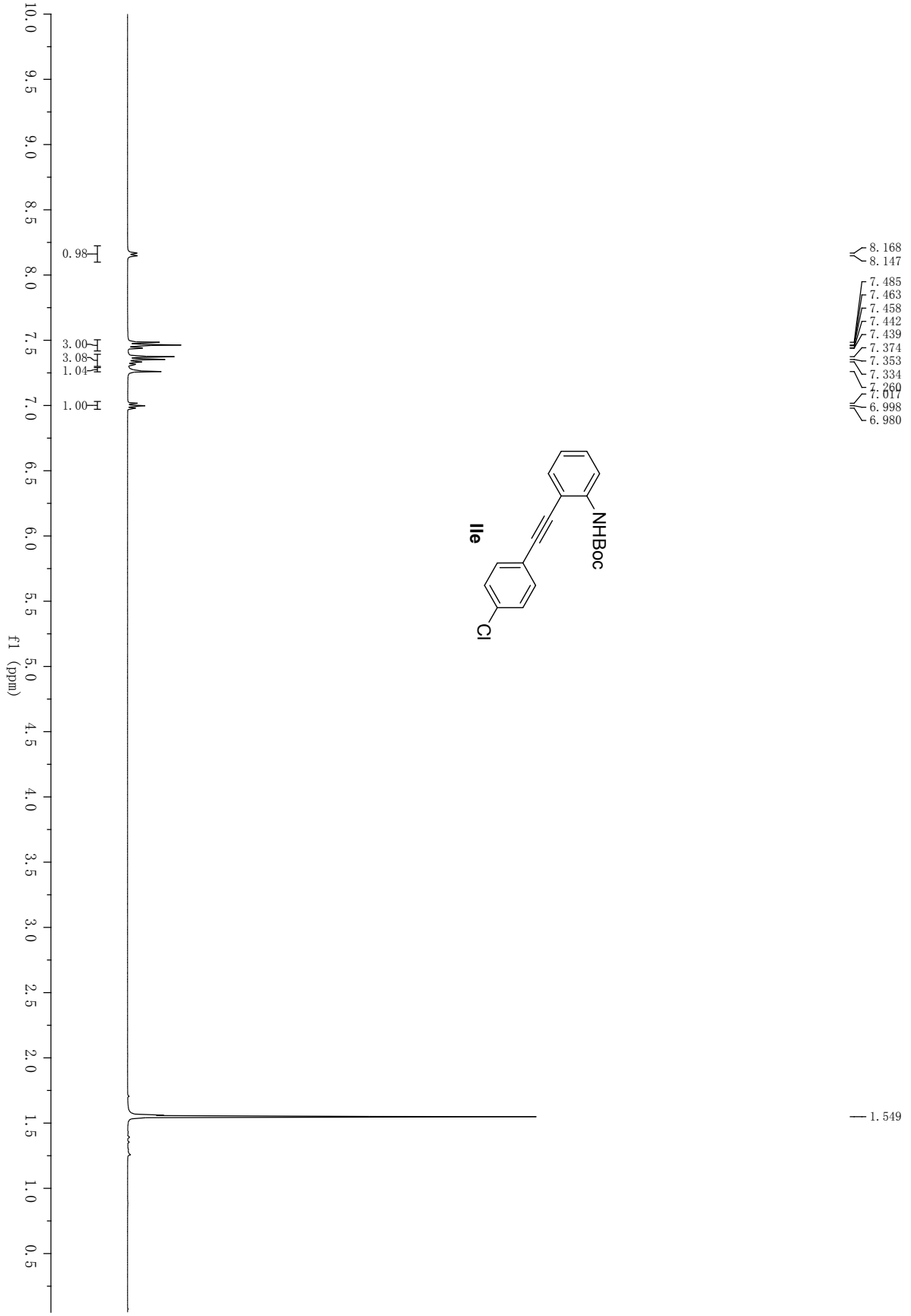
161.188
152.358
139.613
131.836
130.158
130.072
130.033
127.409
127.378
124.494
124.399
122.195
118.416
117.731
116.154
115.944
110.671
94.705
94.671
85.497
80.960
28.306
IIc
NHBoc
F
f1 (ppm)


8.167
8.146
7.548
7.534
7.527
7.513
7.458
7.438
7.346
7.327
7.307
7.277
7.106
7.085
7.064
7.013
6.995
6.976
1.548
NHBoc
F
IId
0.98
2.01
1.00
1.10
0.95
2.00
1.00
9.23
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)


163.979
161.490
152.387
139.466
133.497
133.413
131.724
129.748
122.161
118.758
118.723
117.668
115.962
115.742
110.981
94.902
84.286
80.893
28.312
f1 (ppm)
IId
NHBoc
F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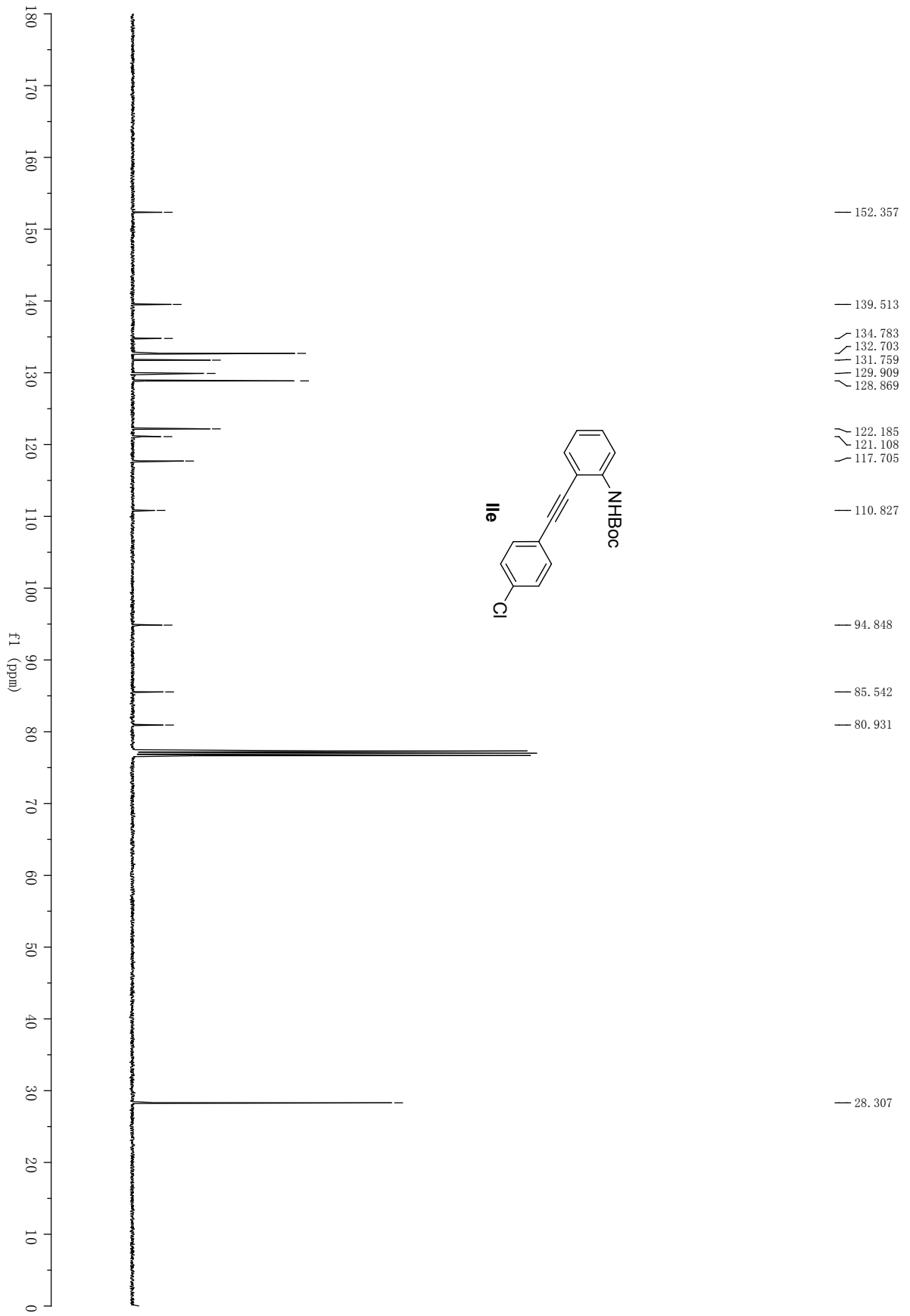
8.147
7.485
7.463
7.458
7.442
7.439
7.374
7.353
7.334
7.260
7.017
6.998
6.980
1.549
0.98
3.00
3.08
1.04
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
NHBoc
Cl
IIe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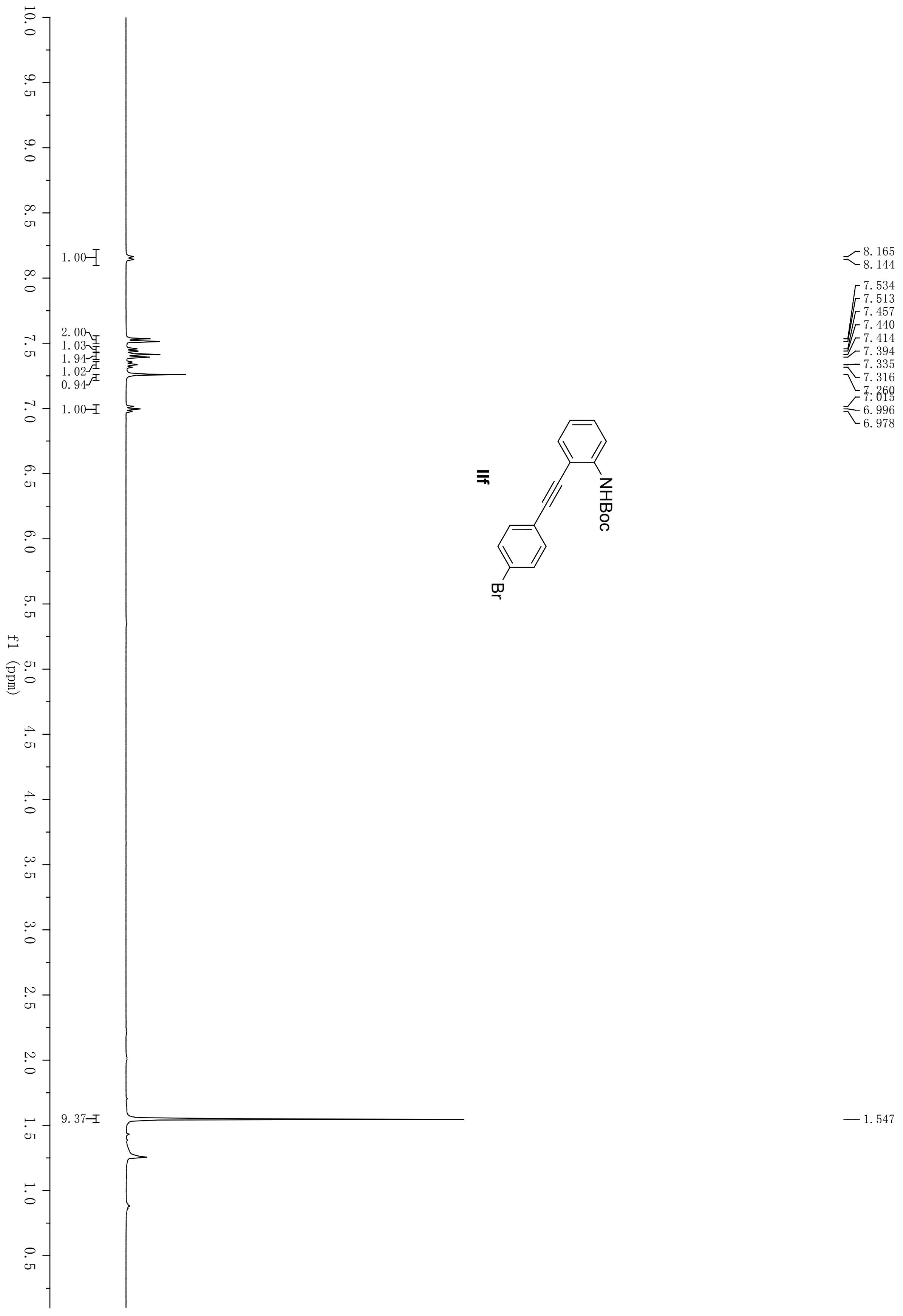
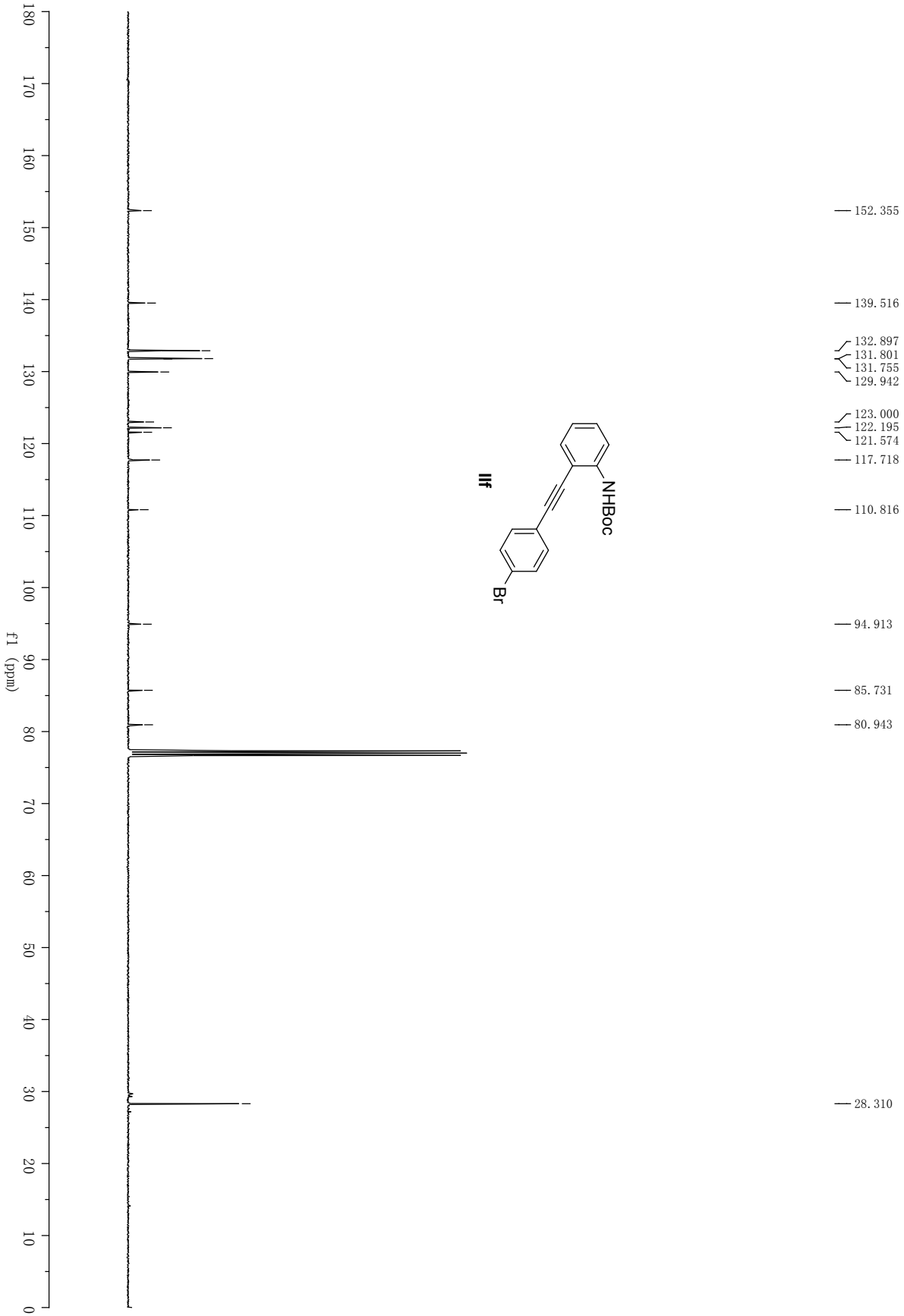
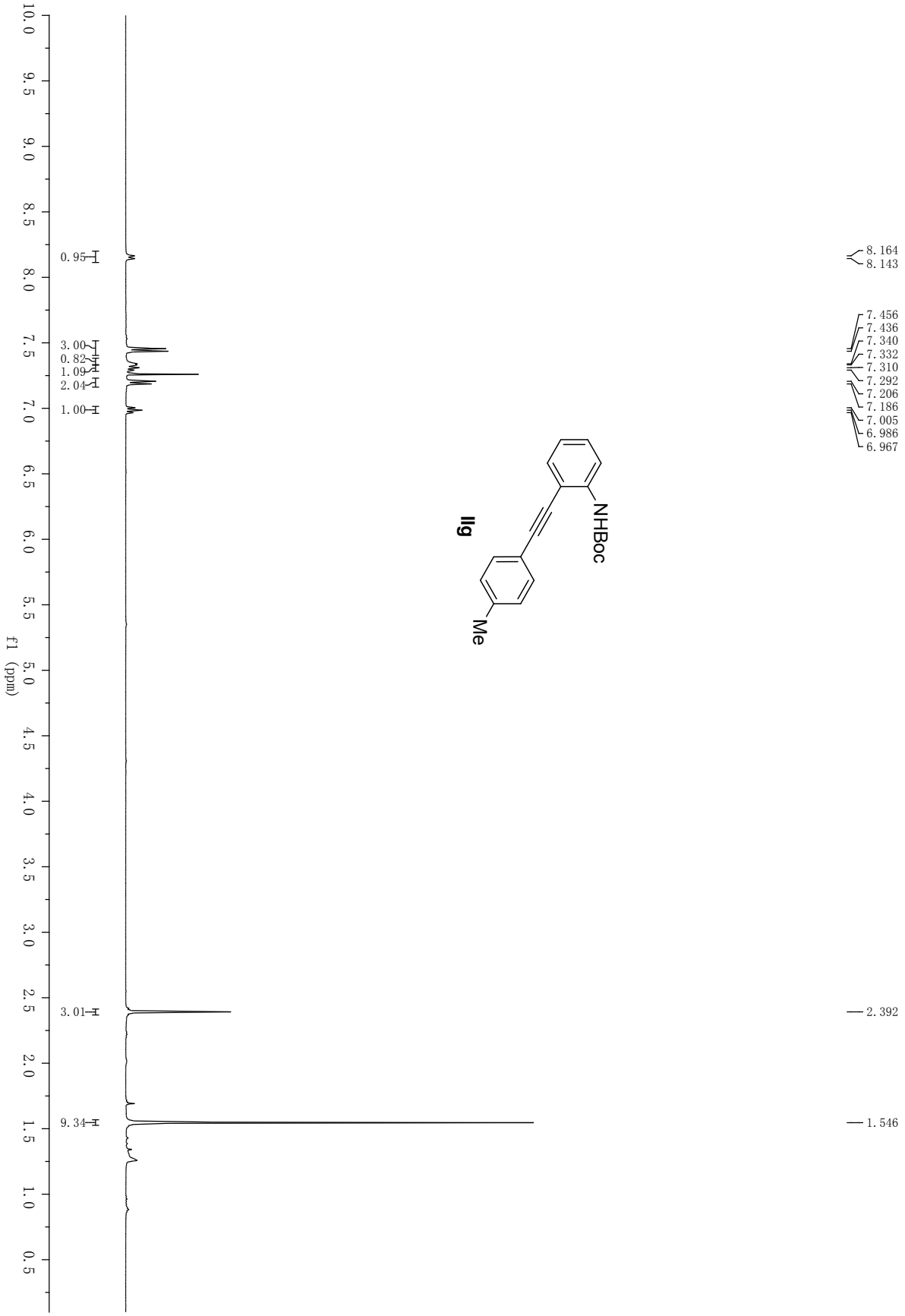
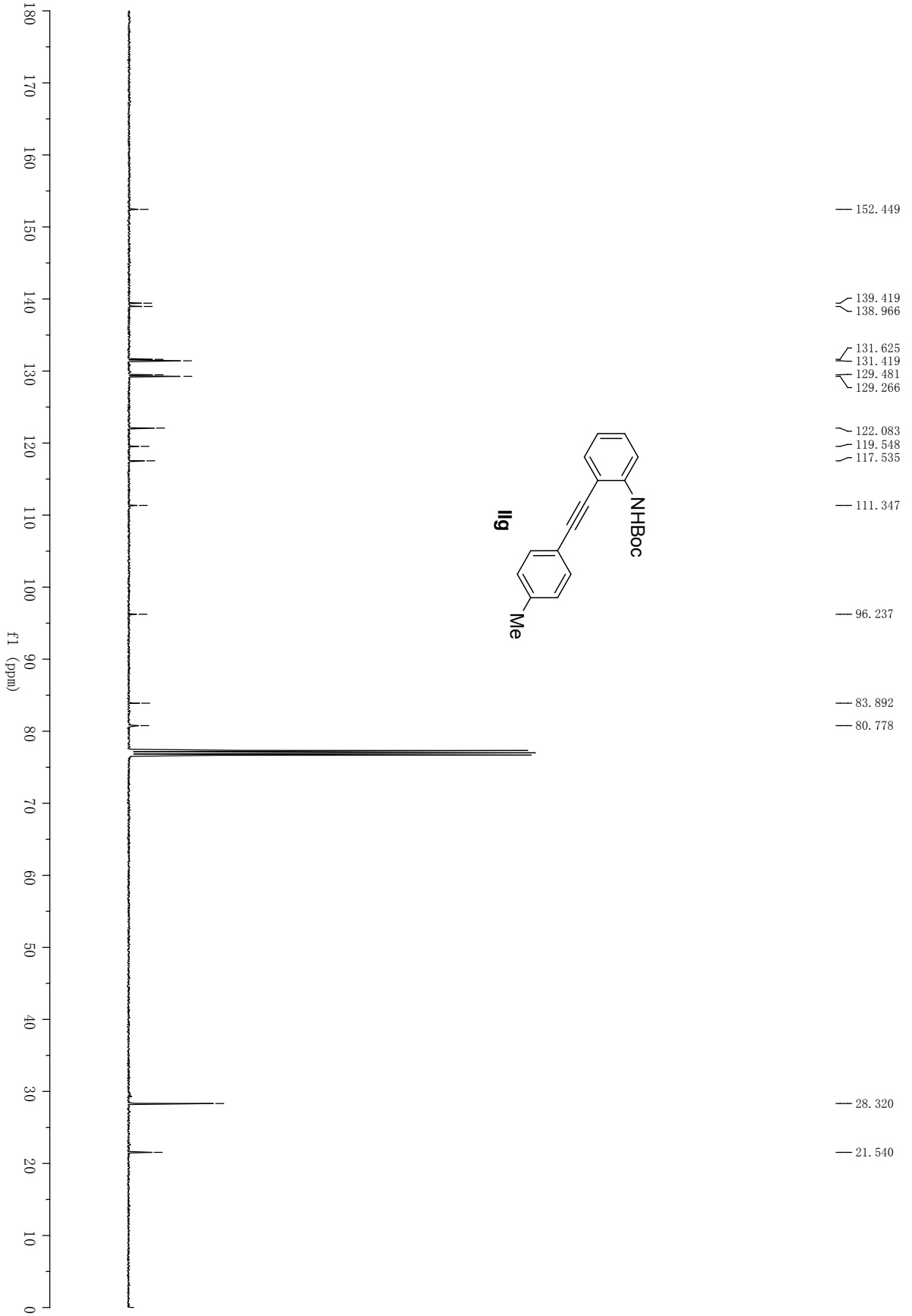
134.783
132.703
131.759
129.909
128.869
122.185
121.108
117.705
110.827
94.848
85.542
80.931
28.307
IIe
NHBoc
Cl
f1 (ppm)


8.165
8.144
7.534
7.513
7.457
7.440
7.414
7.394
7.335
7.316
7.260
7.015
6.996
6.978
1.547
NHBoc
Br
IIf
1.00
2.00
1.03
1.94
1.02
0.94
1.00
9.37
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)


152.355
139.516
132.897
131.801
131.755
129.942
123.000
122.195
121.574
117.718
110.816
94.913
85.731
80.943
28.310
IIIf
NHBoc
Br
f1 (ppm)


8.164
8.143
7.456
7.436
7.340
7.332
7.310
7.292
7.206
7.186
7.005
6.986
6.967
2.392
1.546
0.95
3.00
0.82
1.09
2.04
1.00
3.01
9.34
NHBoc
Me
IIg
f1 (ppm)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139.419
138.966
131.625
131.419
129.481
129.266
122.083
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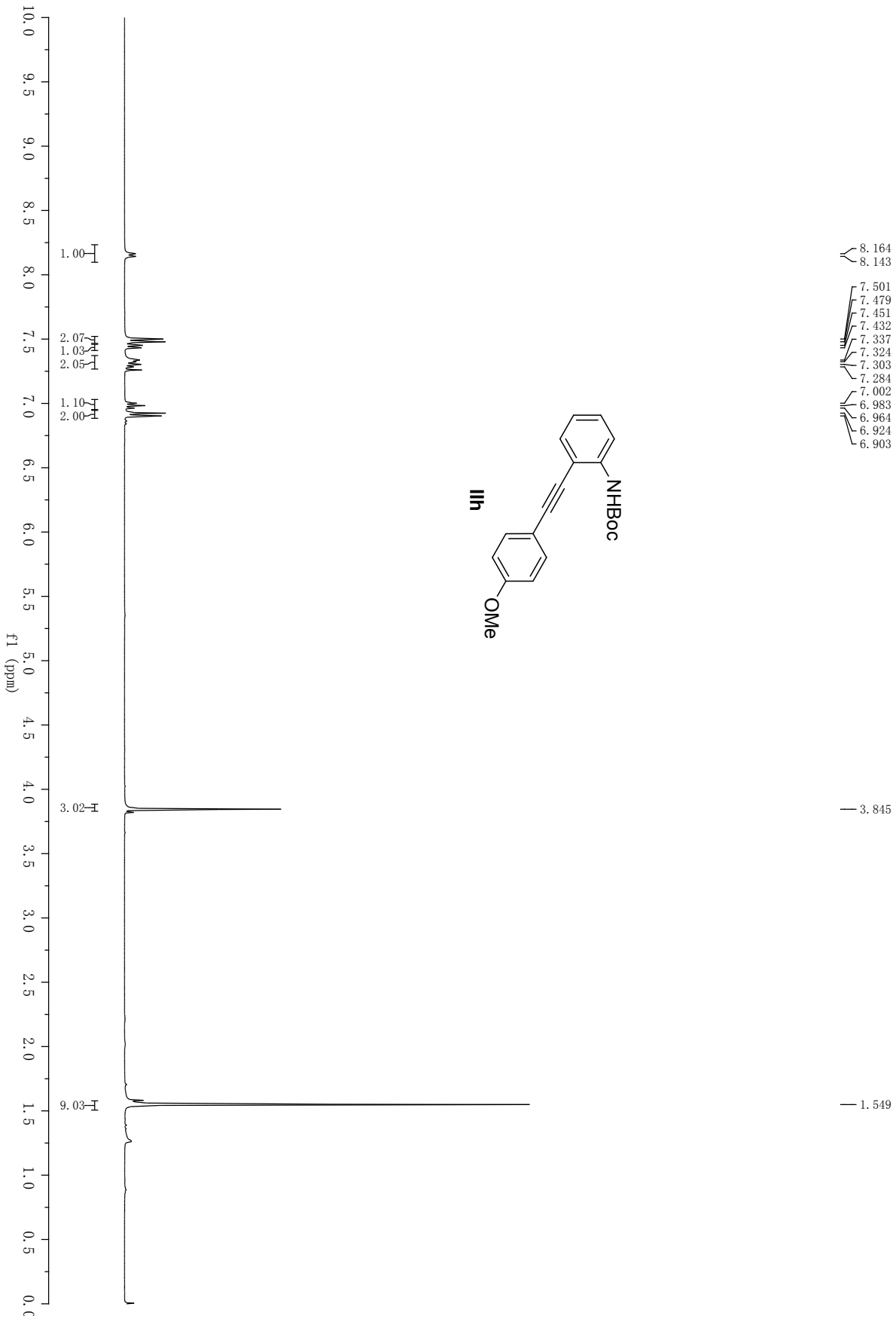
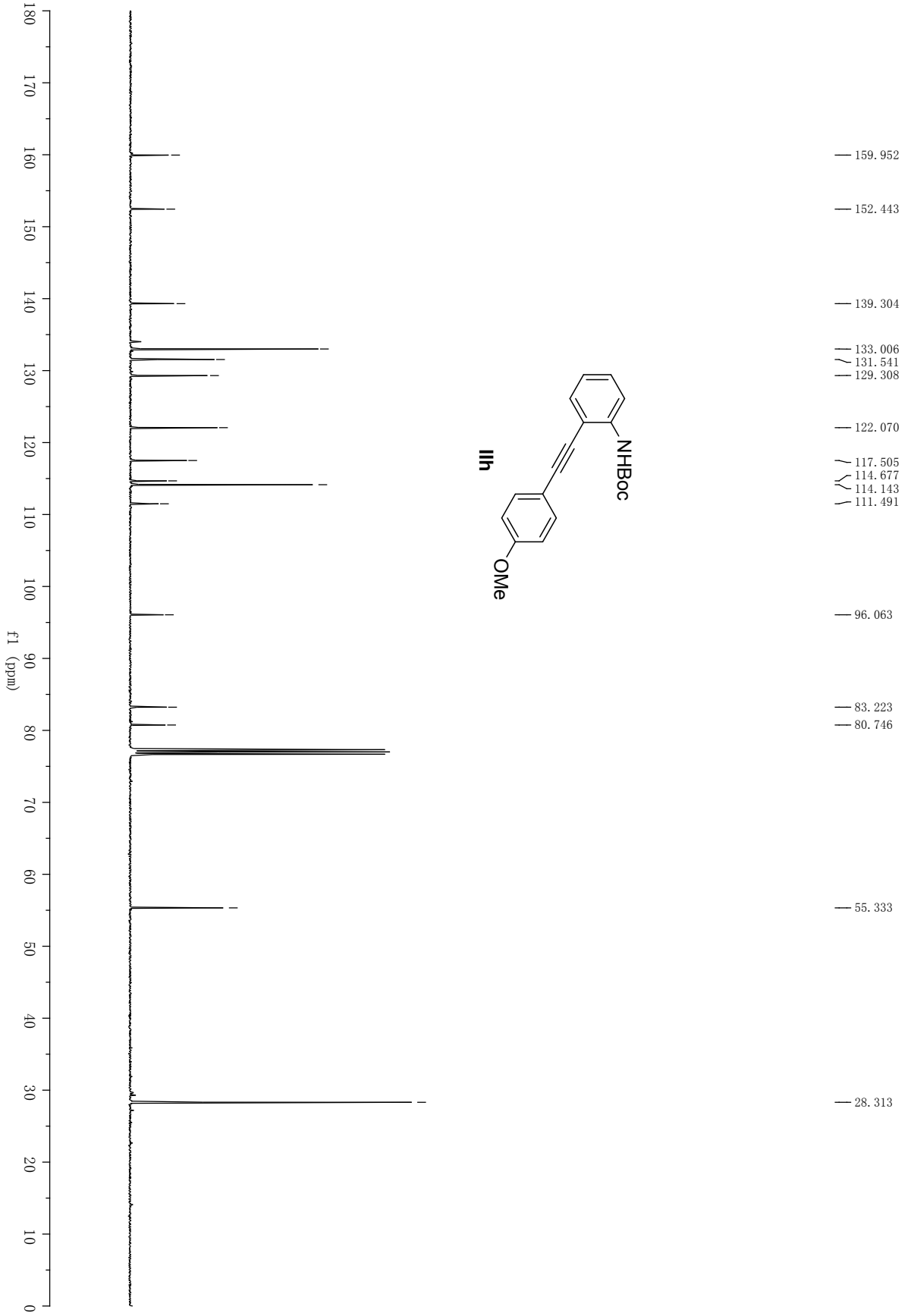
111.347
96.237
83.892
80.778
28.320
21.540
NHBoc
Me
Ilg
f1 (ppm)


IIh
NHBoc
OMe
8.164
8.143
7.501
7.479
7.451
7.432
7.337
7.324
7.303
7.284
7.002
6.983
6.964
6.924
6.903
3.845
1.549
1.00
2.07
1.03
2.05
1.10
2.00
3.02
9.03
f1 (ppm)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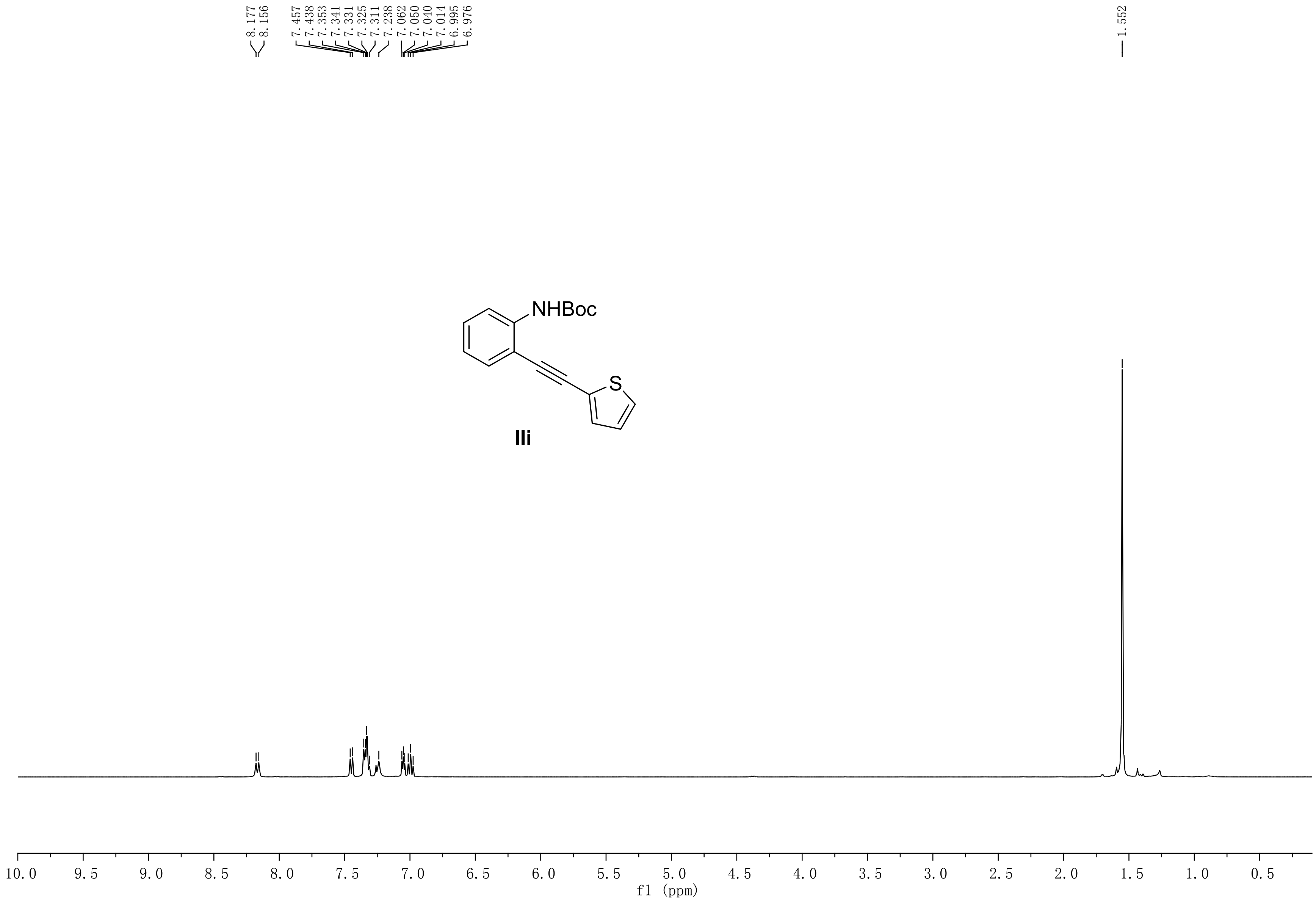
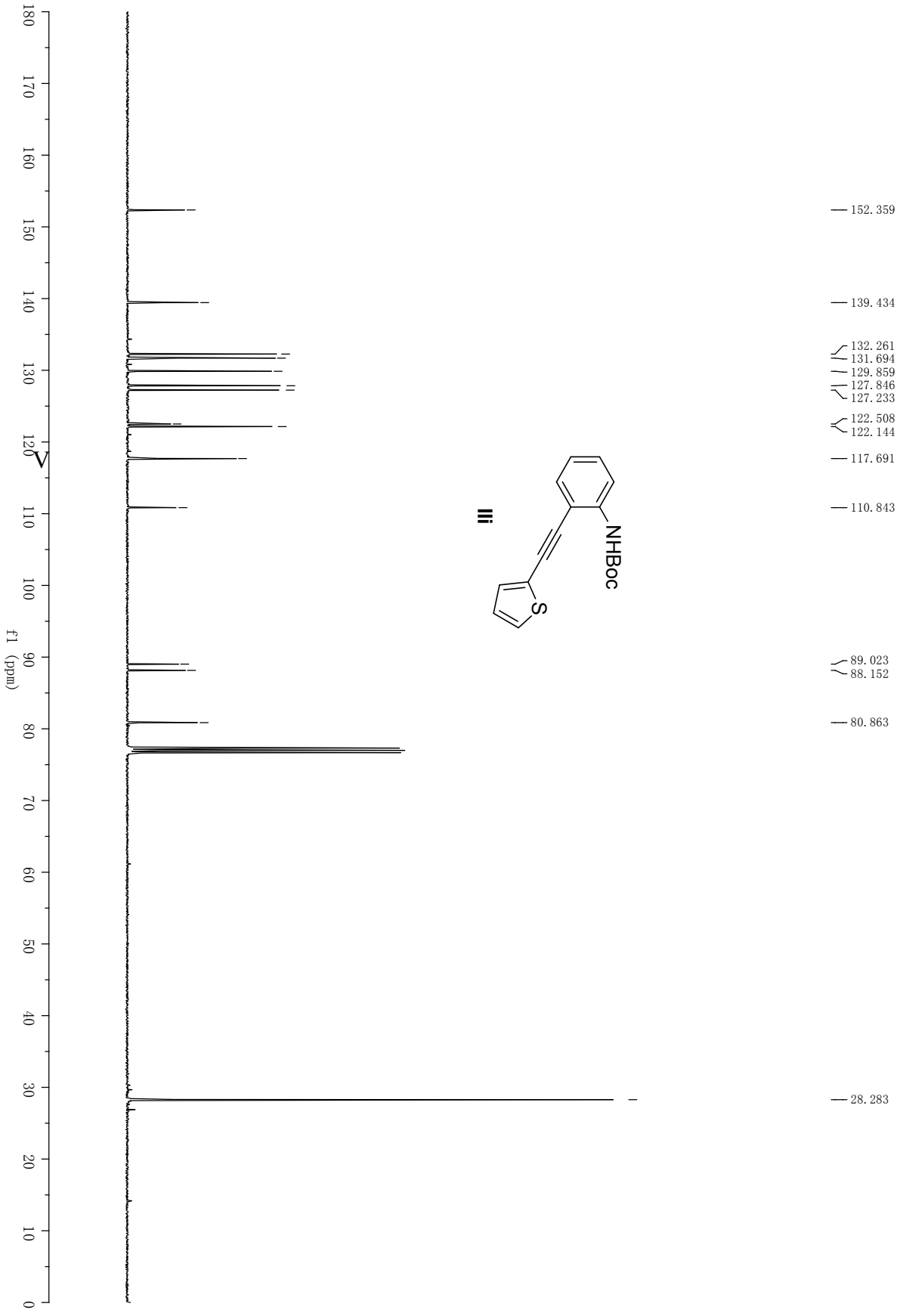
139.304
133.006
131.541
129.308
122.070
117.505
114.677
114.143
111.491
96.063
83.223
80.746
55.333
28.313
f1 (ppm)
IIh
NHBoc
OMe



