Supporting Information

Highly Chemo- and Site-selective C(sp^2)-H Bond Functionalization of Aniline and Phenol Derivatives with Aryl/Aryl Diazo Compounds

Yu-Zhu Wang,[a] Xiaoyan Wei, Yinuo Chen, Yueyue Liu and Lu Liu[*abc]

[a]*School of Chemistry and Molecular Engineering, East China Normal University, 500 Dongchuan Road, Shanghai 200241, P. R. China*

[b]*Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, East China Normal University, Shanghai 200062, P. R. China*

[c]*School of Chemistry and Chemical Engineering, Shihezi University, Shihezi, 832003, P. R. China*

E-mail : lliu@chem.ecnu.edu.cn

Contents

1. General Information S2

2. Optimization of reaction conditions..... S3

3. General procedure for the synthesis of compounds S5

4. Gram scale reaction and synthetic spplication S25

5. References S28

6. NMR and HRMS spectra of new compounds..... S28

1. General Information

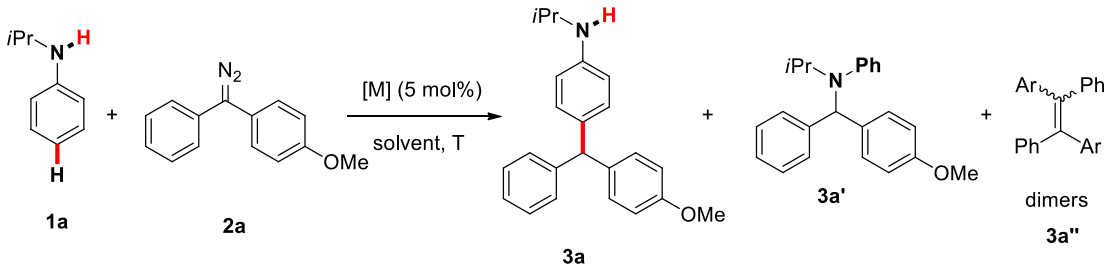
Unless otherwise noted, all reactions were carried out in standard Schlenk techniques with magnetic stirring bar under air. Materials obtained from commercial suppliers were used directly without further purification. ^{1}H NMR spectra were recorded on a BRUKER 500 (500 MHz) or BRUKER 600 (600 MHz) spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with tetramethylsilane (TMS: 0 ppm) with the solvent resonance as the internal standard. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, quint = quintus, sext = sextus, sept = septimum, m = multiplet), coupling constants (Hz), and integration. $^{13}C\{^{1}H\}$ NMR spectra were recorded on a BRUKER 500 (126 MHz) or BRUKER 600 (151 MHz) spectrometer in $CDCl_3$ with complete proton decoupling. Chemical shifts are reported in ppm with the deuterium solvent as the internal standard (e.g. $CDCl_3$: 77.0 ppm). HRMS spectra were recorded on BRUKER maXis impact, Source type is electrospray ionization (ESI-TOF).

Anhydrous toluene were distilled from sodium and benzophenone to use. Anhydrous hexane, $Bi(OTf)_3$, and $(PhO)_2POOH$ were purchased from Energy Chemical Company and used directly.

Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed on silica gel 60 (particle size 200-400 mesh ASTM, purchased from Yantai, China) and eluted with petroleum ether/ethyl acetate (PE/EtOAc) or petroleum ether/ diethyl ether (PE/ DCM). Without special instructions, heating reactions are carried out through an oil bath.

2. Optimization of reaction conditions

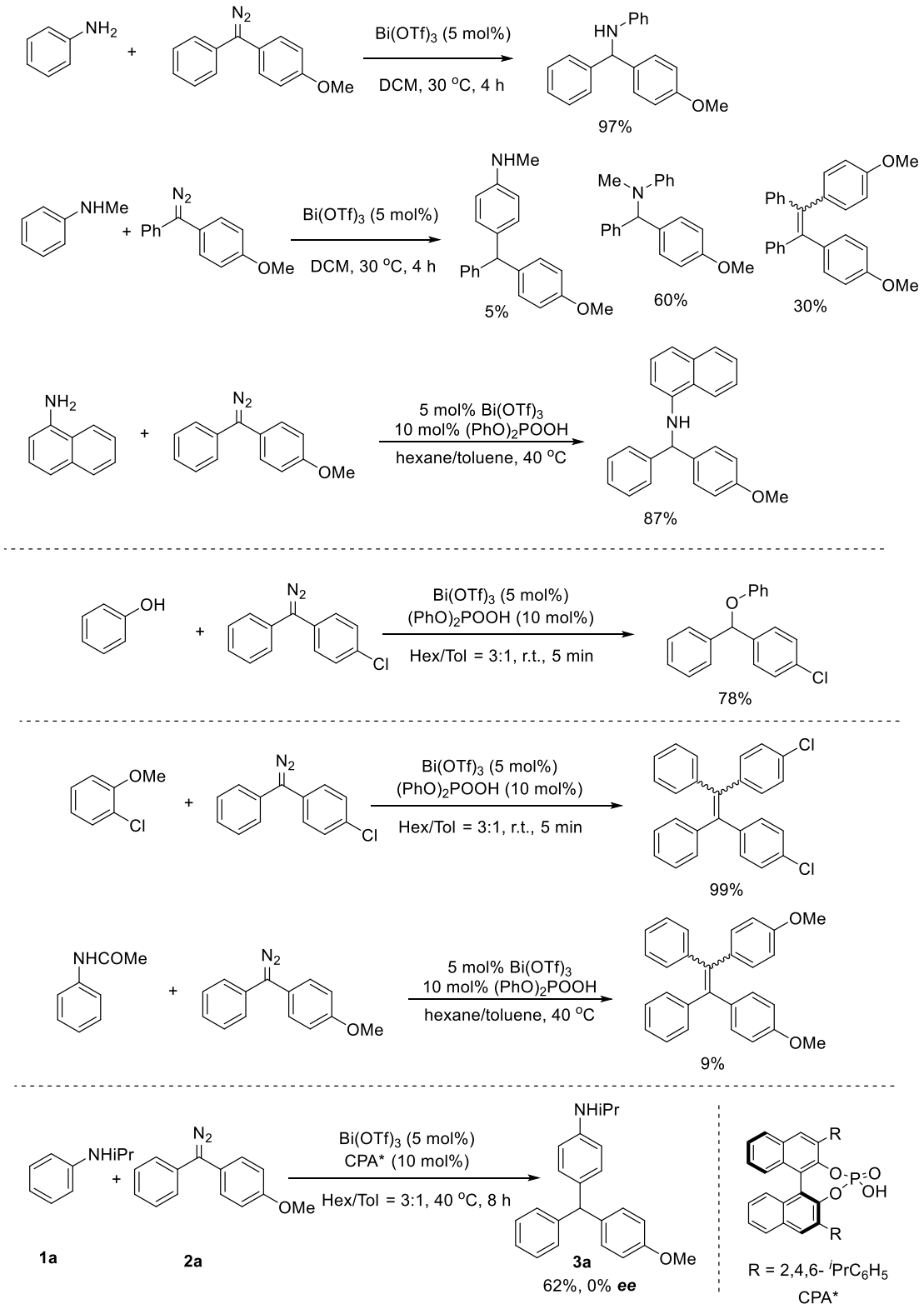
Table S1. Optimization of reaction conditions with N-isopropyl aniline[a]



Entry	[M]	Solvent	T/ °C	t/h	Additive	Yield (%)[b]		
						3a	**3a'**	**3a''**
1	$Bi(OTf)_3$	DCM	30	8	--	52	0	45
2	$Rh_2(OAc)_4$	DCM	30	--	--	0	0	97
3	$Ph_3PAuOTf$	DCM	30	--	--	0	21	74
4	AgOTf	DCM	30	--	--	0	11	87
5	$B(C_6F_5)_3$	DCM	30	2	--	42	12	41
6	$Sc(OTf)_3$	DCM	30	12	--	32	7	56
7	HOTf	DCM	30	--	--	0	93	2
8	$(PhO)_2PO_2H$	DCM	30	36	--	0	8	88
9	$Bi(OTf)_3$	hexane	30	48	--	58	0	40
10	$Bi(OTf)_3$	toluene	30	14	--	50	0	47
11	$Bi(OTf)_3$	THF	30	48	--	0	0	94
12	$Bi(OTf)_3$	MeCN	30	36	--	0	0	96
13	$Bi(OTf)_3$	hex:tol	30	14	--	63	0	32
14	$Bi(OTf)_3$	hex:tol	40	12	--	63	0	32
15	$Bi(OTf)_3$	hex:tol	50	122	--	60	0	37
17[c]	**$Bi(OTf)_3$**	**hex:tol**	**40**	**12**	**$(PhO)_2PO_2H$**	**79**	**0**	**12**
18	$Bi(OTf)_3$	hex:tol	40	12	$C_6H_5CO_2H$	62	0	33
19[d]	$Bi(OTf)_3$	hex:tol	40	12	$(PhO)_2PO_2H$	75	0	22
20[e]	$Bi(OTf)_3$	hex:tol	40	12	$(PhO)_2PO_2H$	77	0	25
21[f]	$Bi(OTf)_3$	hex:tol	40	12	$(PhO)_2PO_2H$	75	0	23

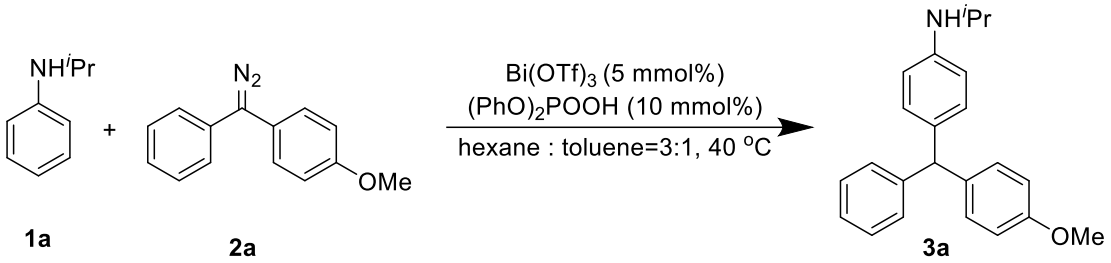
[a]Reaction conditions: **1** (0.2 mmol), **2** (0.1 mmol) and [M] (5 mol %), solvent (2.0 mL), at 30 °C for 24h; [b]Yields were determined by crude ^1H NMR using CH_2Br_2 as internal standard. [c]$(PhO)_2PO_2H$ (10 mol%). [d] $(PhO)_2PO_2H$ (5 mol%). [e] $(PhO)_2PO_2H$ (15 mol%). [f]$(PhO)_2PO_2H$ (20 mol%)

Table S2. Unsuccessful results.



3. General procedure for the synthesis of compounds

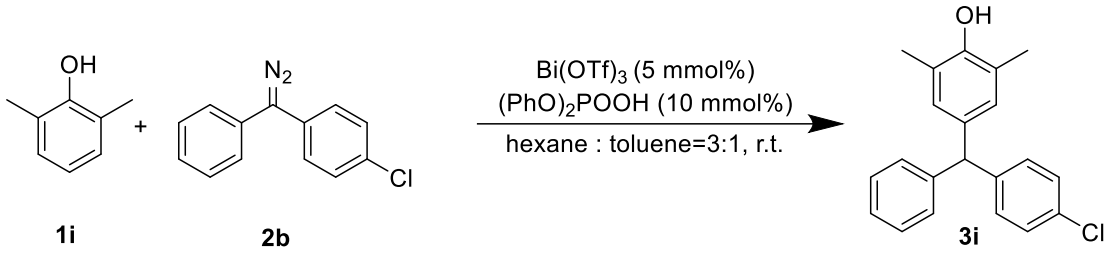
General procedure for synthesis aniline compounds



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

General procedure: aniline **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%) and $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) were introduced into a dried glass tube under Argon protection, and add 1mL dry hexane and 1mL dry toluene as solvent, then the diazo **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) was dissolved in 2 ml of hexane and add dropwise in 10 min at 40 °C. After the addition, continue to react for 12 h consumed diazo completely determined by TLC analysis. The mixture was purified by column chromatography on silica gel using PE/EtOAc = 20:1 as the eluent and concentrated to obtain the product **3a** (101.8 mg, 79%). Unless otherwise specified, the synthesis of other aniline compounds refers to this method.

General procedure for synthesis phenol compounds

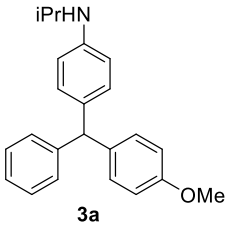


1i **2b** **3i**

General procedure: phenol **1i** (97.7 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%) and $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) were introduced into a dried glass tube under Argon protection, and add 1mL dry hexane and 1mL dry toluene as solvent, then the diazo **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) was dissolved in 2 ml of hexane and add dropwise in 10 min at room temperature. After the addition, continue to react for 1 minute consumed diazo completely determined by TLC analysis. The mixture was purified by column chromatography on silica gel using PE/EtOAc =

30:1 as the eluent and concentrated to obtain the product **3i** (96.3 mg, 75%). Unless otherwise specified, the synthesis of other phenol compounds refers to this method.

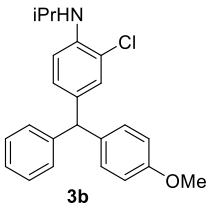
1) *N*-isopropyl-4-((4-methoxyphenyl)(phenyl)methyl)aniline (3a)



3a

The general procedure was followed using **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.4, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3a** (102.3 mg, 77%) was obtained as colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (d, *J* = 6.2 Hz, 2H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 2H), 6.88 (d, *J* = 8.1 Hz, 2H), 6.80 (d, *J* = 8.2 Hz, 2H), 6.50 (d, *J* = 8.1 Hz, 2H), 5.38 (s, 1H), 3.77 (s, 3H), 3.58 (hept, *J* = 6.3 Hz, 1H), 3.39 (br, 1H), 1.19 (d, *J* =6.2 Hz, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 157.8, 145.8, 145.0, 136.9, 132.7, 130.3, 130.1, 129.3, 128.1, 125.9, 113.5, 113.0, 55.2, 55.2, 44.3, 23.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{23}H_{26}NO$ 332.2009, found 332.2006.

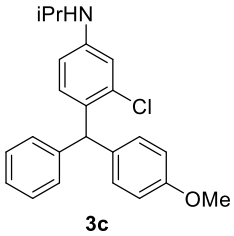
2) 2-chloro-*N*-isopropyl-4-((4-methoxyphenyl)(phenyl)methyl)aniline (3b)



3b

The general procedure was followed using **1b** (135.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.42, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3b** (95.2 mg, 65%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.3 Hz, 1H), 7.26 (s, 1H), 7.22-7.17 (m, 1H), 7.10 (d, *J* = 7.1 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 2H), 6.98 (d, *J* = 2.1 Hz, 1H), 6.85 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.82 (d, *J* = 8.7 Hz, 2H), 6.58 (d, *J* = 8.4 Hz, 1H), 5.35 (s, 1H), 3.78 (s, 3H), 3.62 (p, *J* = 6.3 Hz, 1H), 1.23 (d, *J* = 6.3 Hz, 6H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$) δ 157.9, 144.4, 141.5, 136.2, 130.2, 129.9, 129.2, 128.6, 128.2, 126.1, 118.9, 113.6, 111.4, 55.2, 54.8, 44.2, 22.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{23}H_{25}ClNO$ 366.1619, found 366.1614.

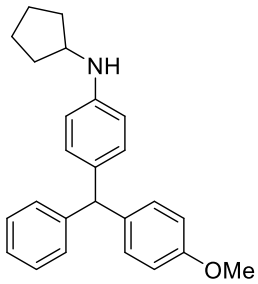
3) 3-chloro-*N*-isopropyl-4-((4-methoxyphenyl)(phenyl)methyl)aniline (3c)



3c

The general procedure was followed using **1c** (135.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.45, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3c** (114.2 mg, 78%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.7 Hz, 2H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 7.5 Hz, 2H), 6.98 (d, *J* = 8.3 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 6.67 (d, *J* = 8.5 Hz, 1H), 6.59 (d, *J* = 2.1 Hz, 1H), 6.36 (dd, *J* = 8.5, 2.5 Hz, 1H), 5.77 (s, 1H), 3.77 (s, 3H), 3.55 (hept, *J* = 6.3 Hz, 1H), 3.46 (br, 1H), 1.18 (d, *J* = 6.2 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 157.9, 146.8, 143.9, 135.6, 135.0, 131.4, 130.4, 129.8, 129.4, 128.1, 126.1, 113.6, 113.3, 111.6, 55.2, 51.7, 44.3, 22.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{23}H_{25}ClNO$ 366.1619, found 366.1614.

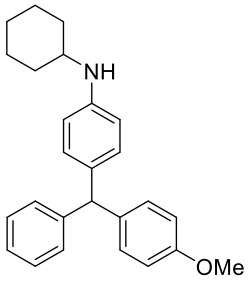
4) *N*-cyclopentyl-4-((4-methoxyphenyl)(phenyl)methyl)aniline (3d)



3d

The general procedure was followed using **1d** (128.9 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.41, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3d** (103.2 mg, 72%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.23 (m, 2H), 7.17 (t, *J* = 6.6 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 2H), 7.03 (d, *J* = 7.4 Hz, 2H), 6.88 (d, *J* = 6.8 Hz, 2H), 6.80 (d, *J* = 6.9 Hz, 2H), 6.52 (d, *J* = 8.4 Hz, 2H), 5.38 (s, 1H), 3.77 (s, 3H), 3.76 – 3.71 (quint, J = 5.5 Hz, 1H), 3.63 (br, 1H), 2.03 – 1,94 (m, 2H), 1.75 – 1.66 (m, 2H), 1.63 – 1.57 (m, 2H), 1.49 – 1.41 (m, 2H); ^{13}C NMR{^{1}H} (126 MHz, $CDCl_3$) δ 157.8, 146.3, 145.0, 136.9, 132.7, 130.3, 130.0, 129.3, 128.1, 125.9, 113.5, 113.0, 55.2, 55.2, 54.8, 33.6, 24.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{25}H_{28}NO$ 358.2165, found 358.2160.

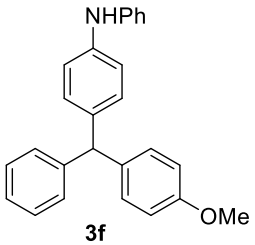
5) *N*-cyclohexyl-4-((4-methoxyphenyl)(phenyl)methyl)aniline (3e)



3e

The general procedure was followed using **1e** (140.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.41, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3e** (108.7 mg, 73%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 – 7.22 (m, 2H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 7.0 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 6.50 (d, *J* = 7.0 Hz, 2H), 5.37 (s, 1H), 3.77 (d, *J* = 1.5 Hz, 3H), 3.46 (br, 1H), 3.24 – 3.15 (m, 1H), 2.07 – 1.98 (m, 2H), 1.76 – 1.69 (m, 2H), 1.41 – 1.06 (m, 6H); ^{13}C {^{1}H}NMR (126 MHz, $CDCl_3$) δ 157.8, 145.7, 145.1, 136.9, 132.6, 130.3, 130.1, 129.3, 128.1, 125.9, 113.5, 112.9, 55.2, 55.1, 51.8, 33.5, 25.9, 25.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{26}H_{30}NO$ 372.2322, found 372.2319.

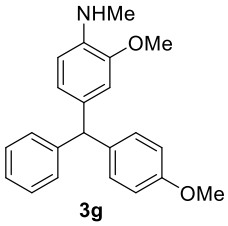
6) 4-((4-methoxyphenyl)(phenyl)methyl)-*N*-phenylaniline (3f)



3f

The general procedure was followed using **1f** (138.4 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.39, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3f** (96.8 mg, 72%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.17 (m, 5H), 7.12 (d, *J* = 7.2 Hz, 2H), 7.05 – 7.02 (m, 4H), 6.98 (s, 4H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.82 (d, *J* = 8.8 Hz, 2H), 5.64 (br, 1H), 5.43 (s, 1H), 3.77 (s, 3H); ^{13}C NMR {^{1}H} (126 MHz, $CDCl_3$) δ 157.9, 144.6, 143.3, 141.2, 137.0, 136.4, 130.3, 130.2, 129.3, 129.3, 128.2, 126.1, 120.7, 117.8, 117.5, 113.6, 55.3, 55.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{26}H_{24}NO$ 366.1852, found 366.1840.

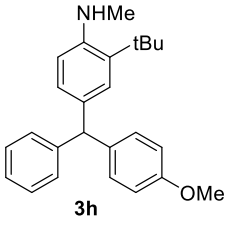
7) 2-methoxy-4-((4-methoxyphenyl)(phenyl)methyl)-*N*-methylaniline (3g)



3g

The general procedure was followed using **1g** (109.7 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.32, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3g** (97.8 mg, 71%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.22 (m, 2H), 7.18 (t, *J* = 6.6 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 8.3 Hz, 2H), 6.81 (d, *J* = 7.2 Hz, 2H), 6.56 (d, *J* = 7.9 Hz, 1H), 6.53 (s, 1H), 6.49 (d, *J* = 7.9 Hz, 1H), 5.41 (s, 1H), 4.12 (br, 1H), 3.77 (s, 3H), 3.70 (s, 3H), 2.82 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 157.8, 146.8, 145.0, 137.6, 136.9, 132.3, 130.3, 129.3, 128.1, 126.9, 121.9, 113.5, 110.7, 108.9, 55.6, 55.3, 55.2, 30.4.; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{22}H_{24}NO_2$ 334.1802, found 334.1795.

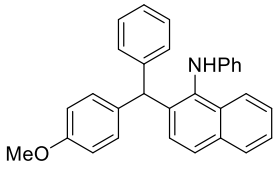
8) 2-(tert-butyl)-4-((4-methoxyphenyl)(phenyl)methyl)-*N*-methylaniline (3h)



3h

The general procedure was followed using **1h** (130.5 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.32, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3h** (103.7 mg, 72%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.22 (m, 3H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 6.9 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 2.2 Hz, 1H), 6.83 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.80 (d, *J* = 8.7 Hz, 2H), 6.57 (d, *J* = 8.3 Hz, 1H), 5.39 (s, 1H), 3.68 (br, 1H), 3.76 (s, 3H), 2.87 (s, 3H), 1.33 (s, 9H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 157.7, 145.6, 145.3, 137.2, 133.1, 132.2, 130.3, 129.3, 128.1, 127.7, 127.5, 126.8, 113.4, 110.9, 55.5, 55.2, 34.1, 31.3, 29.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{25}H_{30}NO$ 360.2322, found 360.2317.

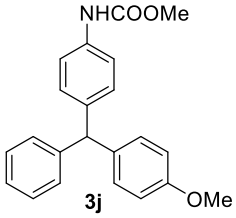
9) 2-((4-methoxyphenyl)(phenyl)methyl)-N-phenylnaphthalen-1-amine (3i)



3i

The general procedure was followed using **1i** (175.4 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.32, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3i** (150.7 mg, 86%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 7.8, 2.0 Hz, 1H), 8.00 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.29 – 7.27 (m, 1H), 7.26 – 7.17 (m, 5H), 7.12 (d, *J* = 7.1 Hz, 2H), 7.03 (d, *J* = 8.7 Hz, 2H), 6.95 (d, *J* = 7.6 Hz, 2H), 6.90 – 6.78 (m, 4H), 6.17 (s, 1H), 5.87 (br, 1H), 3.77 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.0, 144.9, 144.2, 137.6, 136.0, 135.1, 132.8, 130.5, 129.5, 129.2, 128.3, 127.6, 126.2, 126.2, 125.2, 125.0, 122.4, 120.2, 117.1, 115.5, 113.7, 55.1, 52.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{30}H_{25}NNaO$ 438.1826, found 438.1828.

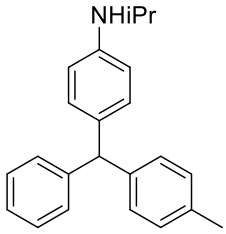
10) methyl (4-((4-methoxyphenyl)(phenyl)methyl)phenyl)carbamate (3j)



3j

The general procedure was followed using **1j** (120.9 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.7 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.28, PE/EtOAc = 20:1). After purification by column chromatography (PE/EtOAc = 30:1), **3j** (44.4 mg, 30%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 4H), 7.22 – 7.16 (m, 1H), 7.09 (d, *J* = 7.4 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.59 (br, 1H), 5.45 (s, 1H), 3.77 (s, 3H), 3.75 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 158.0, 154.0, 144.2, 139.4, 136.0, 135.9, 130.2, 129.9, 129.2, 128.2, 126.2, 113.6, 55.3, 55.2, 52.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ calculated for $C_{22}H_{21}NNaO_3$ 370.1417, found 370.1414.

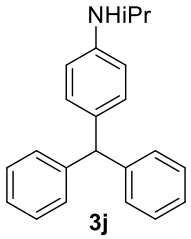
11) *N*-isopropyl-4-(phenyl(p-tolyl)methyl) aniline (3m)



3i

The general procedure was followed using **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2c** (83.2 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.3, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **3m** (94.6 mg, 70%) was obtained as white semi-solid. ^1H NMR (500 MHz, $CDCl_3$) δ 7.26 – 7.22 (m, 2H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 2H), 7.07 (d, *J* = 7.9 Hz, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.50 (d, *J* = 8.6 Hz, 2H), 5.39 (s, 1H), 3.58 (hept, *J* = 6.3 Hz, 1H), 2.31 (s, 3H), 1.18 (d, *J* = 6.3 Hz, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ145.77, 144.9, 141.7, 135.4, 132.5, 130.1, 129.3, 129.2, 128.5, 128.1, 125.9, 113.0, 55.6, 44.2, 23.0, 20.9; HRMS (ESI-TOF) m/z: [M+Na]+ calculated for $C_{23}H_{25}NNa$ 338.1885, found 338.1882.

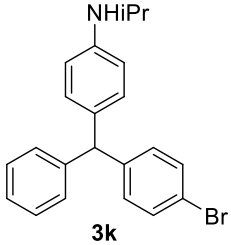
12) 4-benzhydryl-*N*-isopropylaniline (3n)



3j

The general procedure was followed using **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2d** (77.6 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.5, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **3n** (54.2 mg, 45%) was obtained as white semi-solid. ^1H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.4 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 3H), 7.20 (t, *J* = 7.3 Hz, 1H), 7.11 – 7.07 (m, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 6.50 (d, *J* = 8.5 Hz, 2H), 5.37 (s, 1H), 3.59 (hept, *J* = 6.3 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 6H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 143.8, 131.2, 131.1, 130.1, 129.2, 128.2, 126.2, 113.0, 55.4, 44.2, 23.0; HRMS (ESI-TOF) m/z: $[M+H]^-$ calculated for $C_{22}H_{23}N$ 301.1830, found 301.1834.

13) 4-((4-bromophenyl)(phenyl)methyl)-*N*-isopropylaniline (3o)

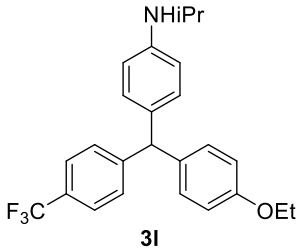


3k

The general procedure was followed using **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2e** (108.8 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.5, PE/DCM

= 2:1). After purification by column chromatography (PE/DCM = 3:1), **3o** (104.1 mg, 37%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.5 Hz, 4H), 7.18 (t, *J* = 7.3 Hz, 2H), 7.12 (d, *J* = 7.2 Hz, 4H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.51 (d, *J* = 8.6 Hz, 2H), 5.43 (s, 1H), 3.58 (hept, *J* = 6.3 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 6H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 145.7, 144.6, 132.3, 130.2, 129.3, 129.3, 128.6, 128.1, 128.0, 127.8, 126.0, 113.0, 55.9, 44.3, 23.0; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{22}H_{22}BrNNa$ 402.0833, found 402.0837.

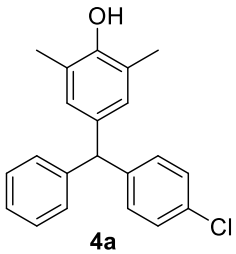
14) 4-((4-ethoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)-*N*-isopropylaniline (3p)



3l

The general procedure was followed using **1a** (108.1 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2h** (122.5 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.2, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **3p** (92.3 mg, 56%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 2H), 7.24 – 7.18 (m, 2H), 7.00 – 6.96 (m, 2H), 6.87 – 6.84 (m, 2H), 6.83 – 6.78 (m, 2H), 6.51 (dd, *J* = 8.5, 1.1 Hz, 2H), 5.41 (s, 1H), 3.99 (q, *J* = 6.9 Hz, 2H), 1.39 (t, *J* = 6.9 Hz, 3H), 1.19 (d, *J* = 6.3 Hz, 6H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ157.4, 149.2, 146.02, 135.7, 131.6, 130.2, 130.0, 129.6, 128.8 (q, *J* = 31.8 Hz), 125.8 (q, *J* = 3.8 Hz), 125.0, 125.0, 125.0, 124.9, 124.3 (q, *J* = 271.6 Hz), 114.2, 113.0, 63.3, 54.9, 44.2, 23.0, 14.8; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{25}H_{26}F_3NO$ 412.1996, found 412.1996.

15) 4-((4-chlorophenyl)(phenyl)methyl)-2,6-dimethylphenol (4a)

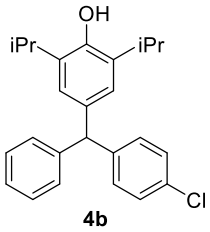


4a

The general procedure was followed using **1i** (97.7 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.4, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **3i** (96.3 mg, 75%) was obtained as colorless oil. ^{1}H NMR (500

MHz, $CDCl_3$) δ 7.29 – 7.17 (m, 6H), 7.07 (d, *J* = 7.2 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.68 (s, 2H), 5.37 (s, 1H), 4.54 (s, 1H), 2.17 (s, 6H); ^{13}C {^1H} NMR (126 MHz, $CDCl_3$) δ 150.7, 143.8, 143.0, 135.0, 131.9, 130.7, 129.4, 129.2, 128.3, 126.3, 122.9, 55.4, 16.0; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{21}H_{18}ClO$ 321.1052, found 321.1060.

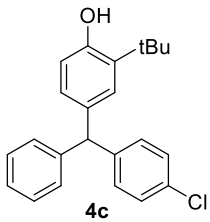
16) 4-((4-chlorophenyl)(phenyl)methyl)-2,6-diisopropylphenol (4b)



4b

The general procedure was followed using **1j** (142.6 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.4, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **4b**(119.2 mg, 79%) was obtained as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.17 (m, 5H), 7.08 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.75 (s, 2H), 5.43 (s, 1H), 4.69 (s, 1H), 3.09 (hept, *J* = 6.9 Hz, 2H), 1.17 (d, *J* = 6.9 Hz, 12H); ^{13}C {^1H} NMR (126 MHz, $CDCl_3$) δ 148.5, 144.1, 143.3, 135.0, 133.5, 131.8, 130.7, 129.3, 128.3, 126.3, 124.5, 56.0, 27.3, 22.7, 22.7; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{25}H_{26}ClO$ 377.1678, found 377.1678.

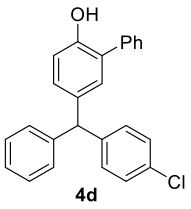
17) 2-(tert-butyl)-4-((4-chlorophenyl)(phenyl)methyl)phenol (4c)



4c

The general procedure was followed using **1k** (120.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.43, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **4c** (103.6 mg, 74%) was obtained as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.17 (m, 5H), 7.08 (d, *J* = 7.6 Hz, 2H), 7.03 (d, *J* = 9.3 Hz, 3H), 6.71 (d, *J* = 7.9 Hz, 1H), 6.57 (d, *J* = 8.1 Hz, 1H), 5.43 (s, 1H), 4.74 (s, 1H), 1.33 (s, 9H); ^{13}C {^1H} NMR (126 MHz, $CDCl_3$) δ 152.7, 144.0, 143.1, 136.0, 135.2, 131.9, 130.7, 129.3, 128.3, 128.3, 127.5, 126.3, 116.3, 55.7, 34.5, 29.5; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{23}H_{22}ClO$ 349.1365, found 349.1368.

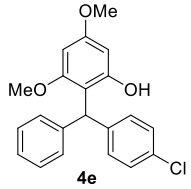
18) 5-((4-chlorophenyl)(phenyl)methyl)-[1,1'-biphenyl]-2-ol (4d)



4d

The general procedure was followed using **1l** (136.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.43, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **4d**(107.8 mg, 73%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 5H), 7.31 – 7.22 (m, 5H), 7.11 (d, *J* = 7.1 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 2.3 Hz, 1H), 6.96 (dd, *J* = 8.3, 2.4 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.48 (s, 1H), 5.15 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 151.0, 143.8, 142.7, 136.9, 135.8, 132.1, 131.0, 130.7, 129.9, 129.3, 129.0, 128.4, 127.9, 126.5, 115.8, 55.5; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{25}H_{18}ClO$ 369.1052, found 369.1052.

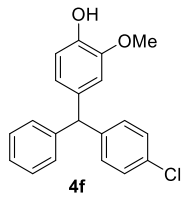
19) 4-((4-chlorophenyl)(phenyl)methyl)-3,5-dimethoxyphenol (4e)



4e

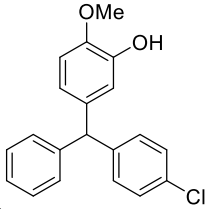
The general procedure was followed using **1m** (123.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.43, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **4e**(128.2 mg, 85%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.23 (m, 5H), 7.19 – 7.14 (m, 4H), 6.12 (d, J = 2.4 Hz, 1H), 6.02 (d, J = 2.8 Hz, 2H), 4.80 (s, 1H), 3.75 (s, 3H), 3.70 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 160.3, 158.8, 155.9, 142.1, 140.8, 132.3, 130.4, 128.8 128.7, 128.6, 126.9, 110.4, 94.7, 91.9, 55.8, 55.2, 44.4; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{21}H_{19}ClNaO_3$ 377.0915, found 377.0907.

20) 4-((4-chlorophenyl)(phenyl)methyl)-2-methoxyphenol (4f)



4f

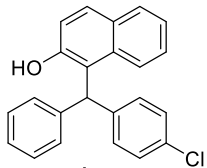
and



C4 : C5 = 3 : 1

The general procedure was followed using **1n** (99.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.35, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **4f** (93.0 mg, 72%) was obtained as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.17 (m 6H), 7.09 (d, J = 9.7 Hz, 2H), 7.04 (d, J = 9.8 Hz, 2H), [6.83 (d, J = 10.3 Hz, 0.77H) (C4), 6.76 (d, J = 10.4 Hz, 0.26H) (C5)], [6.68 (s, 0.25H) (C5), 6.60 (s, 0.78H) (C4)], [6.56 (d, J = 10.0 Hz, 0.23H) (C5), 6.54 (d, J = 10.0 Hz, 0.80H) (C4)], [5.55 (s, 0.25H) (C5), 5.52 (s, 0.75H) (C4)], [5.44 (s, 0.76H) (C4), 5.41 (s, 0.27H) (C5)], [3.86 (s, 0.77H) (C5), 3.76 (s, 2.36H) (C4)]; $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) : [146.4 (C5), 145.5 (C4)], [145.1 (C5), 144.2 (C4)], [143.6 (C4), 143.5 (C5)], [142.7 (C4), 142.6 (C5)], [136.7 (C5), 135.3 (C4)], [132.1 (C4), 130.7 (C5)], [132.0 (C5), 129.2 (C4)], [128.63 (C4), 128.58 (C5)], 128.38 (C4), 128.36 (C4), 127.9 (C4), 126.49(C5),126.47(C5), 126.4 (C5), [122.1 (C4), 120.8 (C5)], [115. 6 (C5), 114.1 (C4)], [111.9 (C5), 110.4 (C4)], 55.9 (C5), 55.84 (C5), 55.78 (C4), 55.5 (C4); HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{20}H_{16}ClO_2$ 323.0844, found 323.0844.

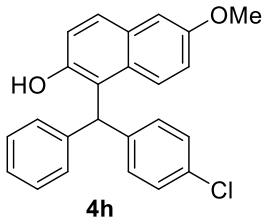
21) 1-((4-chlorophenyl)(phenyl)methyl)naphthalen-2-ol (4g)[1]



4g

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.2, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4g** (110.1 mg, 80%) was obtained as white semi-solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 10.5 Hz, 1H), 7.77 (d, *J* = 10.0 Hz, 1H), 7.72 (d, *J* = 11.0 Hz, 1H), 7.39 (t, *J* = 9.8 Hz, 1H), 7.32-7.26 (m, 6H), 7.22-7.17 (m, 4H), 7.04 (d, *J* = 11.0 Hz, 1H), 6.37 (s, 1H), 5.12 (s, 1H); 1H NMR spectrum is consistent with literature reports.

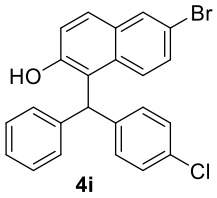
22) 1-((4-chlorophenyl)(phenyl)methyl)-6-methoxynaphthalen-2-ol (4h)



4h

The general procedure was followed using **1p** (139.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.23, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4h** (112.2 mg, 75%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 9.3 Hz, 1H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.32 (t, *J* = 7.3 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 3H), 7.25 – 7.16 (m, 4H), 7.11 (d, *J* = 2.7 Hz, 1H), 7.07 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.02 (d, *J* = 8.8 Hz, 1H), 6.32 (s, 1H), 4.89 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.7, 150.9, 141.5, 140.1, 132.8, 130.7, 130.4, 129.2, 129.0, 128.8, 128.5, 128.4, 127.3, 124.4, 120.3, 120.2, 119.1, 107.2, 55.3, 48.0; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{24}H_{18}ClO_2$ 373.1001, found 373.1005.

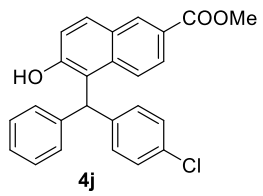
23) 6-bromo-1-((4-chlorophenyl)(phenyl)methyl)naphthalen-2-ol (4i)[2]



4i

The general procedure was followed using **1q** (178.5 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.25, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4i** (148.2 mg, 88%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 2.2 Hz, 1H), 7.76 (d, *J* = 9.1 Hz, 1H), 7.63 (d, *J* = 8.9 Hz, 1H), 7.44 (dd, *J* = 9.1, 2.1 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 3H), 7.21 – 7.14 (m, 4H), 7.07 (d, *J* = 8.9 Hz, 1H), 6.31 (s, 1H), 5.11 (s, 1H); 1H NMR spectrum is consistent with literature reports.

24) methyl 5-((4-chlorophenyl)(phenyl)methyl)-6-hydroxy-2-naphthoate (4j)

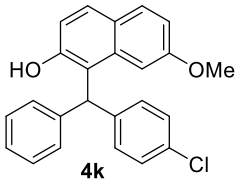


4j

The general procedure was followed using **1r** (161.8 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.1, PE/DCM = 1:1). After purification by column chromatography (PE/DCM = 1:1), **4j** (122.2 mg, 76%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53

(s, 1H), 7.99 – 7.93 (m, 2H), 7.85 (d, *J* = 8.9 Hz, 1H), 7.34 (t, *J* = 7.0 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 7.23 – 7.16 (m, 4H), 7.12 (d, *J* = 8.8 Hz, 1H), 6.37 (s, 1H), 5.29 (s, 1H), 3.95 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 167.1, 154.7, 141.0, 139.6, 133.1, 131.8, 131.3, 130.4, 129.4, 129.2, 128.8, 128.7, 127.6, 126.4, 124.9, 123.0, 120.5, 120.0, 52.1, 47.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{25}H_{19}ClNaO_3$ 425.0915, found 425.0905.

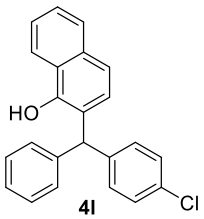
25) 1-((4-chlorophenyl)(phenyl)methyl)-7-methoxynaphthalen-2-ol (4k)



4k

The general procedure was followed using **1s** (139.4 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.23, PE/DCM = 3:1). After purification by column chromatography (PE/DCM = 3:1), **4k** (119.7 mg, 80%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (t, *J* = 9.5 Hz, 2H), 7.34 – 7.30 (m, 3H), 7.29 – 7.26 (m, 2H), 7.25 – 7.15 (m, 4H), 7.14 (s, 1H), 6.97 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 1H), 6.30 (s, 1H), 5.05 (s, 1H), 3.68 (s, 3H); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 158.3, 153.0, 141.7, 140.3, 134.6, 132.7, 130.5, 130.2, 129.5, 129.1, 129.0, 128.9, 127.2, 126.0, 119.2, 116.7, 115.1, 103.1, 55.1, 47.9; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{24}H_{18}ClO_2$ 373.1001, found 373.1005.

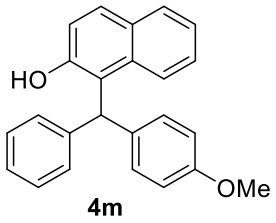
26) 2-((4-chlorophenyl)(phenyl)methyl)naphthalen-1-ol (4l)[4]



4l

The general procedure was followed using **1t** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.3, PE/DCM = 2:1). After purification by column chromatography PE/DCM = 3:1), **4l** (83.9 mg, 61%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.14- 8.12 (m, 1H), 7.83-7.81 (m, 1H), 7.52-7.50 (m, 2H), 7.43-7.32 (m, 6H), 7.20 (d, *J* = 9.4 Hz, 2H), 7.15 (d, *J* = 9.8 Hz, 2H), 7.00 (d, *J* = 10.6 Hz, 1H), 5.89 (s, 1H), 5.23 (s, 1H); 1H NMR spectrum is consistent with literature reports.

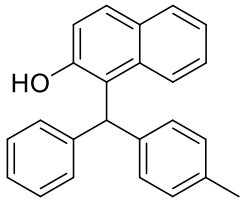
27) 1-((4-methoxyphenyl)(phenyl)methyl)naphthalen-2-ol (4m)[2]



4m

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.6 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.23, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4m** (78,9 mg, 58%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.31 (q, *J* = 6.9, 6.2 Hz, 3H), 7.28 – 7.23 (m, 3H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 1H), 6.86 (d, *J* = 7.7 Hz, 2H), 6.34 (s, 1H), 5.24 (s, 1H), 3.77 (s, 3H); 1H NMR spectrum is consistent with literature reports.

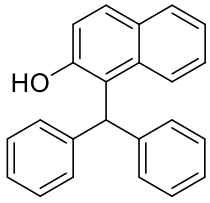
28) 1-(phenyl(*p*-tolyl)methyl)naphthalen-2-ol (4n)



4n

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2c** (83.2 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.3, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4n** (102.4 mg, 79%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.32 (q, *J* = 7.4 Hz, 3H), 7.28 – 7.23 (m, 3H), 7.13 (s, 3H), 7.06 (d, *J* = 8.9 Hz, 1H), 6.36 (s, 1H), 5.20 (s, 1H), 2.32 (s, 3H); 1H NMR spectrum is consistent with literature reports.

29) 1-benzhydrylnaphthalen-2-ol (4o)[1]

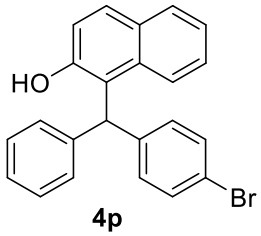


4o

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2d** (77.6 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.4, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4o** (97.9 mg, 73%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.7 Hz, 1H),

7.39 (t, *J* = 8.2 Hz, 2H), 7.35 – 7.22 (m, 12H), 7.08 – 7.03 (m, 1H), 6.41 (s, 1H), 5.17 (s, 1H); 1H NMR spectrum is consistent with literature reports.

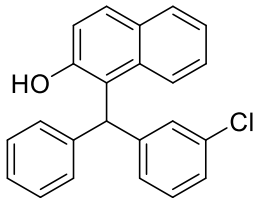
30) 1-((4-bromophenyl)(phenyl)methyl)naphthalen-2-ol (4p)



4p

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2e** (108.8 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.35, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4p** (134.4 mg, 87%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.42 (d, *J* = 6.8 Hz, 2H), 7.39 (d, *J* = 8.6 Hz, 1H), 7.34 – 7.29 (m, 3H), 7.27 (d, *J* = 6.3 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 7.4 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.35 (s, 1H), 5.05 (s, 1H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 152.5, 141.4, 140.5, 133.2, 132.0, 130.8, 129.9, 129.6, 129.2, 128.9, 128.8, 127.4, 126.9, 123.3, 122.7, 121.0, 119.8, 119.7, 47.9; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{23}H_{15}BrNaO$ 409.0198, found 409.0191.

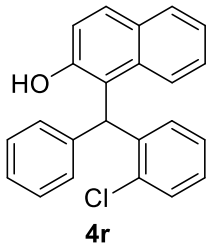
31) 1-((3-chlorophenyl)(phenyl)methyl)naphthalen-2-ol (4q)



4q

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2f** (91.2 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.3, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4q** (93.6 mg, 68%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.6 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.9 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.36 – 7.31 (m, 3H), 7.30 – 7.20 (m, 6H), 7.16 – 7.13 (m, 1H), 7.07 (d, *J* = 8.8 Hz, 1H), 6.38 (s, 1H), 5.06 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.6, 143.7, 141.2, 134.9, 133.3, 130.1, 129.9, 129.6, 129.3, 129.2, 128.9, 128.8, 127.4, 127.3, 127.2, 126.9, 123.3, 122.7, 119.7, 119.6, 48.2; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{23}H_{17}ClNaO$ 367.0860, found 367.0842.

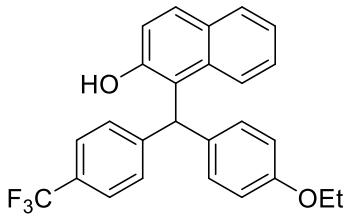
32) 1-((2-chlorophenyl)(phenyl)methyl)naphthalen-2-ol (4r)



4r

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2g** (91.2 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.3, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4r** (112.9 mg, 82%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.7 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.34 – 7.26 (m, 5H)), 7.15 – 7.11 (m, 3H), 7.05 (dd, *J* = 8.9, 1.5 Hz, 1H), 6.71 (s, 1H), 5.16 (s, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 153.2, 140.7, 138.5, 134.6, 133.4, 1307, 130.0, 129.9, 129.6, 129.5, 128.7, 128.6, 128.5, 127.6, 127.5, 127.1, 123.3, 122.6, 119.8, 119.2, 46.2; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{22}H_{17}ClNaO_2Se$ 450.9980, found 450.9961.

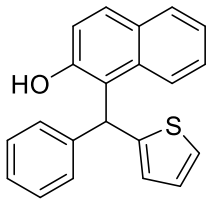
33) 1-((4-ethoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)naphthalen-2-ol (4s)



4s

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2h** (122.5 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.25, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4s** (135.1 mg, 80%) was obtained as white semi-solid. ^{1}H NMR (500 MHz, $CDCl_3$) ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.96 – 7.88 (m, 1H), 7.79 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.75 (dd, *J* = 8.9, 3.8 Hz, 1H), 7.56 (dd, *J* = 8.2, 4.2 Hz, 2H), 7.45 – 7.37 (m, 3H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.15 – 7.03 (m, 3H), 6.87 (dq, *J* = 8.7, 2.7, 2.1 Hz, 2H), 6.40 (s, 1H), 5.15 (s, 1H), 4.01 (q, *J* = 7.0 Hz, 2H), 1.40 (t, *J* = 7.0 Hz, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, CDCl3) δ 158.3, 152.6, 146.1, 133.2, 132.6, 129.9, 129.9, 129.7, 129.7, 128.8 (q, *J* = 31.8 Hz), 126.9, 125.8 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 271.6 Hz), 123.3, 123.1, 122.6, 119.7, 119.7, 115.3, 63.5, 47.5, 14.8; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for $C_{26}H_{20}F_3O_2$ 421.1421, found 421.1432.

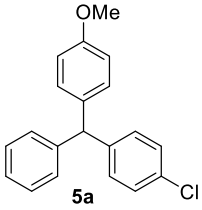
34) 1-(phenyl(thiophen-2-yl)methyl)naphthalen-2-ol (4t)



4t

The general procedure was followed using **1o** (115.3 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2i** (80.4 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.4, PE/DCM = 2:1). After purification by column chromatography (PE/DCM = 3:1), **4t** (93.6 mg, 74%) was obtained as white semi-solid. ^1H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.6 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.41 (d, *J* = 7.1 Hz, 1H), 7.37 – 7.31 (m, 5H), 7.28 (d, *J* = 4.8 Hz, 2H), 7.09 (d, *J* = 8.8 Hz, 1H), 6.96 – 6.92 (m, 1H), 6.83 (d, *J* = 3.3 Hz, 1H), 6.56 (s, 1H), 5.50 (s, 1H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 152.8, 146.0, 141.4, 132.8, 129.9, 129.5, 129.0, 128.8, 128.4, 127.4, 127.0, 127.0, 126.9, 126.0, 123.3, 122.5, 119.9, 119.8, 43.8; HRMS (ESI-TOF) m/z: $[M-H]^-$ calculated for C21H15OS 315.0849, found 315.0853.

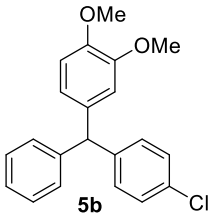
35) 1-chloro-4-((4-methoxyphenyl)(phenyl)methyl)benzene (5a)[3]



5a

The general procedure was followed using **1u** (86.4 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.6, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5a** (99.8 mg, 81%) was obtained as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.18 (m, 5H), 7.08 (d, *J* = 7.4 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 5.46 (s, 1H), 3.77 (s, 3H); 1H NMR spectrum is consistent with literature reports.

36) 4-((4-chlorophenyl)(phenyl)methyl)-1,2-dimethoxybenzene (5b)[5]

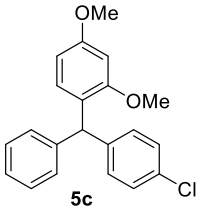


5b

The general procedure was followed using **1v** (110.5 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.5, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5a** (94.7 mg, 70%) was obtained as white solid; m .p. 75.4-77.1 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.20

(m, 5H), 7.09 (d, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.63 (s, 1H), 6.57 (d, *J* = 8.1 Hz, 1H), 5.46 (s, 1H), 3.85 (s, 3H), 3.76 (s, 3H); 1H NMR spectrum is consistent with literature reports.

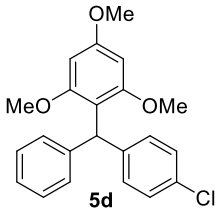
37) 1-((4-chlorophenyl)(phenyl)methyl)-2,4-dimethoxybenzene (5c)



5c

The general procedure was followed using **1w** (110.5 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.5, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5c**(105.5 mg, 78%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 – 7.17 (m, 5H), 7.05 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 6.5 Hz, 2H), 6.69 (d, *J* = 8.5 Hz, 1H), 6.46 (s, 1H), 6.39 (d, *J* = 8.4 Hz, 1H), 5.78 (s, 1H), 3.78 (s, 3H), 3.68 (s, 3H); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 159.6, 157.9, 143.7, 142.8, 131.7, 130.7, 130.6, 129.3, 128.2, 126.1, 124.7, 103.8, 98.7, 55.5, 55.3, 48.6; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{21}H_{19}ClNaO_2$ 361.0966, found 361.0957.

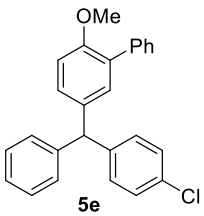
38) 2-((4-chlorophenyl)(phenyl)methyl)-1,3,5-trimethoxybenzene (5d)[6]



5d

The general procedure was followed using **1x** (134.5 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.43, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5d** (119.3 mg, 81%) was obtained as white solid; m. p. 103.2-104.5 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.25–7.20 (m, 2H), 7.19–7.14 (m, 5H), 7.13–7.09 (m, 2H), 6.14 (s, 2H), 6.00 (s, 1H), 3.80 (s, 3H), 3.59 (s, 6H). 1H NMR spectrum is consistent with literature reports.

39) 5-((4-chlorophenyl)(phenyl)methyl)-2-methoxy-1,1'-biphenyl (5e)

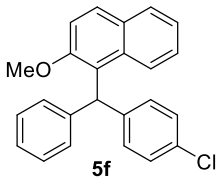


5e

The general procedure was followed using **1y** (136.2 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0

equiv) at room temperature, TLC (R_f = 0.5, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5e** (116.8 mg, 76%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 6.6 Hz, 2H), 7.40 – 7.31 (m, 6H), 7.21 (d, *J* = 7.3 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 3H), 7.08 (d, *J* = 8.5 Hz, 1H), 6.98 (dd, *J* = 8.5, 2.3 Hz, 1H), 5.59 (s, 1H), 3.87 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 155.1, 143.6, 142.7, 138.3, 135.7, 132.1, 131.8, 130.7, 130.6 129.5, 129.3, 129.2, 128.4, 127.9, 126.9, 126.5, 111.1, 55.6, 55.5; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{26}H_{21}ClNaO$ 407.1173, found 407.1160.

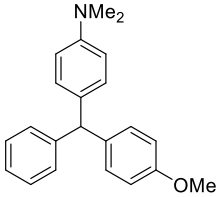
40) 1-((4-chlorophenyl)(phenyl)methyl)-2-methoxynaphthalene (5f)[2]



5f

The general procedure was followed using **1z** (126.6 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2b** (91.3 mg, 0.4 mmol, 1.0 equiv) at room temperature, TLC (R_f = 0.5, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5f** (103.1 mg, 72%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 – 7.85 (m, 1H), 7.81 (d, *J* = 9.0 Hz, 1H), 7.80 – 7.76 (m, 1H), 7.33 – 7.27 (m, 3H), 7.26 – 7.21 (m, 2H), 7.21 – 7.16 (m, 5H), 7.14 (d, *J* = 8.3 Hz, 2H), 6.49 (s, 1H), 3.60 (s, 3H); 1H NMR spectrum is consistent with literature reports.

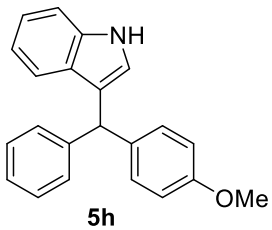
41) 4-((4-methoxyphenyl)(phenyl)methyl)-N,N-dimethylaniline (5g)[7]



5g

The general procedure was followed using **1aa** (96.9 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.6 mg, 0.4 mmol, 1.0 equiv) at 40 °C, TLC (R_f = 0.4, PE/EtOAc = 50:1). After purification by column chromatography (PE/EtOAc = 80:1), **5g** (96.4 mg, 76%) was obtained as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 (d, *J* = 7.5 Hz, 2H), 7.20 – 7.15 (m, 1H), 7.11 (d, *J* = 7.3 Hz, 2H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 6.66 (d, *J* = 8.5 Hz, 2H), 5.41 (s, 1H), 3.77 (s, 3H), 2.91 (s, 6H); 1H NMR spectrum is consistent with literature reports.

42) 3-((4-methoxyphenyl)(phenyl)methyl)-1*H*-indole (5h)[2]

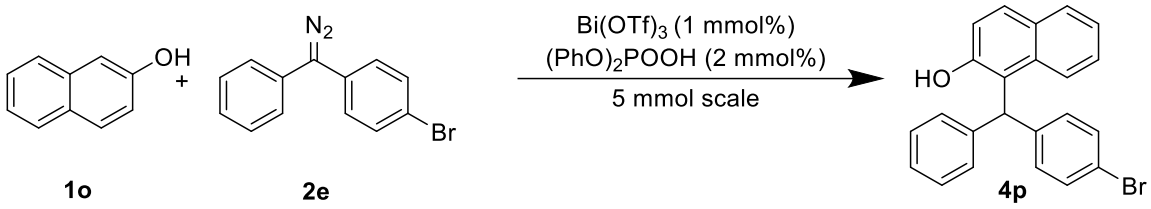


5h

The general procedure was followed using **1ab** (93.6 mg, 0.8 mmol, 2.0 equiv), $Bi(OTf)_3$ (13.1 mg, 0.02 mmol, 5.0 mol%), $(PhO)_2POOH$ (10.0 mg, 0.04 mmol, 10.0 mol%) and **2a** (89.6 mg, 0.4 mmol, 1.0 equiv) at 40 ^oC, TLC (R_f = 0.5, PE/EtOAc = 30:1). After purification by column chromatography (PE/EtOAc = 50:1), **5h** (102.6 mg, 81%) was obtained as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.91 (br, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.11 (m, 9H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.81 (d, *J* = 8.3 Hz, 2H), 6.54 (s, 1H), 5.61 (s, 1H), 3.77 (s, 3H); 1H NMR spectrum is consistent with literature reports.

4. Gram scale reaction and synthetic spplication

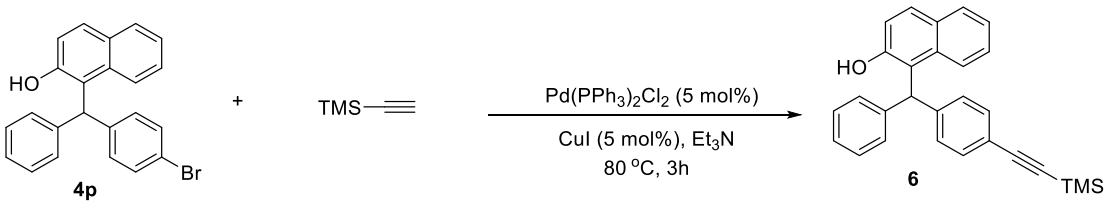
4.1 Gram scale preparation of 6e



1o 2e 4p

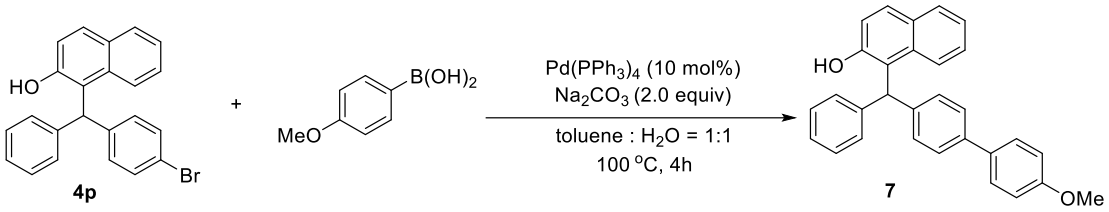
naphthol **1o** (1.4 g, 10.0 mmol, 2.0 equiv), $Bi(OTf)_3$ (32.8 mg, 0.05 mmol, 1.0 mol%) and $(PhO)_2POOH$ (25.0 mg, 0.10 mmol, 2.0 mol%) were introduced into a dried glass tube under Argon protection, and add 5 mL dry hexane and 5 mL dry toluene as solvent, then the diazo **2e** (1.4 g, 5.0 mmol, 1.0 equiv) was dissolved in 10 ml of hexane and add dropwise in 10 min at room temperature. After the addition, continue to react for 5 minute consumed diazo completely determined by TLC analysis. The mixture was purified by column chromatography on silica gel using PE/DCM = 3:1 as the eluent and concentrated to obtain the product **4p** (1.6 g, 85%).

4.2 Synthetic Application

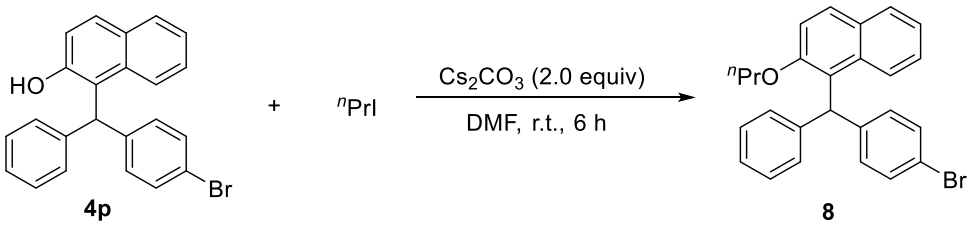


4p (154.4 mg, 0.4 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (14.0 mg, 0.02 mmol, 5 mol%), CuI (3.8 mg, 0.02 mmol, 5 mol%) and trimethylsilylacetylene (78.6 mg, 0.8 mmol, 2.0 equiv) were introduced into a 25 mL dried Schlenk tube under N_2 protection. Then add 2mL dry Et_3N as solvent and react at 80 °C for 3 hours. Consumed completely determined by TLC analysis (R_f = 0.52, PE/EtOAc = 20:1). Concentrate the solvent and then the mixture was purified by column chromatography on silica gel using PE/EtOAc (30:1) as the eluent and concentrated to obtain the product **6** (121.8 mg, 75%) as colorless oil. ^1H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.6 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.39 – 7.34 (m, 3H), 7.34 – 7.31 (m,, 1H), 7.29 – 7.22 (m, 4H), 7.10 (d, *J* = 8.9 Hz, 1H), 6.43 (s, 1H), 5.12 (s, 1H), 0.29 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.6, 142.2, 141.3, 133.3, 132.6, 132.0, 130.8,

129.8, 129.2, 128.9, 128.7, 127.3, 126.9, 123.3, 122.8, 121.9, 119.8, 119.7, 104.7, 94.5, 48.4. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{28}H_{26}NaOSi$ 429.1645, found 429.1647.

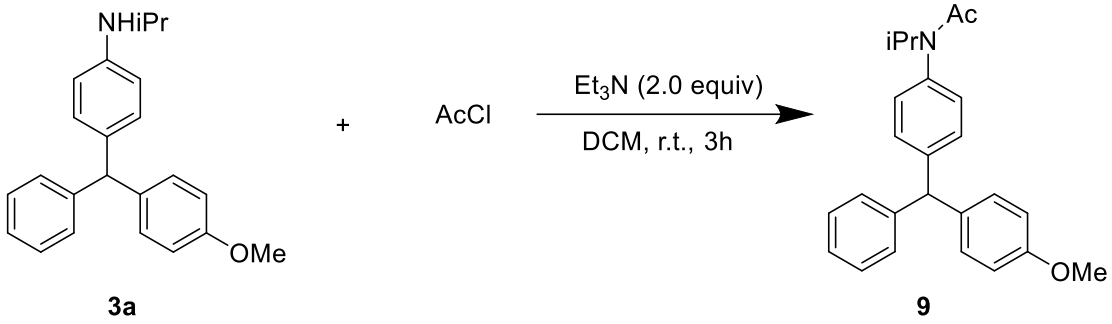


4p (154.4 mg, 0.4 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (46.2 mg, 0.04 mmol, 10 mol%), Na_2CO_3 (84.8 mg, 0.8 mmol, 2.0 equiv) and phenylboronic acid (91.2 mg, 0.6 mmol, 1.5 equiv) were introduced into a 25mL dried Schlenk tube under N_2 protection. Then add 4.0 mL solvent (toluene: H_2O = 1:1) and react at 100°C in oil bath for 4 hours. Consumed completely determined by TLC analysis (R_f = 0.23, PE/EtOAc = 10:1). Concentrate the solvent and then the mixture was purified by column chromatography on silica gel using PE/EtOAc (10:1) as the eluent and concentrated to obtain the product **7** (131.5 mg, 79%) as colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.50 (dd, *J* = 8.2, 5.7 Hz, 4H), 7.44 – 7.39 (m, 1H), 7.36 – 7.30 (m, 3H), 7.29 (d, *J* = 8.1 Hz, 5H), 7.08 (d, *J* = 8.8 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.43 (s, 1H), 5.23 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2, 152.8, 141.6, 139.8, 139.6, 129.7, 129.6, 129.4, 129.2, 129.0, 128.7, 128.0, 127.3, 127.2, 126.9, 123.2, 122.8, 120.1, 119.8, 114.2, 55.3, 48.2. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{30}H_{24}NaO_2$ 439.1669, found 439.1678.



