Supporting Information

DBU-promoted Decomposition of Difluorocarbene and the Subsequent Trifluoromethylation*

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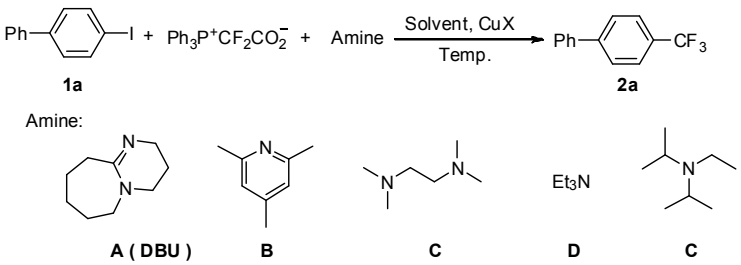
Contents

1. General information:

Solvents and reagents were purchased from commercial sources and used as received unless otherwise noted. ^{1}H, ^{13}C and ^{19}F NMR spectra were detected on a 500 MHz, 400 MHz or 300 MHz NMR spectrometer. Data for ^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, coupling constant (s) in Hz). Mass spectra were obtained on a GC-MS. High resolution mass data were recorded on a high resolution mass spectrometer in the EI or ESI mode.

2. Screening of reaction conditions with the use of PDFA

Table 1. Screening of reaction conditions with the use of PDFA[a]



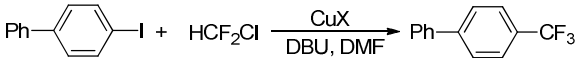
Entry	Temp. (°C)	Solvent	CuX	Amine	Molar Ratio[b]	Yield(%)[c]
1	80	DMF	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	29
2	80	DMSO	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	0
3	80	1,4-Dioxane	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	12
4	80	DCE	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	13
5	80	*p*-Xylene	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	17
6	80	NMP	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	23
7	80	DMA	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	25
8	80	EA	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	14
9	80	THF	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	10
10	80	Methyl benzoate	$[Cu(MeCN)_4]PF_4$	A	1:1.5:1:1	15
11	80	DMF	$[Cu(MeCN)_4]BF_4$	A	1:1.5:1:1	21
12	80	DMF	CuOAc	A	1:1.5:1:1	3
13	50	DMF	CuI	A	1:1.5:1:1	8
14[d]	50	DMF	CuI	--	1:1.5:1:--	0
15	80	DMF	$[Cu(MeCN)_4]PF_4$	B	1:1.5:1:1	trace
16	80	DMF	$[Cu(MeCN)_4]PF_4$	C	1:1.5:1:1	3
17	80	DMF	$[Cu(MeCN)_4]PF_4$	D	1:1.5:1:1	8
18	80	DMF	$[Cu(MeCN)_4]PF_4$	E	1:1.5:1:1	2
19	80	DMF	$[Cu(MeCN)_4]PF_4$	A	1:3:3:3	82
20	80	DMF	$[Cu(MeCN)_4]PF_4$	A	1:3.5:3.5:4	89

21[e]	55	DMF	$[Cu(MeCN)_4]PF_4$	A	1:3.5:3.5:4	94

[a]Reaction conditions: 1a (0.2 mmol), $Ph_3P^+CF_2CO_2^-$, CuX and amine in solvent (1 mL) for 3.5 h. [b] Molar ratio of **1a**:$Ph_3P^+CF_2CO_2^-$:CuX:base. [c]Determined by ^{19}F NMR. [d] The reaction was conducted for 4 h without the addition of DBU. [e]The reaction system was stirred for 36 h in 3 mL of DMF.

3. Screening of reaction conditions with the use of HCF_2Cl.

Table 2. Screening of reaction conditions with the use of HCF_2Cl[a]

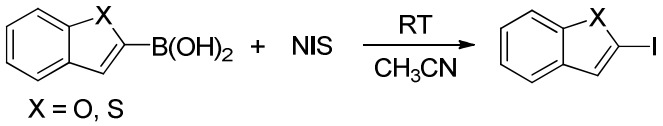


1a **2a**

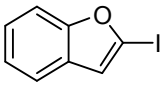
Entry	Solv.	CuX	DBU (eq.)	T (°C)	T (h)	Yield (%)[b]
1	DMF	$[Cu(MeCN)_4]PF_6$	2	80	3	13
2	DMF	$[Cu(MeCN)_4]BF_4$	2	80	3	20
3	DMF	CuBr	2	80	3	<1
4	DMF	CuI	2	80	3	3
5	DMF	CuOAc	2	80	3	<1
6	DMF	$[Cu(MeCN)_4]BF_4$	2	40	3	5
7	DMF	$[Cu(MeCN)_4]BF_4$	2	100	3	37
8	DMF	$[Cu(MeCN)_4]BF_4$	3	100	3	0
9	DMF	$[Cu(MeCN)_4]BF_4$	1.5	100	3	3
10	DMF	$[Cu(MeCN)_4]BF_4$	2	100	5	48
11	DMF	$[Cu(MeCN)_4]BF_4$[c]	7	100	5	80
12	DMF	$[Cu(MeCN)_4]BF_4$[c]	7	110	5	89
13	DMF	$[Cu(MeCN)_4]BF_4$[c]	7	120	5	93
14	*p*-xylene	$[Cu(MeCN)_4]BF_4$[c]	7	120	5	38
15	1,4-dioxane	$[Cu(MeCN)_4]BF_4$[c]	7	120	5	46
16	DMF	$[Cu(MeCN)_4]BF_4$[c]	DBN(7)[d]	120	5	33
17	DMF	$[Cu(MeCN)_4]BF_4$[c]	PO[e]	120	5	0

[a]Reaction conditions: into the solution of HCF_2Cl in DMF (2.43 M, 1.5 mL) was added 4-phenyl iodobenzene (0.2 mmol), CuX (1 equiv.) and DBU. [b]Determined by ^{19}F NMR with the addition of trifluoromethylbenzene as an internal standard. [c]3.5 equiv. of $[Cu(MeCN)_4]BF_4$ was used. [d]DBN = 1,5-diazabicyclo[4.3.0]non-5-ene. [e]The system composed of $^nBu_4NCl$ (0.2 eq), PO (abbreviate for propylene epoxide, 7 eq) and 4 Å MS (75 mg) was used as base.

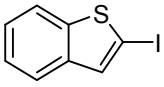
4. Synthesis of 2-iodobenzofuran and 2-iodobenzo[b]thiophene[1].



Into the solution of arylboronic acid (1 mmol) in dry acetonitrile (5 mL) was added *N*-iodosuccinimide (1.0 mmol, 225 mg). The mixture was stirred at room temperature protected from air and light until the completion of the reaction, as monitored by TLC. The solvent was removed by concentration. And the residue was further purified by column chromatography (petroleum ether) to afford the pure product.



2-iodobenzofuran: yellow oil, 240 mg, 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.43 (m, 2H), 7.24 – 7.16 (m, 2H), 6.96 (d, *J* = 0.9 Hz, 1H). GC-MS (EI) calcd. for C_8H_5IO $[M]^+$ 243.9; found 243.9.

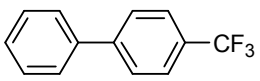


2-iodobenzo[b]thiophene: white solid, 227 mg, 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 1H), 7.73 – 7.67 (m, 1H), 7.53 (d, *J* = 0.5 Hz, 1H), 7.33 – 7.26 (m, 2H). GC-MS (EI) calcd. for C_8H_5IS $[M]^+$ 259.9; found 259.9.