8.177
8.156
7.457
7.438
7.353
7.341
7.331
7.325
7.311
7.238
7.062
7.050
7.040
7.014
6.995
6.976
1.552
NHBoc
S
IIi
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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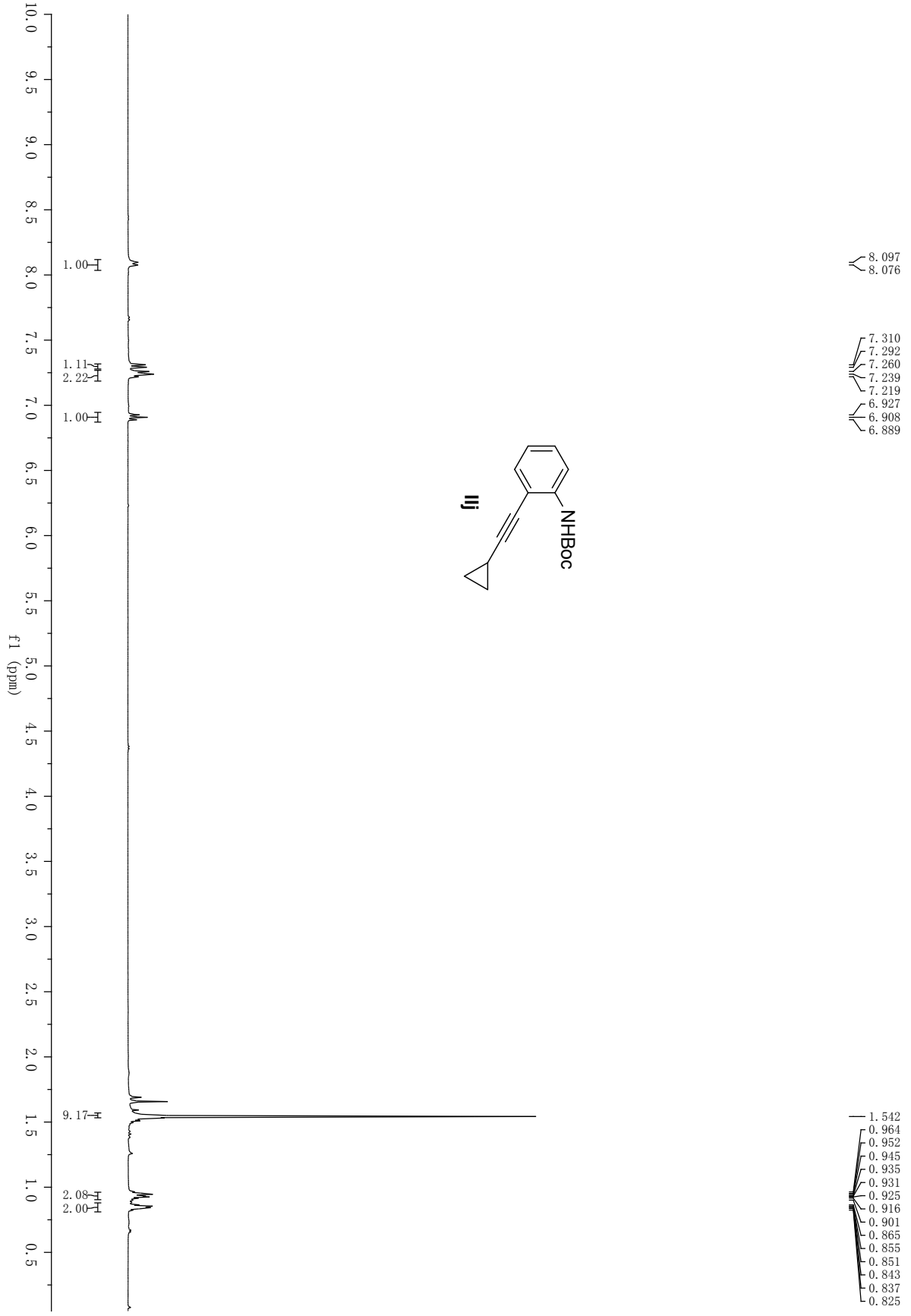
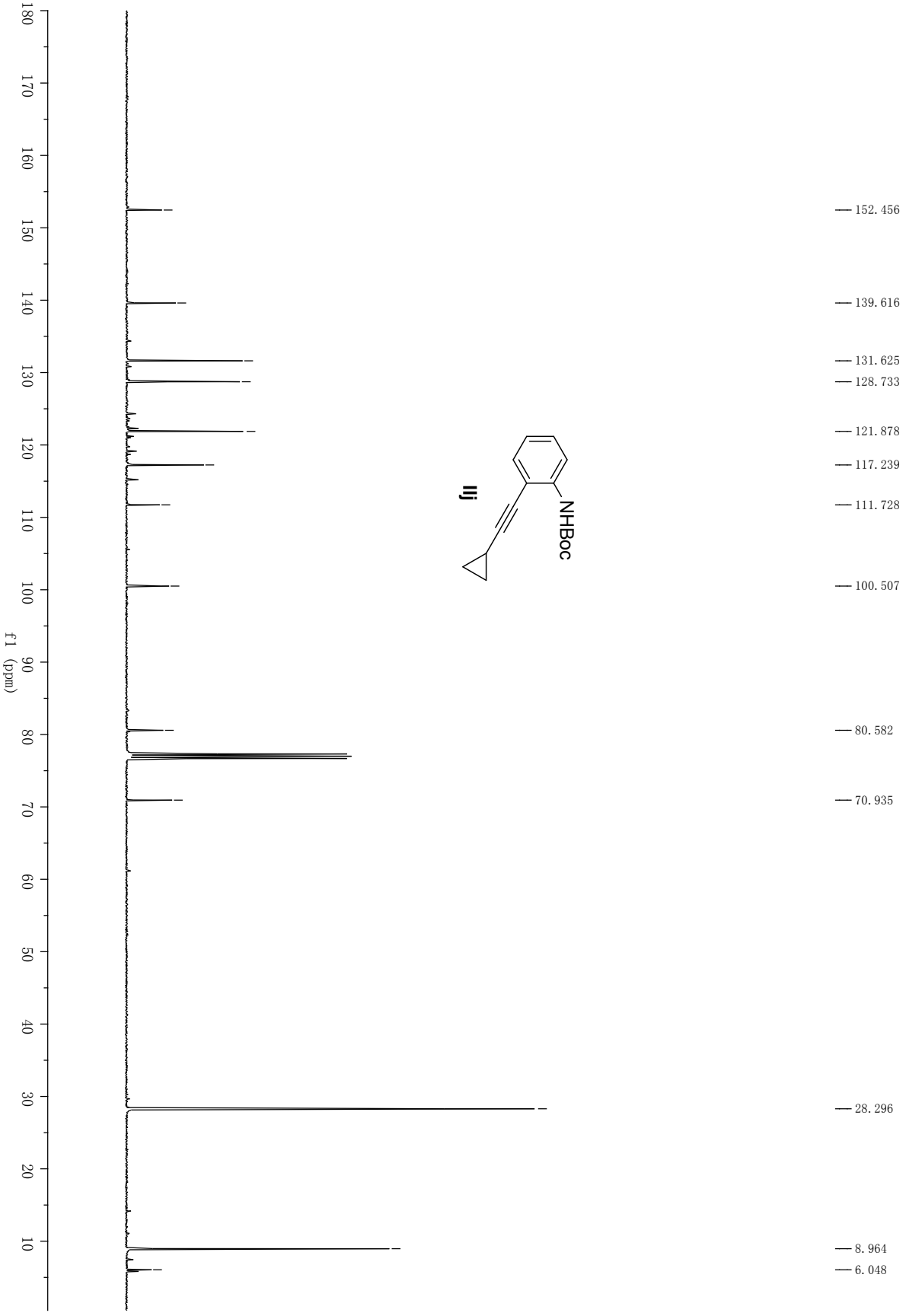
139.434
132.261
131.694
129.859
127.846
127.233
122.508
122.144
117.691
110.843
89.023
88.152
80.863
28.283
f1 (ppm)
NHBoc
S


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)
1.00
1.11
2.22
1.00
9.17
2.08
2.00
8.097
8.076
7.310
7.292
7.260
7.239
7.219
6.927
6.908
6.889
1.542
0.964
0.952
0.945
0.935
0.931
0.925
0.916
0.901
0.865
0.855
0.851
0.843
0.837
0.825
NHBoc
IIj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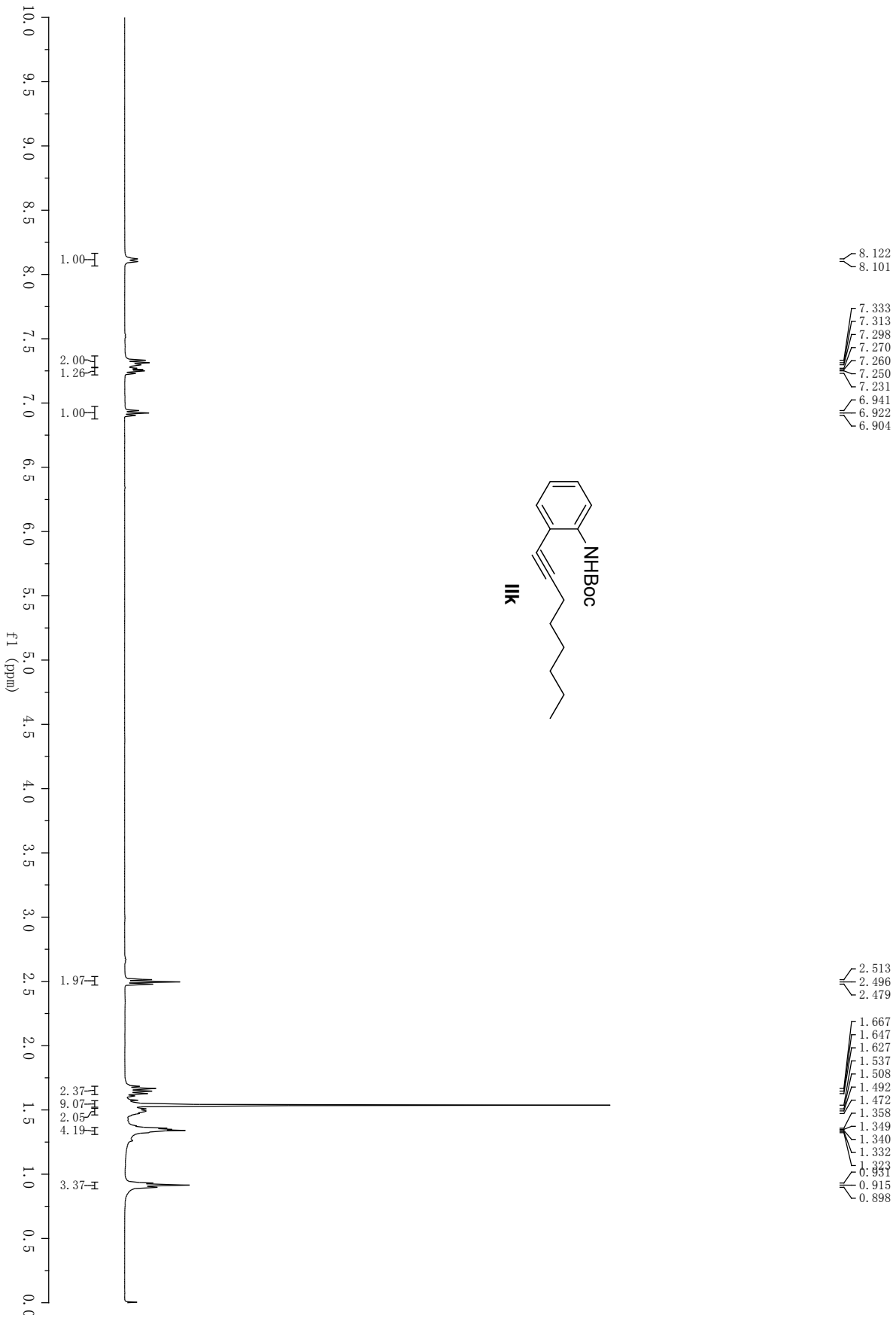
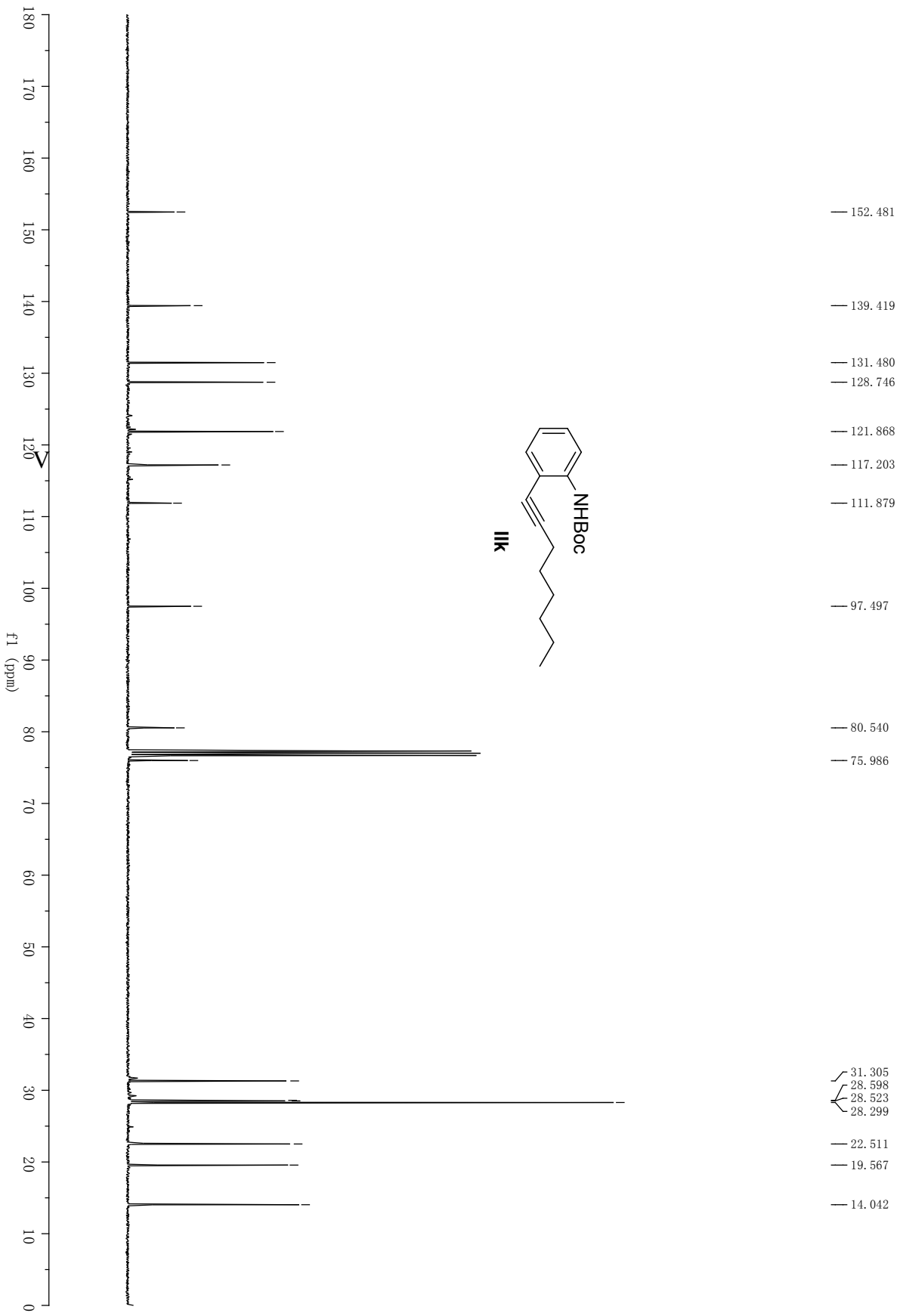
139.616
131.625
128.733
121.878
117.239
111.728
100.507
80.582
70.935
28.296
8.964
6.048
f1 (ppm)
NHBoc
IIj


8.122
8.101
7.333
7.313
7.298
7.270
7.260
7.250
7.231
6.941
6.922
6.904
NHBoc
IIk
2.513
2.496
2.479
1.667
1.647
1.627
1.537
1.508
1.492
1.472
1.358
1.349
1.340
1.332
1.323
0.931
0.915
0.898
1.00
2.00
1.26
1.00
1.97
2.37
9.07
2.05
4.19
3.37
f1 (ppm)


152.481
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131.480
128.746
121.868
117.203
111.879
97.497
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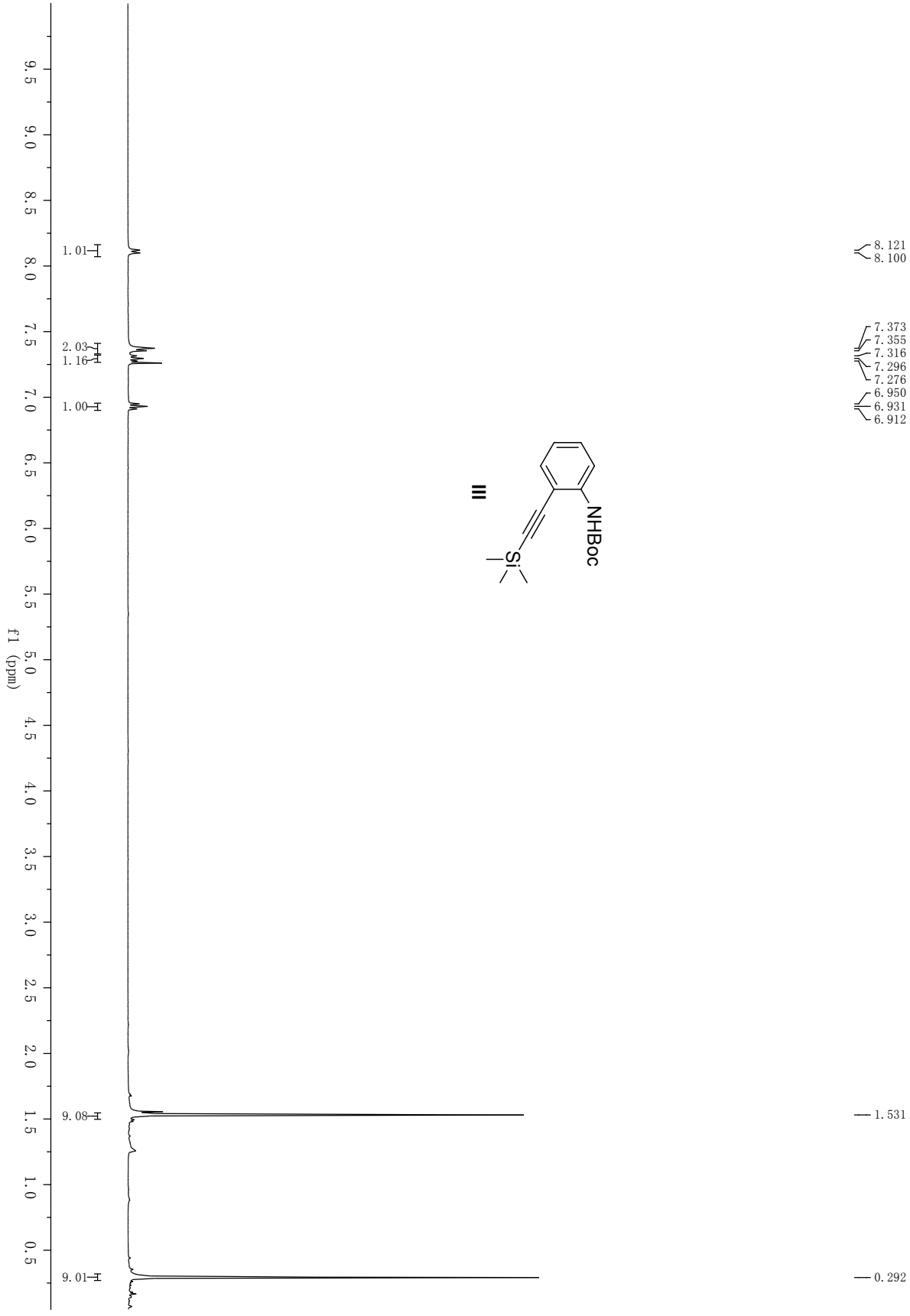
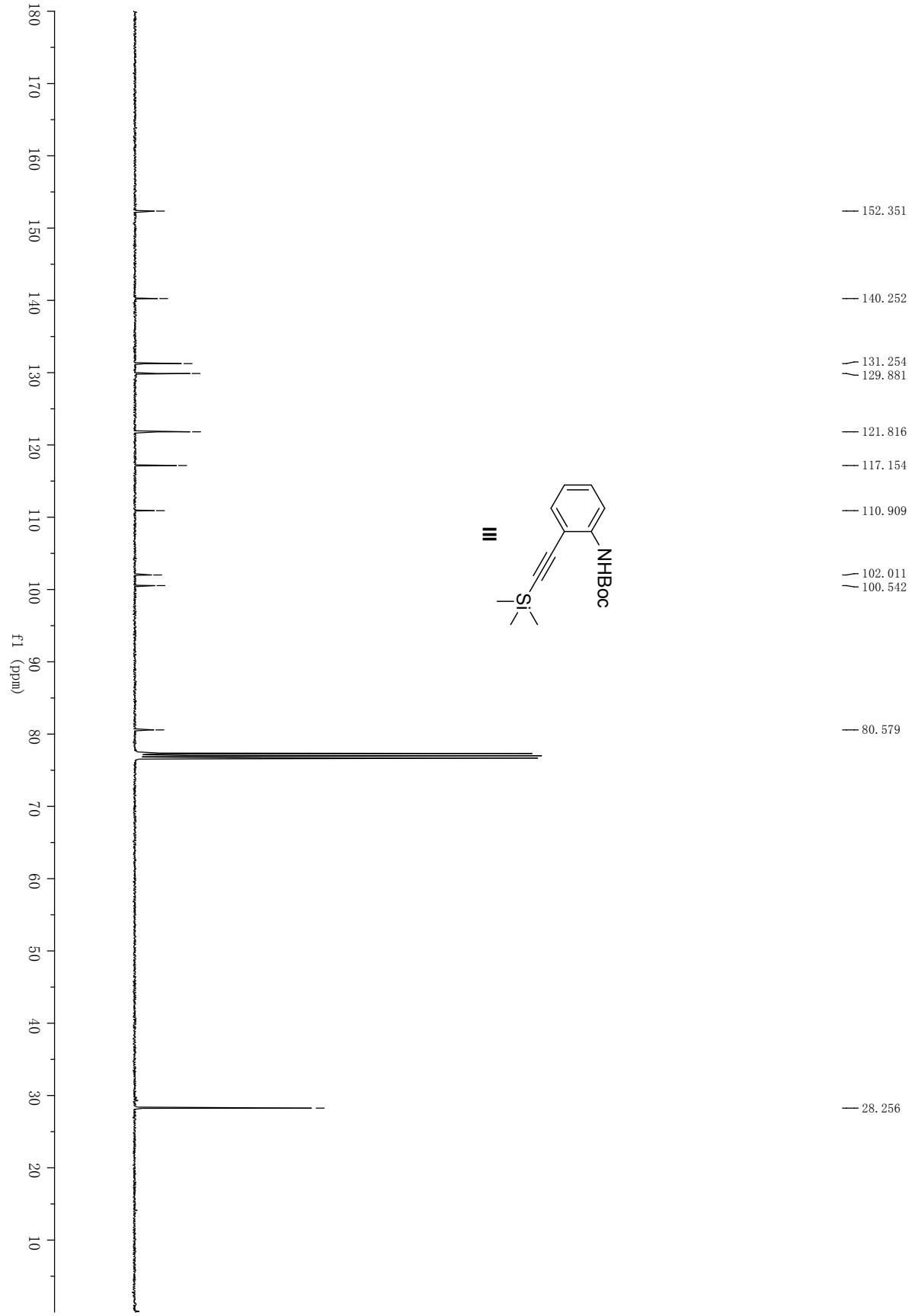
75.986
31.305
28.598
28.523
28.299
22.511
19.567
14.042
NHBoc
f1 (ppm)


f1 (ppm)
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
1.01
2.03
1.16
1.00
9.08
9.01
8.121
8.100
7.373
7.355
7.316
7.296
7.276
6.950
6.931
6.912
1.531
0.292
NHBoc
Si


152.351
140.252
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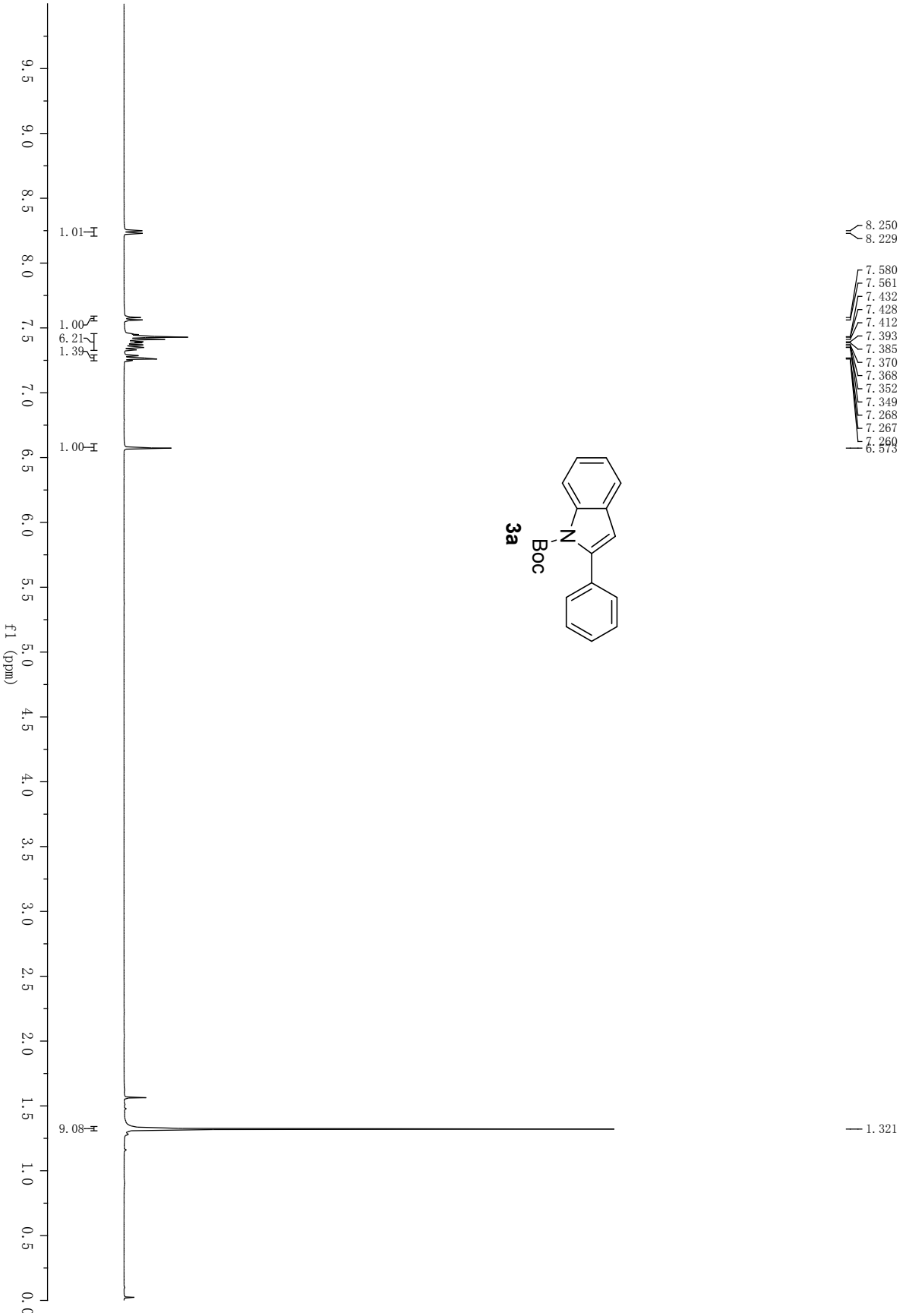
121.816
117.154
110.909
102.011
100.542
80.579
28.256
NHBoc
Si
f1 (ppm)


8.250
8.229
7.580
7.561
7.432
7.428
7.412
7.393
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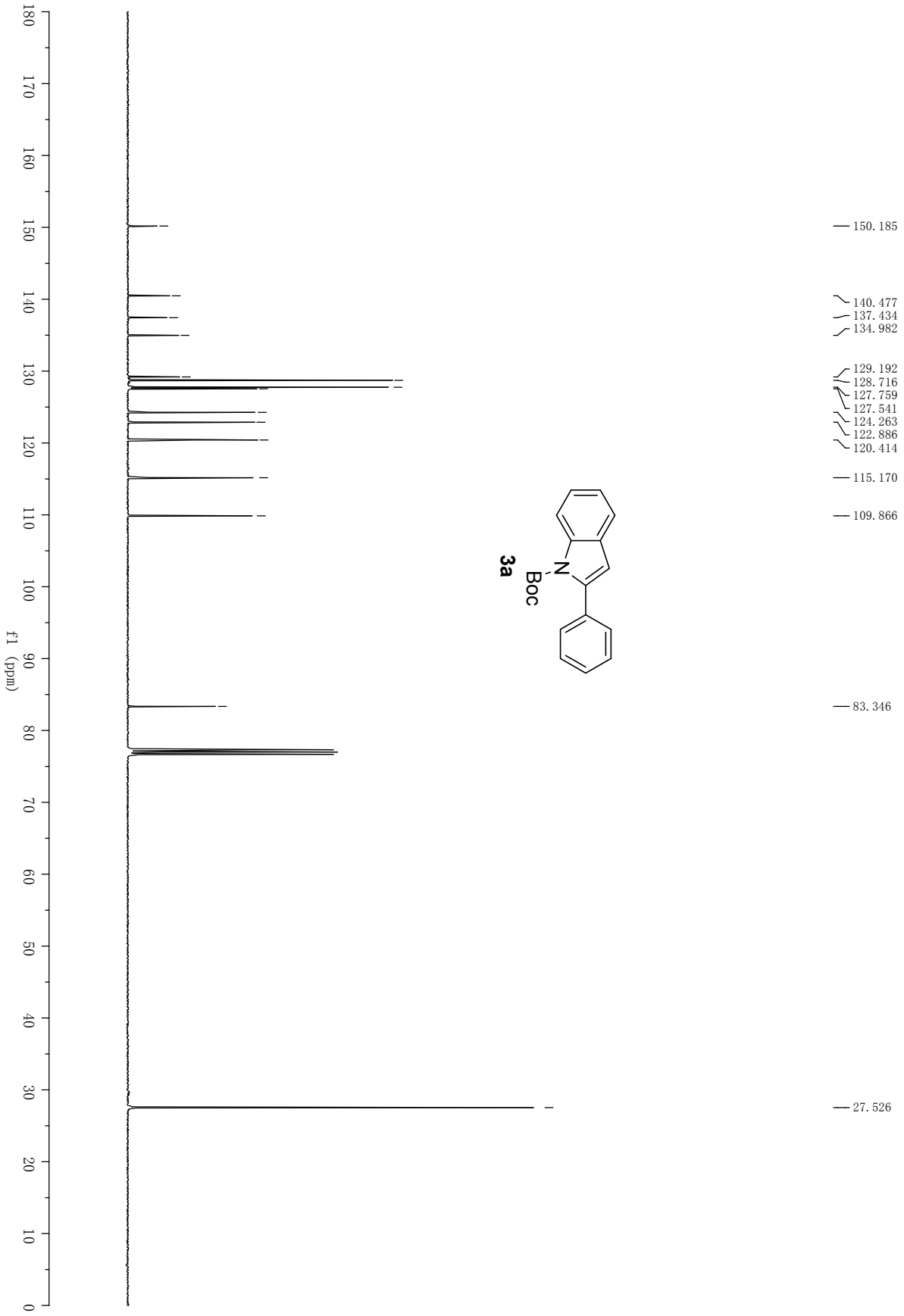
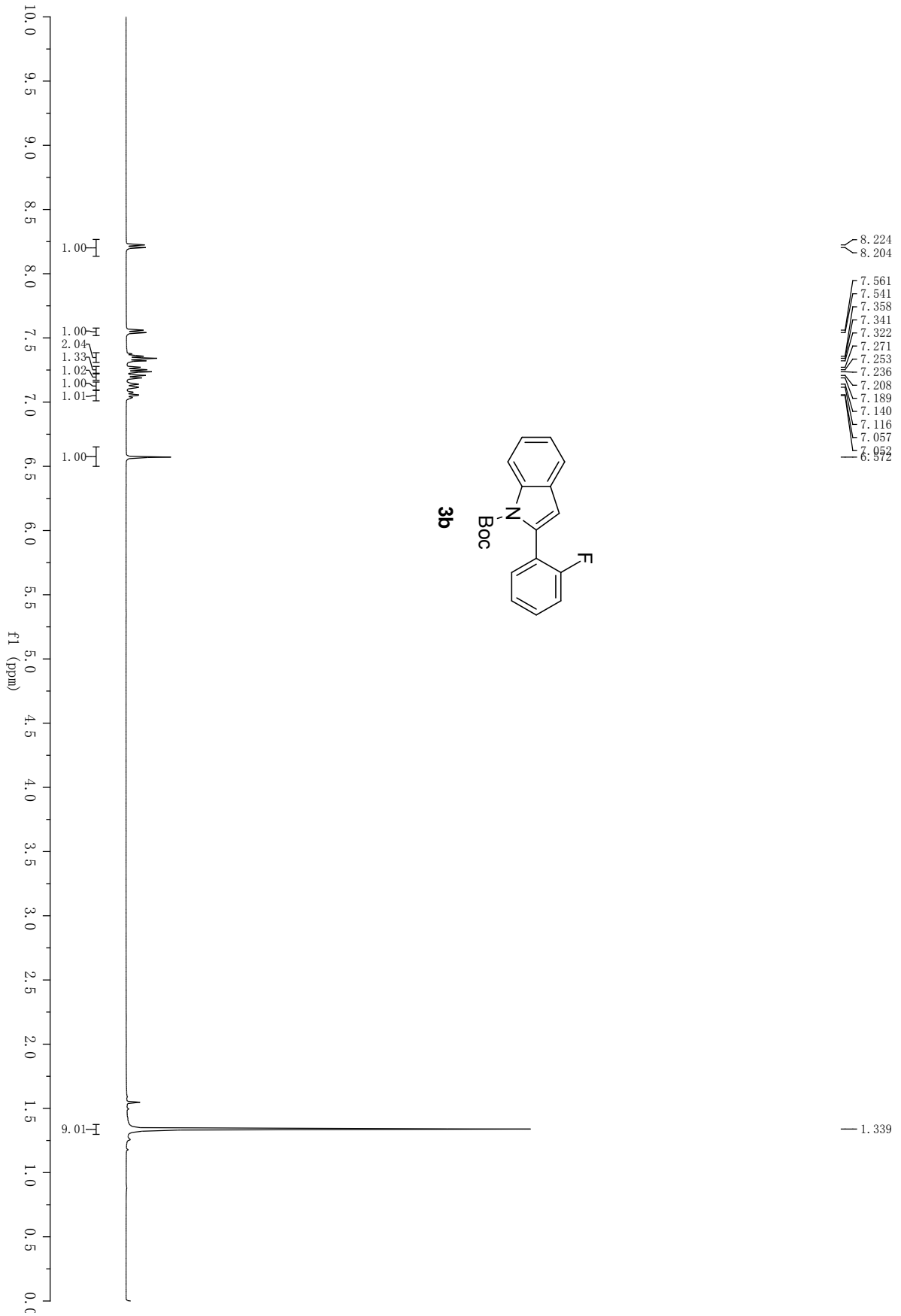
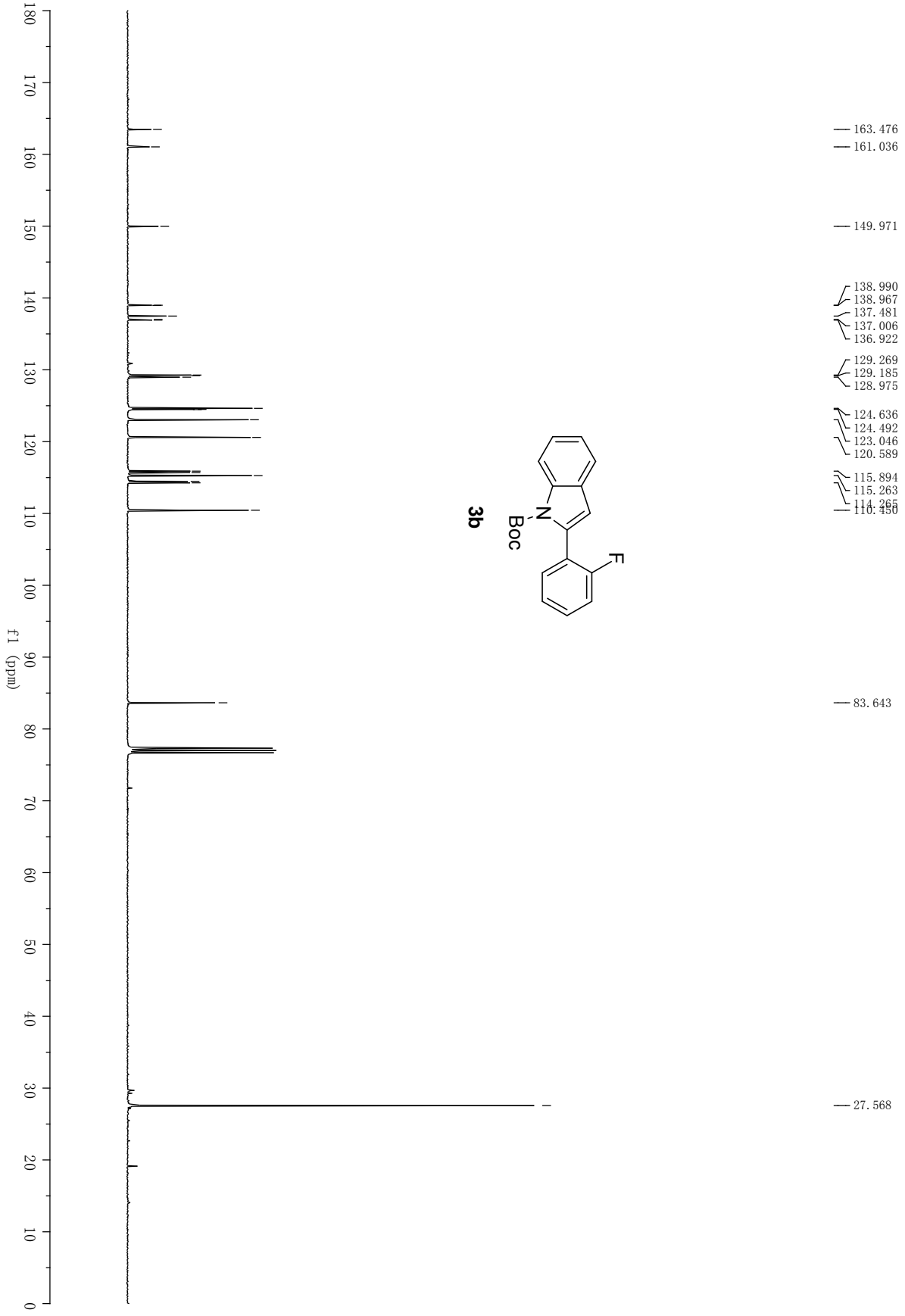
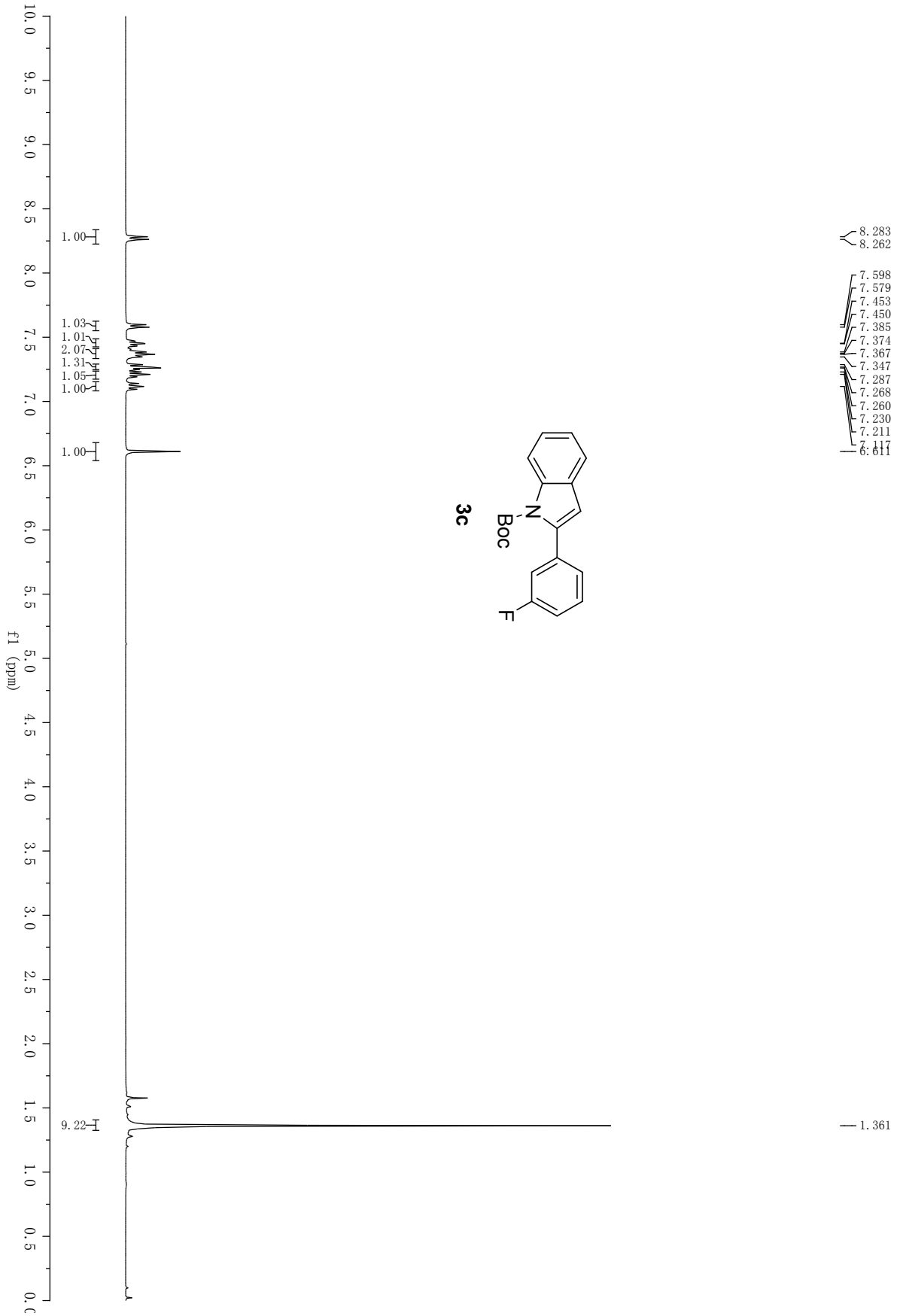
7.370
7.368
7.352
7.349
7.268
7.267
7.260
6.573
1.321
1.01
1.00
6.21
1.39
1.00
9.08
3a
Boc
N
f1 (ppm)