4p (154.4 mg, 0.4 mmol, 1.0 equiv), nPrI (101.9mg, 0.6 mmol, 1.5 equiv) and Cs_2CO_3 (46.2 mg, 0.8 mmol, 2.0 equiv) were introduced into a 50 mL glass bottle under air. Then add 2.0 mL DMF and react at r.t. for 6 hours. Consumed completely determined

by TLC analysis (R_f = 0.4, PE/EtOAc = 20:1). Concentrate the solvent and then the mixture was purified by column chromatography on silica gel using PE/EtOAc (40:1) as the eluent and concentrated to obtain the product **8** (170.3 mg, 99%) as colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 9.4 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.30 – 7.26 (m, 3H), 7.25 – 7.14 (m, 5H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.49 (s, 1H), 3.83 (t, *J* = 6.6 Hz, 2H), 1.50 (h, *J* = 7.0 Hz, 2H), 0.86 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.72, 142.90, 142.79, 133.19, 131.00, 130.89, 129.65, 129.33, 129.00, 128.67, 128.11, 126.22, 125.95, 124.41, 124.29, 123.13, 114.99, 70.82, 47.20, 22.59, 10.55. HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{26}H_{23}BrNaO$ 453.0824, found 453.0838.



3a (132.8mg, 0.4 mmol, 1.0 equiv), AcCl (62.8mg, 0.8 mmol, 2.0 equiv) and Et_3N (80.9 mg, 0.8 mmol, 2.0 equiv) were introduced into a 50 mL glass bottle under air. Then add 2.0 mL DCM and react at r.t. for 3 hours. Consumed completely determined by TLC analysis (R_f = 0.5, PE/EtOAc = 20:1). Concentrate the solvent and then the mixture was purified by column chromatography on silica gel using PE/EtOAc (20:1) as the eluent and concentrated to obtain the product **9** (150.5 mg, 95%) as colorless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.16 – 7.09 (m, 4H), 7.01 (dd, *J* = 11.1, 8.5 Hz, 4H), 6.85 (d, *J* = 8.7 Hz, 2H), 5.53 (s, 1H), 4.99 (hept, *J* = 6.8 Hz, 1H), 3.79 (s, 3H), 1.75 (s, 4H), 1.04 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.04, 158.17, 144.34, 143.72, 137.30, 135.53, 130.25, 130.05, 129.90, 129.24, 128.40, 126.45, 113.79, 55.55, 55.20, 45.73, 23.54, 20.99; HRMS (ESI-TOF) m/z: $[M+Na]^+$ calculated for $C_{25}H_{27}NNaO_2$ 396.1939, found 396.1942.

5. References

[1] Ash, J.; Ahmed, E.; Le, N.; Huang, H.; Kang, J. Y., Catalytic, regioselective Friedel–Crafts alkylation of beta-naphthol. *New J. Chem.* **2024,** *48*, 4224-4228.

[2] Yang, G.-P.; Dilixiati, D.; Yang, T.; Liu, D.; Yu, B.; Hu, C.-W., Phosphomolybdic acid as a bifunctional catalyst for Friedel–Crafts type dehydrative coupling reaction. *Appl. Organomet. Chem.* **2018,** *32*, e4450.

[3] Lee, M.; Davies, H. M. L., Enantioselective Synthesis of Triarylmethanes via Intermolecular C–H Functionalization of Cyclohexadienes with Diaryldiazomethanes. *Org. Lett.* **2023,** *25*, 4000-4004.

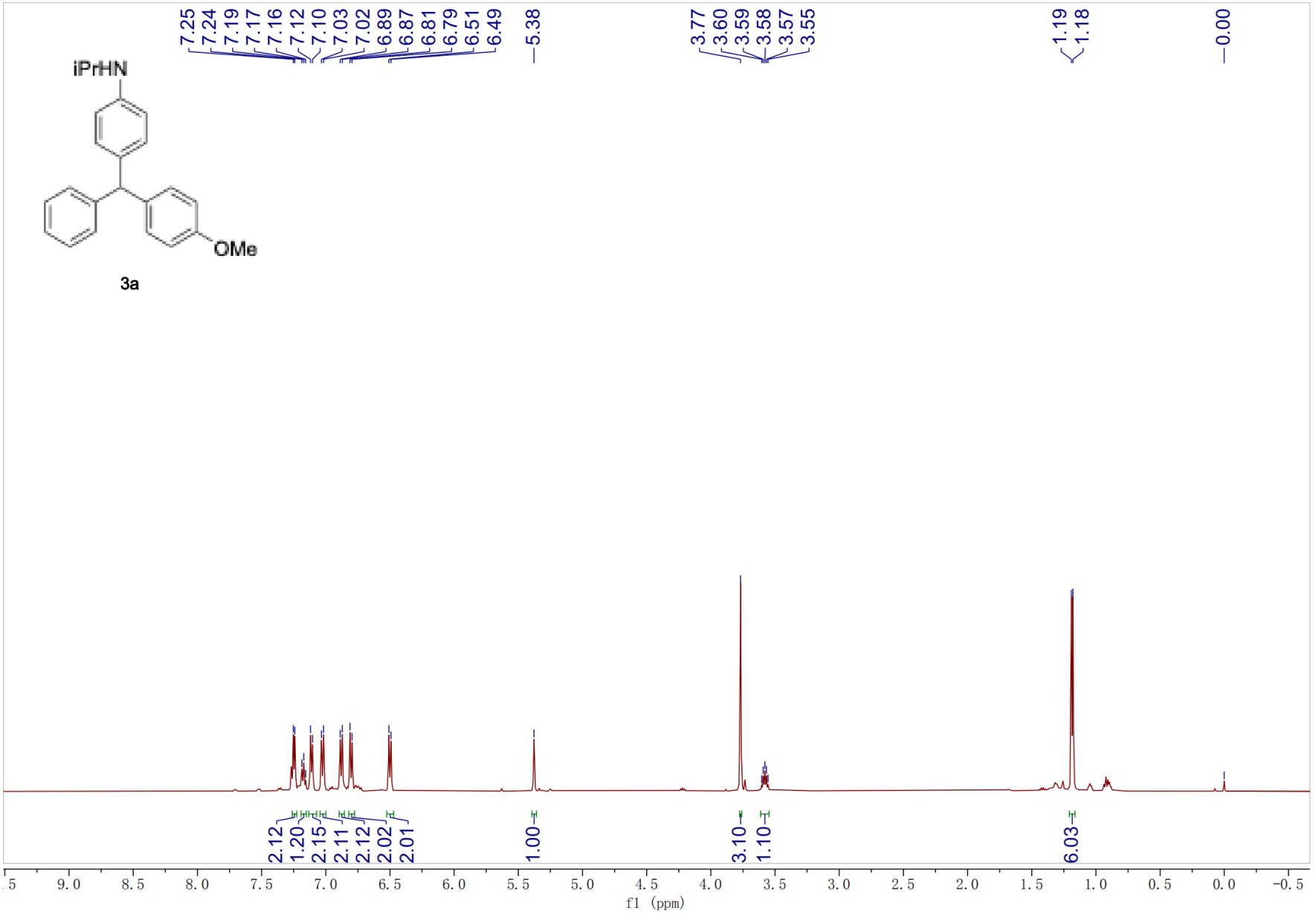
[4] Sankar, R.; Bhattacharya, D.; Arulananda Babu, S., Synthesis of 1-Naphthol-based Unsymmetrical Triarylmethanes: Heck-type Desulfitative Reaction of Arylsulfonyl Chlorides with Tetralone-derived Chalcones. *Asian J. Org. Chem.* **2021,** *10*, 576-581.

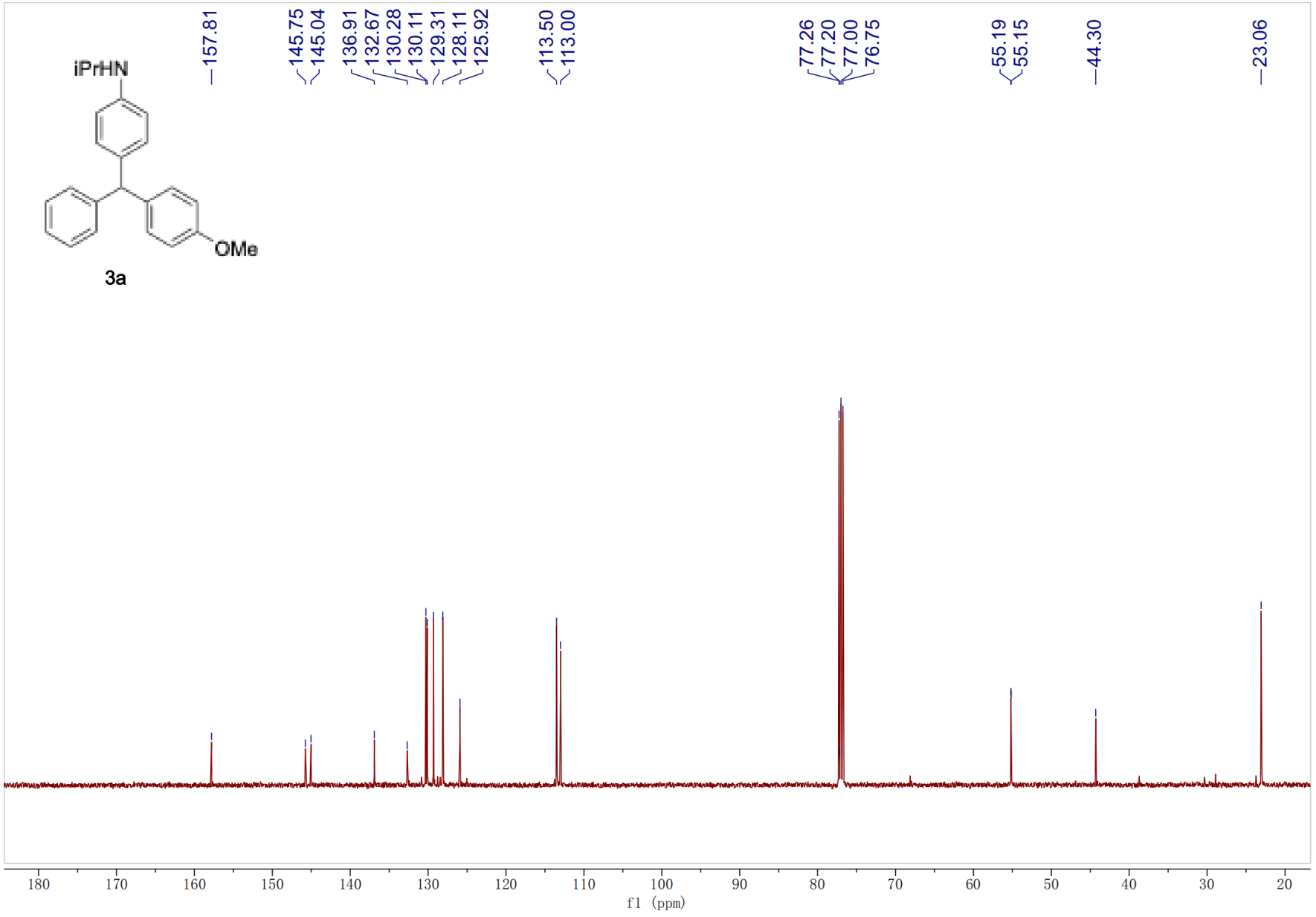
[5] Sato, Y.; Aoyama, T.; Takido, T.; Kodomari, M., Direct alkylation of aromatics using alcohols in the presence of NaHSO4/SiO2. *Tetrahedron* **2012,** *68*, 7077-7081.

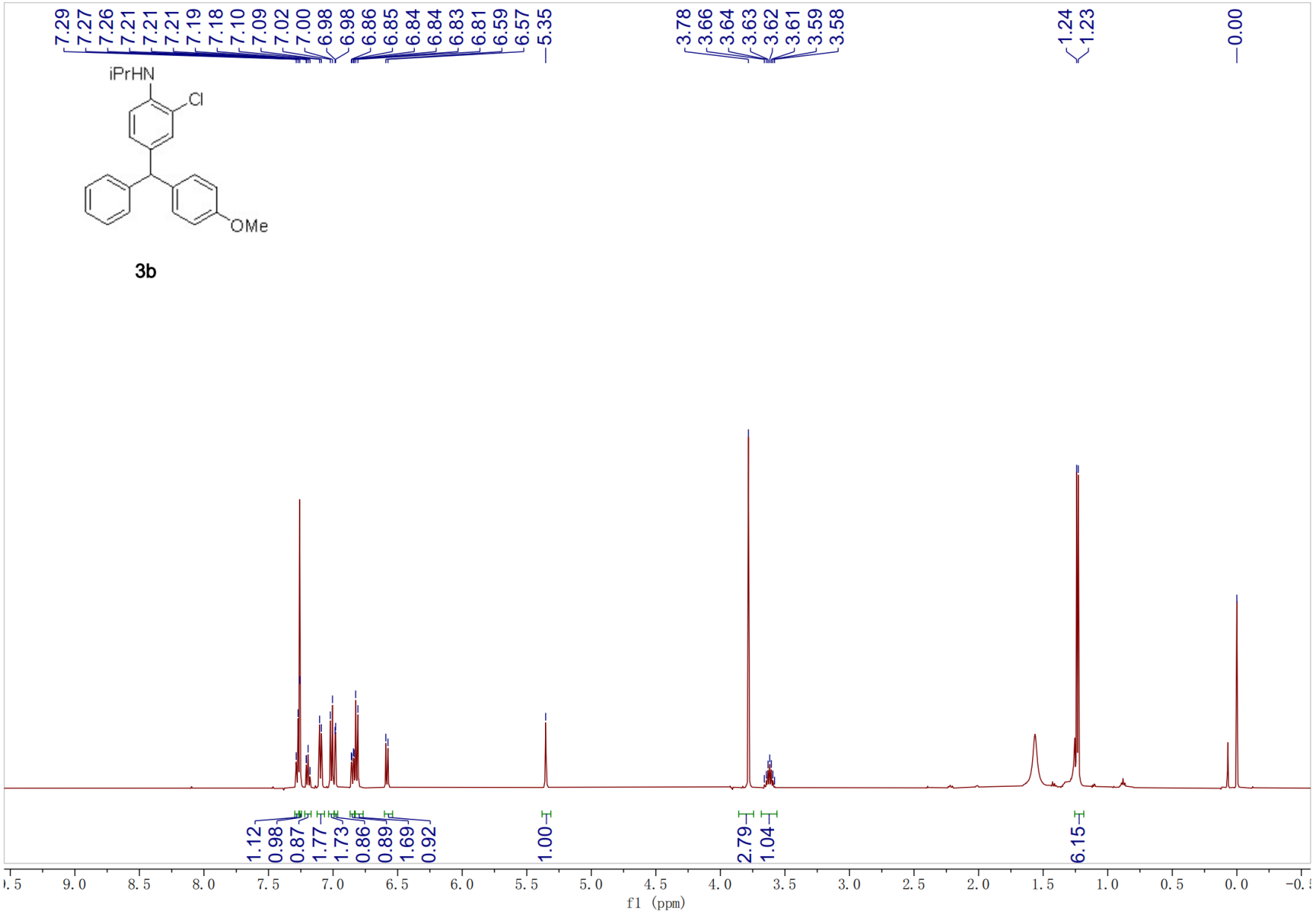
[6] Courant, T.; Lombard, M.; Boyarskaya, D. V.; Neuville, L.; Masson, G., Tritylium assisted iodine catalysis for the synthesis of unsymmetrical triarylmethanes. *Org. Biomol. Chem.* **2020**, *18*, 6502-6508.

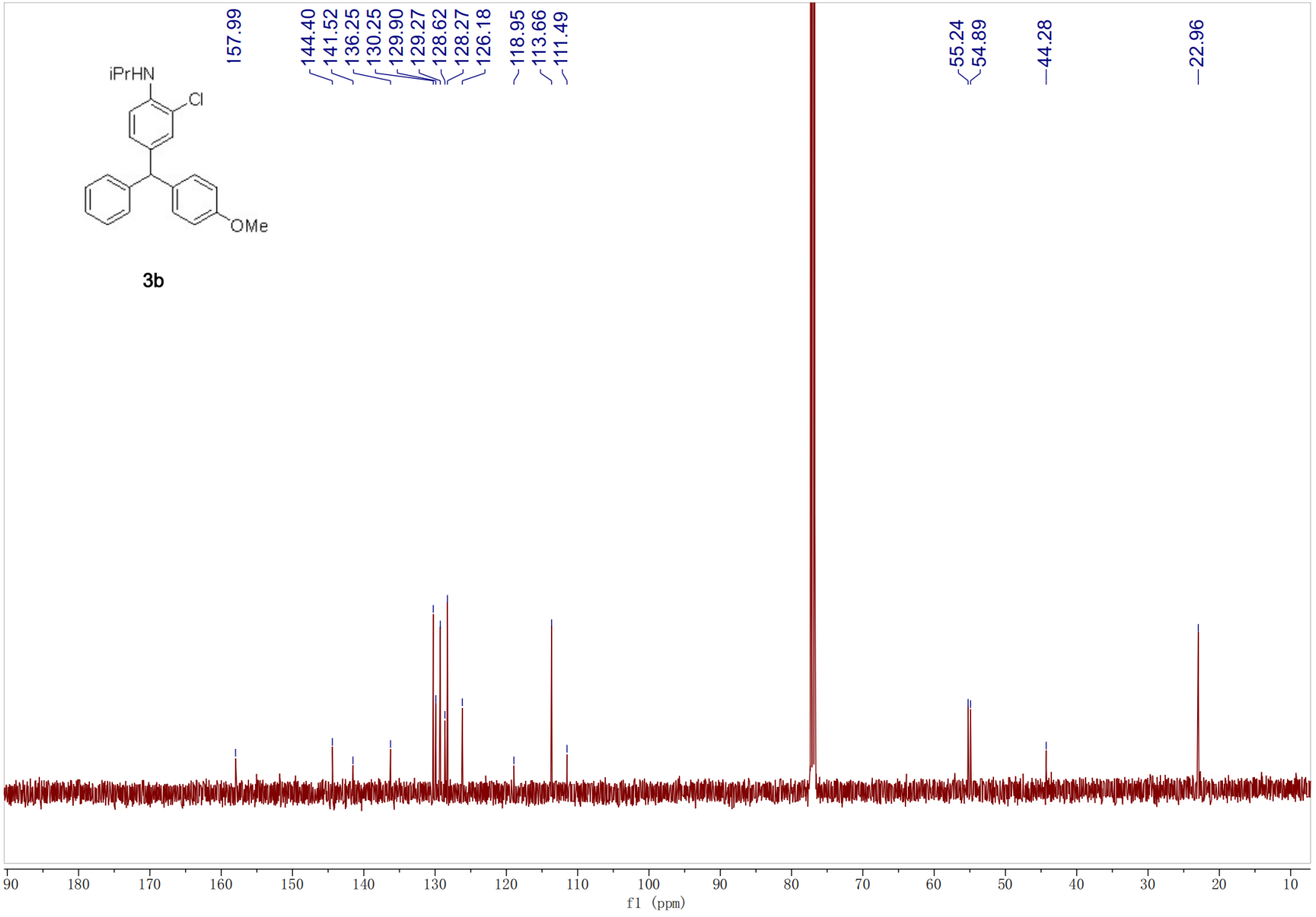
[7] Chen, X.; Tan, Y.; Berionni, G.; Ofial, A. R.; Mayr, H., Di- and Triarylmethylium Ions as Probes for the Ambident Reactivities of Carbanions Derived from 5-Benzylated Meldrum's Acid. *Chem. Eur. J.* **2014,** *20*, 11069-11077.

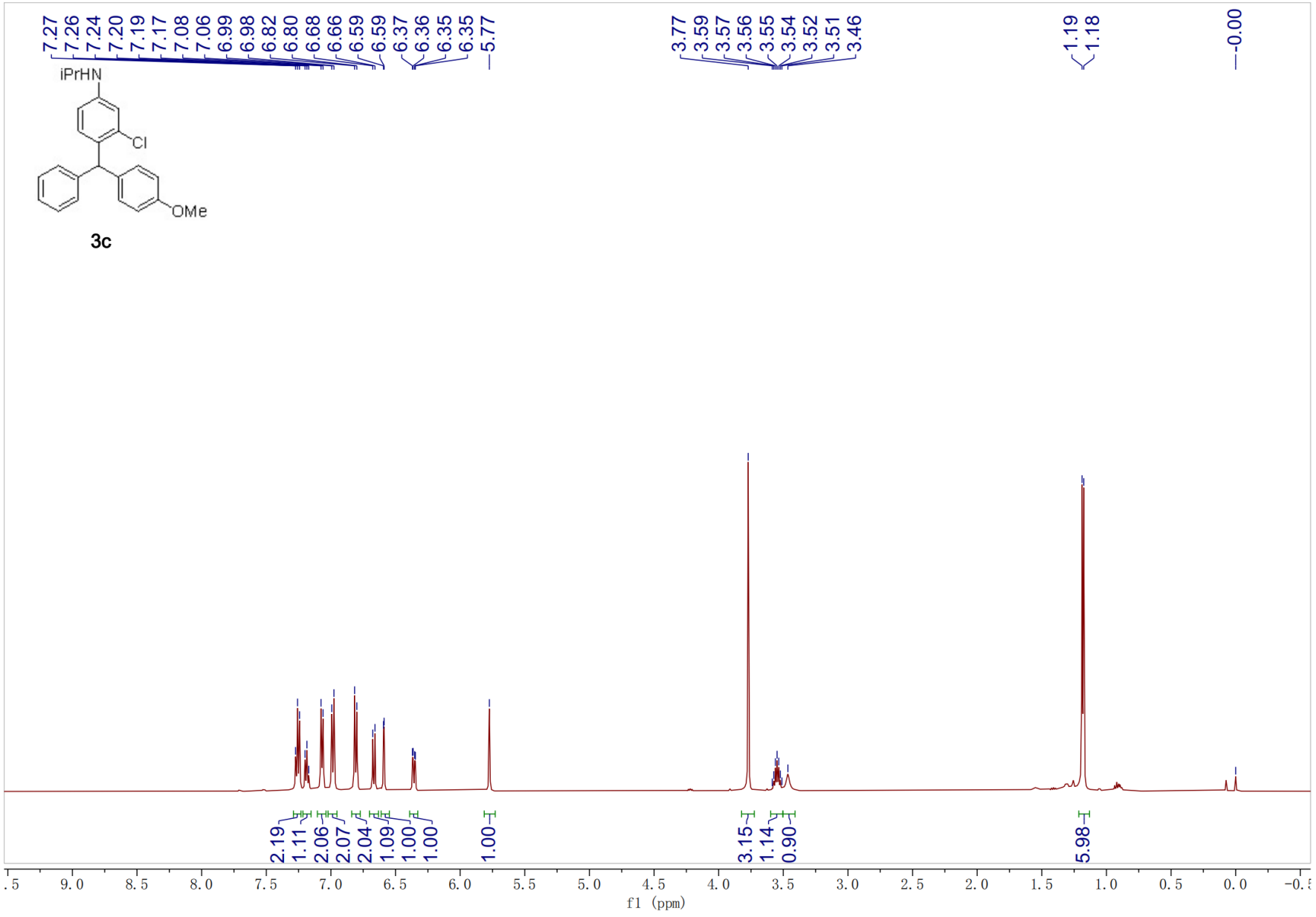
6. NMR and HRMS spectra of new compounds

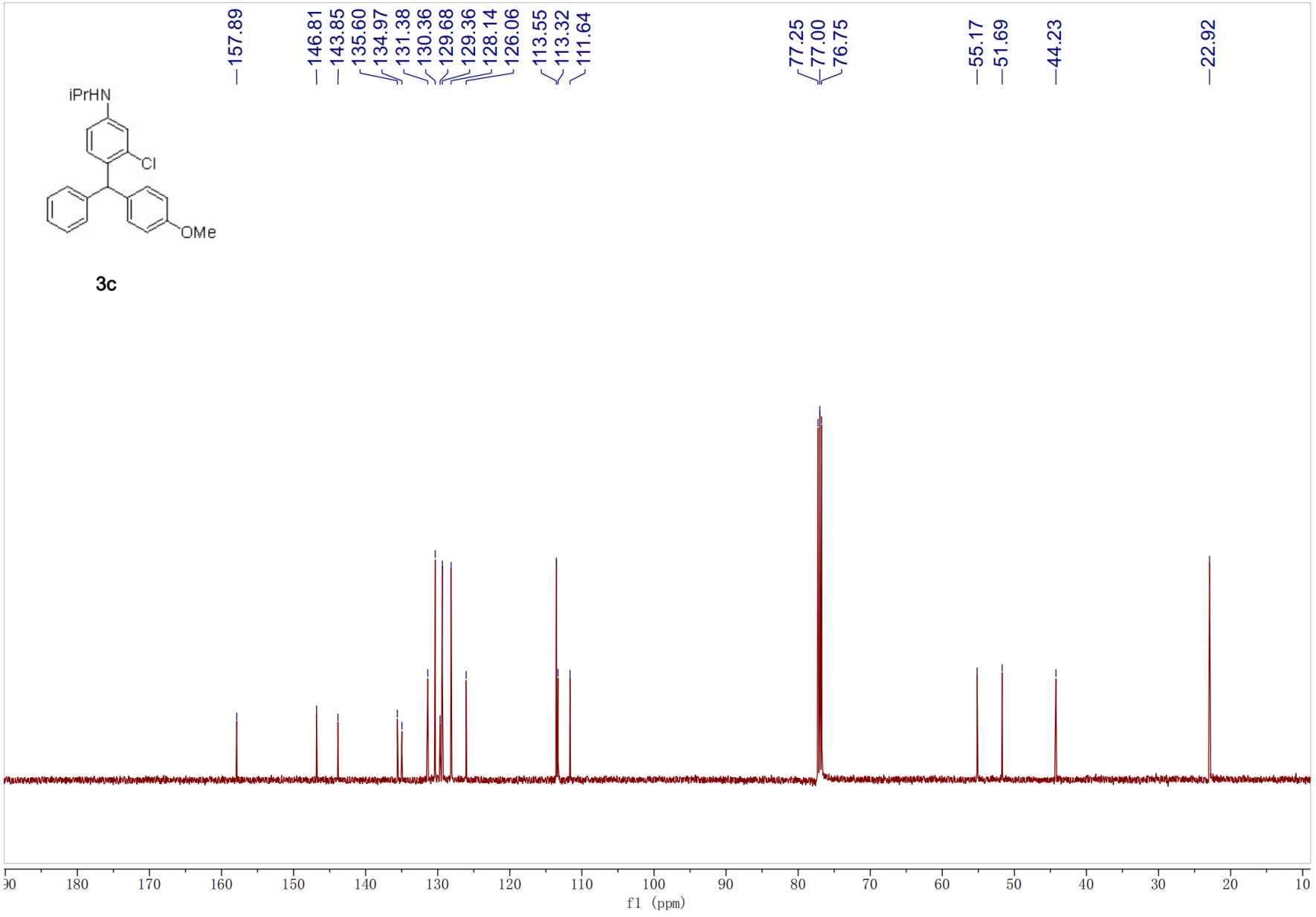

7.25
7.24
7.19
7.17
7.16
7.12
7.10
7.03
7.02
6.89
6.87
6.81
6.79
6.51
6.49
5.38
3.77
3.60
3.59
3.58
3.57
3.55
1.19
1.18
0.00
iPrHN
OMe
3a
2.12
1.20
2.15
2.11
2.12
2.02
2.01
1.00
3.10
1.10
6.03
f1 (ppm)

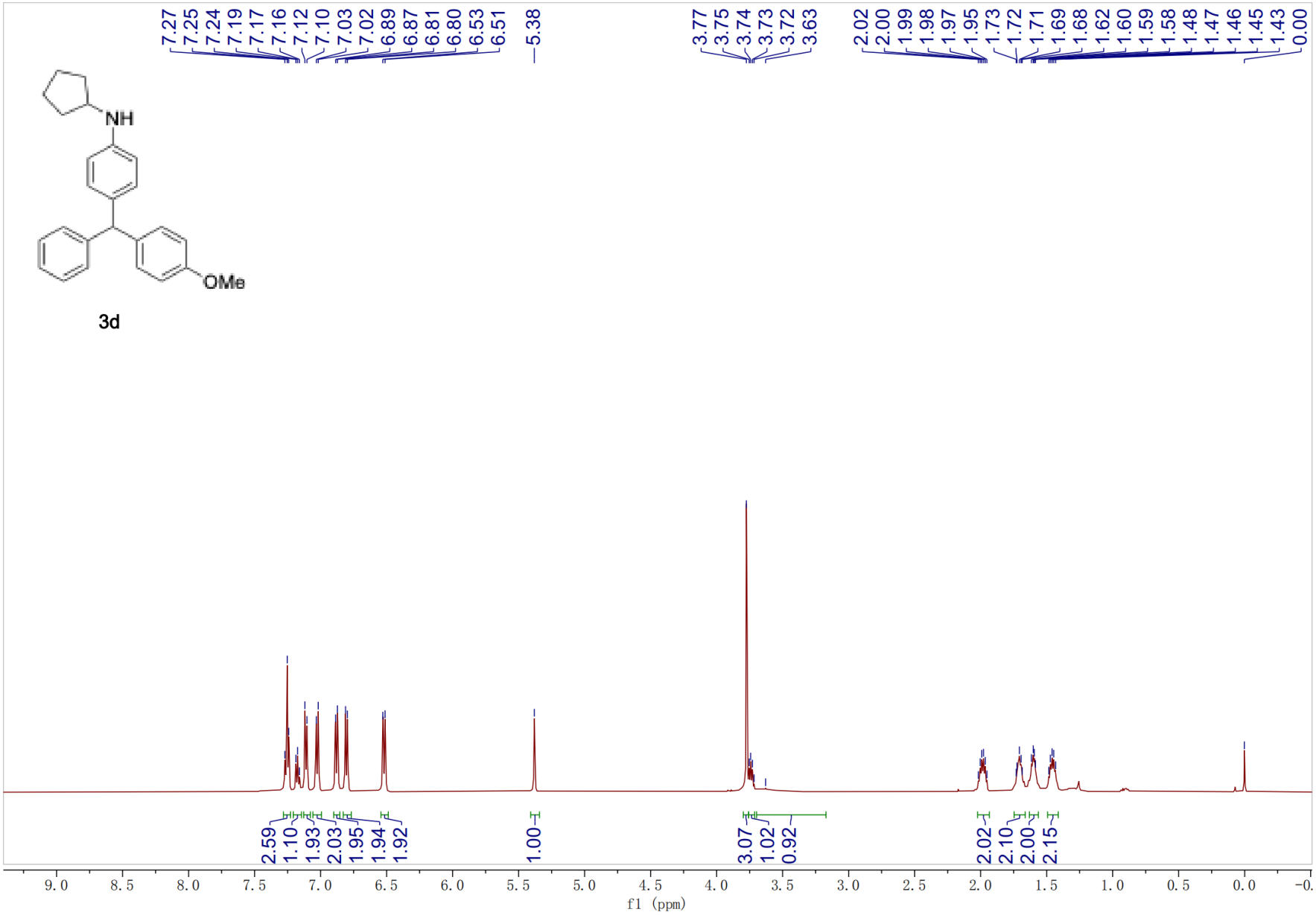

iPrHN
OMe
3a
157.81
145.75
145.04
136.91
132.67
130.28
130.11
129.31
128.11
125.92
113.50
113.00
77.26
77.20
77.00
76.75
55.19
55.15
44.30
23.06
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

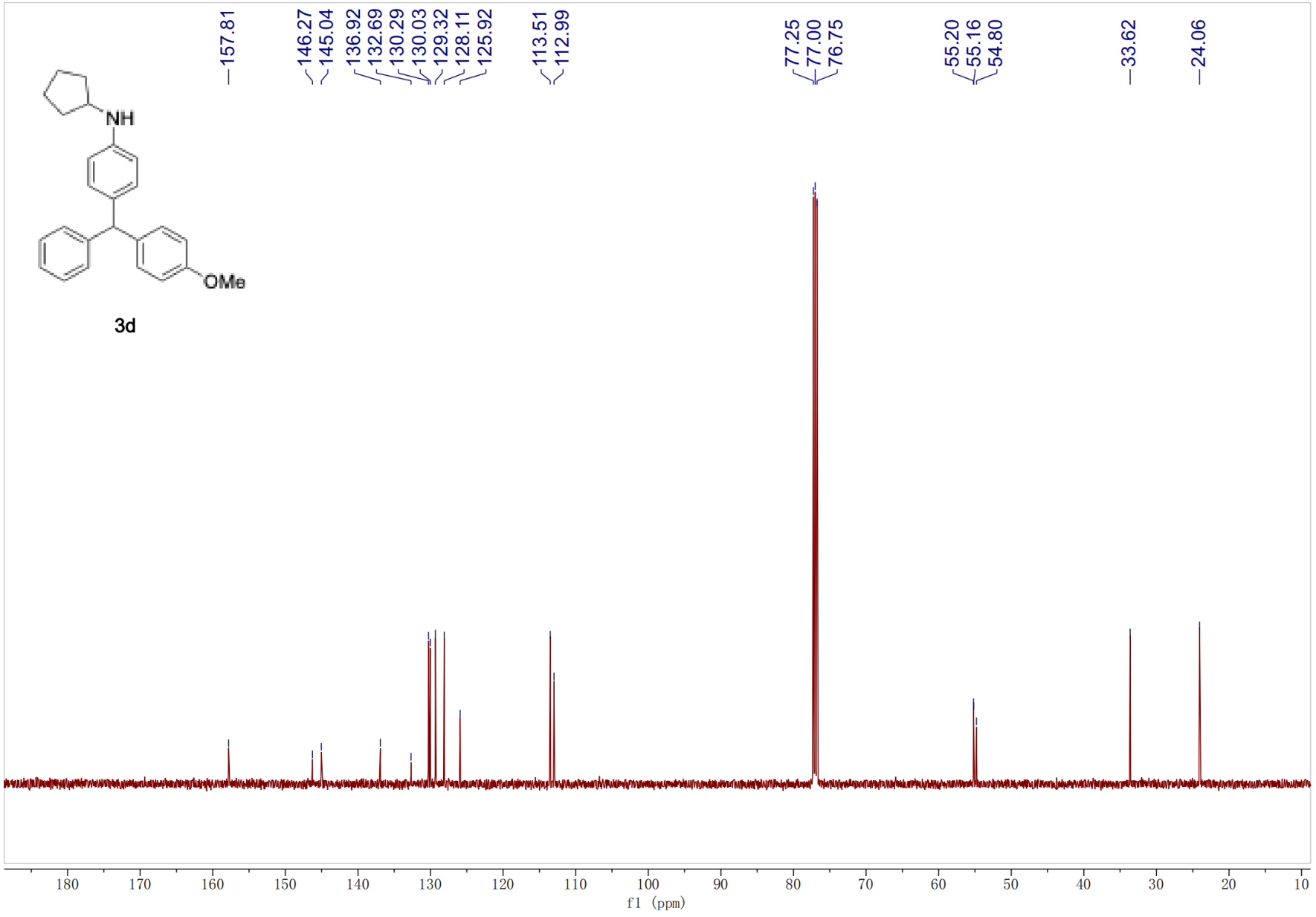

7.29
7.27
7.26
7.21
7.21
7.21
7.19
7.18
7.10
7.09
7.02
7.00
6.98
6.98
6.86
6.85
6.84
6.84
6.83
6.81
6.59
6.57
5.35
3.78
3.66
3.64
3.63
3.62
3.61
3.59
3.58
1.24
1.23
0.00
iPrHN
Cl
OMe
3b
1.12
0.98
0.87
1.77
1.73
0.86
0.89
1.69
0.92
1.00
2.79
1.04
6.15
f1 (ppm)

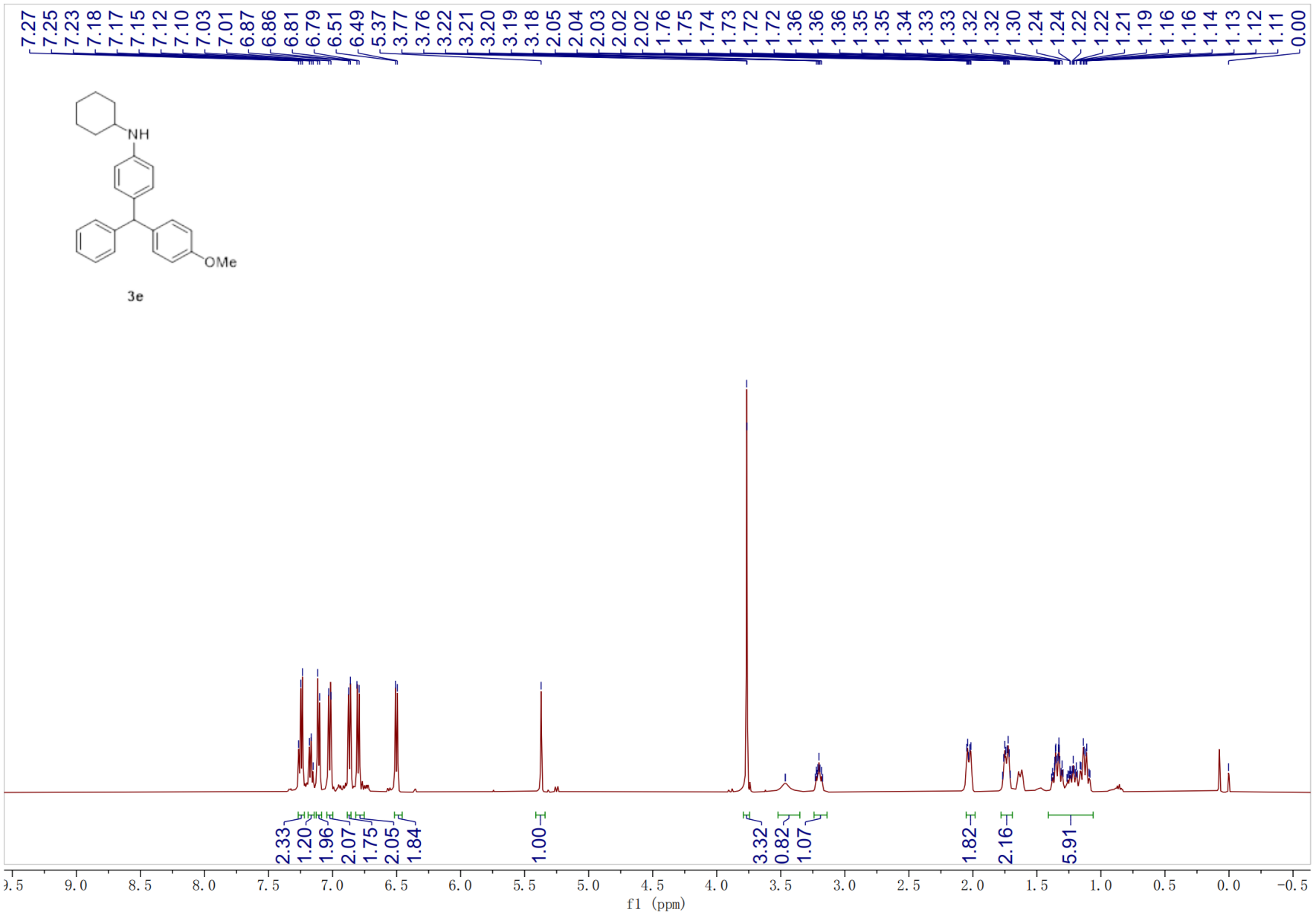

157.99
144.40
141.52
136.25
130.25
129.90
129.27
128.62
128.27
126.18
118.95
113.66
111.49
55.24
54.89
44.28
22.96
iPrHN
Cl
OMe
3b
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

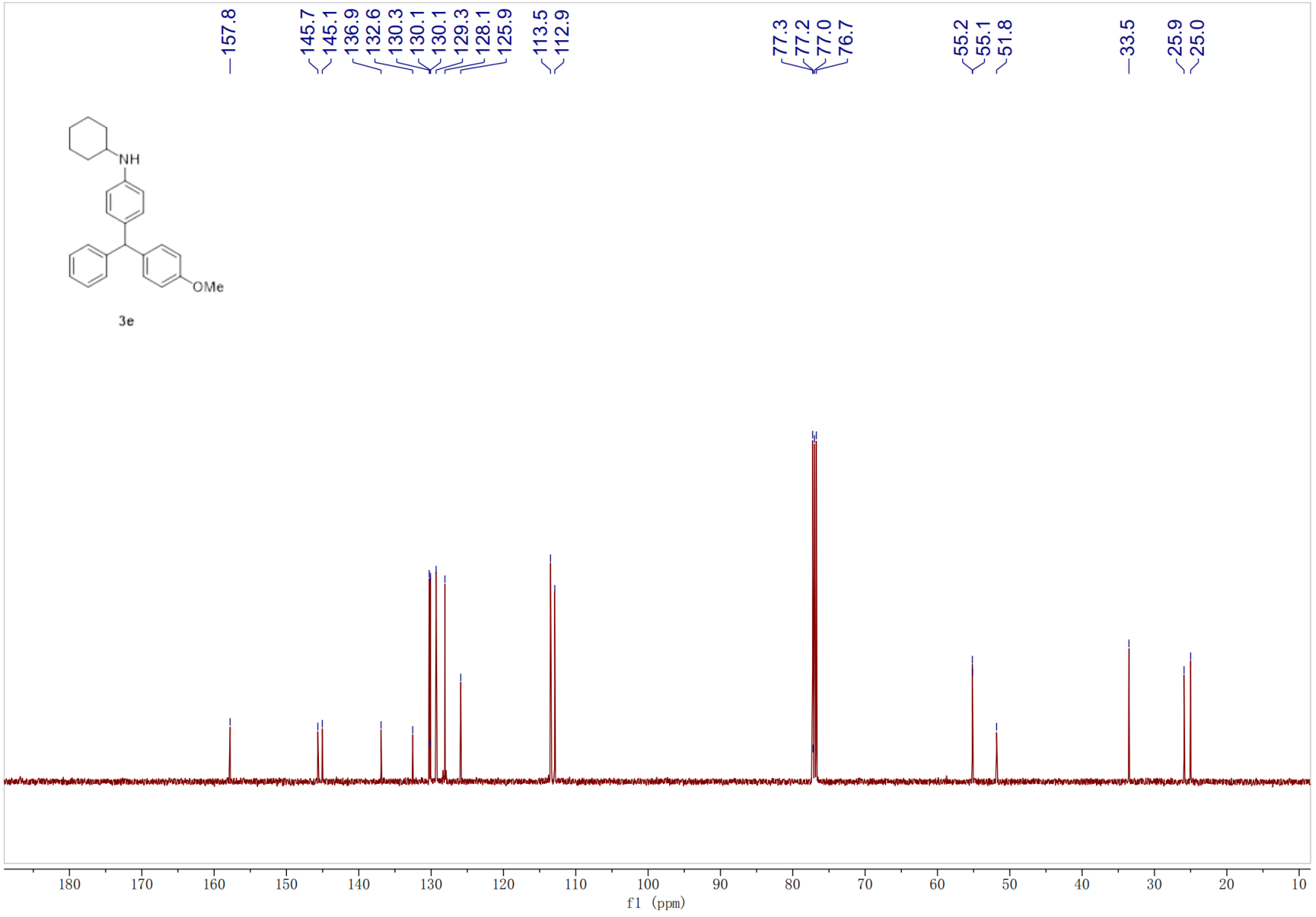

7.27
7.26
7.24
7.20
7.19
7.17
7.08
7.06
6.99
6.98
6.82
6.80
6.68
6.66
6.59
6.59
6.37
6.36
6.35
6.35
5.77
3.77
3.59
3.57
3.56
3.55
3.54
3.52
3.51
3.46
1.19
1.18
0.00
iPrHN
Cl
OMe
3c
2.19
1.11
2.06
2.07
2.04
1.09
1.00
1.00
1.00
3.15
1.14
0.90
5.98
f1 (ppm)

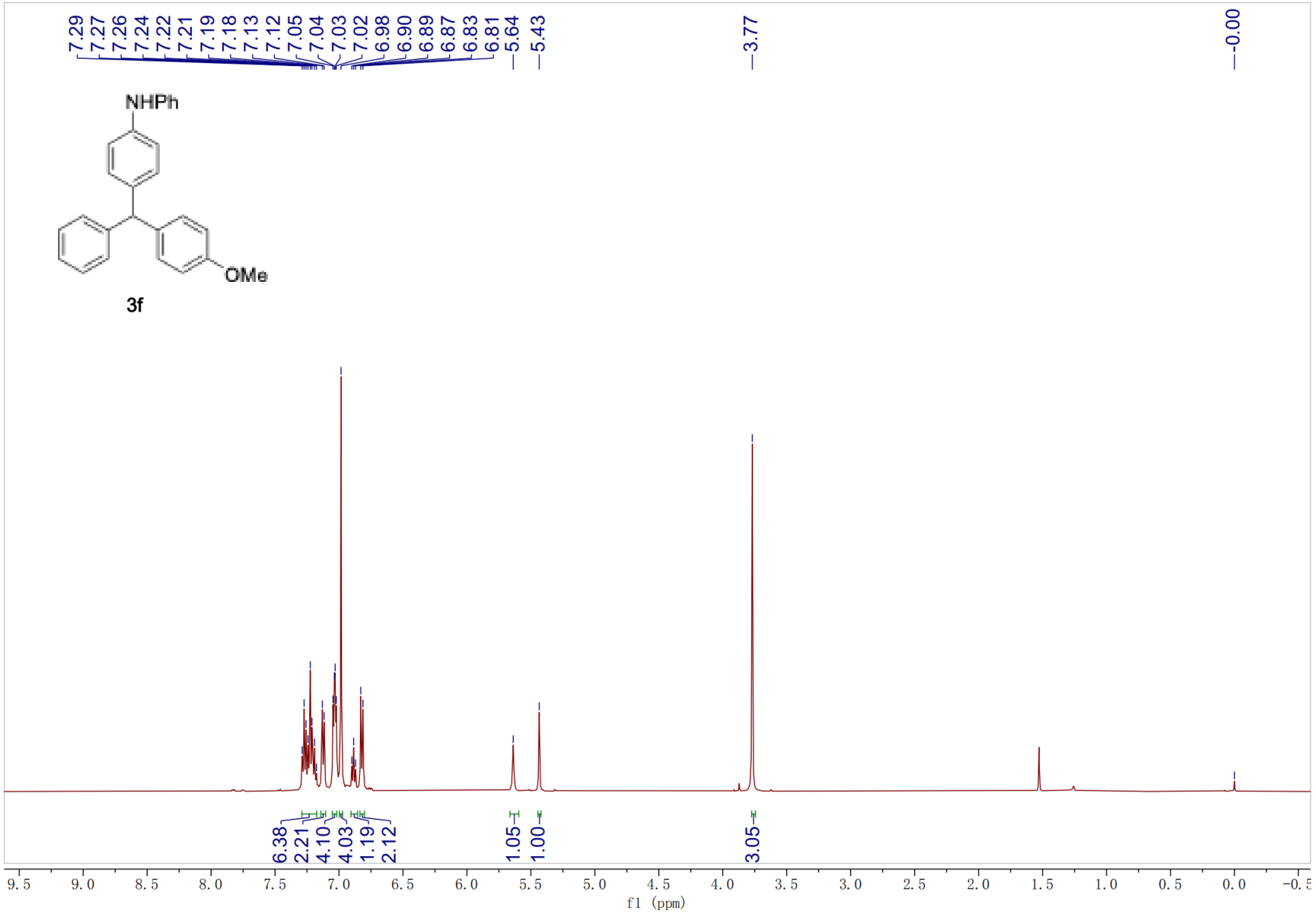

157.89
146.81
143.85
135.60
134.97
131.38
130.36
129.68
129.36
128.14
126.06
113.55
113.32
111.64
77.25
77.00
76.75
55.17
51.69
44.23
22.92
iPrHN
Cl
OMe
3c
f1 (ppm)

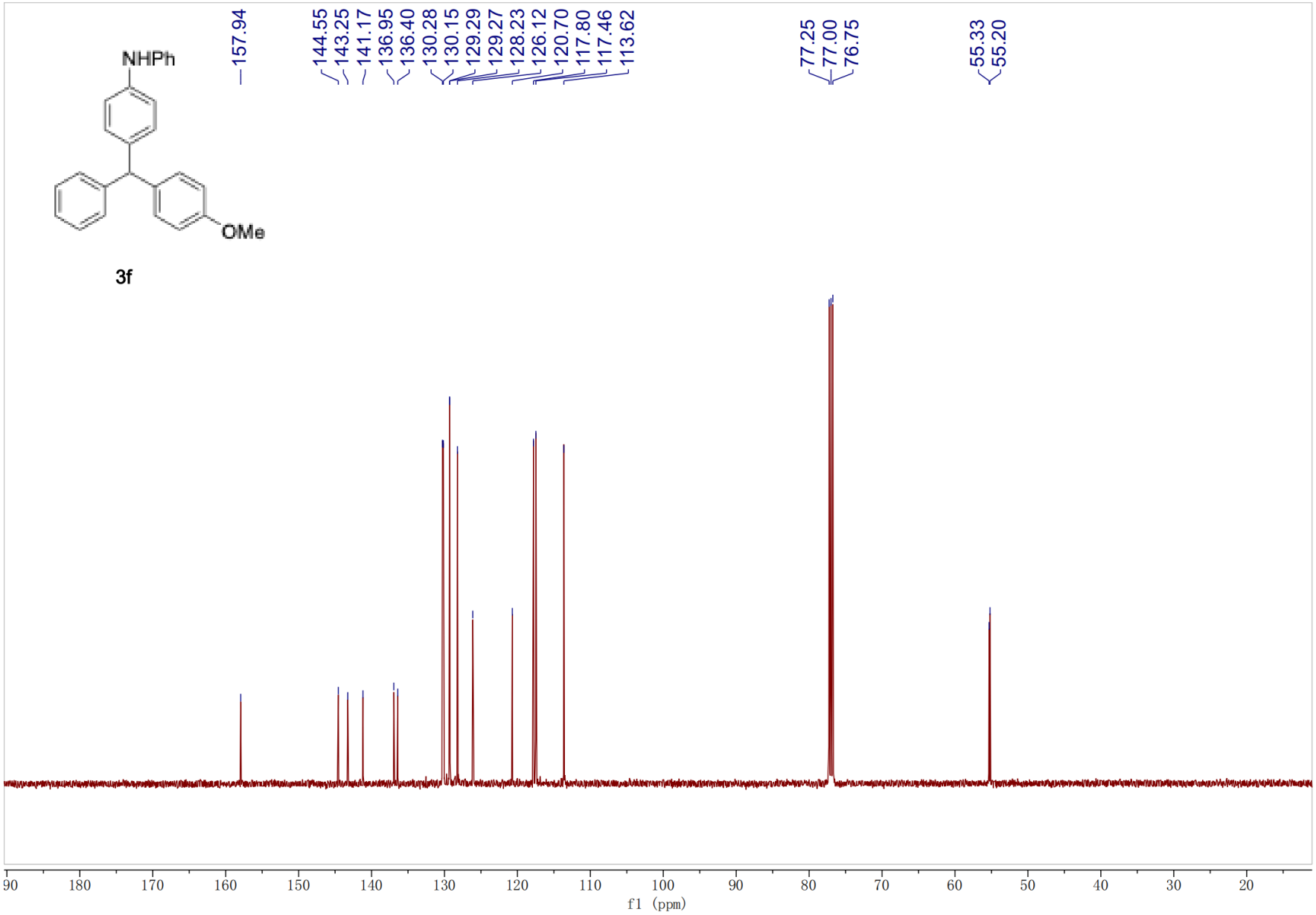

7.27
7.25
7.24
7.19
7.17
7.16
7.12
7.10
7.03
7.02
6.89
6.87
6.81
6.80
6.53
6.51
5.38
3.77
3.75
3.74
3.73
3.72
3.63
2.02
2.00
1.99
1.98
1.97
1.95
1.73
1.72
1.71
1.69
1.68
1.62
1.60
1.59
1.58
1.48
1.47
1.46
1.45
1.43
0.00
NH
OMe
3d
2.59
1.10
1.93
2.03
1.95
1.94
1.92
1.00
3.07
1.02
0.92
2.02
2.10
2.00
2.15
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

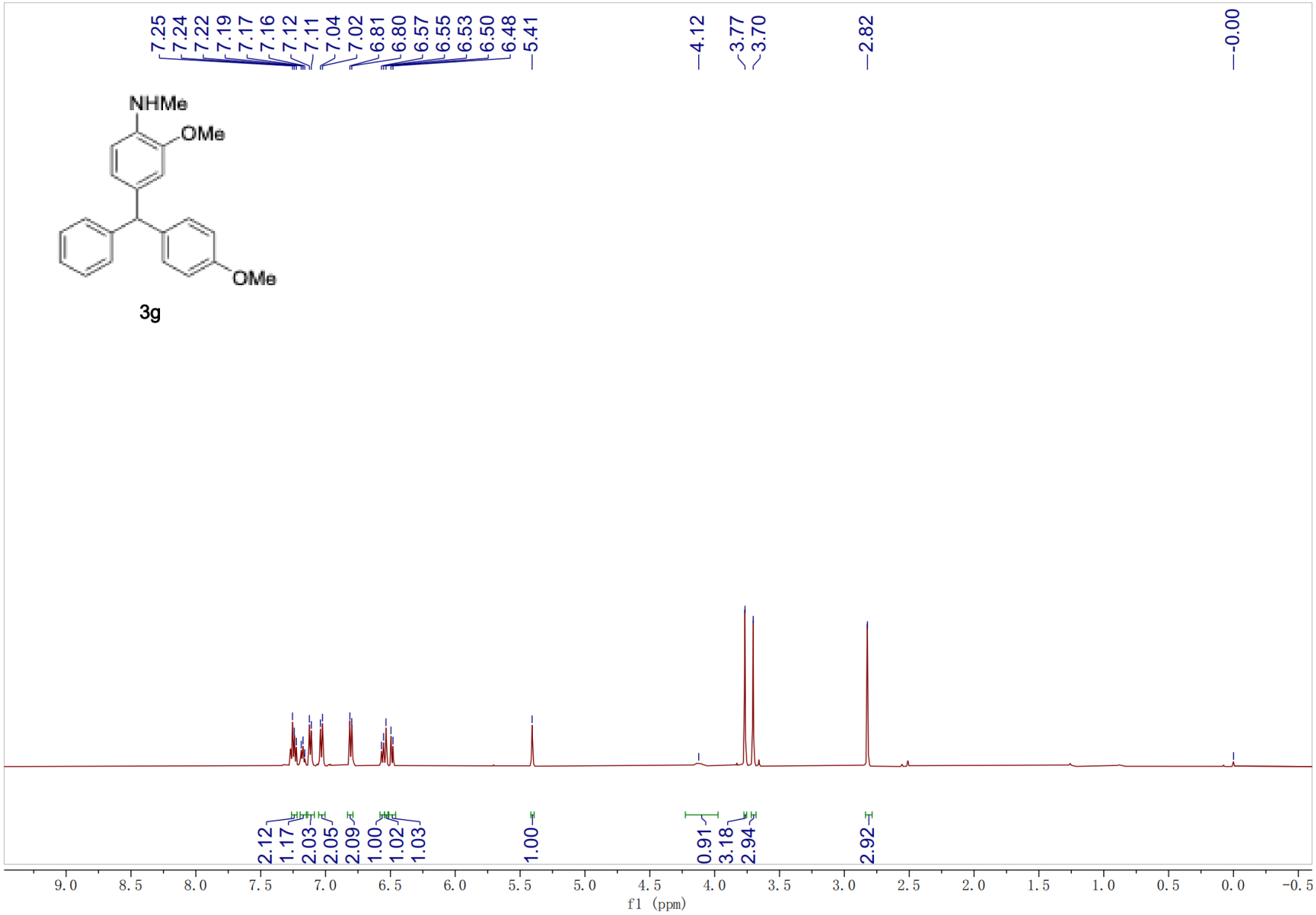

157.81
146.27
145.04
136.92
132.69
130.29
130.03
129.32
128.11
125.92
113.51
112.99
77.25
77.00
76.75
55.20
55.16
54.80
33.62
24.06
NH
OMe
3d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

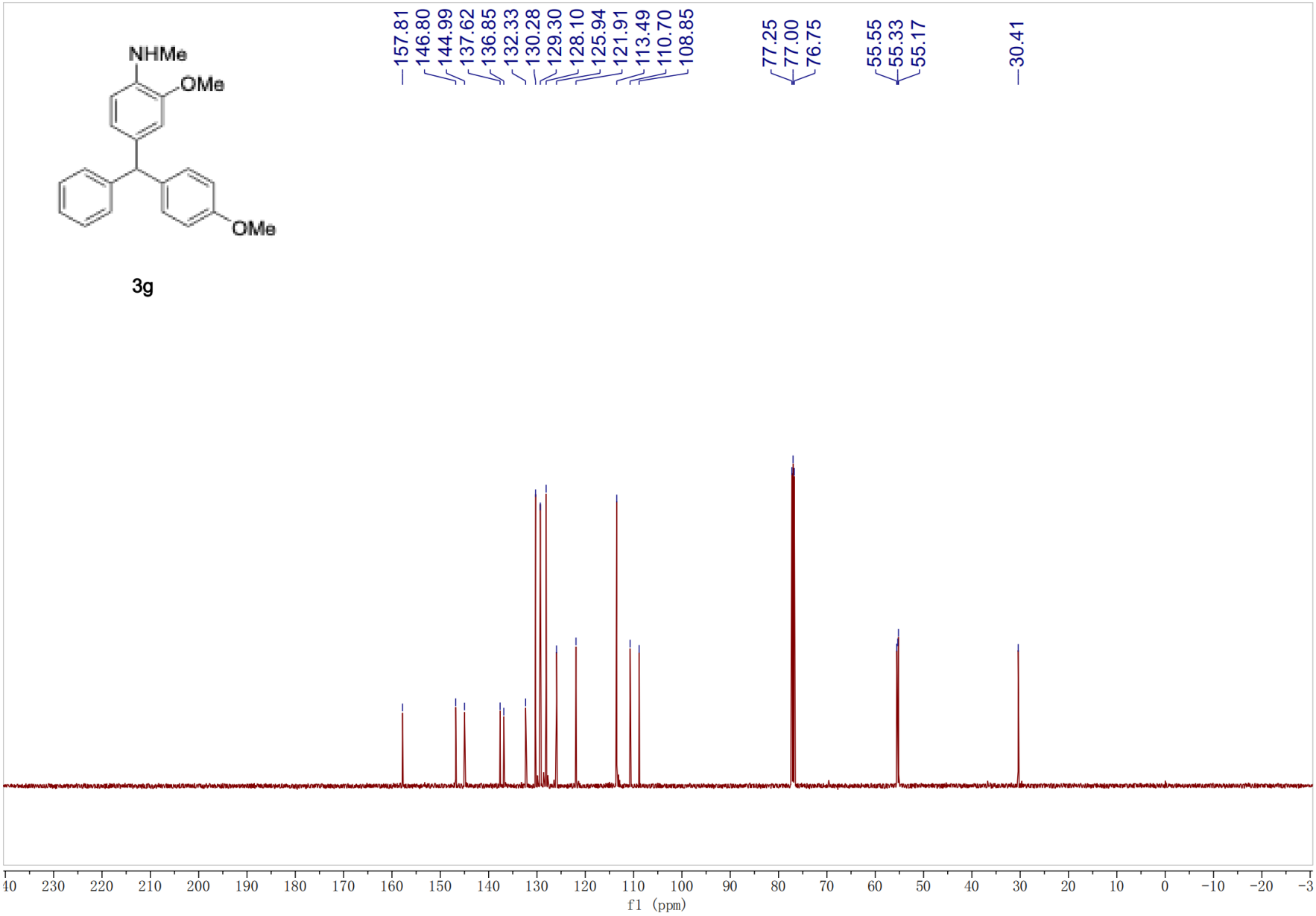

7.27 7.25 7.23 7.18 7.17 7.15 7.12 7.10 7.03 7.01 6.87 6.86 6.81 6.79 6.51 6.49 5.37 3.77 3.76 3.22 3.21 3.20 3.19 3.18 2.05 2.04 2.03 2.02 2.02 1.76 1.75 1.74 1.73 1.72 1.72 1.36 1.36 1.36 1.35 1.35 1.34 1.33 1.33 1.32 1.32 1.30 1.24 1.24 1.22 1.22 1.21 1.19 1.16 1.16 1.14 1.13 1.12 1.11 0.00
NH
OMe
3e
2.33 1.20 1.96 2.07 1.75 2.05 1.84 1.00 3.32 0.82 1.07 1.82 2.16 5.91
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