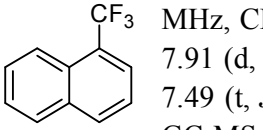
5. Trifluoromethylation of aromatic iodide with HCF_2Cl.

Into a 5 mL sealed tube were added aromatic iodide (0.2 mmol), $[Cu(MeCN)_4]BF_4$ (220.2 mg, 0.7 mmol), DBU(213.1 mg, 1.4 mmol) and the solution of HCF_2Cl in DMF (2.43 M, 1.5 mL) under N_2. The reaction mixture was stirred at 120 ^oC for 5 h. After being cooled to room temperature, the reaction mixture was subjected to flash column chromatography to give the desired product. For the cases that the substrates (aromatic iodide) can't be completely consumed (**2a-2e**, **2j-2k**), the reaction mixture was filtered through a short pad of silica gel and washed with DCM to remove the solid. After evaporation of the solvent, the residue was dissolved in AcOH (1 mL). Into this solution was added *m*-CPBA (68 mg, 0.4 mmol). The resulting mixture was stirred 50 ^oC for 5 h. After being cooled to room temperature, the solution was subjected to flash column chromatography (petroleum ether:EA = 6:1, or petroleum ether) to afford the pure product.

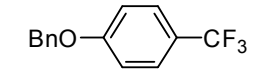
4-(Trifluoromethyl)-1,1'-biphenyl (**2a**): white solid, 40.2 mg, 91%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71-7.67 (m, 4H), 7.65 – 7.54 (m, 2H), 7.52 – 7.44 (m, 2H), 7.41 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.43 (s, 3F). GC-MS (EI) calcd. for $C_{13}H_9F_3$ $[M]^+$ 222.1; found 222.1.



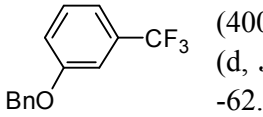
1-(Trifluoromethyl)naphthalene (**2b**): colorless oil, 36.7 mg, 94%; ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, J = 8.5, 0.8 Hz, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.91 (d, J = 7.4 Hz, 1H), 7.87 (d, J = 7.2 Hz, 1H), 7.66 – 7.54 (m, 2H), 7.49 (t, J = 7.6 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -59.71 (s, 3F). GC-MS (EI) calcd. for $C_{11}H_7F_3$ $[M]^+$ 196.0; found 196.1.



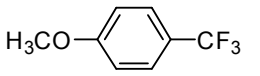
1-(Benzyloxy)-4-(trifluoromethyl)benzene (**2c**): white solid, 40.2 mg, 80%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.6 Hz, 2H), 7.48 – 7.30 (m, 5H), 7.03 (d, J = 8.6 Hz, 2H), 5.10 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.51 (s, 3F). GC-MS (EI) calcd. for $C_{14}H_{11}F_3O$ $[M]^+$ 252.1; found 252.1.



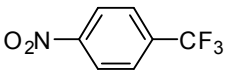
1-(Benzyloxy)-3-(trifluoromethyl)benzene (**2d**): white solid, 42.1 mg, 83%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.30 (m, 6H), 7.23-7.19 (m, 2H), 7.13 (d, J = 7.9 Hz, 1H), 5.08 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.73 (s, 3F). GC-MS (EI) calcd. for $C_{14}H_{11}F_3O$ $[M]^+$ 252.1; found 252.1.



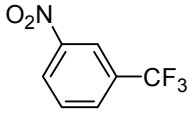
1-Methoxy-4-(trifluoromethyl)benzene (**2e**): colorless oil, 28.2 mg, 80%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 8.5 Hz, 2H), 6.94 (d, J = 8.5 Hz, 2H), 3.83 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.49 (s, 3F). GC-MS (EI) calcd. for $C_8H_7F_3O$ $[M]^+$ 176.0; found 176.1.



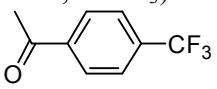
1-Nitro-4-(trifluoromethyl)benzene (**2f**): white solid, 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.4 Hz, 2H), 7.82 (d, *J* = 8.4 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.21 (s, 3F). GC-MS (EI) calcd. for $C_7H_4F_3NO_2$ $[M]^+$ 191.0; found 191.0.



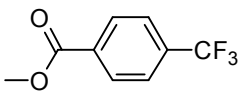
1-Nitro-3-(trifluoromethyl)benzene (**2g**): yellow oil, 37.5 mg, 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.00 (s, 3F). GC-MS (EI) calcd. for $C_7H_4F_3NO_2$ $[M]^+$ 191.0; found 191.0.



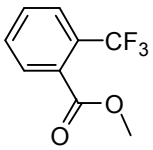
1-(4-(Trifluoromethyl)phenyl)ethanone (**2h**): yellow oil, 34.2 mg, 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 2.29 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.55 (s, 3F). GC-MS (EI) calcd. for $C_9H_7F_3O$ $[M]^+$ 188.0; found 188.0.



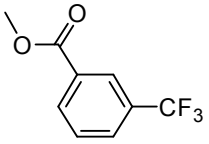
Methyl 4-(trifluoromethyl)benzoate (**2i**): yellow oil, 36.9 mg, 90%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.1 Hz, 2H), 3.96 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.14 (s, 3F). GC-MS (EI) calcd. for $C_9H_7F_3O_2$ $[M]^+$ 204.0; found 204.0.



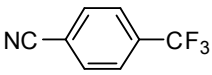
Methyl 2-(trifluoromethyl)benzoate (**2j**): colorless oil, 30.7 mg, 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.71 (m, 2H), 7.68 – 7.53 (m, 2H), 3.93 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.76 (s, 3F). GC-MS (EI) calcd. for $C_9H_7F_3O_2$ $[M]^+$ 204.0; found 204.0.



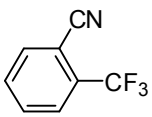
Methyl 3-(trifluoromethyl)benzoate (**2k**): colorless oil, 35.2 mg, 86%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.23 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 3.96 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.85 (s, 3F). GC-MS (EI) calcd. for $C_9H_7F_3O_2$ $[M]^+$ 204.0; found 204.0.



4-(Trifluoromethyl)benzonitrile (**2l**): white solid, 24.4 mg, 71%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.54 (s, 3F). GC-MS (EI) calcd. for $C_8H_4F_3N$ $[M]^+$ 171.0; found 171.0.

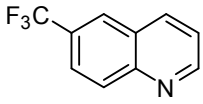


2-(Trifluoromethyl)benzonitrile (**2m**): yellow oil, 23.9 mg, 70%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 – 7.76 (m, 2H), 7.76 – 7.64 (m, 2H). ^{19}F NMR (282

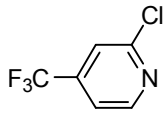


MHz, $CDCl_3$) δ -61.97 (s, 3F). GC-MS (EI) calcd. for $C_8H_4F_3N$ $[M]^+$ 171.0; found 171.1.

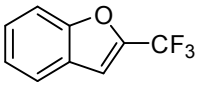
6-(Trifluoromethyl)quinoline (**2n**): white solid, 36.3 mg, 92%; ^1H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, J = 4.2 Hz, 1H), 8.32 – 8.15 (m, 2H), 8.12 (s, 1H), 7.86 (d, J = 8.3 Hz, 1H), 7.49 (dd, J = 8.3, 4.2 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.40 (s, 3F). GC-MS (EI) calcd. for $C_{10}H_6F_3N$ $[M]^+$ 197.0; found 197.1.