150.185
140.477
137.434
134.982
129.192
128.716
127.759
127.541
124.263
122.886
120.414
115.170
109.866
83.346
27.526
f1 (ppm)
3a
Boc
N

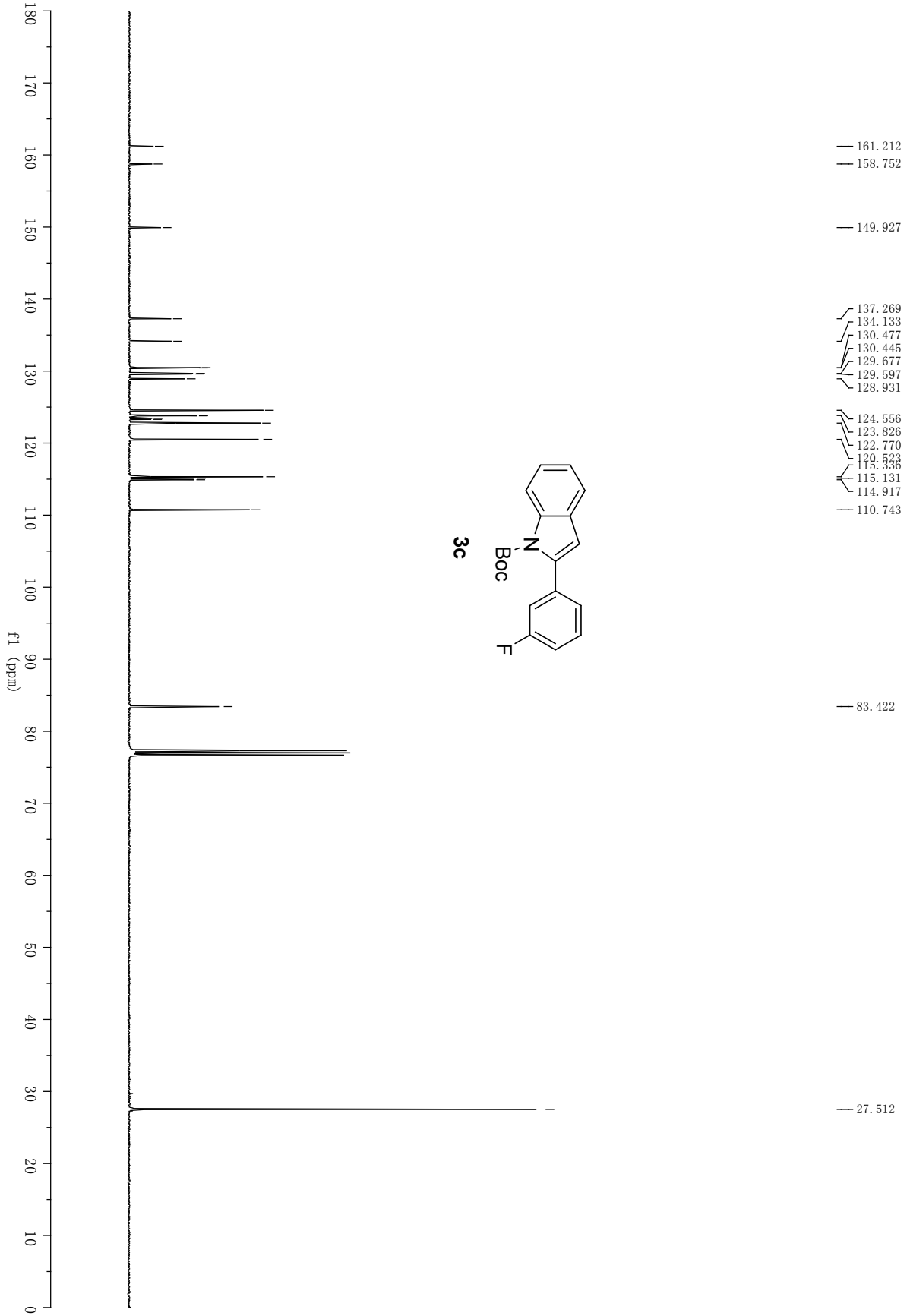

8.224
8.204
7.561
7.541
7.358
7.341
7.322
7.271
7.253
7.236
7.208
7.189
7.140
7.116
7.057
7.052
6.872
1.339
1.00
1.00
2.04
1.33
1.02
1.00
1.01
1.00
9.01
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
N
Boc
F

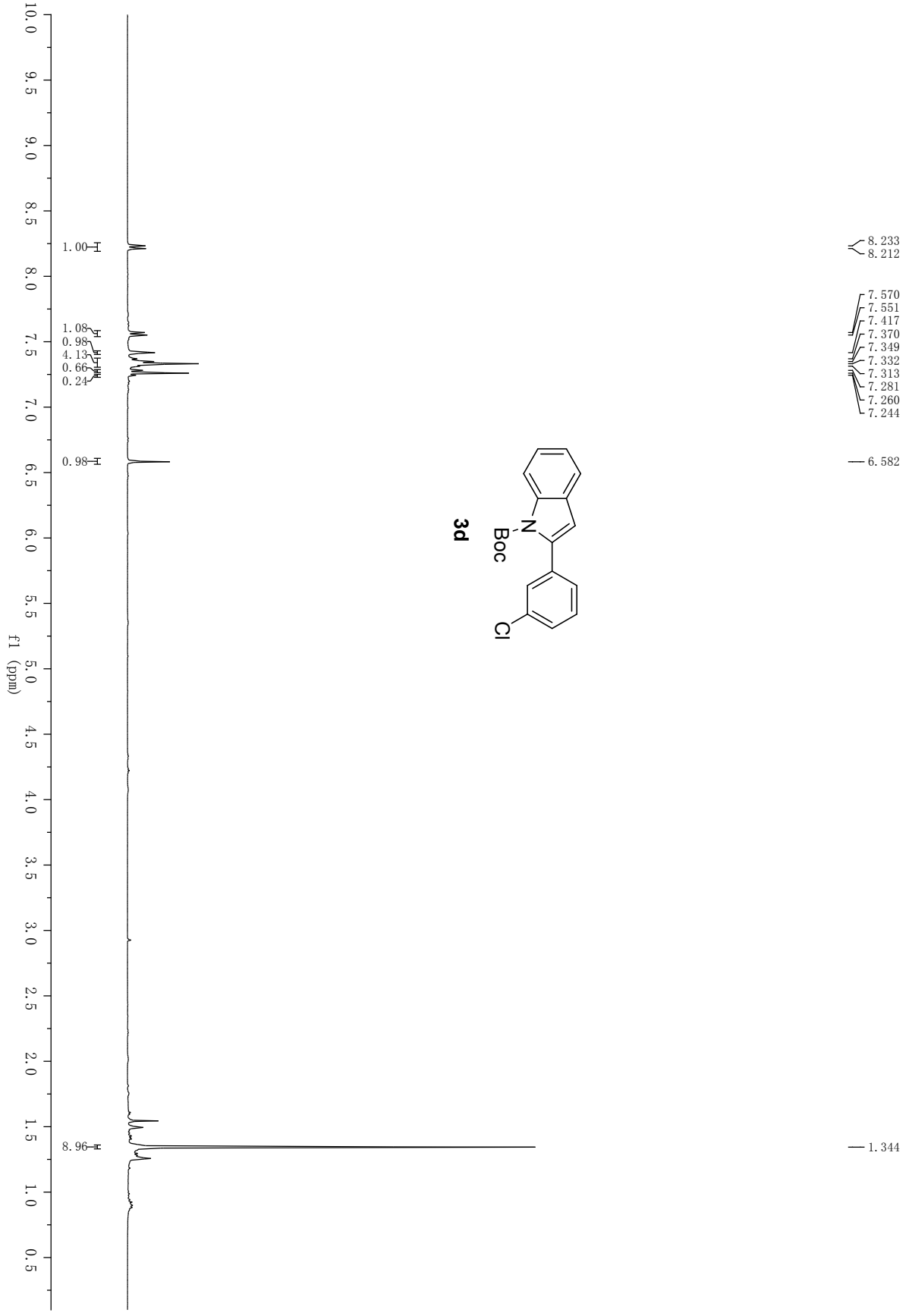
3b

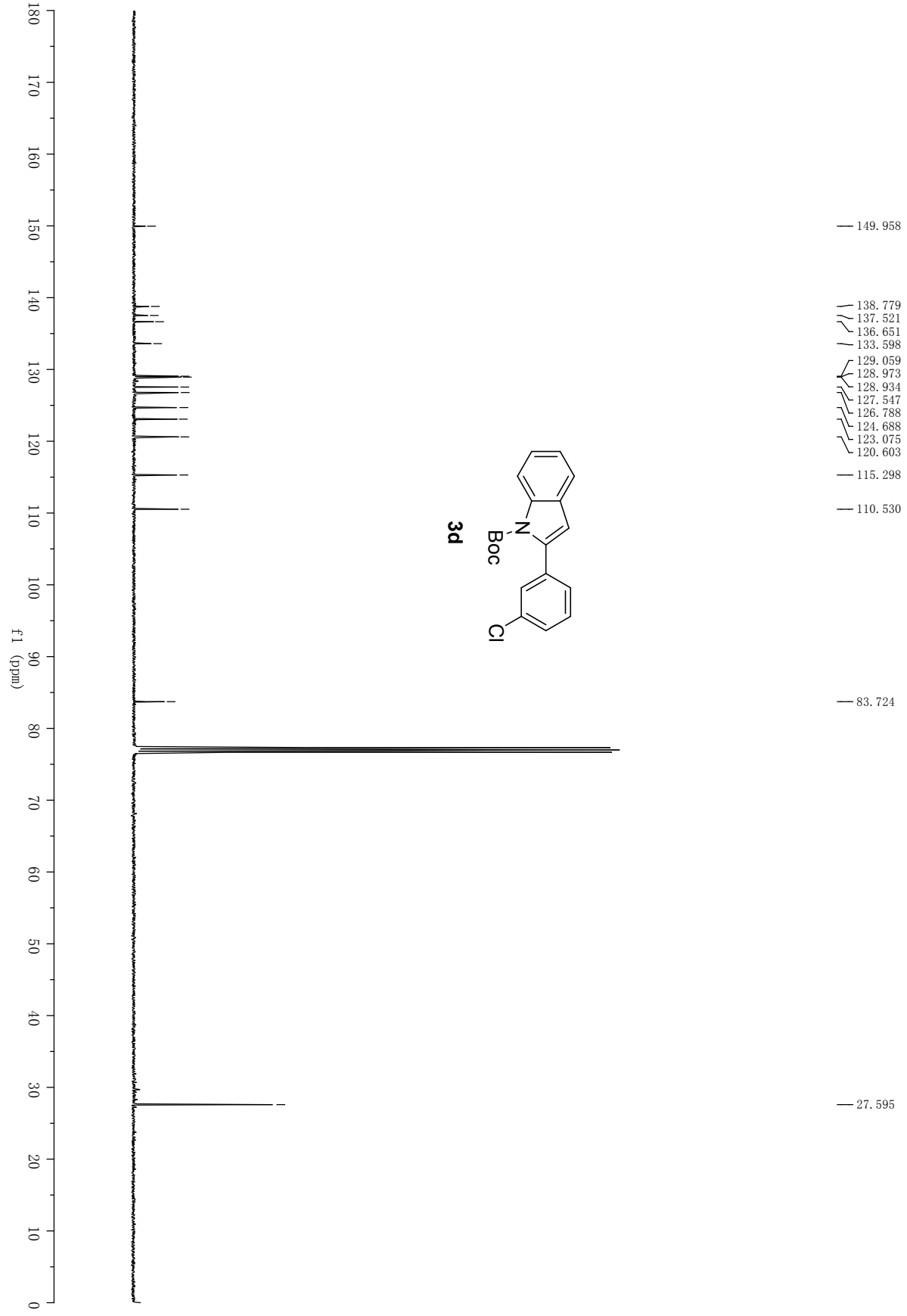

163.476
161.036
149.971
138.990
138.967
137.481
137.006
136.922
129.269
129.185
128.975
124.636
124.492
123.046
120.589
115.894
115.263
114.265
110.450
83.643
27.568
f1 (ppm)
3b
N
Boc
F

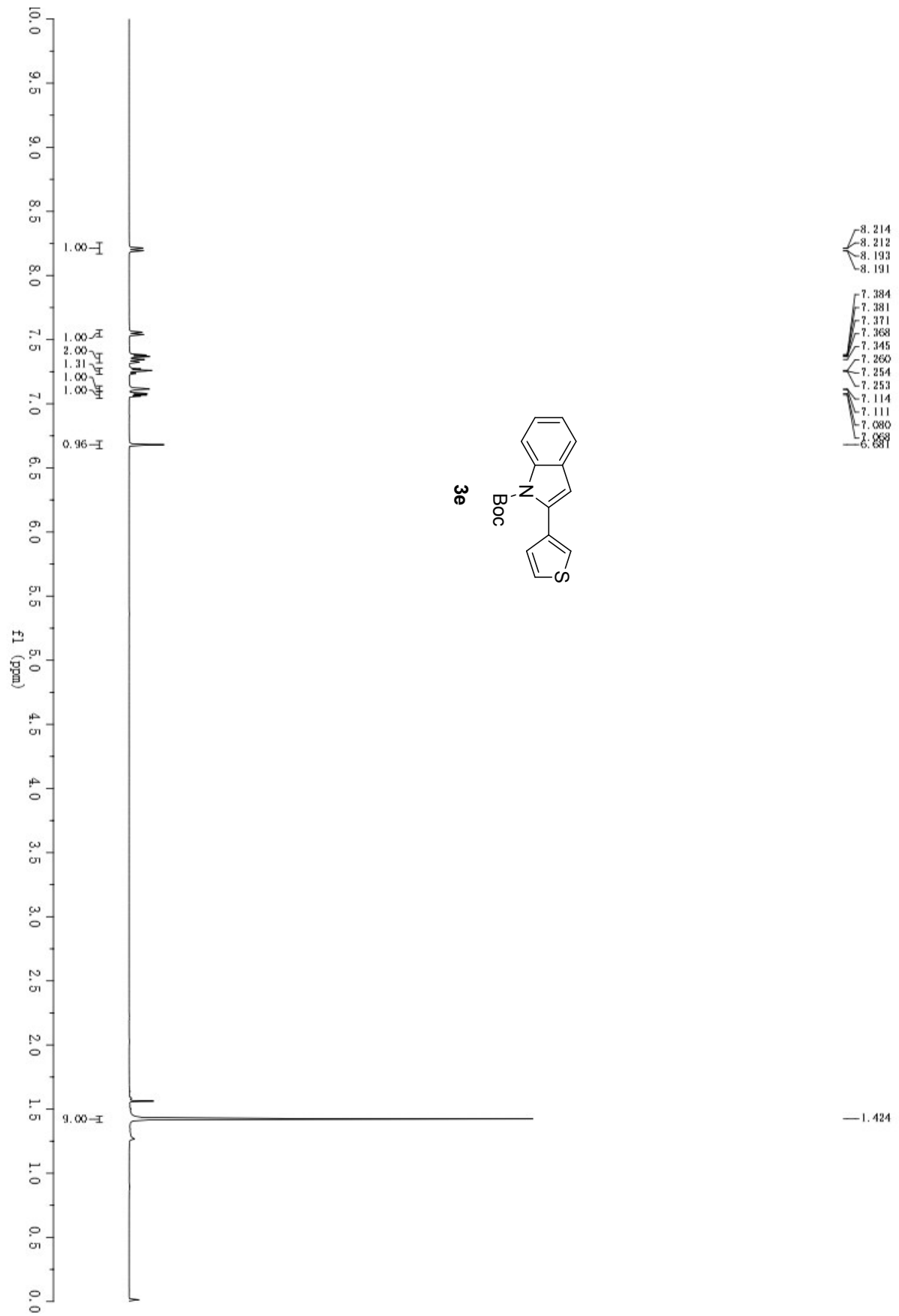

8.283
8.262
7.598
7.579
7.453
7.450
7.385
7.374
7.367
7.347
7.287
7.268
7.260
7.230
7.211
7.117
6.611
1.361
1.00
1.03
1.01
2.07
1.31
1.05
1.00
1.00
9.22
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
N
Boc
F

3c

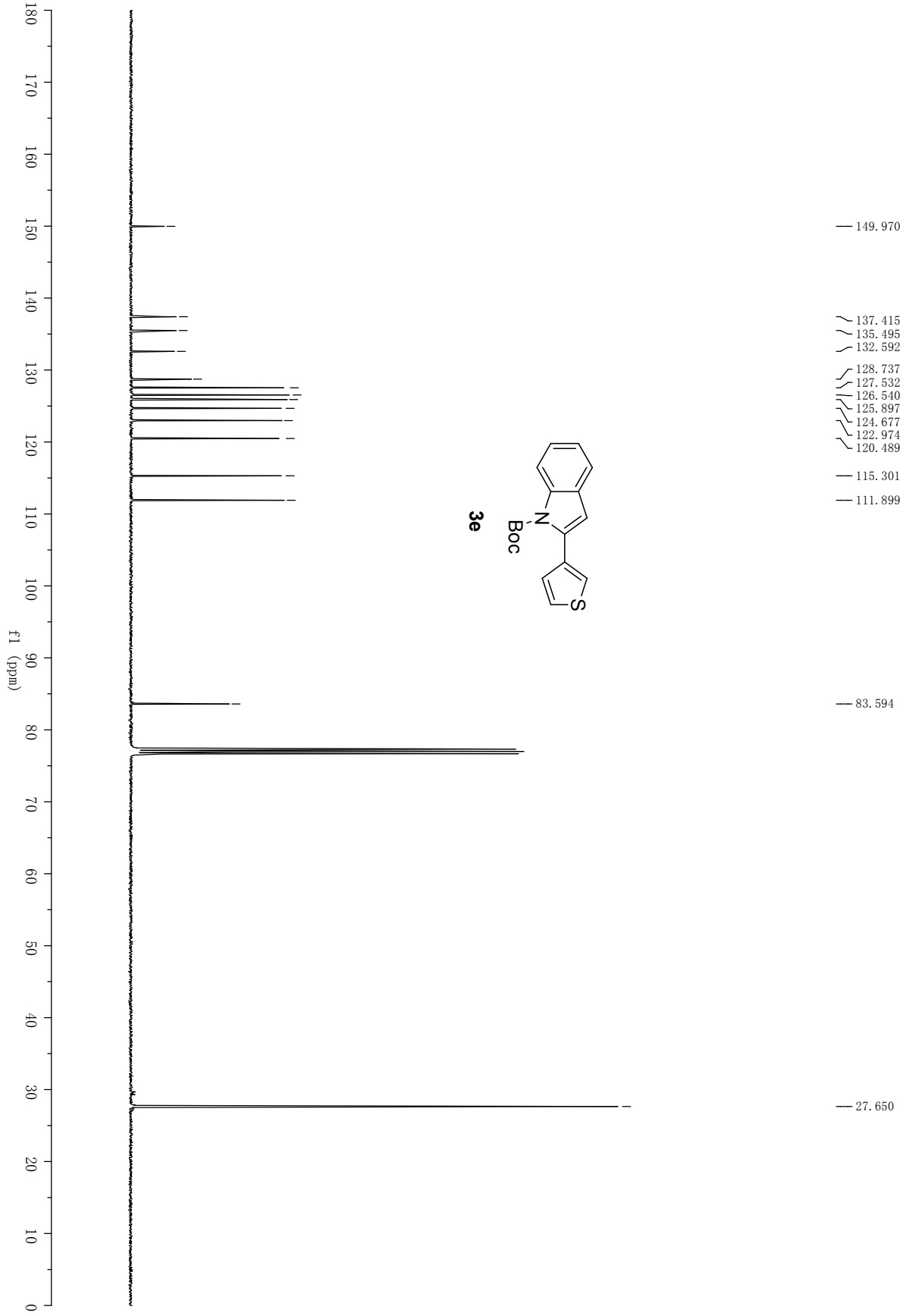

161.212
158.752
149.927
137.269
134.133
130.477
130.445
129.677
129.597
128.931
124.556
123.826
122.770
120.523
115.336
115.131
114.917
110.743
83.422
27.512
f1 (ppm)
3c
N
Boc
F


8.233
8.212
7.570
7.551
7.417
7.370
7.349
7.332
7.313
7.281
7.260
7.244
6.582
1.344
1.00
1.08
0.98
4.13
0.66
0.24
0.98
8.96
f1 (ppm)
3d
N
Boc
Cl


149.958
138.779
137.521
136.651
133.598
129.059
128.973
128.934
127.547
126.788
124.688
123.075
120.603
115.298
110.530
83.724
27.595
f1 (ppm)
3d
Boc
N
Cl

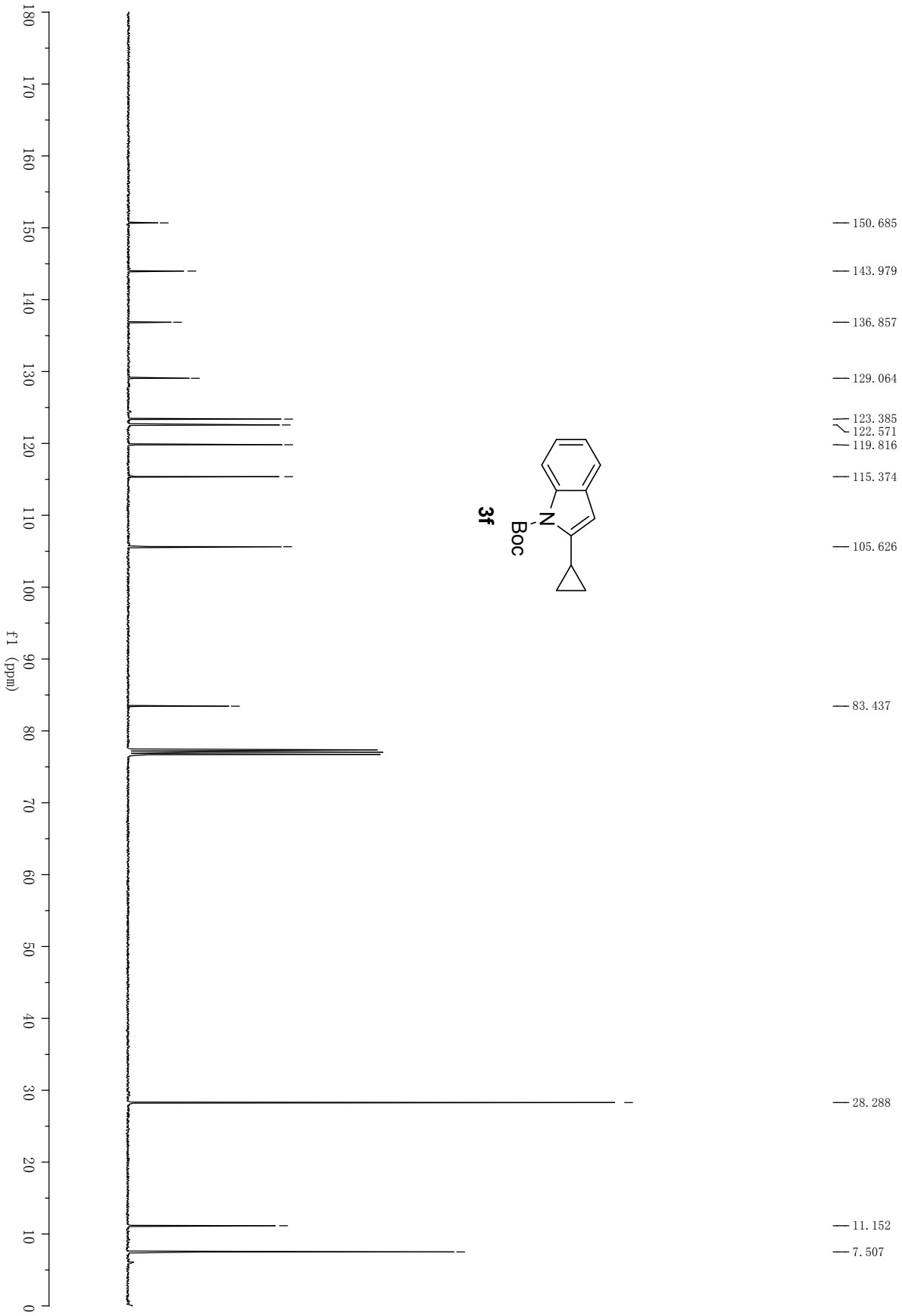

8.214
8.212
8.193
8.191
7.384
7.381
7.371
7.368
7.345
7.260
7.254
7.253
7.114
7.111
7.080
7.068
6.981
1.424
1.00
1.00
2.00
1.31
1.00
1.00
0.96
9.00
f1 (ppm)
N
Boc
S

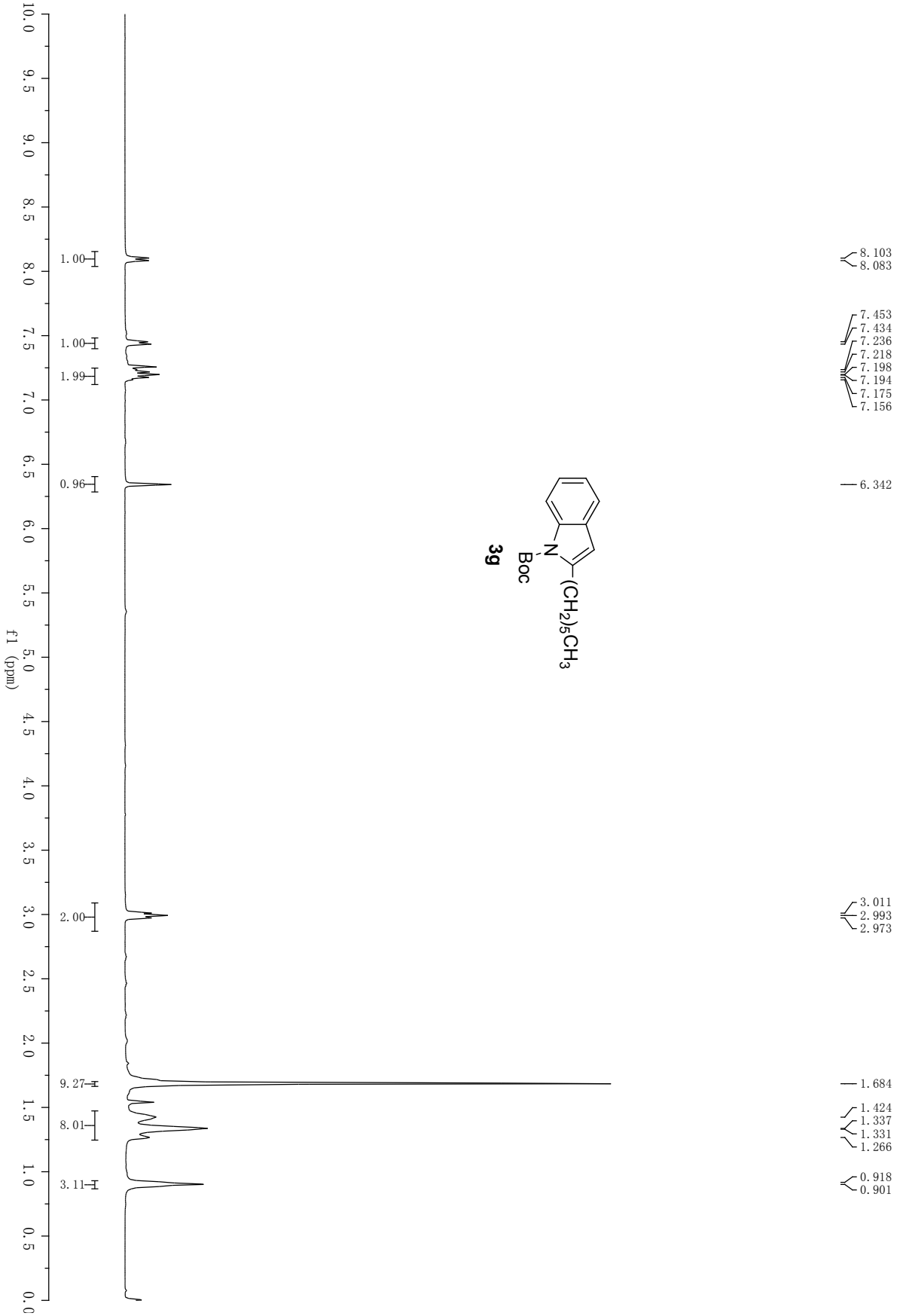
3e

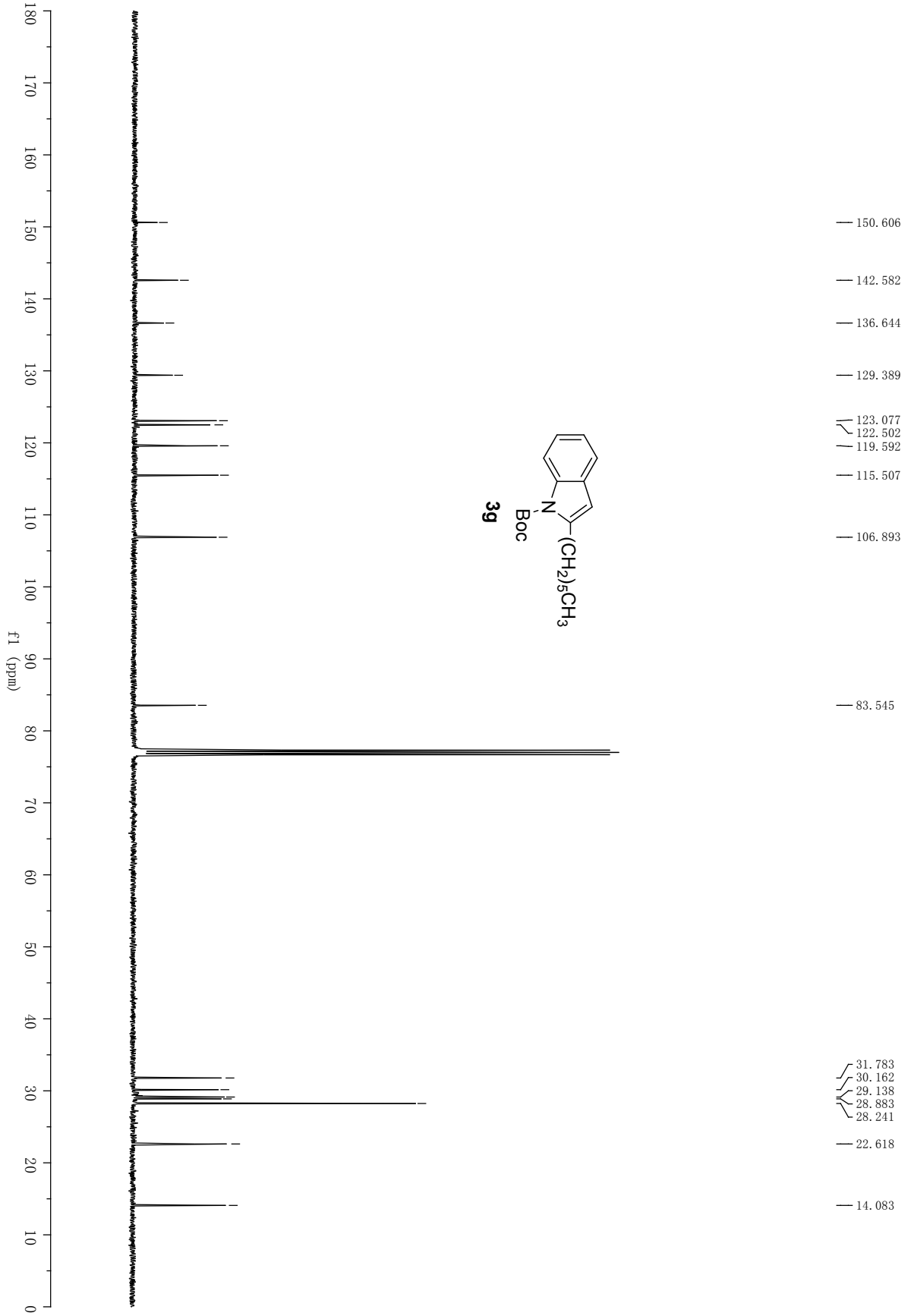

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
149.970
137.415
135.495
132.592
128.737
127.532
126.540
125.897
124.677
122.974
120.489
115.301
111.899
83.594
27.650
3e
N
Boc
S