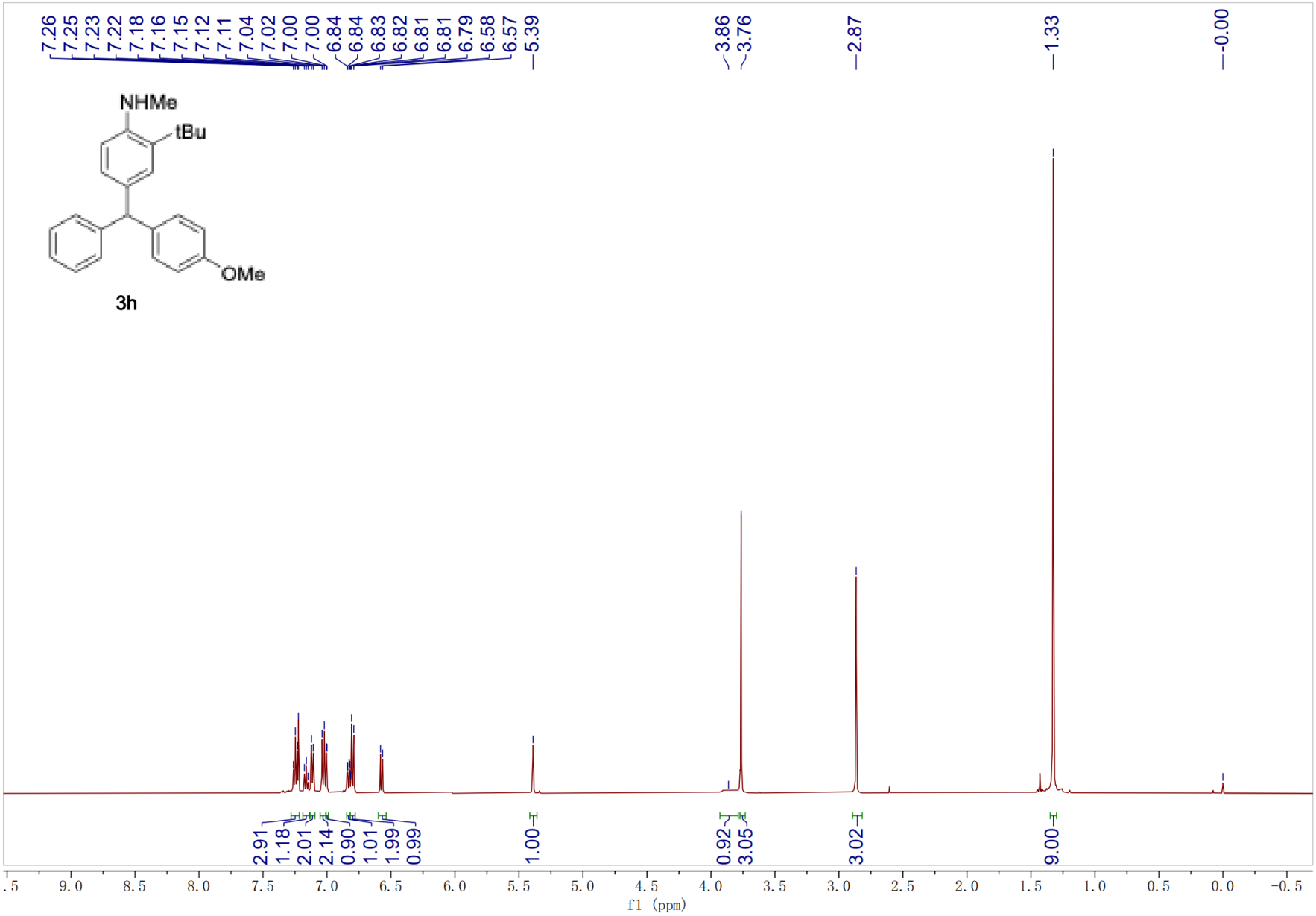

157.8
145.7
145.1
136.9
132.6
130.3
130.1
130.1
129.3
128.1
125.9
113.5
112.9
77.3
77.2
77.0
76.7
55.2
55.1
51.8
33.5
25.9
25.0
NH
OMe
3e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

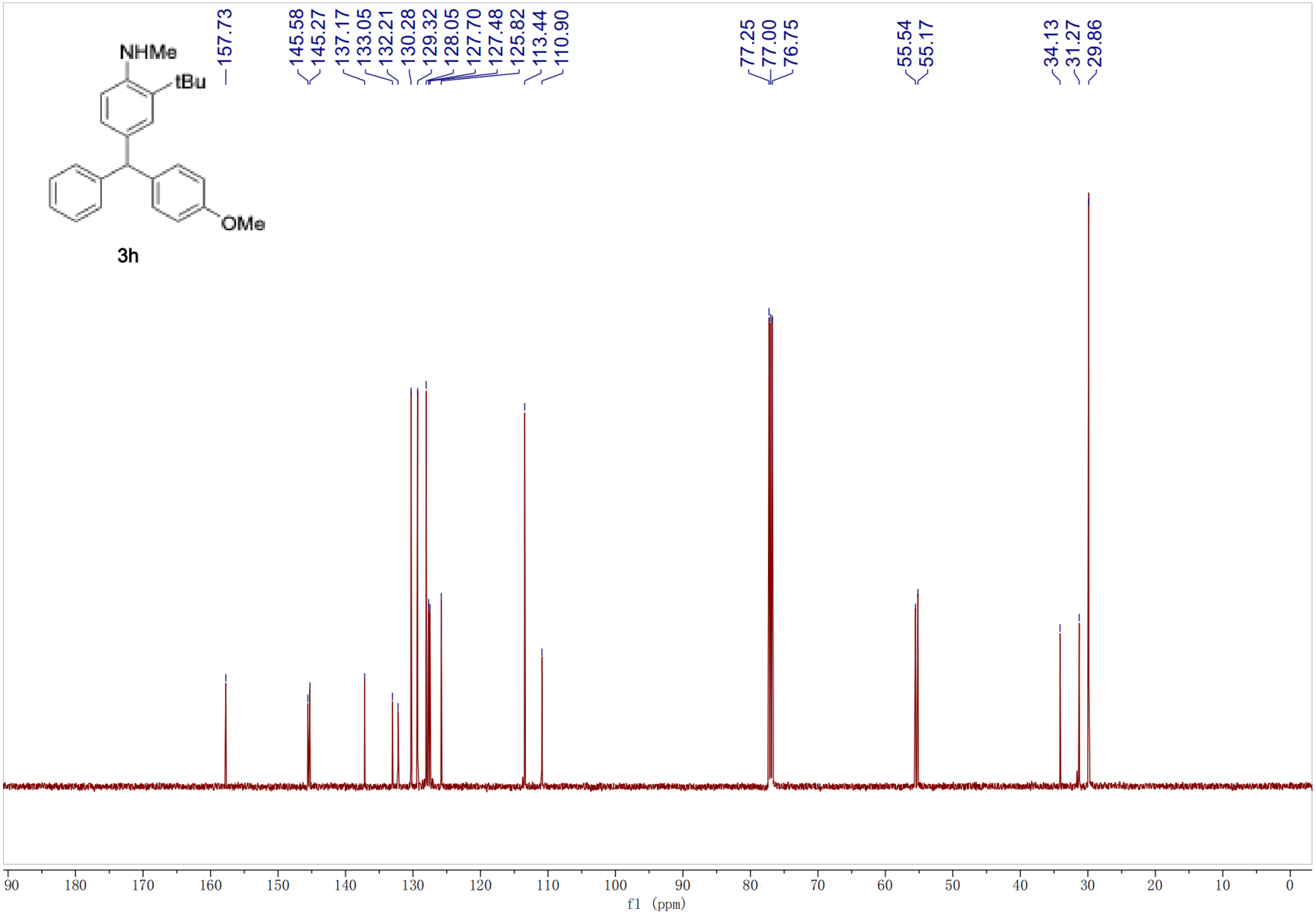

7.29
7.27
7.26
7.24
7.22
7.21
7.19
7.18
7.13
7.12
7.05
7.04
7.03
7.02
6.98
6.90
6.89
6.87
6.83
6.81
5.64
5.43
3.77
0.00
NHPh
OMe
3f
6.38
2.21
4.10
4.03
1.19
2.12
1.05
1.00
3.05
f1 (ppm)

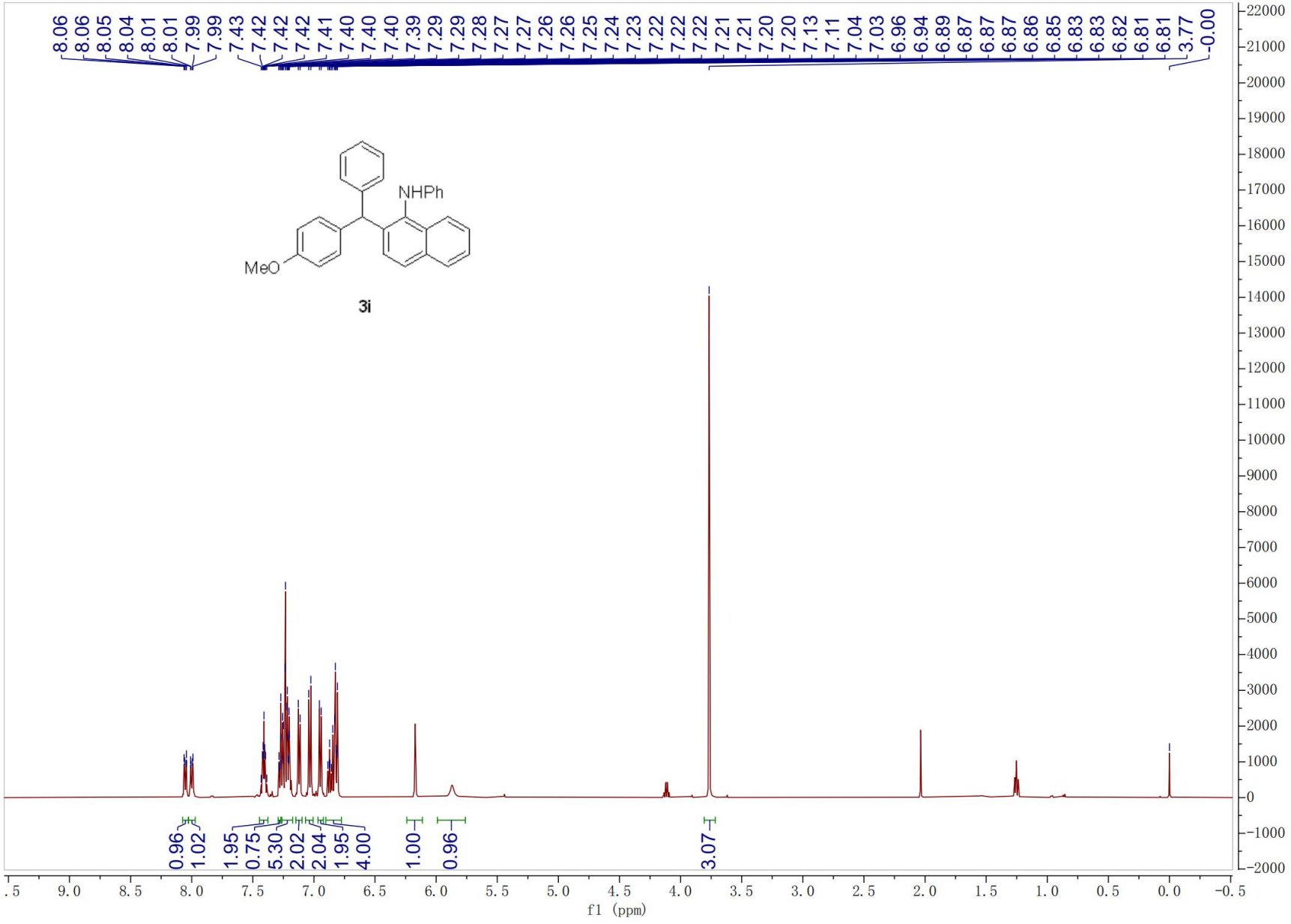

NHPh
OMe
3f
157.94
144.55
143.25
141.17
136.95
136.40
130.28
130.15
129.29
129.27
128.23
126.12
120.70
117.80
117.46
113.62
77.25
77.00
76.75
55.33
55.20
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

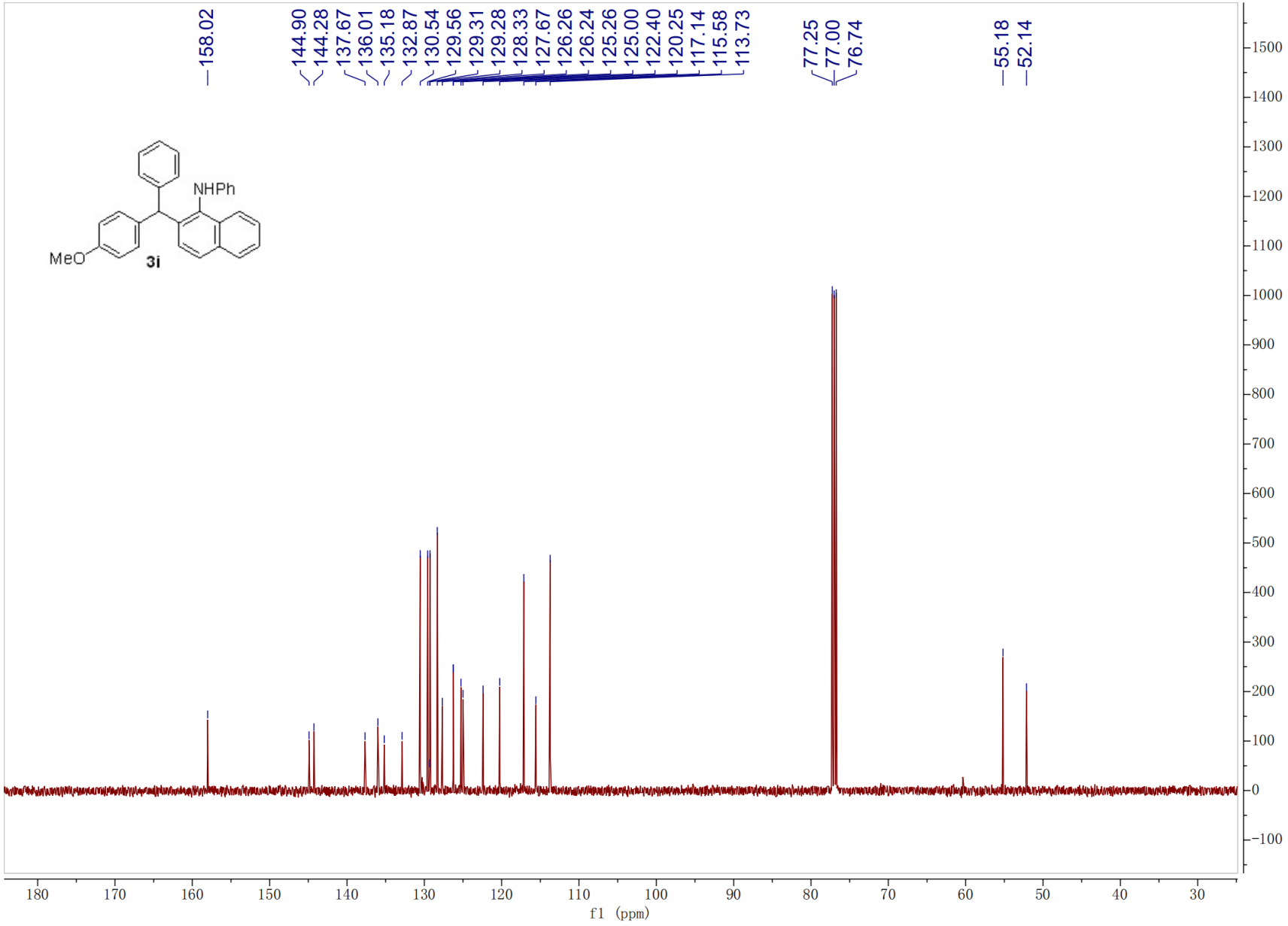

7.25
7.24
7.22
7.19
7.17
7.16
7.12
7.11
7.04
7.02
6.81
6.80
6.57
6.55
6.53
6.50
6.48
5.41
4.12
3.77
3.70
2.82
0.00
NHMe
OMe
OMe
3g
2.12
1.17
2.03
2.05
2.09
1.00
1.02
1.03
1.00
0.91
3.18
2.94
2.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

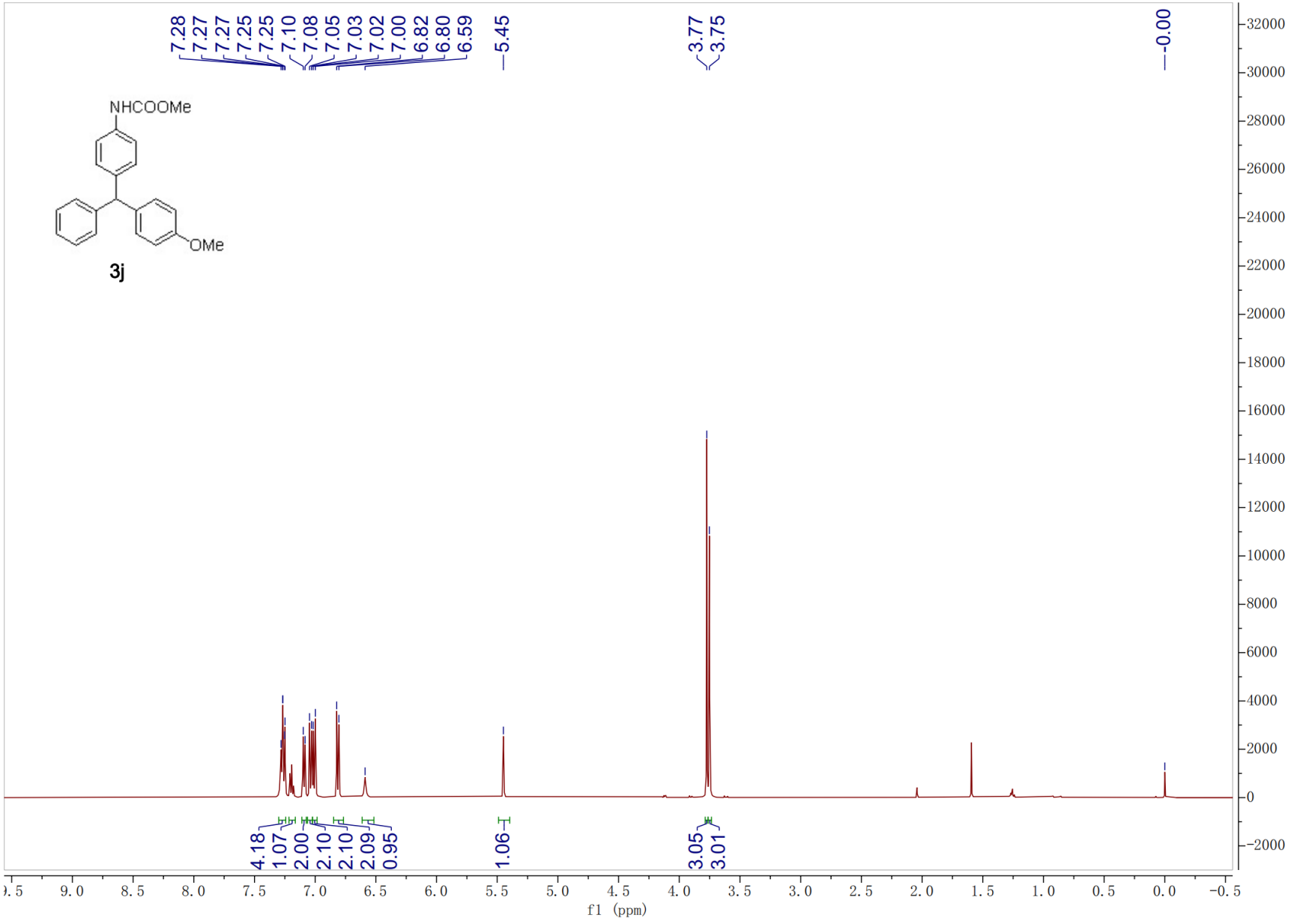

NHMe
OMe
OMe
3g
157.81
146.80
144.99
137.62
136.85
132.33
130.28
129.30
128.10
125.94
121.91
113.49
110.70
108.85
77.25
77.00
76.75
55.55
55.33
55.17
30.41
f1 (ppm)

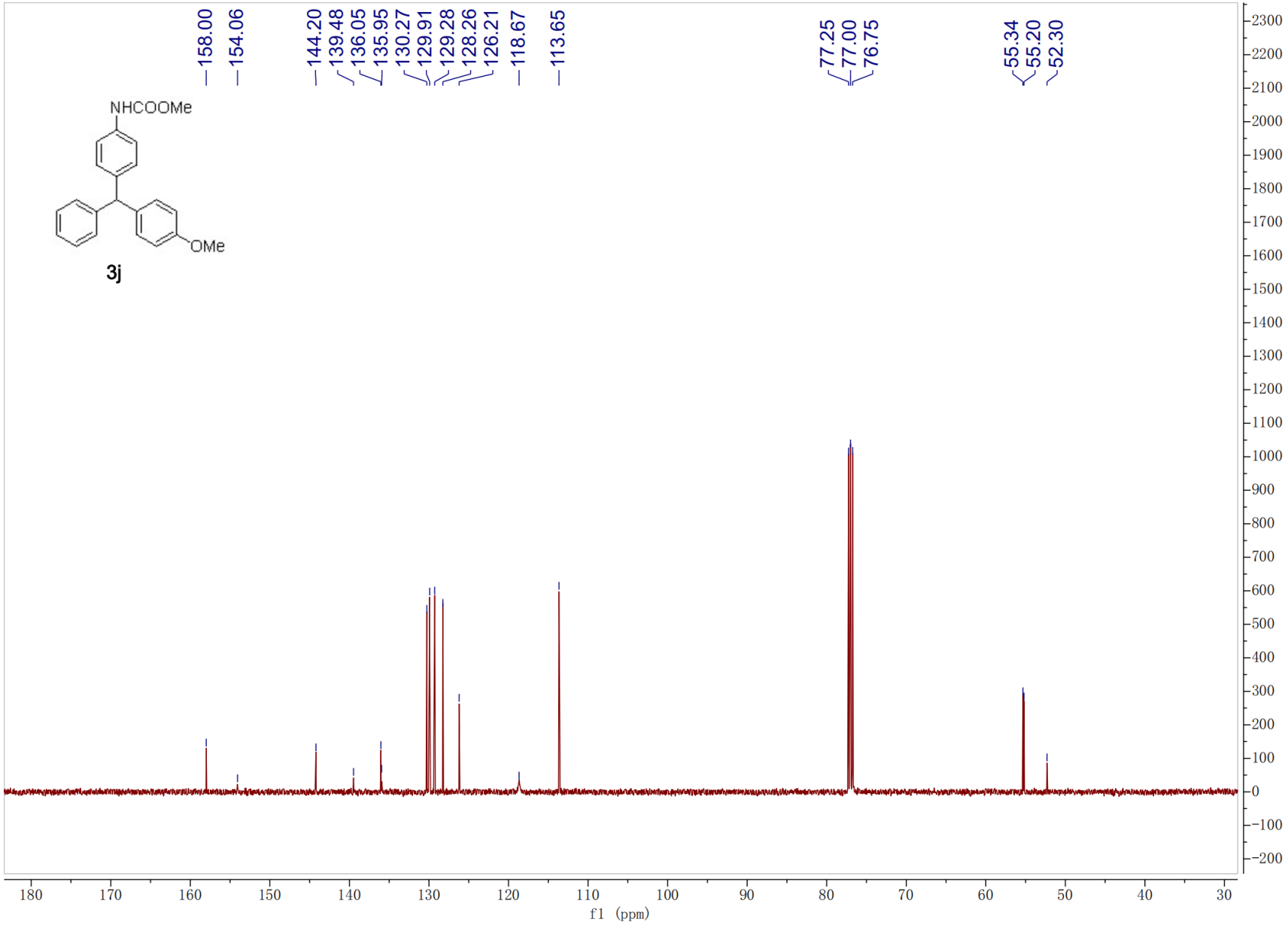

7.26
7.25
7.23
7.22
7.18
7.16
7.15
7.12
7.11
7.04
7.02
7.00
7.00
6.84
6.84
6.83
6.82
6.81
6.81
6.79
6.58
6.57
5.39
3.86
3.76
2.87
1.33
0.00
NHMe
tBu
OMe
3h
2.91
1.18
2.01
2.14
0.90
1.01
1.99
0.99
1.00
0.92
3.05
3.02
9.00
f1 (ppm)

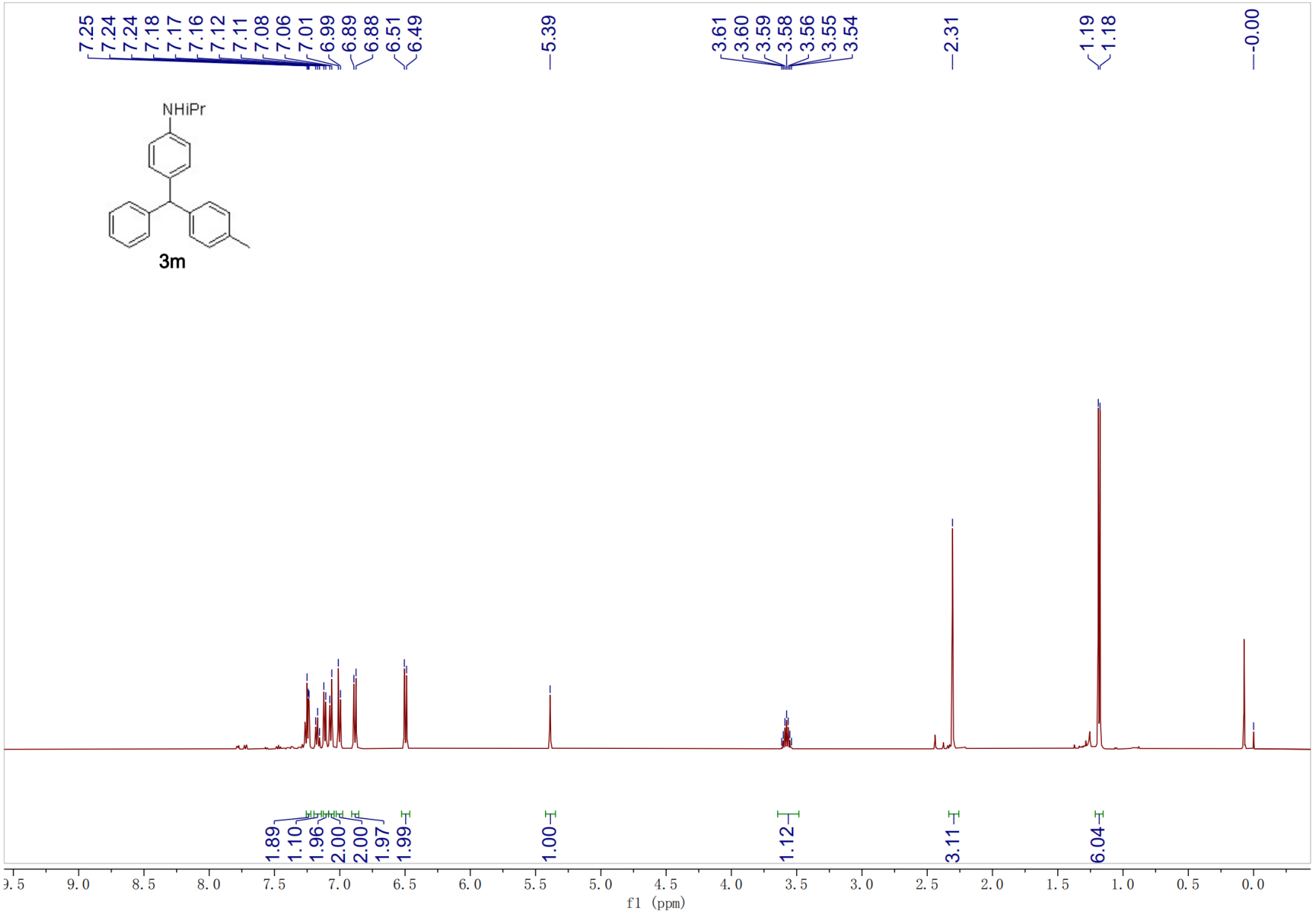

NHMe
tBu
OMe
3h
157.73
145.58
145.27
137.17
133.05
132.21
130.28
129.32
128.05
127.70
127.48
125.82
113.44
110.90
77.25
77.00
76.75
55.54
55.17
34.13
31.27
29.86
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

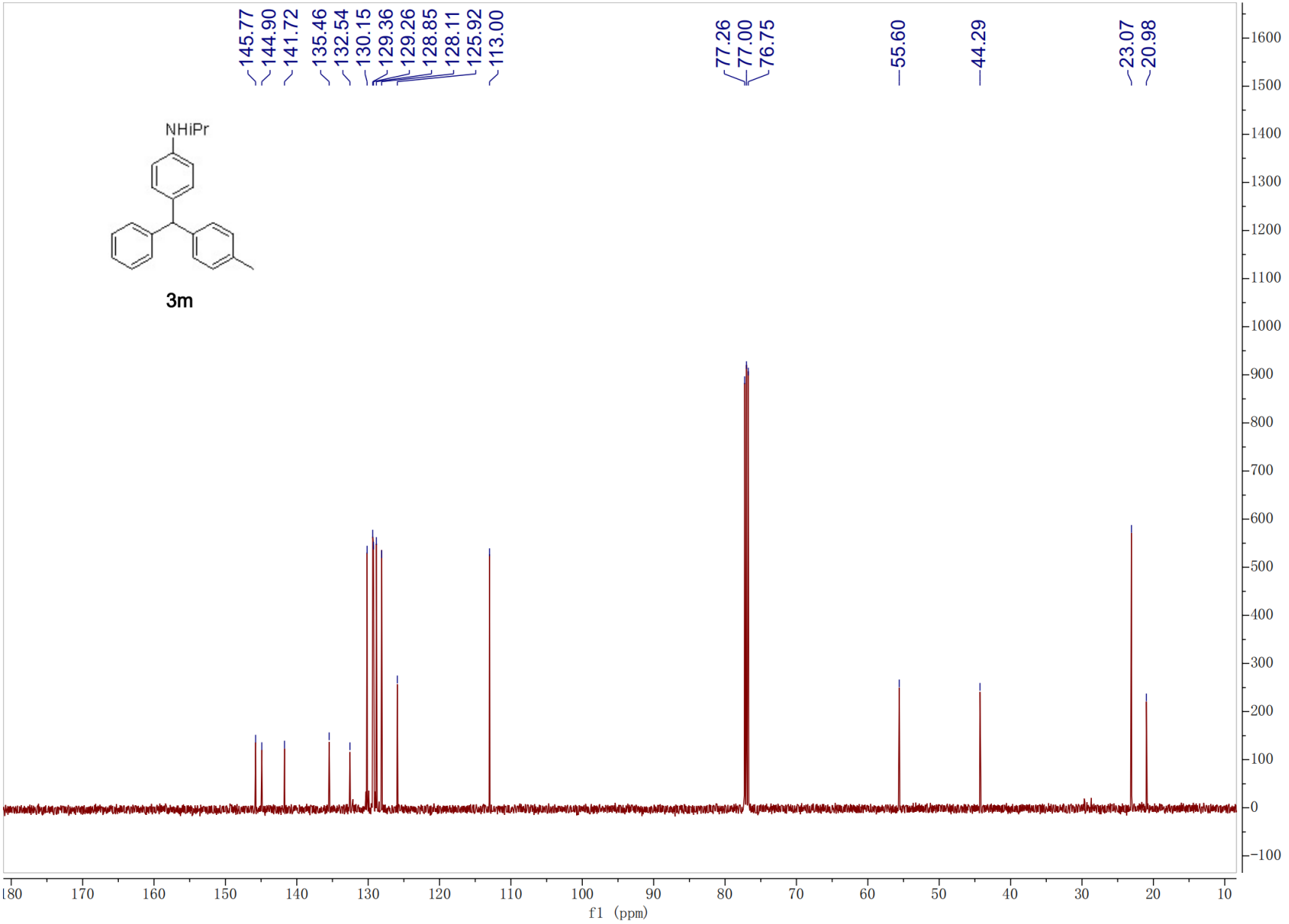

8.06 8.06 8.05 8.04 8.01 8.01 7.99 7.99 7.43 7.42 7.42 7.42 7.41 7.40 7.40 7.40 7.39 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.25 7.24 7.23 7.22 7.22 7.22 7.21 7.21 7.20 7.20 7.13 7.11 7.04 7.03 6.96 6.94 6.89 6.87 6.87 6.87 6.86 6.85 6.83 6.83 6.82 6.81 6.81 3.77 0.00
NHPh
MeO
3i
0.96 1.02 1.95 0.75 5.30 2.02 2.04 1.95 4.00 1.00 0.96 3.07
f1 (ppm)

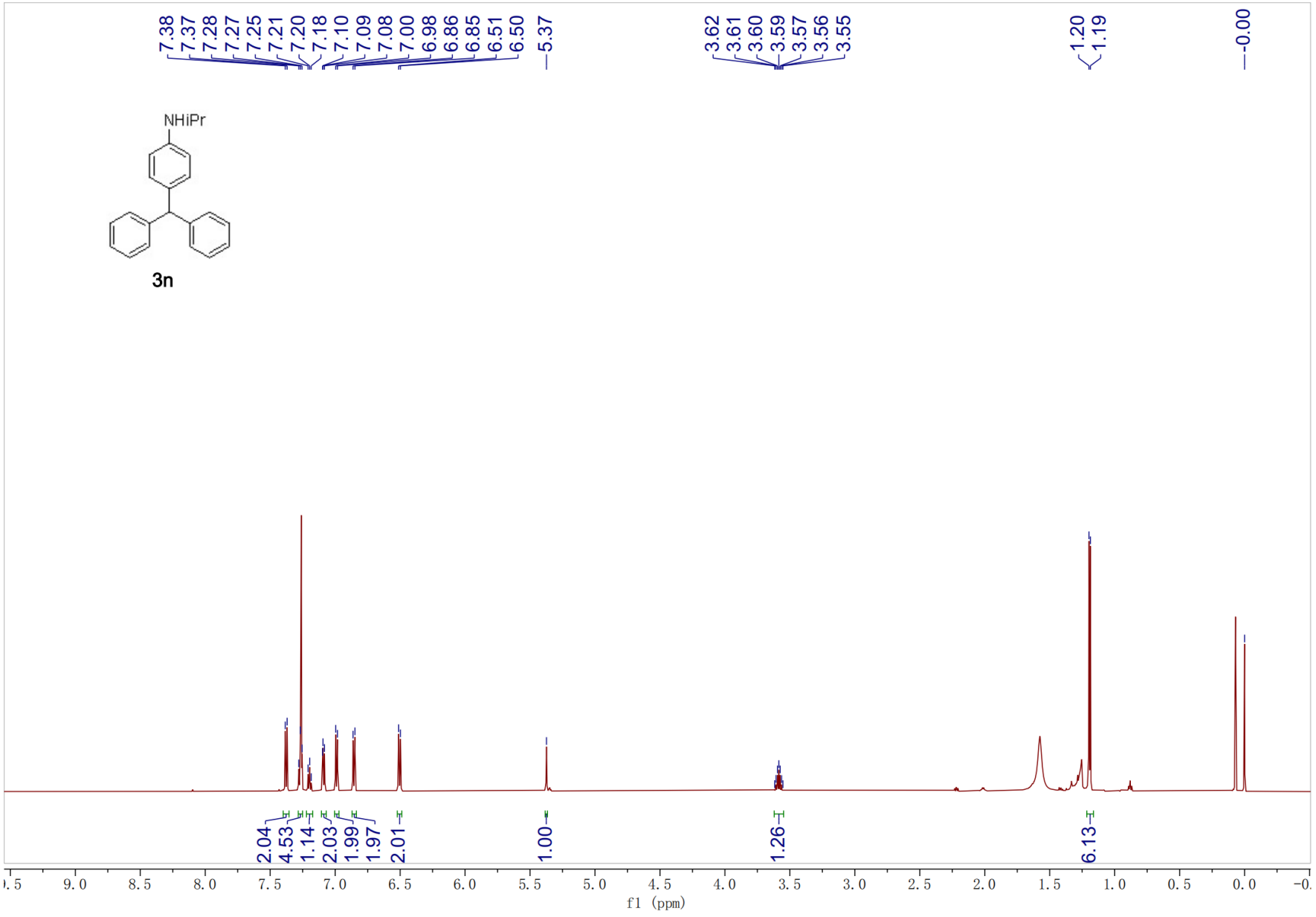

158.02
144.90
144.28
137.67
136.01
135.18
132.87
130.54
129.56
129.31
129.28
128.33
127.67
126.26
126.24
125.26
125.00
122.40
120.25
117.14
115.58
113.73
77.25
77.00
76.74
55.18
52.14
NHPh
MeO
3i
f1 (ppm)

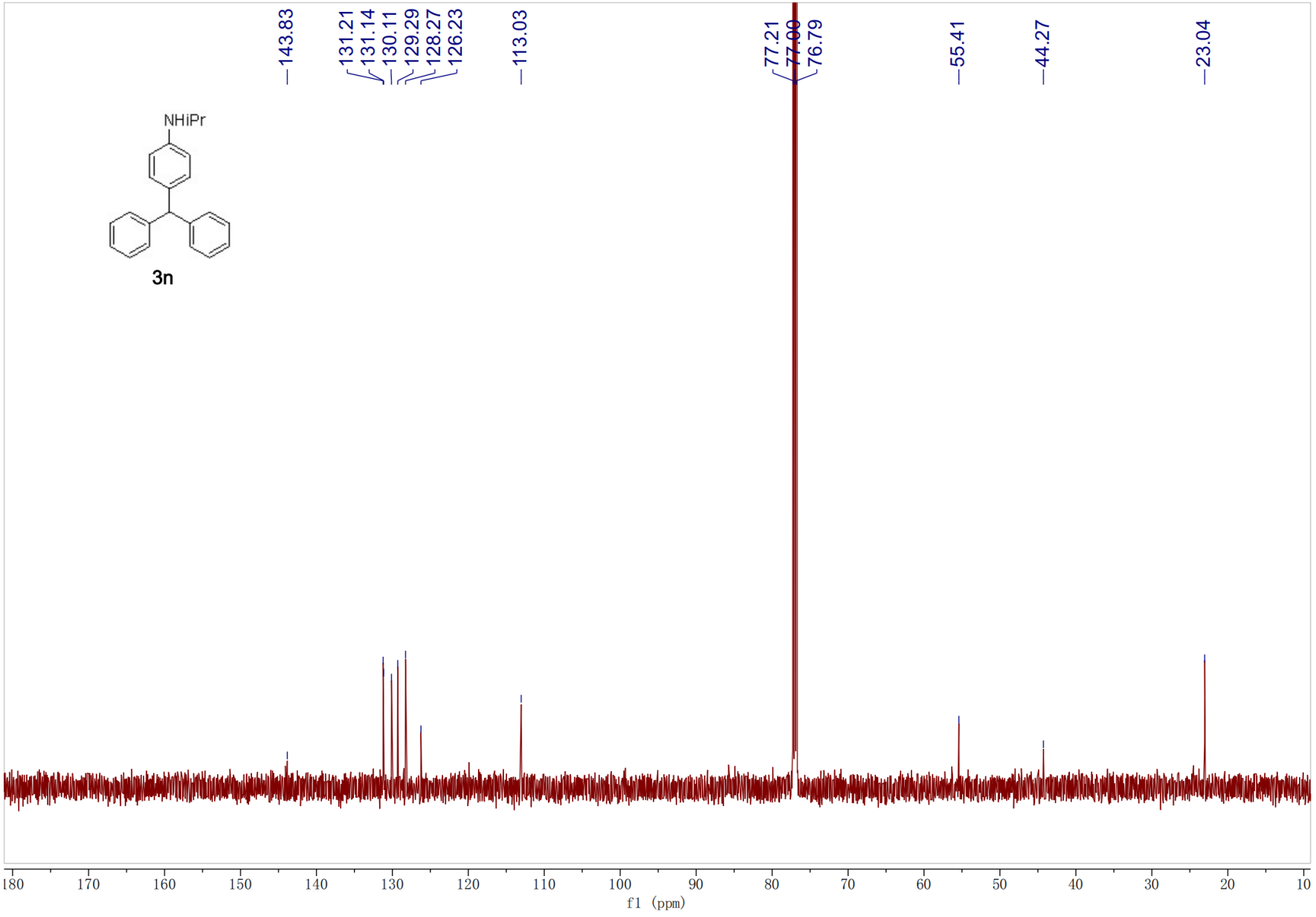

7.28
7.27
7.27
7.25
7.25
7.10
7.08
7.05
7.03
7.02
7.00
6.82
6.80
6.59
5.45
3.77
3.75
0.00
NHCOOMe
OMe
3j
4.18
1.07
2.00
2.10
2.10
2.09
0.95
1.06
3.05
3.01
f1 (ppm)

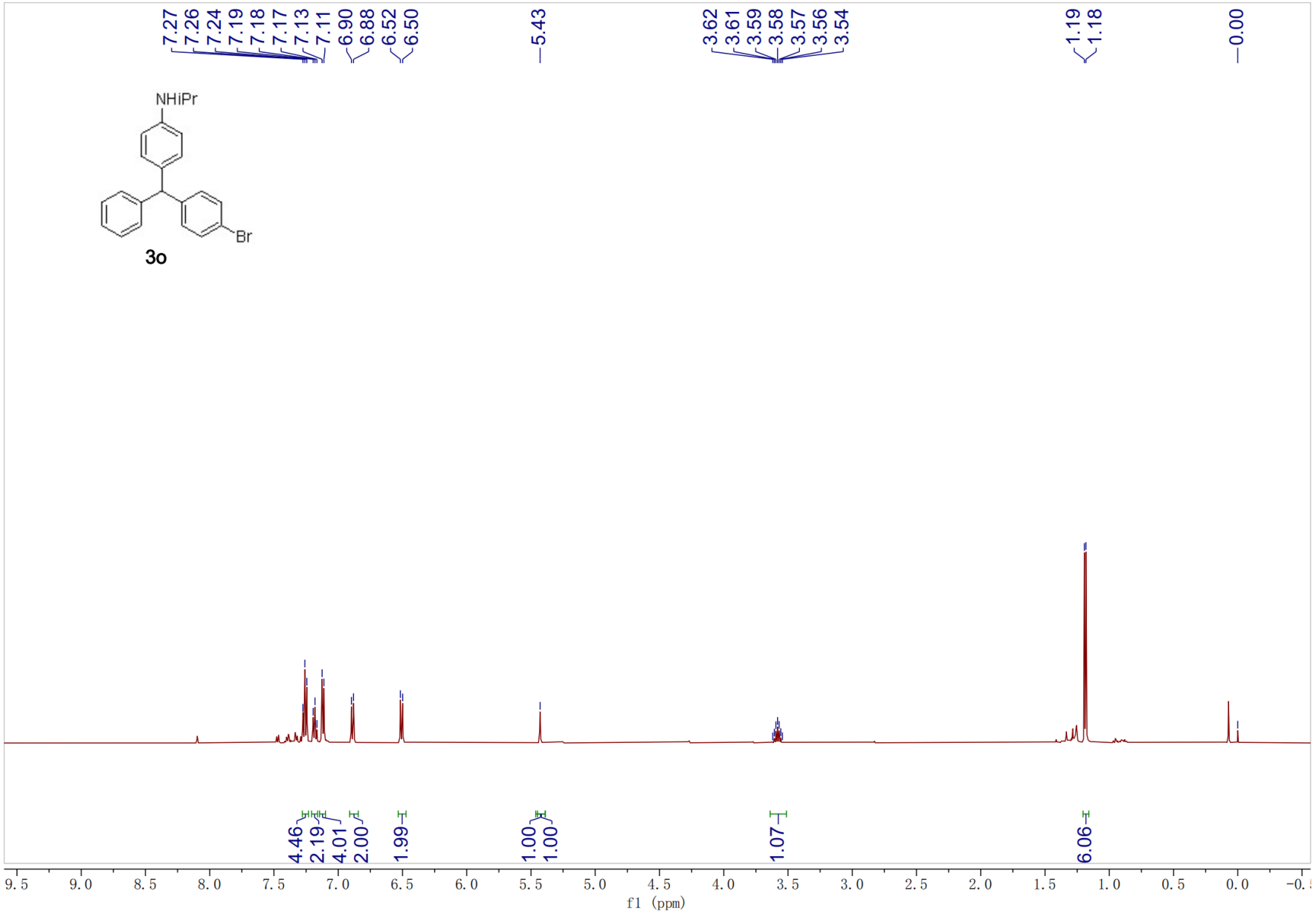

158.00
154.06
144.20
139.48
136.05
135.95
130.27
129.91
129.28
128.26
126.21
118.67
113.65
77.25
77.00
76.75
55.34
55.20
52.30
NHCOOMe
OMe
3j
f1 (ppm)

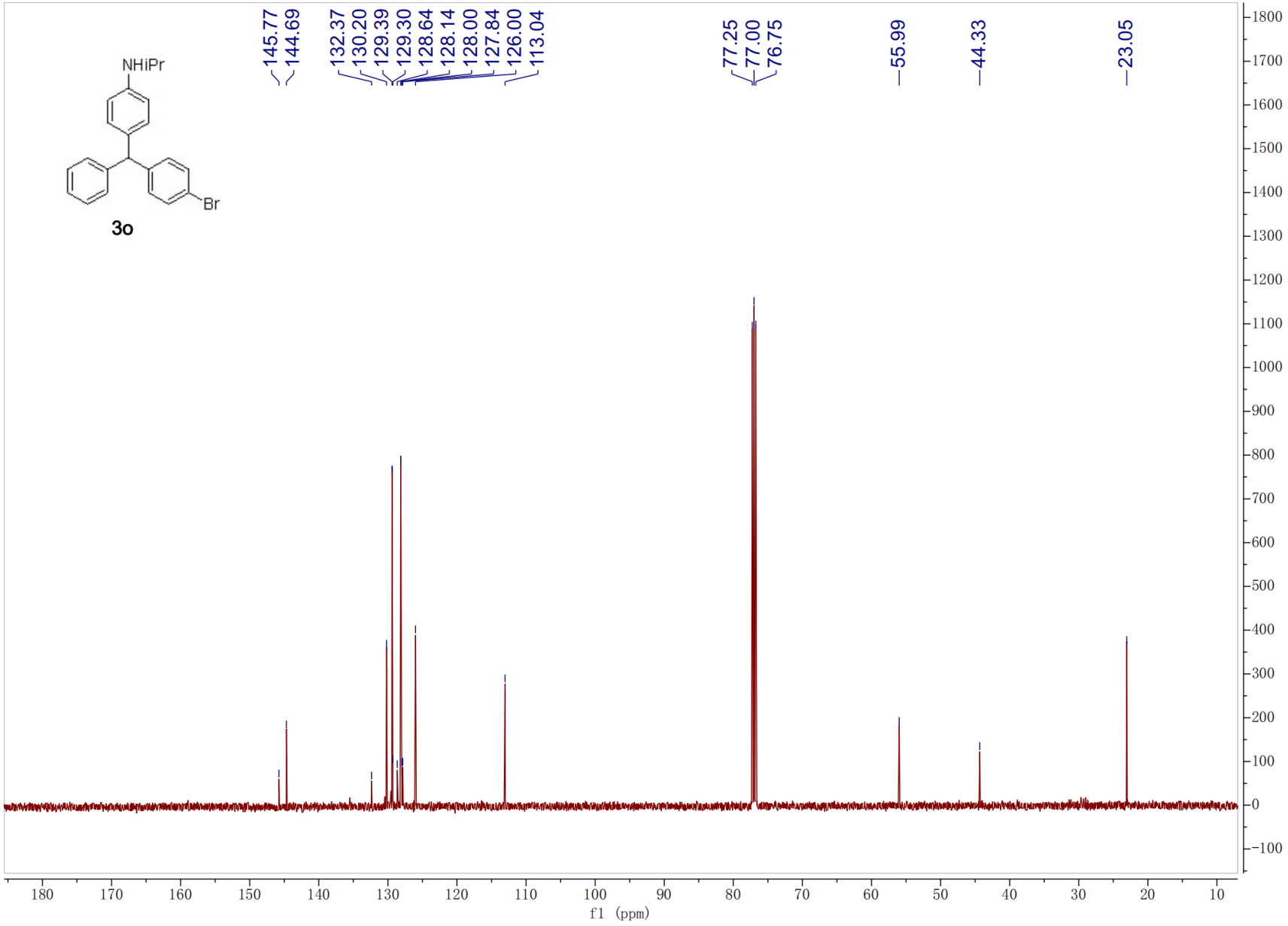

7.25
7.24
7.24
7.18
7.17
7.16
7.12
7.11
7.08
7.06
7.01
6.99
6.89
6.88
6.51
6.49
5.39
3.61
3.60
3.59
3.58
3.56
3.55
3.54
2.31
1.19
1.18
0.00
NHiPr
3m
1.89
1.10
1.96
2.00
2.00
1.97
1.99
1.00
1.12
3.11
6.04
f1 (ppm)

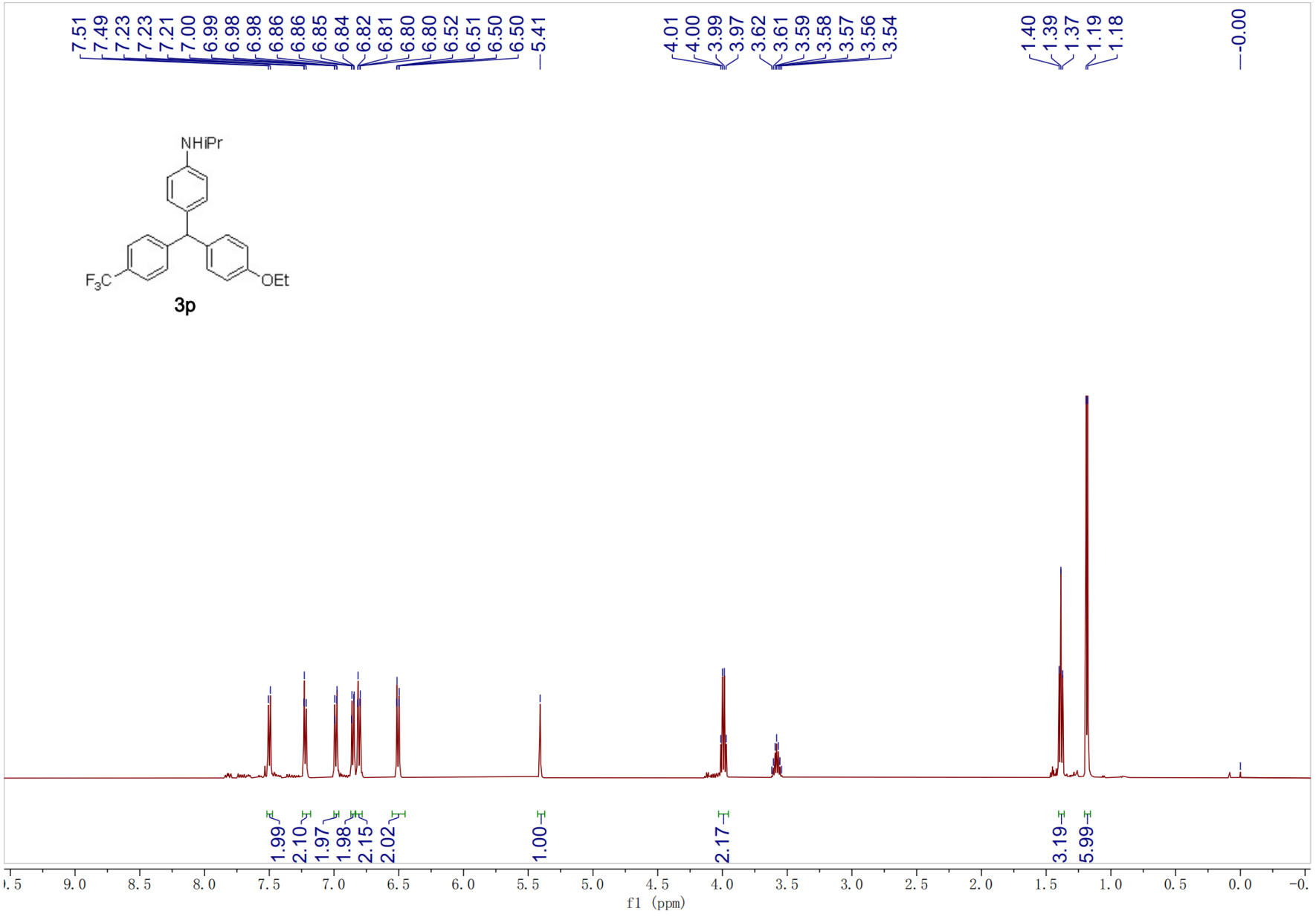

145.77
144.90
141.72
135.46
132.54
130.15
129.36
129.26
128.85
128.11
125.92
113.00
77.26
77.00
76.75
55.60
44.29
23.07
20.98
NHiPr
3m
f1 (ppm)

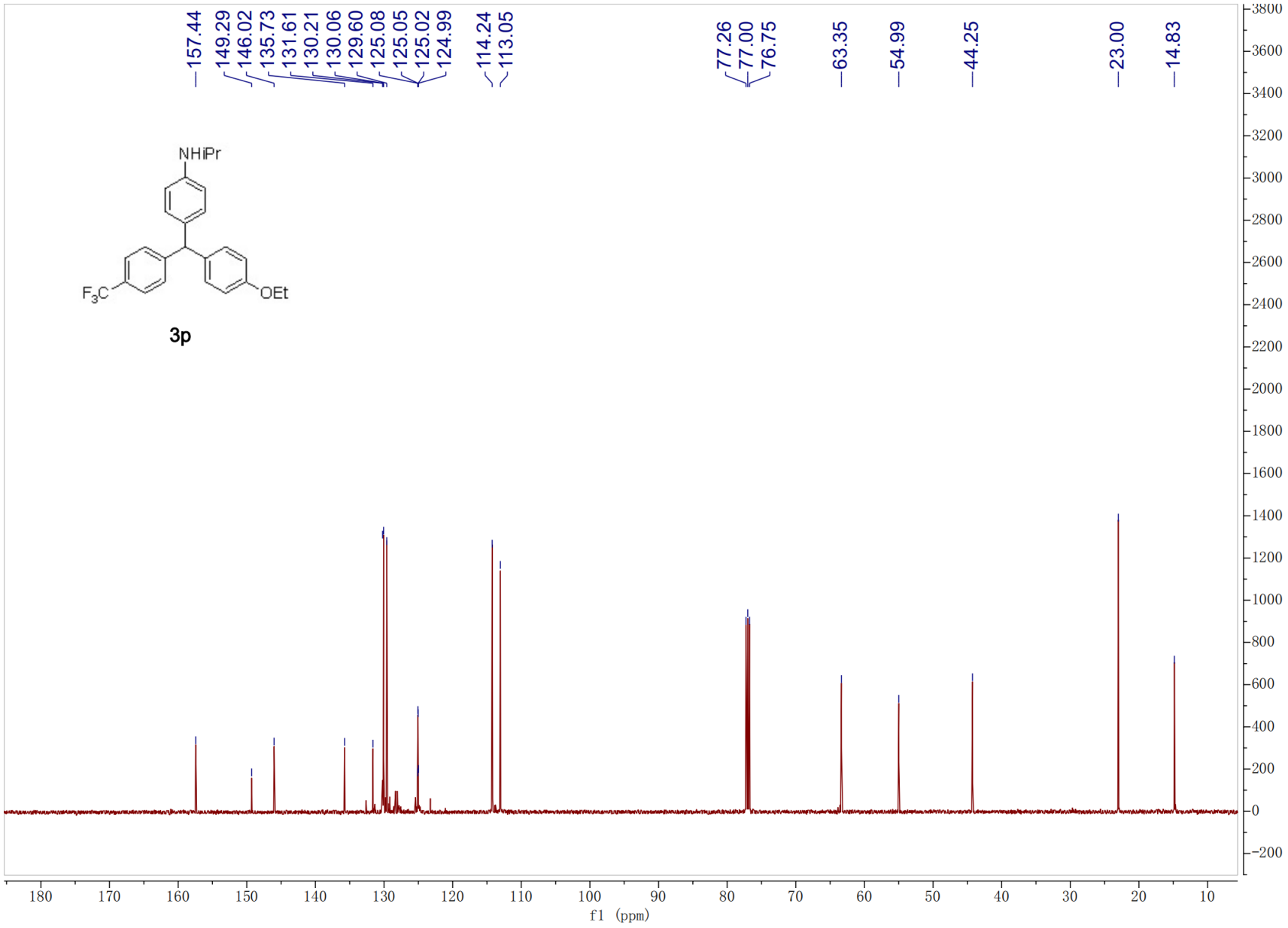

7.38
7.37
7.28
7.27
7.25
7.21
7.20
7.18
7.10
7.09
7.08
7.00
6.98
6.86
6.85
6.51
6.50
5.37
3.62
3.61
3.60
3.59
3.57
3.56
3.55
1.20
1.19
0.00
NHiPr
3n
2.04
4.53
1.14
2.03
1.99
1.97
2.01
1.00
1.26
6.13
f1 (ppm)

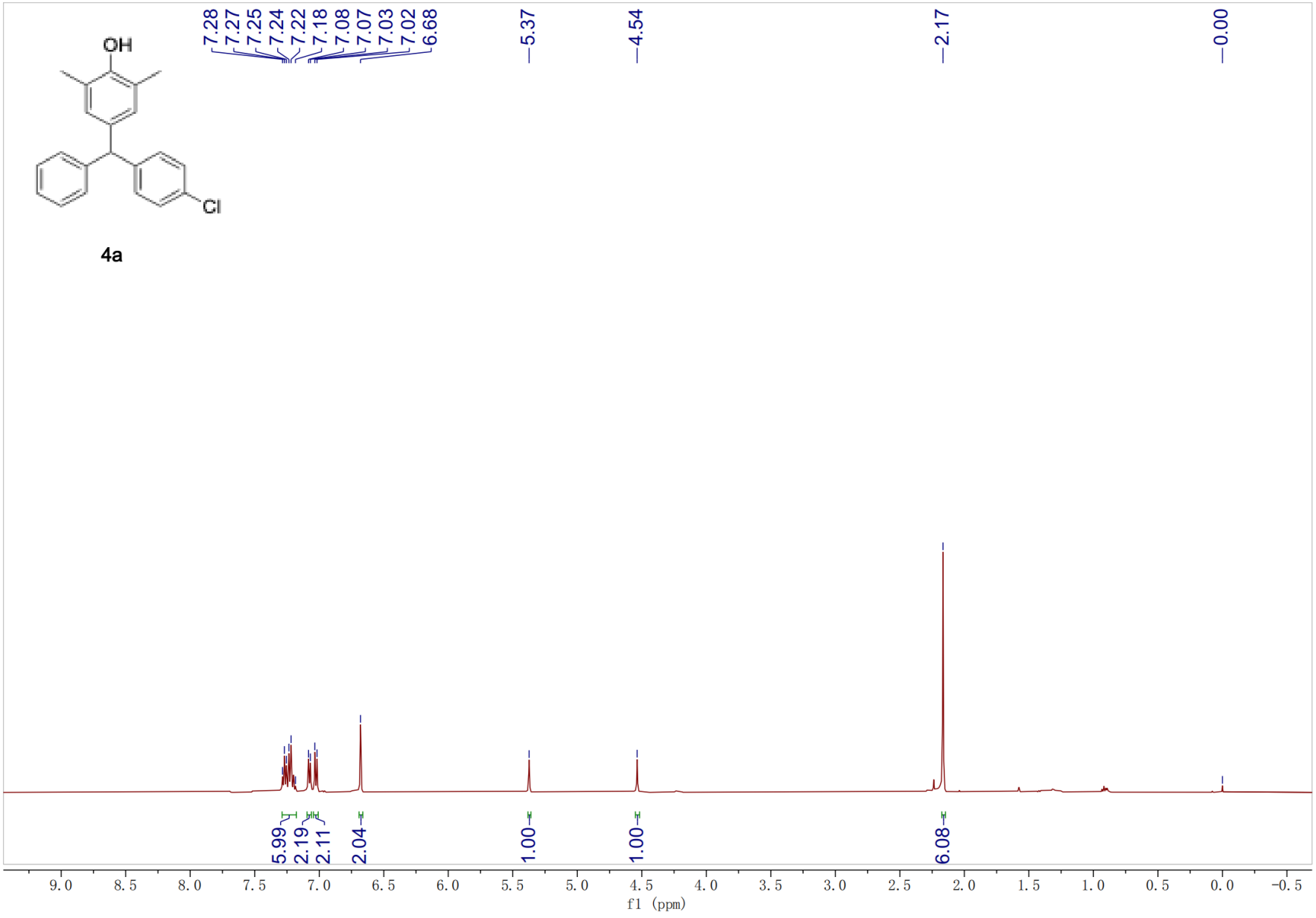

143.83
131.21
131.14
130.11
129.29
128.27
126.23
113.03
77.21
77.00
76.79
55.41
44.27
23.04
NHiPr
3n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

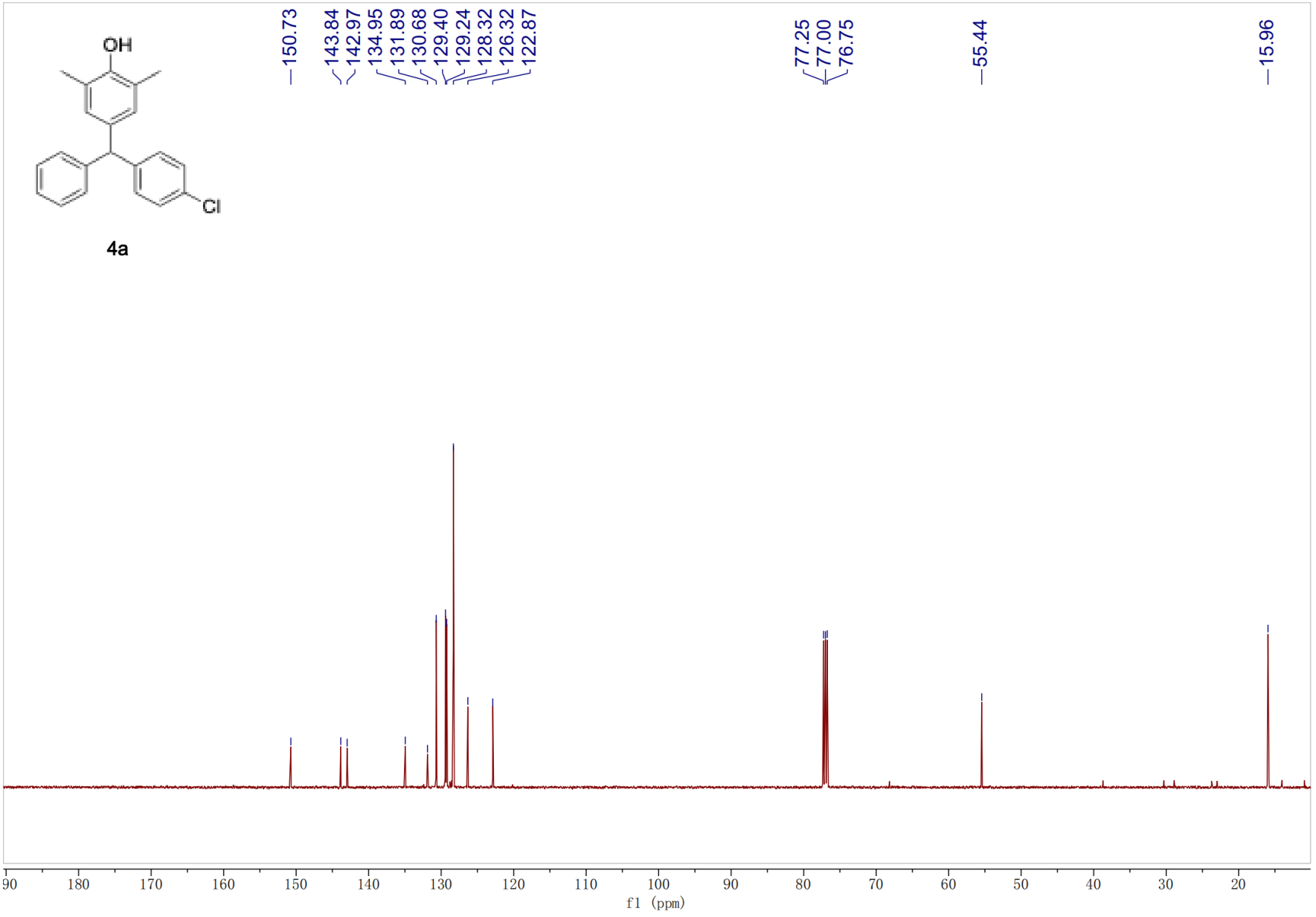

7.27
7.26
7.24
7.19
7.18
7.17
7.13
7.11
6.90
6.88
6.52
6.50
5.43
3.62
3.61
3.59
3.58
3.57
3.56
3.54
1.19
1.18
0.00
NHiPr
Br
3o
4.46
2.19
4.01
2.00
1.99
1.00
1.00
1.07
6.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