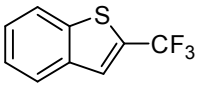
2-Chloro-4-(trifluoromethyl)pyridine (**2o**): colorless oil, 32.8 mg, 90%; ^1H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, J = 4.4 Hz, 1H), 7.59 (s, 1H), 7.47 (d, J = 4.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.80 (s, 3F). GC-MS (EI) calcd. for $C_6H_3ClF_3N$ $[M]^+$ 181.0; found 181.0.



2-(Trifluoromethyl)benzofuran (**2p**): colorless oil, 30.2 mg, 81%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 7.8 Hz, 1H), 7.58 (dd, J = 8.4, 0.7 Hz, 1H), 7.50 – 7.41 (m, 1H), 7.37 – 7.30 (m, 1H), 7.21 – 7.14 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -64.85 (s, 3F). GC-MS (EI) calcd. for $C_9H_5F_3O$ $[M]^+$ 186.0; found 186.0.



2-(Trifluoromethyl)benzo[b]thiophene (**2q**): white solid, 32.7 mg, 81%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.82 (m, 2H), 7.70 (s, 1H), 7.52 – 7.39 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.31 (s, 3F). GC-MS (EI) calcd. for $C_9H_5F_3O$ $[M]^+$ 186.0; found 186.0.



References:

[1] C. Thiebes, C. Thiebes, G. K. S. Prakash, N. A. Petasis, G. A. Olah, *Synlett* **1998**, *1998*, 141-142.

6. Investigation of the mechanism of the trifluoromethylation with HCF_2Cl.

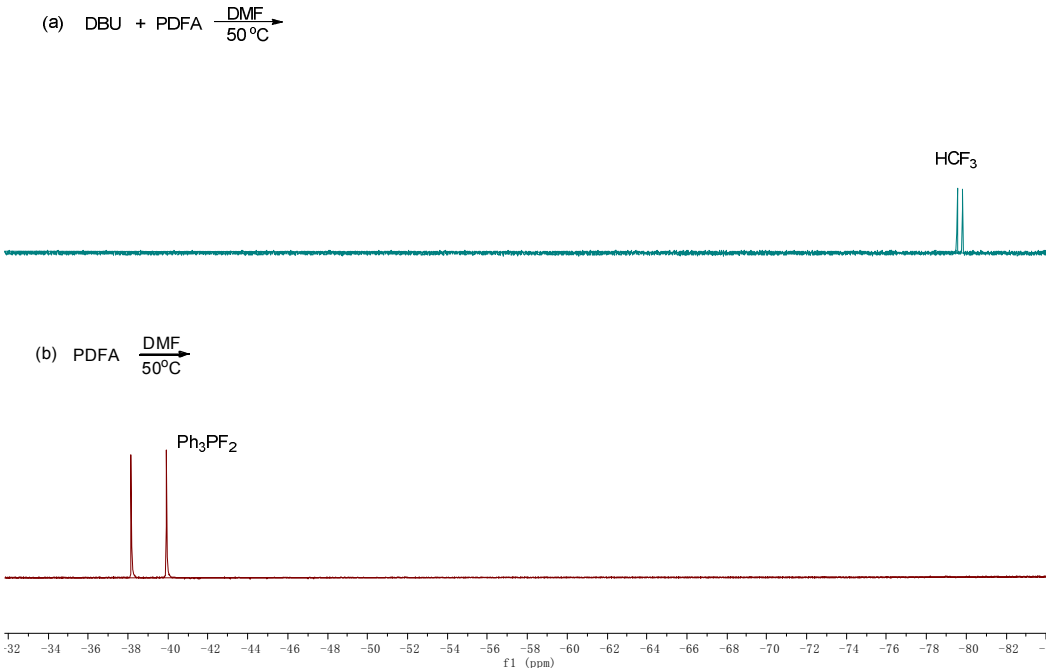


Figure 1. ^{19}F NMR measurement of the reaction of PDFA with DBU.

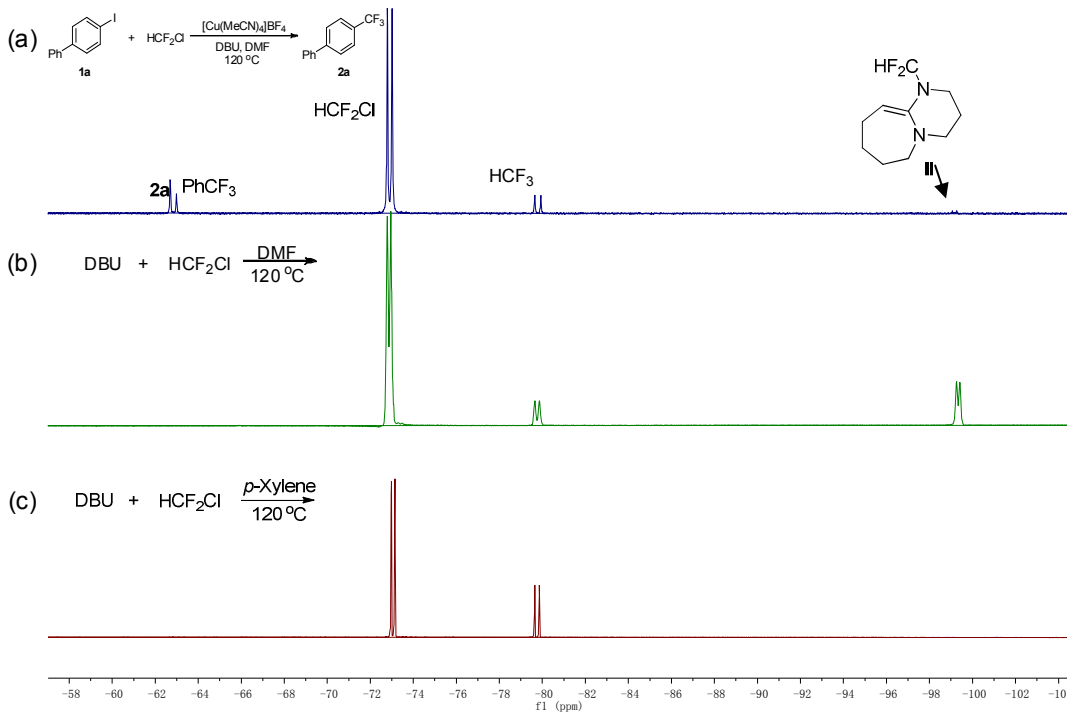


Figure 2. ^{19}F NMR measurement of the reaction of HCF_2Cl with DBU.