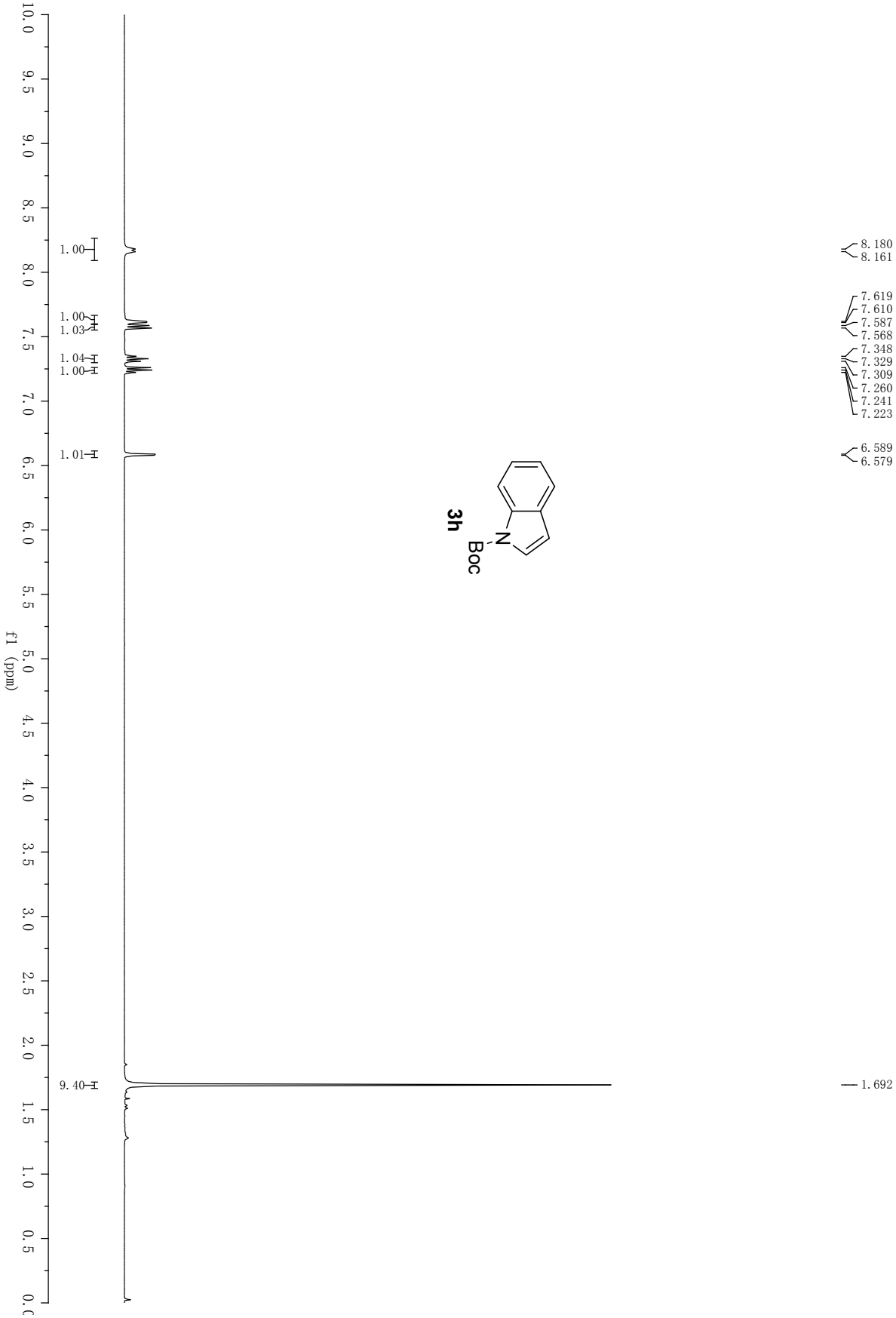

8.142
8.121
7.440
7.422
7.421
7.260
7.244
7.242
7.224
7.221
7.199
7.196
7.180
7.178
7.162
7.160
2.405
2.391
2.387
2.384
2.373
2.371
2.360
2.357
2.352
2.339
2.337
1.703
0.987
0.976
0.971
0.961
0.955
0.950
0.940
0.765
0.755
0.750
0.741
0.737
0.726
N
Boc
1.00
1.01
1.10
1.01
1.00
1.00
9.03
2.05
2.03
f1 (ppm)

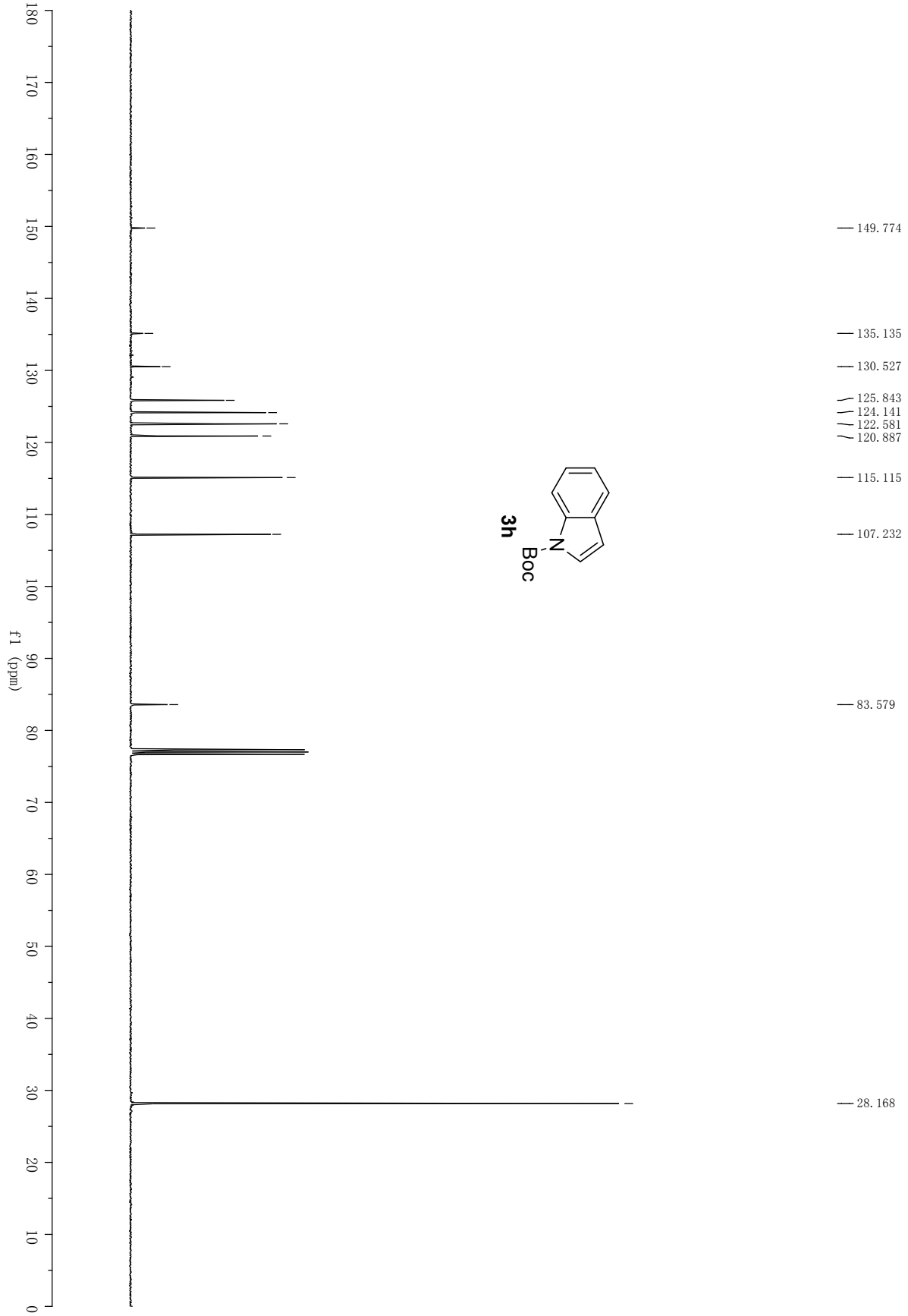
3f

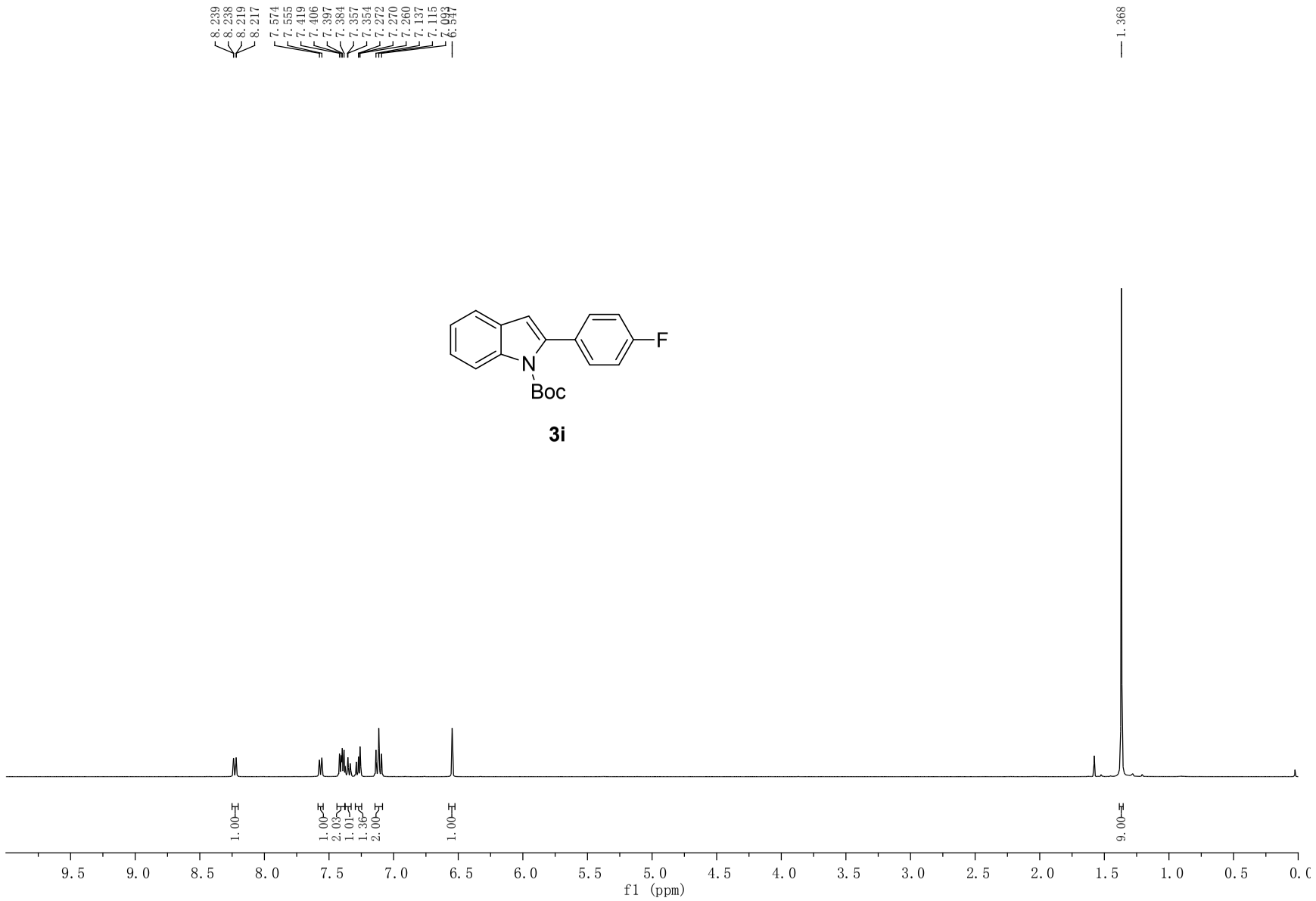

150.685
143.979
136.857
129.064
123.385
122.571
119.816
115.374
105.626
83.437
28.288
11.152
7.507
f1 (ppm)
3f
N
Boc

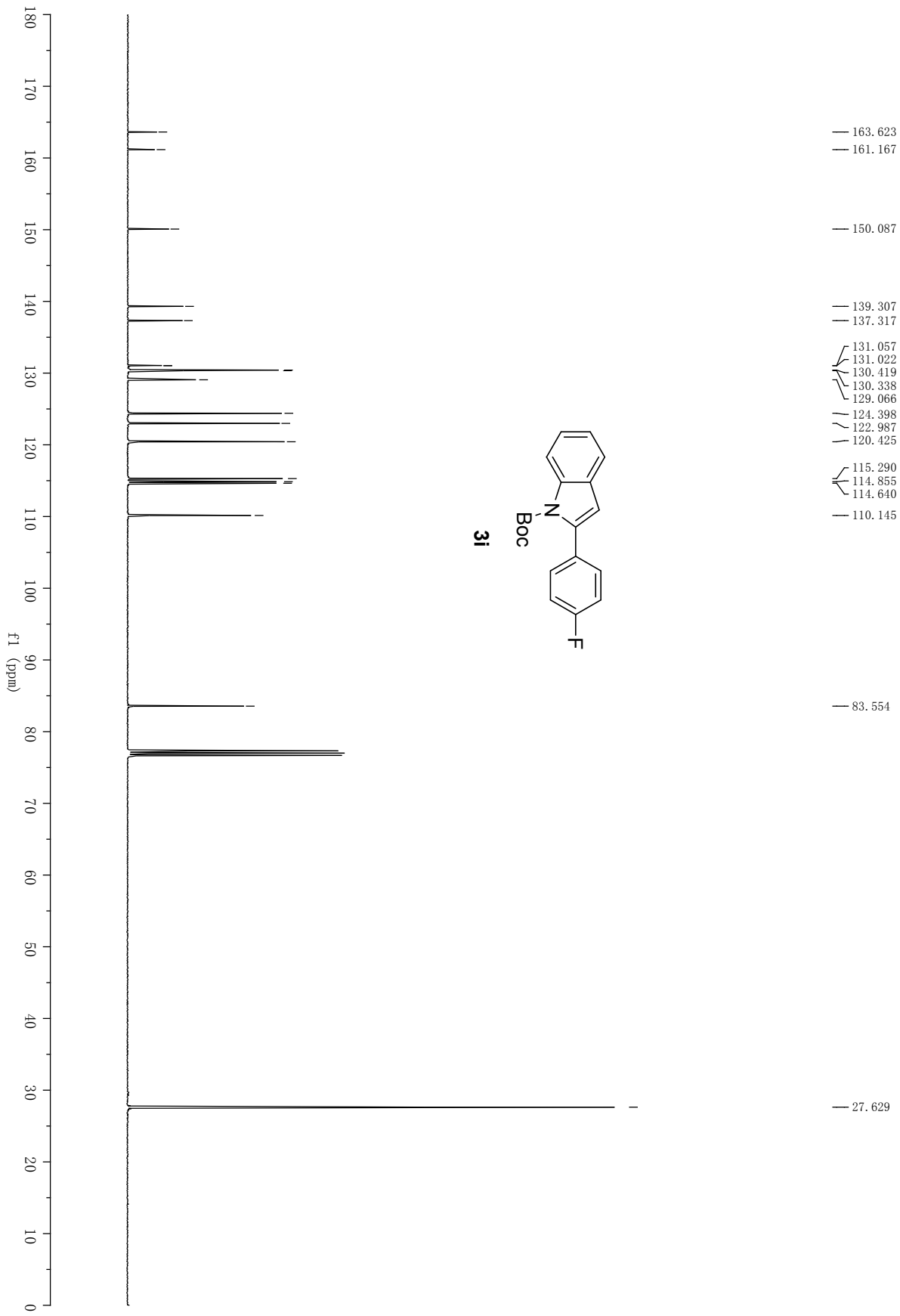

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.00
1.00
1.99
0.96
2.00
9.27
8.01
3.11
8.103
8.083
7.453
7.434
7.236
7.218
7.198
7.194
7.175
7.156
6.342
3.011
2.993
2.973
1.684
1.424
1.337
1.331
1.266
0.918
0.901
N
Boc
(CH2)5CH3
3g

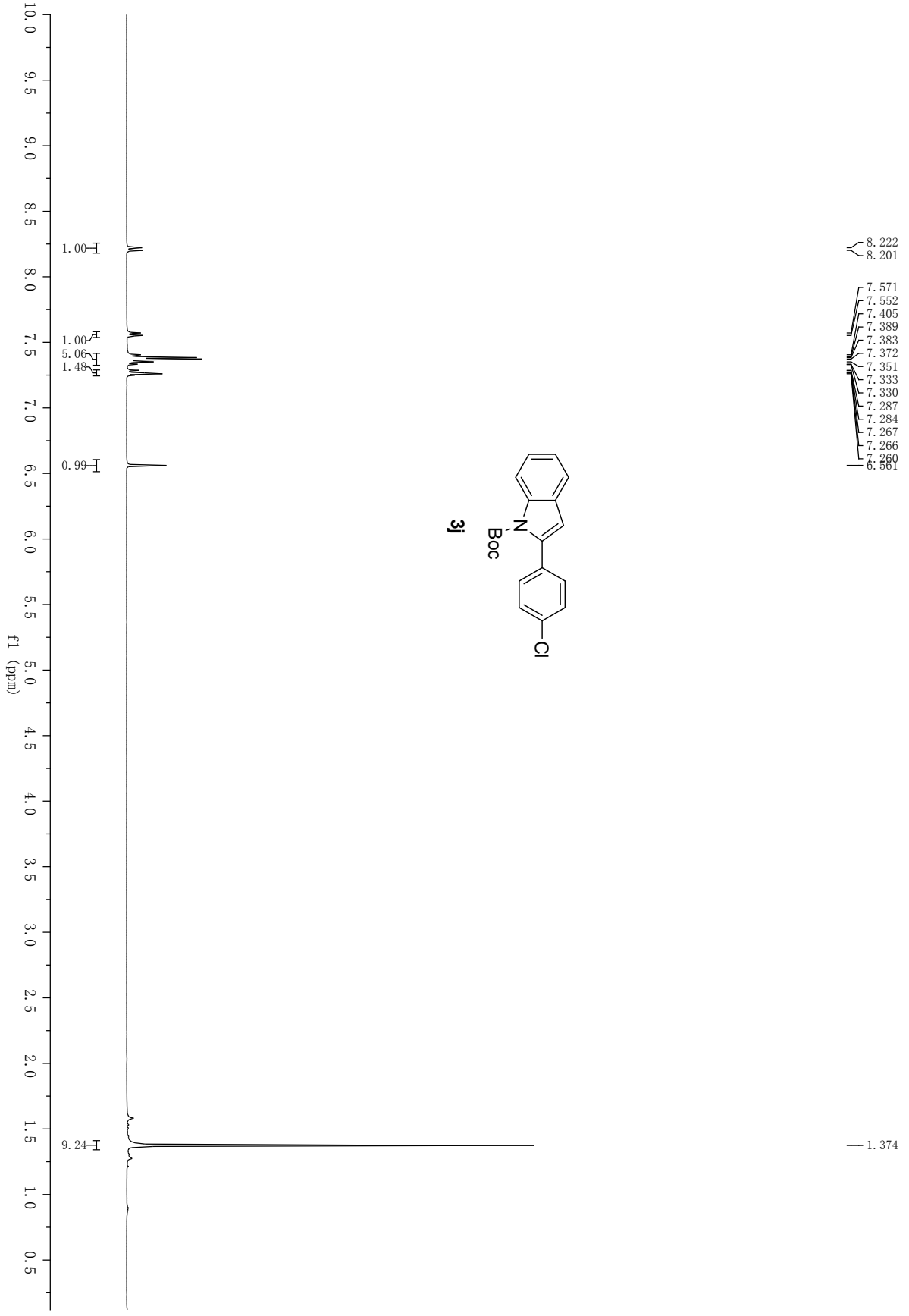

150.606
142.582
136.644
129.389
123.077
122.502
119.592
115.507
106.893
83.545
31.783
30.162
29.138
28.883
28.241
22.618
14.083
f1 (ppm)
Boc
(CH2)5CH3
3g

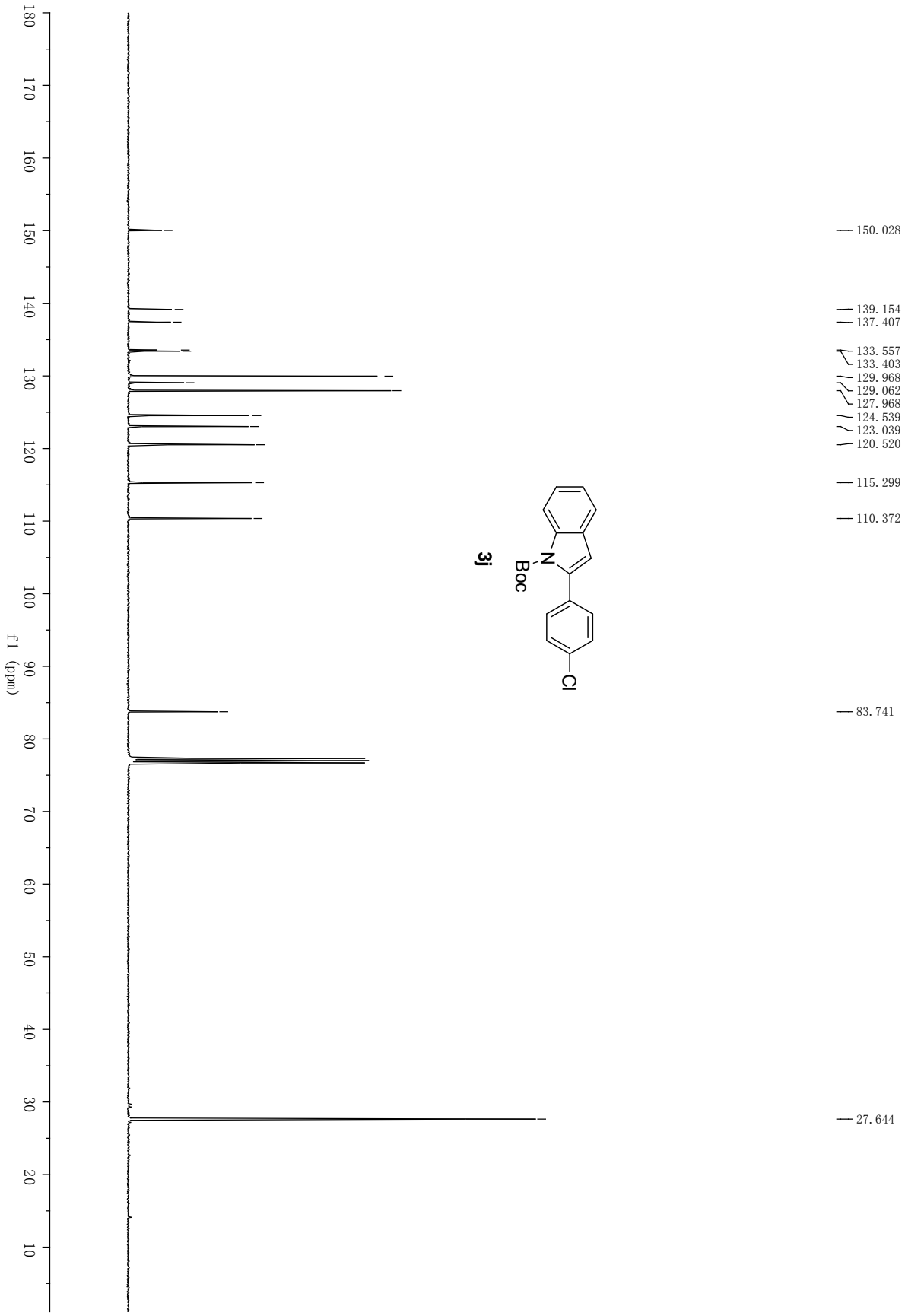

8.180
8.161
7.619
7.610
7.587
7.568
7.348
7.329
7.309
7.260
7.241
7.223
6.589
6.579
1.692
1.00
1.00
1.03
1.04
1.00
1.01
9.40
3h
N
Boc
f1 (ppm)

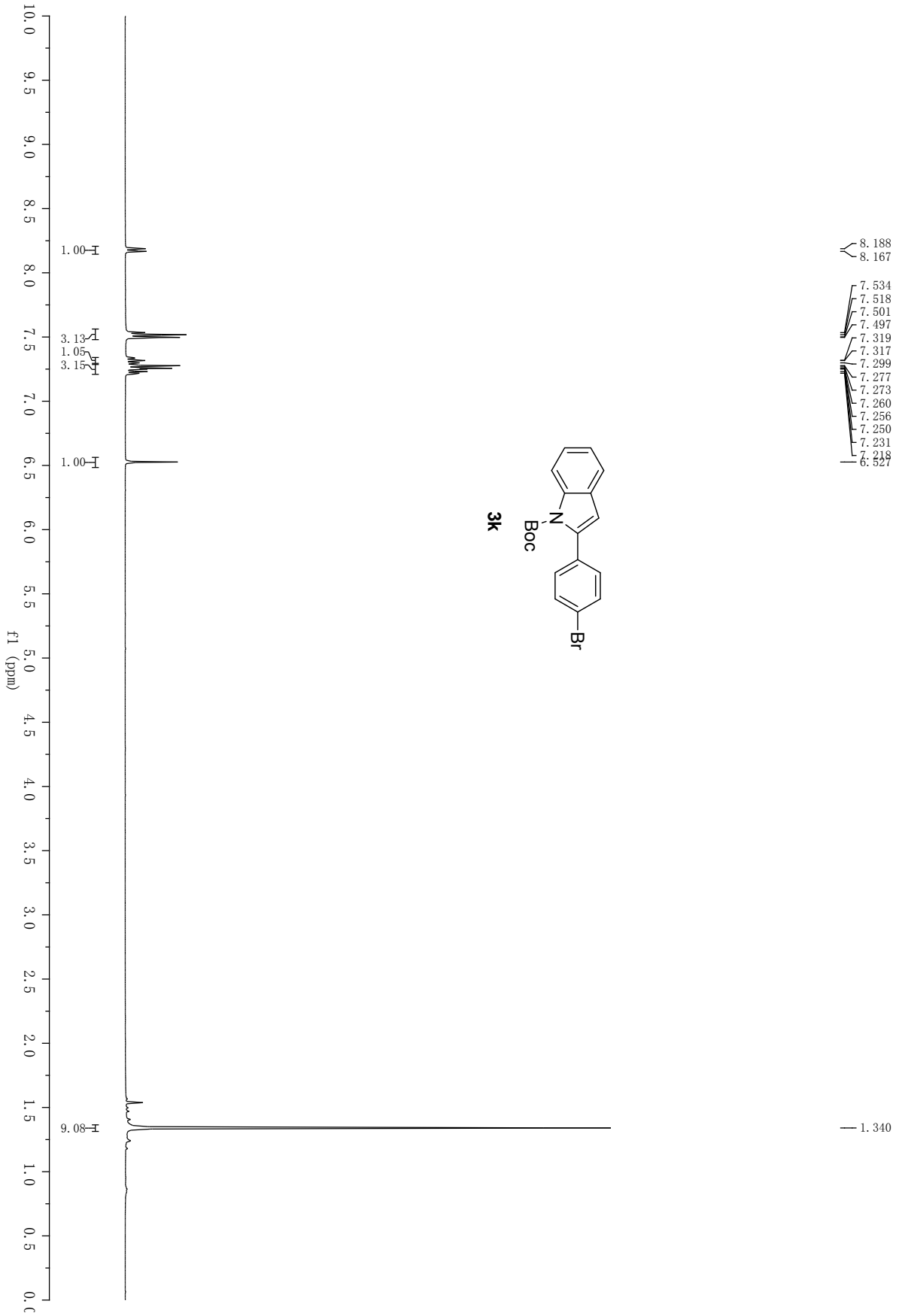

149.774
135.135
130.527
125.843
124.141
122.581
120.887
115.115
107.232
83.579
28.168
3h
N
Boc
f1 (ppm)

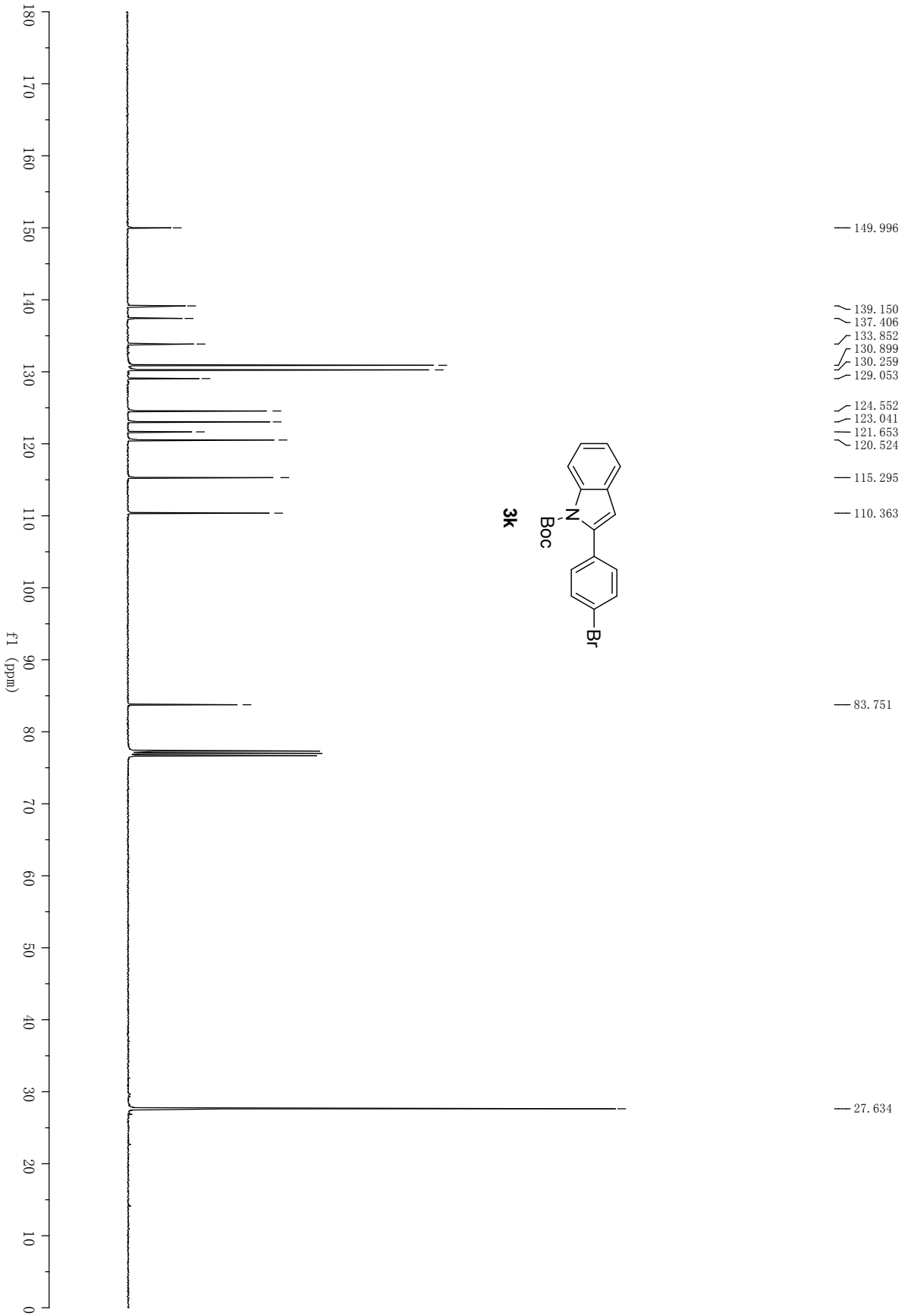

8.239
8.238
8.219
8.217
7.574
7.555
7.419
7.406
7.397
7.384
7.357
7.354
7.272
7.270
7.260
7.137
7.115
6.917
1.368
F
N
Boc
3i
1.00
1.00
2.03
1.01
1.36
2.00
1.00
9.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

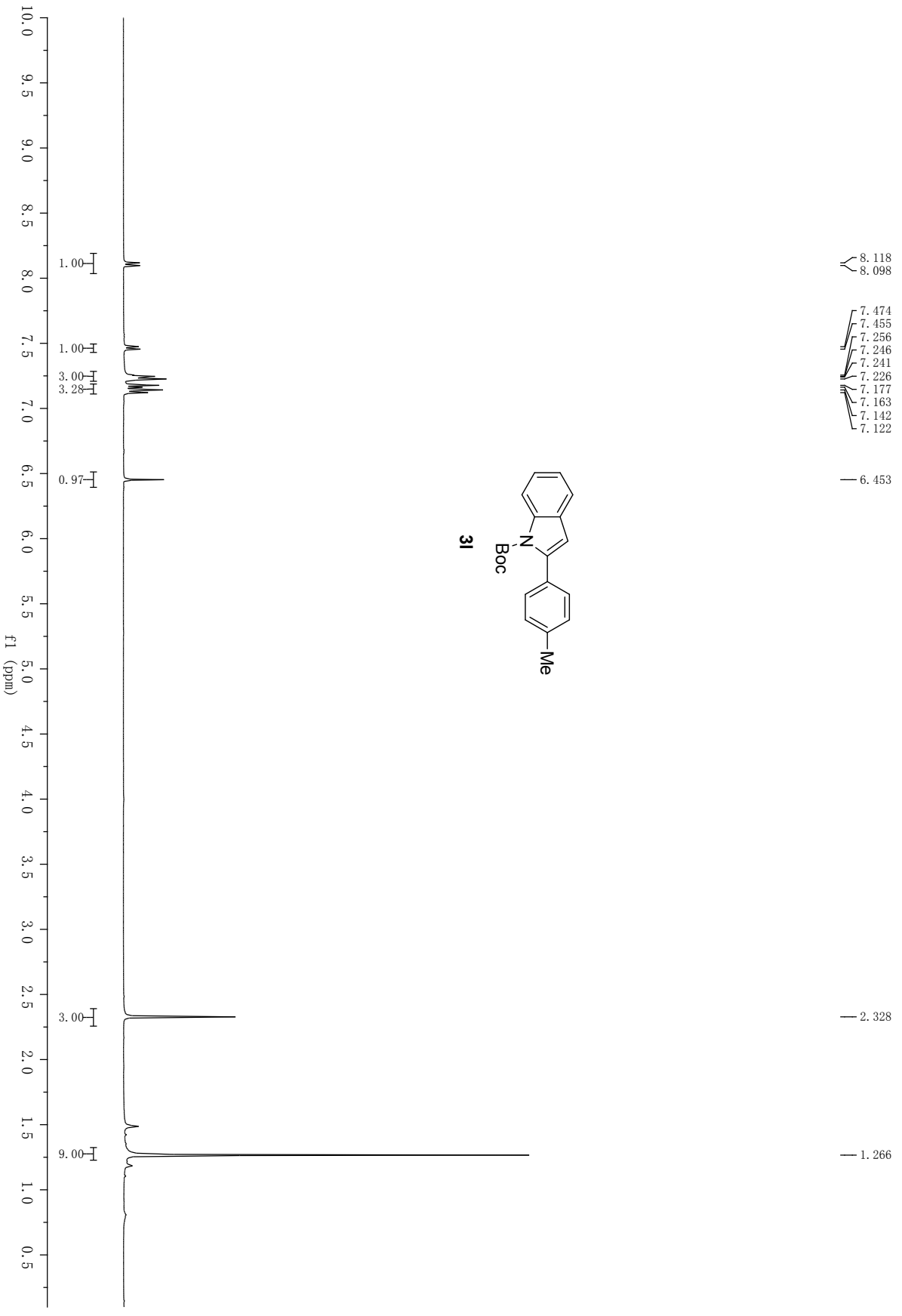

163.623
161.167
150.087
139.307
137.317
131.057
131.022
130.419
130.338
129.066
124.398
122.987
120.425
115.290
114.855
114.640
110.145
83.554
27.629
f1 (ppm)
N
Boc
F
3i

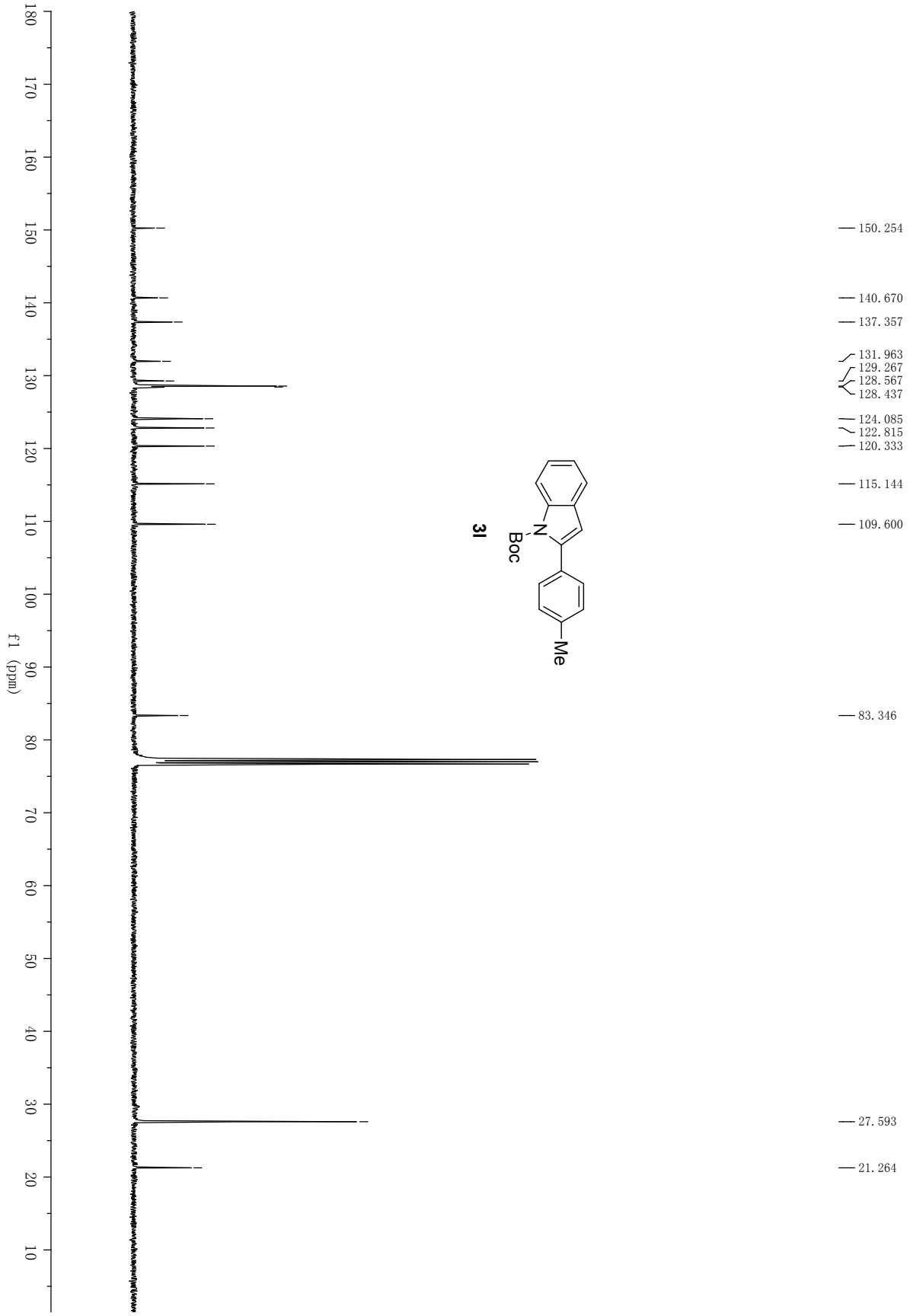

8.222
8.201
7.571
7.552
7.405
7.389
7.383
7.372
7.351
7.333
7.330
7.287
7.284
7.267
7.266
7.260
6.561
1.374
1.00
1.00
5.06
1.48
0.99
9.24
f1 (ppm)
3j
N
Boc
Cl