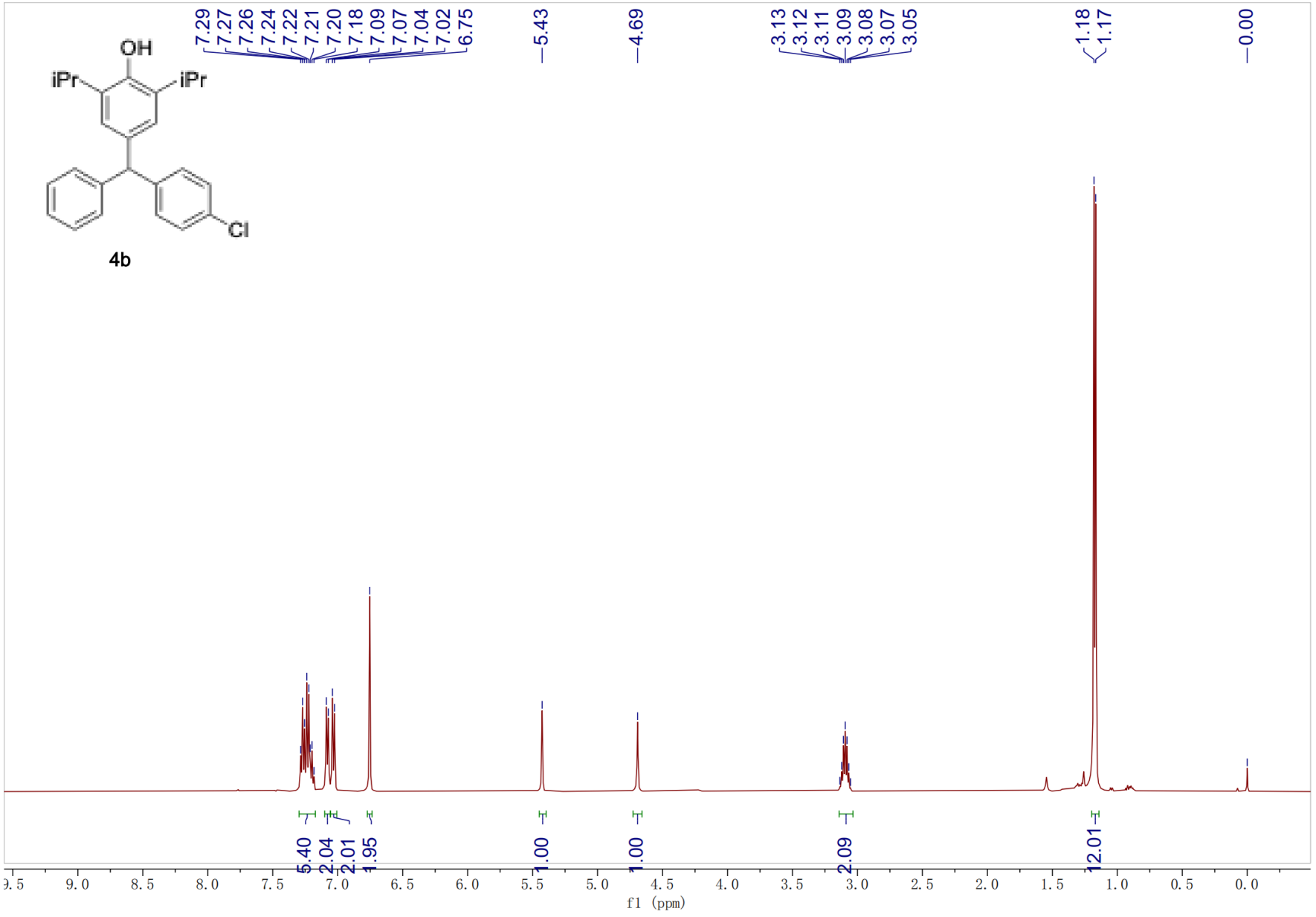

NHiPr
Br
3o
145.77
144.69
132.37
130.20
129.39
129.30
128.64
128.14
128.00
127.84
126.00
113.04
77.25
77.00
76.75
55.99
44.33
23.05
f1 (ppm)

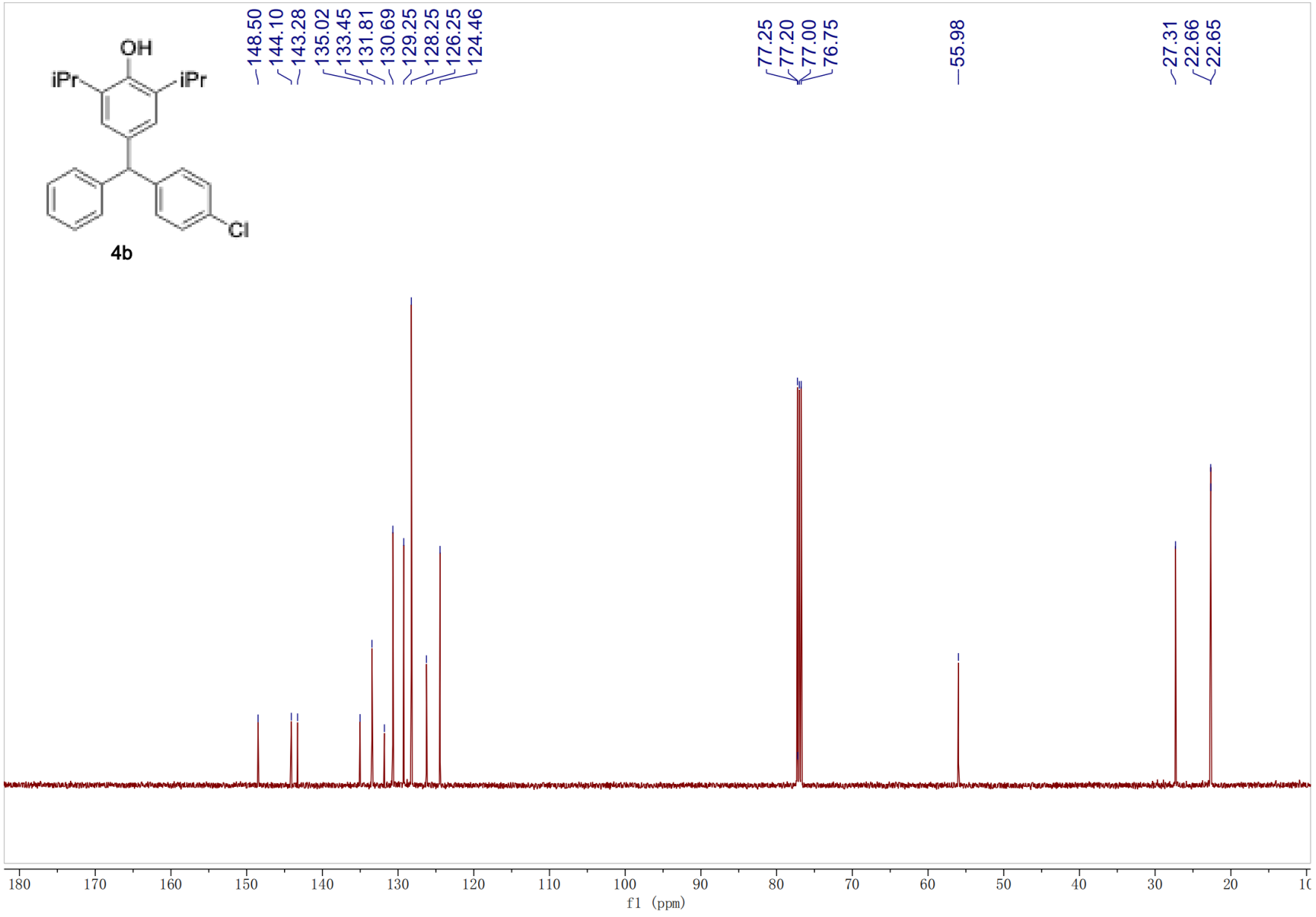

7.51
7.49
7.23
7.23
7.21
7.00
6.99
6.98
6.98
6.86
6.86
6.85
6.84
6.82
6.81
6.80
6.80
6.52
6.51
6.50
6.50
5.41
4.01
4.00
3.99
3.97
3.62
3.61
3.59
3.58
3.57
3.56
3.54
1.40
1.39
1.37
1.19
1.18
0.00
NHiPr
F3C
OEt
3p
1.99
2.10
1.97
1.98
2.15
2.02
1.00
2.17
3.19
5.99
f1 (ppm)

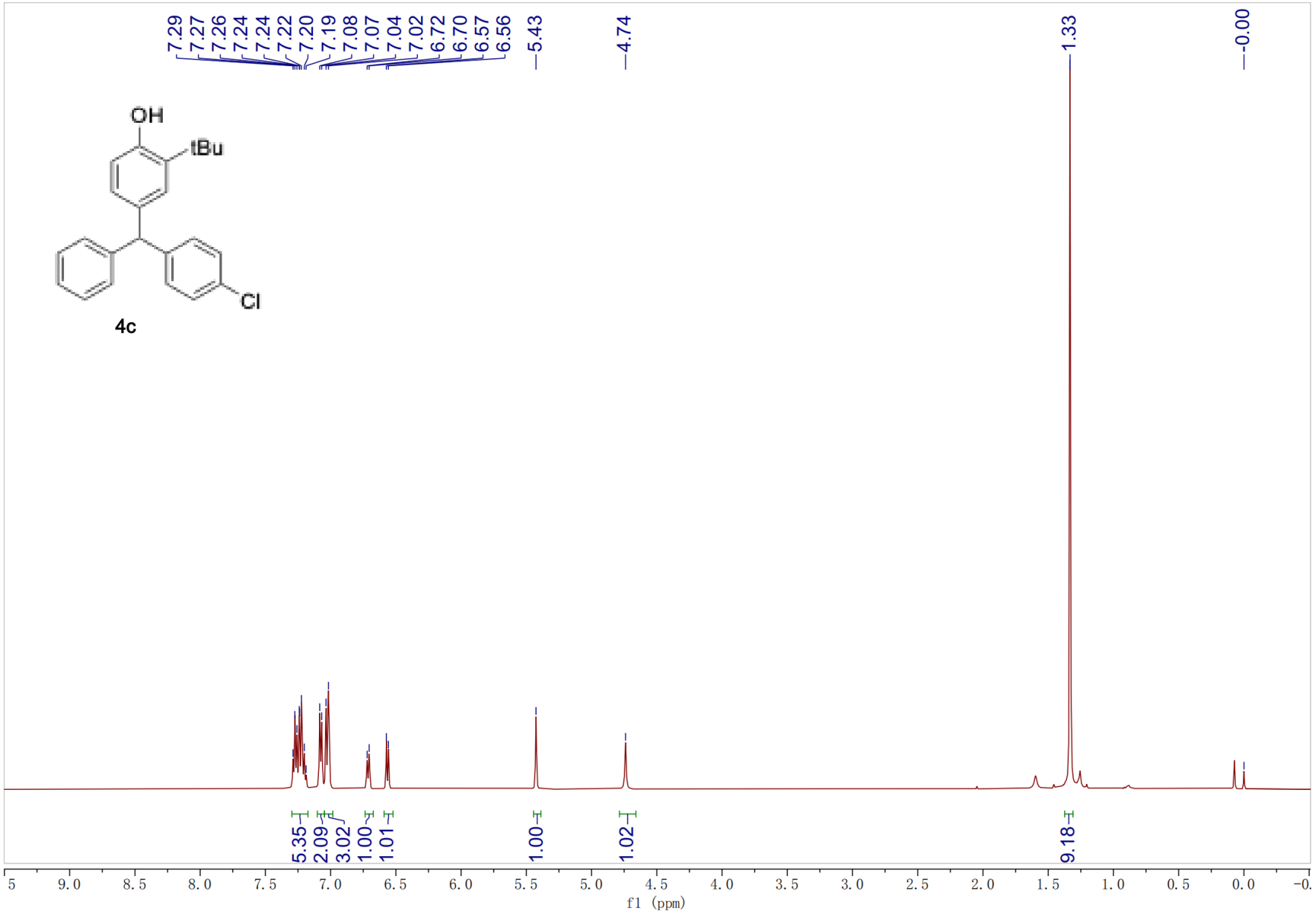

157.44
149.29
146.02
135.73
131.61
130.21
130.06
129.60
125.08
125.05
125.02
124.99
114.24
113.05
77.26
77.00
76.75
63.35
54.99
44.25
23.00
14.83
NHiPr
F3C
OEt
3p
f1 (ppm)

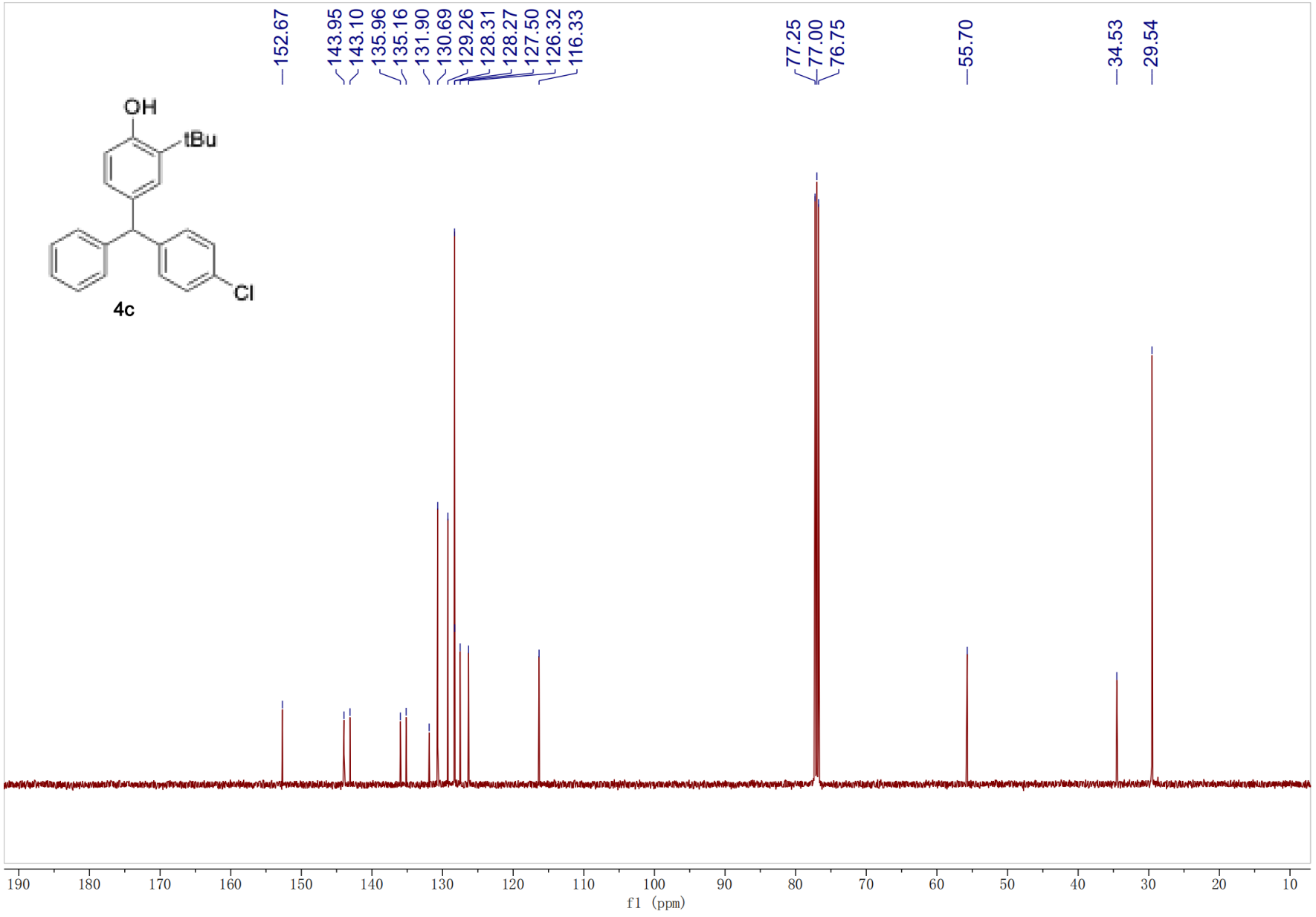

OH
Cl
4a
7.28
7.27
7.25
7.24
7.22
7.18
7.08
7.07
7.03
7.02
6.68
5.37
4.54
2.17
0.00
5.99
2.19
2.11
2.04
1.00
1.00
6.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

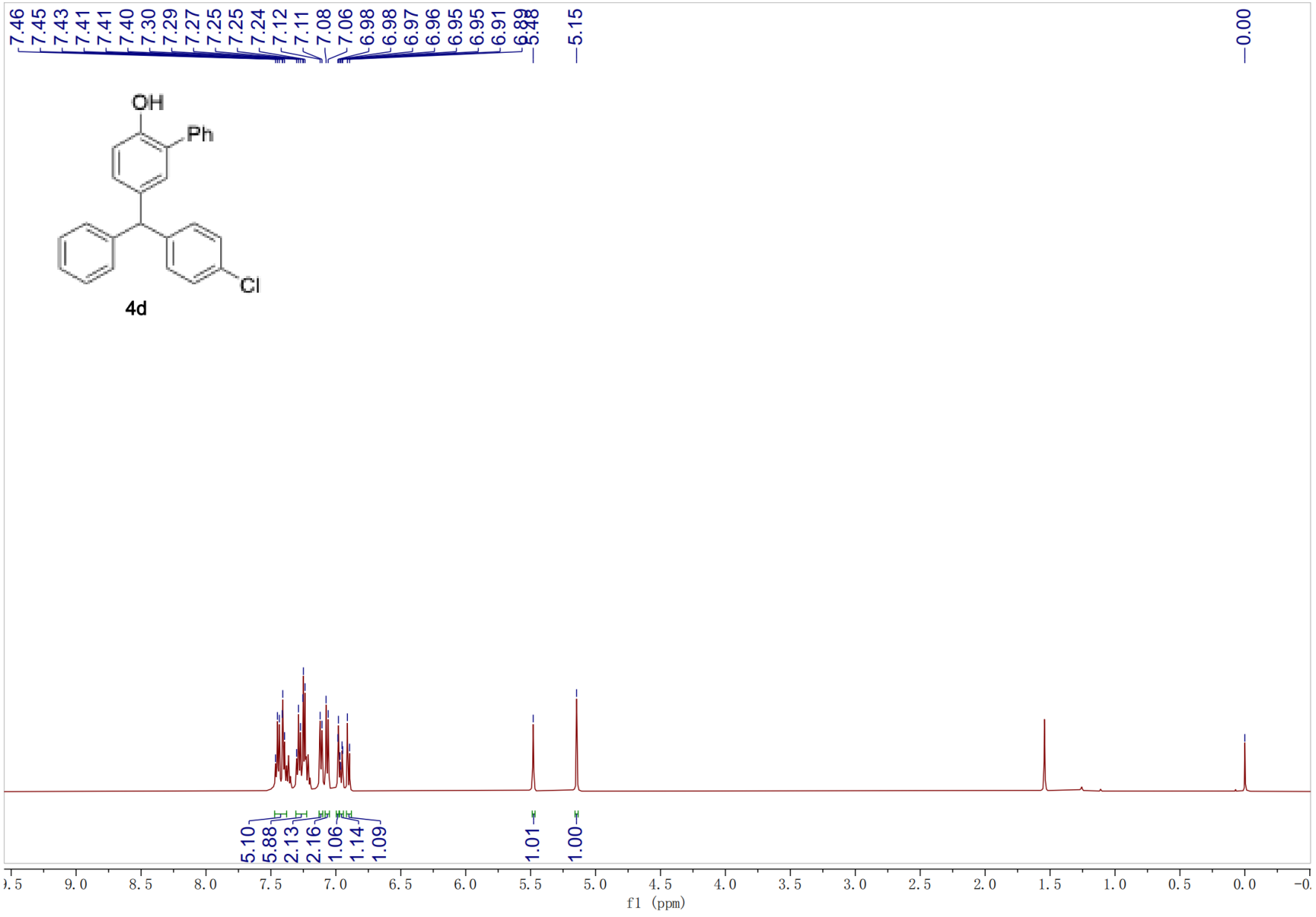

OH
Cl
4a
150.73
143.84
142.97
134.95
131.89
130.68
129.40
129.24
128.32
126.32
122.87
77.25
77.00
76.75
55.44
15.96
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

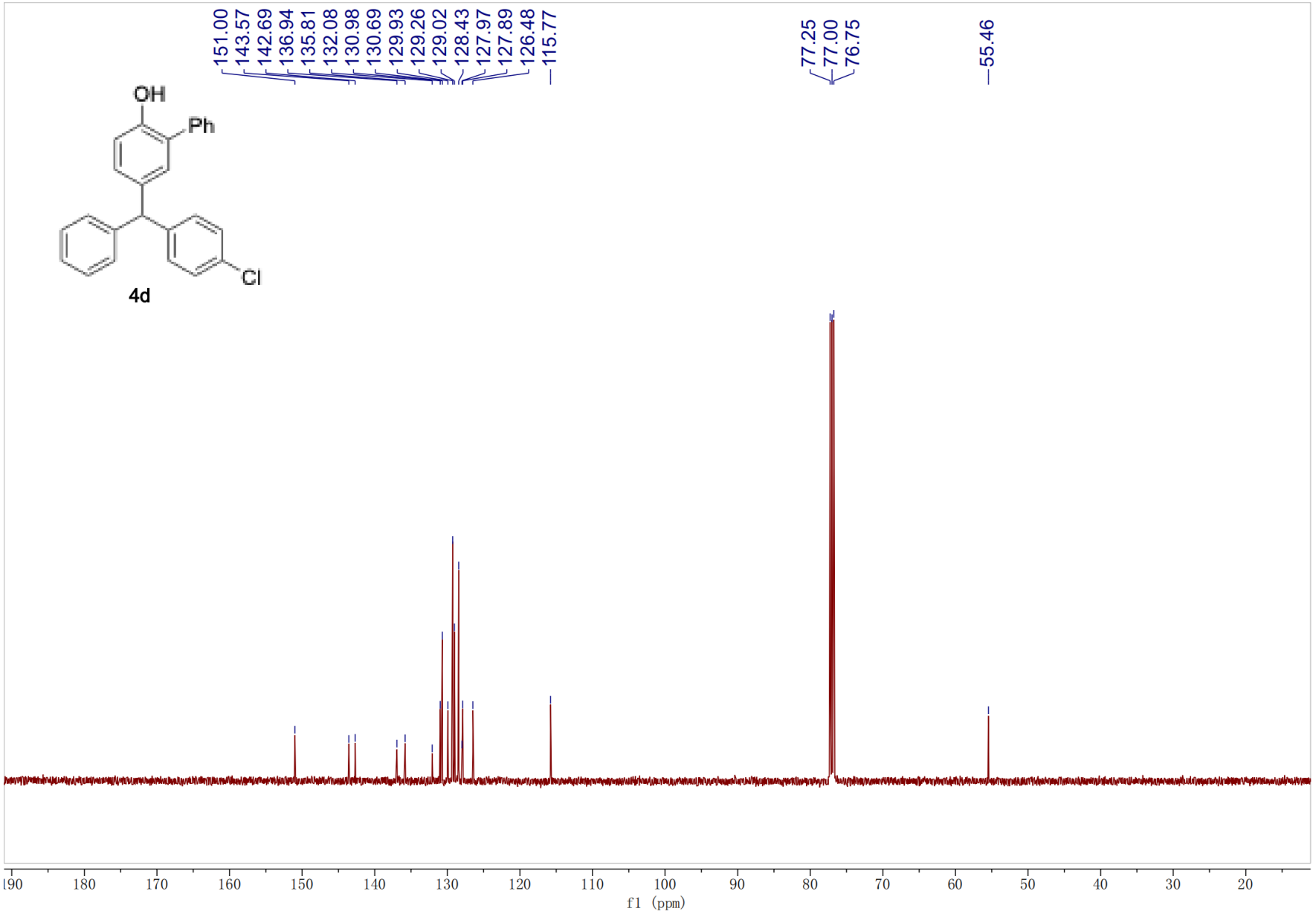

OH
iPr
iPr
Cl
4b
7.29
7.27
7.26
7.24
7.22
7.21
7.20
7.18
7.09
7.07
7.04
7.02
6.75
5.43
4.69
3.13
3.12
3.11
3.09
3.08
3.07
3.05
1.18
1.17
0.00
5.40
2.04
2.01
1.95
1.00
1.00
2.09
12.01
f1 (ppm)

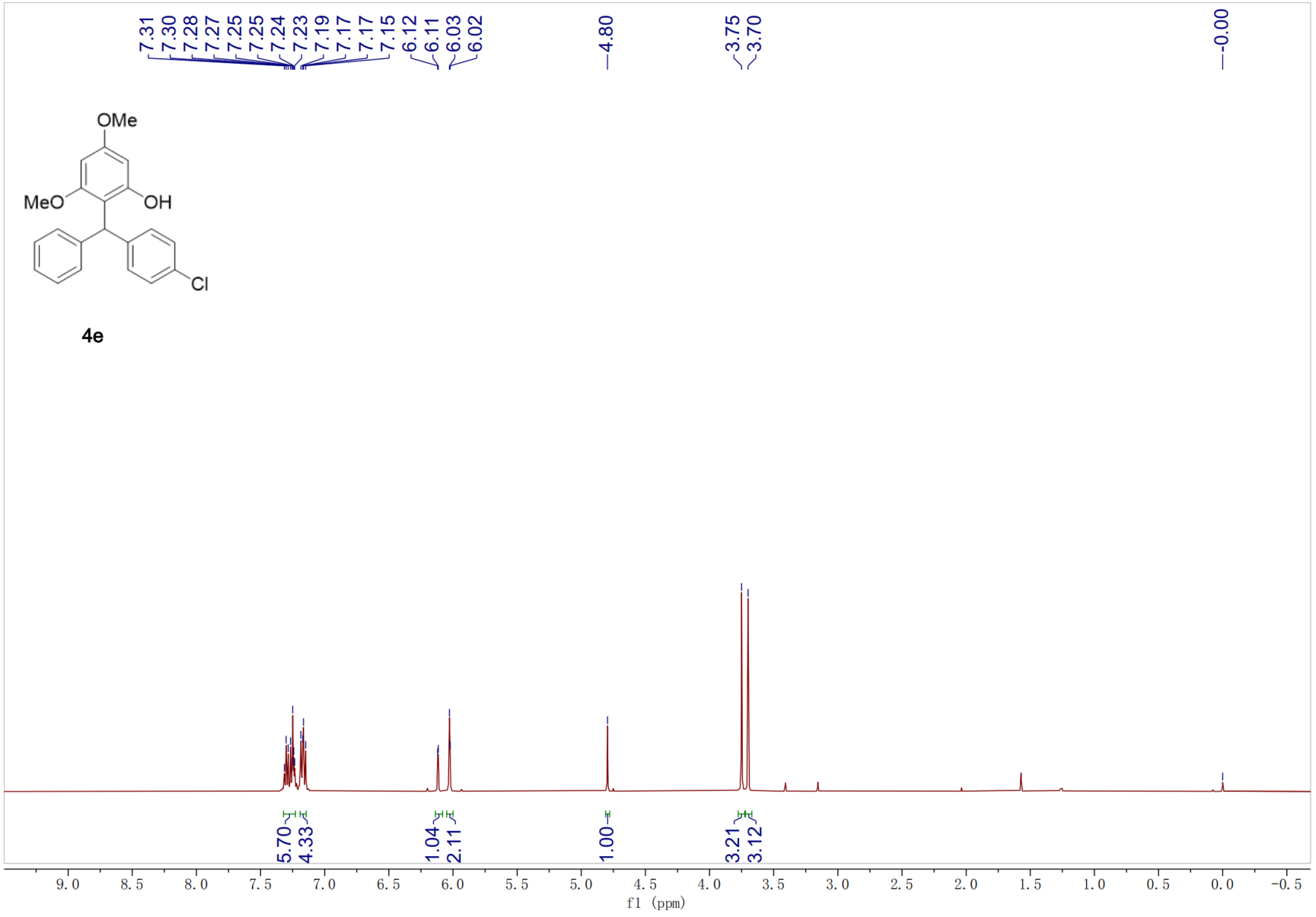

OH
iPr
iPr
Cl
4b
148.50
144.10
143.28
135.02
133.45
131.81
130.69
129.25
128.25
126.25
124.46
77.25
77.20
77.00
76.75
55.98
27.31
22.66
22.65
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

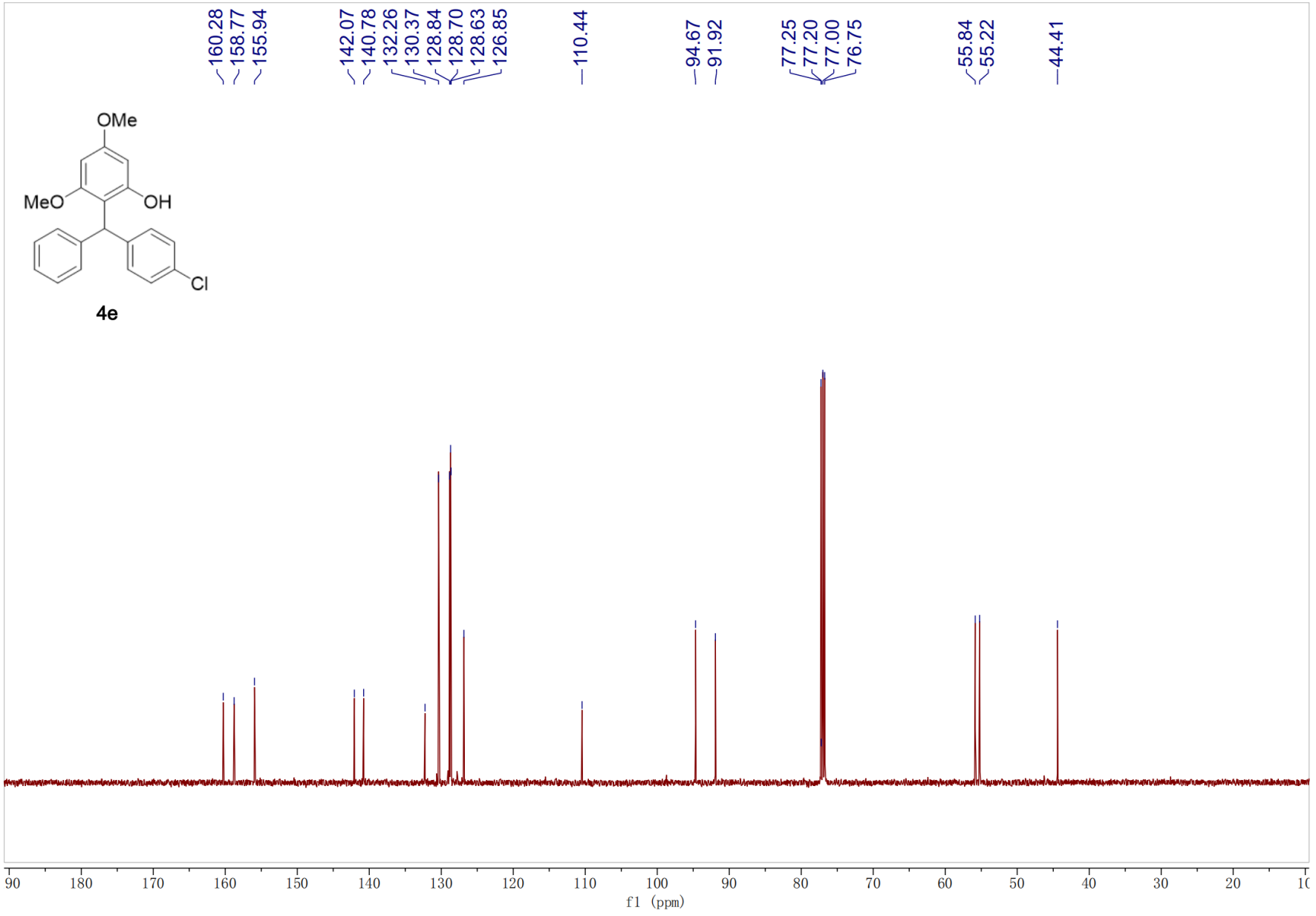

7.29
7.27
7.26
7.24
7.24
7.22
7.20
7.19
7.08
7.07
7.04
7.02
6.72
6.70
6.57
6.56
5.43
4.74
1.33
0.00
OH
tBu
Cl
4c
5.35
2.09
3.02
1.00
1.01
1.00
1.02
9.18
f1 (ppm)

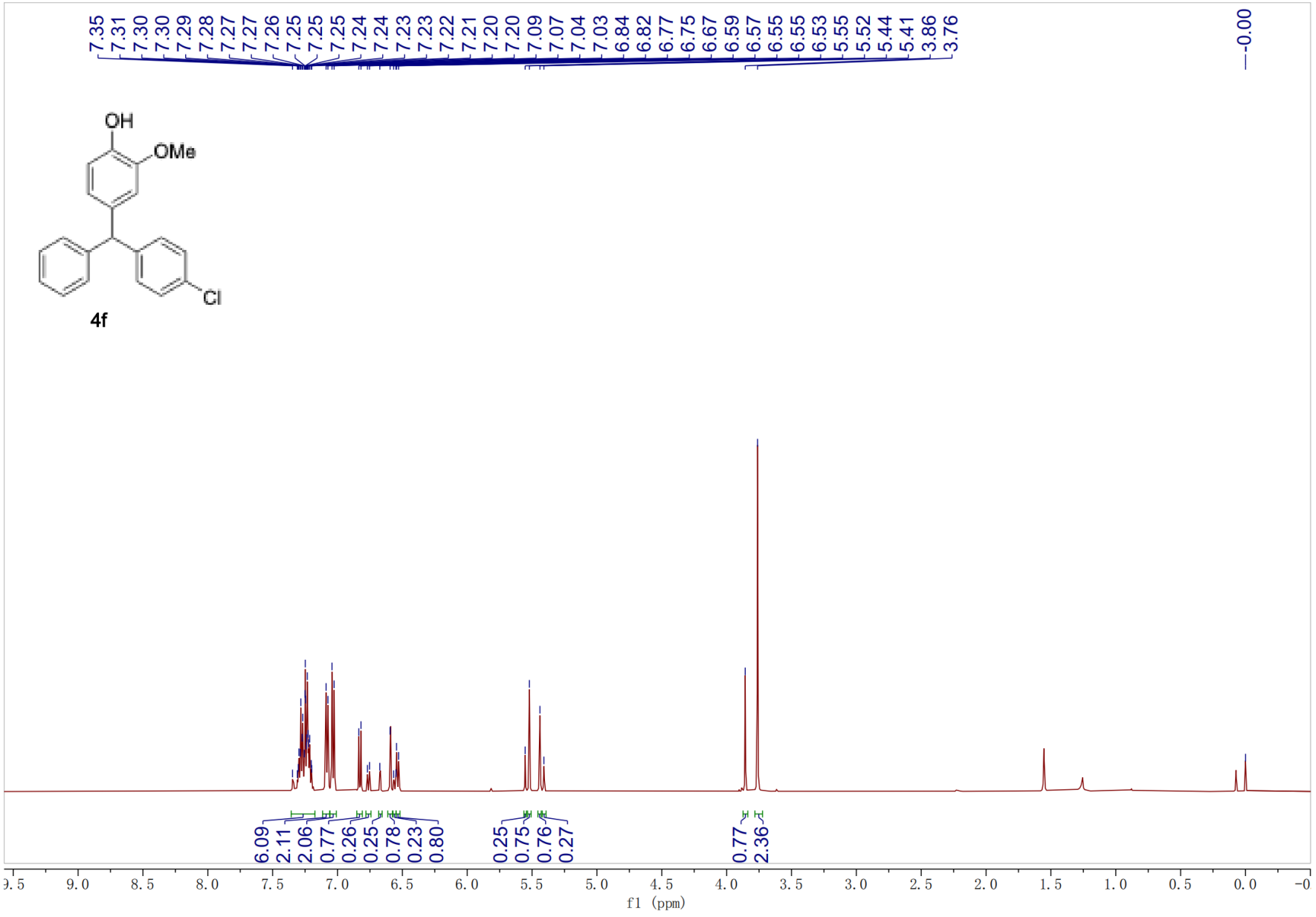

152.67
143.95
143.10
135.96
135.16
131.90
130.69
129.26
128.31
128.27
127.50
126.32
116.33
77.25
77.00
76.75
55.70
34.53
29.54
OH
tBu
Cl
4c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

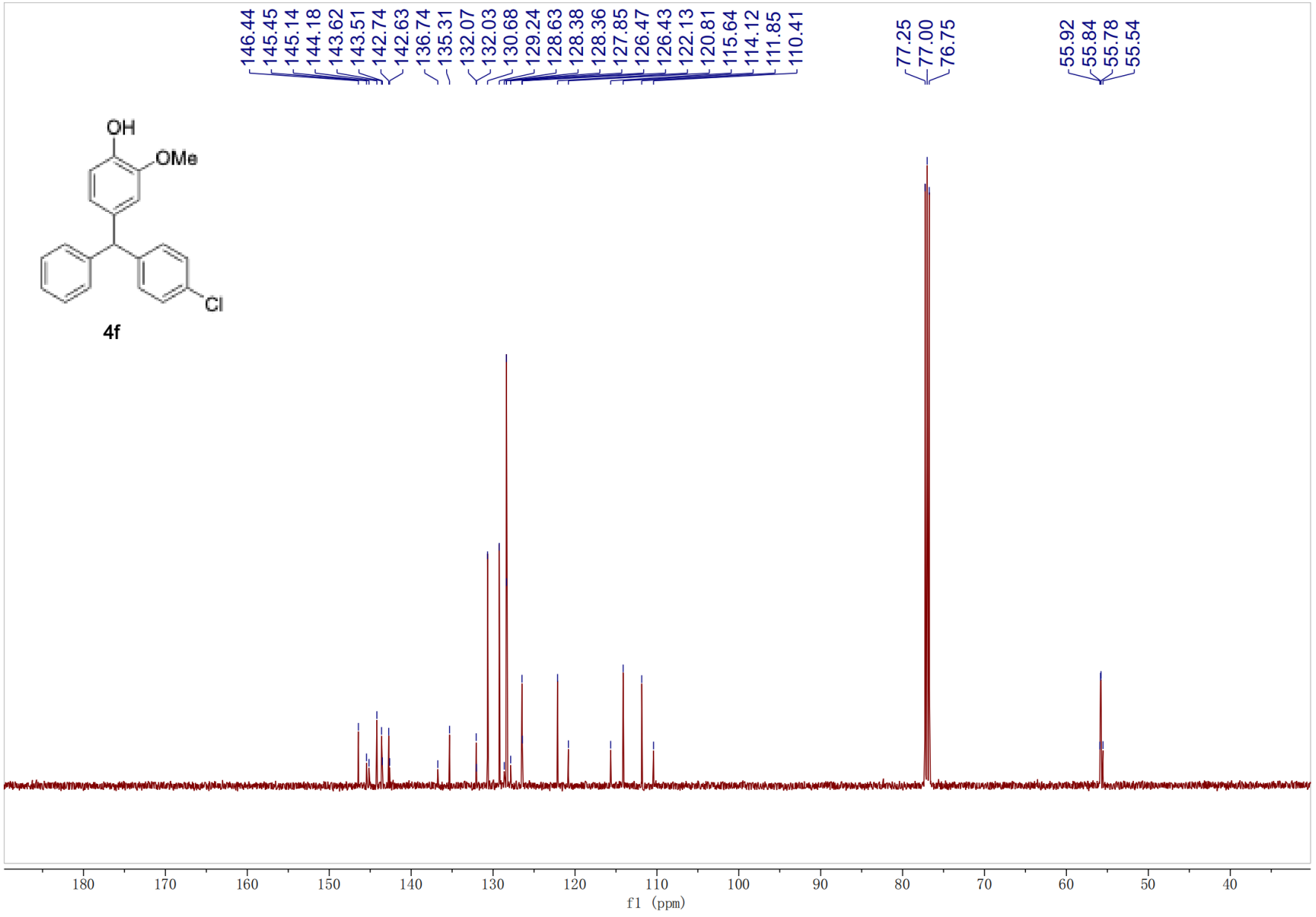

7.46
7.45
7.43
7.41
7.41
7.40
7.30
7.29
7.27
7.25
7.25
7.24
7.12
7.11
7.08
7.06
6.98
6.98
6.97
6.96
6.95
6.95
6.91
5.15
0.00
OH
Ph
Cl
4d
5.10
5.88
2.13
2.16
1.06
1.14
1.09
1.01
1.00
f1 (ppm)

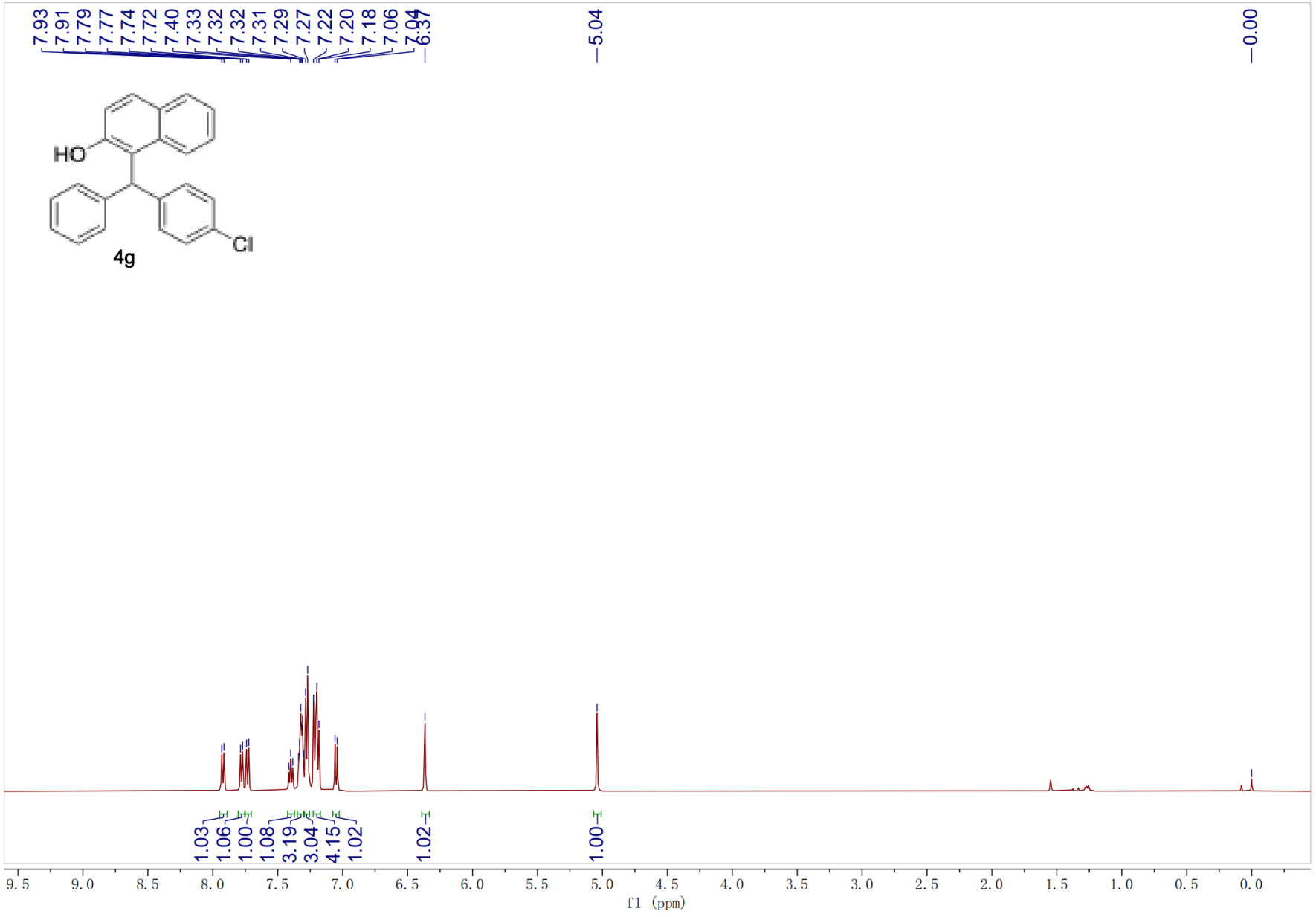

151.00
143.57
142.69
136.94
135.81
132.08
130.98
130.69
129.93
129.26
129.02
128.43
127.97
127.89
126.48
115.77
77.25
77.00
76.75
55.46
OH
Ph
Cl
4d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

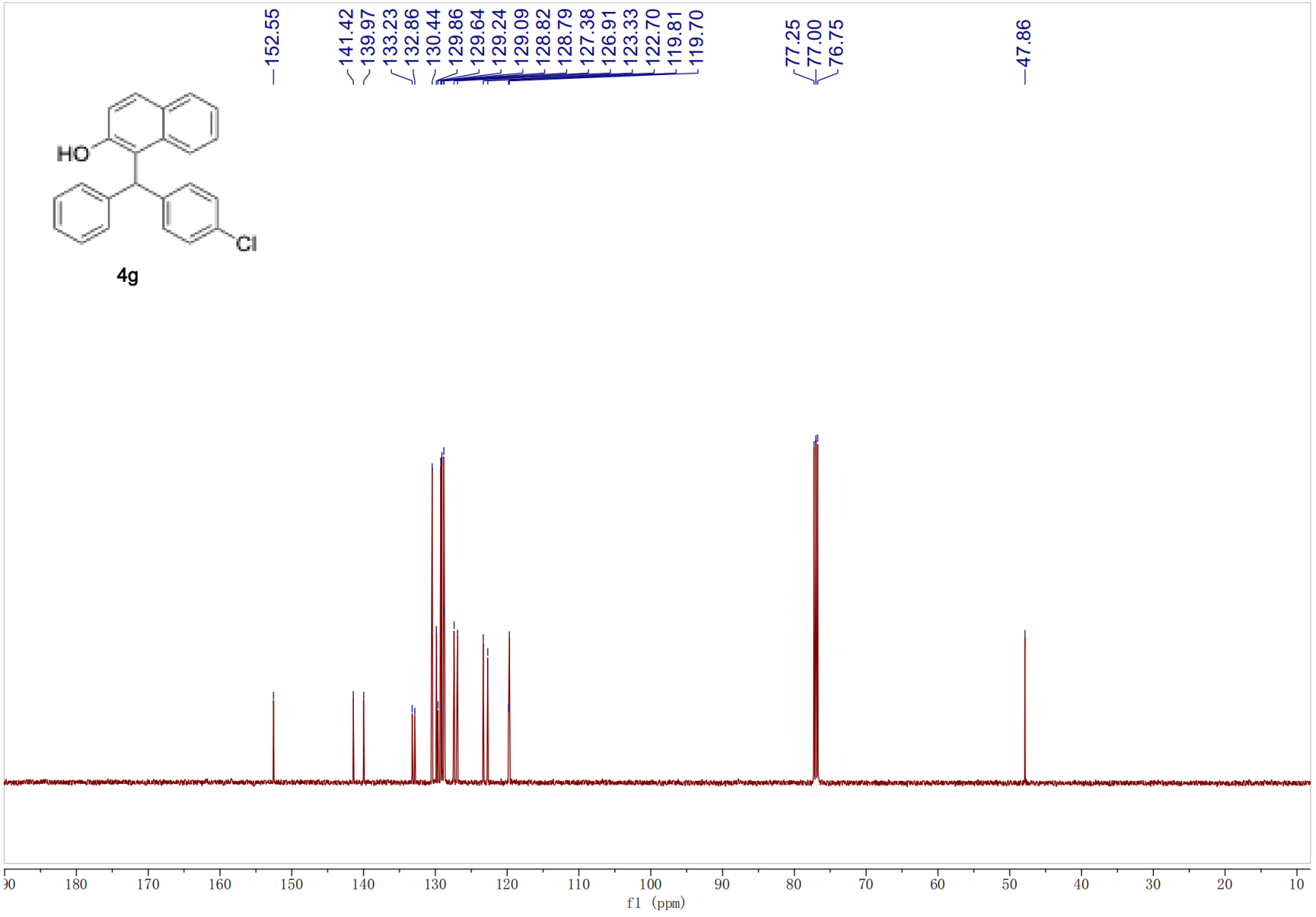

7.31
7.30
7.28
7.27
7.25
7.25
7.24
7.23
7.19
7.17
7.17
7.15
6.12
6.11
6.03
6.02
4.80
3.75
3.70
0.00
OMe
MeO
OH
Cl
4e
5.70
4.33
1.04
2.11
1.00
3.21
3.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

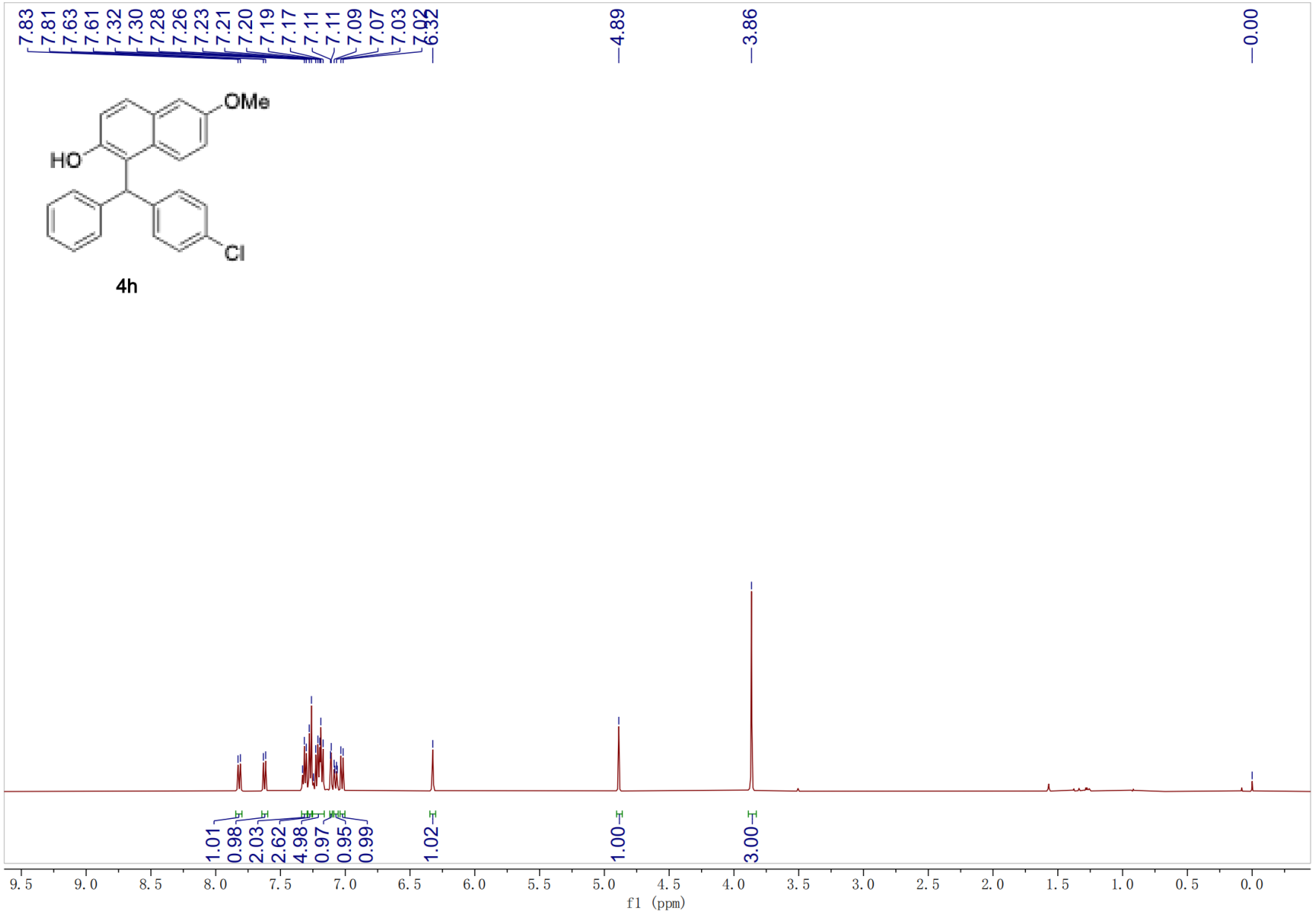

160.28
158.77
155.94
142.07
140.78
132.26
130.37
128.84
128.70
128.63
126.85
110.44
94.67
91.92
77.25
77.20
77.00
76.75
55.84
55.22
44.41
OMe
MeO
OH
Cl
4e
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

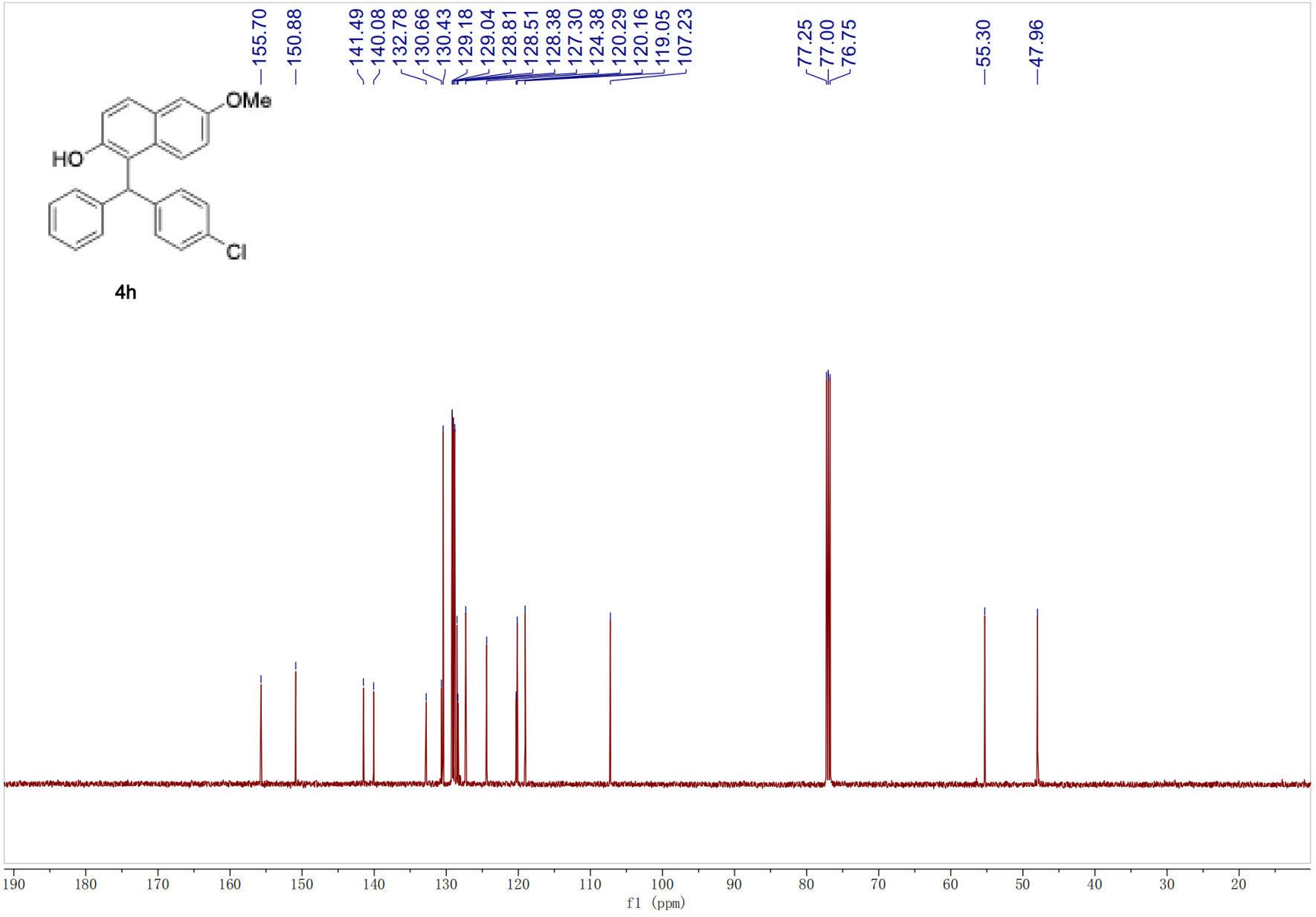

7.35
7.31
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.20
7.20
7.09
7.07
7.04
7.03
6.84
6.82
6.77
6.75
6.67
6.59
6.57
6.55
6.55
6.53
5.55
5.52
5.44
5.41
3.86
3.76
-0.00
OH
OMe
Cl
4f
6.09
2.11
2.06
0.77
0.26
0.25
0.78
0.23
0.80
0.25
0.75
0.76
0.27
0.77
2.36
f1 (ppm)

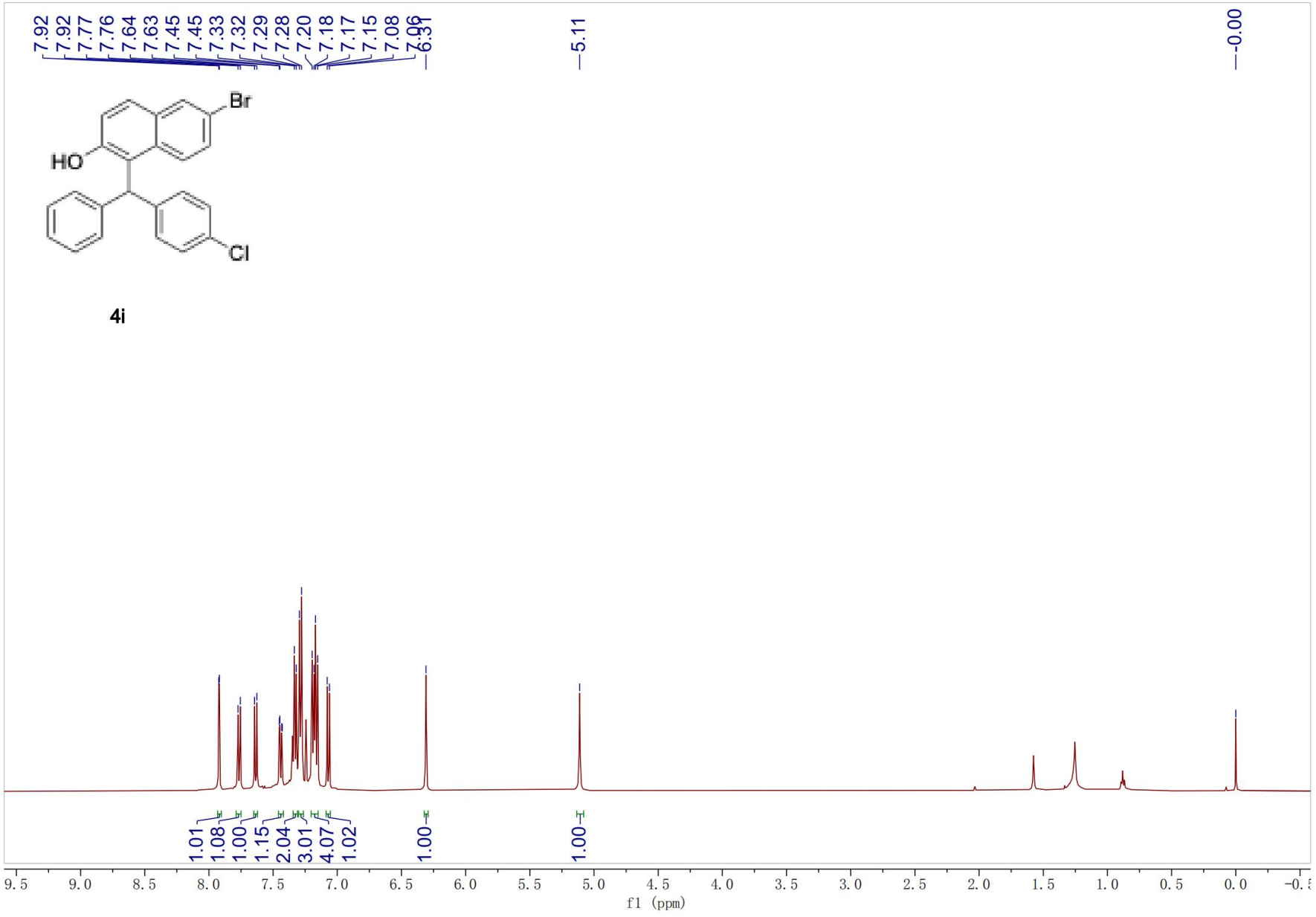

146.44
145.45
145.14
144.18
143.62
143.51
142.74
142.63
136.74
135.31
132.07
132.03
130.68
129.24
128.63
128.38
128.36
127.85
126.47
126.43
122.13
120.81
115.64
114.12
111.85
110.41
77.25
77.00
76.75
55.92
55.84
55.78
55.54
OH
OMe
Cl
4f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)