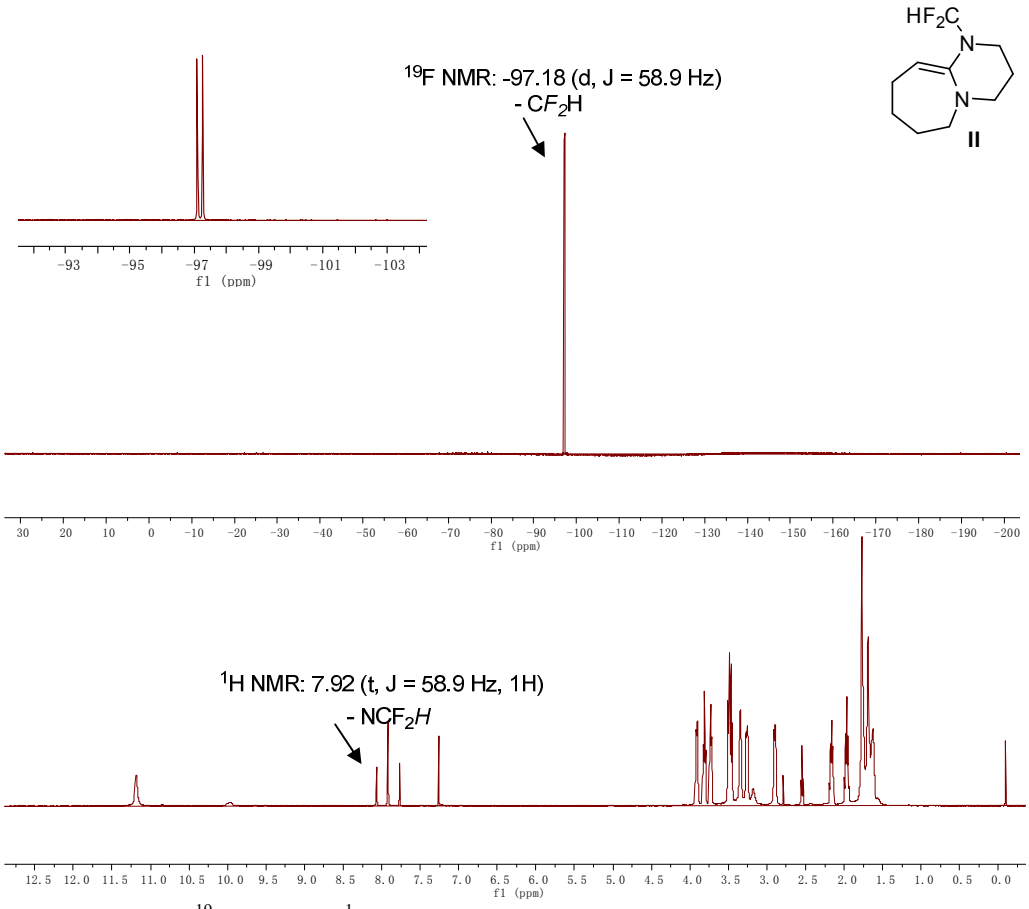


Figure 3. ^{19}F NMR and ^{1}H NMR of the impure intermediate Ⅱ after flash column chromatography.

Shanghai Mass Spectrometry Center

Shanghai Institute of Organic Chemistry

Chinese Academy of Sciences

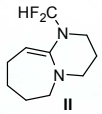
High Resolution MS Data Report

Instrument

Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number	E140034
Analysis Name	D:\Data\zfj2013\20131225_000046.d
Sample Name	2011167-54-HR
Acquisition Date	4/26/2013 1:57:25 PM
Operator:	zfj
Ionization Mode	ESI-Positive
Ion Mass (Measured)	203.1358

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 10 H 17 F 2 N 2	0.007	203.1354	-1.93	-2.02	-0.39	2.50	ok	even
C 6 H 21 N 1 O 6	0.022	203.1363	2.54	2.57	0.52	-3.00	ok	odd



II

Bruker Daltonics DataAnalysis 3.4 printed: 4/26/2013 1:58:40 PM Pag1 of 1

Figure 4. HRMS-ESI of intermediate **II**.

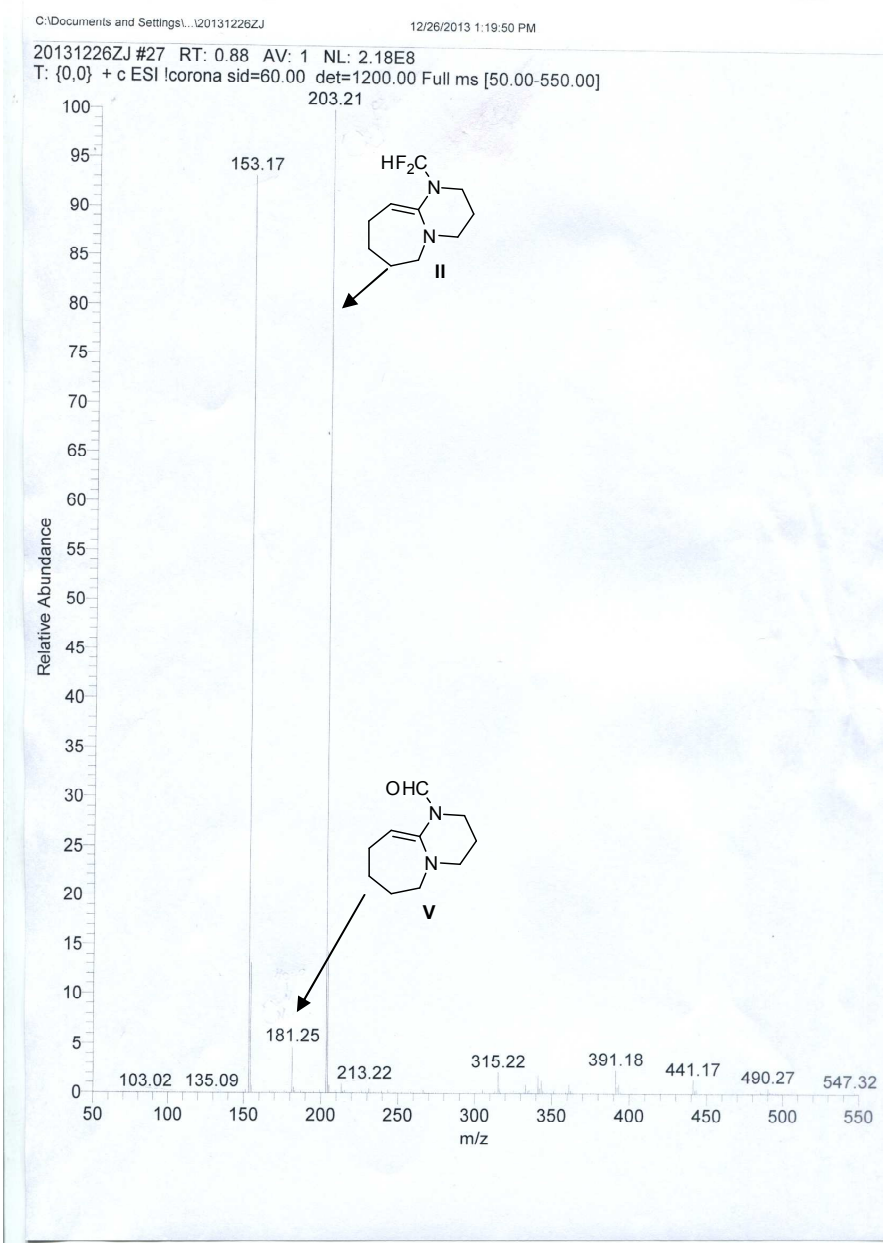


Figure 5. LRMS-ESI of intermediate Ⅱ and Ⅴ.