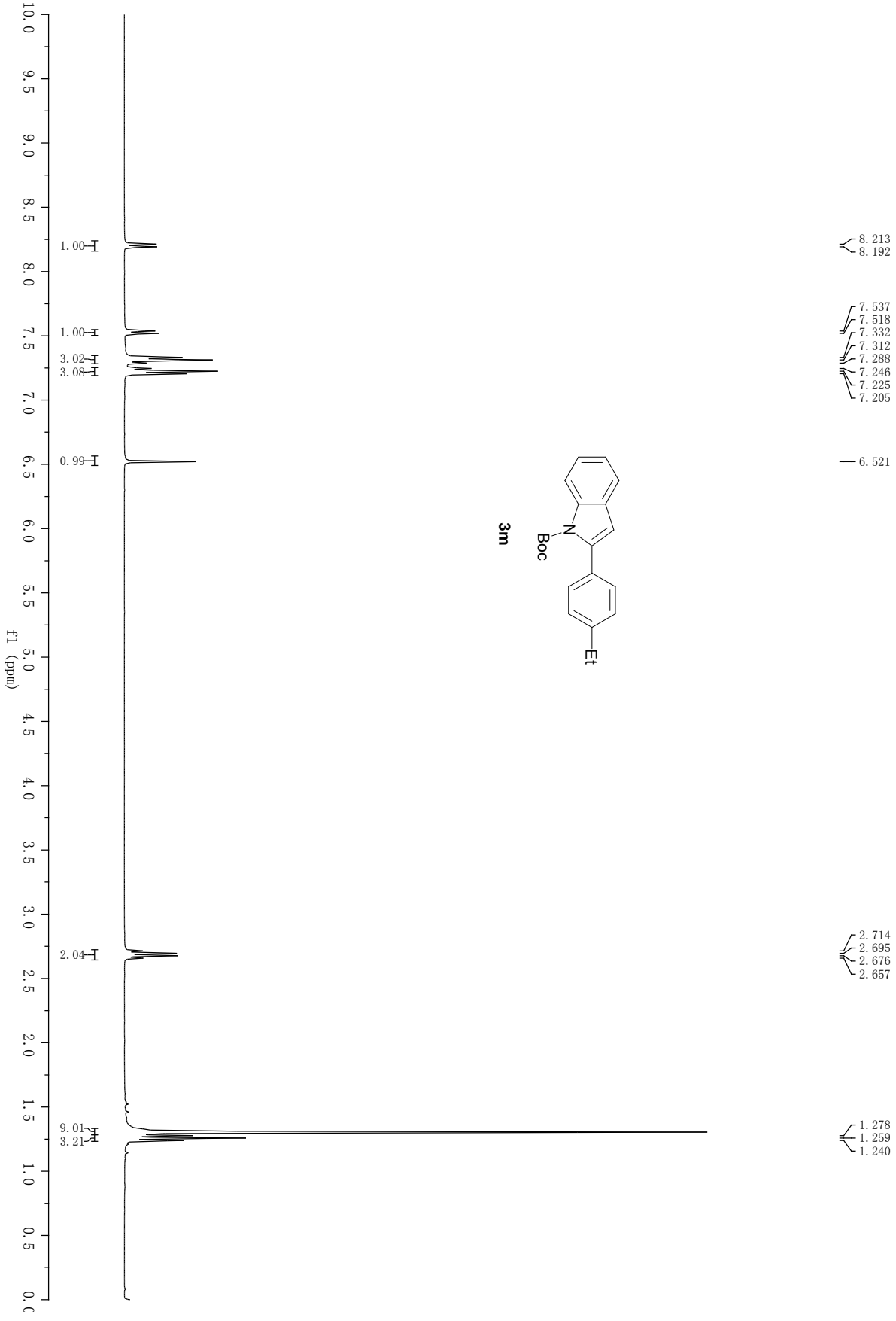

150.028
139.154
137.407
133.557
133.403
129.968
129.062
127.968
124.539
123.039
120.520
115.299
110.372
83.741
27.644
f1 (ppm)
3j
Boc
N
Cl

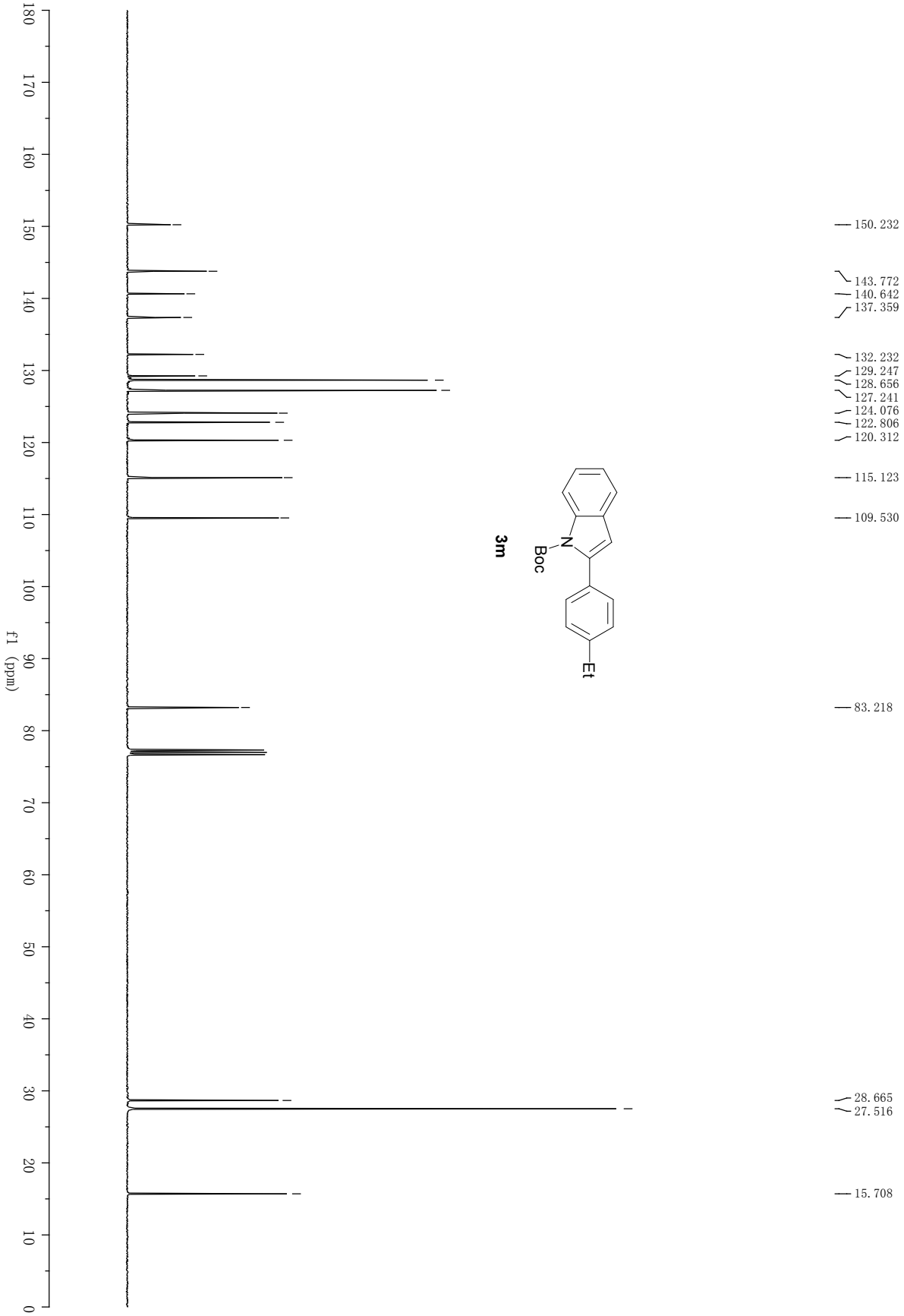

8.188
8.167
7.534
7.518
7.501
7.497
7.319
7.317
7.299
7.277
7.273
7.260
7.256
7.250
7.231
7.218
6.527
1.340
1.00
3.13
1.05
3.15
1.00
9.08
N
Boc
Br
3k
f1 (ppm)

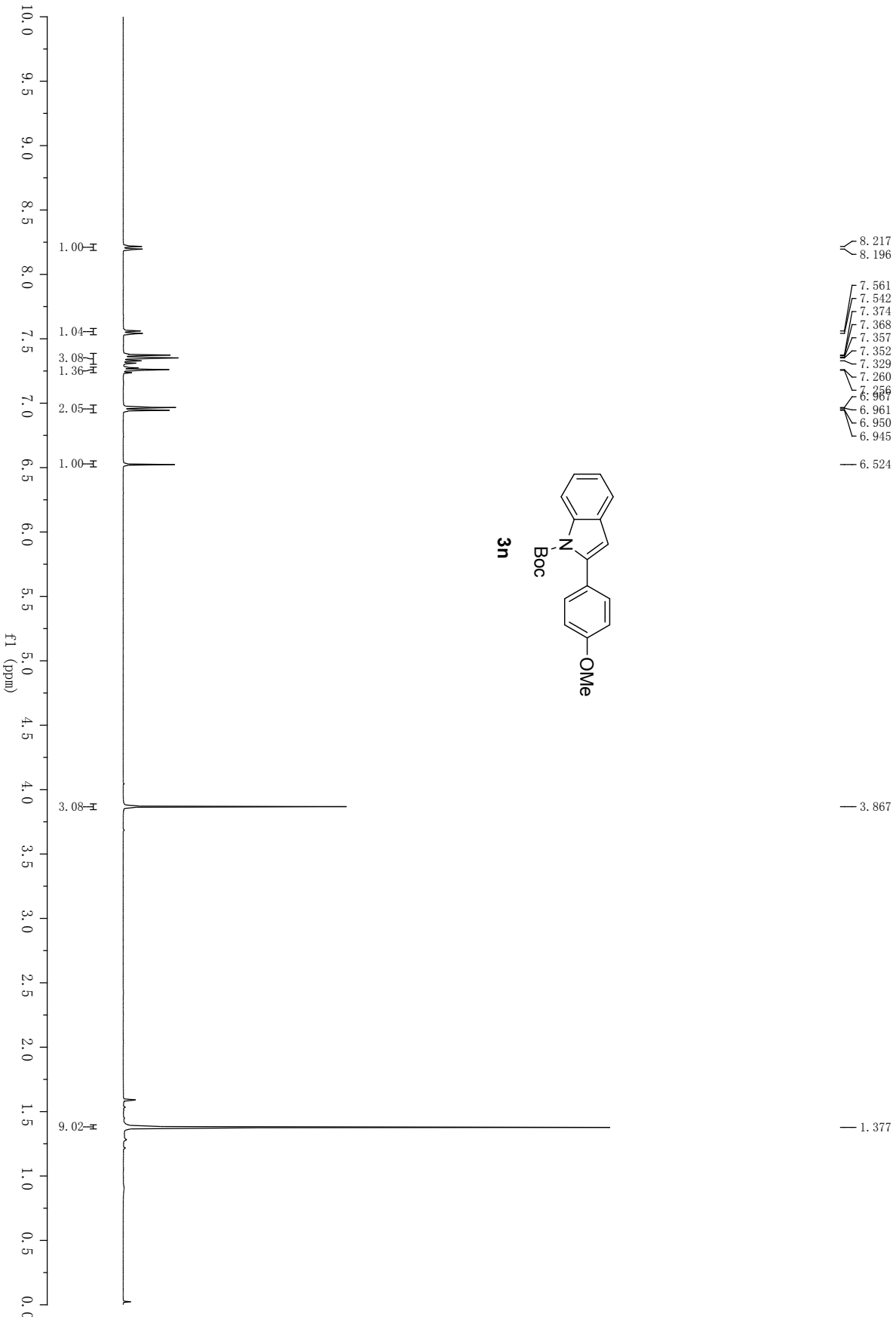

149.996
139.150
137.406
133.852
130.899
130.259
129.053
124.552
123.041
121.653
120.524
115.295
110.363
83.751
27.634
f1 (ppm)
3k
Boc
N
Br

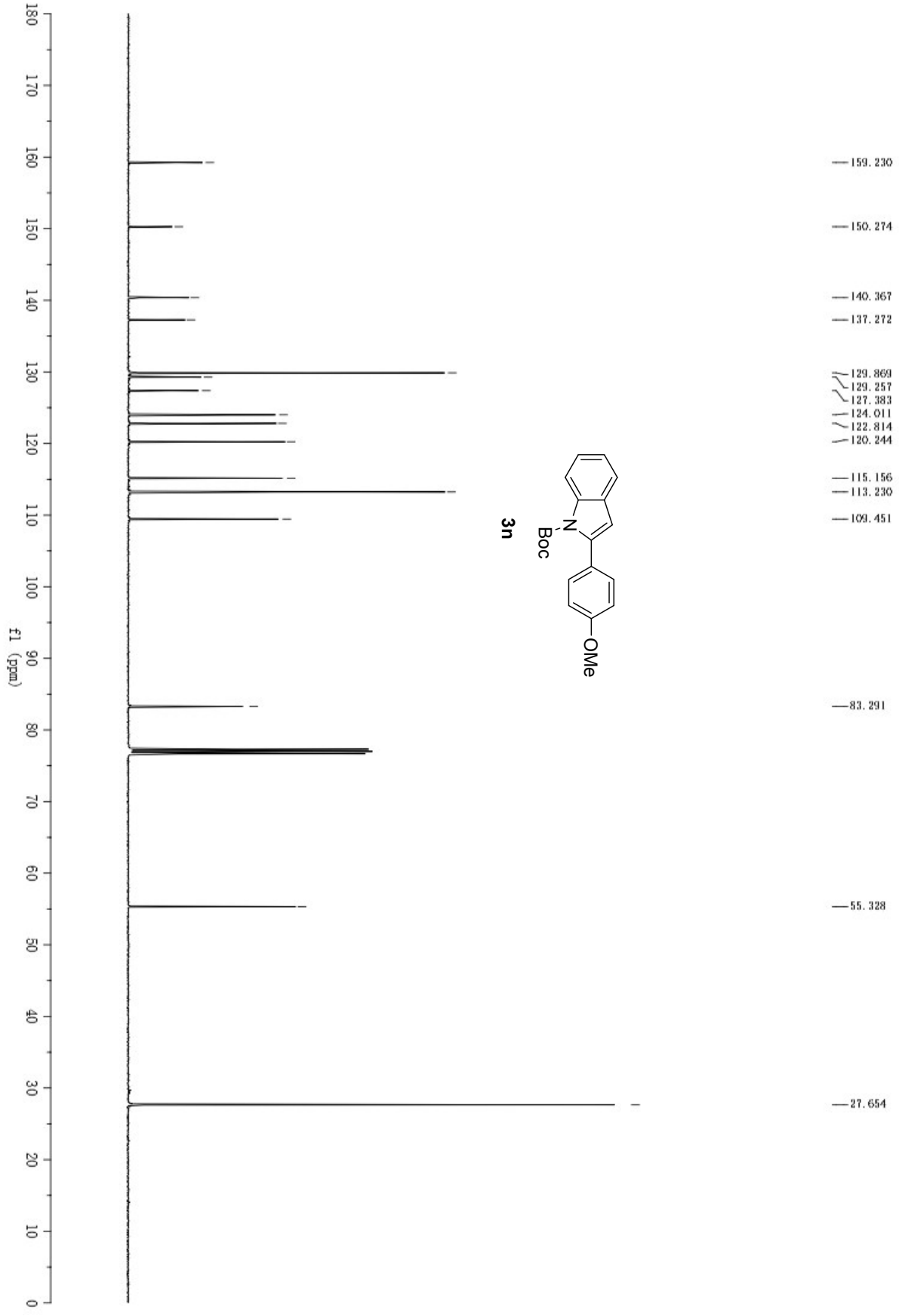

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
1.00
1.00
3.00
3.28
0.97
3.00
9.00
8.118
8.098
7.474
7.455
7.256
7.246
7.241
7.226
7.177
7.163
7.142
7.122
6.453
2.328
1.266
N
Boc
Me
3l

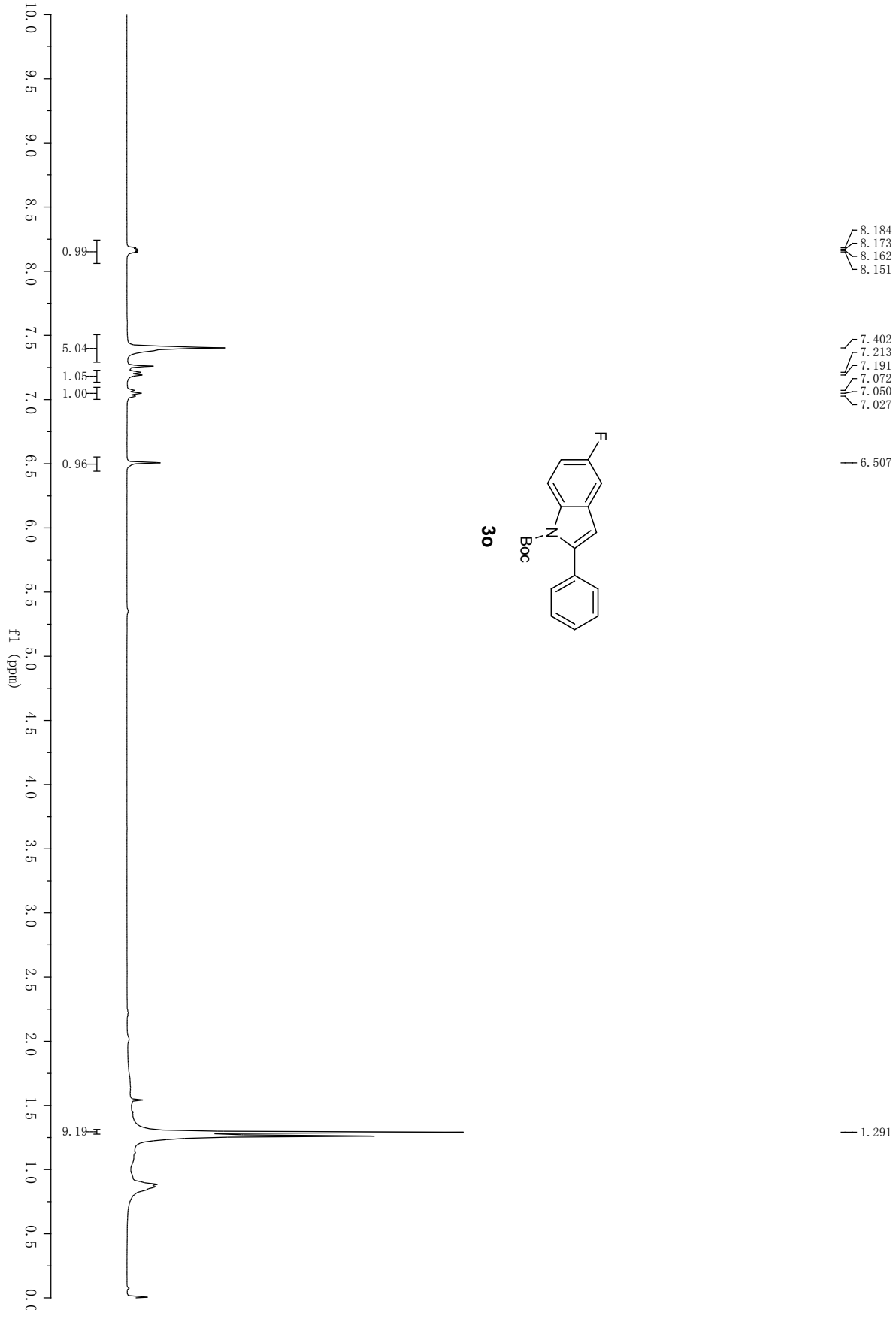

150.254
140.670
137.357
131.963
129.267
128.567
128.437
124.085
122.815
120.333
115.144
109.600
83.346
27.593
21.264
f1 (ppm)
N
Boc
Me
3l

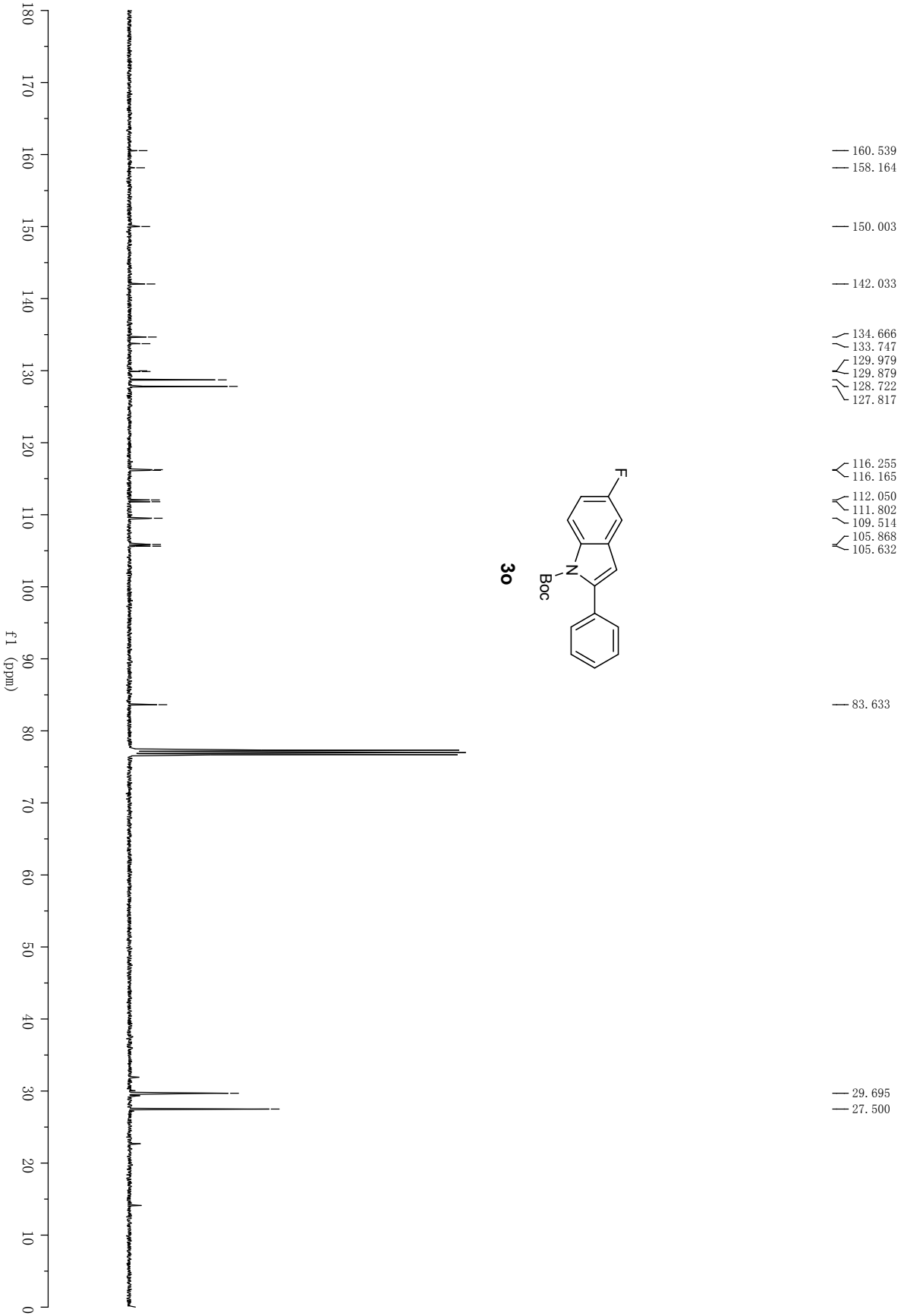

8.213
8.192
7.537
7.518
7.332
7.312
7.288
7.246
7.225
7.205
6.521
2.714
2.695
2.676
2.657
1.278
1.259
1.240
1.00
1.00
3.02
3.08
0.99
2.04
9.01
3.21
f1 (ppm)
3m
N
Boc
Et

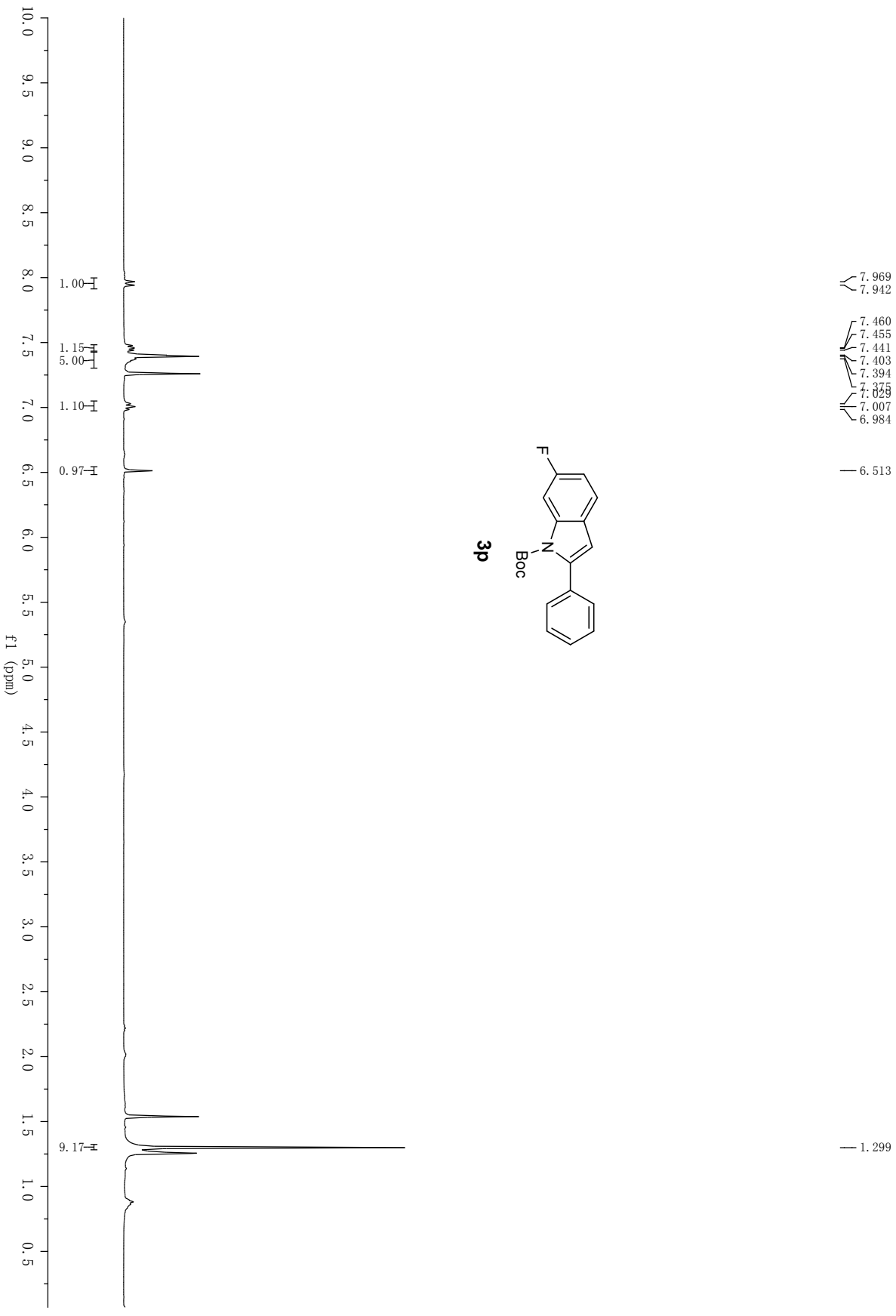

150.232
143.772
140.642
137.359
132.232
129.247
128.656
127.241
124.076
122.806
120.312
115.123
109.530
83.218
28.665
27.516
15.708
3m
N
Boc
Et
f1 (ppm)


8.217
8.196
7.561
7.542
7.374
7.368
7.357
7.352
7.329
7.260
7.256
6.967
6.961
6.950
6.945
6.524
3.867
1.377
1.00
1.04
3.08
1.36
2.05
1.00
3.08
9.02
f1 (ppm)
N
Boc
OMe
3n

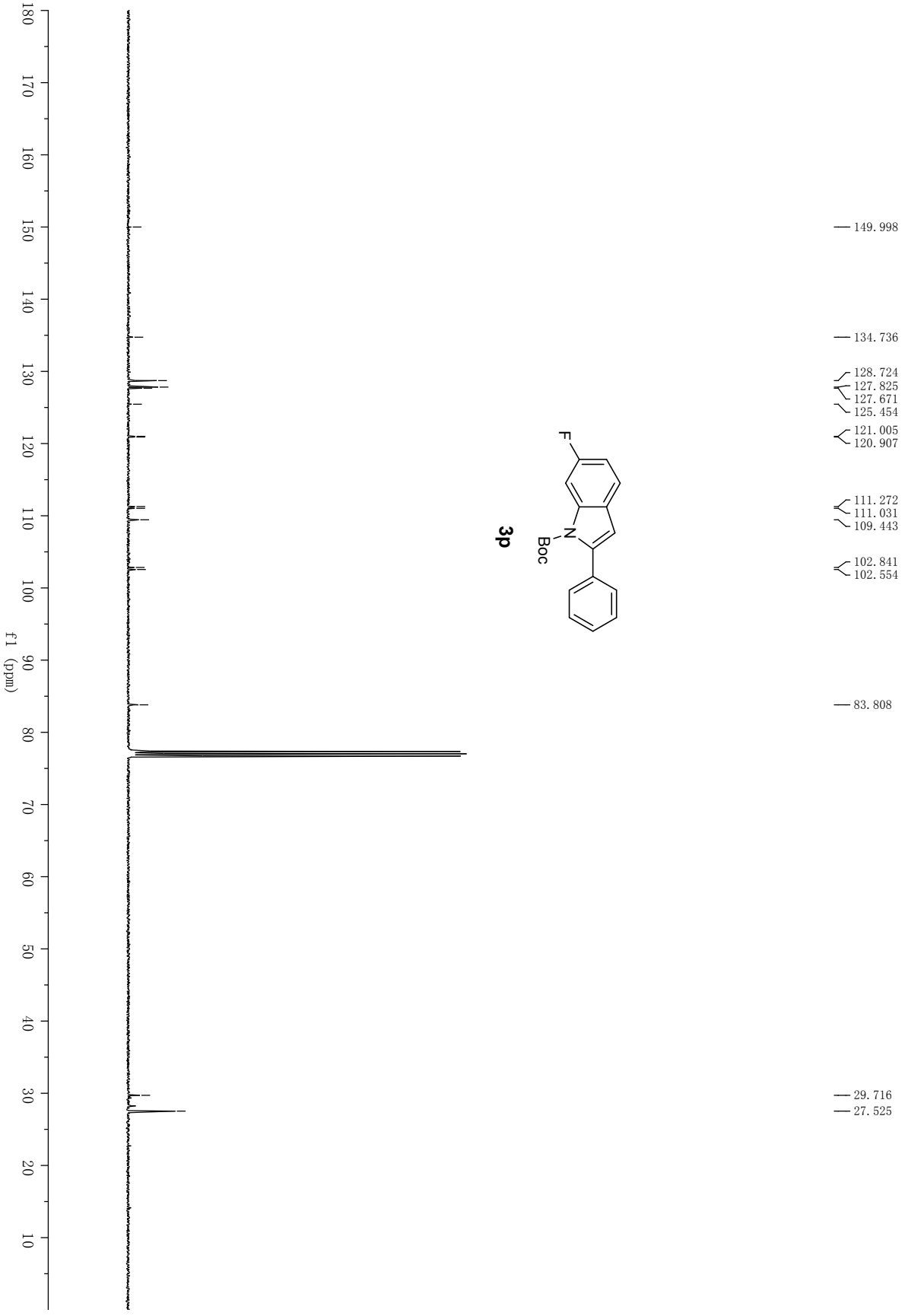

159.230
150.274
140.367
137.272
129.869
129.257
127.383
124.011
122.814
120.244
115.156
113.230
109.451
83.291
55.328
27.654
f1 (ppm)
N
Boc
OMe
3n

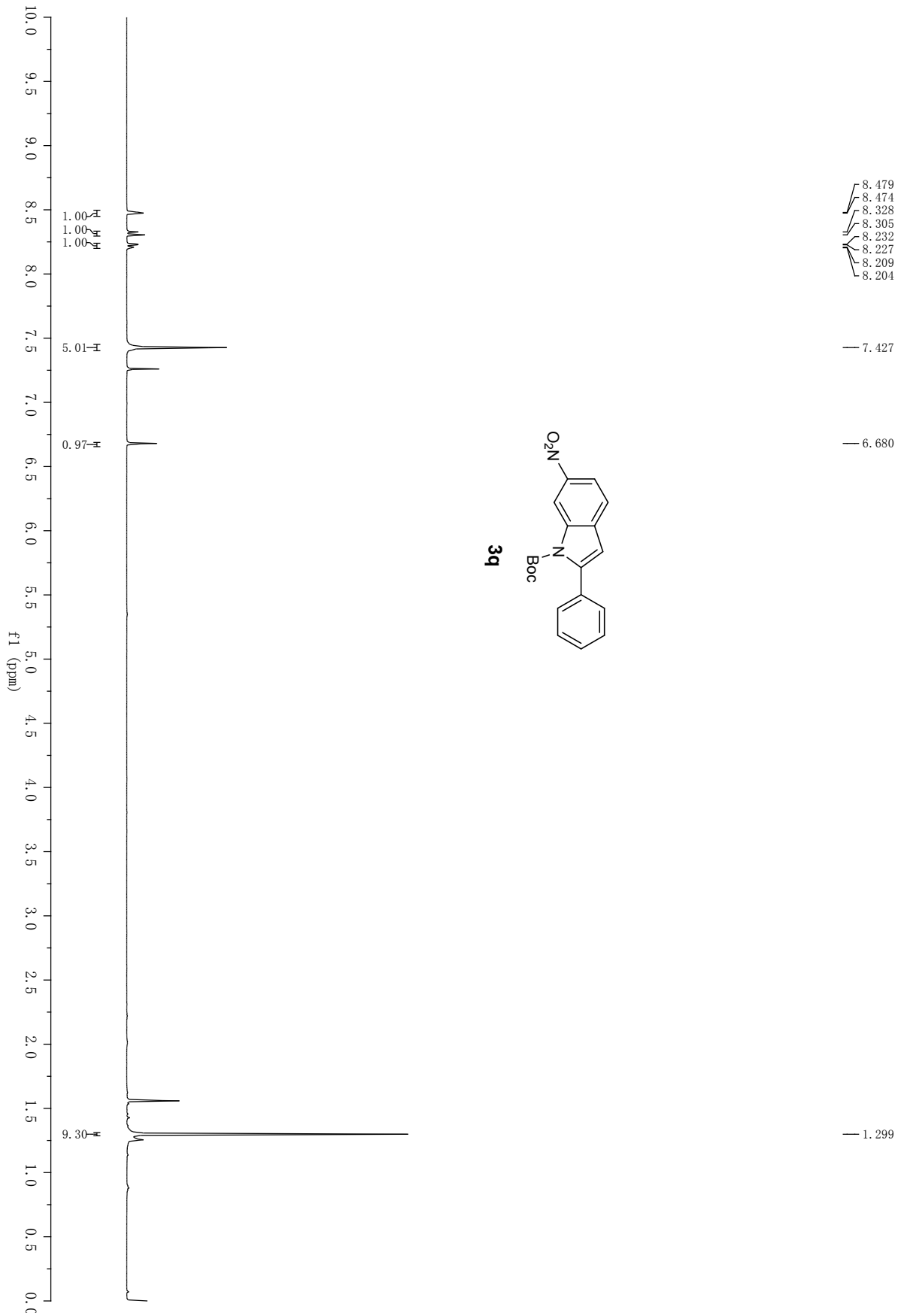

8.184
8.173
8.162
8.151
7.402
7.213
7.191
7.072
7.050
7.027
6.507
1.291
0.99
5.04
1.05
1.00
0.96
9.19
F
N
Boc
3o
f1 (ppm)