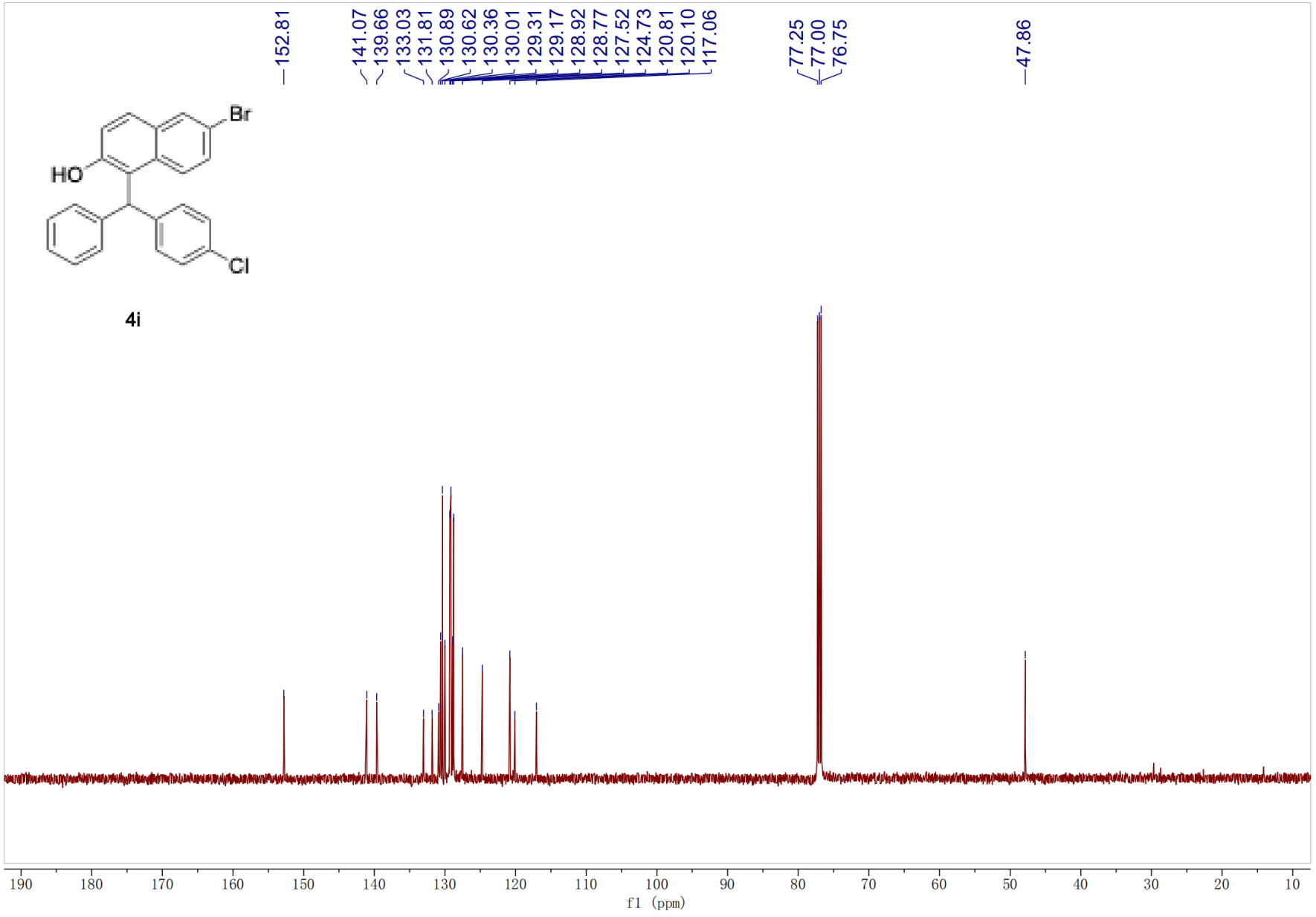

7.93
7.91
7.79
7.77
7.74
7.72
7.40
7.33
7.32
7.32
7.31
7.29
7.27
7.22
7.20
7.18
7.06
7.04
6.37
5.04
0.00
HO
Cl
4g
1.03
1.06
1.00
1.08
3.19
3.04
4.15
1.02
1.02
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

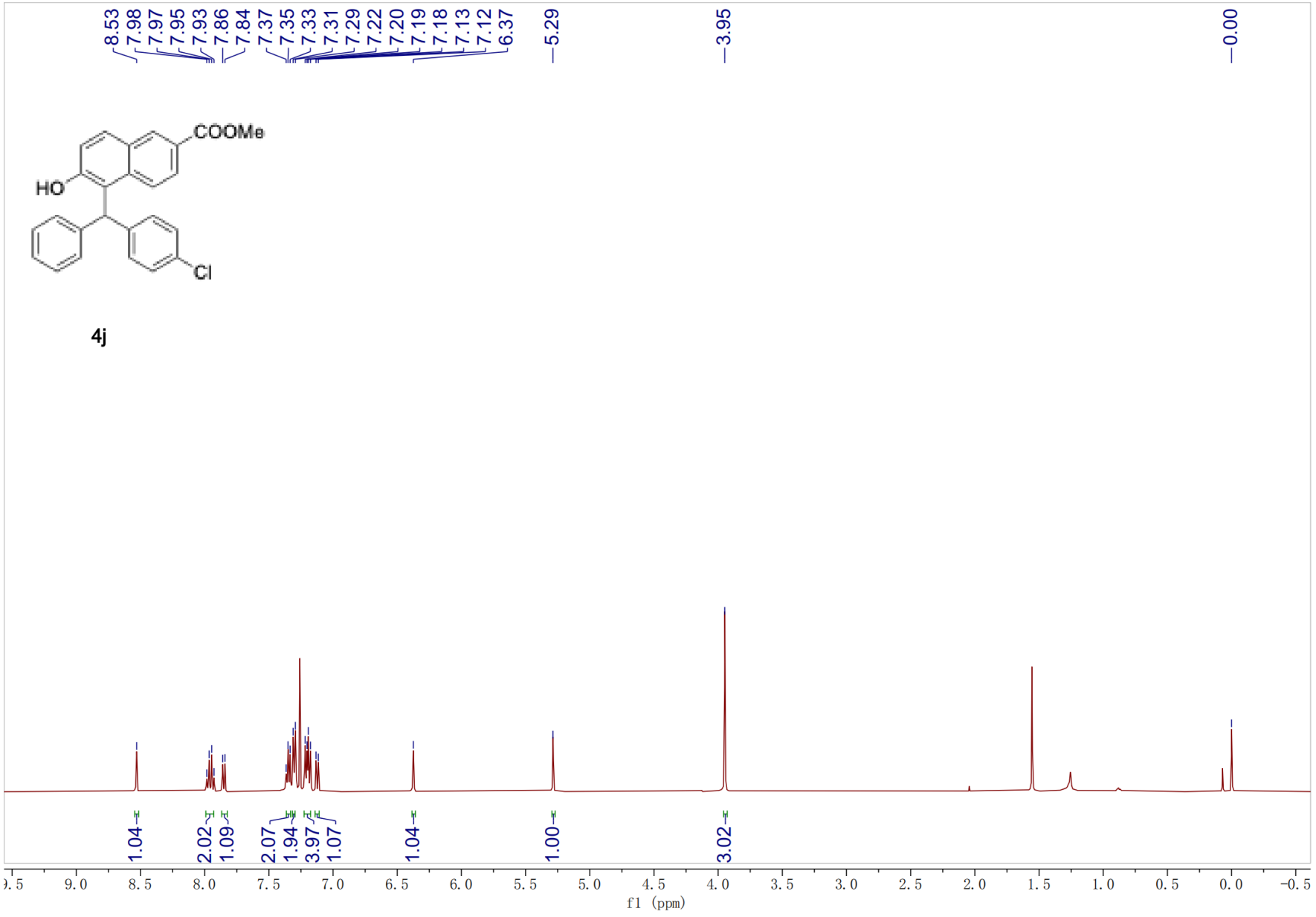

152.55
141.42
139.97
133.23
132.86
130.44
129.86
129.64
129.24
129.09
128.82
128.79
127.38
126.91
123.33
122.70
119.81
119.70
77.25
77.00
76.75
47.86
HO
Cl
4g
f1 (ppm)

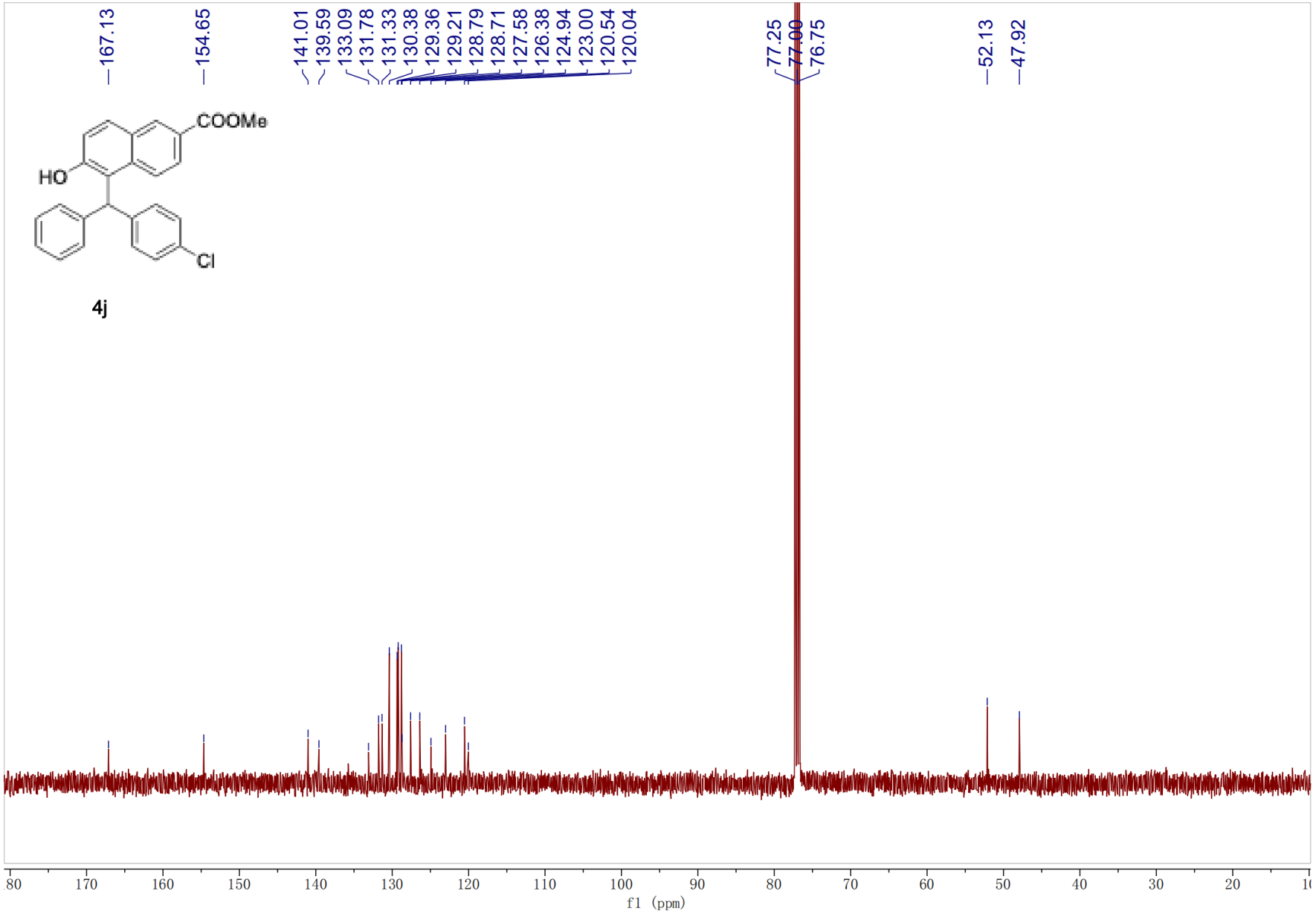

7.83
7.81
7.63
7.61
7.32
7.30
7.28
7.26
7.23
7.21
7.20
7.19
7.17
7.11
7.11
7.09
7.07
7.03
7.02
6.32
4.89
3.86
0.00
OMe
HO
Cl
4h
1.01
0.98
2.03
2.62
4.98
0.97
0.95
0.99
1.02
1.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

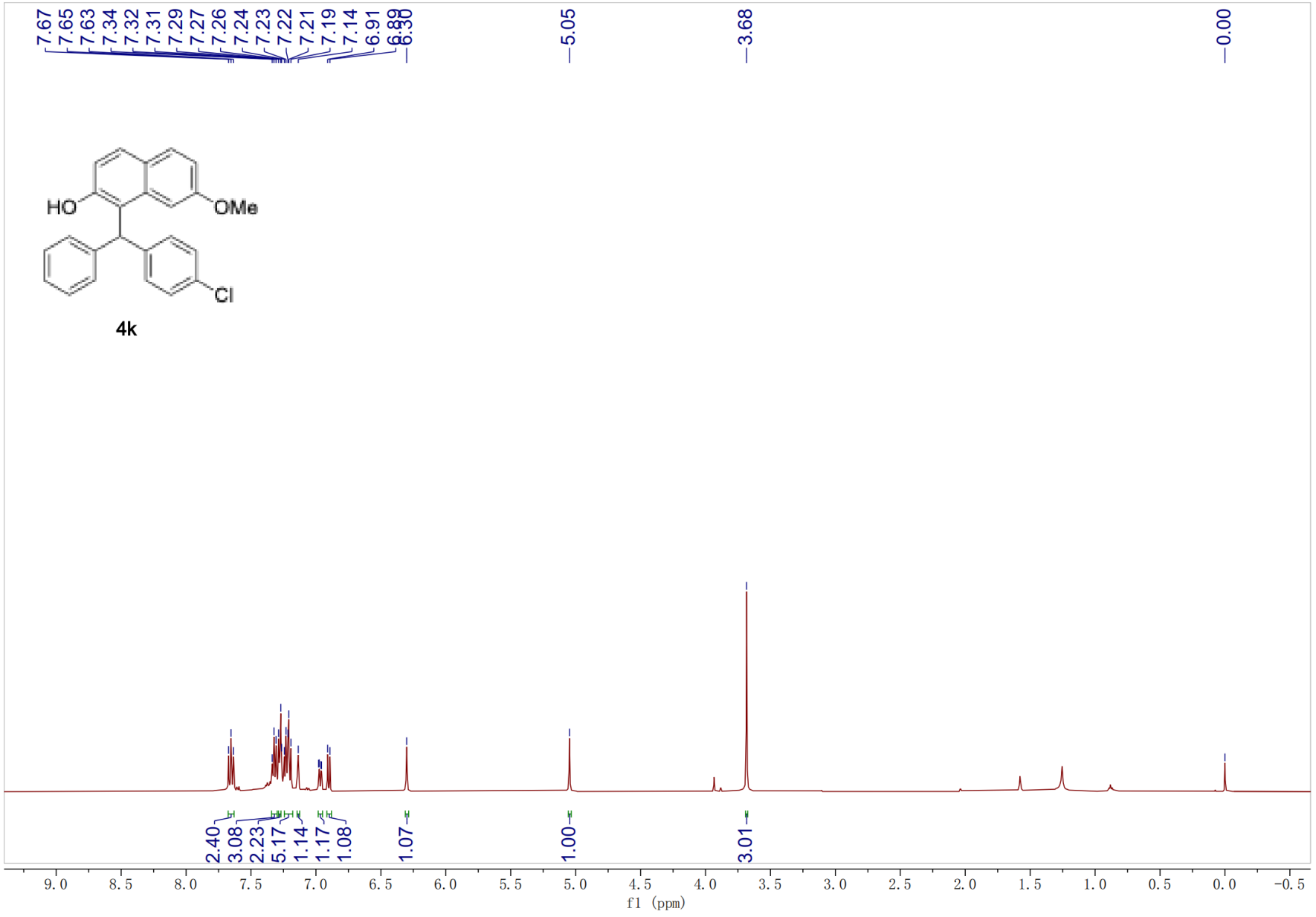

155.70
150.88
141.49
140.08
132.78
130.66
130.43
129.18
129.04
128.81
128.51
128.38
127.30
124.38
120.29
120.16
119.05
107.23
77.25
77.00
76.75
55.30
47.96
OMe
HO
Cl
4h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

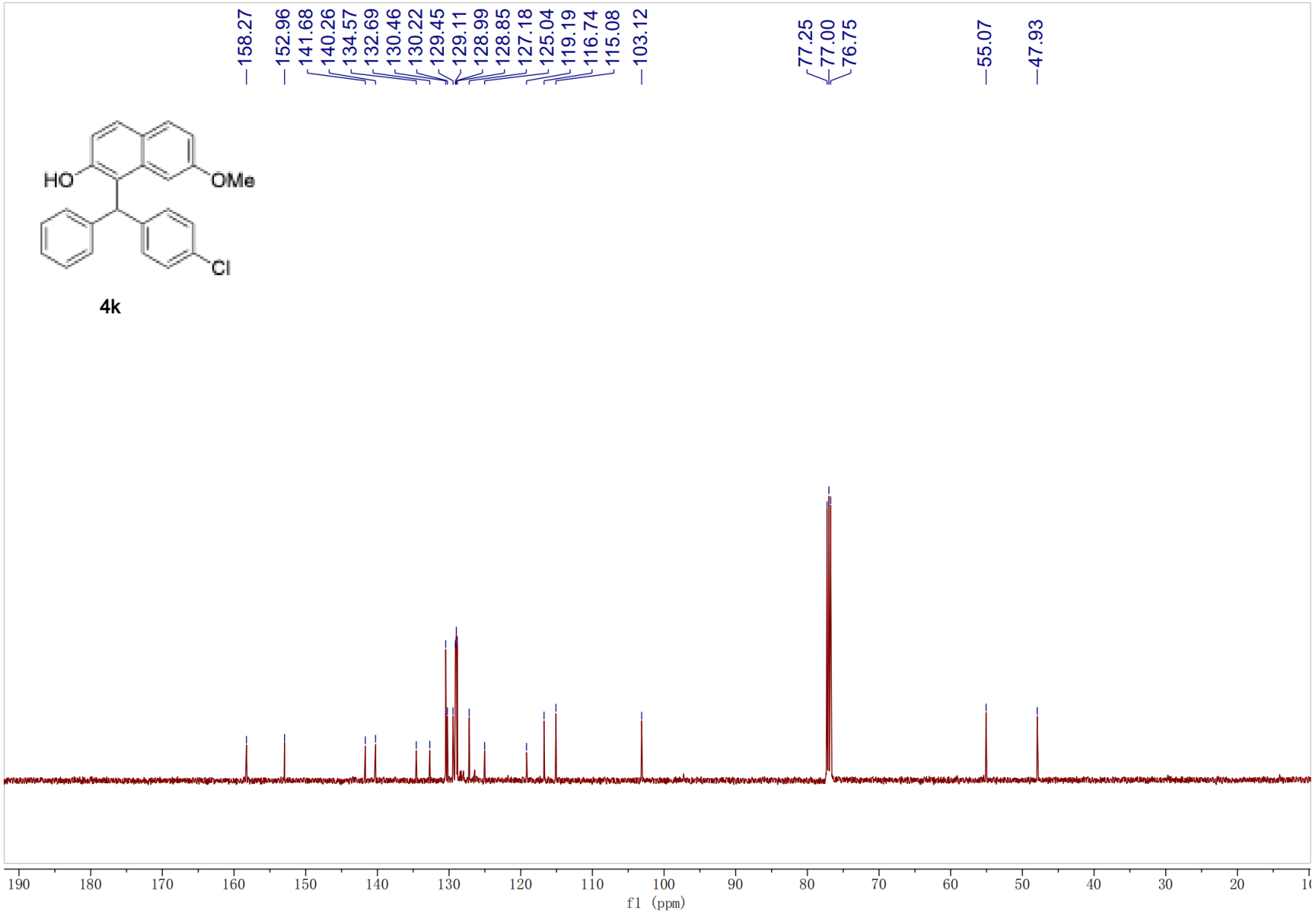

7.92
7.92
7.77
7.76
7.64
7.63
7.45
7.45
7.33
7.32
7.29
7.28
7.20
7.18
7.17
7.15
7.08
7.06
6.31
5.11
0.00
Br
HO
Cl
4i
1.01
1.08
1.00
1.15
2.04
3.01
4.07
1.02
1.00
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

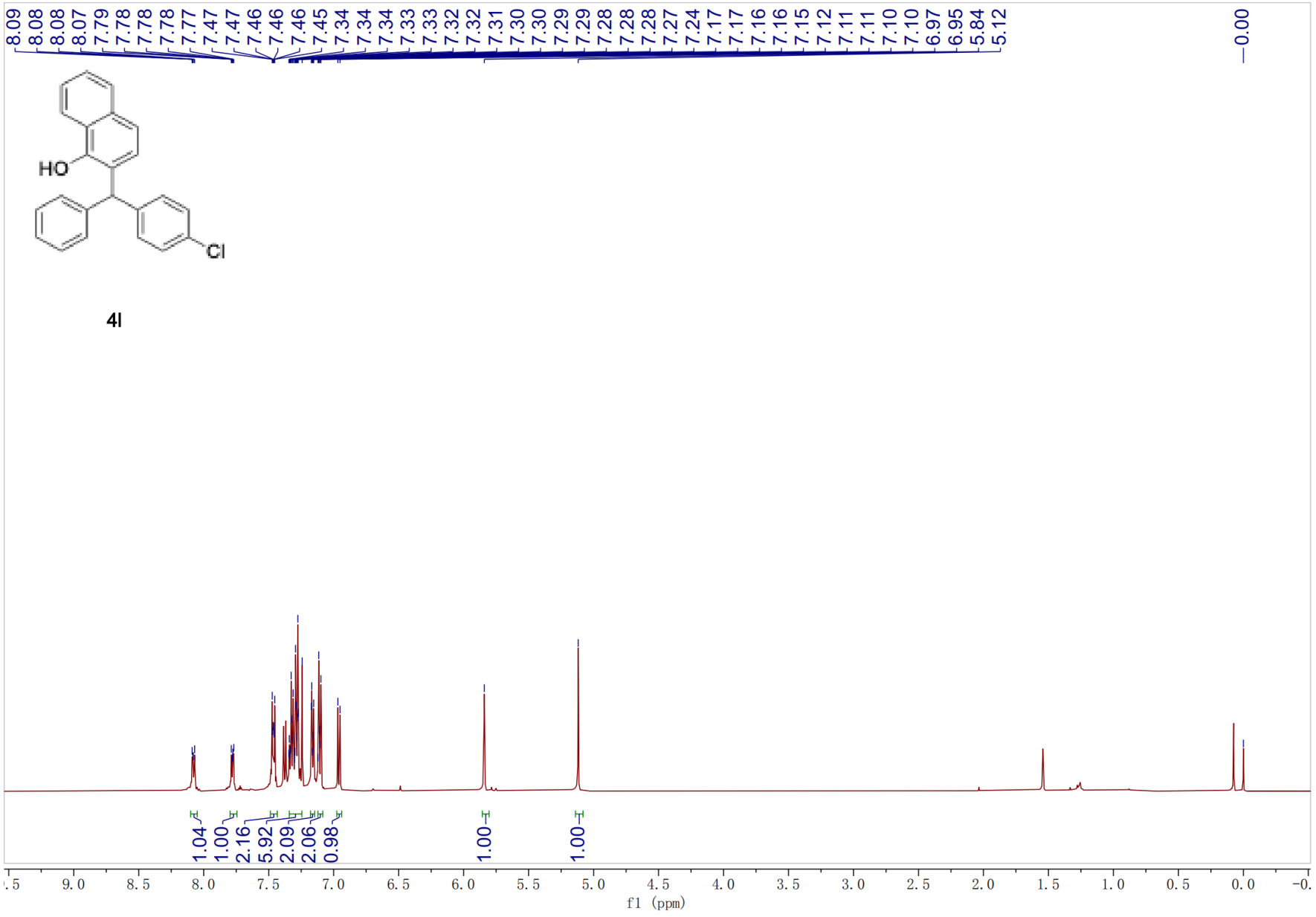

152.81
141.07
139.66
133.03
131.81
130.89
130.62
130.36
130.01
129.31
129.17
128.92
128.77
127.52
124.73
120.81
120.10
117.06
77.25
77.00
76.75
47.86
Br
HO
Cl
4i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

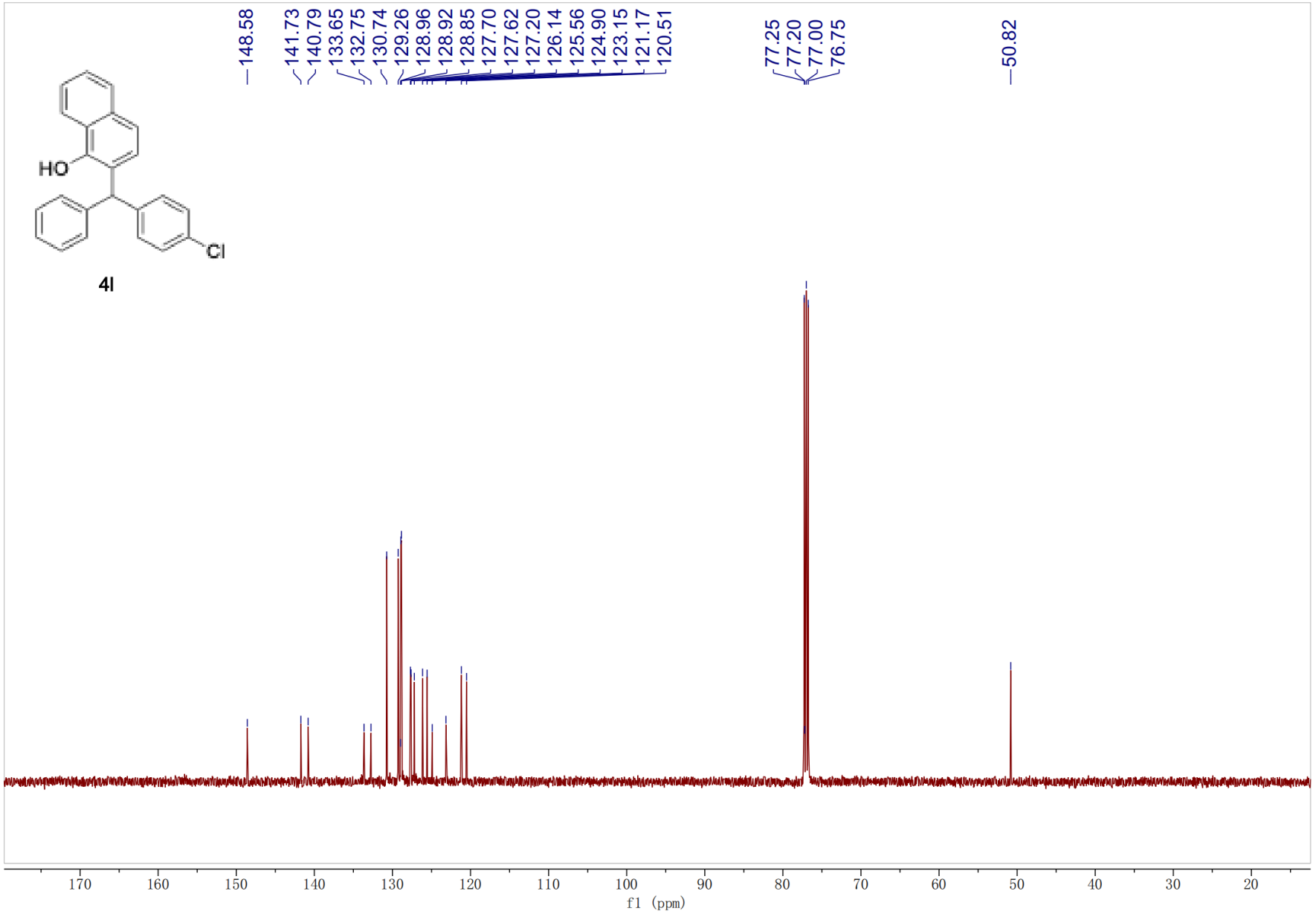

8.53
7.98
7.97
7.95
7.93
7.86
7.84
7.37
7.35
7.33
7.31
7.29
7.22
7.20
7.19
7.18
7.13
7.12
6.37
5.29
3.95
0.00
COOMe
HO
Cl
4j
1.04
2.02
1.09
2.07
1.94
3.97
1.07
1.04
1.00
3.02
f1 (ppm)

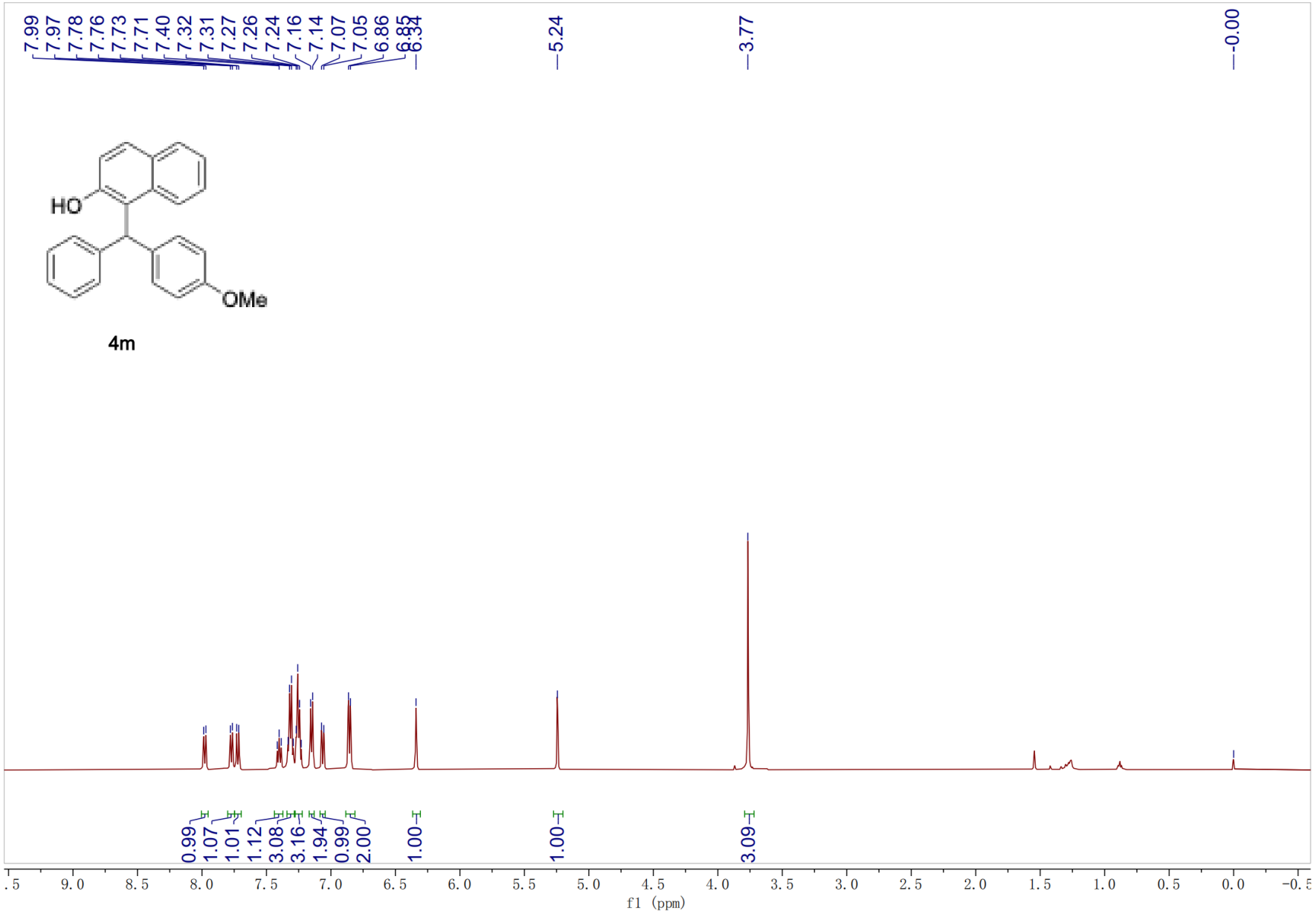

167.13
154.65
141.01
139.59
133.09
131.78
131.33
130.38
129.36
129.21
128.79
128.71
127.58
126.38
124.94
123.00
120.54
120.04
77.25
77.00
76.75
52.13
47.92
COOMe
HO
Cl
4j
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

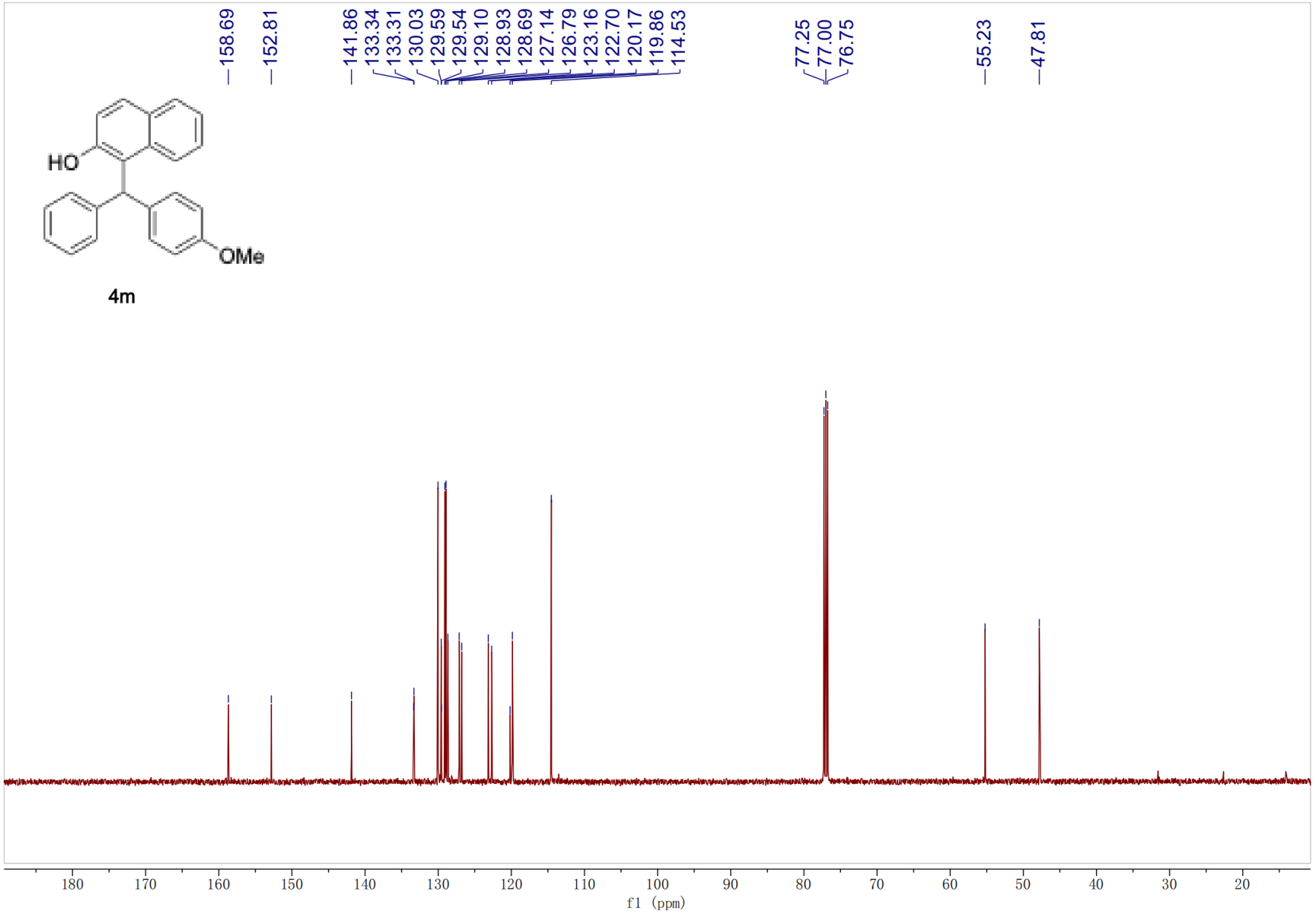

7.67
7.65
7.63
7.34
7.32
7.31
7.29
7.27
7.26
7.24
7.23
7.22
7.21
7.19
7.14
6.91
6.89
6.30
5.05
3.68
0.00
HO
OMe
Cl
4k
2.40
3.08
2.23
5.17
1.14
1.17
1.08
1.07
1.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

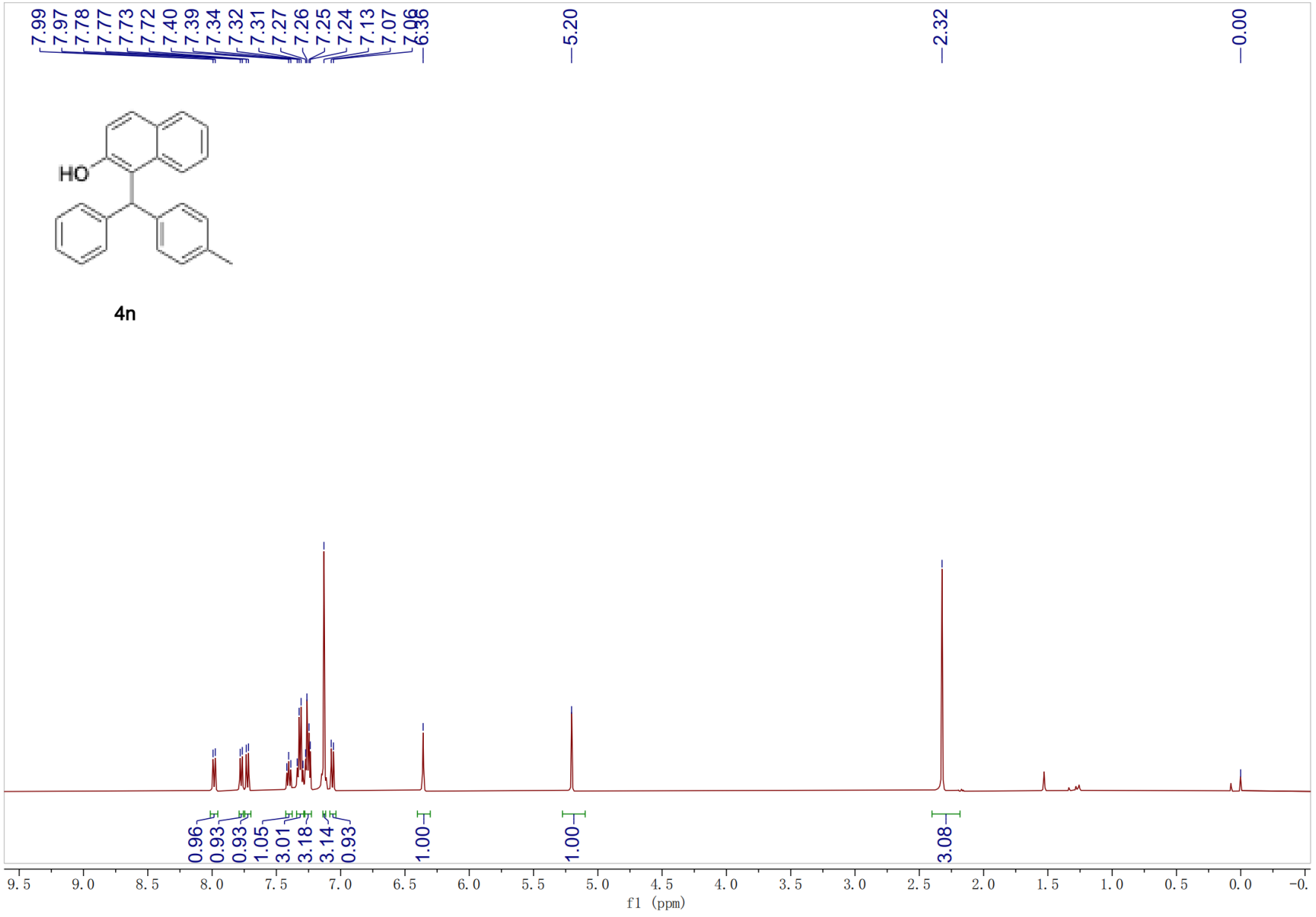

158.27
152.96
141.68
140.26
134.57
132.69
130.46
130.22
129.45
129.11
128.99
128.85
127.18
125.04
119.19
116.74
115.08
103.12
77.25
77.00
76.75
55.07
47.93
HO
OMe
Cl
4k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

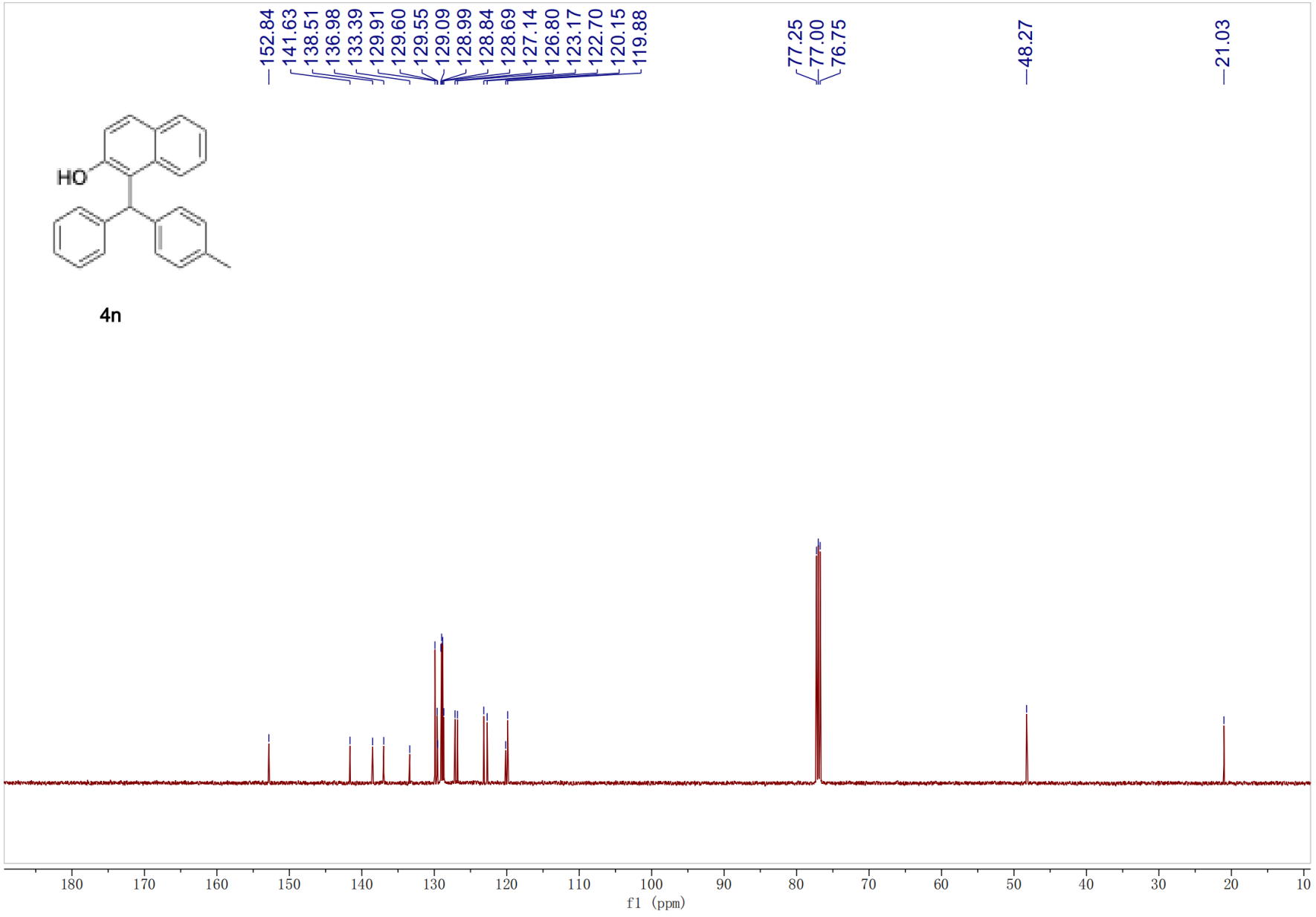

8.09
8.08
8.08
8.07
7.79
7.78
7.78
7.78
7.77
7.47
7.47
7.46
7.46
7.46
7.45
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.27
7.24
7.17
7.17
7.16
7.16
7.15
7.12
7.11
7.11
7.10
7.10
6.97
6.95
5.84
5.12
0.00
HO
Cl
4l
1.04
1.00
2.16
5.92
2.09
2.06
0.98
1.00
1.00
f1 (ppm)

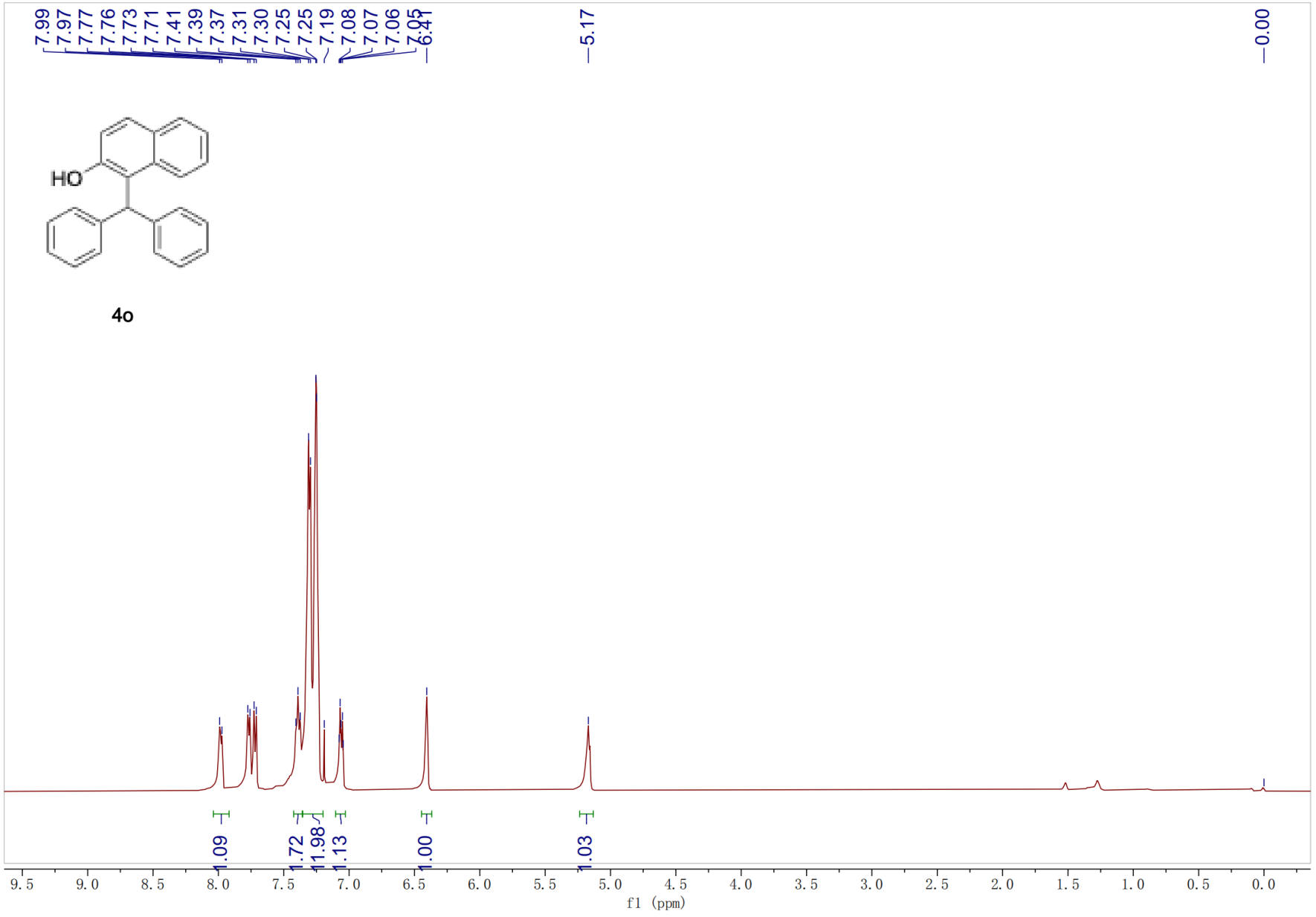

148.58
141.73
140.79
133.65
132.75
130.74
129.26
128.96
128.92
128.85
127.70
127.62
127.20
126.14
125.56
124.90
123.15
121.17
120.51
77.25
77.20
77.00
76.75
50.82
HO
Cl
4l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

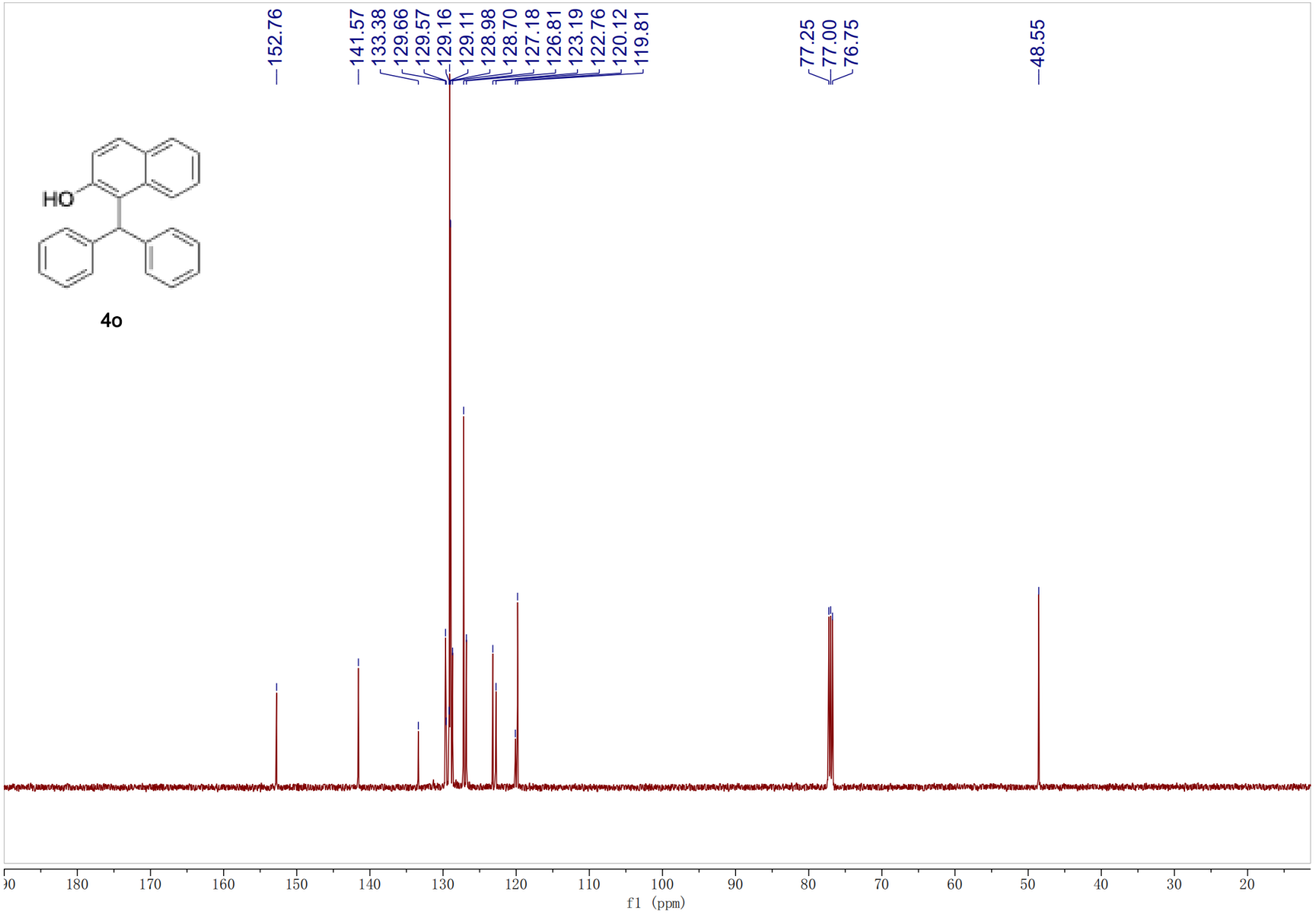

7.99
7.97
7.78
7.76
7.73
7.71
7.40
7.32
7.31
7.27
7.26
7.24
7.16
7.14
7.07
7.05
6.86
6.85
6.84
5.24
3.77
0.00
HO
OMe
4m
0.99
1.07
1.01
1.12
3.08
3.16
1.94
0.99
2.00
1.00
1.00
3.09
f1 (ppm)

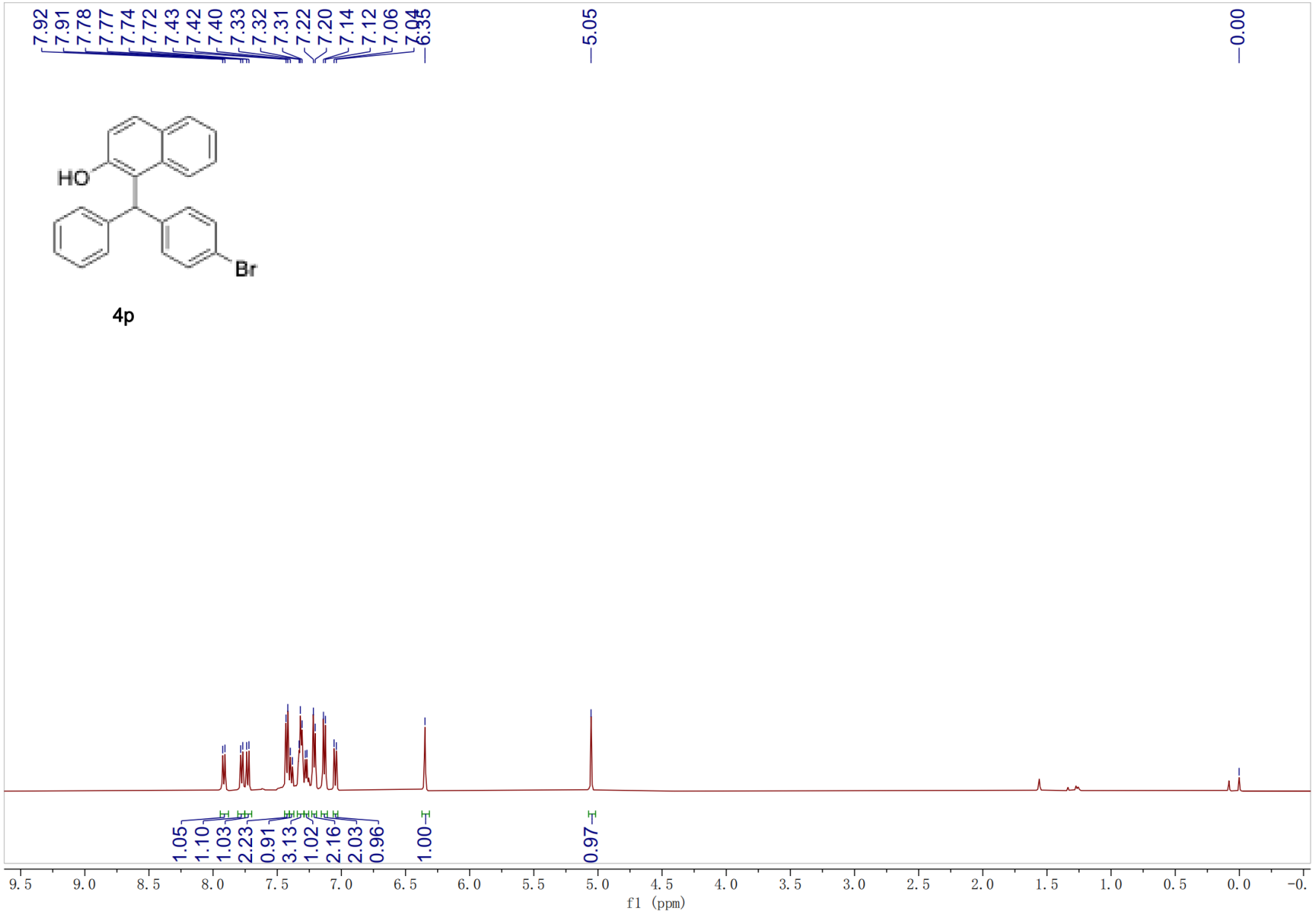

158.69
152.81
141.86
133.34
133.31
130.03
129.59
129.54
129.10
128.93
128.69
127.14
126.79
123.16
122.70
120.17
119.86
114.53
77.25
77.00
76.75
55.23
47.81
HO
OMe
4m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

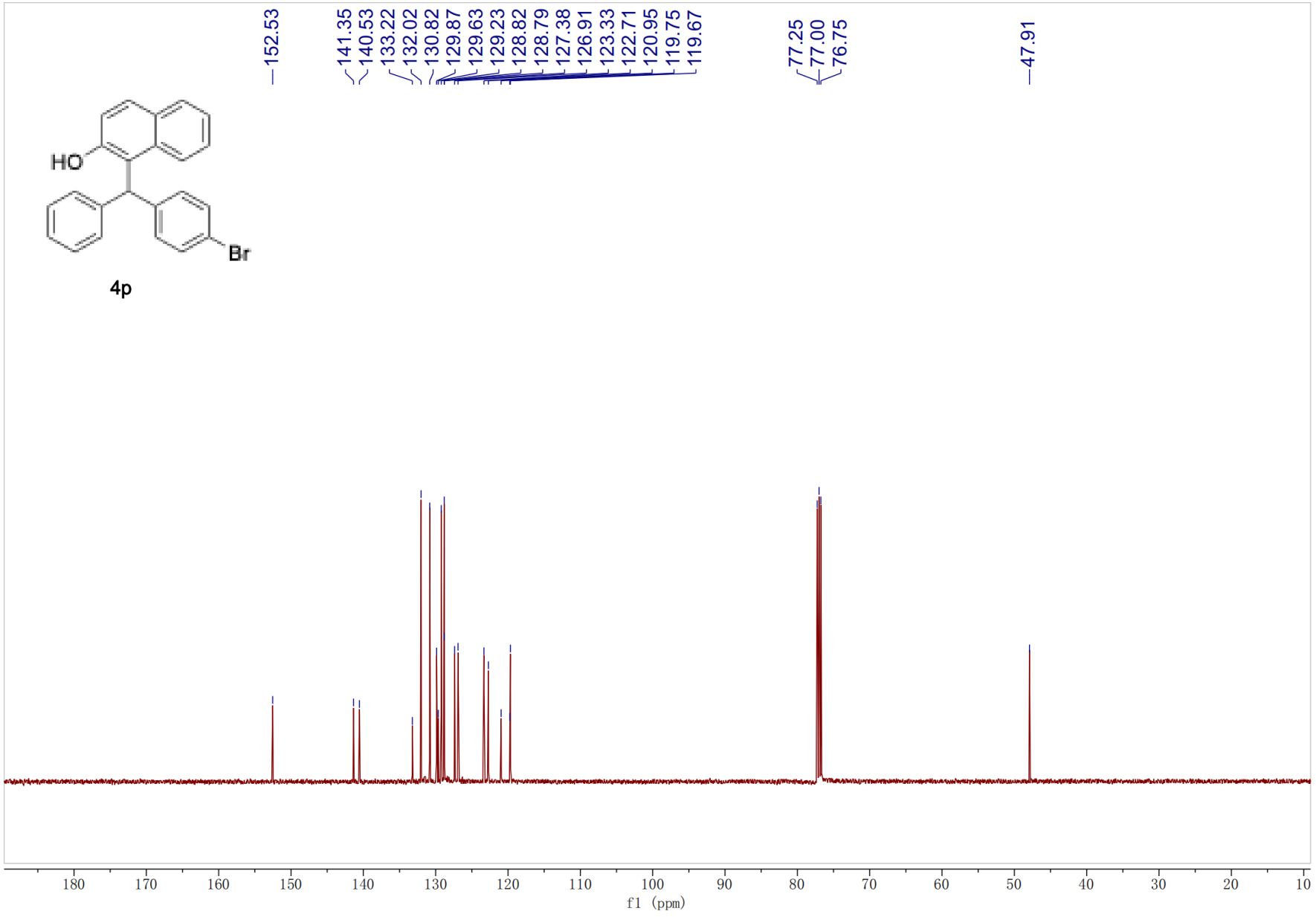

7.99
7.97
7.78
7.77
7.73
7.72
7.40
7.39
7.34
7.32
7.31
7.27
7.26
7.25
7.24
7.13
7.07
7.06
6.36
5.20
2.32
0.00
HO
4n
0.96
0.93
0.93
1.05
3.01
3.18
3.14
0.93
1.00
1.00
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

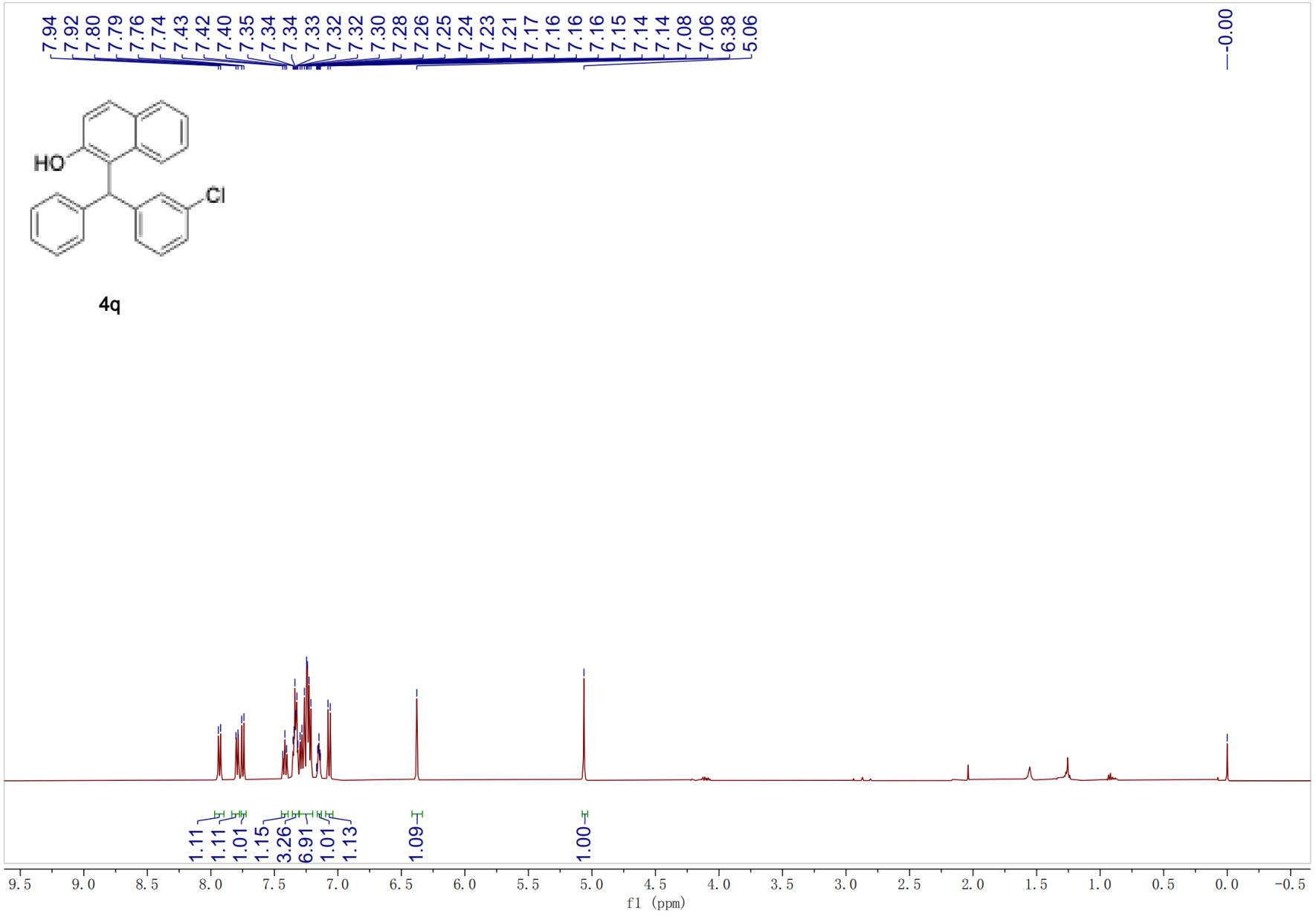

152.84
141.63
138.51
136.98
133.39
129.91
129.60
129.55
129.09
128.99
128.84
128.69
127.14
126.80
123.17
122.70
120.15
119.88
77.25
77.00
76.75
48.27
21.03
HO
4n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