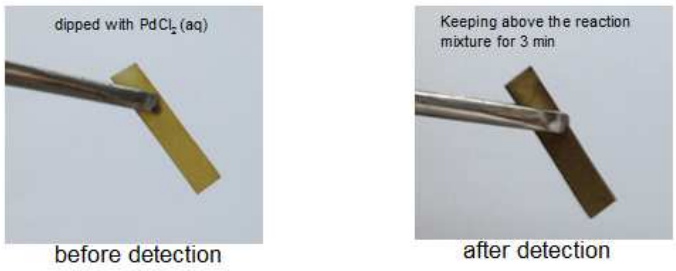
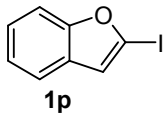
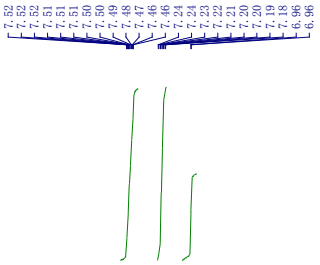


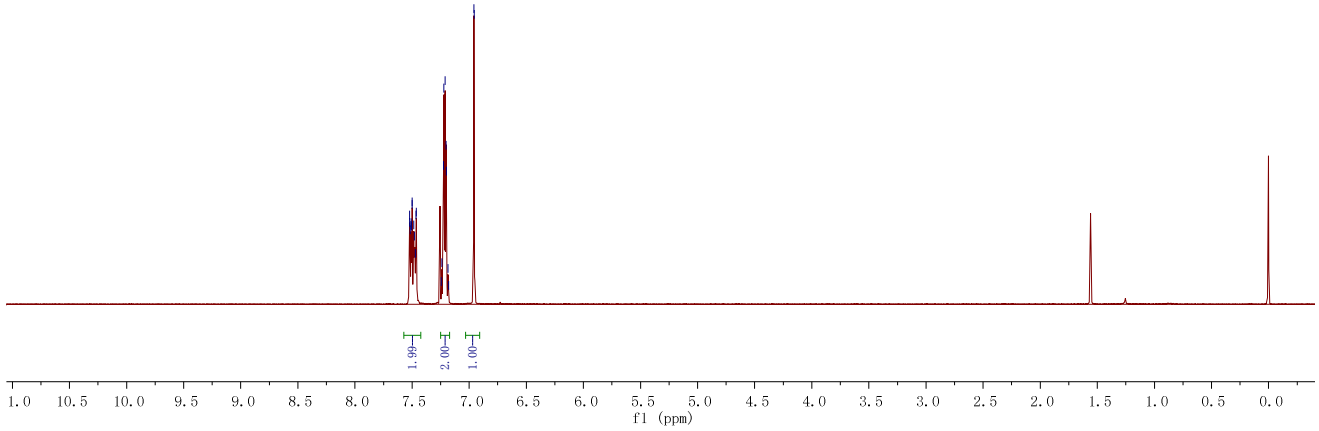
Figure 6. Detection of CO released from the reaction system.

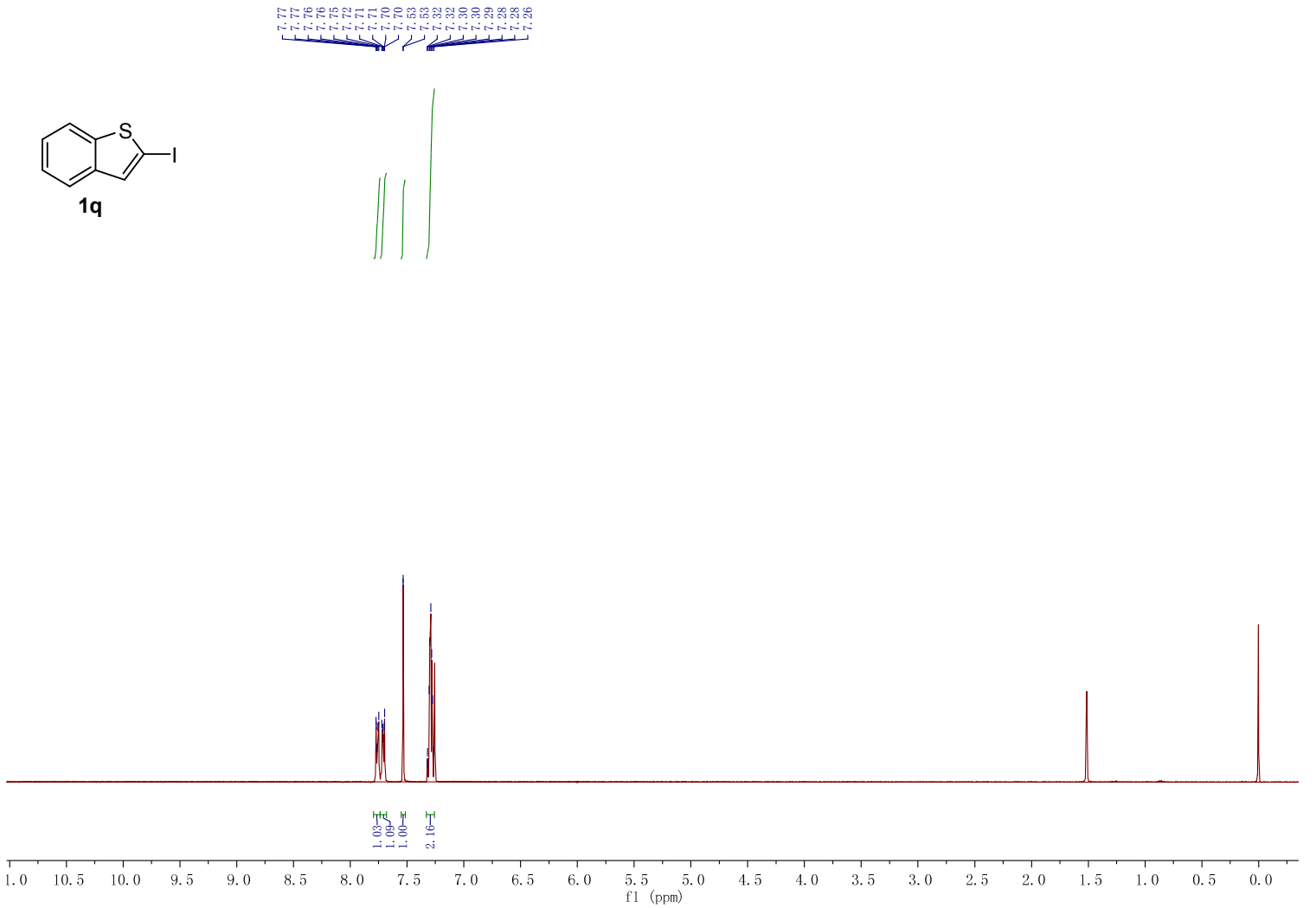
7. Copies of ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra.