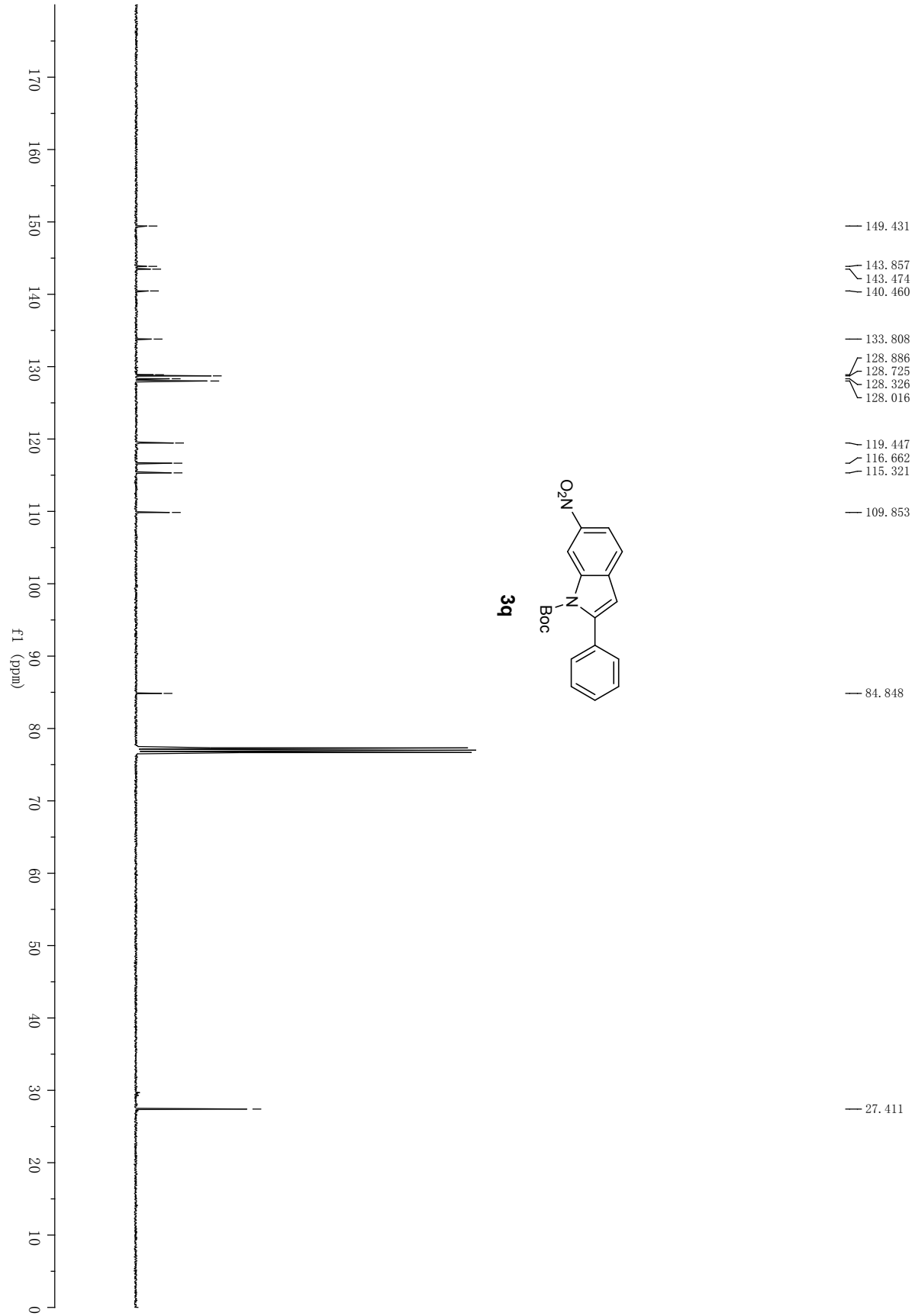

160.539
158.164
150.003
142.033
134.666
133.747
129.979
129.879
128.722
127.817
116.255
116.165
112.050
111.802
109.514
105.868
105.632
83.633
29.695
27.500
F
N
Boc
3o
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

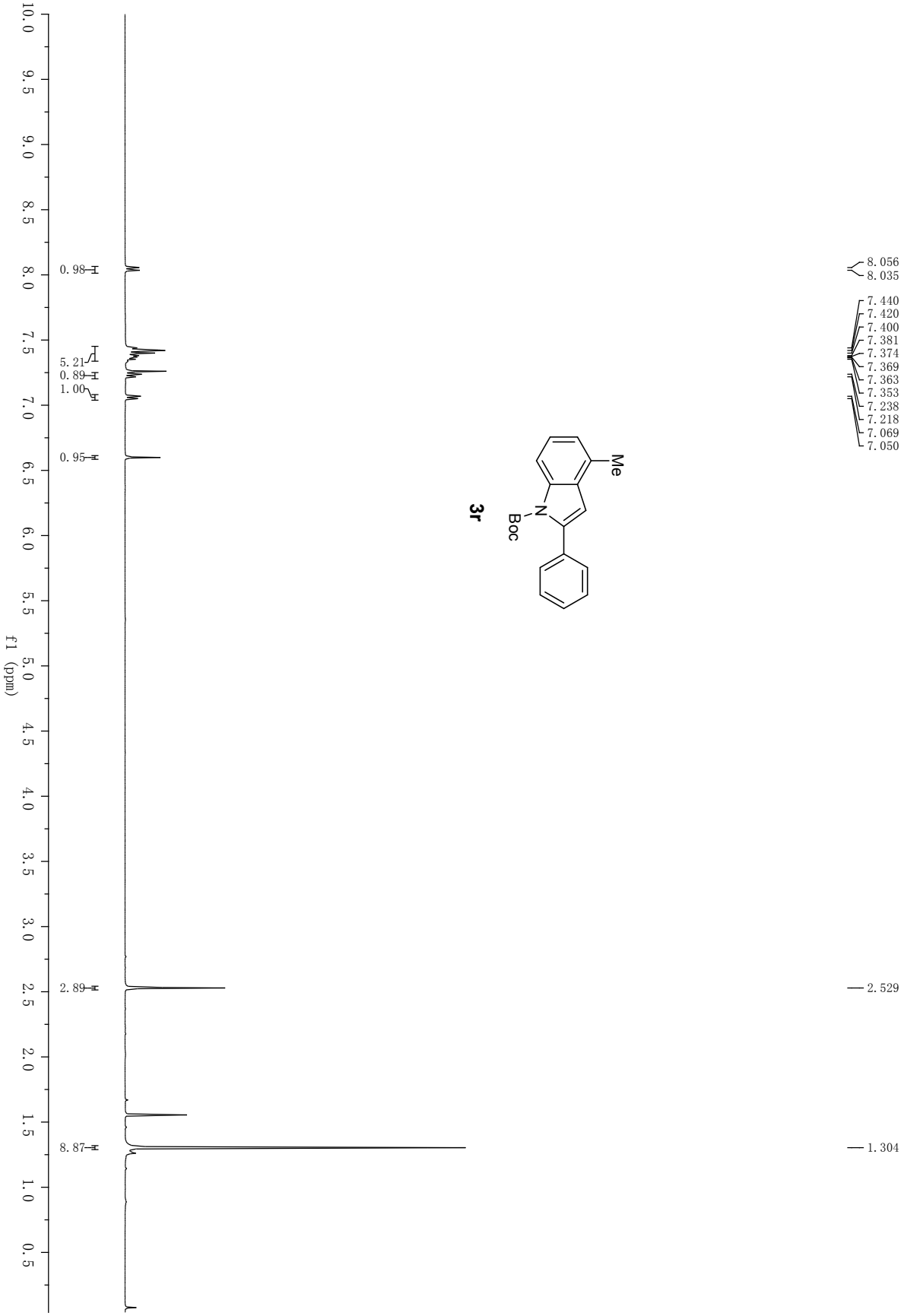

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
1.00
1.15
5.00
1.10
0.97
9.17
7.969
7.942
7.460
7.455
7.441
7.403
7.394
7.375
7.029
7.007
6.984
6.513
1.299
F
N
Boc

3p

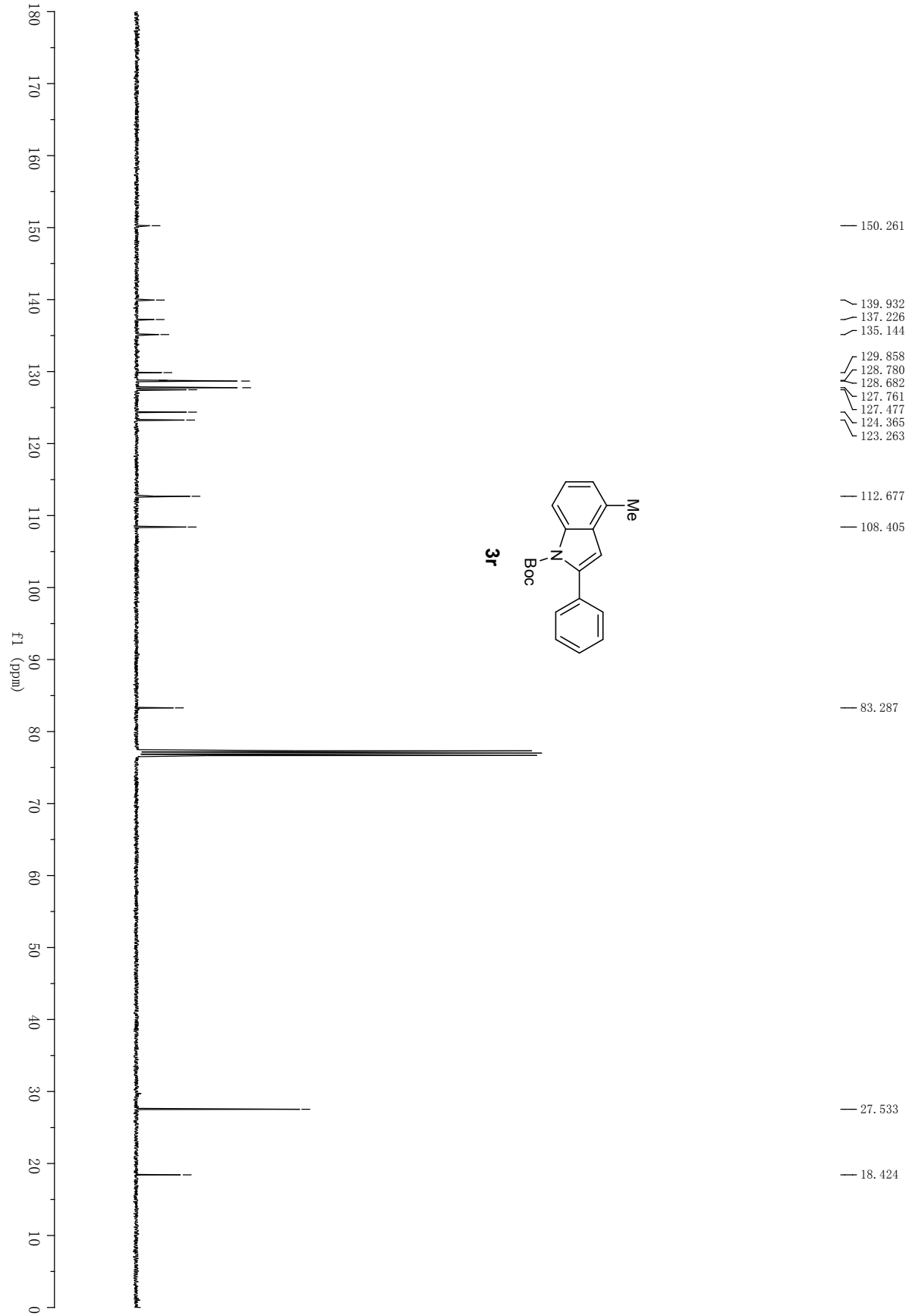

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
149.998
134.736
128.724
127.825
127.671
125.454
121.005
120.907
111.272
111.031
109.443
102.841
102.554
83.808
29.716
27.525
F
N
Boc
3p

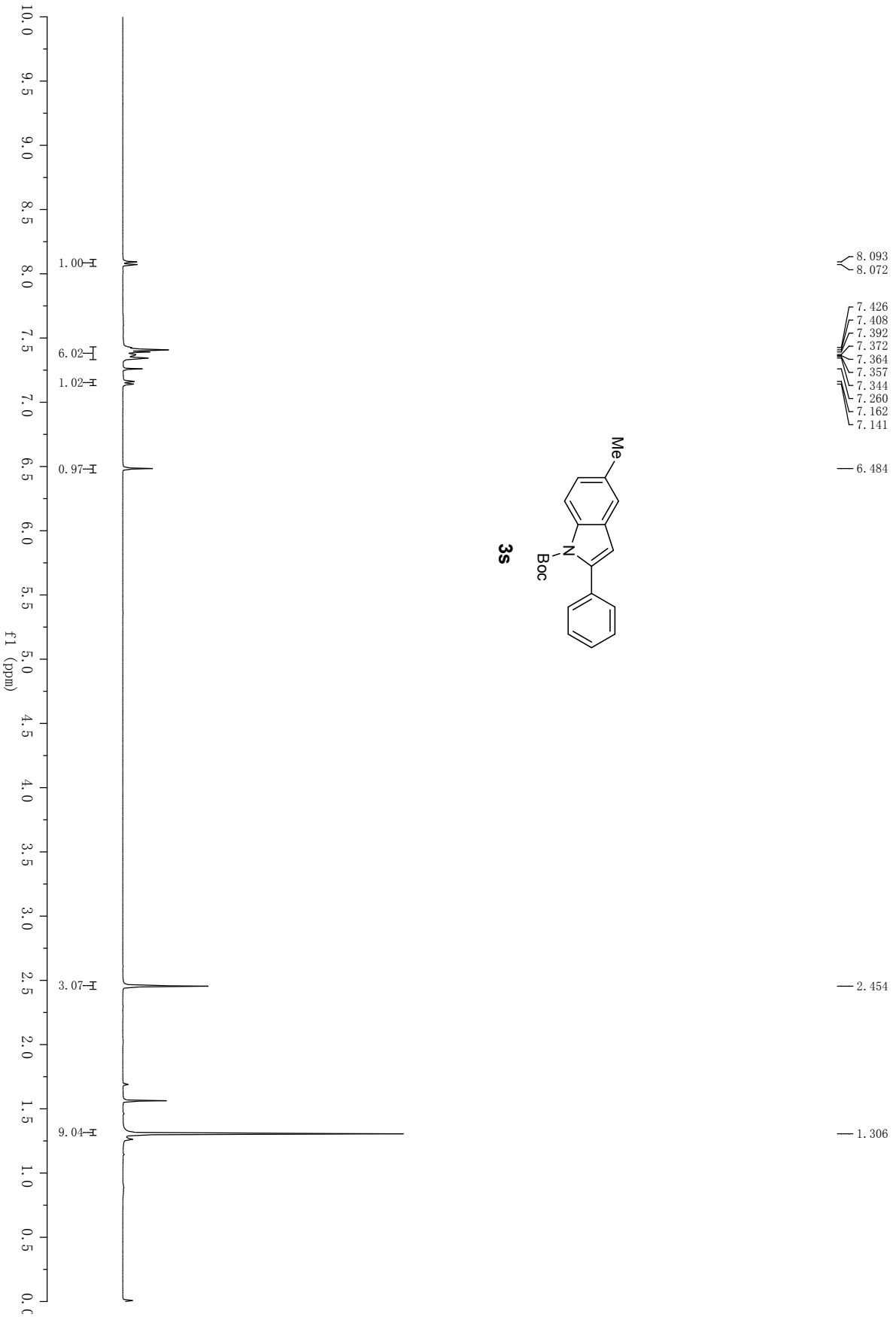

8.479
8.474
8.328
8.305
8.232
8.227
8.209
8.204
7.427
6.680
1.299
1.00
1.00
1.00
5.01
0.97
9.30
f1 (ppm)
O2N
N
Boc
3q

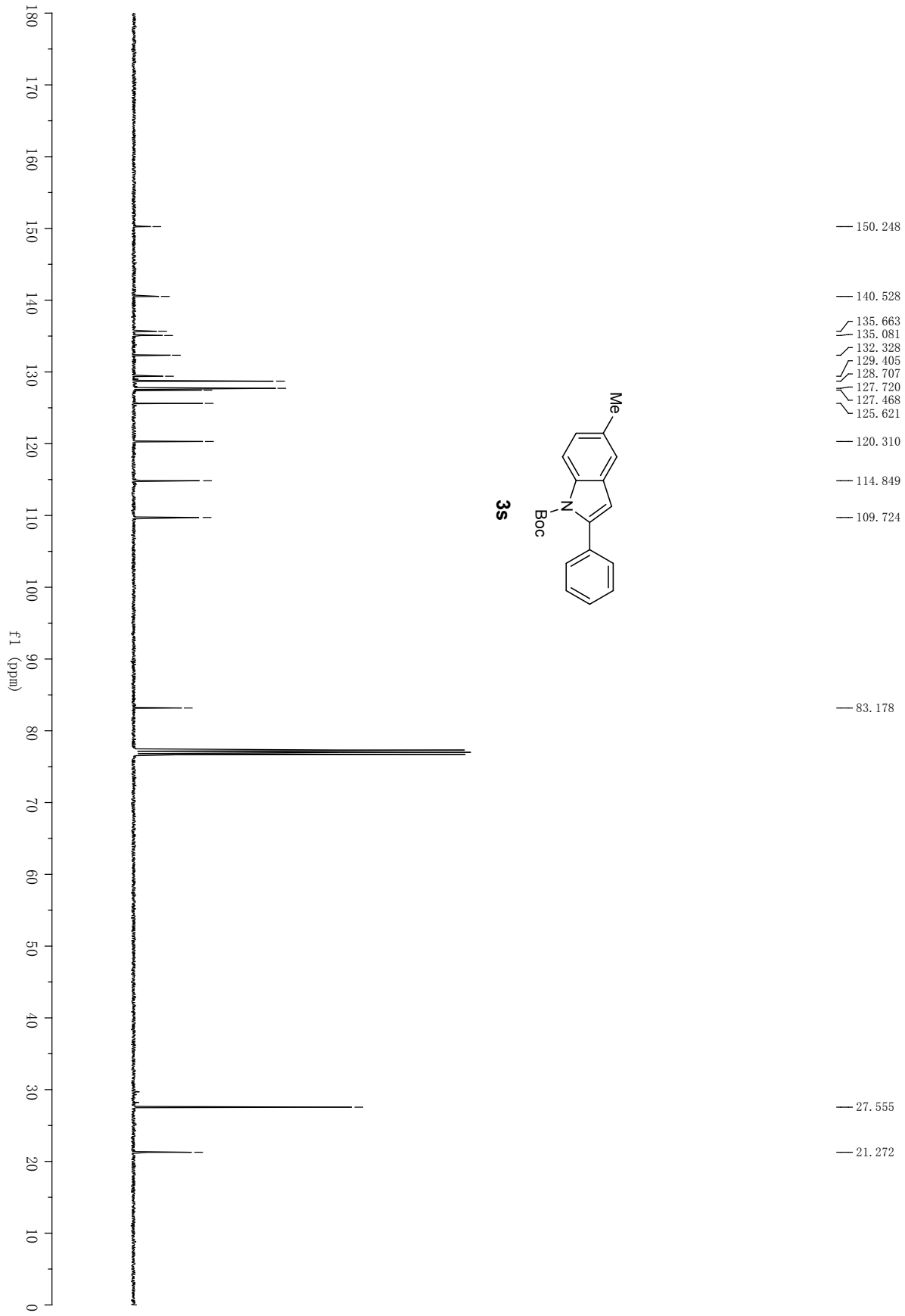

149.431
143.857
143.474
140.460
133.808
128.886
128.725
128.326
128.016
119.447
116.662
115.321
109.853
84.848
27.411
f1 (ppm)
O2N
N
Boc
3q

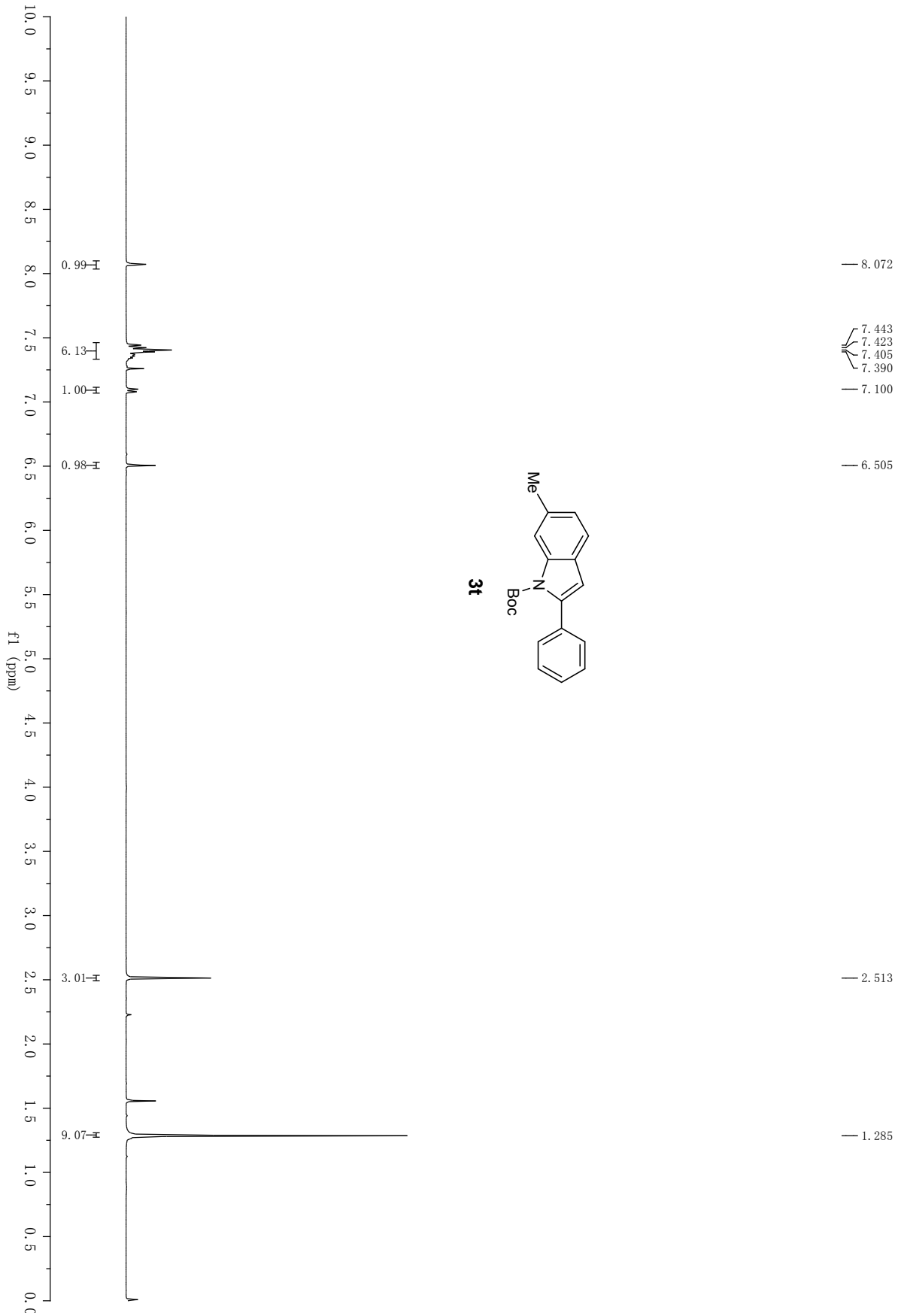

8.056
8.035
7.440
7.420
7.400
7.381
7.374
7.369
7.363
7.353
7.238
7.218
7.069
7.050
2.529
1.304
0.98H
5.21
0.89H
1.00H
0.95H
2.89H
8.87H
f1 (ppm)
Me
N
Boc

3r

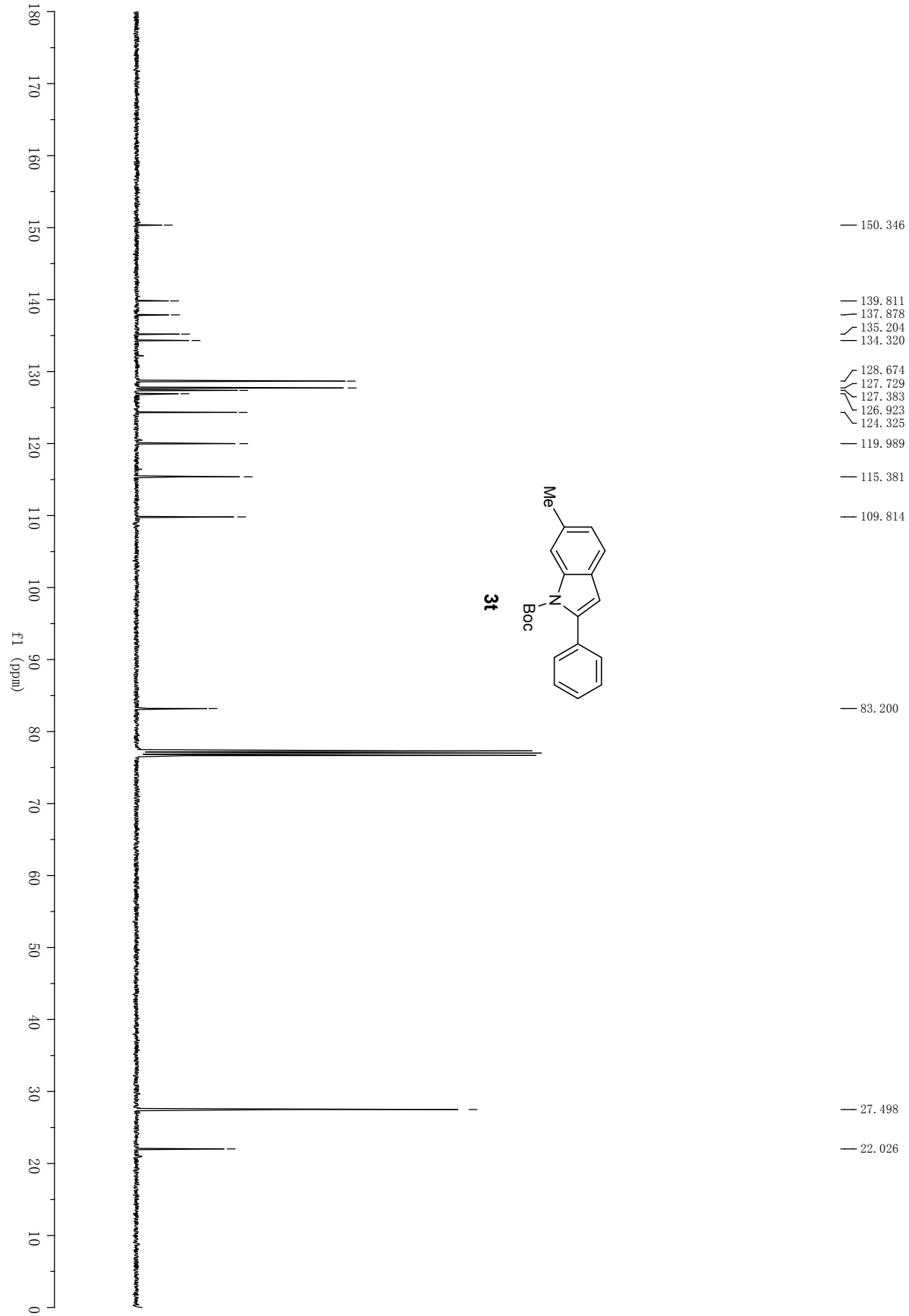

150.261
139.932
137.226
135.144
129.858
128.780
128.682
127.761
127.477
124.365
123.263
112.677
108.405
83.287
27.533
18.424
f1 (ppm)
Me
N
Boc
3r

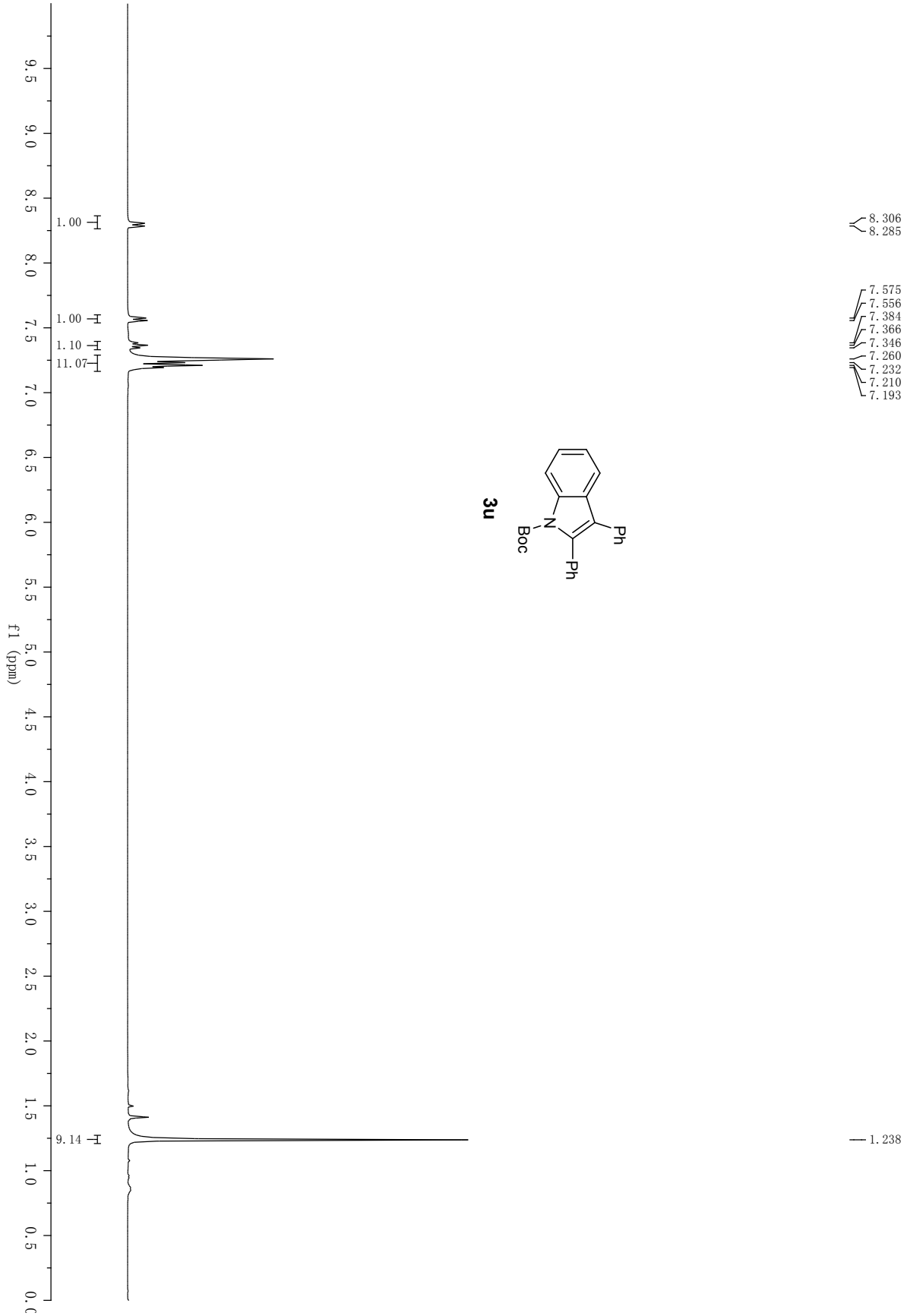

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
1.00
6.02
1.02
0.97
3.07
9.04
8.093
8.072
7.426
7.408
7.392
7.372
7.364
7.357
7.344
7.260
7.162
7.141
6.484
2.454
1.306
Me
N
Boc
3s

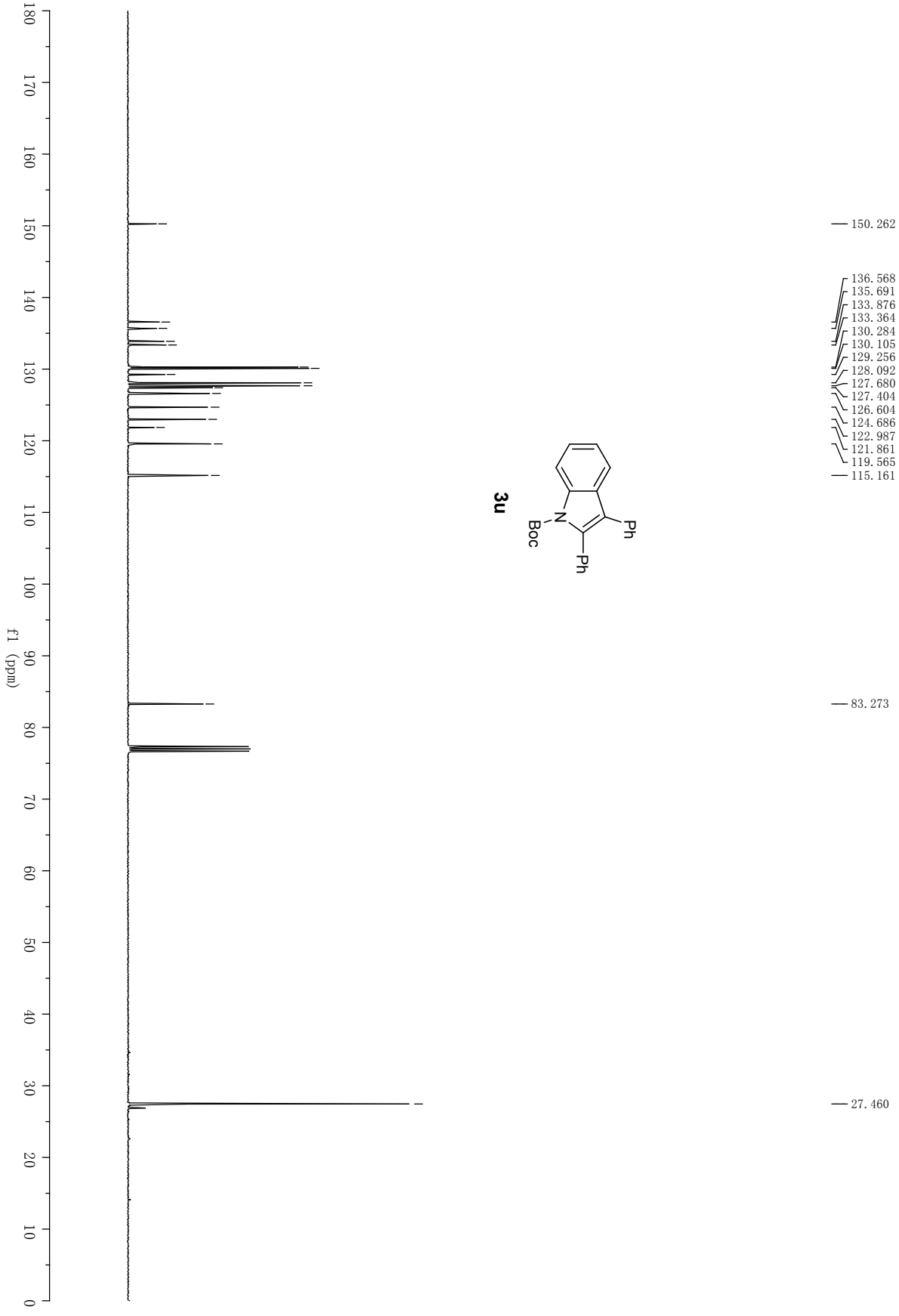

150.248
140.528
135.663
135.081
132.328
129.405
128.707
127.720
127.468
125.621
120.310
114.849
109.724
83.178
27.555
21.272
f1 (ppm)
Me
N
Boc
3s

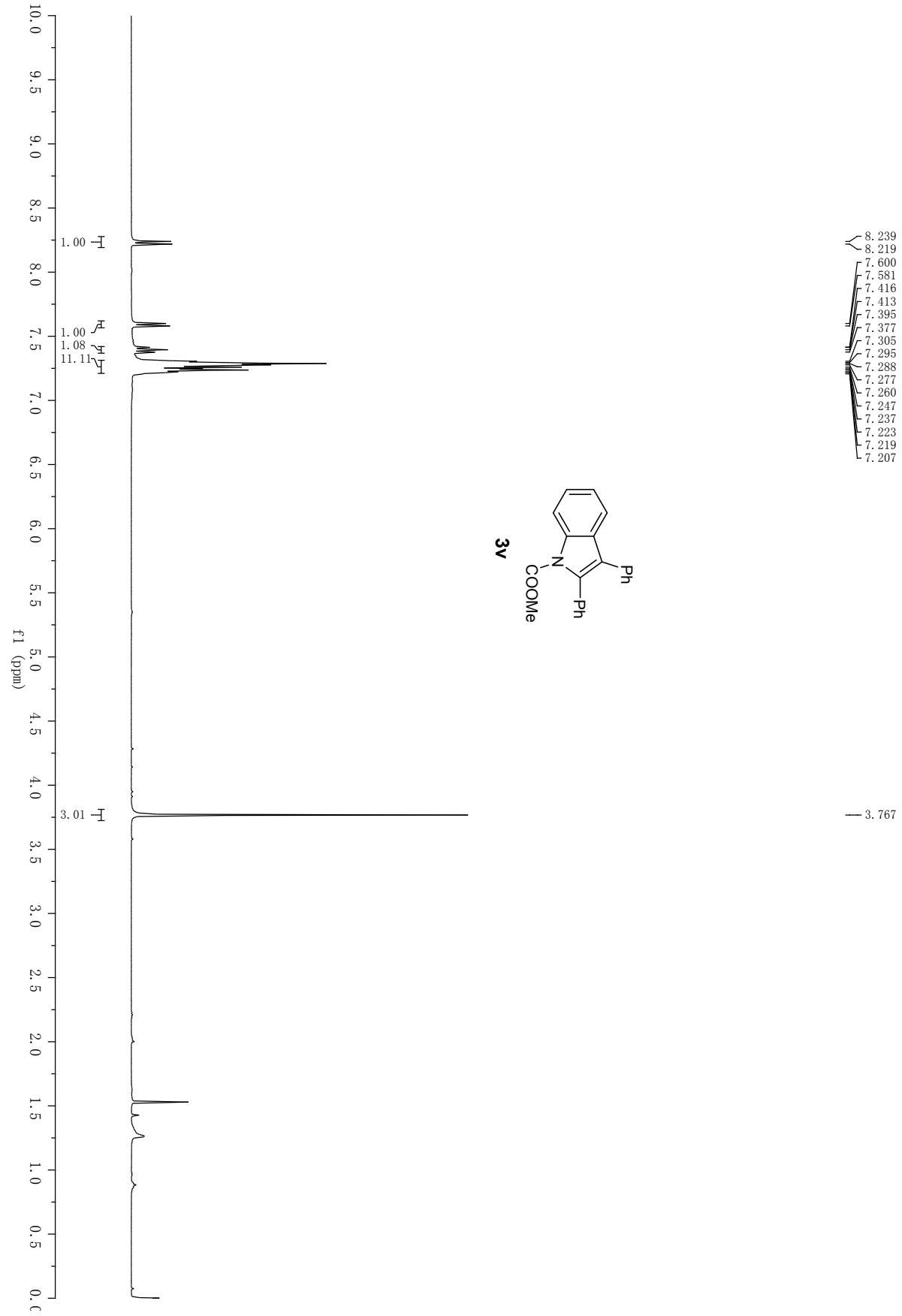

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
0.99
6.13
1.00
0.98
3.01
9.07
8.072
7.443
7.423
7.405
7.390
7.100
6.505
2.513
1.285
Me
N
Boc