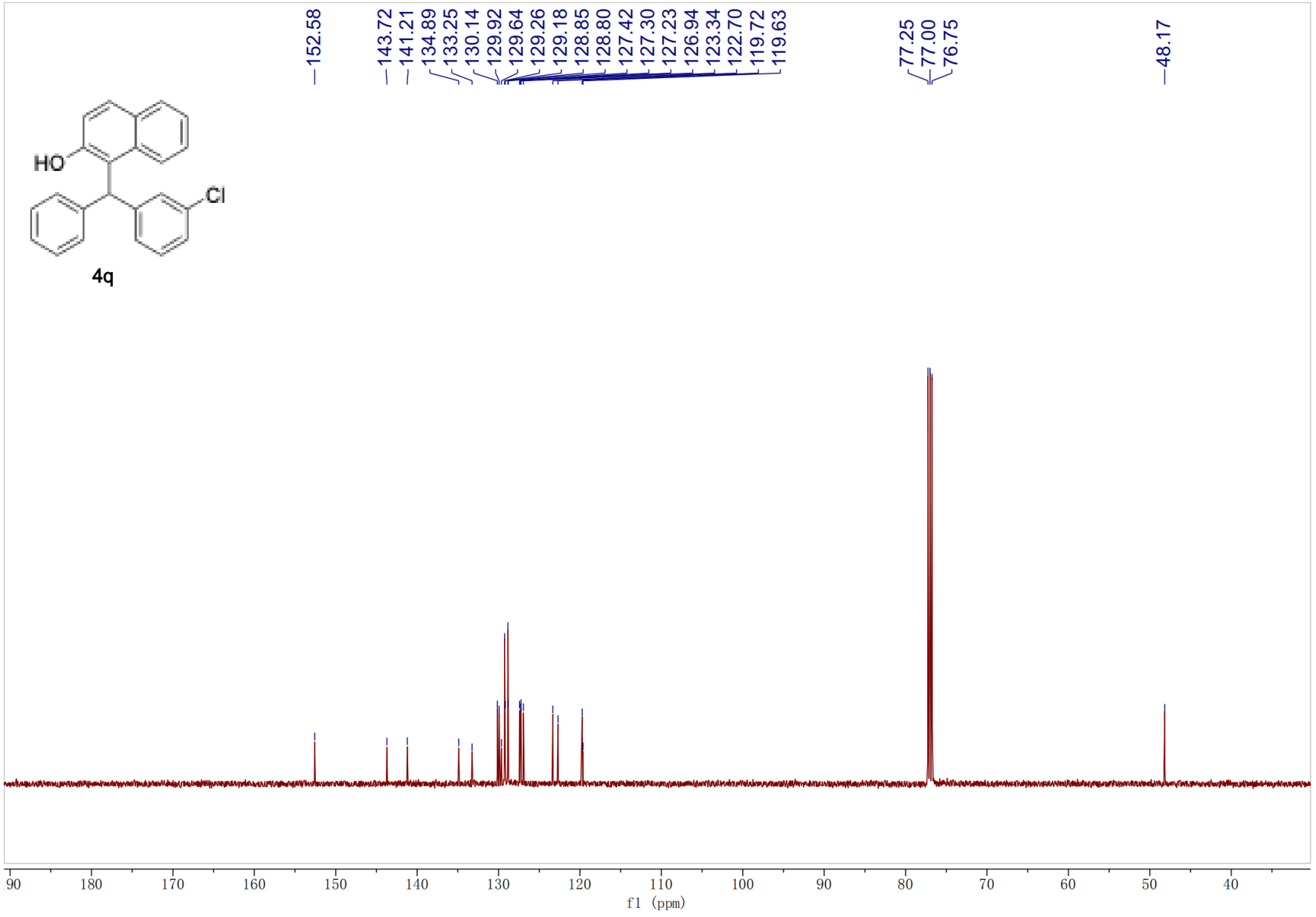

7.99
7.97
7.77
7.76
7.73
7.71
7.41
7.39
7.37
7.31
7.30
7.25
7.25
7.19
7.08
7.07
7.06
7.05
6.41
5.17
0.00
HO
4o
1.09
1.72
11.98
1.13
1.00
1.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

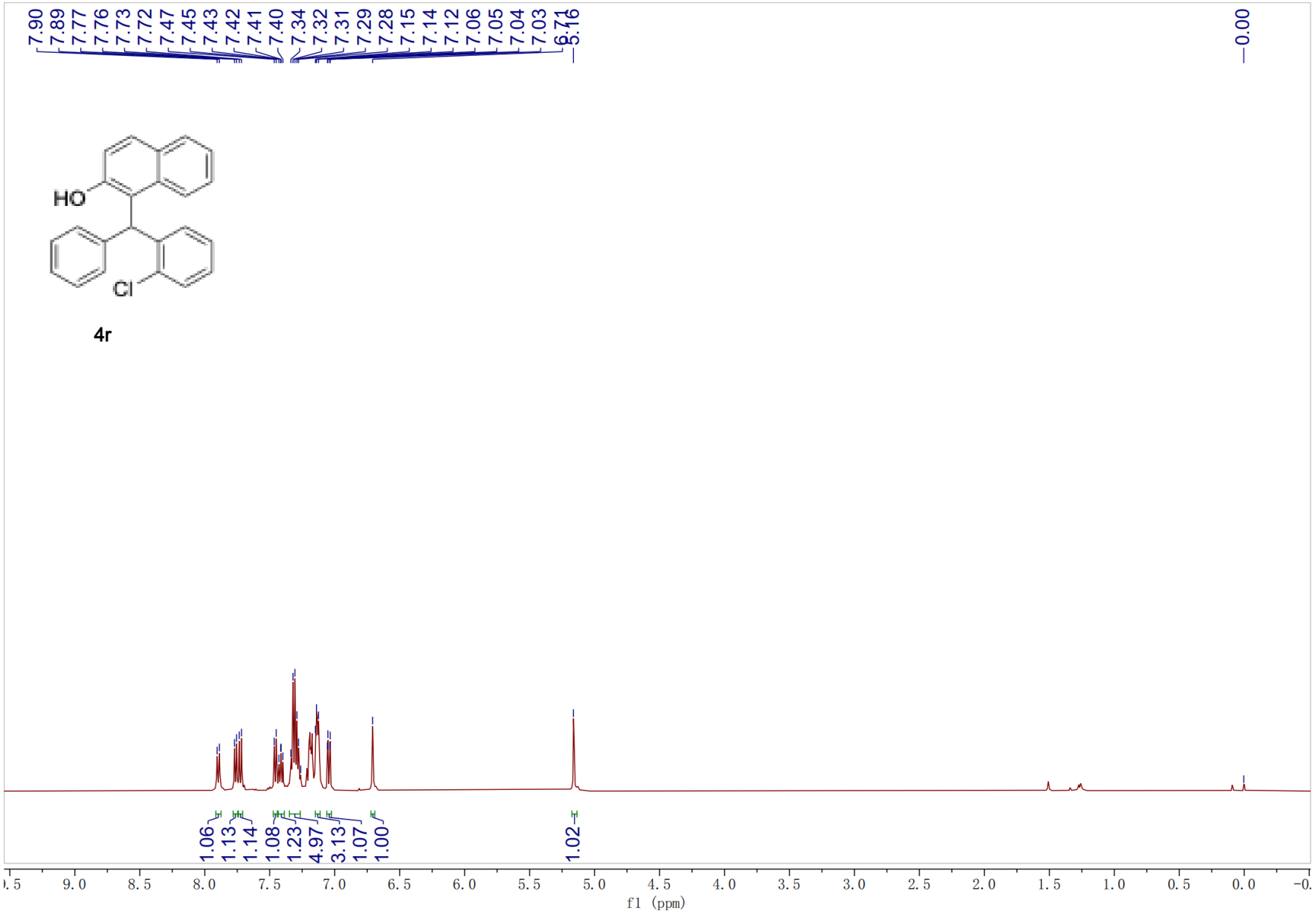

152.76
141.57
133.38
129.66
129.57
129.16
129.11
128.98
128.70
127.18
126.81
123.19
122.76
120.12
119.81
77.25
77.00
76.75
48.55
HO
4o
f1 (ppm)

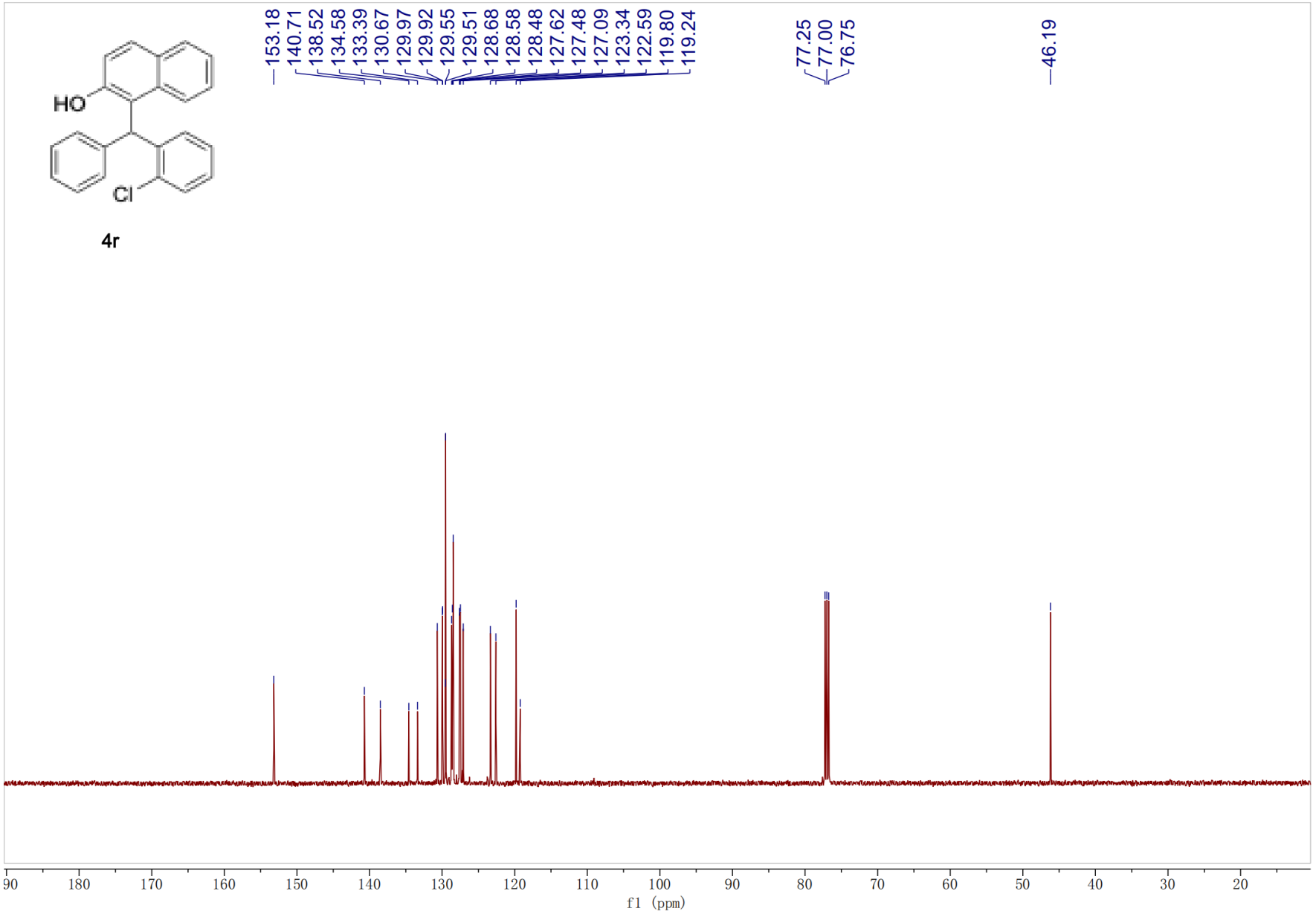

7.92
7.91
7.78
7.77
7.74
7.72
7.43
7.42
7.40
7.33
7.32
7.31
7.22
7.20
7.14
7.12
7.06
6.35
5.05
0.00
HO
Br
4p
1.05
1.10
1.03
2.23
0.91
3.13
1.02
2.16
2.03
0.96
1.00
0.97
f1 (ppm)


152.53
141.35
140.53
133.22
132.02
130.82
129.87
129.63
129.23
128.82
128.79
127.38
126.91
123.33
122.71
120.95
119.75
119.67
77.25
77.00
76.75
47.91
HO
Br
4p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

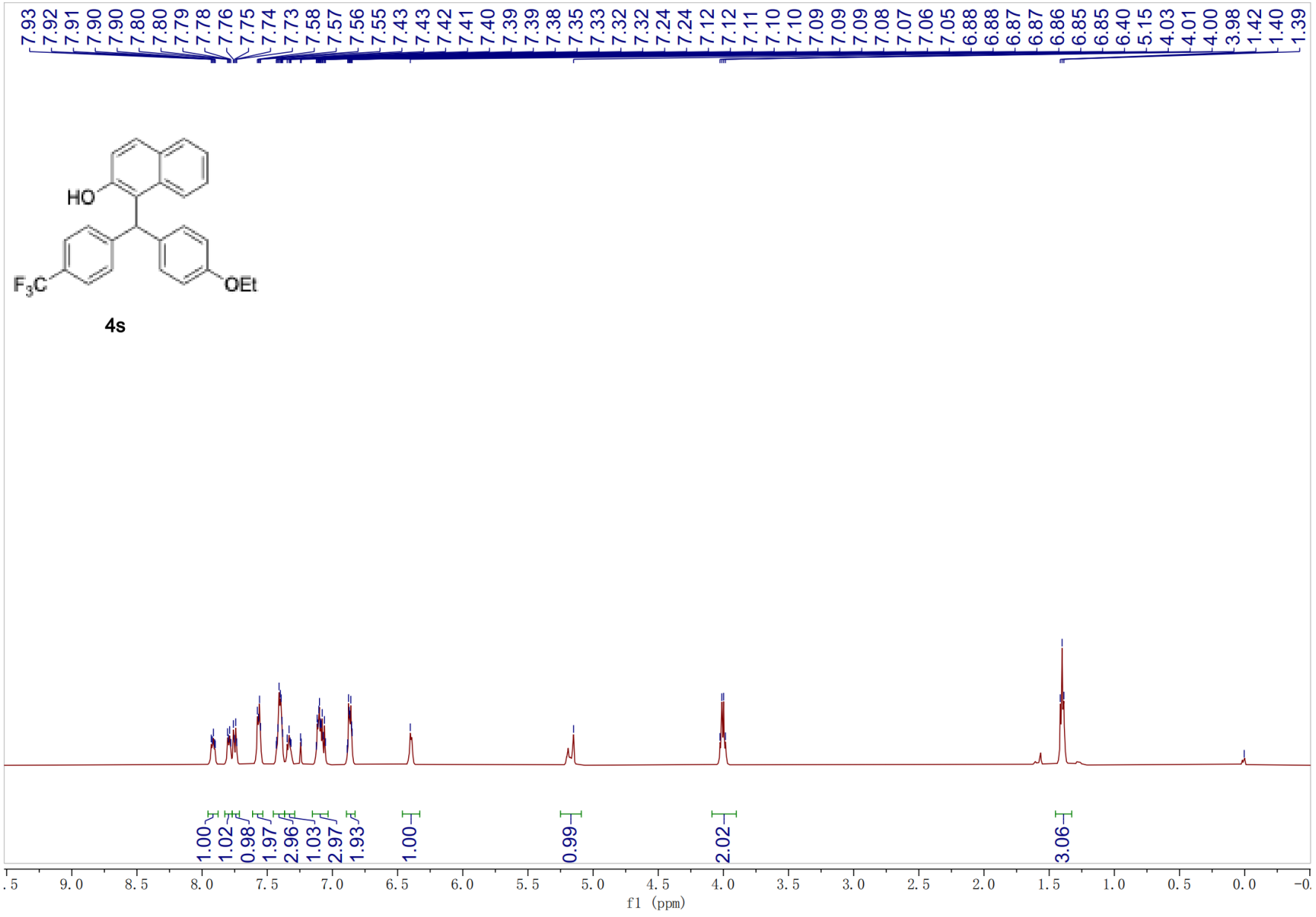

7.94
7.92
7.80
7.79
7.76
7.74
7.43
7.42
7.40
7.35
7.34
7.34
7.33
7.32
7.32
7.30
7.28
7.26
7.25
7.24
7.23
7.21
7.17
7.16
7.16
7.16
7.15
7.14
7.14
7.08
7.06
6.38
5.06
-0.00
HO
Cl
4q
1.11
1.11
1.01
1.15
3.26
6.91
1.01
1.13
1.09
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

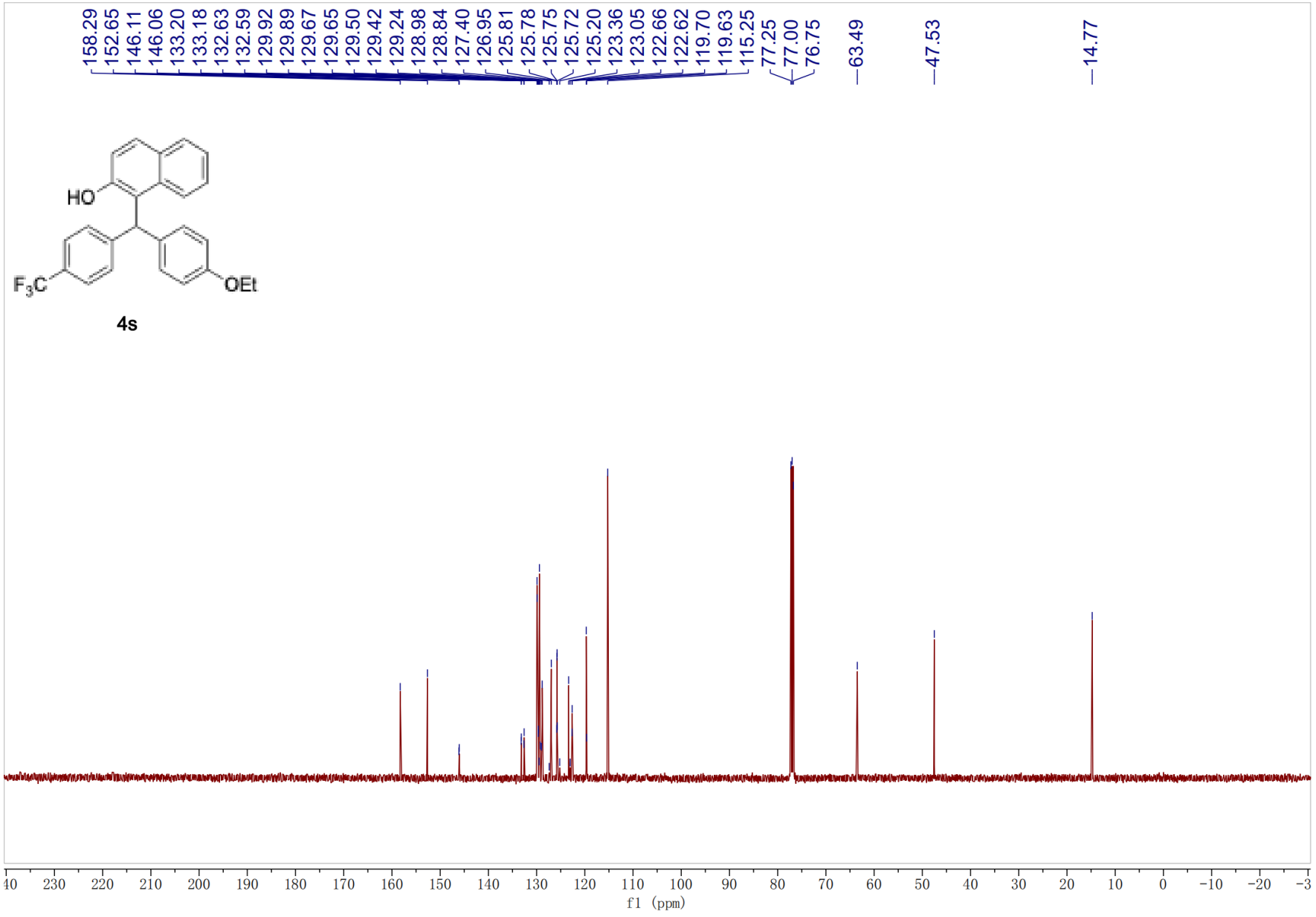

152.58
143.72
141.21
134.89
133.25
130.14
129.92
129.64
129.26
129.18
128.85
128.80
127.42
127.30
127.23
126.94
123.34
122.70
119.72
119.63
77.25
77.00
76.75
48.17
HO
Cl
4q
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)

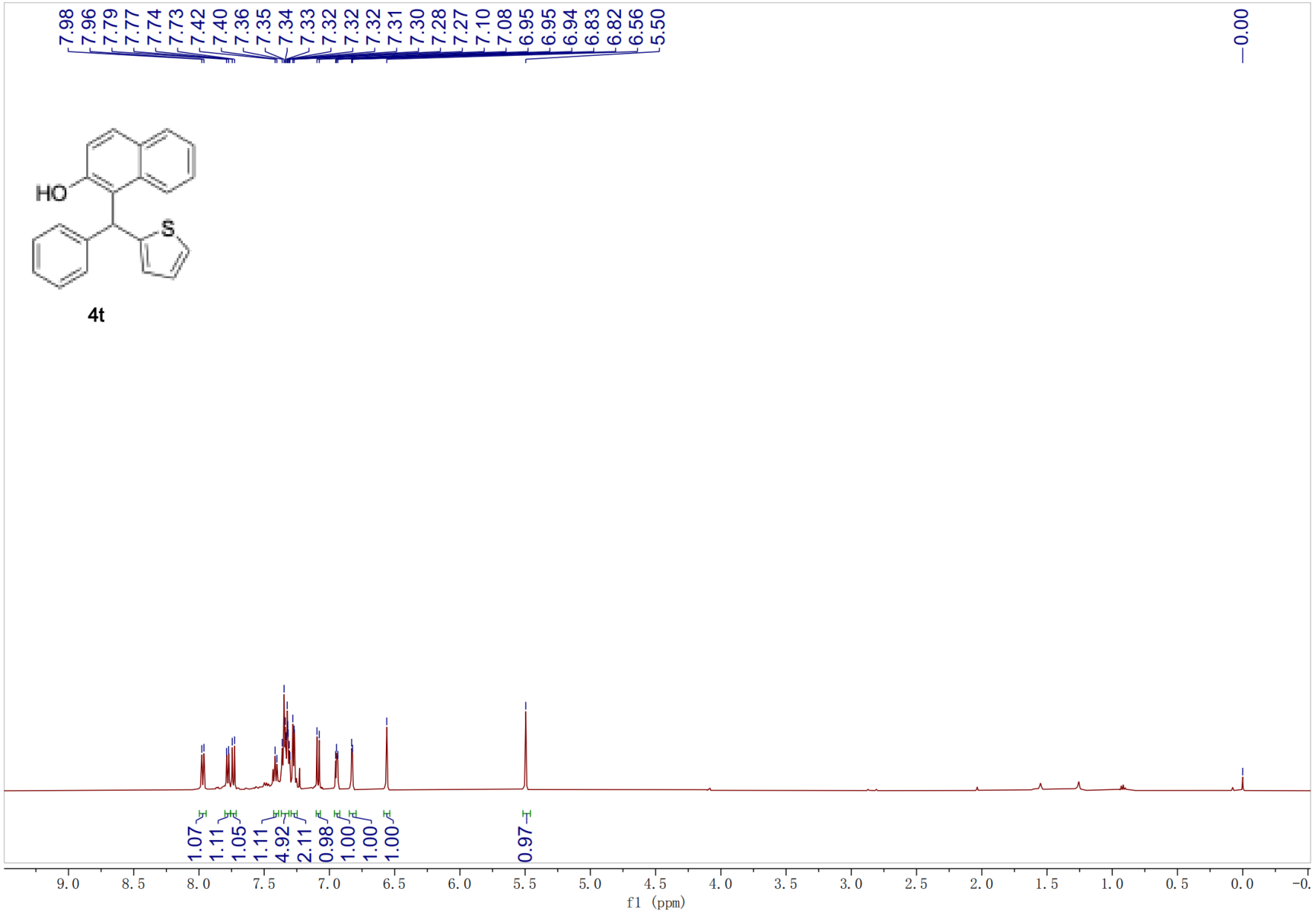

7.90
7.89
7.77
7.76
7.73
7.72
7.47
7.45
7.43
7.42
7.41
7.40
7.34
7.32
7.31
7.29
7.28
7.15
7.14
7.12
7.06
7.05
7.04
7.03
6.71
5.16
0.00
HO
Cl
4r
1.06
1.13
1.14
1.08
1.23
4.97
3.13
1.07
1.00
1.02
f1 (ppm)

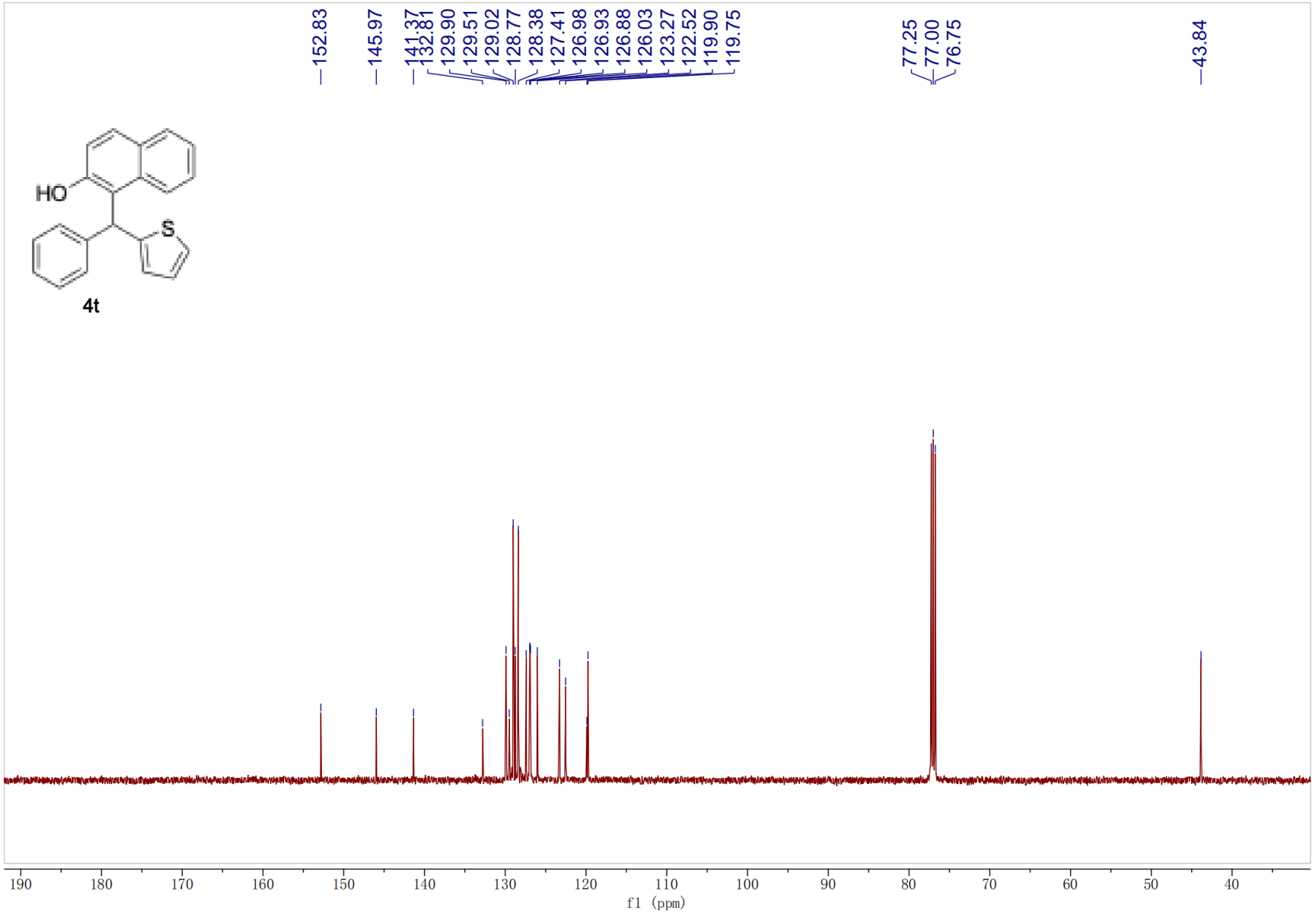

HO
Cl
153.18
140.71
138.52
134.58
133.39
130.67
129.97
129.92
129.55
129.51
128.68
128.58
128.48
127.62
127.48
127.09
123.34
122.59
119.80
119.24
77.25
77.00
76.75
46.19
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

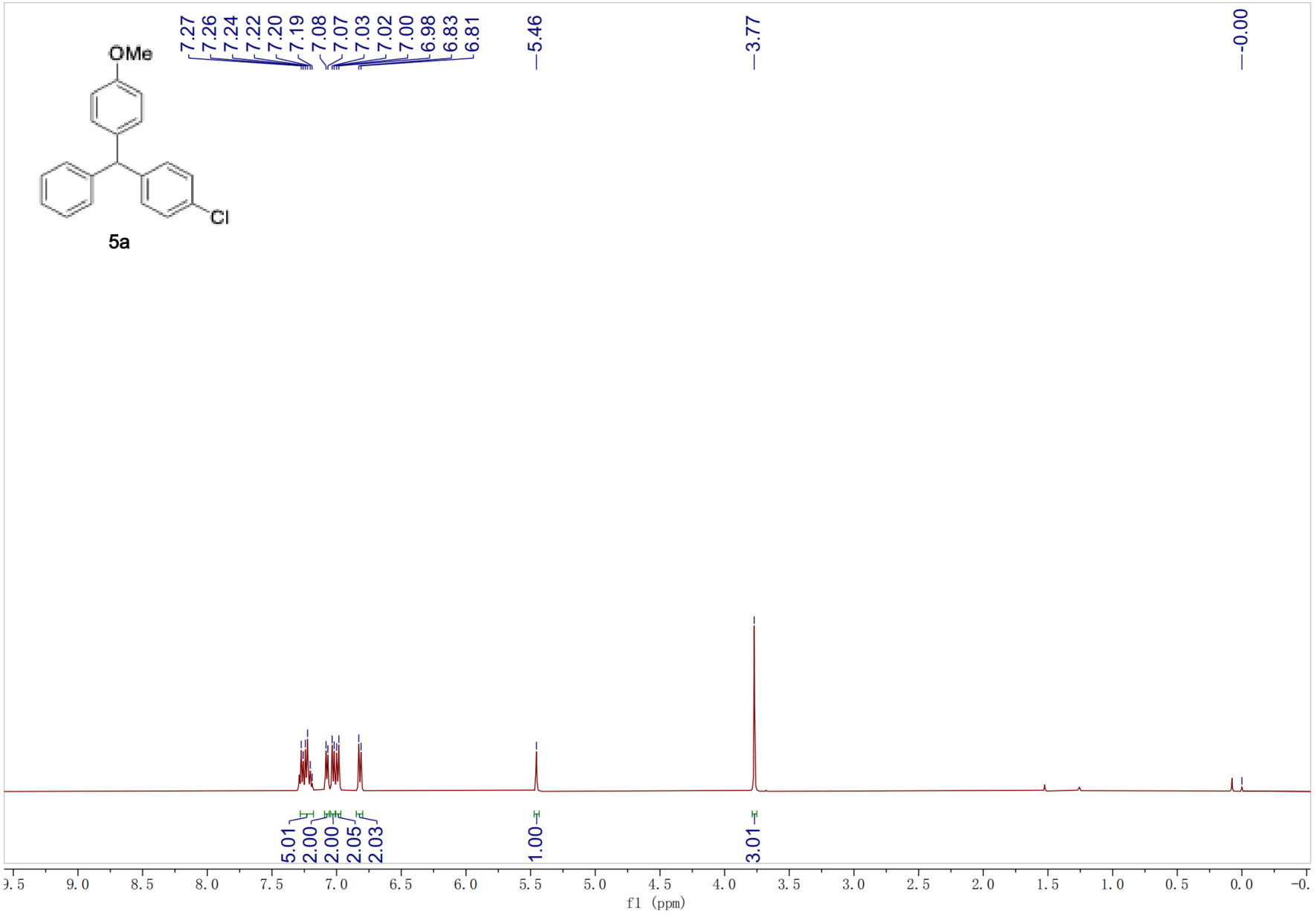
4r

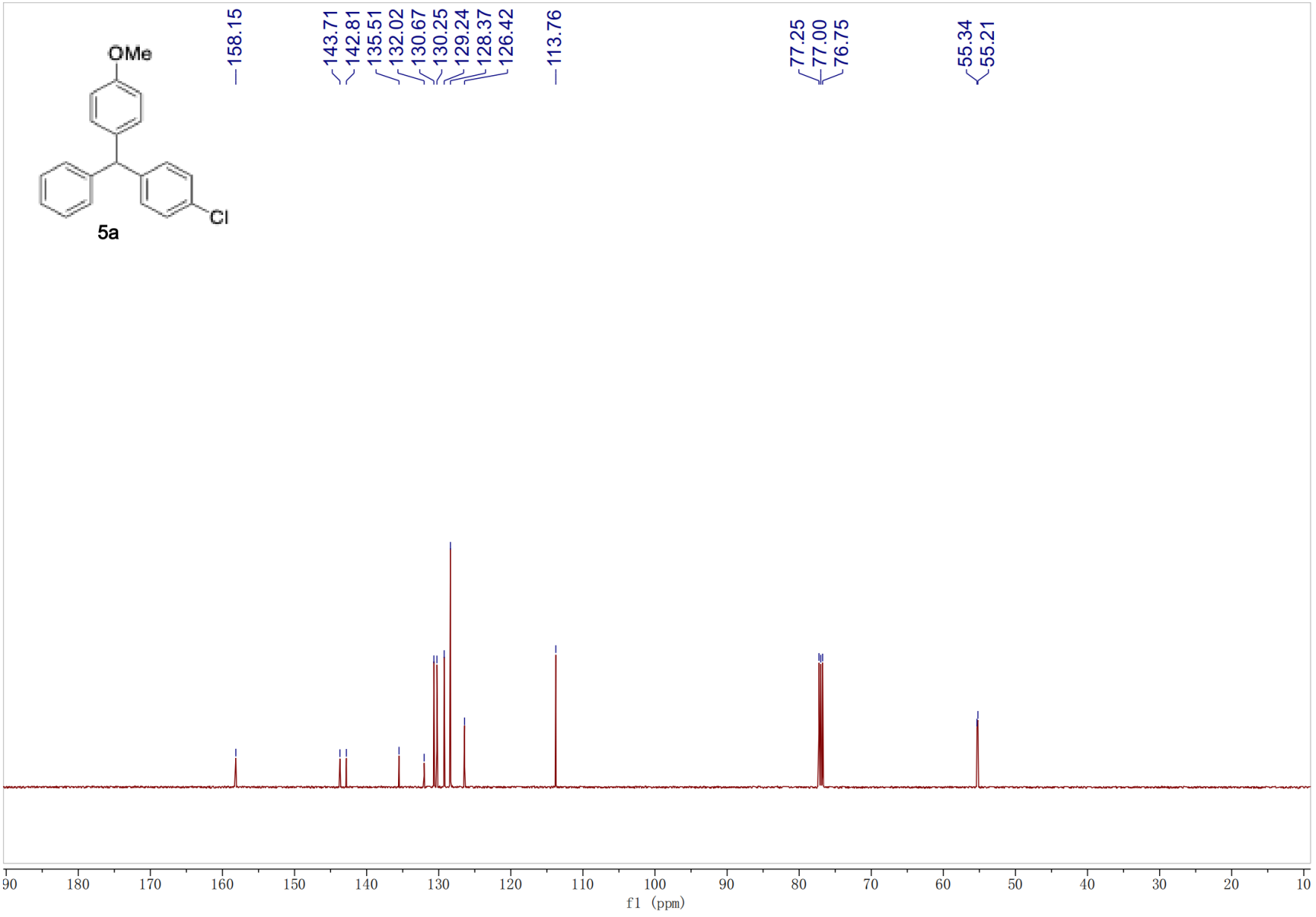

7.93 7.92 7.91 7.90 7.90 7.80 7.80 7.79 7.78 7.76 7.75 7.74 7.73 7.58 7.57 7.56 7.55 7.43 7.43 7.42 7.41 7.40 7.39 7.39 7.38 7.35 7.33 7.32 7.32 7.24 7.24 7.12 7.12 7.11 7.10 7.10 7.09 7.09 7.09 7.08 7.07 7.06 7.05 6.88 6.88 6.87 6.87 6.86 6.85 6.85 6.40 5.15 4.03 4.01 4.00 3.98 1.42 1.40 1.39
HO
F3C
OEt
4s
1.00 1.02 0.98 1.97 2.96 1.03 2.97 1.93 1.00 0.99 2.02 3.06
f1 (ppm)

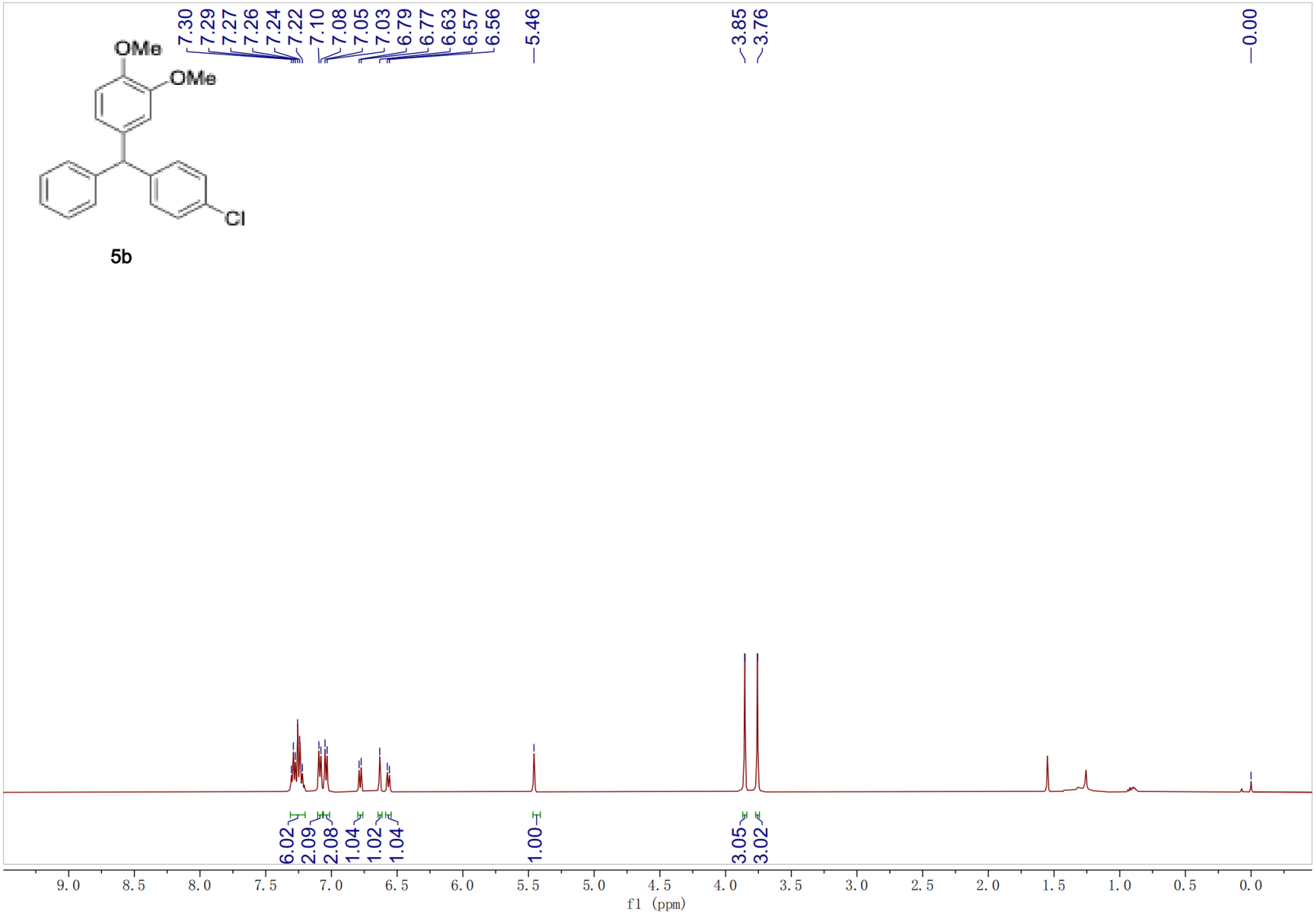

158.29
152.65
146.11
146.06
133.20
133.18
132.63
132.59
129.92
129.89
129.67
129.65
129.50
129.42
129.24
128.98
128.84
127.40
126.95
125.81
125.78
125.75
125.72
125.20
123.36
123.05
122.66
122.62
119.70
119.63
115.25
77.25
77.00
76.75
63.49
47.53
14.77
HO
F3C
OEt
4s
f1 (ppm)

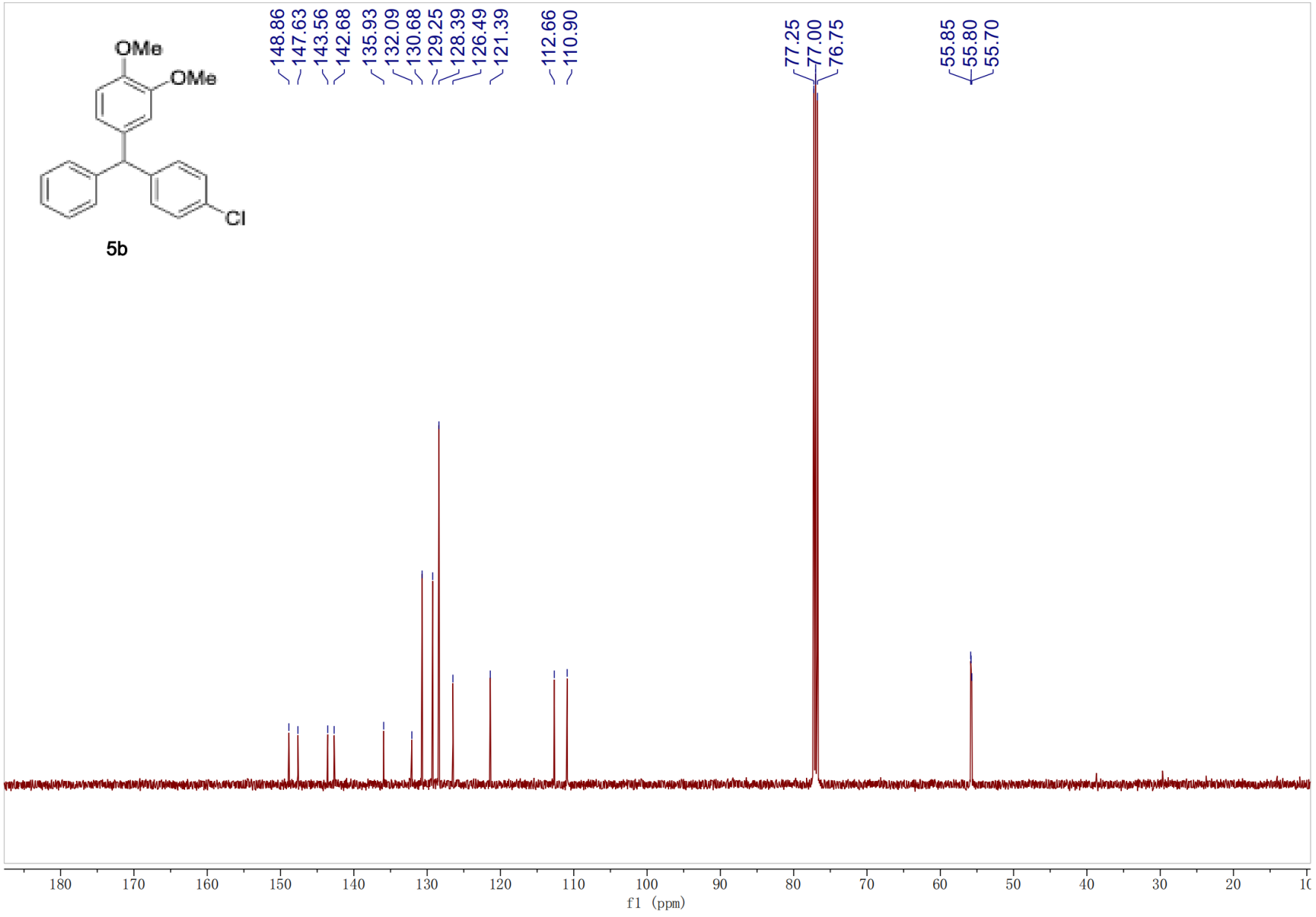

7.98
7.96
7.79
7.77
7.74
7.73
7.42
7.40
7.36
7.35
7.34
7.33
7.32
7.32
7.32
7.31
7.30
7.28
7.27
7.10
7.08
6.95
6.95
6.94
6.83
6.82
6.56
5.50
0.00
HO
S
4t
1.07
1.11
1.05
1.11
4.92
2.11
0.98
1.00
1.00
1.00
0.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)

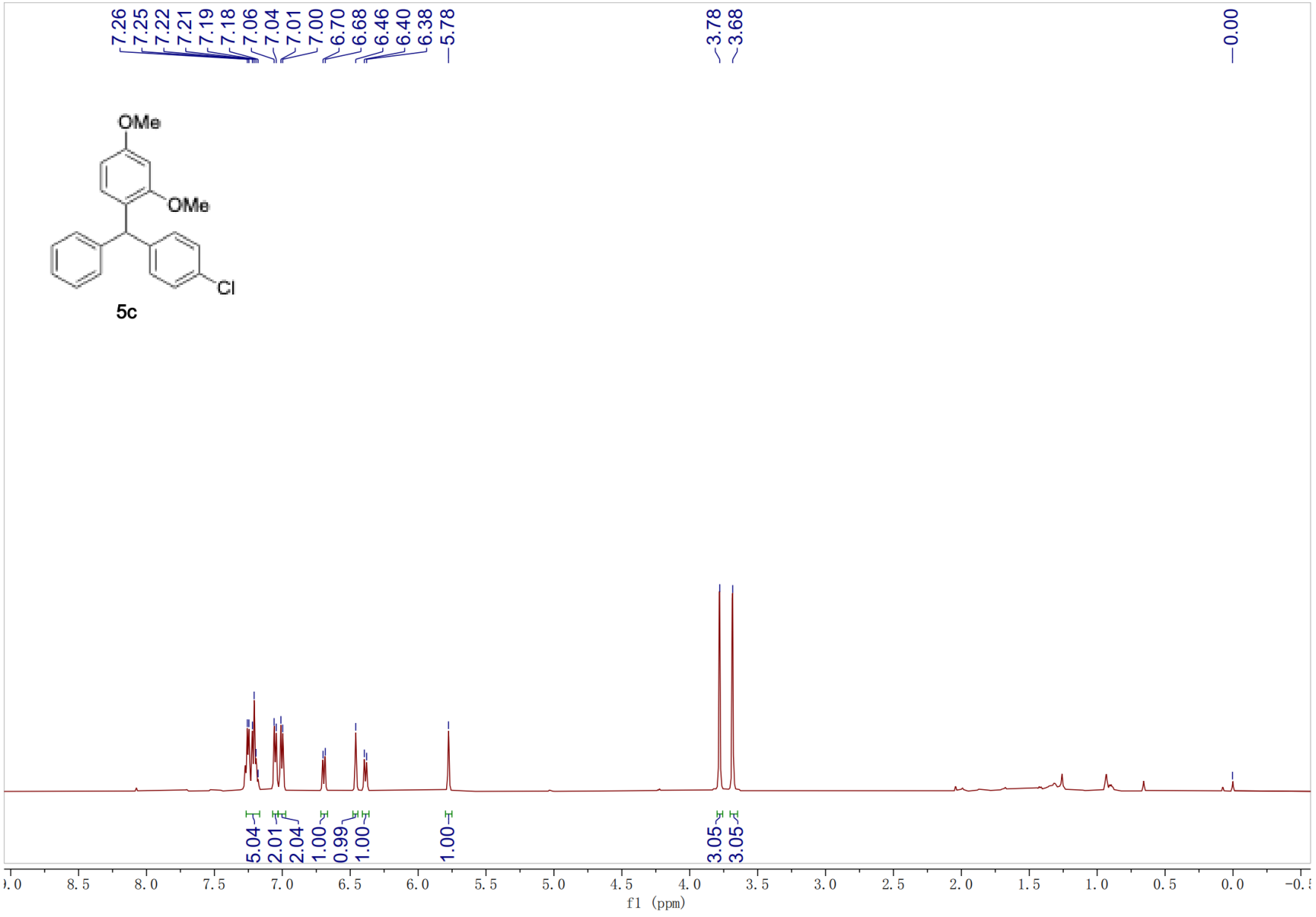

152.83
145.97
141.37
132.81
129.90
129.51
129.02
128.77
128.38
127.41
126.98
126.93
126.88
126.03
123.27
122.52
119.90
119.75
77.25
77.00
76.75
43.84
HO
S
4t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)

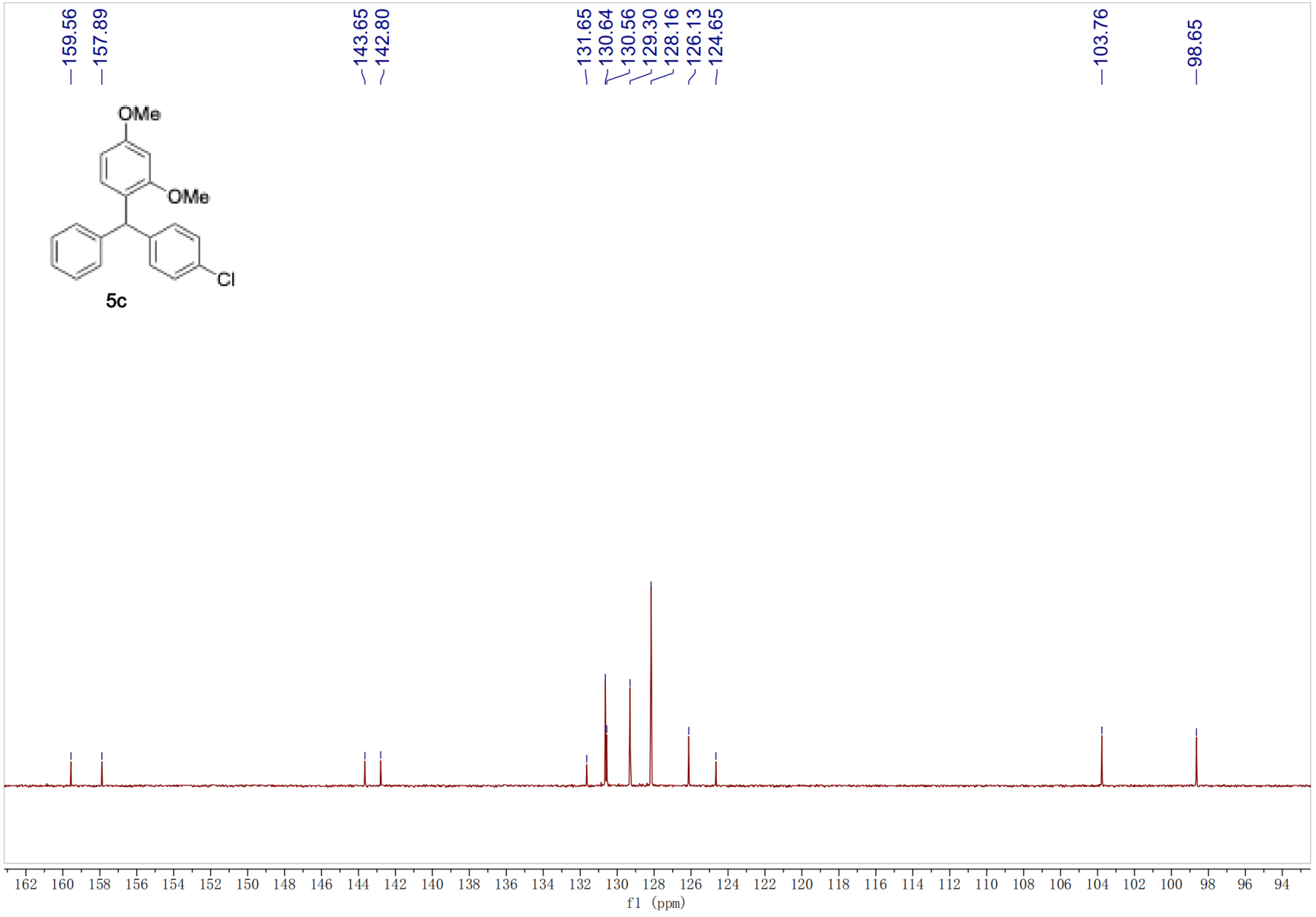

OMe
Cl
5a
7.27
7.26
7.24
7.22
7.20
7.19
7.08
7.07
7.03
7.02
7.00
6.98
6.83
6.81
5.46
3.77
0.00
5.01
2.00
2.00
2.05
2.03
1.00
3.01
f1 (ppm)

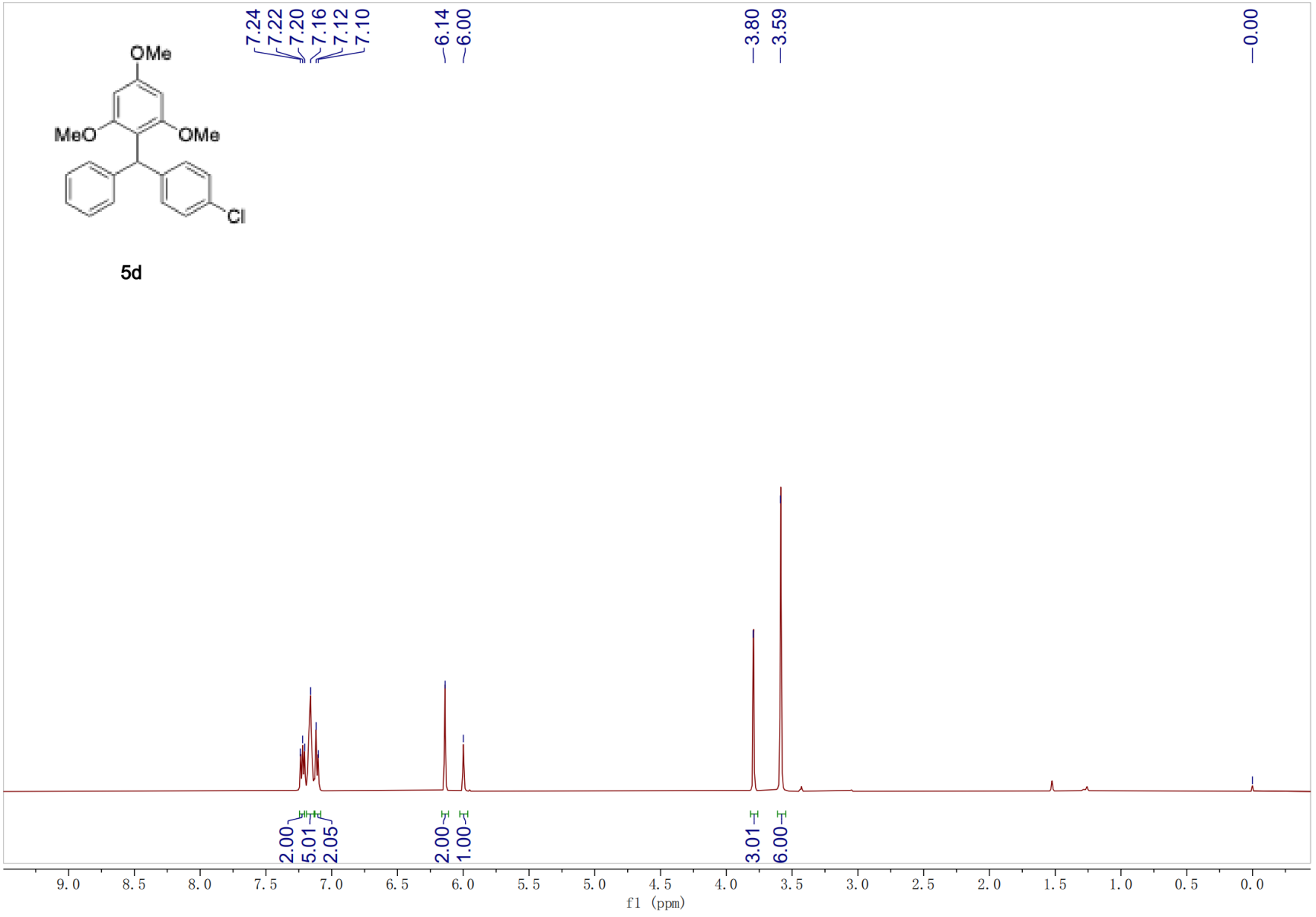

OMe
Cl
5a
158.15
143.71
142.81
135.51
132.02
130.67
130.25
129.24
128.37
126.42
113.76
77.25
77.00
76.75
55.34
55.21
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

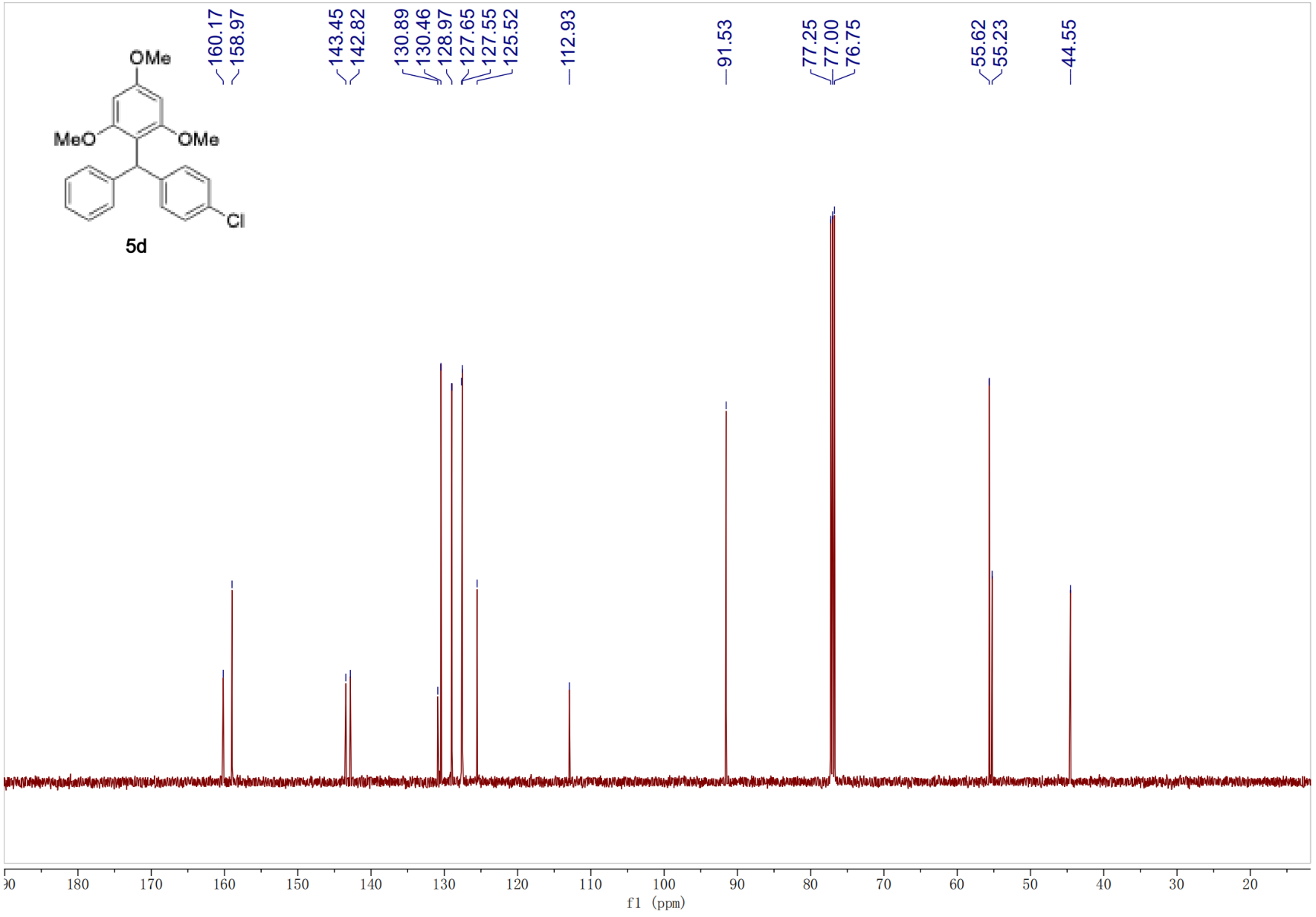

7.30
7.29
7.27
7.26
7.24
7.22
7.10
7.08
7.05
7.03
6.79
6.77
6.63
6.57
6.56
5.46
3.85
3.76
0.00
OMe
OMe
Cl
5b
6.02
2.09
2.08
1.04
1.02
1.04
1.00
3.05
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