1p



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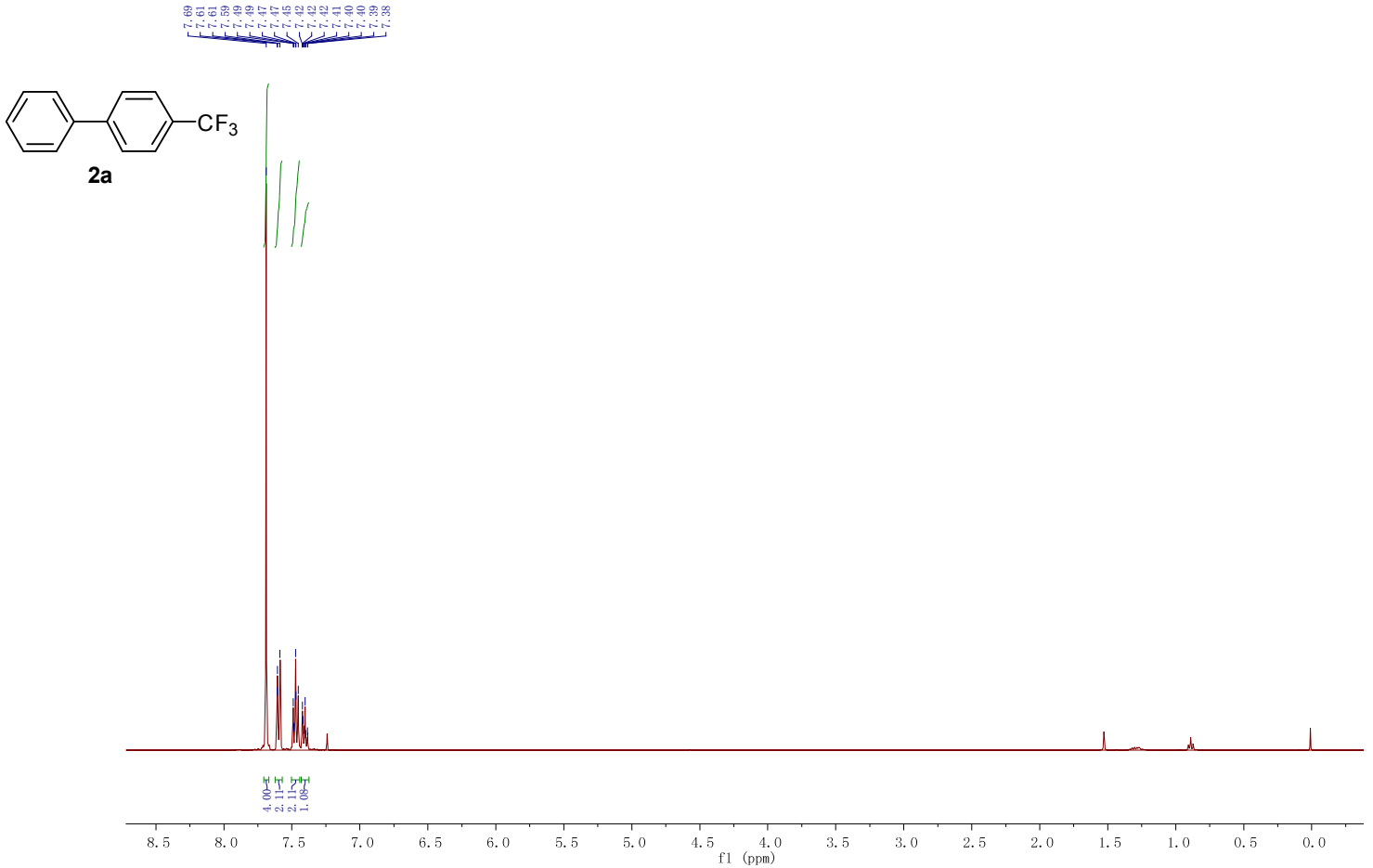
7.75
7.72
7.71
7.71
7.70
7.70
7.53
7.32
7.32
7.30
7.30
7.29
7.28
7.28
7.26
S
I
1q
1.03
1.09
1.00
2.16
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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7.61
7.59
7.49
7.49
7.47
7.47
7.45
7.42
7.42
7.41
7.40
7.40
7.39
7.38
CF3
2a
4.00
2.11
2.11
1.08
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
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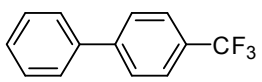
0.0
f1 (ppm)


CF3

2a

-62.43
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
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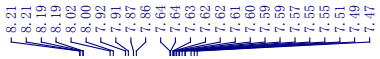
-180
-190
-200
f1 (ppm)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8.21
8.19
8.19
8.02
8.00
7.92
7.91
7.87
7.86
7.64
7.64
7.63
7.62
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7.60
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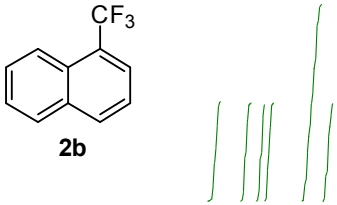
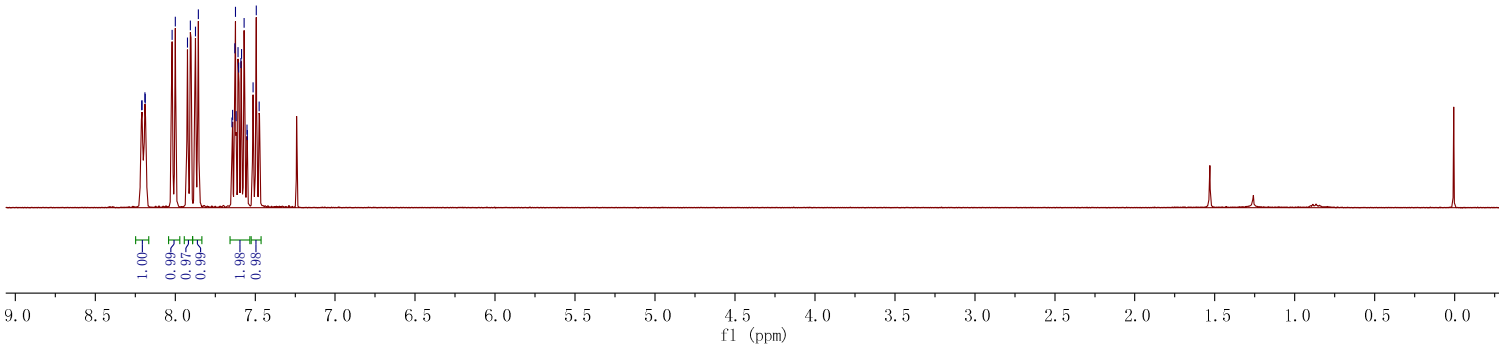
7.57
7.55
7.55
7.51
7.49
7.47


CF3

2b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0.99
1.98
0.98
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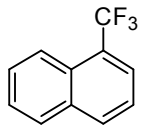
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CF3

2b

-59.71
10
0
-10
-20
-30
-40
-50
-60
-70
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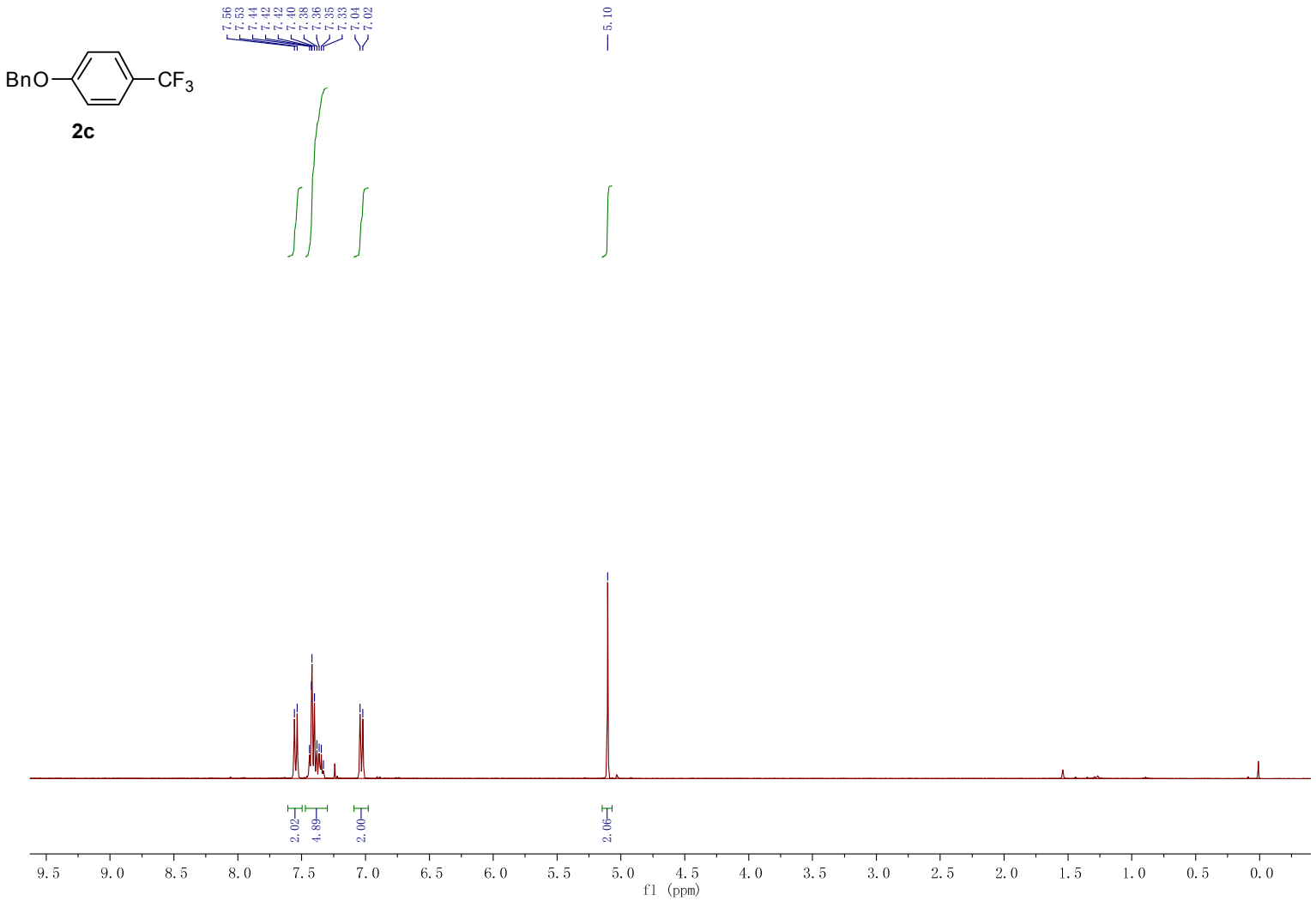
-170
-180
-190
-200
-210
f1 (ppm)