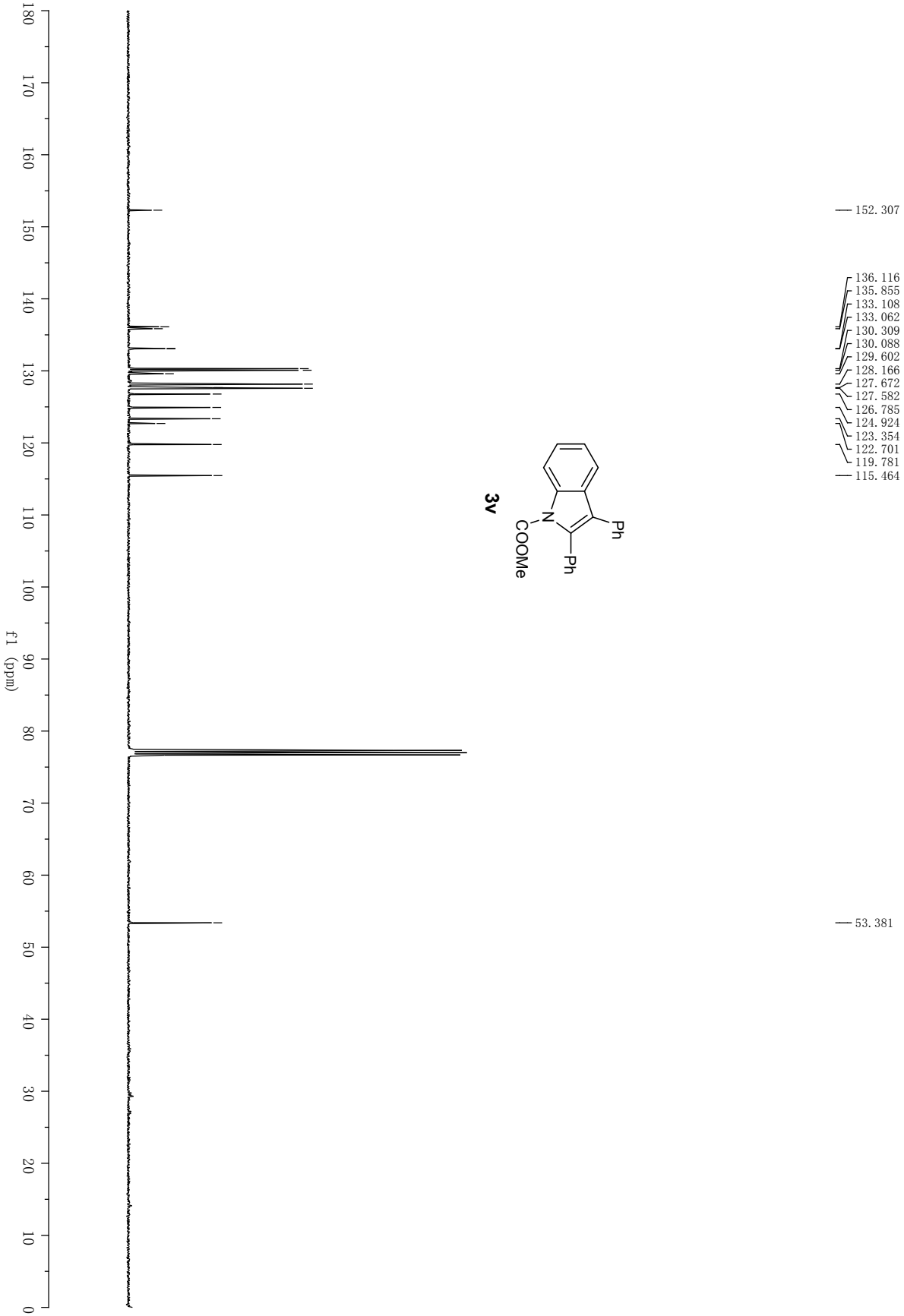
3t

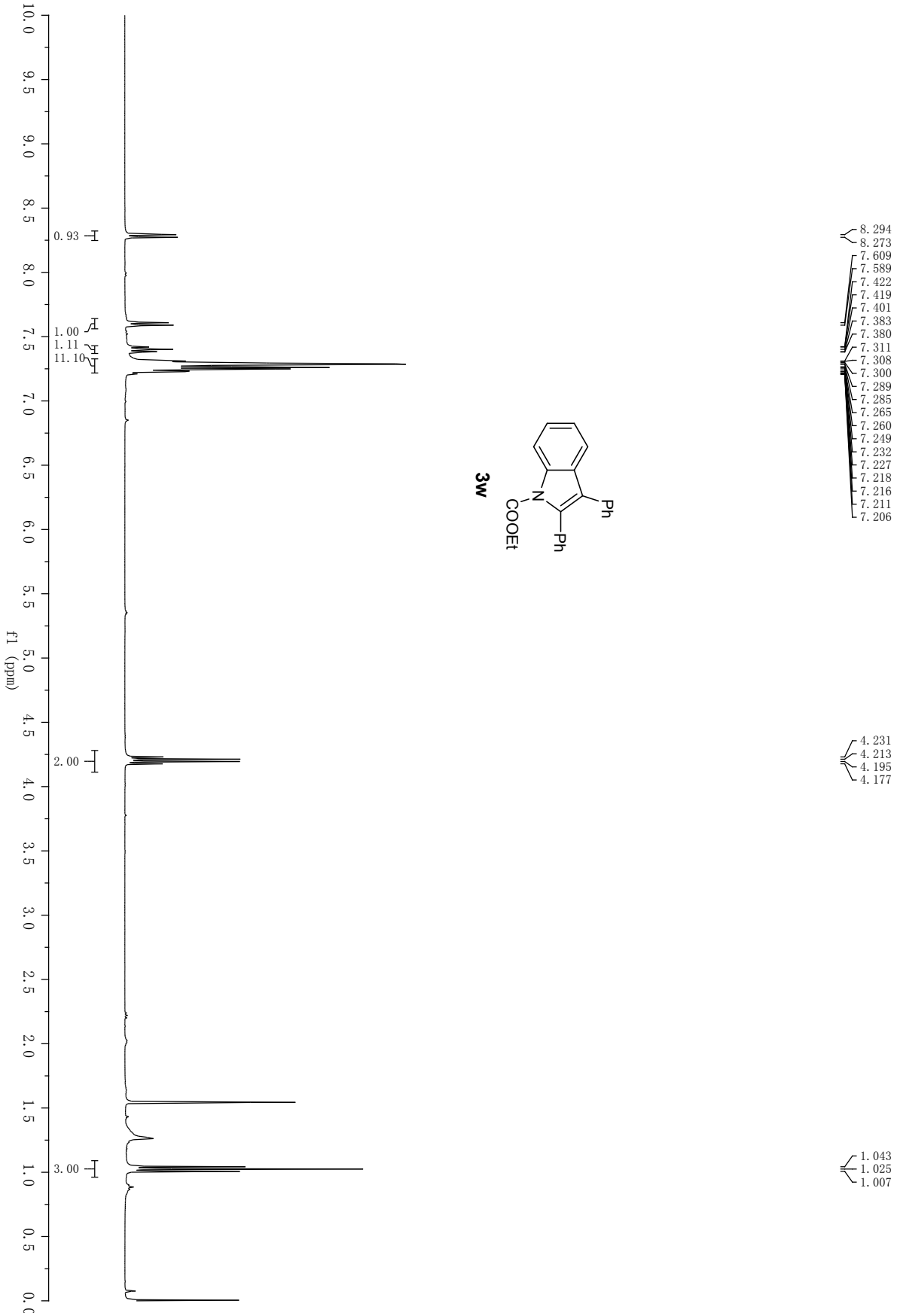

150.346
139.811
137.878
135.204
134.320
128.674
127.729
127.383
126.923
124.325
119.989
115.381
109.814
83.200
27.498
22.026
f1 (ppm)
Me
N
Boc
3t

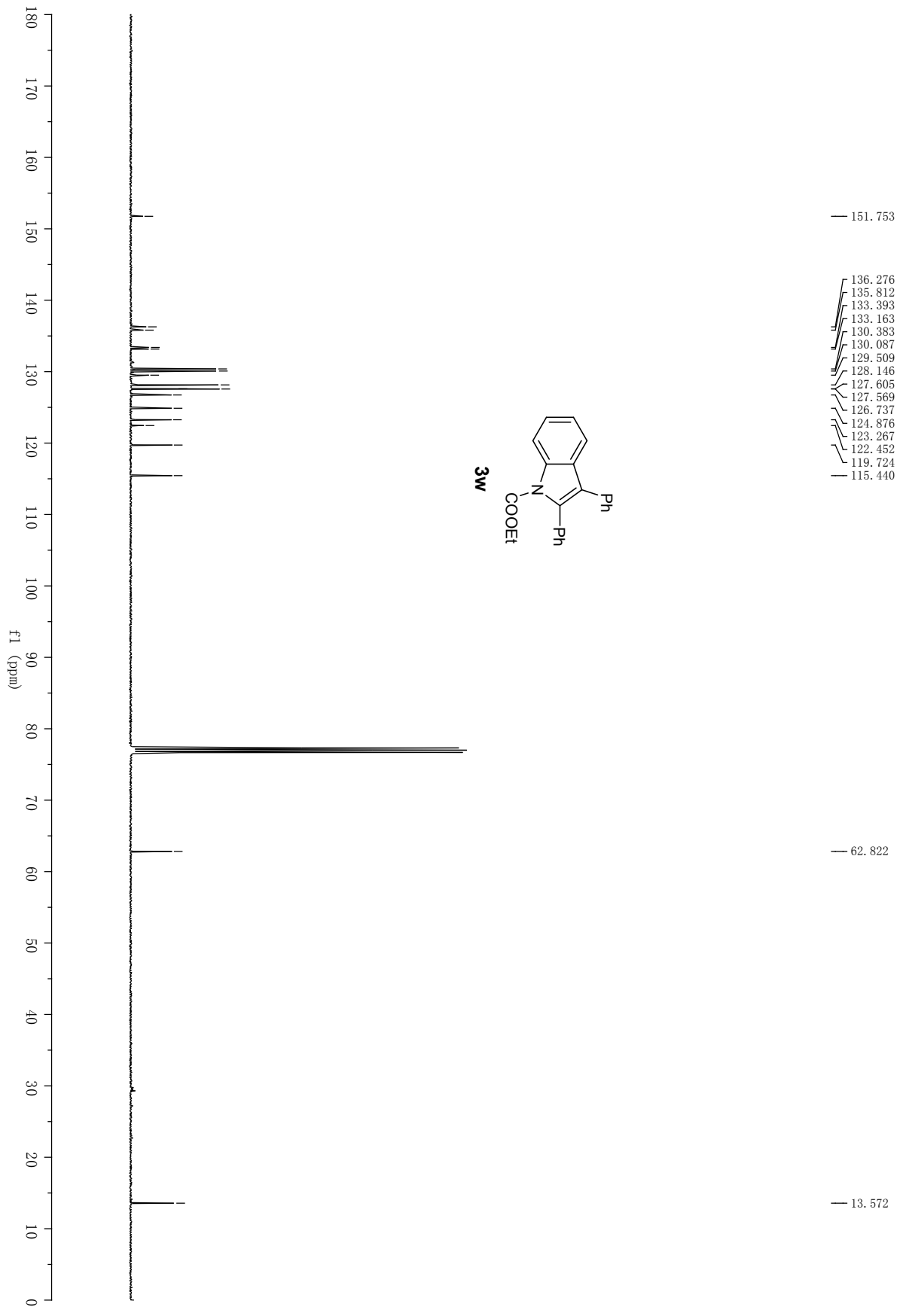

8.306
8.285
7.575
7.556
7.384
7.366
7.346
7.260
7.232
7.210
7.193
1.238
1.00
1.00
1.10
11.07
9.14
f1 (ppm)
3u
N
Boc
Ph
Ph

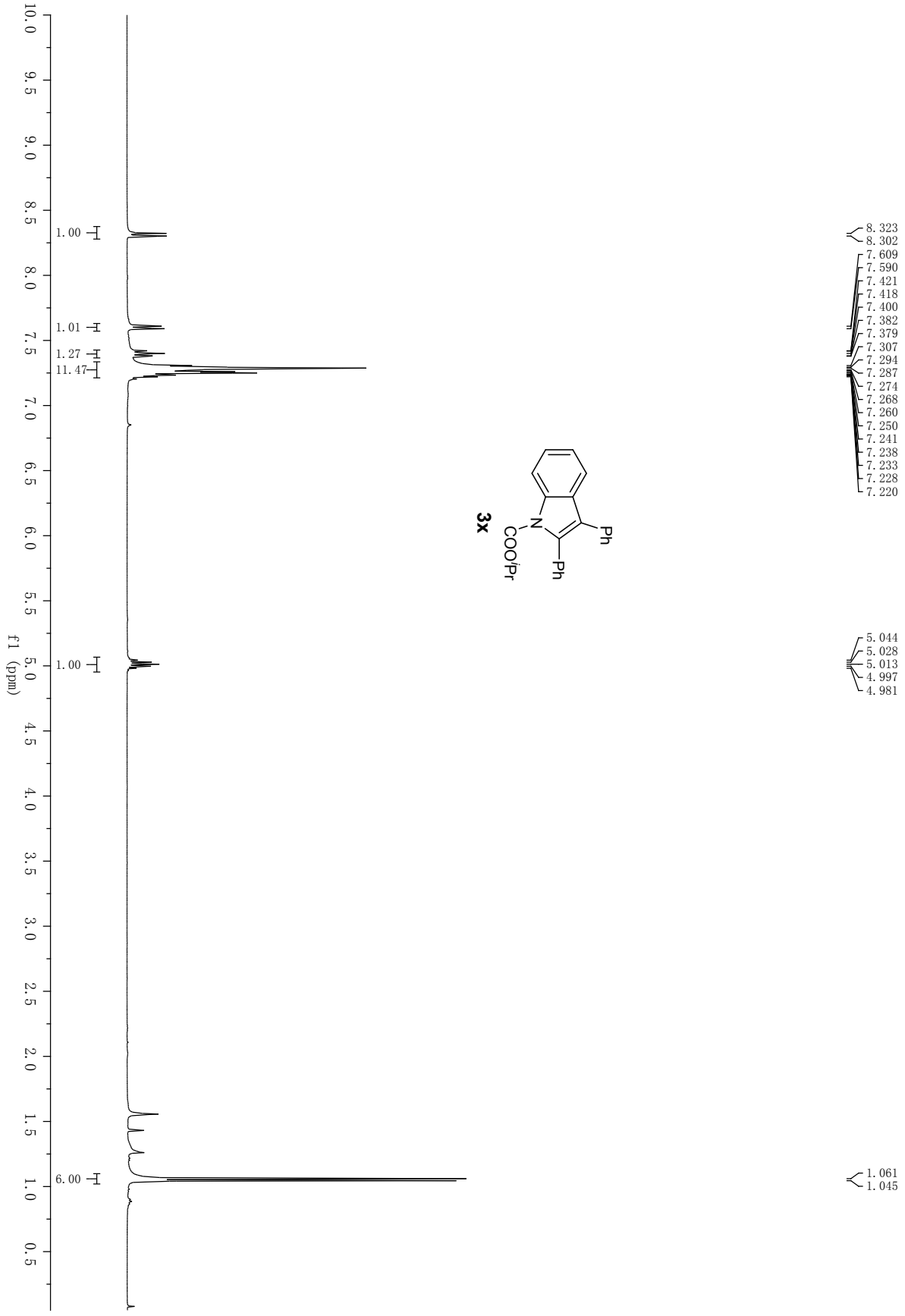

150.262
136.568
135.691
133.876
133.364
130.284
130.105
129.256
128.092
127.680
127.404
126.604
124.686
122.987
121.861
119.565
115.161
83.273
27.460
f1 (ppm)
3u
N
Boc
Ph
Ph

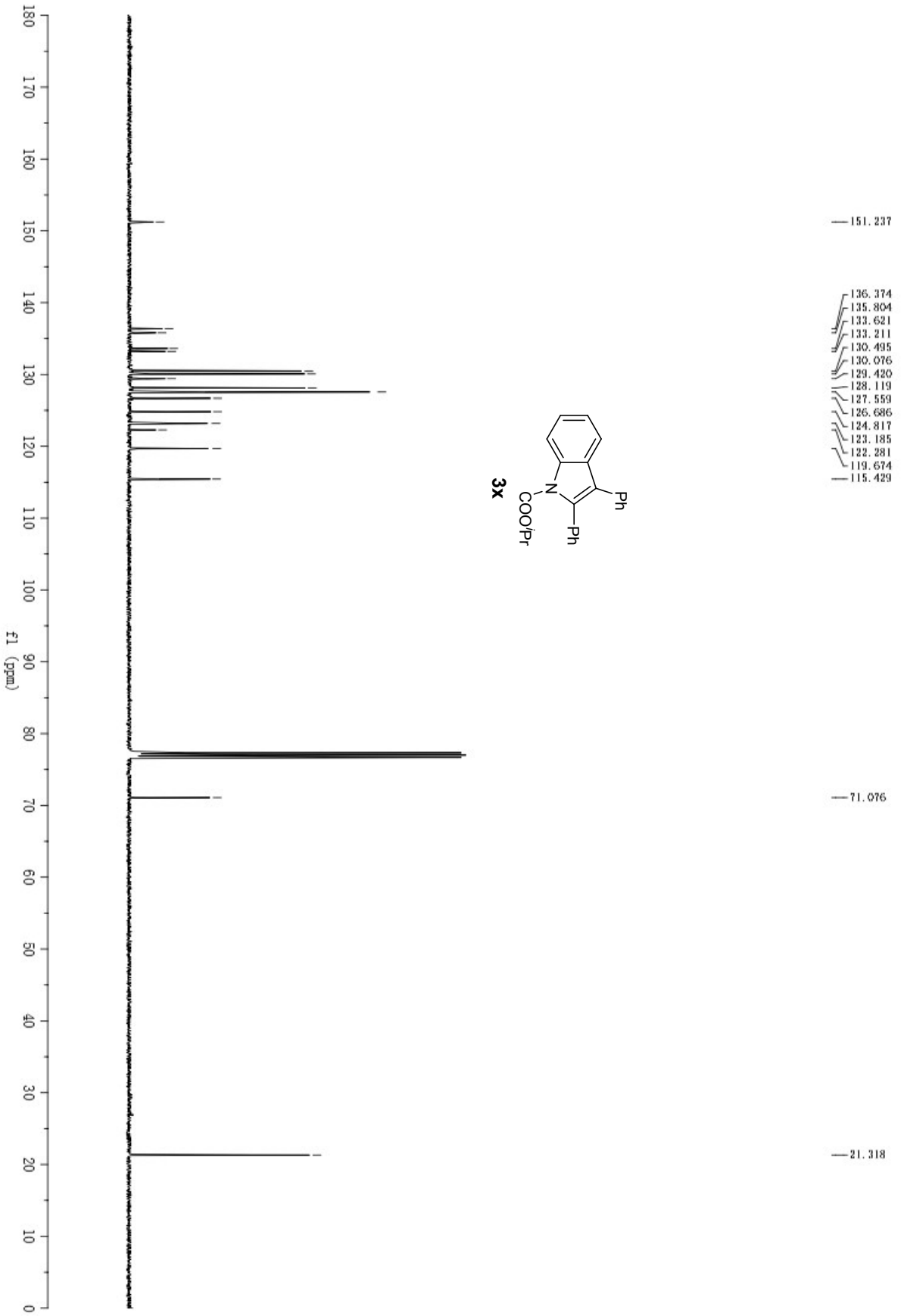

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
1.00
1.00
1.08
11.11
3.01
8.239
8.219
7.600
7.581
7.416
7.413
7.395
7.377
7.305
7.295
7.288
7.277
7.260
7.247
7.237
7.223
7.219
7.207
3.767
3v
N
COOMe
Ph
Ph

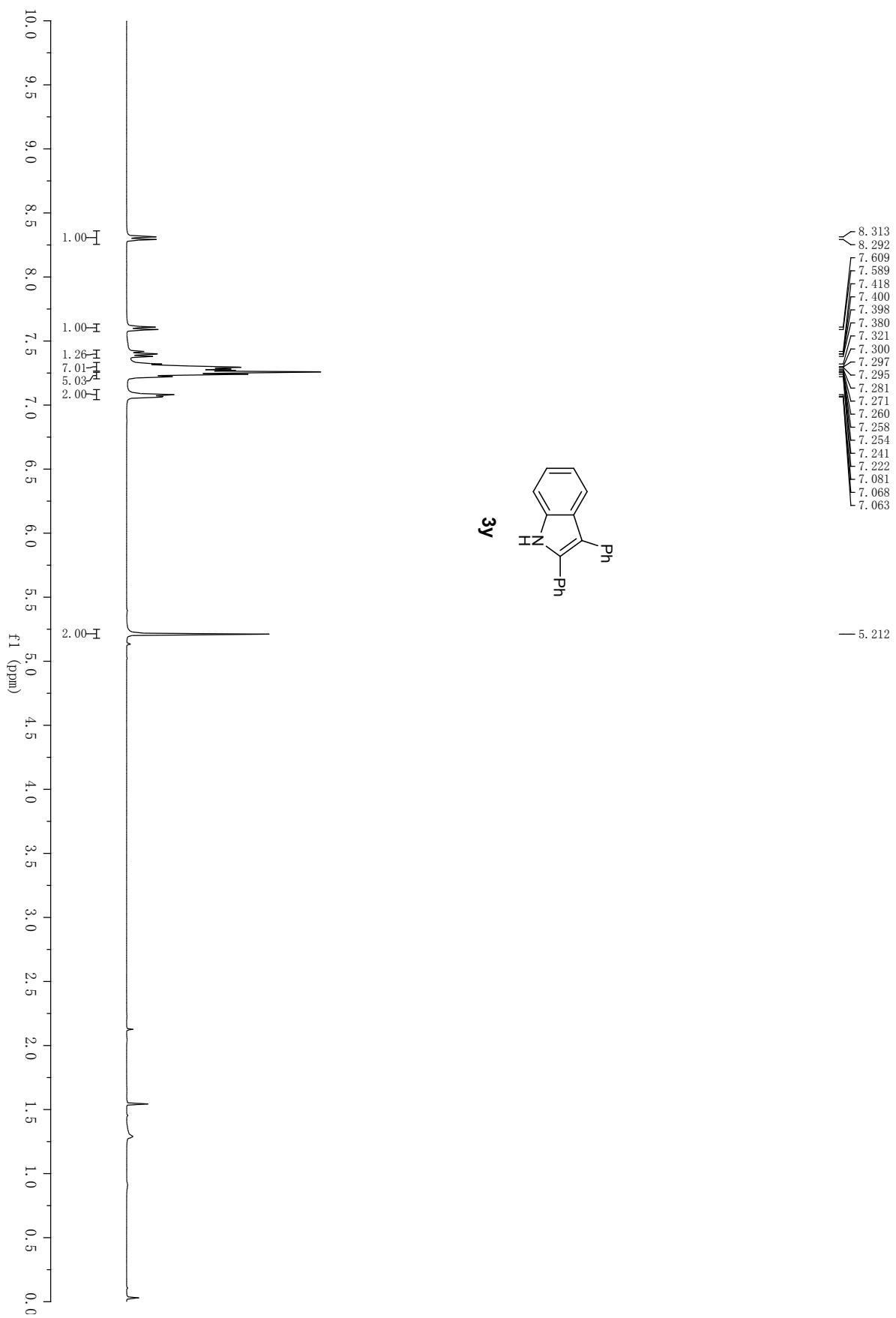

152.307
136.116
135.855
133.108
133.062
130.309
130.088
129.602
128.166
127.672
127.582
126.785
124.924
123.354
122.701
119.781
115.464
53.381
3v
N
COOMe
Ph
Ph
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

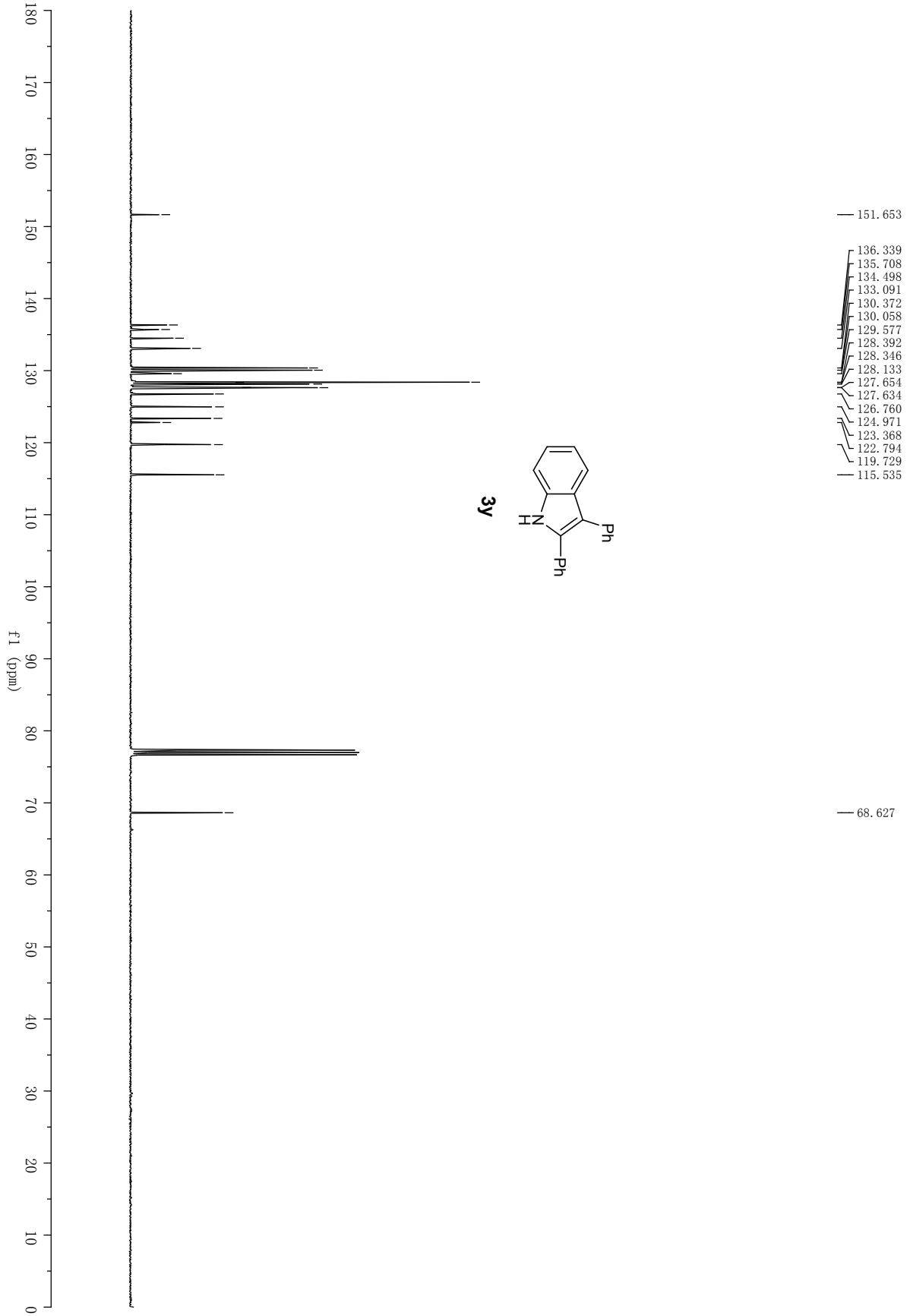

8.294
8.273
7.609
7.589
7.422
7.419
7.401
7.383
7.380
7.311
7.308
7.300
7.289
7.285
7.265
7.260
7.249
7.232
7.227
7.218
7.216
7.211
7.206
4.231
4.213
4.195
4.177
1.043
1.025
1.007
0.93
1.00
1.11
11.10
2.00
3.00
f1 (ppm)
3w
N
COOEt
Ph
Ph

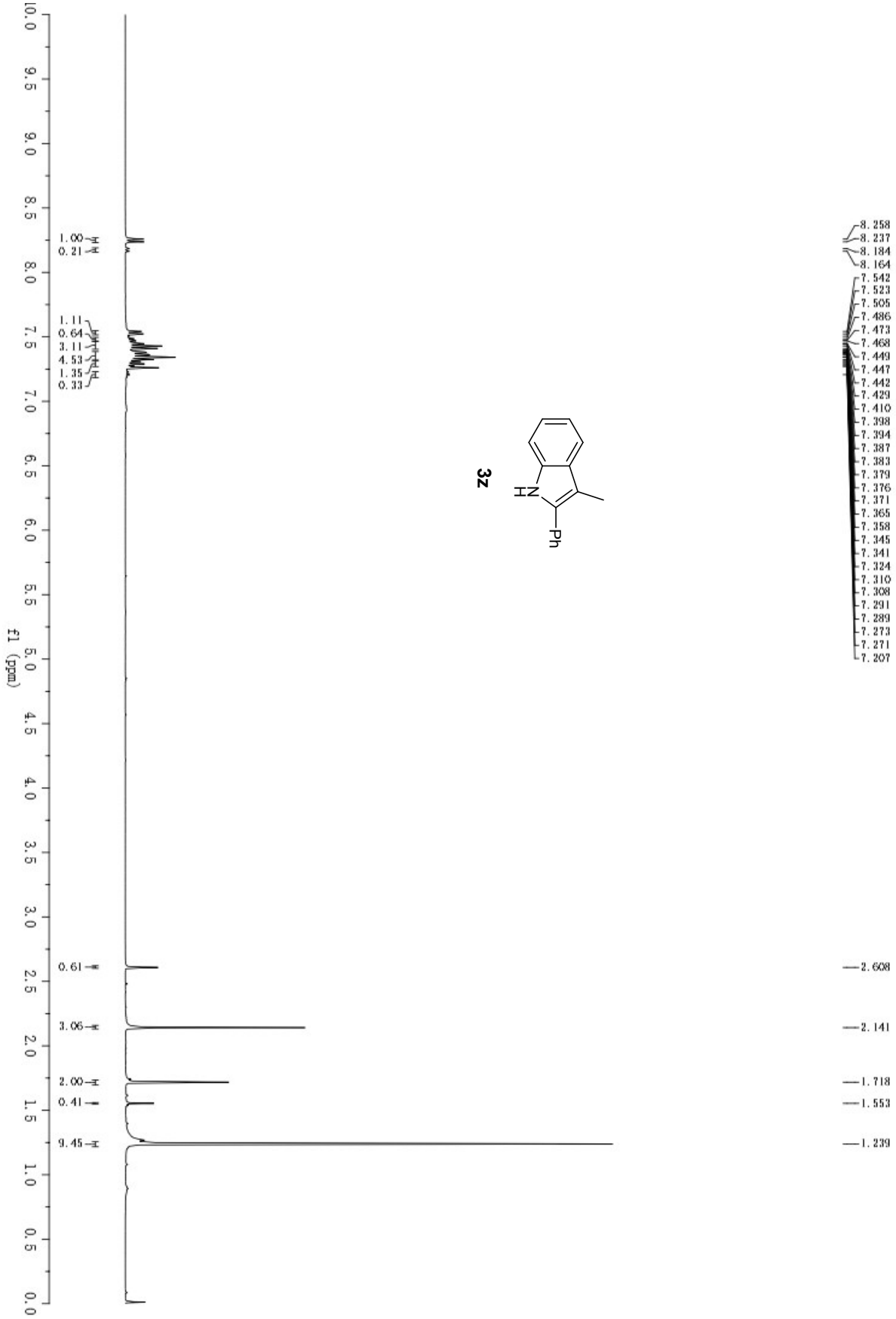

151.753
136.276
135.812
133.393
133.163
130.383
130.087
129.509
128.146
127.605
127.569
126.737
124.876
123.267
122.452
119.724
115.440
62.822
13.572
3w
COOEt
N
Ph
Ph
f1 (ppm)

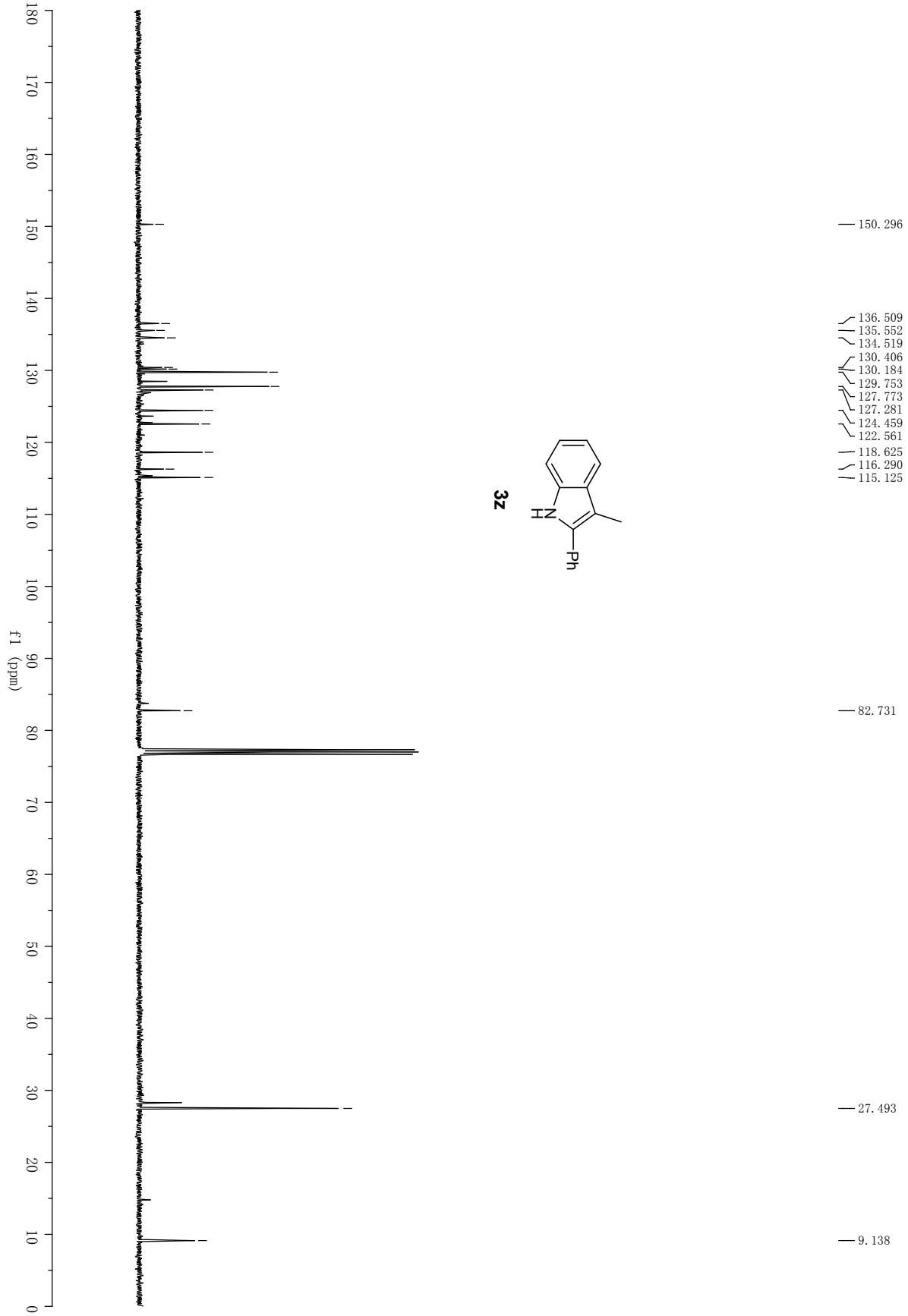

8.323
8.302
7.609
7.590
7.421
7.418
7.400
7.382
7.379
7.307
7.294
7.287
7.274
7.268
7.260
7.250
7.241
7.238
7.233
7.228
7.220
5.044
5.028
5.013
4.997
4.981
1.061
1.045
1.00
1.01
1.27
11.47
1.00
6.00
f1 (ppm)
3x
N
COO/Pr
Ph
Ph

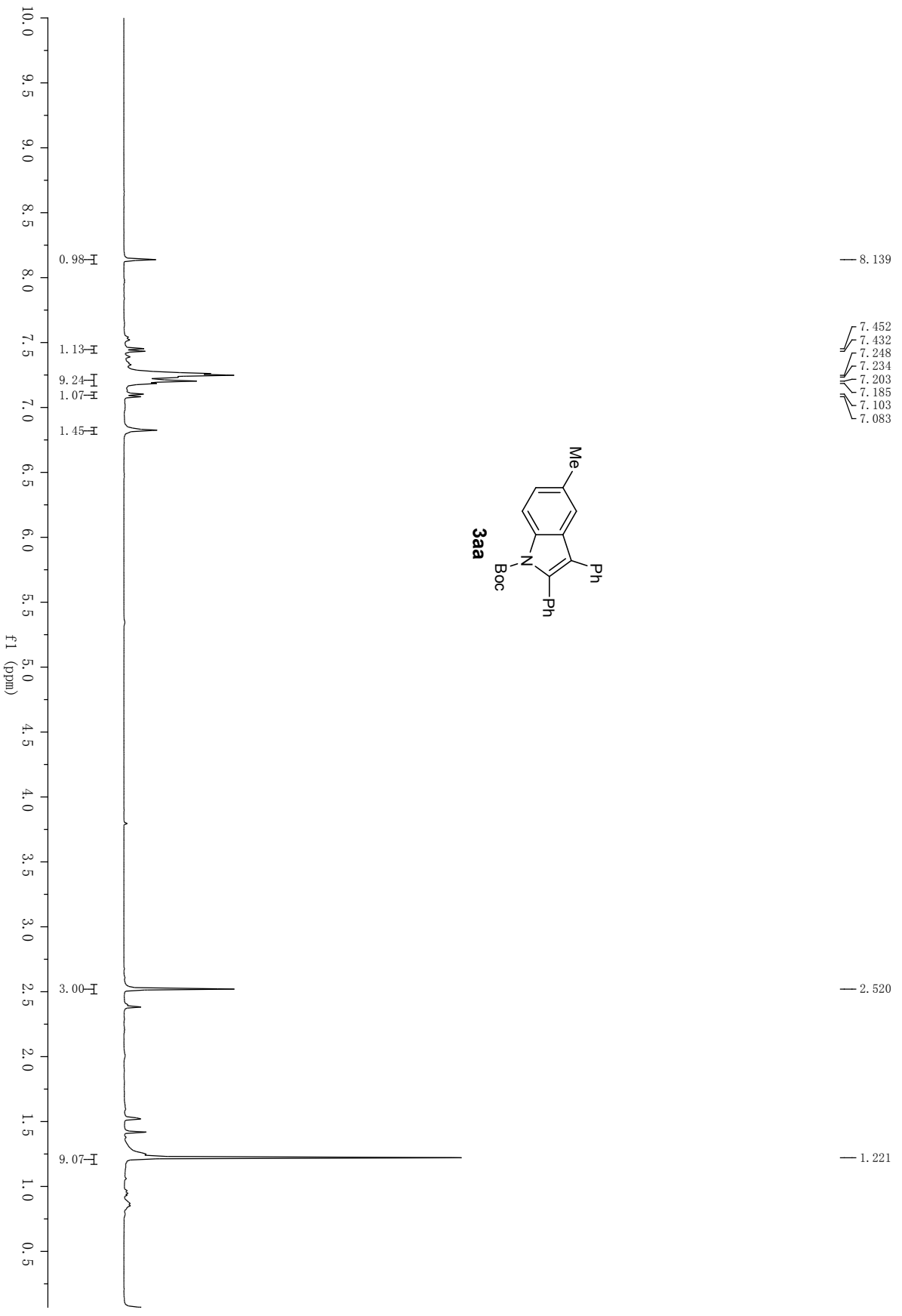

151.237
136.374
135.804
133.621
133.211
130.495
130.076
129.420
128.119
127.559
126.686
124.817
123.185
122.281
119.674
115.429
71.076
21.318
f1 (ppm)
3x
N
COO/Pr
Ph
Ph