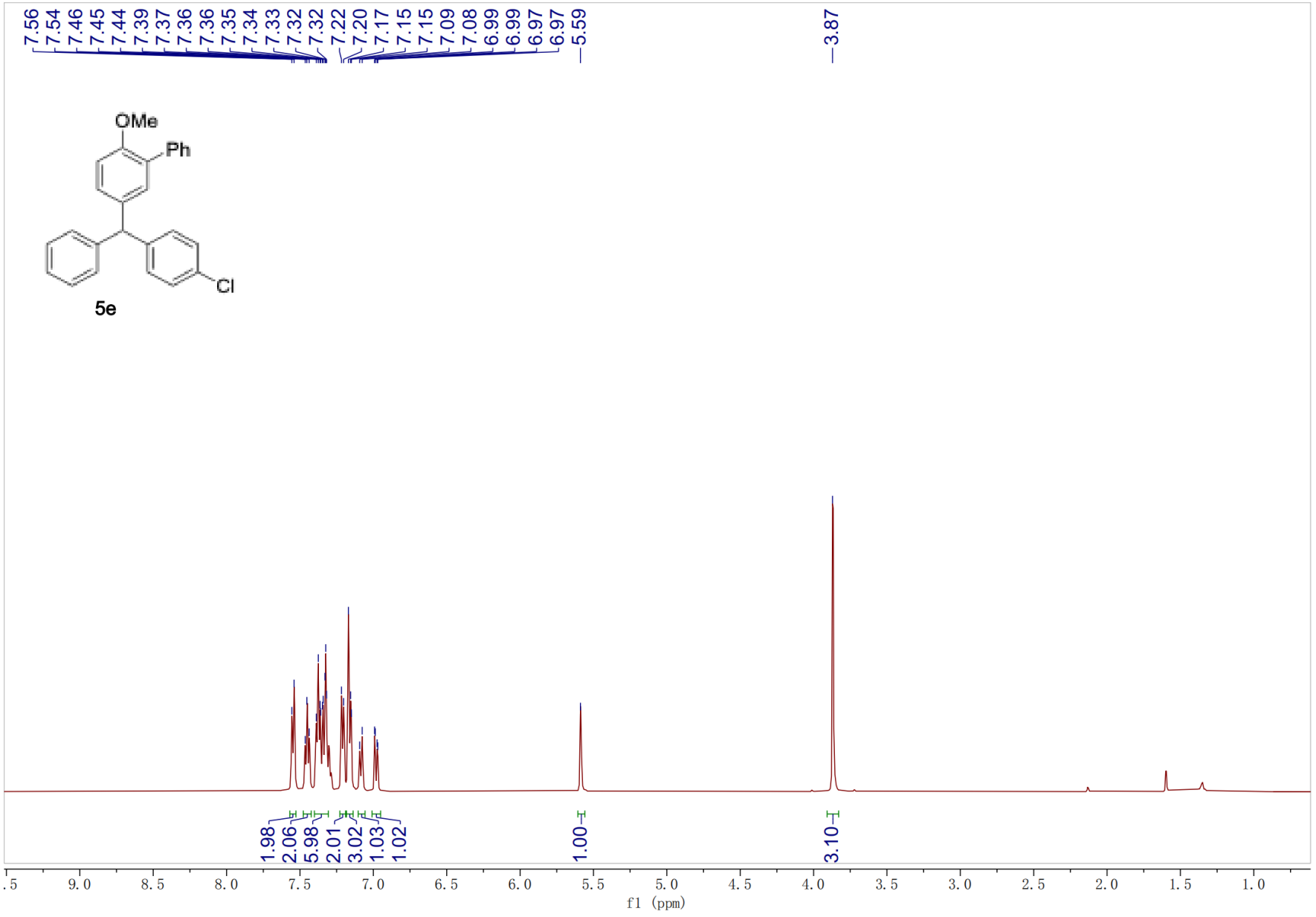

OMe
OMe
Cl
5b
148.86
147.63
143.56
142.68
135.93
132.09
130.68
129.25
128.39
126.49
121.39
112.66
110.90
77.25
77.00
76.75
55.85
55.80
55.70
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

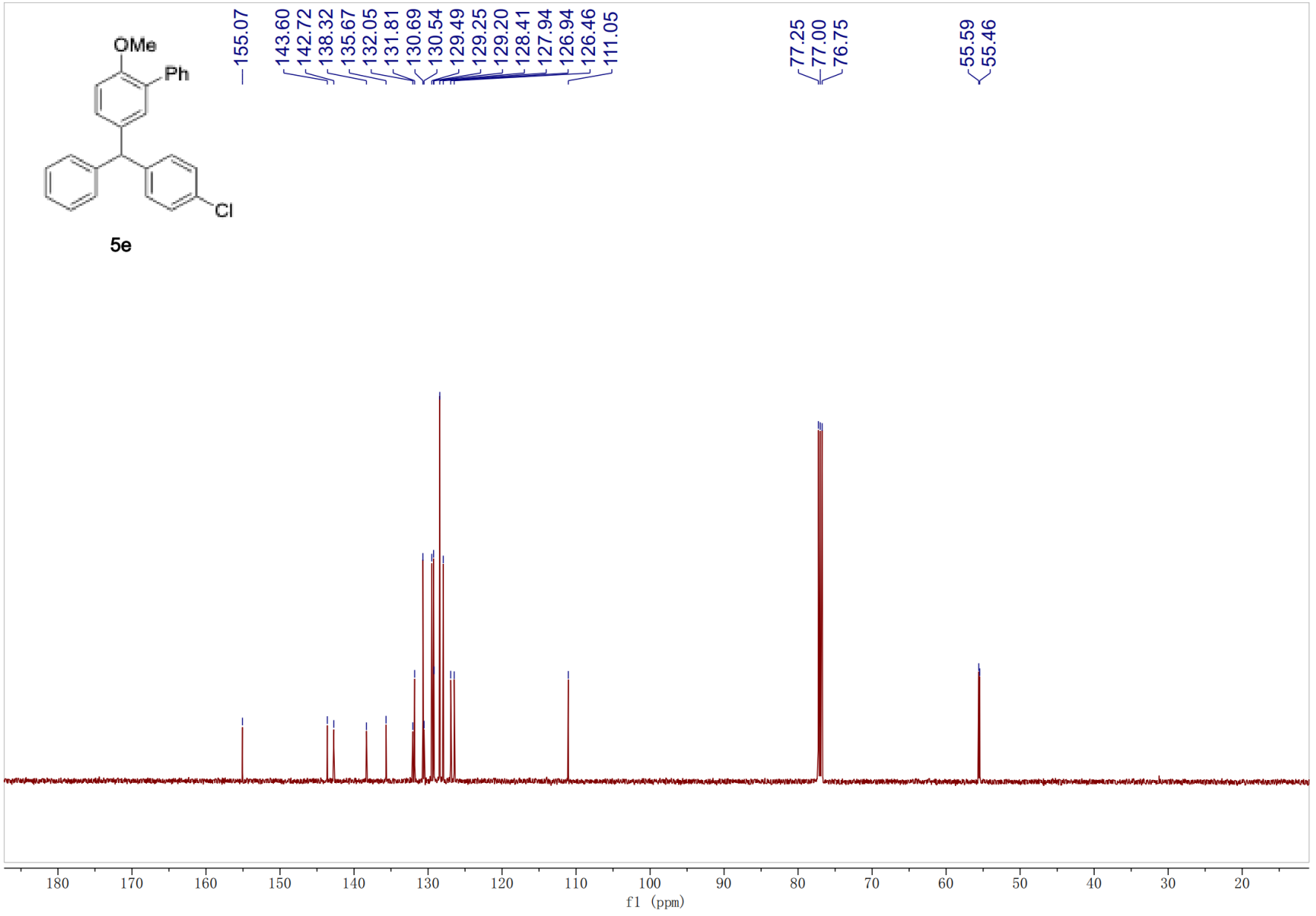

7.26
7.25
7.22
7.21
7.19
7.18
7.06
7.04
7.01
7.00
6.70
6.68
6.46
6.40
6.38
5.78
3.78
3.68
0.00
OMe
OMe
Cl
5c
5.04
2.01
2.04
1.00
0.99
1.00
1.00
3.05
3.05
f1 (ppm)

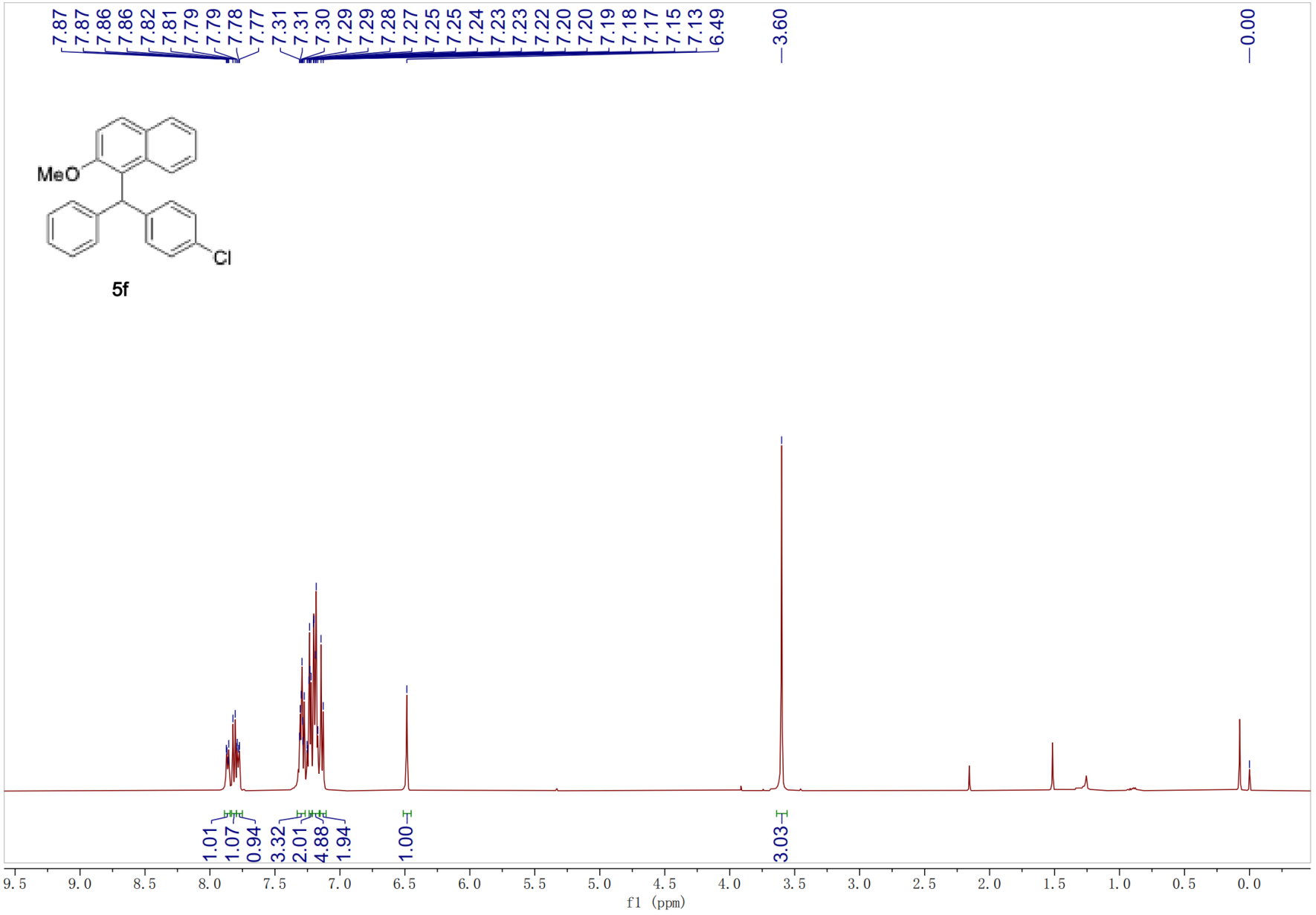

159.56
157.89
143.65
142.80
131.65
130.64
130.56
129.30
128.16
126.13
124.65
103.76
98.65
OMe
OMe
Cl
5c
162 160 158 156 154 152 150 148 146 144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108 106 104 102 100 98 96 94
f1 (ppm)

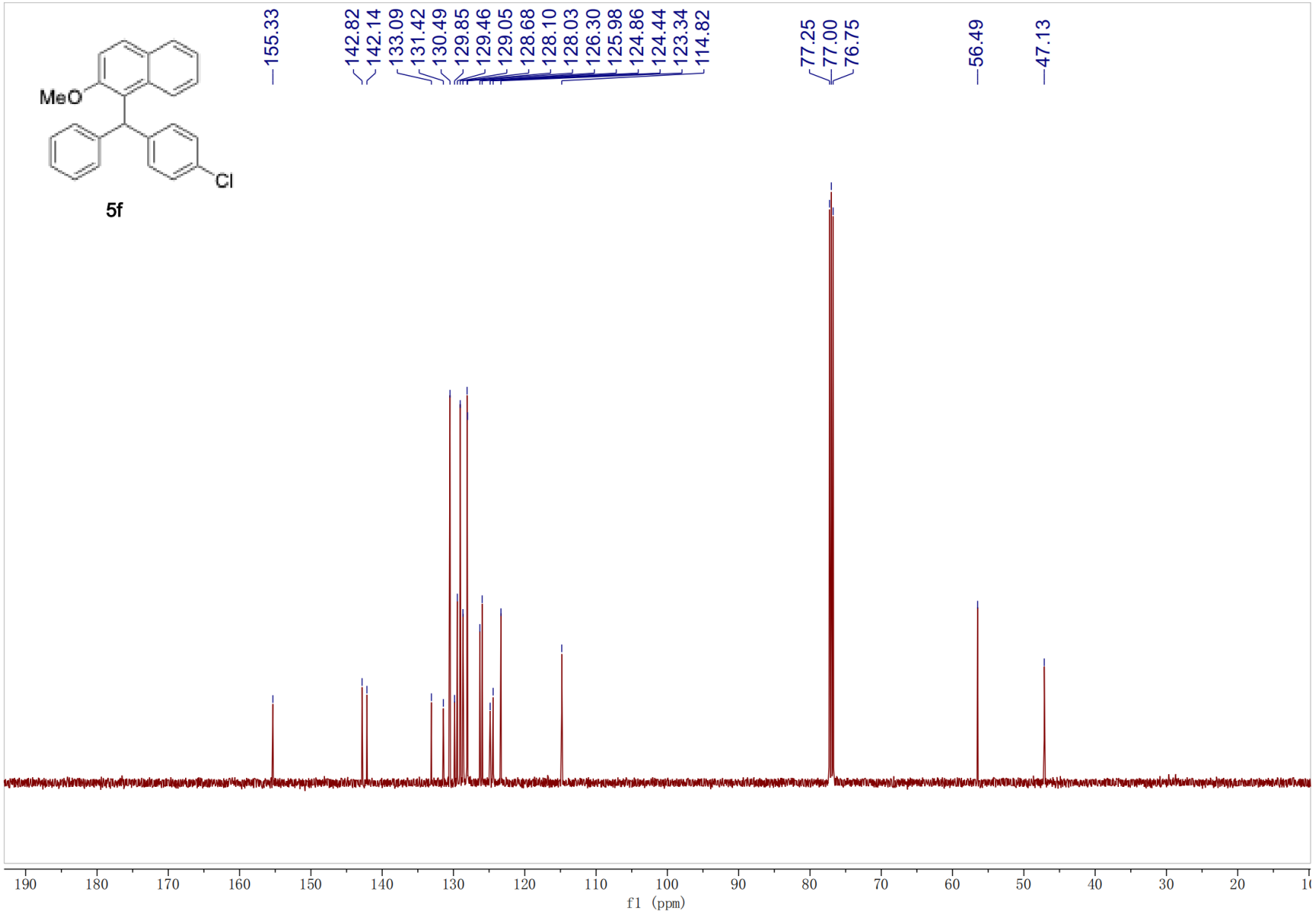

7.24
7.22
7.20
7.16
7.12
7.10
6.14
6.00
3.80
3.59
0.00
OMe
MeO
OMe
Cl
5d
2.00
5.01
2.05
2.00
1.00
3.01
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

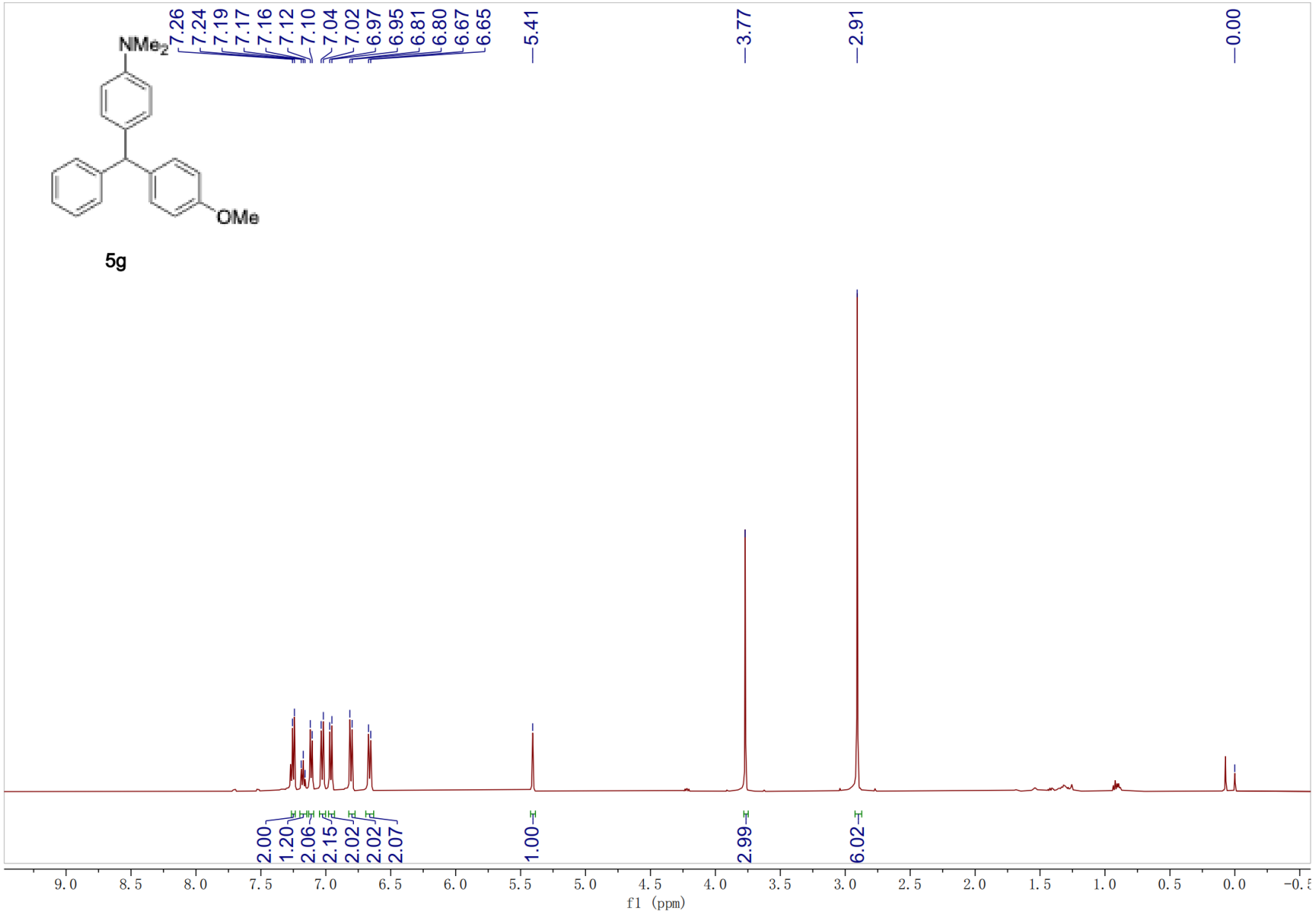

OMe
MeO
OMe
Cl
5d
160.17
158.97
143.45
142.82
130.89
130.46
128.97
127.65
127.55
125.52
112.93
91.53
77.25
77.00
76.75
55.62
55.23
44.55
f1 (ppm)


7.56
7.54
7.46
7.45
7.44
7.39
7.37
7.36
7.36
7.35
7.34
7.33
7.32
7.32
7.22
7.20
7.17
7.15
7.15
7.09
7.08
6.99
6.99
6.97
6.97
5.59
3.87
OMe
Ph
Cl
5e
1.98
2.06
5.98
2.01
3.02
1.03
1.02
1.00
3.10
f1 (ppm)

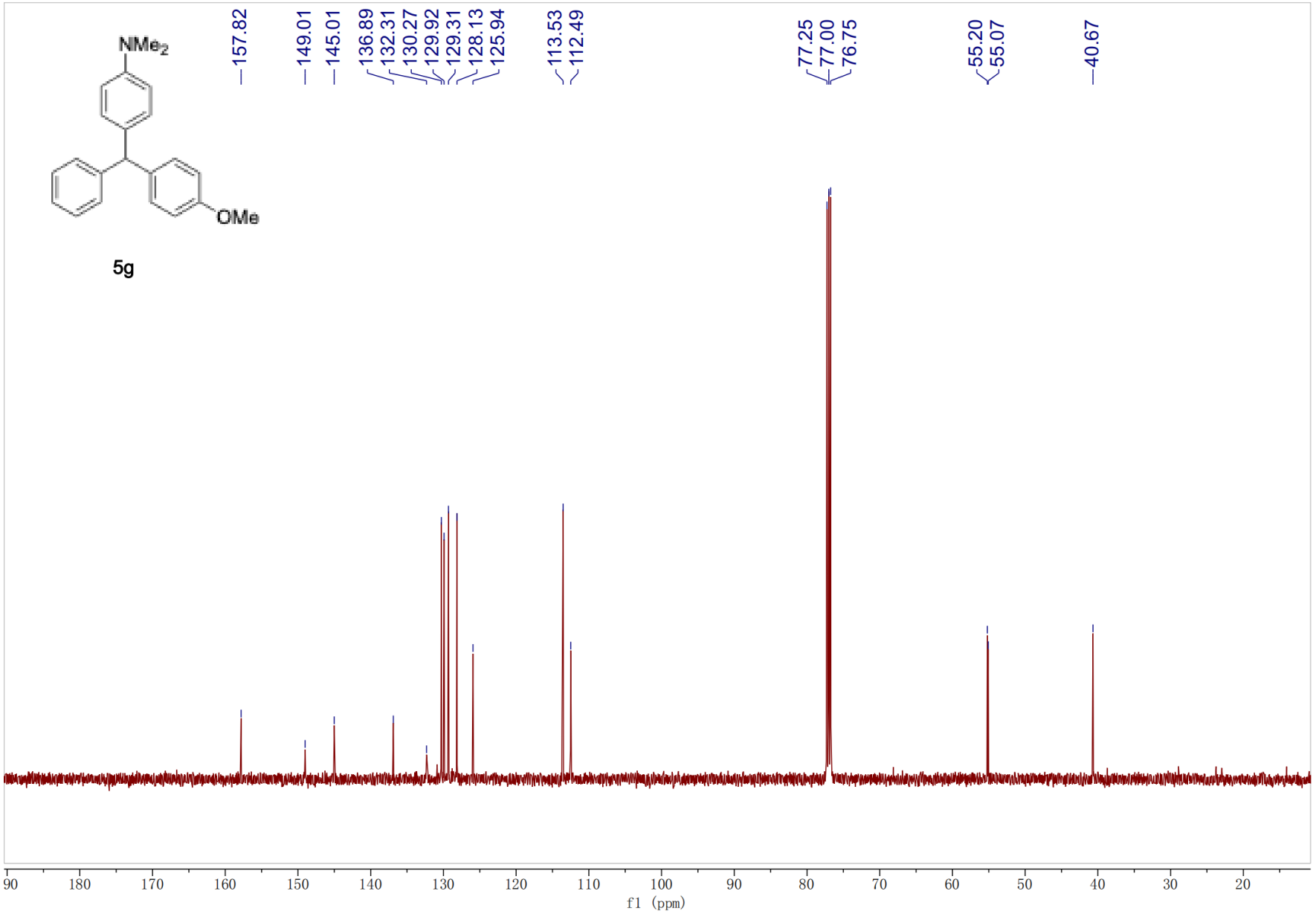

OMe
Ph
Cl
5e
155.07
143.60
142.72
138.32
135.67
132.05
131.81
130.69
130.54
129.49
129.25
129.20
128.41
127.94
126.94
126.46
111.05
77.25
77.00
76.75
55.59
55.46
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

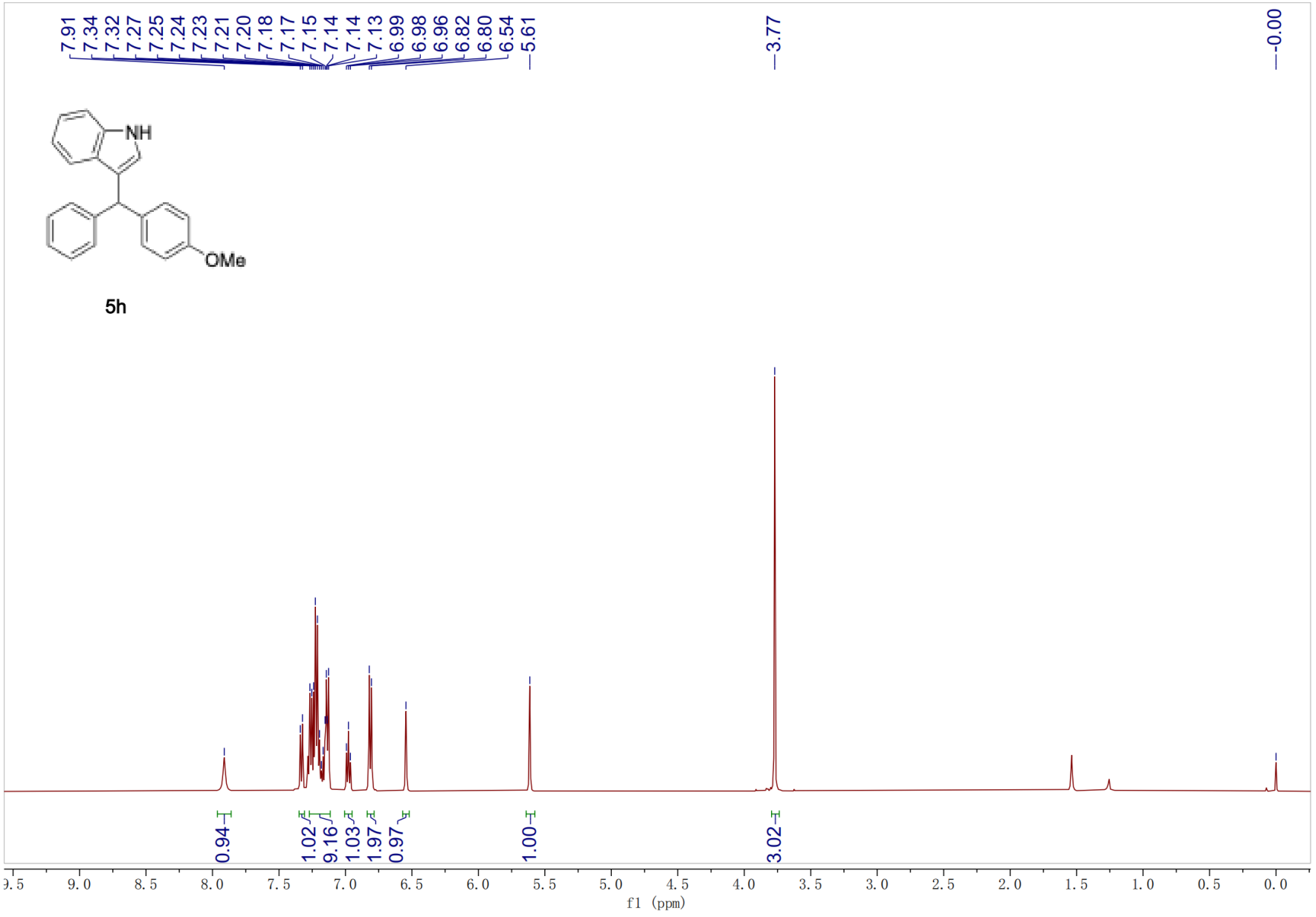

7.87
7.87
7.86
7.86
7.82
7.81
7.79
7.79
7.78
7.77
7.31
7.31
7.30
7.29
7.29
7.28
7.27
7.25
7.25
7.24
7.23
7.23
7.22
7.20
7.20
7.19
7.18
7.17
7.15
7.13
6.49
3.60
0.00
MeO
Cl
5f
1.01
1.07
0.94
3.32
2.01
4.88
1.94
1.00
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

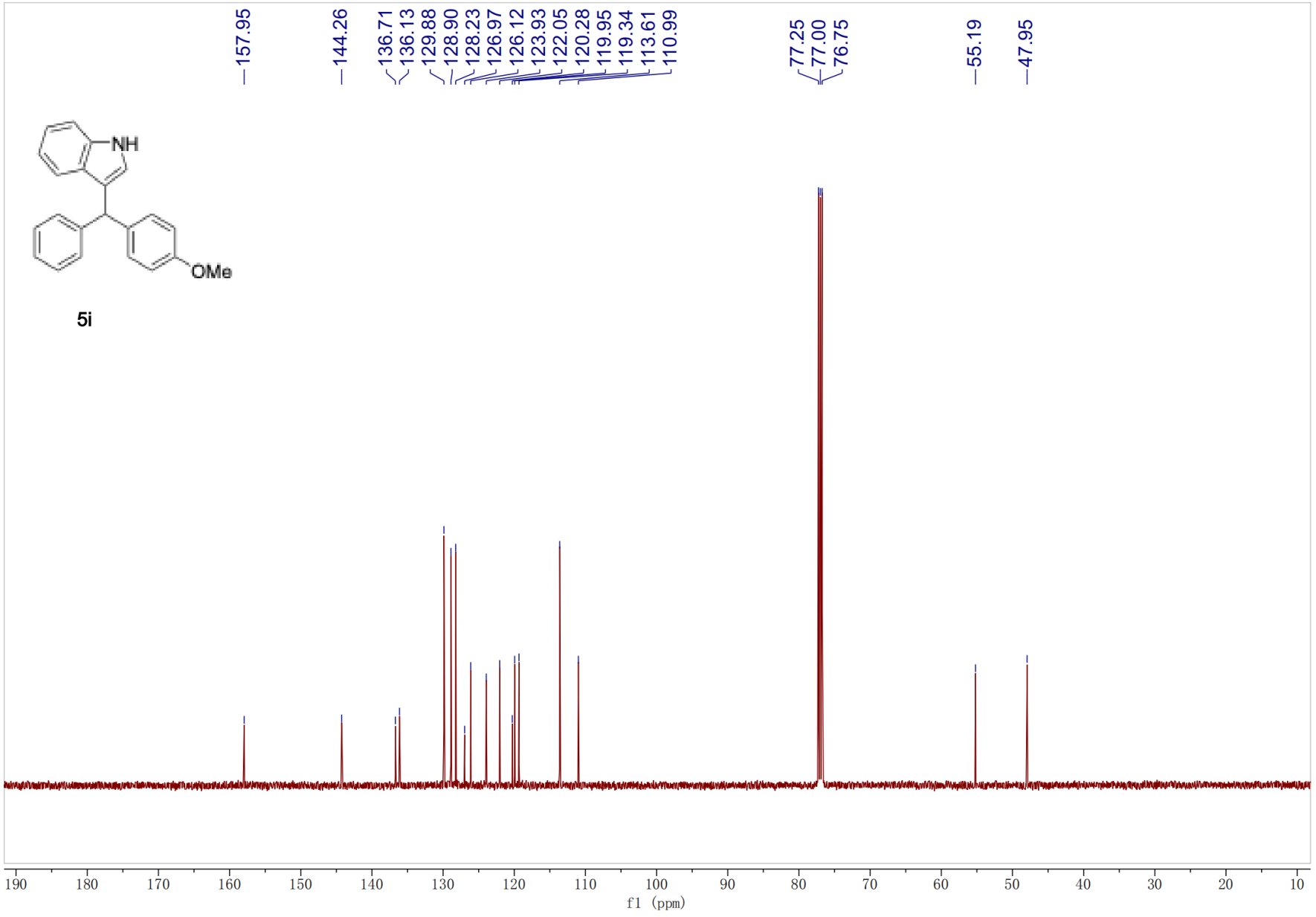

MeO
Cl
5f
155.33
142.82
142.14
133.09
131.42
130.49
129.85
129.46
129.05
128.68
128.10
128.03
126.30
125.98
124.86
124.44
123.34
114.82
77.25
77.00
76.75
56.49
47.13
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

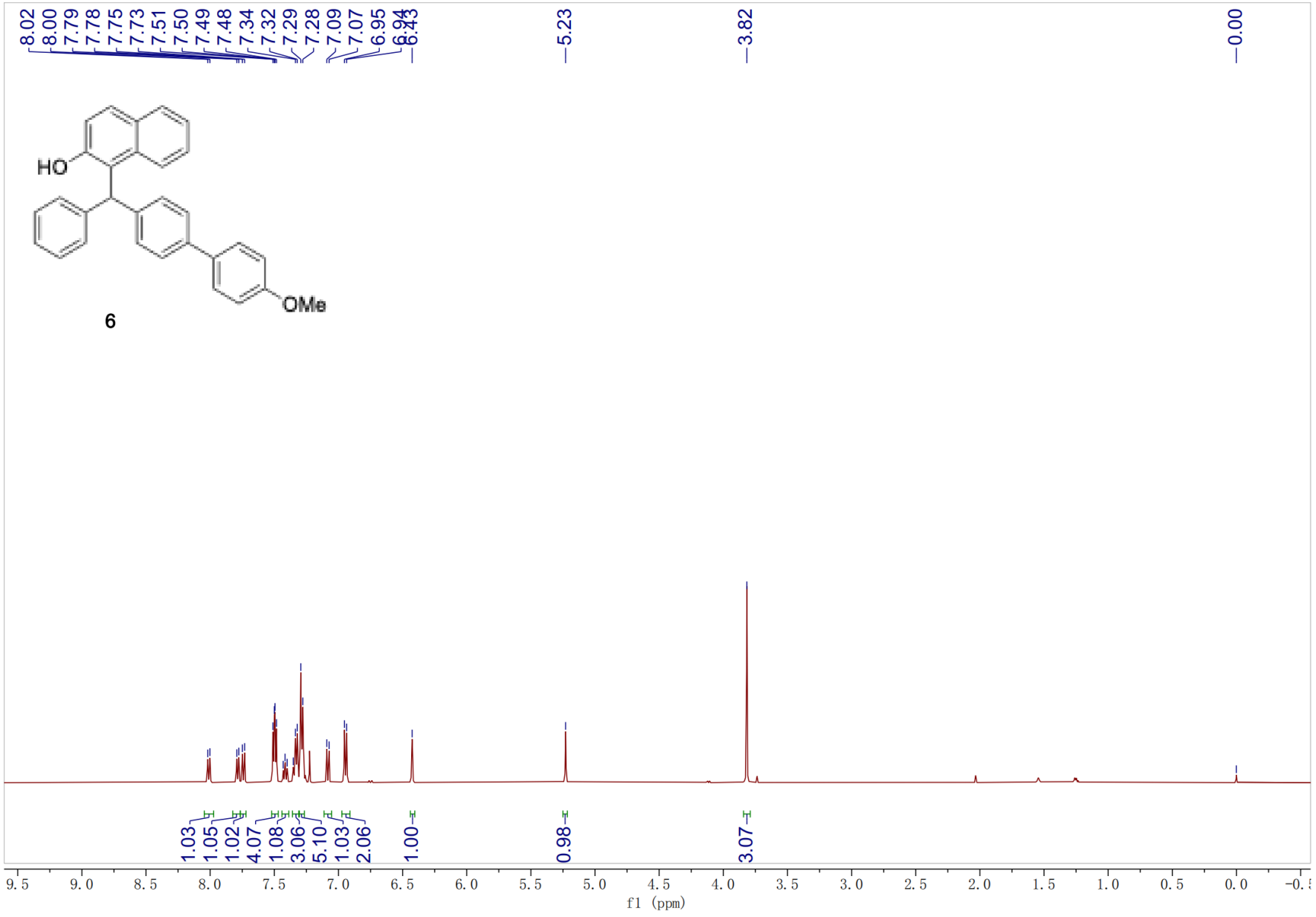

NMe2
OMe
7.26
7.24
7.19
7.17
7.16
7.12
7.10
7.04
7.02
6.97
6.95
6.81
6.80
6.67
6.65
5.41
3.77
2.91
0.00
2.00
1.20
2.06
2.15
2.02
2.02
2.07
1.00
2.99
6.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

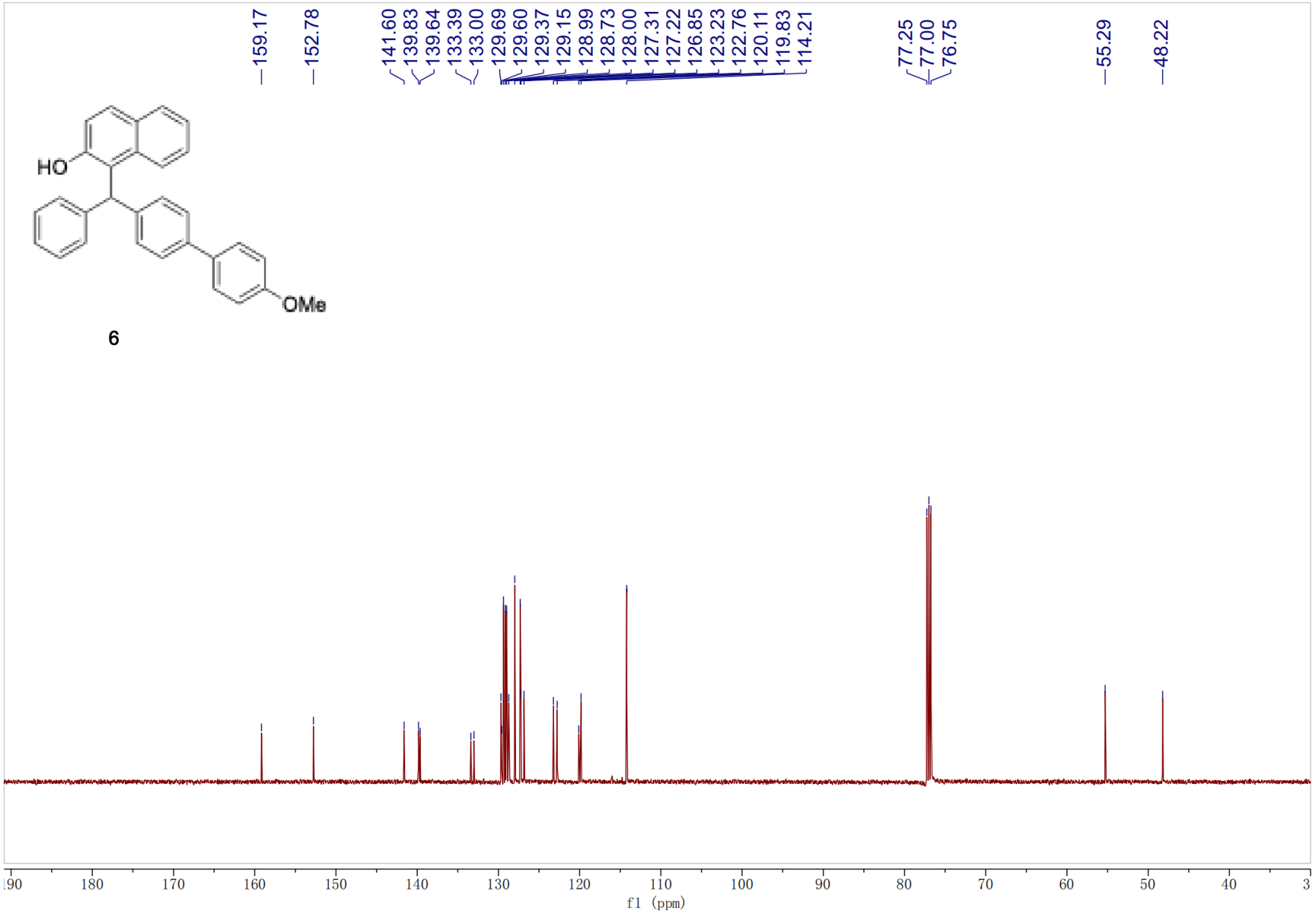
5g

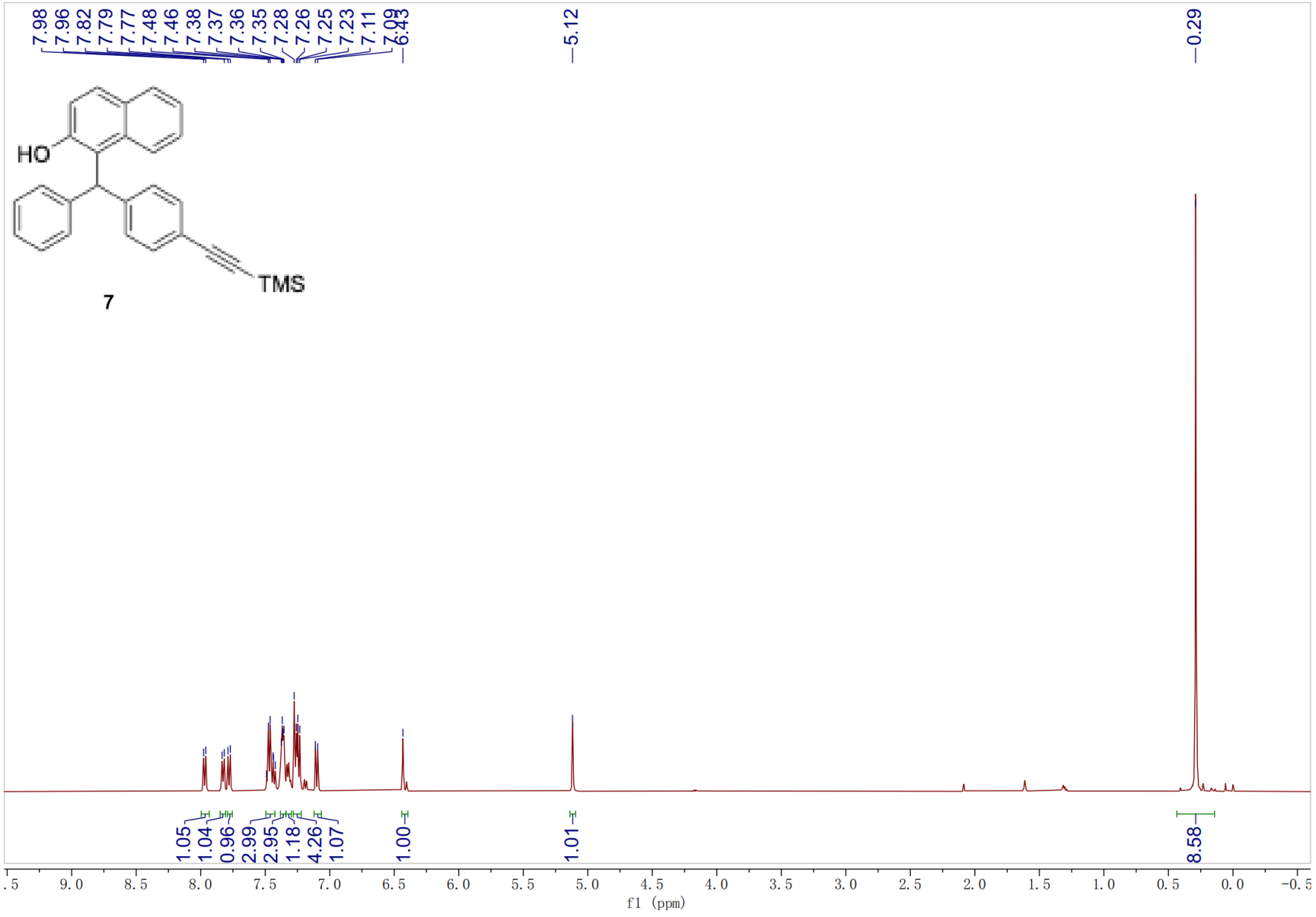

NMe2
OMe
5g
157.82
149.01
145.01
136.89
132.31
130.27
129.92
129.31
128.13
125.94
113.53
112.49
77.25
77.00
76.75
55.20
55.07
40.67
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

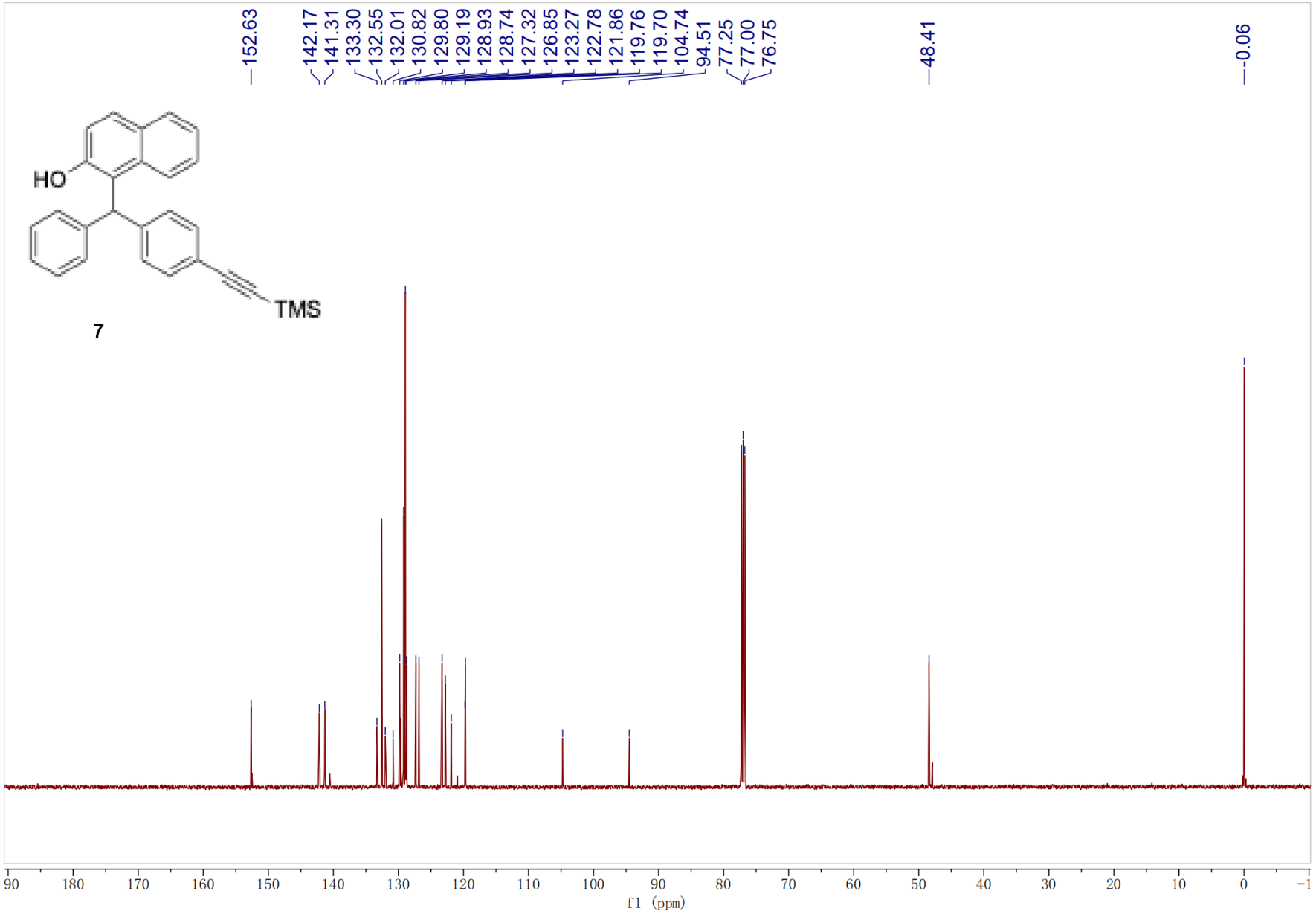

7.91
7.34
7.32
7.27
7.25
7.24
7.23
7.21
7.20
7.18
7.17
7.15
7.14
7.14
7.13
6.99
6.98
6.96
6.82
6.80
6.54
5.61
3.77
0.00
NH
OMe
5h
0.94
1.02
9.16
1.03
1.97
0.97
1.00
3.02
f1 (ppm)

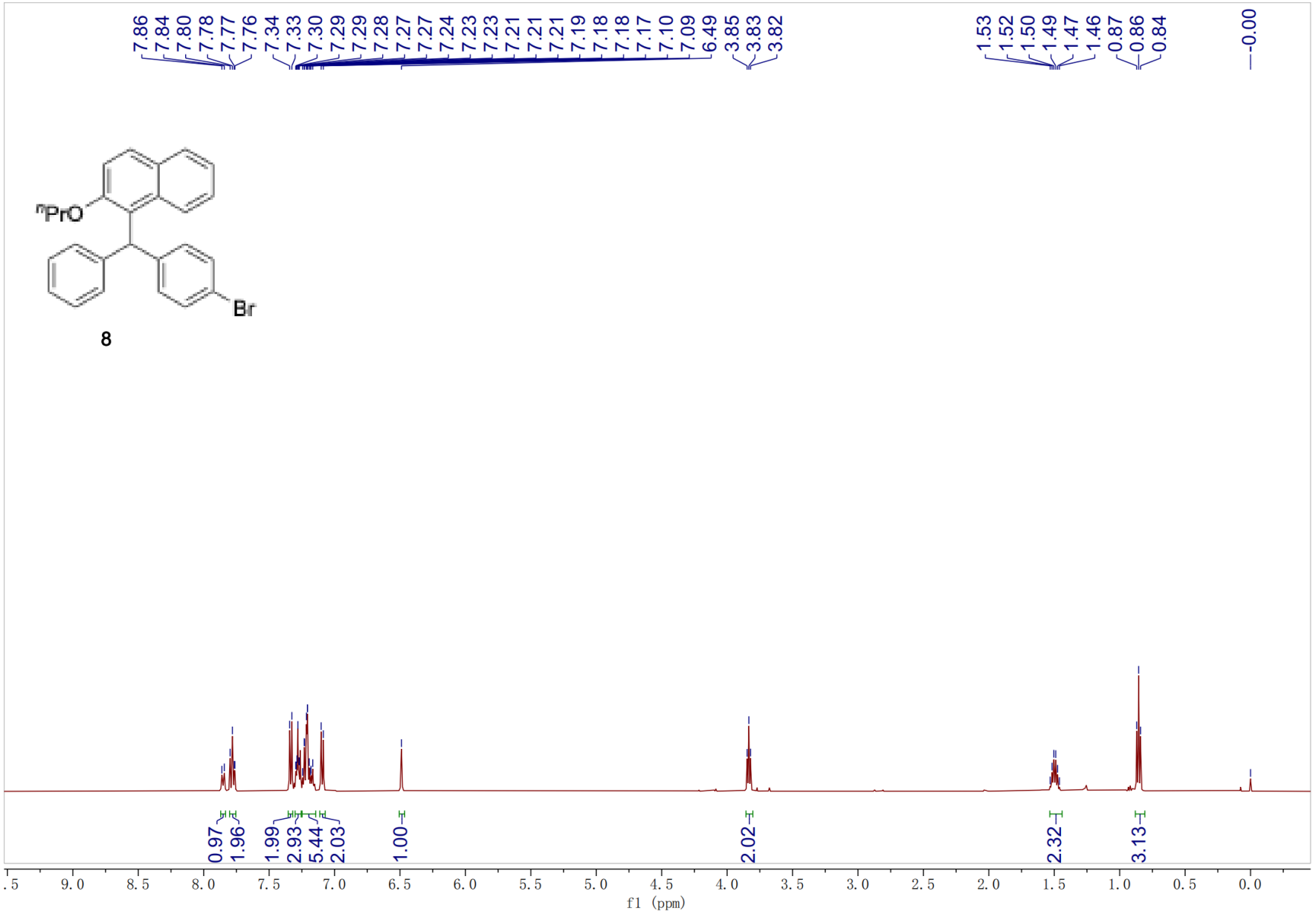

157.95
144.26
136.71
136.13
129.88
128.90
128.23
126.97
126.12
123.93
122.05
120.28
119.95
119.34
113.61
110.99
77.25
77.00
76.75
55.19
47.95
NH
OMe
5i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

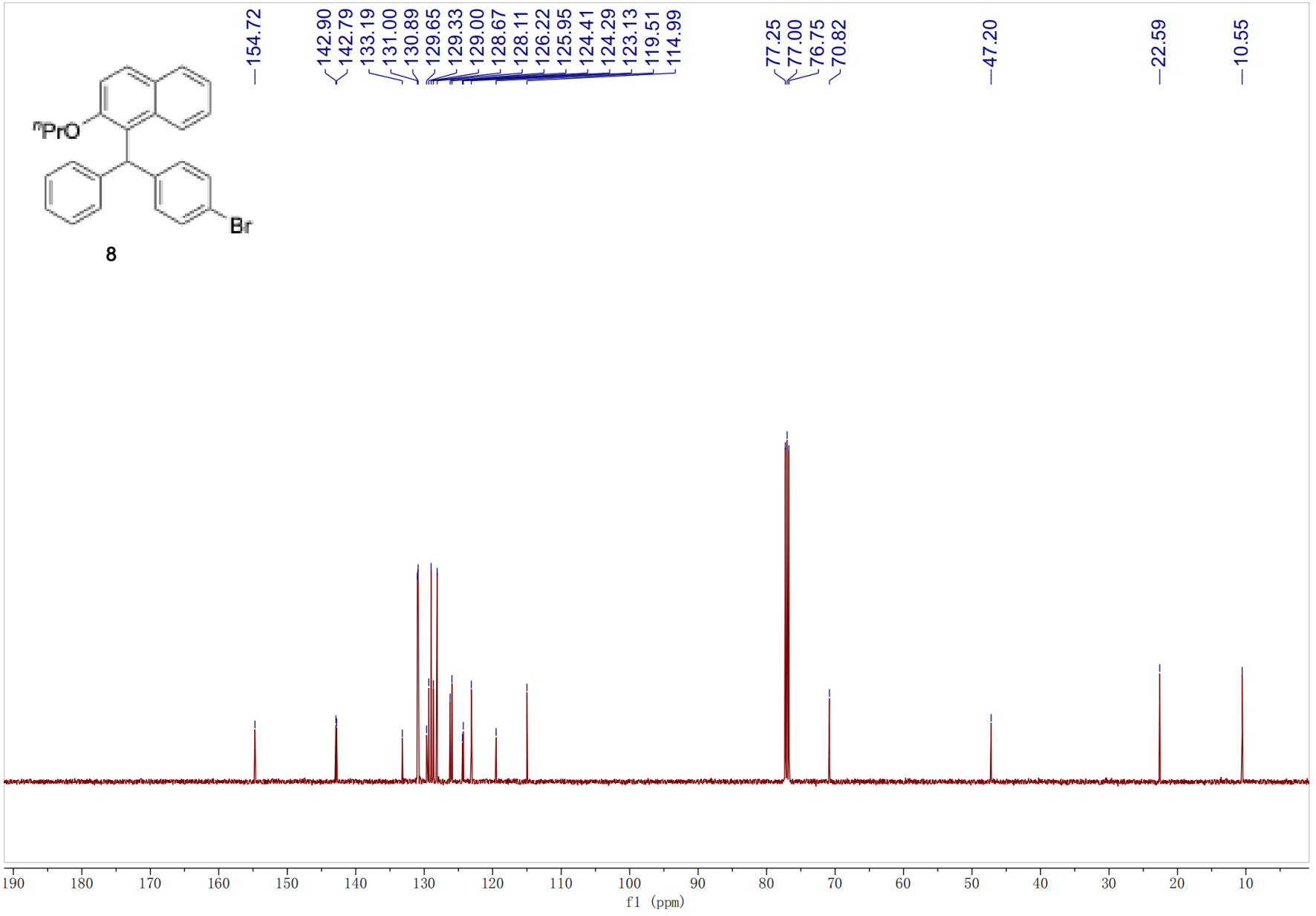

8.02
8.00
7.79
7.78
7.75
7.73
7.51
7.50
7.49
7.48
7.34
7.32
7.29
7.28
7.09
7.07
6.95
6.94
6.43
5.23
3.82
0.00
HO
OMe
6
1.03
1.05
1.02
4.07
1.08
3.06
5.10
1.03
2.06
1.00
0.98
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

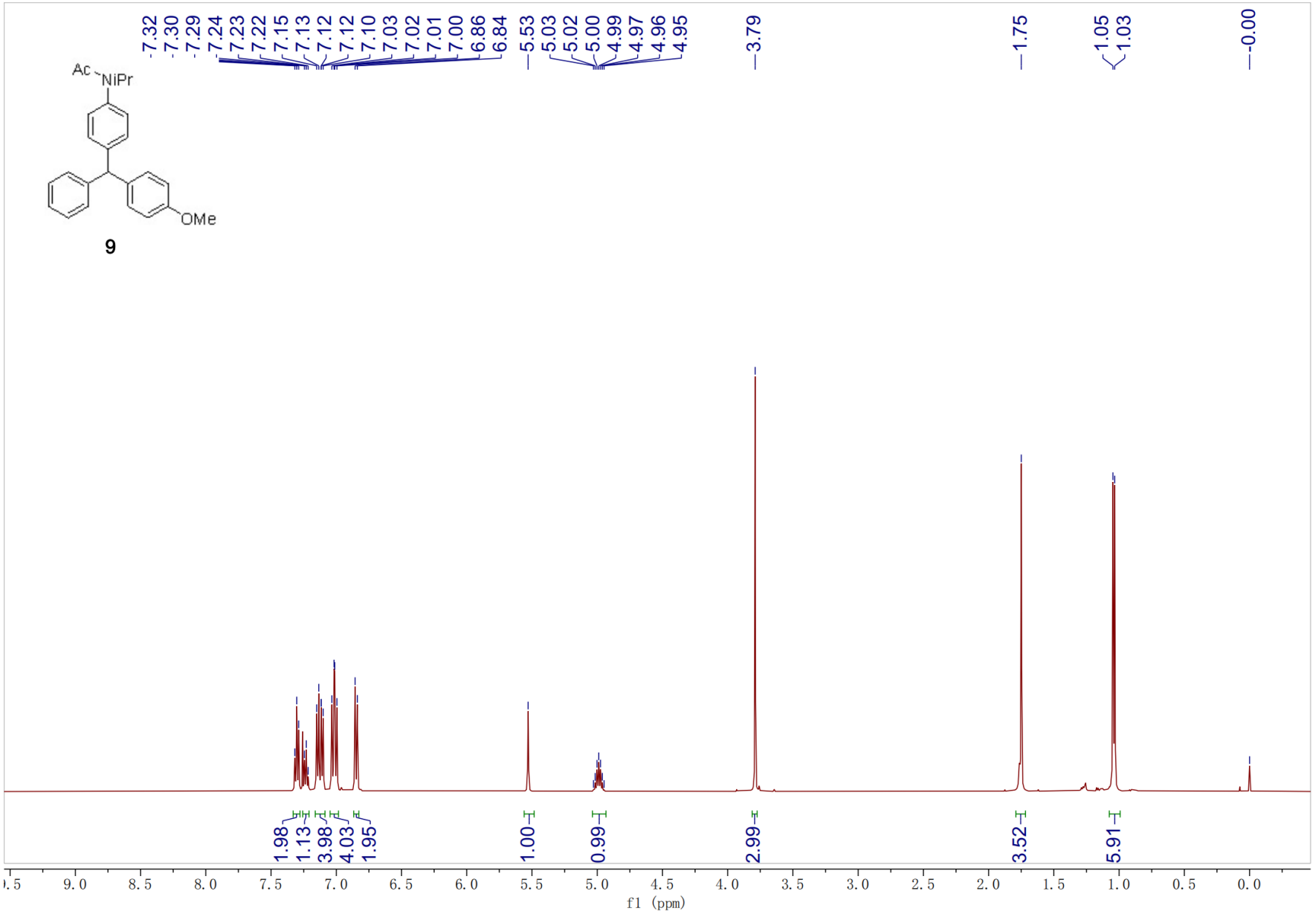

159.17
152.78
141.60
139.83
139.64
133.39
133.00
129.69
129.60
129.37
129.15
128.99
128.73
128.00
127.31
127.22
126.85
123.23
122.76
120.11
119.83
114.21
77.25
77.00
76.75
55.29
48.22
HO
OMe
6
f1 (ppm)

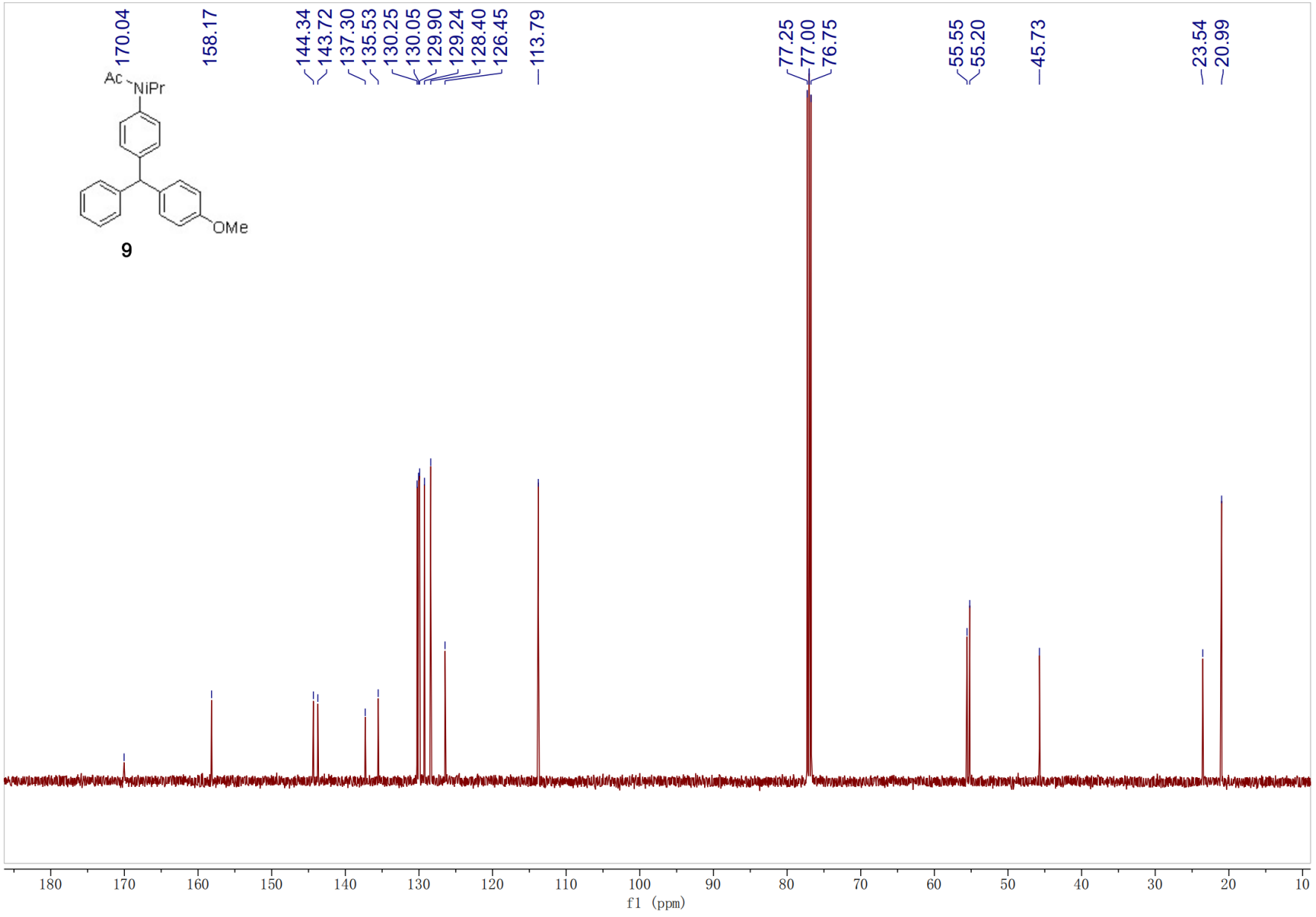

7.98
7.96
7.82
7.79
7.77
7.48
7.46
7.38
7.37
7.36
7.35
7.28
7.26
7.25
7.23
7.11
7.09
6.43
5.12
0.29
HO
TMS
7
1.05
1.04
0.96
2.99
2.95
1.18
4.26
1.07
1.00
1.01
8.58
f1 (ppm)


152.63
142.17
141.31
133.30
132.55
132.01
130.82
129.80
129.19
128.93
128.74
127.32
126.85
123.27
122.78
121.86
119.76
119.70
104.74
94.51
77.25
77.00
76.75
48.41
-0.06
HO
TMS
7
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