BnO
CF3
2c
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7.44
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7.04
7.02
5.10
2.02
4.89
2.00
2.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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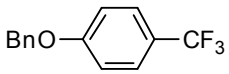
f1 (ppm)


BnO
CF3

2c

-61.51
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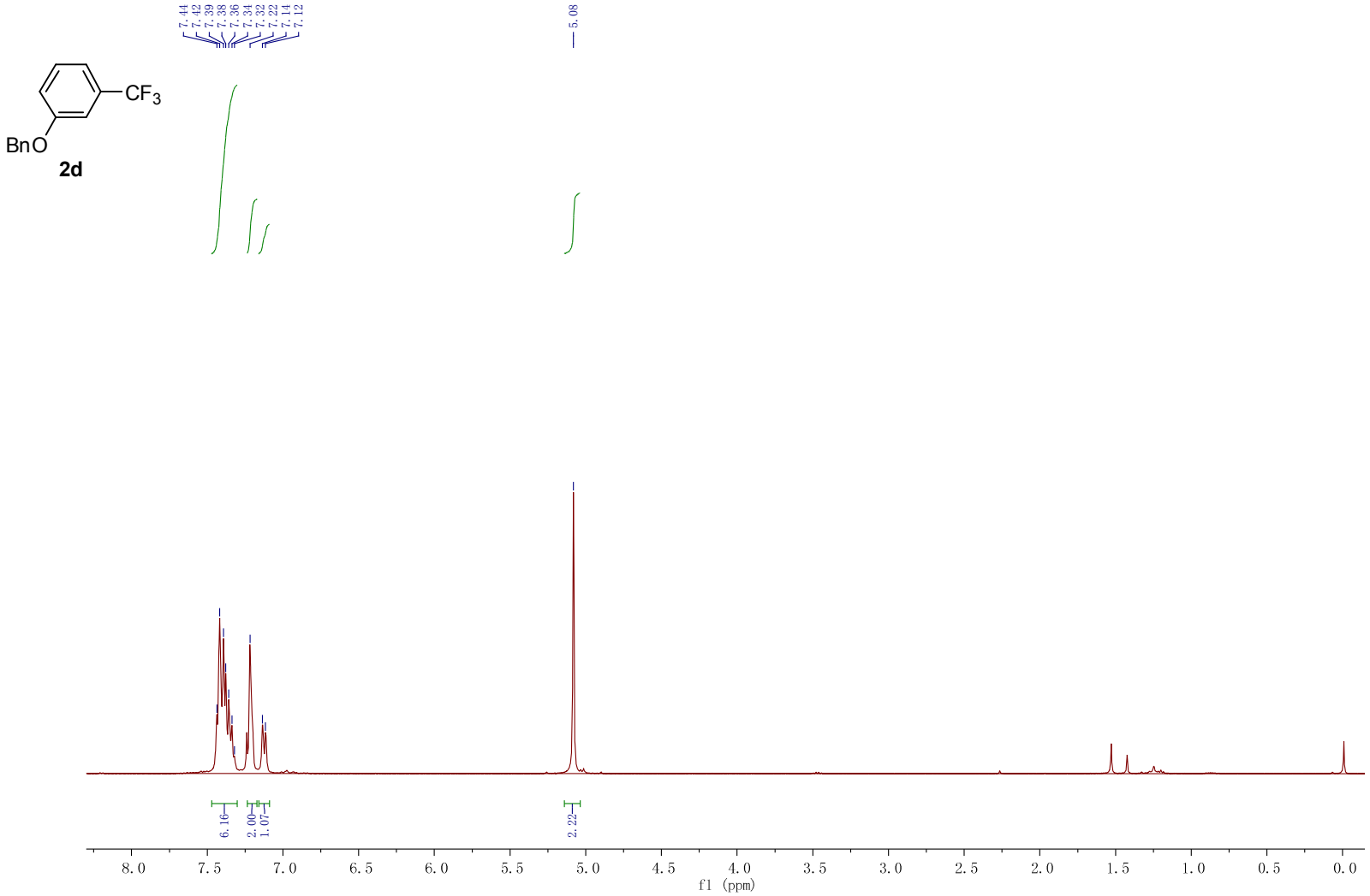
f1 (ppm)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7.14
7.12
5.08
CF3
BnO
2d
6.16
2.00
1.07
2.22
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
1.5
1.0
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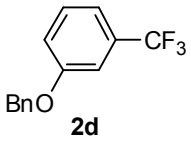
f1 (ppm)