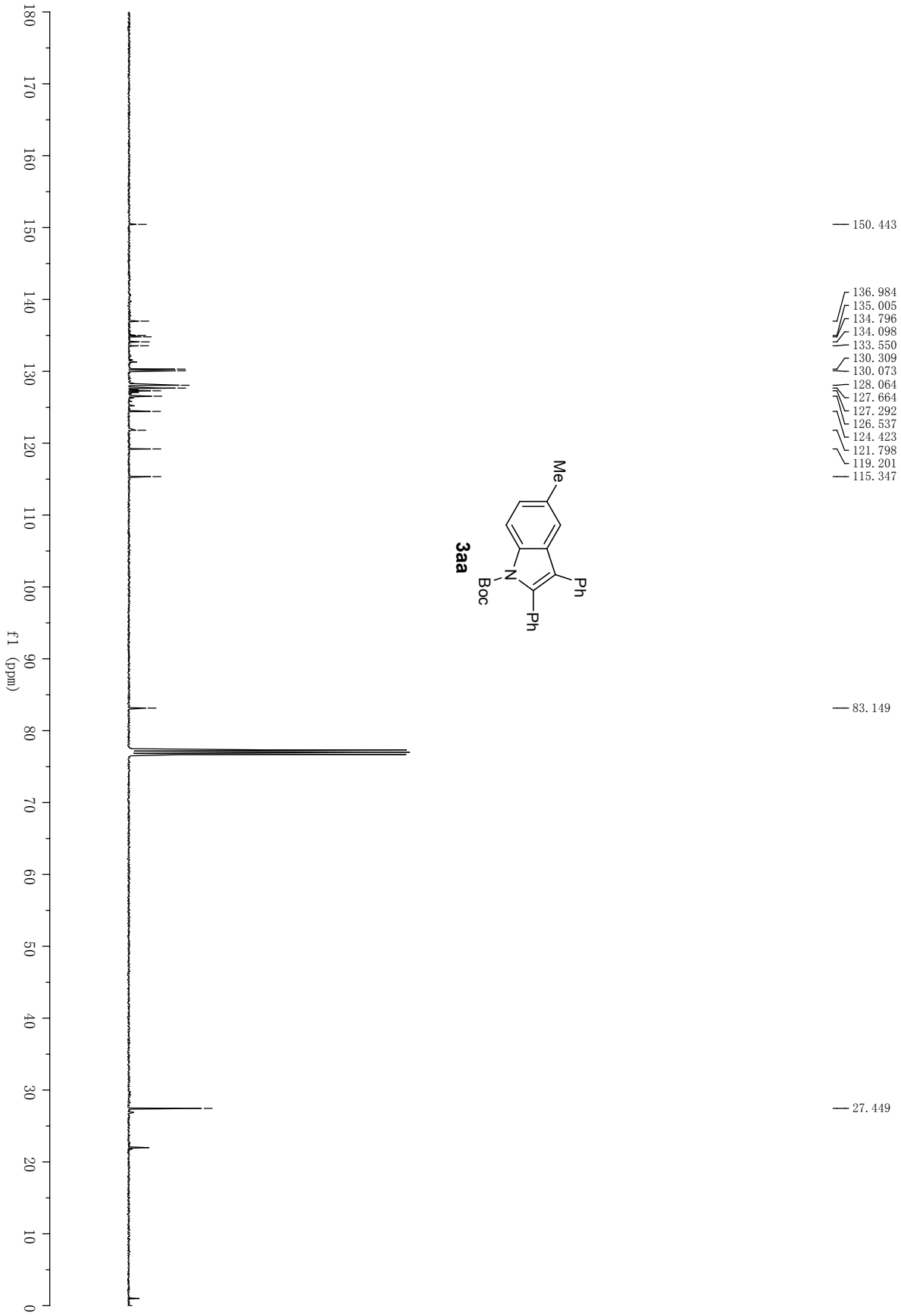

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.00
1.00
1.26
7.01
5.03
2.00
2.00
8.313
8.292
7.609
7.589
7.418
7.400
7.398
7.380
7.321
7.300
7.297
7.295
7.281
7.271
7.260
7.258
7.254
7.241
7.222
7.081
7.068
7.063
5.212
3y
N
H
Ph
Ph

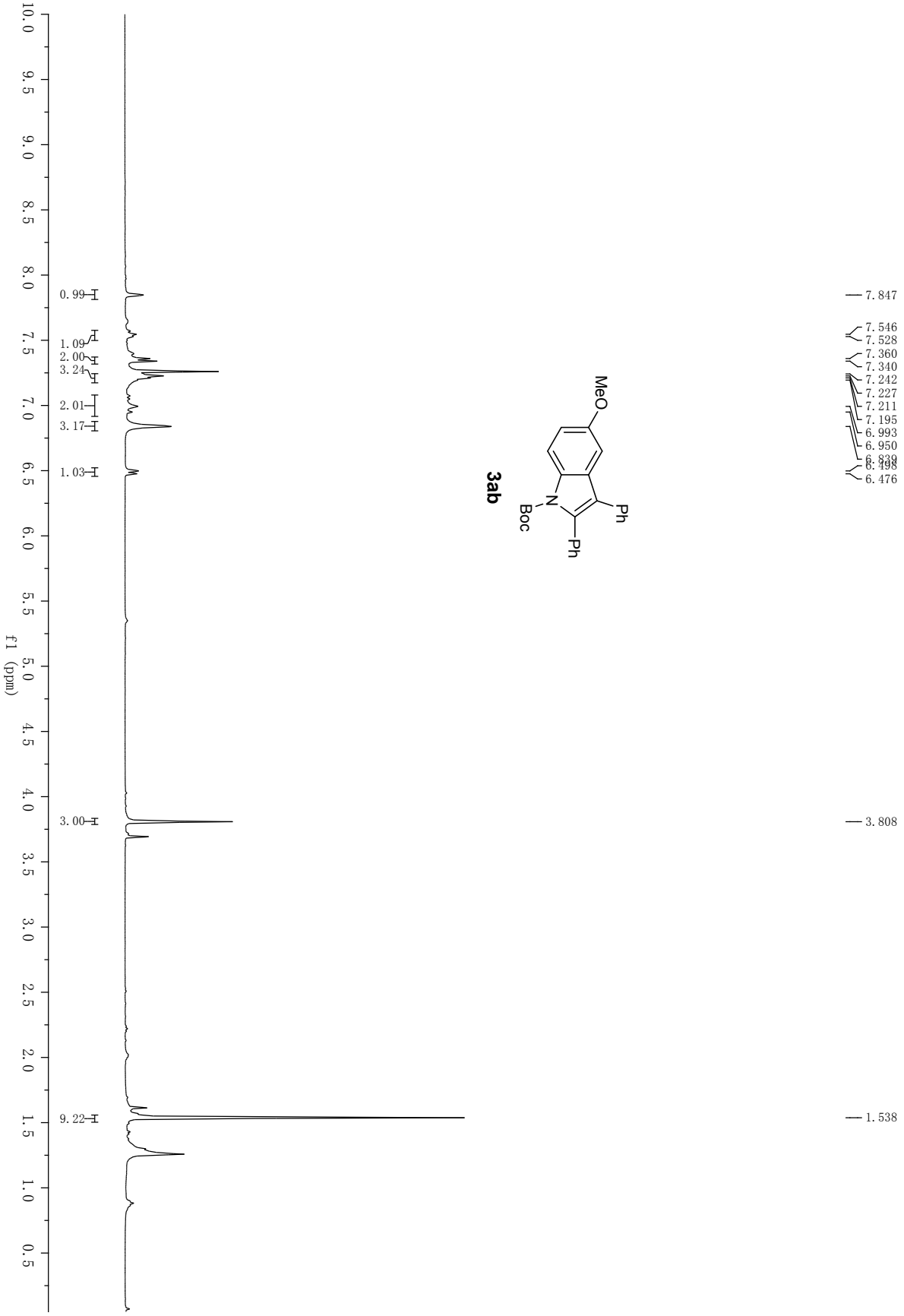

151.653
136.339
135.708
134.498
133.091
130.372
130.058
129.577
128.392
128.346
128.133
127.654
127.634
126.760
124.971
123.368
122.794
119.729
115.535
68.627
f1 (ppm)
3y
N
H
Ph
Ph

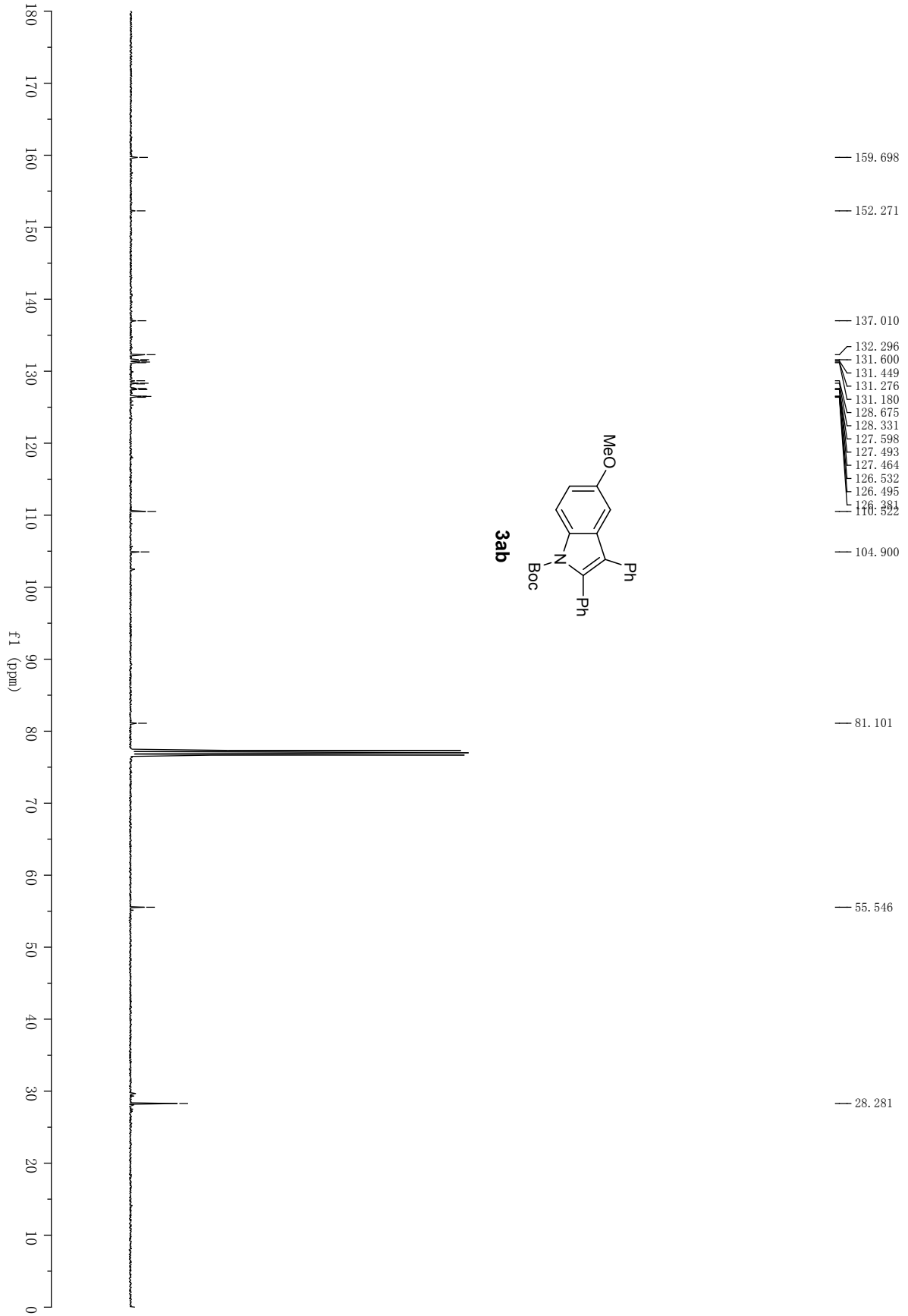

3z
Ph
f1 (ppm)
8.258
8.237
8.184
8.164
7.542
7.523
7.505
7.486
7.473
7.468
7.449
7.447
7.442
7.429
7.410
7.398
7.394
7.387
7.383
7.379
7.376
7.371
7.365
7.358
7.345
7.341
7.324
7.310
7.308
7.291
7.289
7.273
7.271
7.207
2.608
2.141
1.718
1.553
1.239

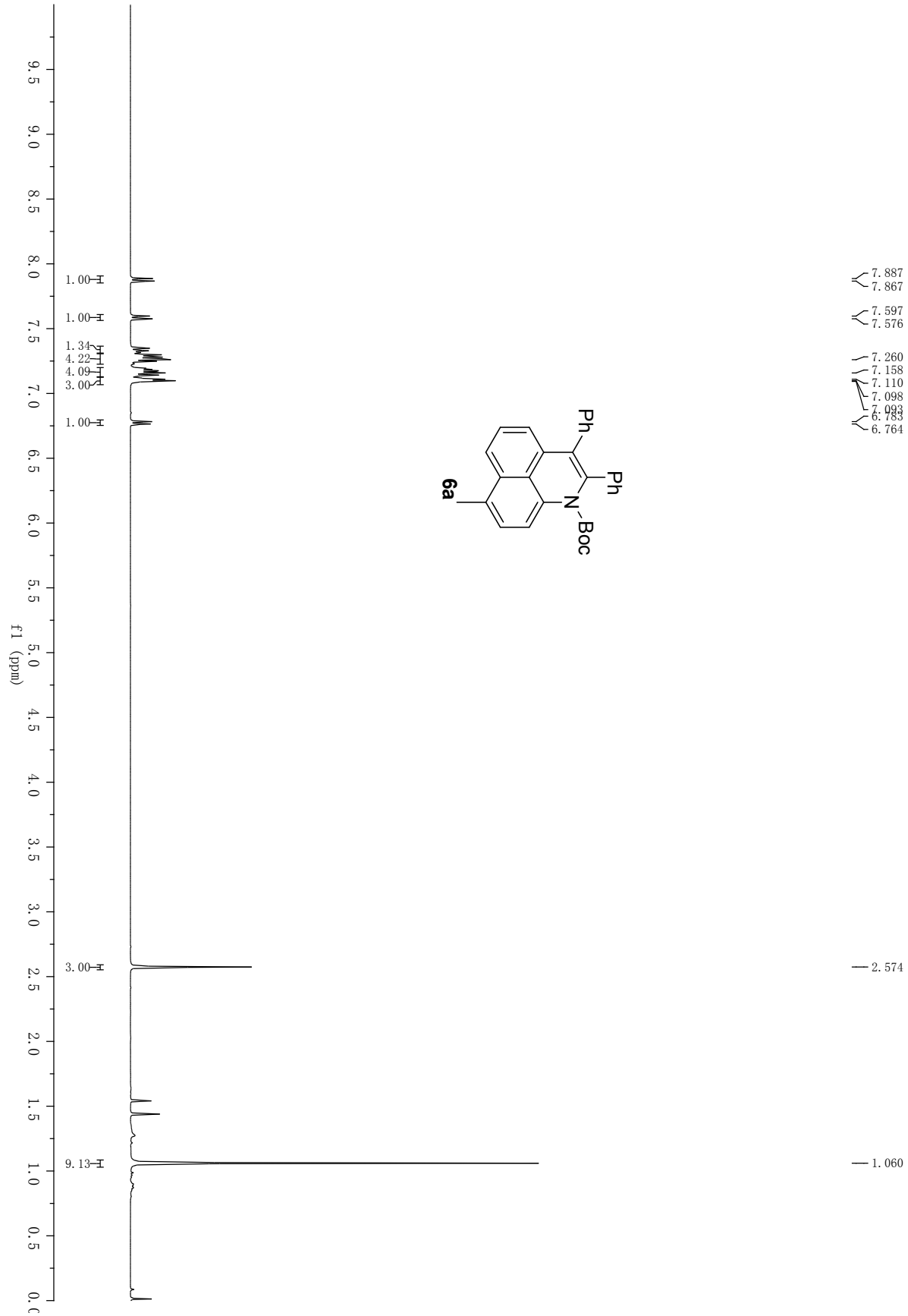

150.296
136.509
135.552
134.519
130.406
130.184
129.753
127.773
127.281
124.459
122.561
118.625
116.290
115.125
82.731
27.493
9.138
f1 (ppm)
3z
N
H
Ph

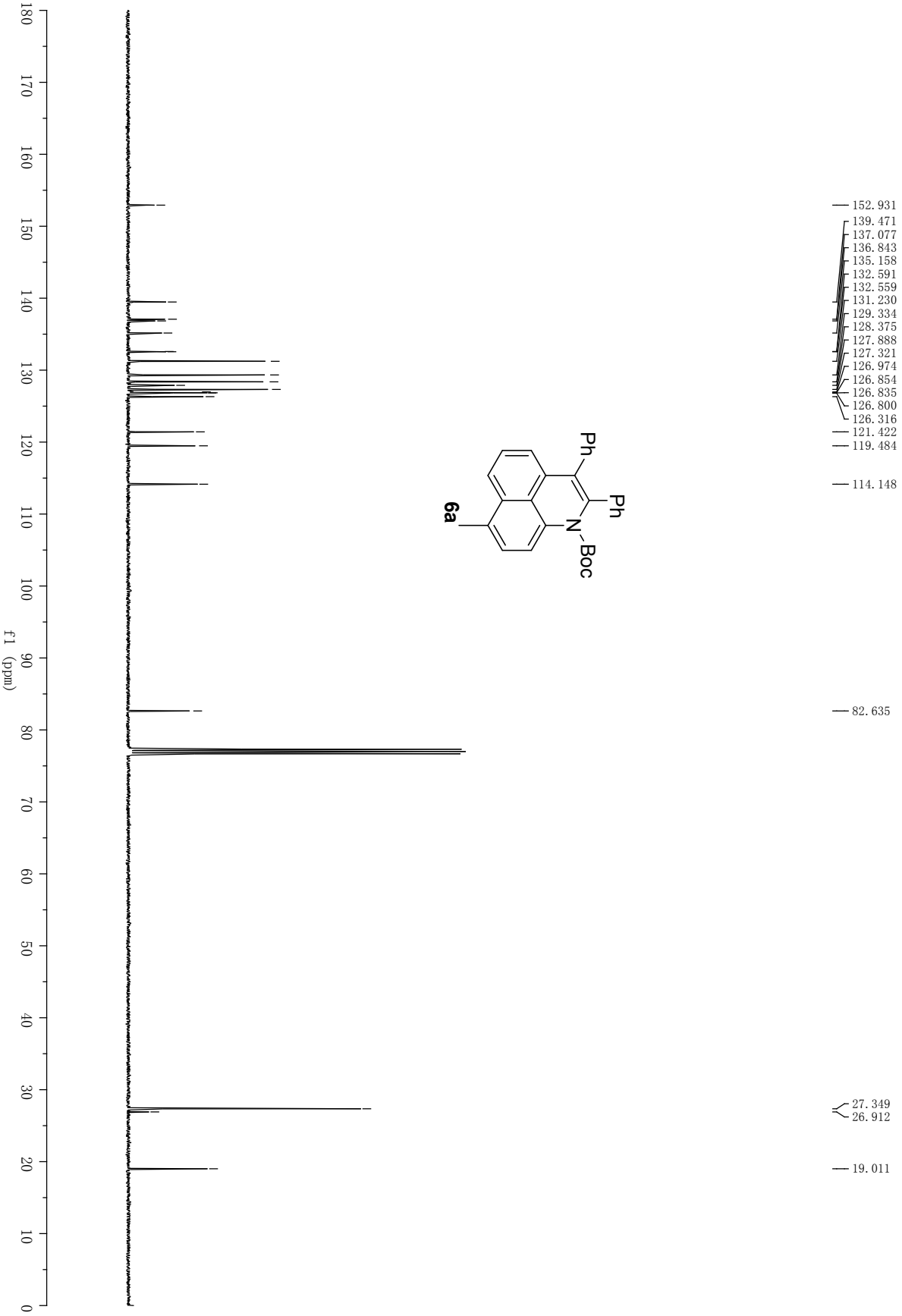

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
0.98
1.13
9.24
1.07
1.45
3.00
9.07
8.139
7.452
7.432
7.248
7.234
7.203
7.185
7.103
7.083
2.520
1.221
Me
Ph
N
Boc
Ph
3aa

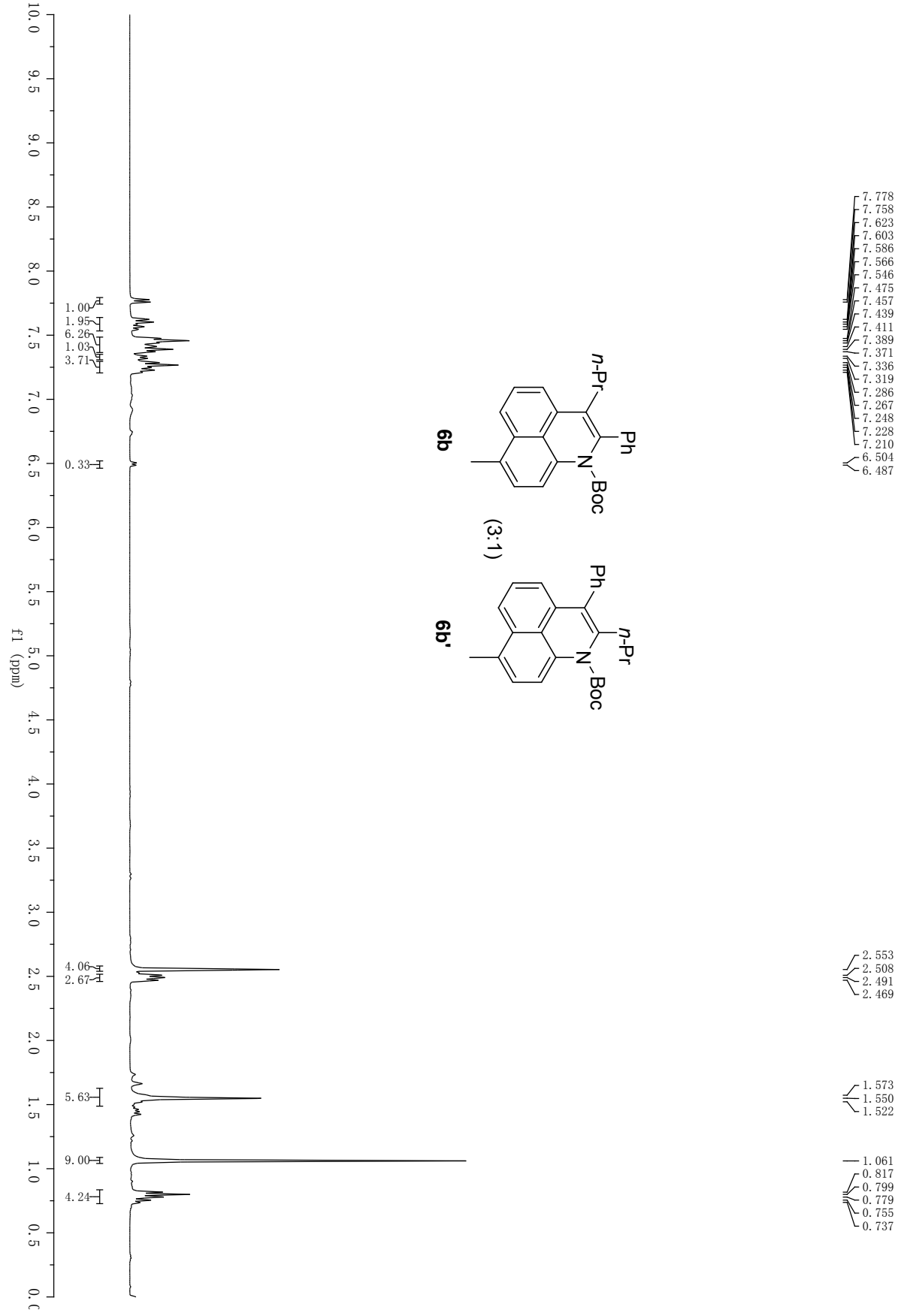

150.443
136.984
135.005
134.796
134.098
133.550
130.309
130.073
128.064
127.664
127.292
126.537
124.423
121.798
119.201
115.347
83.149
27.449
Me
Ph
N
Boc
Ph
3aa
f1 (ppm)

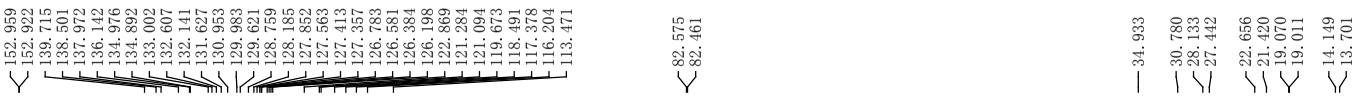

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
0.99
1.09
2.00
3.24
2.01
3.17
1.03
3.00
9.22
MeO
N
Boc
Ph
Ph
3ab
7.847
7.546
7.528
7.360
7.340
7.242
7.227
7.211
7.195
6.993
6.950
6.476
3.808
1.538

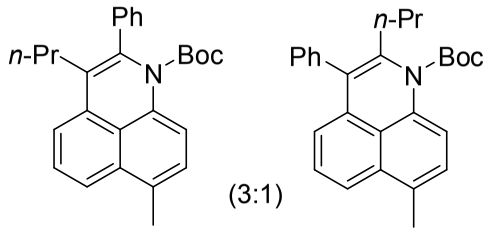

159.698
152.271
137.010
132.296
131.600
131.449
131.276
131.180
128.675
128.331
127.598
127.493
127.464
126.532
126.495
126.381
110.522
104.900
81.101
55.546
28.281
f1 (ppm)
MeO
Ph
Ph
N
Boc
3ab


1.00
1.00
1.34
4.22
4.09
3.00
1.00
3.00
9.13
f1 (ppm)
7.887
7.867
7.597
7.576
7.260
7.158
7.110
7.098
7.093
6.783
6.764
2.574
1.060
Ph
Ph
N
Boc
6a

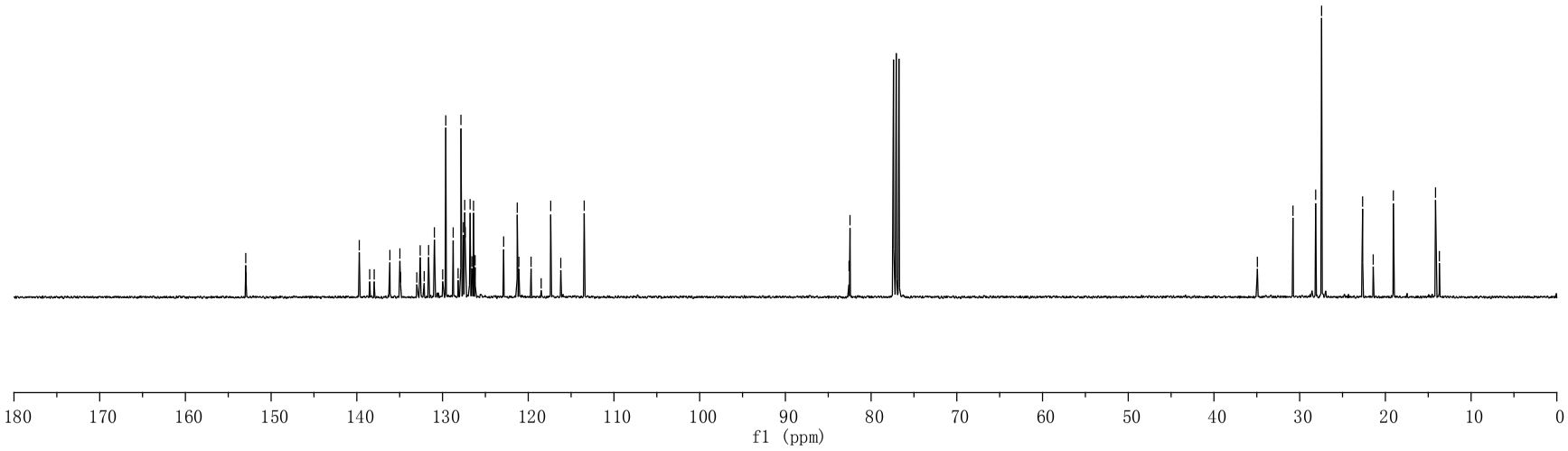

152.931
139.471
137.077
136.843
135.158
132.591
132.559
131.230
129.334
128.375
127.888
127.321
126.974
126.854
126.835
126.800
126.316
121.422
119.484
114.148
82.635
27.349
26.912
19.011
Ph
Ph
N
Boc
6a
f1 (ppm)

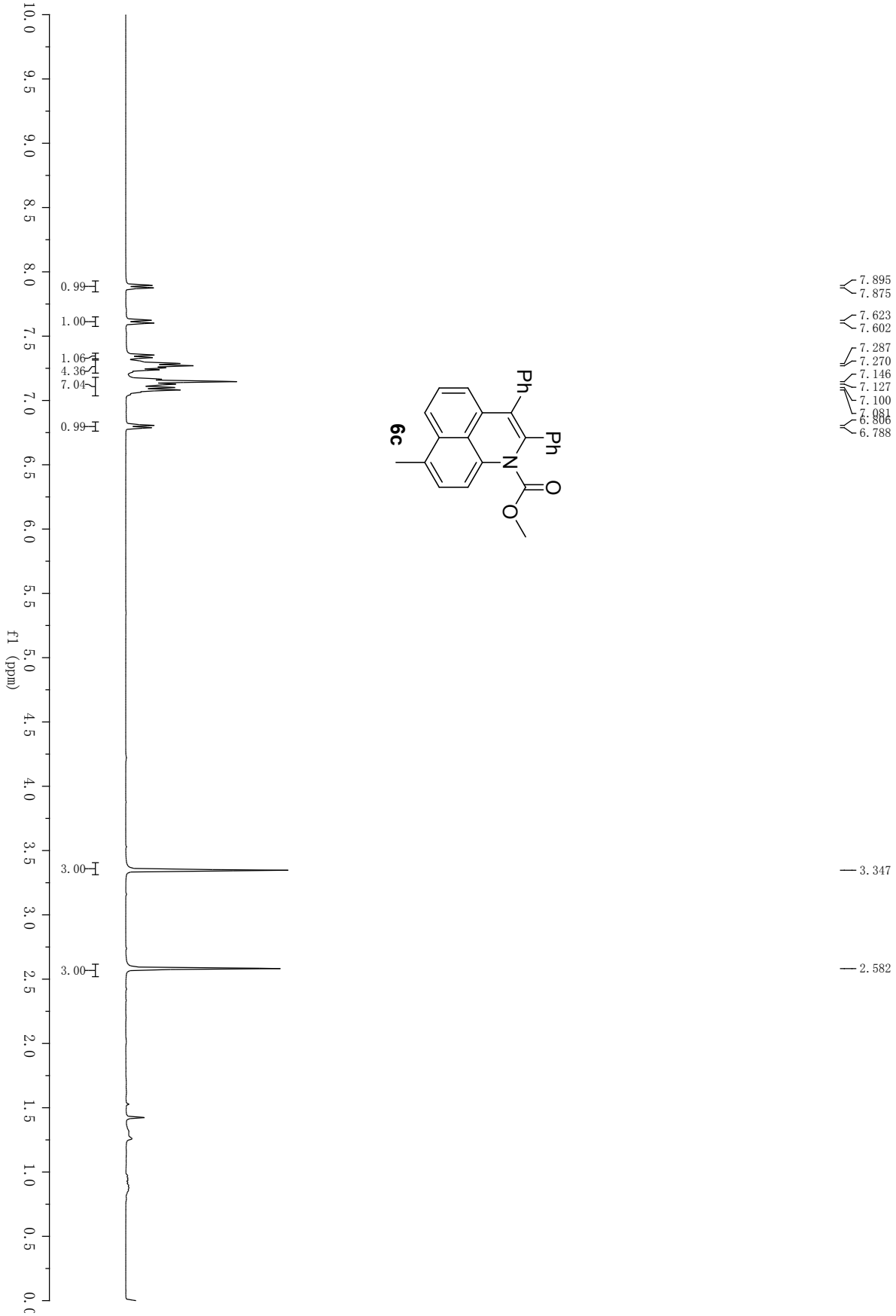

7.778
7.758
7.623
7.603
7.586
7.566
7.546
7.475
7.457
7.439
7.411
7.389
7.371
7.336
7.319
7.286
7.267
7.248
7.228
7.210
6.504
6.487
2.553
2.508
2.491
2.469
1.573
1.550
1.522
1.061
0.817
0.799
0.779
0.755
0.737
1.00
1.95
6.26
1.03
3.71
0.33
4.06
2.67
5.63
9.00
4.24
f1 (ppm)
n-Pr
Ph
N
Boc
6b
(3:1)
6b'

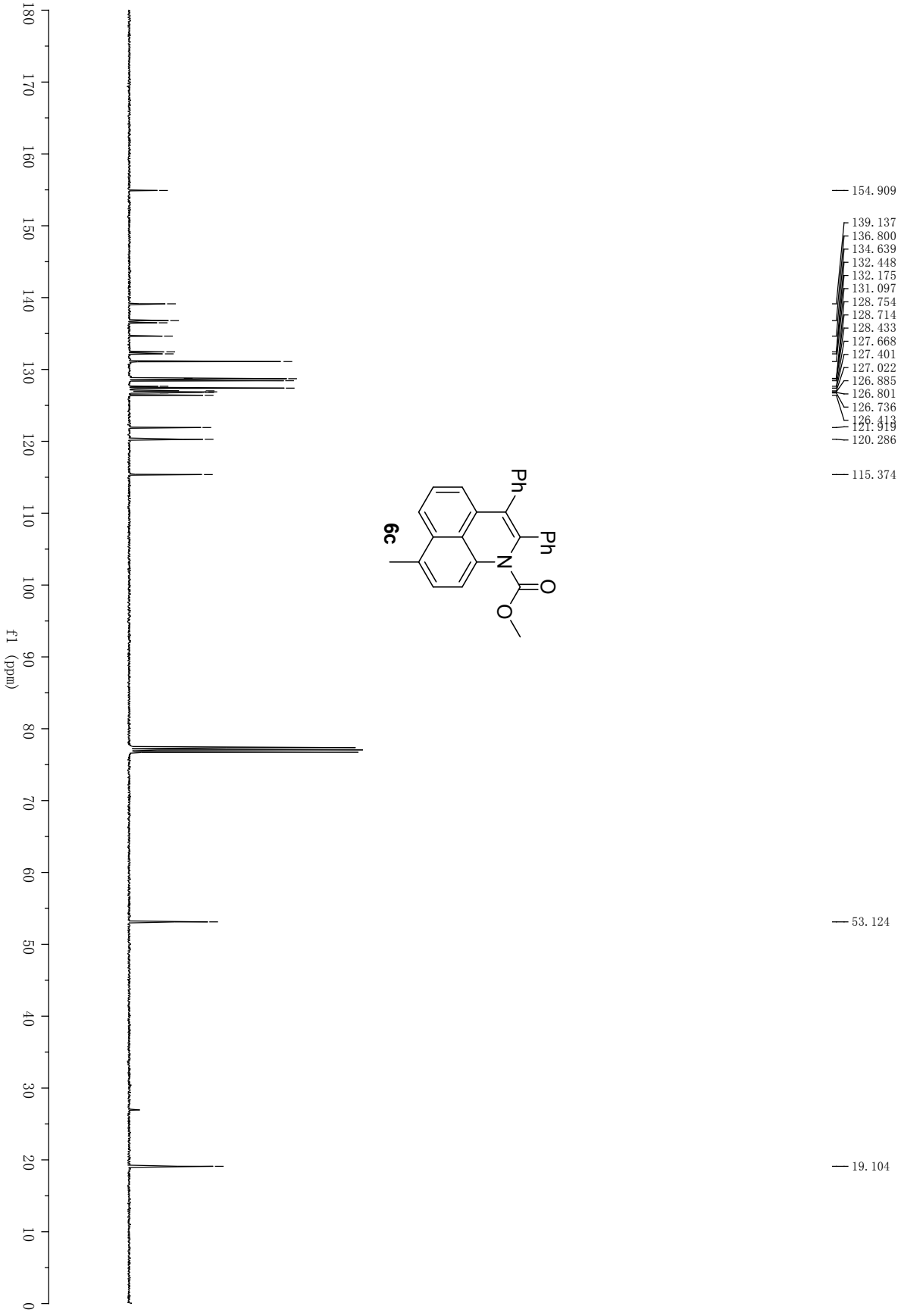

152. 959
152. 922
139. 715
138. 501
137. 972
136. 142
134. 976
134. 892
133. 002
132. 607
132. 141
131. 627
130. 953
129. 983
129. 621
128. 759
128. 185
127. 852
127. 563
127. 413
127. 357
126. 783
126. 581
126. 384
126. 198
122. 869
121. 284
121. 094
119. 673
118. 491
117. 378
116. 204
113. 471
82. 575
82. 461
34. 933
30. 780
28. 133
27. 442
22. 656
21. 420
19. 070
19. 011
14. 149
13. 701


Ph
n-Pr
N
Boc
(3:1)
n-Pr
Ph
N
Boc

6b **6b'**


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


f1 (ppm)
0.99
1.00
1.06
4.36
7.04
0.99
3.00
3.00
6c
Ph
Ph
N
O
O
7.895
7.875
7.623
7.602
7.287
7.270
7.146
7.127
7.100
7.081
6.806
6.788
3.347
2.582


154.909
139.137
136.800
134.639
132.448
132.175
131.097
128.754
128.714
128.433
127.668
127.401
127.022
126.885
126.801
126.736
126.413
121.919
120.286
115.374
53.124
19.104
f1 (ppm)
6c
Ph
Ph
N
O
O