7.86
7.84
7.80
7.78
7.77
7.76
7.34
7.33
7.30
7.29
7.29
7.28
7.27
7.27
7.24
7.23
7.23
7.21
7.21
7.21
7.19
7.18
7.18
7.17
7.10
7.09
6.49
3.85
3.83
3.82
1.53
1.52
1.50
1.49
1.47
1.46
0.87
0.86
0.84
0.00
nPrO
Br
8
0.97
1.96
1.99
2.93
5.44
2.03
1.00
2.02
2.32
3.13
f1 (ppm)


154.72
142.90
142.79
133.19
131.00
130.89
129.65
129.33
129.00
128.67
128.11
126.22
125.95
124.41
124.29
123.13
119.51
114.99
77.25
77.00
76.75
70.82
47.20
22.59
10.55
nPrO
Br
8
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.32
7.30
7.29
7.24
7.23
7.22
7.15
7.13
7.12
7.12
7.10
7.03
7.02
7.01
7.00
6.86
6.84
5.53
5.03
5.02
5.00
4.99
4.97
4.96
4.95
3.79
1.75
1.05
1.03
0.00
Ac
NiPr
OMe
9
1.98
1.13
3.98
4.03
1.95
1.00
0.99
2.99
3.52
5.91
f1 (ppm)


170.04
158.17
144.34
143.72
137.30
135.53
130.25
130.05
129.90
129.24
128.40
126.45
113.79
77.25
77.00
76.75
55.55
55.20
45.73
23.54
20.99
Ac
NiPr
OMe
9
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

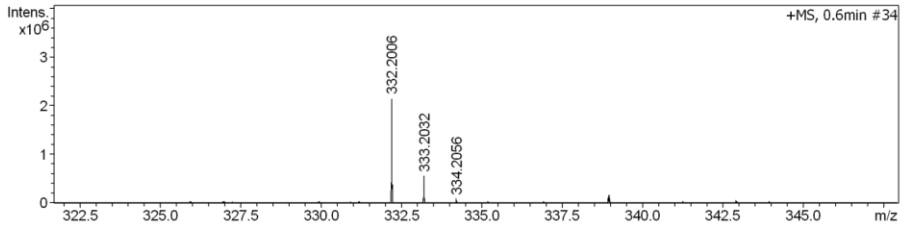
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-47_P1-A-9_01_37904.d	Acquisition Date	2/13/2023 3:26:01 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-47	Instrument	maXis impact 282001.00122
Comment			

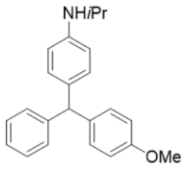
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	332.2006	25135	2110.6	2148556	100.0	0.0132
2	333.2032	25598	538.7	548480	25.5	0.0130
3	334.2056	20166	67.9	69100	3.2	0.0166

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
332.2006	1	C23H26NO	332.2009	0.9	0.8	1	100.00	11.5	even	ok



3a

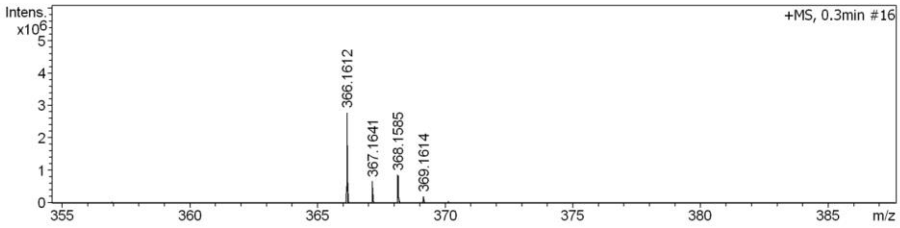
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-101_P1-B-7_01_39422.d	Acquisition Date	3/24/2023 11:39:37 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-101	Instrument	maXis impact 282001.00122
Comment			

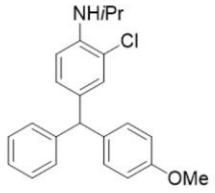
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	366.1612	25462	4246.9	2777816	100.0	0.0144
2	367.1641	27849	1012.9	663304	23.9	0.0132
3	368.1585	27061	1315.2	862596	31.1	0.0136
4	369.1614	22705	303.9	199472	7.2	0.0163

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
366.1612	1	C23H25ClNO	366.1619	1.8	21.4	1	100.00	11.5	even	ok



3b

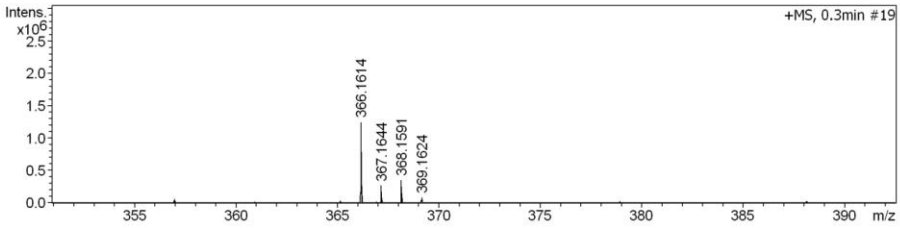
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-84_P1-B-5_01_39420.d	Acquisition Date	3/24/2023 11:33:20 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-84	Instrument	maXis impact 282001.00122
Comment			

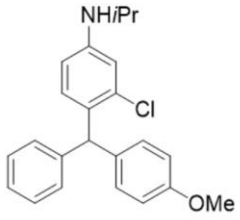
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	366.1614	31387	1930.1	1248216	100.0	0.0117
2	367.1644	21024	409.7	264860	21.2	0.0175
3	368.1591	22088	544.5	352132	28.2	0.0167
4	369.1624	17354	118.7	76776	6.2	0.0213

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
366.1614	1	C23H25ClNO	366.1619	1.5	38.8	1	100.00	11.5	even	ok



3c

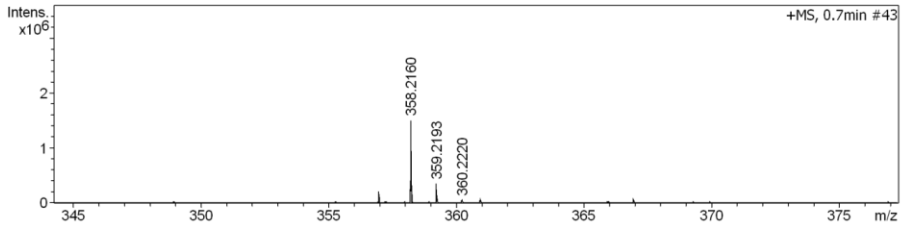
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-48_P1-F-1_01_37905.d	Acquisition Date	2/13/2023 3:29:09 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-48	Instrument	maXis impact 282001.00122
Comment			

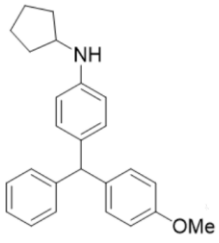
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	358.2160	30073	1479.1	1507508	100.0	0.0119
2	359.2193	20966	337.7	344156	22.8	0.0171
3	360.2220	18050	43.0	43856	2.9	0.0200

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
358.2160	1	C25H28NO	358.2165	1.5	25.2	1	100.00	12.5	even	ok



3d

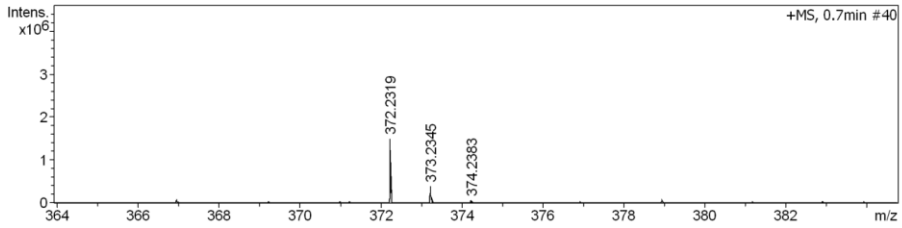
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-49_P1-E-1_01_37866.d	Acquisition Date	2/13/2023 1:19:07 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-49	Instrument	maXis impact 282001.00122
Comment			

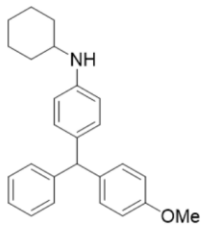
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	372.2319	26745	1412.5	1489028	100.0	0.0139
2	373.2345	20866	361.3	380960	25.6	0.0179
3	374.2383	17482	51.2	54044	3.6	0.0214

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
372.2319	1	C26H30NO	372.2322	0.8	16.7	1	100.00	12.5	even	ok



3e

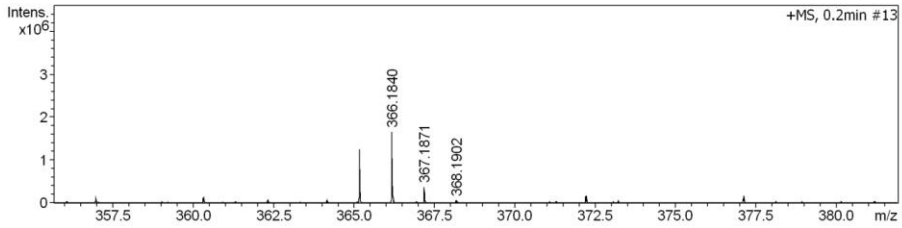
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-12_P1-E-2_01_37867.d	Acquisition Date	2/13/2023 1:22:15 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-12	Instrument	maXis impact 282001.00122
Comment			

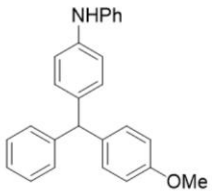
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	366.1840	26472	1159.6	1648996	100.0	0.0138
2	367.1871	20981	260.1	370860	22.5	0.0175
3	368.1902	17230	36.6	52316	3.2	0.0214

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
366.1840	1	C26H24NO	366.1852	3.5	32.0	3	100.00	15.5	even	ok



3f

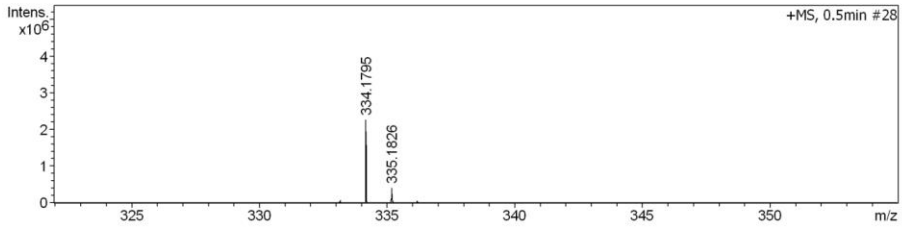
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-28_P1-A-2_01_39491.d	Acquisition Date	3/27/2023 1:46:45 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-28	Instrument	maXis impact 282001.00122
Comment			

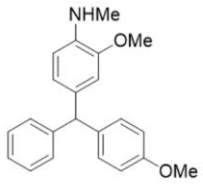
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	334.1795	34347	4826.3	2264320	100.0	0.0097
2	335.1826	23865	882.1	413408	18.3	0.0140
3	336.1852	18372	102.1	47808	2.1	0.0183

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
334.1795	1	C22H24NO2	334.1802	1.8	36.7	1	100.00	11.5	even	ok



3g

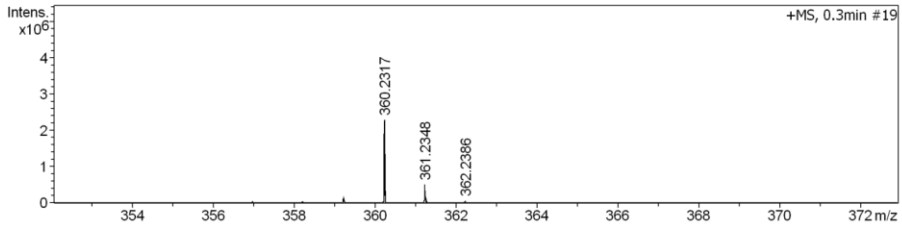
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-85_P1-C-3_01_39425.d	Acquisition Date	3/24/2023 11:49:03 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-85	Instrument	maXis impact 282001.00122
Comment			

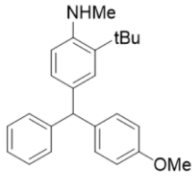
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	360.2317	32906	3455.9	2286248	100.0	0.0109
2	361.2348	25386	776.8	513936	22.5	0.0142
3	362.2386	16271	89.0	58836	2.6	0.0223

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
360.2317	1	C25H30NO	360.2322	1.4	27.4	1	100.00	11.5	even	ok



3h

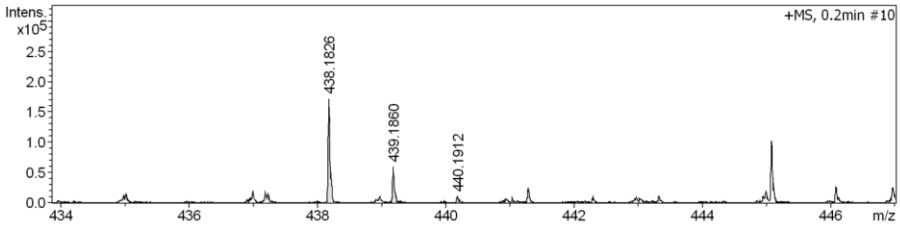
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\LYY-2-89_P2-E-2_01_60281.d	Acquisition Date	3/10/2025 2:21:54 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	LYY-2-89	Instrument	maXis impact 282001.00122
Comment			

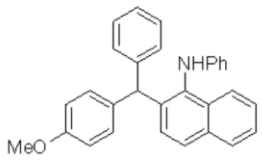
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	438.1826	18081	155.4	172056	100.0	0.0242
2	439.1860	16178	53.8	59680	34.7	0.0271
3	440.1912	15226	9.3	10372	6.0	0.0289

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
438.1826	1	C30H25NNaO	438.1828	0.6	8.5	1	100.00	18.5	even	ok



3i

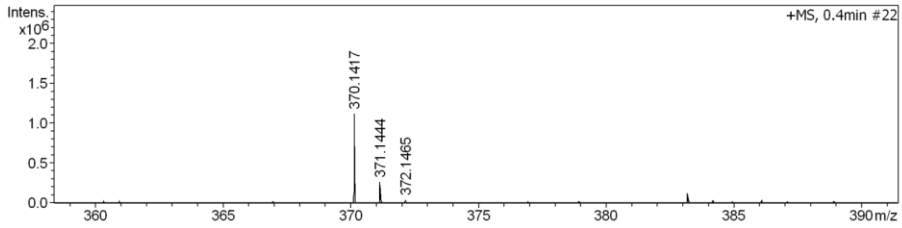
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\LYY-2-85_P2-E-1_01_60280.d	Acquisition Date	3/10/2025 2:18:45 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	LYY-2-85	Instrument	maXis impact 282001.00122
Comment			

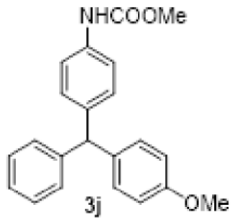
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	370.1417	23536	1297.8	1113892	100.0	0.0157
2	371.1444	18709	306.3	262732	23.6	0.0198
3	372.1465	16232	47.3	40552	3.6	0.0229

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
370.1417	1	C22H21NNaO3	370.1414	-0.9	4.7	1	100.00	12.5	even	ok



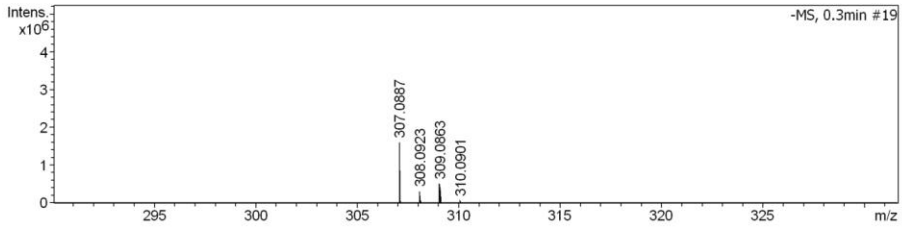
3j

Mass Spectrum List Report

Analysis Info	D:\Data\chem.	Acquisition Date	3/27/2023 11:56:35 AM
Analysis Name	dep\liulu\WYZ-6-112_P1-D-2_01_39486.dTune_neg_low		
Method	_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-112	Instrument	maXis impact 282001.00122
Comment			

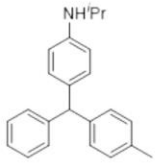
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	307.0887	37222	5679.4	1601848	100.0	0.0083
2	308.0923	32733	1112.4	313816	19.6	0.0094
3	309.0863	33442	1812.8	511448	31.9	0.0092
4	310.0901	23040	212.6	60100	3.8	0.0135

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e⁻ Conf	N-Rule
307.0887	1	C23H25NNa	307.0895	2.6	21.8	21.8	100.00	12.5 even	ok



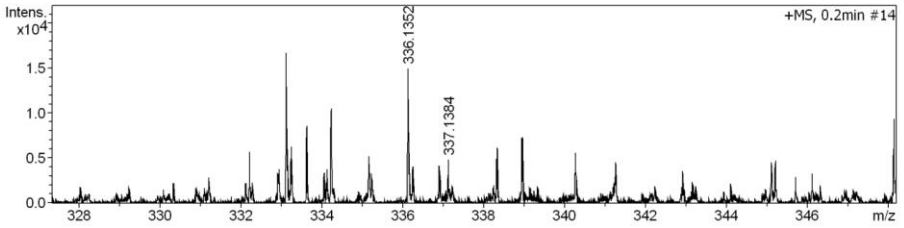
3m

Mass Spectrum List Report

Analysis Info	D:\Data\chem.	Acquisition Date	3/24/2023 11:05:04 AM
Analysis Name	dep\liulu\WYZ-6-123_P1-A-3_01_39411.dTune_pos_low_		
Method	LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-123	Instrument	maXis impact 282001.00122
Comment			

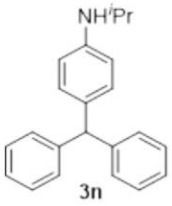
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	336.1352	16388	20.9	14900	100.0	0.0205
2	337.1384	22600	6.7	4820	32.3	0.0149

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e⁻ Conf	N-Rule
336.1352	1	C22H23N	336.1359	2.0	49.1	1	100.00	13.5 even	ok



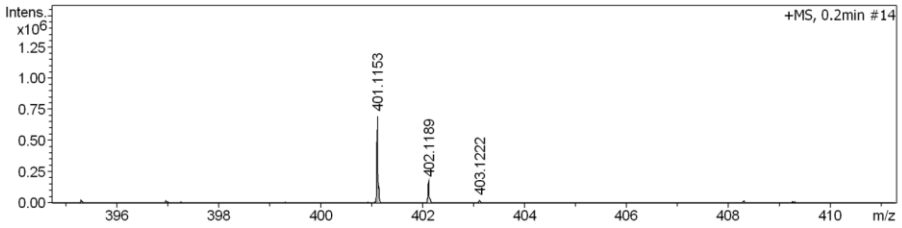
3n

Mass Spectrum List Report

Analysis Info	D:\Data\chem.	Acquisition Date	3/30/2023 5:11:56 PM
Analysis Name	dep\liulu\WYZ-6-109_P1-D-8_01_39668.dTune_pos_low_L		
Method	C with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-109	Instrument	maXis impact 282001.00122
Comment			

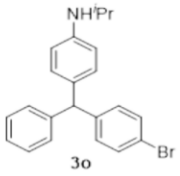
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	401.1153	25153	924.5	697616	100.0	0.0159
2	402.1189	18567	226.5	171112	24.5	0.0217
3	403.1222	15092	32.4	24480	3.5	0.0267

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e⁻ Conf	N-Rule
401.1153	1	C22H22BrNNa	401.1148	-1.3	20.2	1	100.00	17.5 even	ok



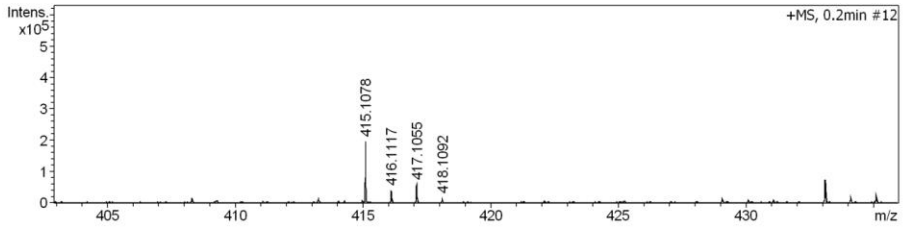
3o

Mass Spectrum List Report

Analysis Info	D:\Data\chem.	Acquisition Date	3/30/2023 5:05:40 PM
Analysis Name	dep\liulu\WYZ-6-110_P1-D-7_01_39666.dTune_pos_low_L		
Method	C with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-110	Instrument	maXis impact 282001.00122
Comment			

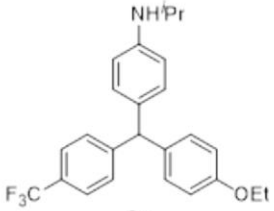
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	415.1078	19960	243.6	195480	100.0	0.0208
2	416.1117	14833	50.3	40404	20.7	0.0281
3	417.1055	16211	72.2	58088	29.7	0.0257
4	418.1092	16023	18.2	14660	7.5	0.0261

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	Score	rdb	e⁻ Conf	N-Rule
415.1078	1	C25H26F3NO	415.1071	-1.6	38.0	1	100.00	13.5 even	ok



3p

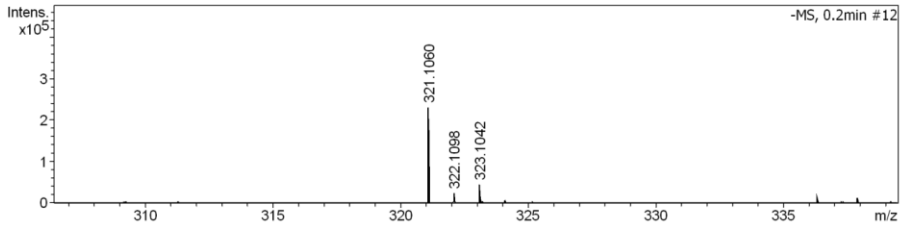
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-25_P1-A-1_01_39469.d	Acquisition Date	3/27/2023 10:01:17 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-25	Instrument	maXis impact 282001.00122
Comment			

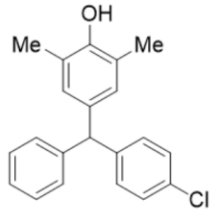
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	321.1060	31101	763.9	231084	100.0	0.0103
2	322.1098	26772	75.4	22820	9.9	0.0120
3	323.1042	24922	147.0	44532	19.3	0.0130

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
321.1060	1	C21H18ClO	321.1052	-2.6	94.2	94.2	28.13	12.5	even	ok



4a

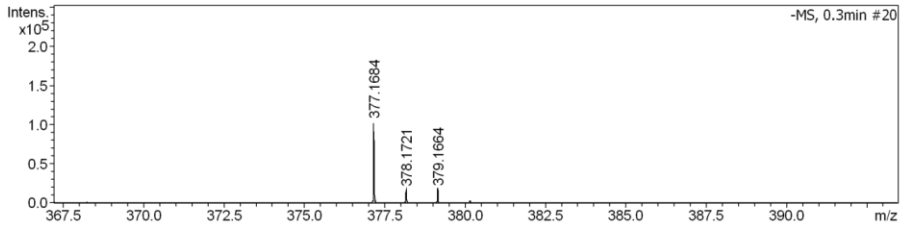
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-38_P1-C-5_01_39481.d	Acquisition Date	3/27/2023 10:46:08 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-38	Instrument	maXis impact 282001.00122
Comment			

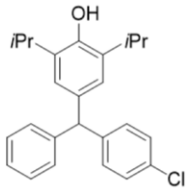
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	377.1684	27808	361.2	102104	100.0	0.0136
2	378.1721	27353	53.8	15212	14.9	0.0138
3	379.1664	17776	57.0	16100	15.8	0.0213

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
377.1684	1	C25H26ClO	377.1678	-1.6	113.3	113.3	19.04	12.5	even	ok



4b

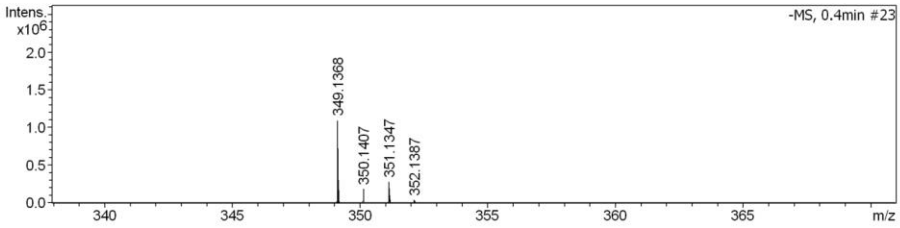
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-26_P1-C-7_01_39483.d	Acquisition Date	3/27/2023 10:52:26 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-26	Instrument	maXis impact 282001.00122
Comment			

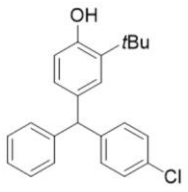
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	349.1368	43493	3883.3	1095556	100.0	0.0080
2	350.1407	28894	650.3	183684	16.8	0.0121
3	351.1347	29957	990.6	279912	25.5	0.0117
4	352.1387	21023	130.3	36840	3.4	0.0168

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
349.1368	1	C23H22ClO	349.1365	-1.0	61.6	61.6	100.00	12.5	even	ok



4c

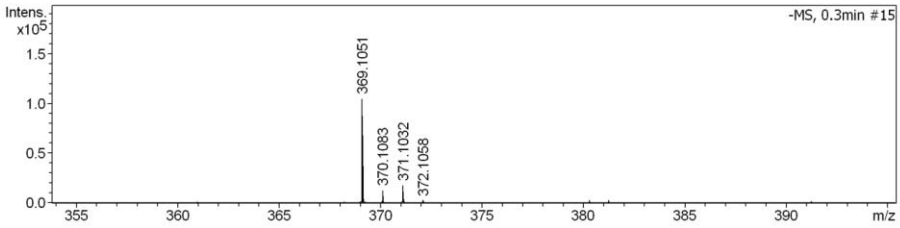
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-27_P1-A-7_01_39474.d	Acquisition Date	3/27/2023 10:24:09 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-27	Instrument	maXis impact 282001.00122
Comment			

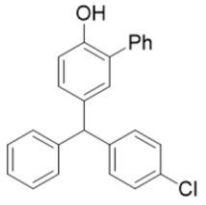
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	369.1051	31328	371.1	104600	100.0	0.0118
2	370.1083	25729	44.1	12424	11.9	0.0144
3	371.1032	23456	63.1	17756	17.0	0.0158
4	372.1058	18605	7.8	2204	2.1	0.0200

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
369.1051	1	C25H18ClO	369.1052	0.3	116.2	116.2	22.26	16.5	even	ok



4d

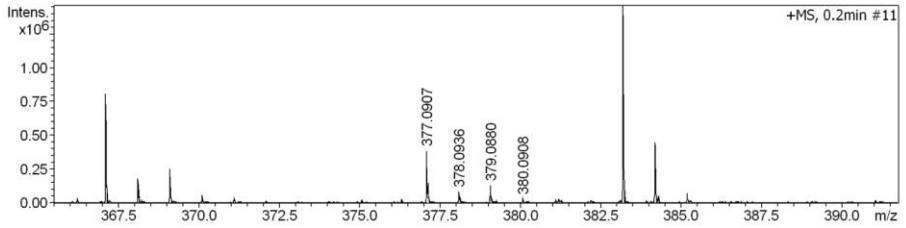
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-5-115_P1-A-5_01_37900.d	Acquisition Date	2/13/2023 3:13:29 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-5-115	Instrument	maXis impact 282001.00122
Comment			

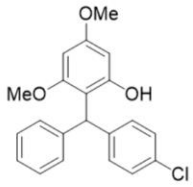
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	377.0907	25109	319.3	386132	100.0	0.0150
2	378.0936	17709	67.1	81556	21.1	0.0214
3	379.0880	20014	105.0	128132	33.2	0.0189
4	380.0908	19865	23.5	28800	7.5	0.0191

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
377.0907	1	C21H19ClNaO3	377.0915	2.2	13.2	2	100.00	11.5	even	ok



4e

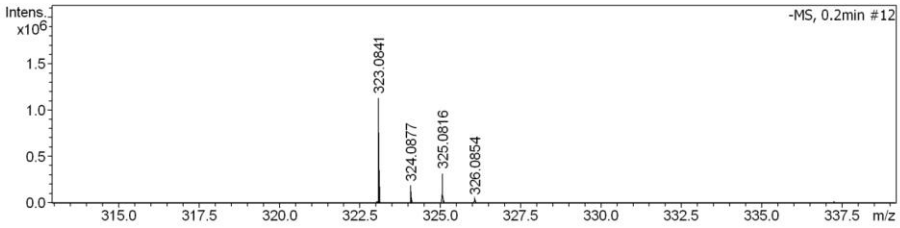
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-64_P1-B-3_01_39477.d	Acquisition Date	3/27/2023 10:33:35 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-64	Instrument	maXis impact 282001.00122
Comment			

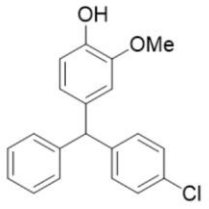
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	323.0841	37615	3741.7	1127480	100.0	0.0086
2	324.0877	30170	621.8	187616	16.6	0.0107
3	325.0816	32285	1068.9	322824	28.6	0.0101
4	326.0854	25274	128.8	38908	3.5	0.0129

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
323.0841	1	C20H16ClO2	323.0844	1.0	39.8	39.8	100.00	12.5	even	ok



4f

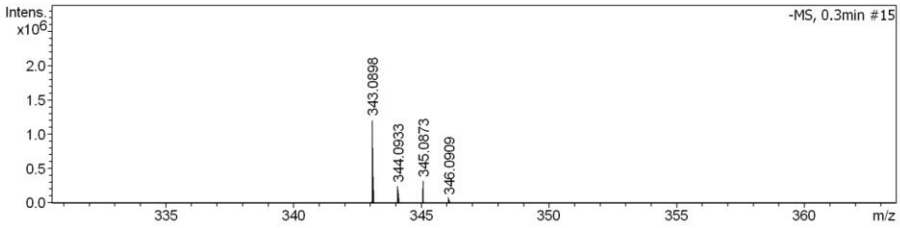
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-39_P1-B-1_01_39475.d	Acquisition Date	3/27/2023 10:27:17 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-39	Instrument	maXis impact 282001.00122
Comment			

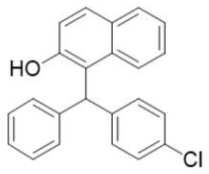
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	343.0898	40048	4118.2	1205584	100.0	0.0086
2	344.0933	33678	827.0	242288	20.1	0.0102
3	345.0873	31473	1078.2	315636	26.2	0.0110
4	346.0909	23635	167.6	49112	4.1	0.0146

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
343.0898	1	C23H16ClO	343.0895	-0.8	50.1	50.1	100.00	15.5	even	ok



4g

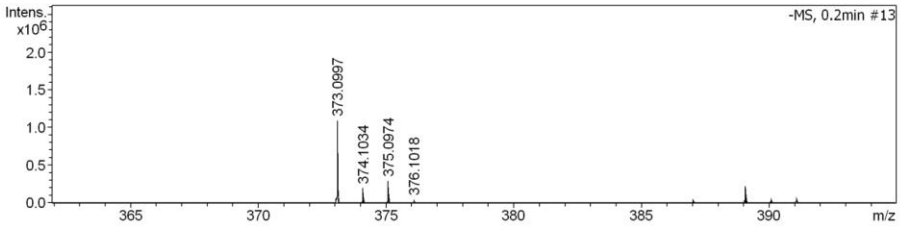
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-40_P1-C-8_01_39484.d	Acquisition Date	3/27/2023 11:50:20 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-40	Instrument	maXis impact 282001.00122
Comment			

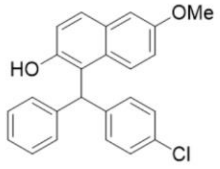
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	373.0997	44750	3727.6	1088156	100.0	0.0083
2	374.1034	19788	662.9	193460	17.8	0.0189
3	375.0974	33890	1007.7	294176	27.0	0.0111
4	376.1018	22092	136.7	39888	3.7	0.0170

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
373.0997	1	C24H18ClO2	373.1001	1.0	59.0	59.0	100.00	15.5	even	ok



4h

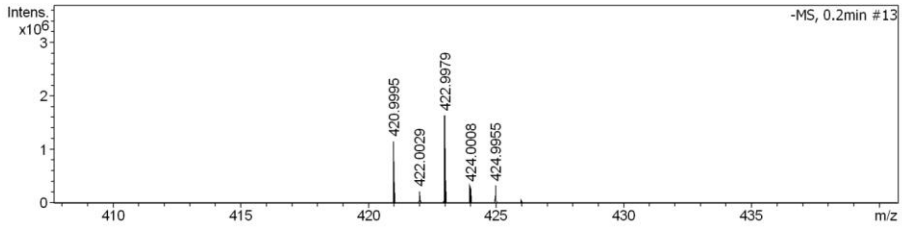
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-42_P1-B-4_01_39478.d	Acquisition Date	3/27/2023 10:36:44 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-42	Instrument	maXis impact 282001.00122
Comment			

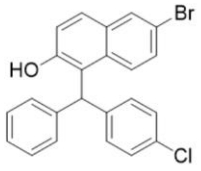
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	420.9995	43434	3995.9	1155308	71.0	0.0097
2	422.0029	33126	757.5	219192	13.5	0.0127
3	422.9979	40985	5625.3	1627652	100.0	0.0103
4	424.0008	36314	1094.0	316728	19.5	0.0117
5	424.9955	35012	1117.8	323668	19.9	0.0121

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e⁻ Conf	N-Rule
420.9995	1	C23H15BrClO	421.0000	1.2	44.0	44.0	100.00	15.5	even	ok



4i

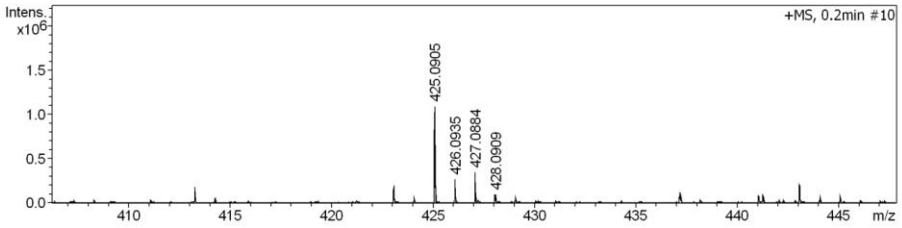
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-43_P1-A-1_01_37896.d	Acquisition Date	2/13/2023 3:00:55 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-43	Instrument	maXis impact 282001.00122
Comment			

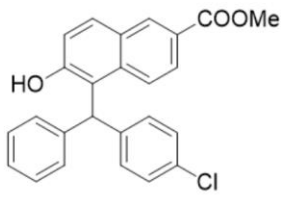
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	425.0905	27953	652.6	1091252	100.0	0.0152
2	426.0935	19944	160.3	269944	24.7	0.0214
3	427.0884	21819	204.2	346132	31.7	0.0196
4	428.0909	17882	53.5	91312	8.4	0.0239

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
425.0905	1	C25H19ClNaO3	425.0915	2.4	28.0	2	100.00	15.5	even	ok



4j

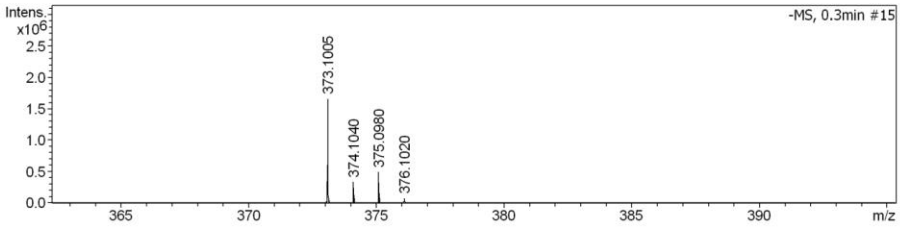
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-41_P1-A-6_01_39473.d	Acquisition Date	3/27/2023 10:20:59 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-41	Instrument	maXis impact 282001.00122
Comment			

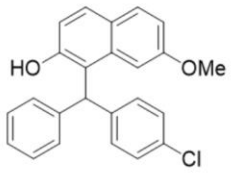
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	373.1005	42345	5727.5	1659344	100.0	0.0088
2	374.1040	33471	1157.6	335448	20.2	0.0112
3	375.0980	37742	1698.6	492144	29.7	0.0099
4	376.1020	26291	267.7	77572	4.7	0.0143

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
373.1005	1	C24H18ClO2	373.1001	-1.2	42.6	42.6	100.00	15.5	even	ok



4k

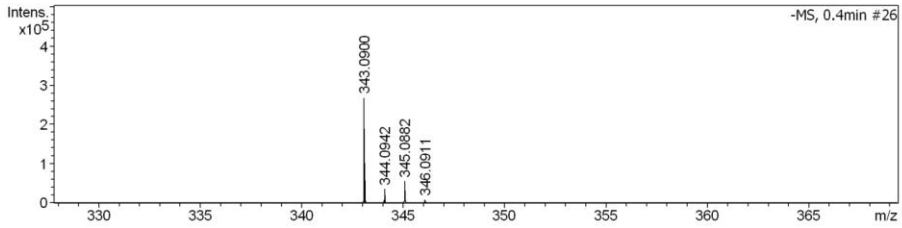
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-44_P1-B-6_01_39479.d	Acquisition Date	3/27/2023 10:39:53 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-44	Instrument	maXis impact 282001.00122
Comment			

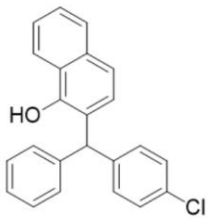
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	343.0900	30794	952.9	266312	100.0	0.0111
2	344.0942	22631	122.7	34296	12.9	0.0152
3	345.0882	16329	194.0	54236	20.4	0.0211
4	346.0911	16702	25.6	7144	2.7	0.0207

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
343.0900	1	C23H16ClO	343.0895	-1.3	89.7	89.7	25.09	15.5	even	ok



4l

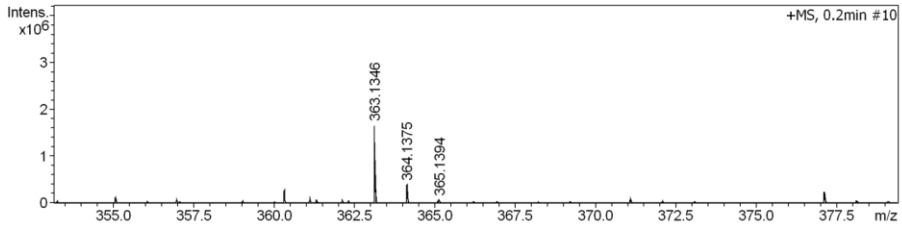
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-59_P1-E-7_01_37872.d	Acquisition Date	2/13/2023 1:37:57 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-59	Instrument	maXis impact 282001.00122
Comment			

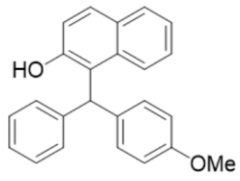
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	363.1346	28677	1320.2	1656528	100.0	0.0127
2	364.1375	22675	310.3	390632	23.6	0.0161
3	365.1394	17524	46.5	58724	3.5	0.0208

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
363.1346	1	C24H20NaO2	363.1356	2.7	13.5	2	100.00	14.5	even	ok



4m

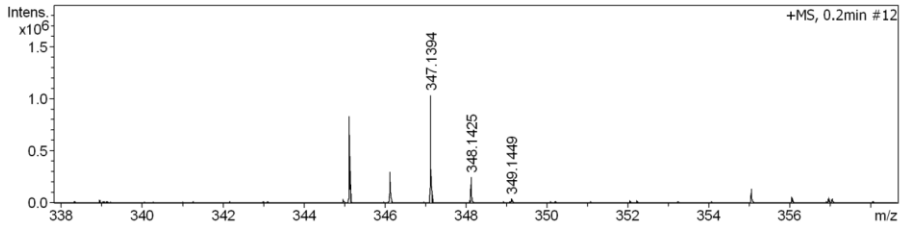
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-62_P1-E-8_01_37873.d	Acquisition Date	2/13/2023 1:41:06 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-62	Instrument	maXis impact 282001.00122
Comment			

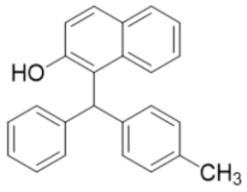
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	347.1394	26733	876.8	1033620	100.0	0.0130
2	348.1425	21152	209.2	246876	23.9	0.0165
3	349.1449	21480	32.9	38896	3.8	0.0163

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
347.1394	1	C24H20NaO	347.1406	3.6	13.6	1	100.00	14.5	even	ok



4n

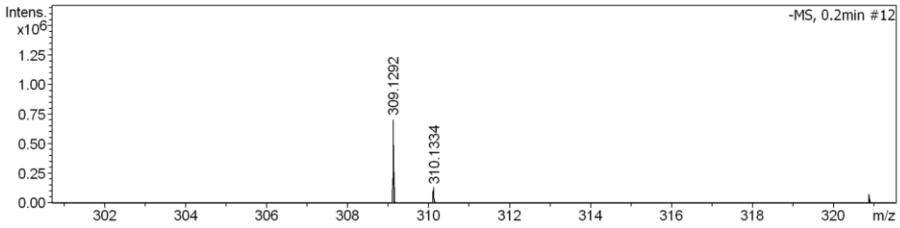
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-57_P1-A-2_01_39470.d	Acquisition Date	3/27/2023 10:09:09 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-57	Instrument	maXis impact 282001.00122
Comment			

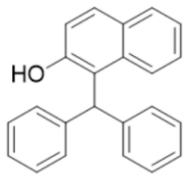
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	309.1292	38390	2575.9	702840	100.0	0.0081
2	310.1334	27516	450.0	122852	17.5	0.0113
3	311.1373	10288	12.0	3284	0.5	0.0302

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
309.1292	1	C23H17O	309.1285	-2.3	47.8	47.8	74.67	15.5	even	ok



4o

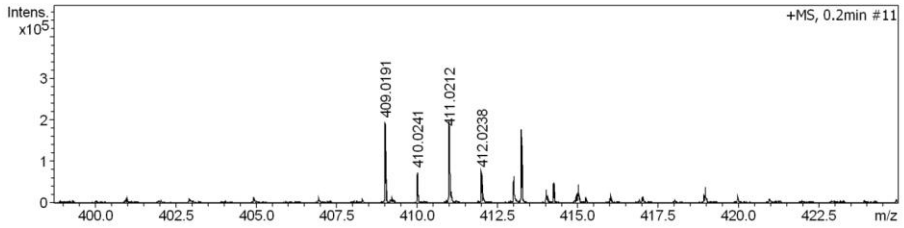
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-58_P1-E-9_01_37874.d	Acquisition Date	2/13/2023 1:44:14 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-58	Instrument	maXis impact 282001.00122
Comment			

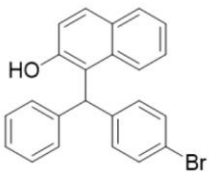
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	409.0191	19529	134.8	193552	100.0	0.0209
2	410.0241	17990	51.2	73708	38.1	0.0228
3	411.0212	11536	120.8	173920	89.9	0.0356
4	412.0238	16673	51.7	74504	38.5	0.0247

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
409.0191	1	C23H15BrNaO	409.0198	1.9	97.9	1	100.00	15.5	even	ok



4p

Bruker Compass DataAnalysis 4.1 printed: 2/13/2023 2:14:43 PM by: ECNU-Chem Page 1 of 1

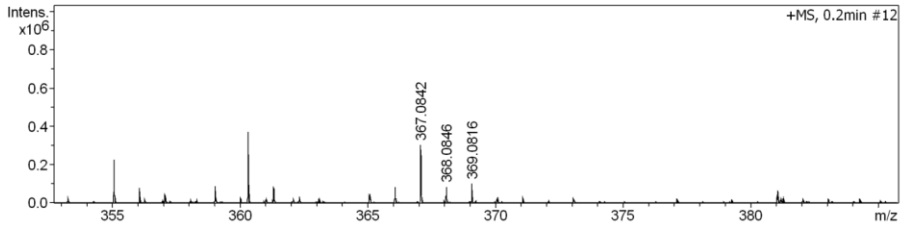
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-60_P2-D-1_01_37913.d	Acquisition Date	2/13/2023 3:54:15 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-60	Instrument	maXis impact 282001.00122
Comment			

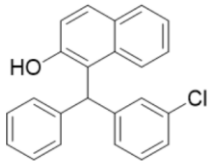
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	367.0842	21593	293.9	303732	100.0	0.0170
2	368.0846	16744	81.2	84028	27.7	0.0220
3	369.0816	17971	95.4	98816	32.5	0.0205

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
367.0842	1	C23H17ClNaO	367.0860	5.0	33.7	1	100.00	14.5	even	ok



4q

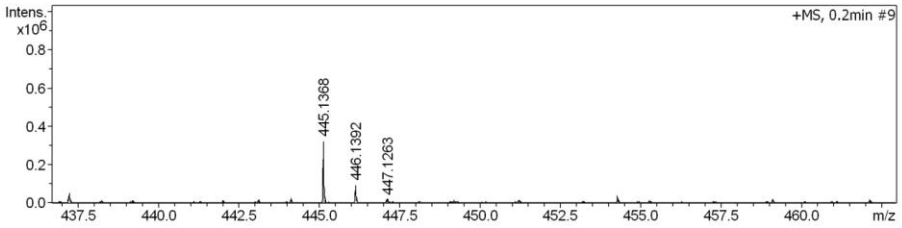
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-63_P2-D-3_01_37915.d	Acquisition Date	2/13/2023 4:00:32 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-63	Instrument	maXis impact 282001.00122
Comment			

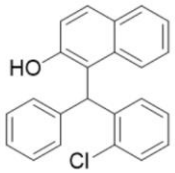
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	445.1368	21514	281.7	323596	100.0	0.0207
2	446.1392	18193	79.6	91488	28.3	0.0245
3	447.1263	107032	13.2	15232	4.7	0.0042

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
445.1368	1	C26H21F3NaO2	445.1386	4.1	21.7	1	48.61	14.5	even	ok



4r

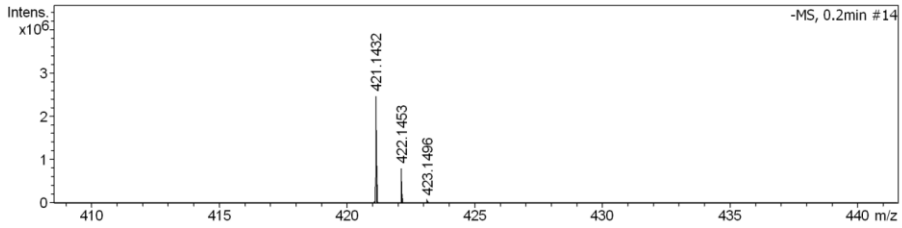
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-63_P1-B-2_01_39476.d	Acquisition Date	3/27/2023 10:30:27 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-63	Instrument	maXis impact 282001.00122
Comment			

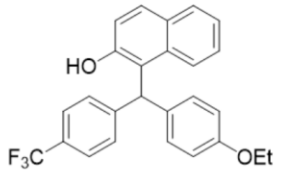
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	421.1432	22230	8805.7	2467464	100.0	0.0189
2	422.1453	42181	2889.4	810468	32.8	0.0100
3	423.1496	25902	216.8	60820	2.5	0.0163

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
421.1432	1	C26H20F3O2	421.1421	-2.7	24.0	24.0	81.18	15.5	even	ok



4s

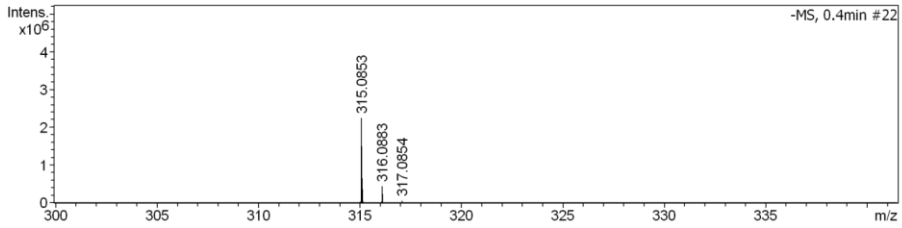
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-96_P1-D-1_01_39485.d	Acquisition Date	3/27/2023 11:53:28 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-96	Instrument	maXis impact 282001.00122
Comment			

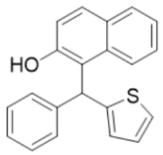
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	315.0853	39029	7998.0	2242060	100.0	0.0081
2	316.0883	34482	1577.1	442560	19.7	0.0092
3	317.0854	13589	212.6	59724	2.7	0.0233

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
315.0853	1	C21H15OS	315.0849	-1.3	31.2	31.2	100.00	14.5	even	ok



4t

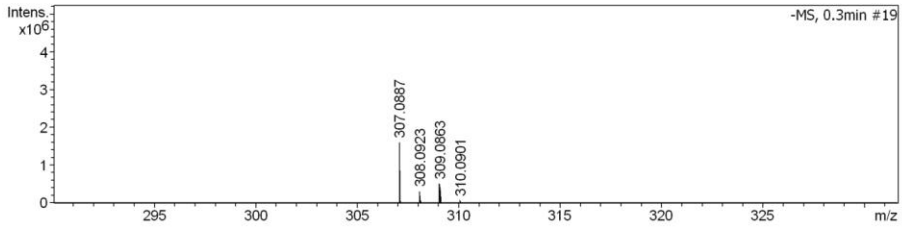
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-30_P1-D-2_01_39486.d	Acquisition Date	3/27/2023 11:56:35 AM
Method	Tune_neg_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-30	Instrument	maXis impact 282001.00122
Comment			

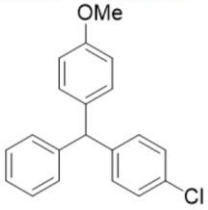
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	307.0887	37222	5679.4	1601848	100.0	0.0083
2	308.0923	32733	1112.4	313816	19.6	0.0094
3	309.0863	33442	1812.8	511448	31.9	0.0092
4	310.0901	23040	212.6	60100	3.8	0.0135

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	mSigma	Score	rdb	e¯ Conf	N-Rule
307.0887	1	C20H16ClO	307.0895	2.6	21.8	21.8	100.00	12.5	even	ok



5a

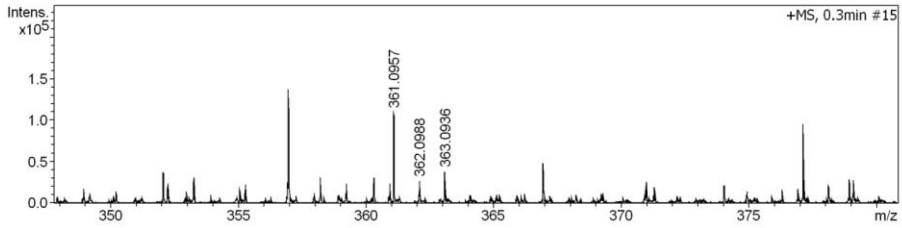
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-31_P1-F-2_01_37877.d	Acquisition Date	2/13/2023 1:53:38 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-31	Instrument	maXis impact 282001.00122
Comment			

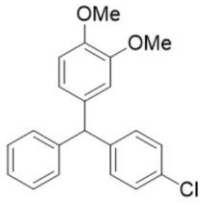
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	361.0957	19943	80.8	108960	100.0	0.0181
2	362.0988	16122	19.9	26828	24.6	0.0225
3	363.0936	18290	28.1	37992	34.9	0.0199

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
361.0957	1	C21H19ClNaO2	361.0966	2.5	8.5	1	100.00	11.5	even	ok



5b

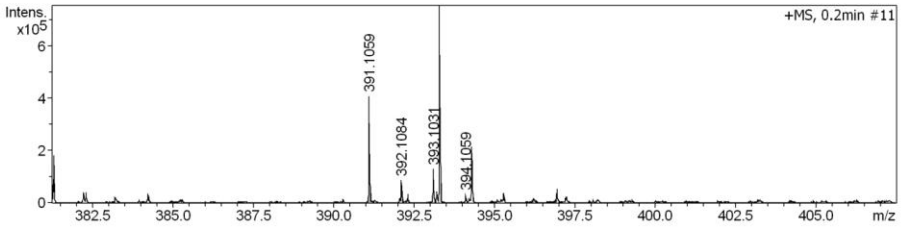
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-33_P1-F-4_01_37879.d	Acquisition Date	2/13/2023 1:59:53 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-33	Instrument	maXis impact 282001.00122
Comment			

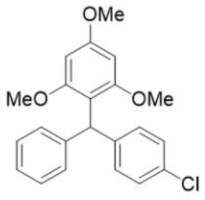
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	391.1059	24824	316.8	405356	100.0	0.0158
2	392.1084	17398	66.4	85384	21.1	0.0225
3	393.1031	18741	100.1	129088	31.8	0.0210
4	394.1059	16824	23.7	30784	7.6	0.0234

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
391.1059	1	C22H21ClNaO3	391.1071	3.3	21.9	3	92.16	11.5	even	ok



5d

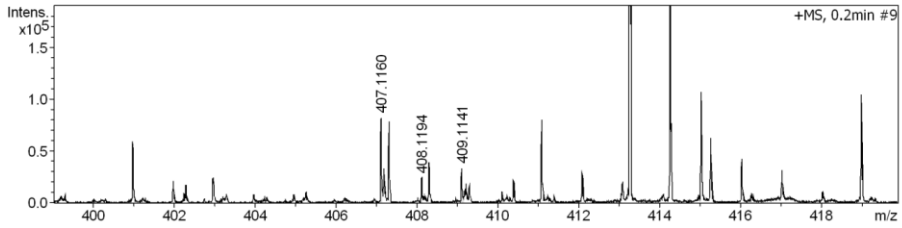
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-36_P2-F-5_01_37925.d	Acquisition Date	2/13/2023 4:31:54 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-36	Instrument	maXis impact 282001.00122
Comment			

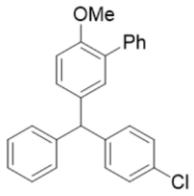
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	407.1160	19408	75.1	82232	100.0	0.0210
2	408.1194	18464	22.0	24252	29.5	0.0221
3	409.1141	20480	30.5	33876	41.2	0.0200

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
407.1160	1	C26H21ClNaO	407.1173	3.3	29.0	1	100.00	15.5	even	ok



5e

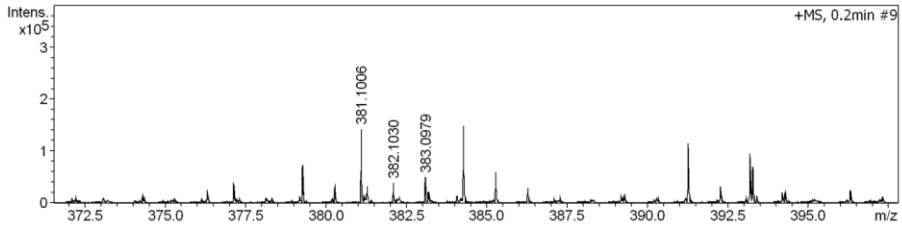
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-37_P2-F-6_01_37926.d	Acquisition Date	2/13/2023 4:35:02 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-37	Instrument	maXis impact 282001.00122
Comment			

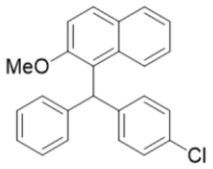
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	381.1006	20525	110.0	142028	100.0	0.0186
2	382.1030	20167	30.2	38972	27.4	0.0189
3	383.0979	18167	38.3	49568	34.9	0.0211

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
381.1006	1	C24H19ClNaO	381.1017	2.9	8.9	1	100.00	14.5	even	ok



5f

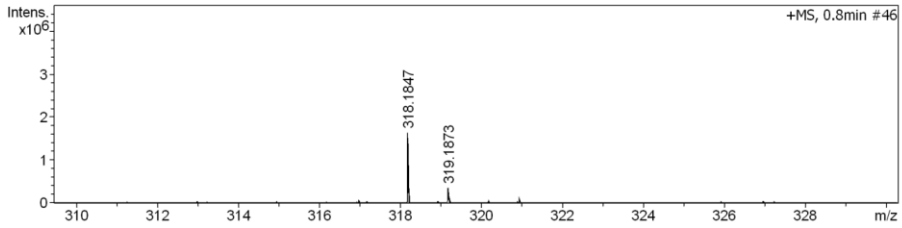
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-46_P1-E-3_01_37868.d	Acquisition Date	2/13/2023 1:25:22 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-46	Instrument	maXis impact 282001.00122
Comment			

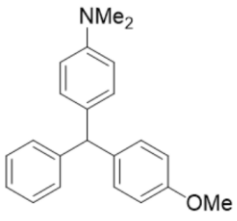
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	318.1847	27246	1657.0	1631608	100.0	0.0117
2	319.1873	22083	357.8	352408	21.6	0.0145
3	320.1899	16545	42.9	42308	2.6	0.0194

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
318.1847	1	C22H24NO	318.1852	1.7	16.8	1	100.00	11.5	even	ok



5g

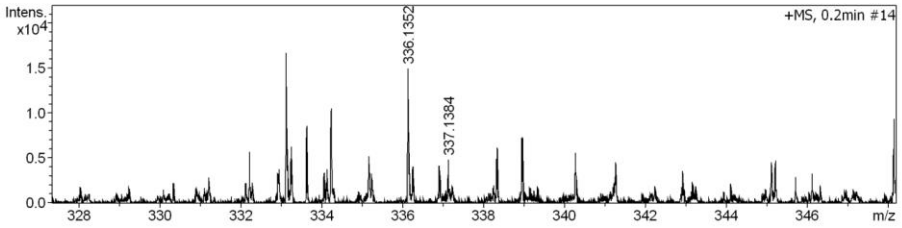
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-5-23_P1-A-3_01_39411.d	Acquisition Date	3/24/2023 11:05:04 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-5-23	Instrument	maXis impact 282001.00122
Comment			

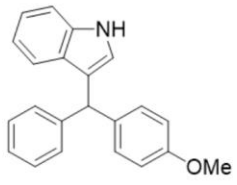
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	336.1352	16388	20.9	14900	100.0	0.0205
2	337.1384	22600	6.7	4820	32.3	0.0149

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
336.1352	1	C22H19NNaO	336.1359	2.0	49.1	1	100.00	13.5	even	ok



5h

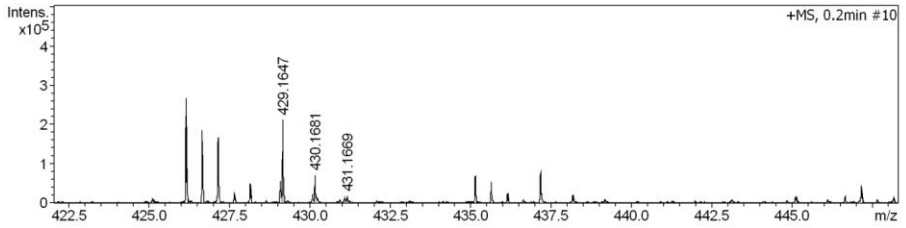
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-80_P1-C-4_01_39426.d	Acquisition Date	3/24/2023 11:52:11 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-80	Instrument	maXis impact 282001.00122
Comment			

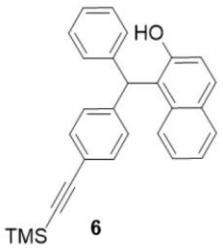
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	429.1647	18448	231.8	211452	100.0	0.0233
2	430.1681	17093	78.7	71744	33.9	0.0252
3	431.1669	14040	19.7	17904	8.5	0.0307

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
429.1647	1	C28H26NaOSi	429.1645	-0.5	10.6	1	100.00	16.5	even	ok



6

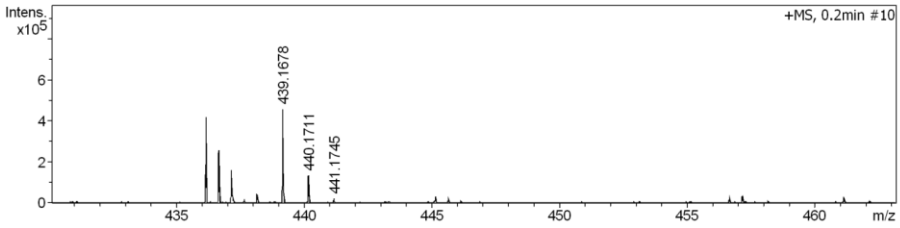
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-79_P1-C-2_01_39424.d	Acquisition Date	3/24/2023 11:45:55 AM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-79	Instrument	maXis impact 282001.00122
Comment			

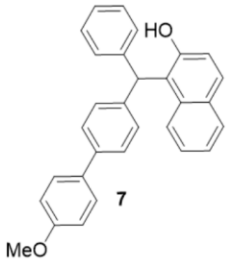
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	439.1678	22241	601.5	457656	100.0	0.0197
2	440.1711	17956	177.9	135276	29.6	0.0245
3	441.1745	13678	26.9	20388	4.5	0.0323

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
439.1678	1	C30H24NaO2	439.1669	-2.1	17.2	1	100.00	18.5	even	ok



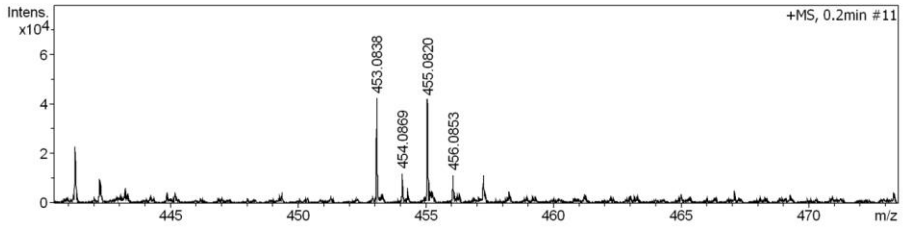
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\chem. dep\liulu\WYZ-6-94_P1-A-1_01_39490.d	Acquisition Date	3/27/2023 1:43:36 PM
Method	Tune_pos_low_LC with calibration_2min_20210727.m	Operator	ECNU-Chem
Sample Name	WYZ-6-94	Instrument	maXis impact 282001.00122
Comment			

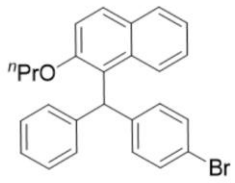
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1350 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	453.0838	15532	50.9	42352	100.0	0.0292
2	454.0869	15509	14.4	12008	28.4	0.0293
3	455.0820	15356	49.7	41356	97.6	0.0296
4	456.0853	14993	13.7	11420	27.0	0.0304

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
453.0838	1	C26H23BrNaO	453.0824	-2.9	19.9	1	100.00	14.5	even	ok



8