CF3
BnO

2d

-62.73
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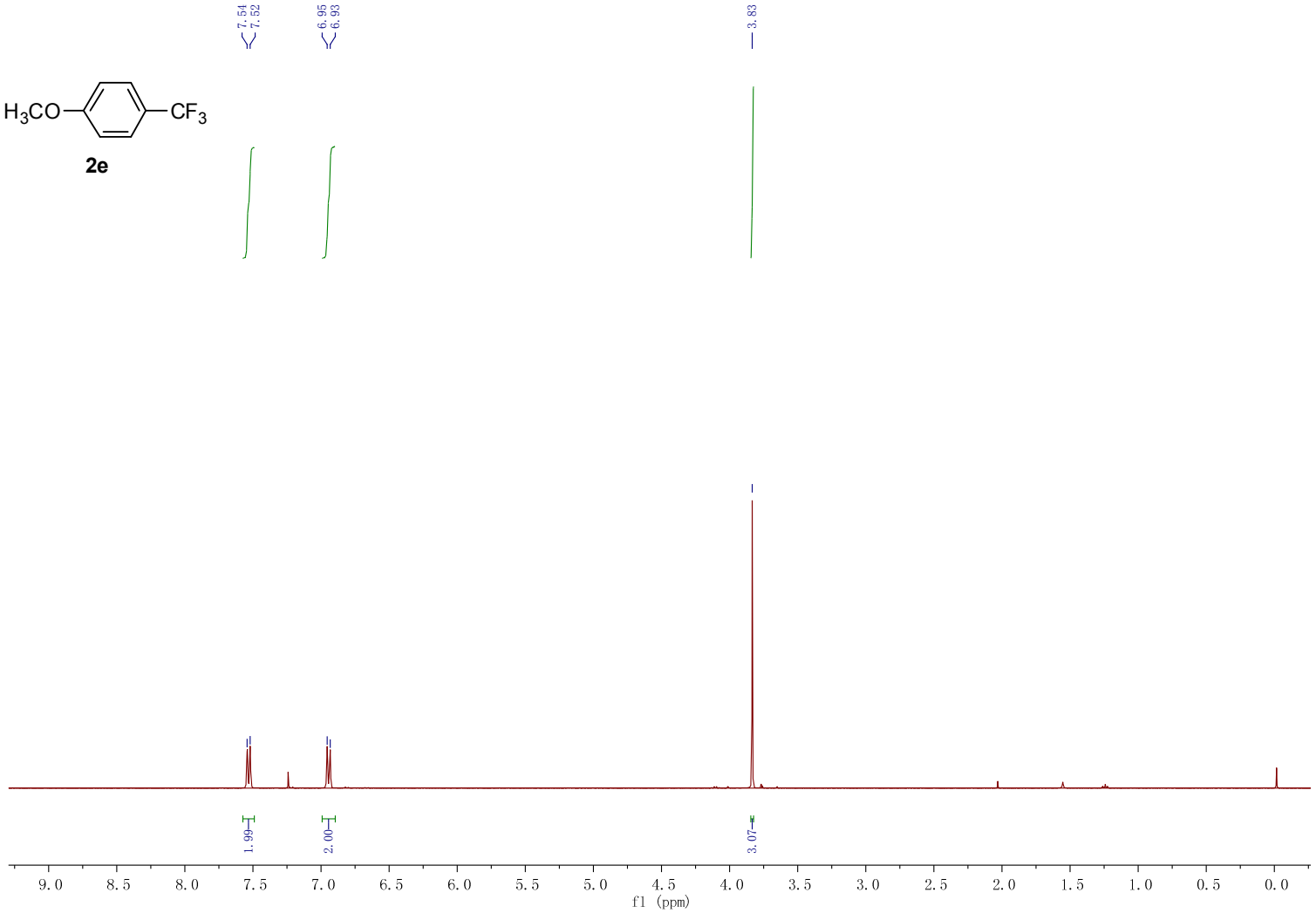
f1 (ppm)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7.52
6.95
6.93
3.83
H3CO
CF3
2e
1.99
2.00
3.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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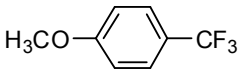
0.0
f1 (ppm)


H3CO
CF3

2e

-61.49
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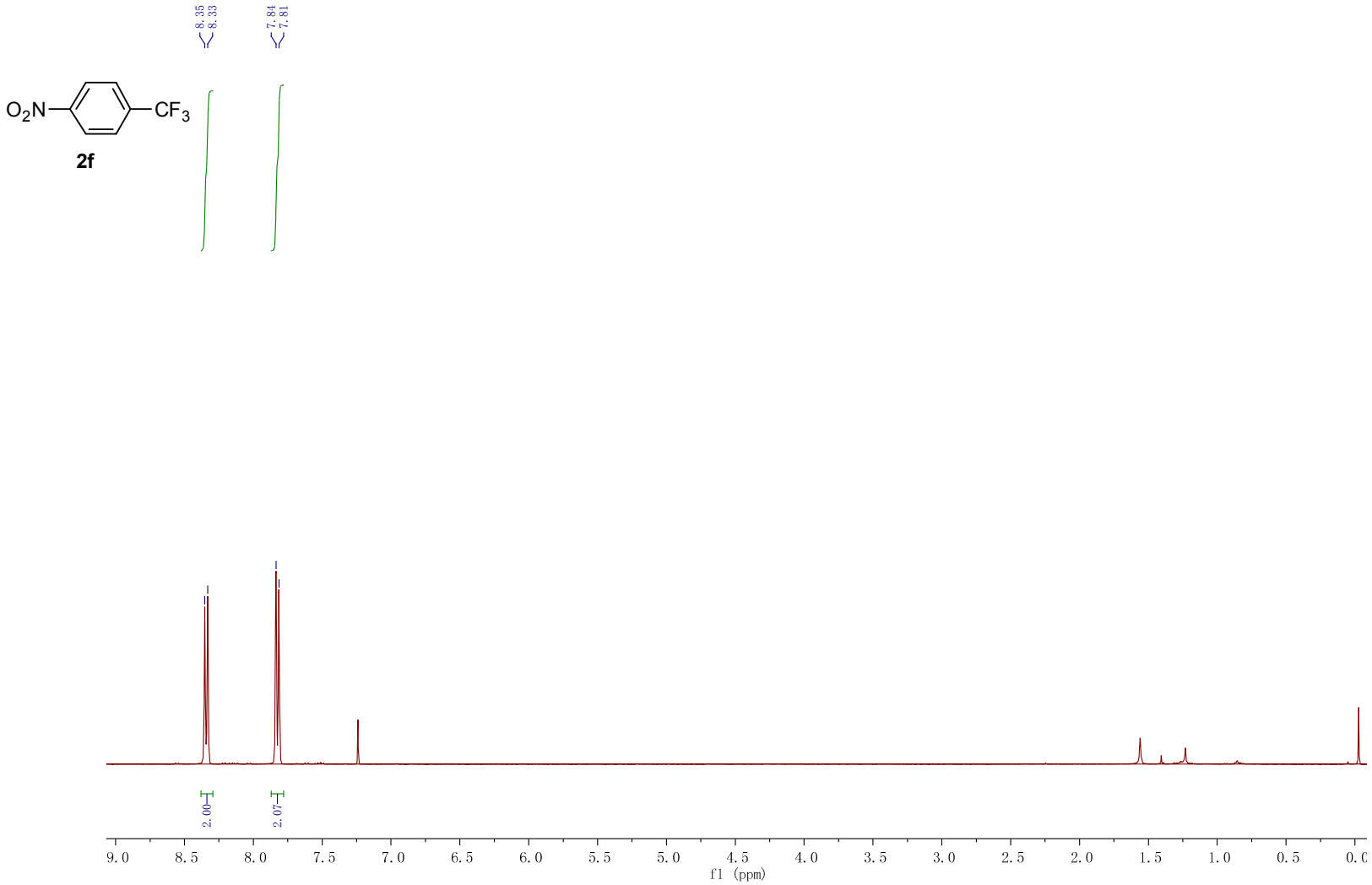
f1 (ppm)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8.33
7.84
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CF3
2f
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2.07
9.0
8.5
8.0
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7.0
6.5
6.0
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4.0
3.5
3.0
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2.0
1.5
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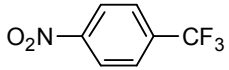
0.5
f1 (ppm)


O_2N
CF_3

2f

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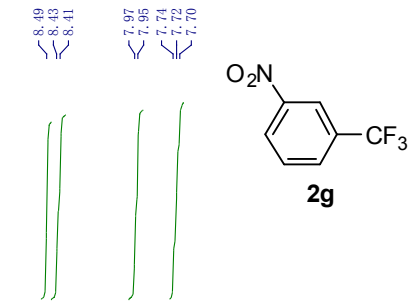
f1 (ppm)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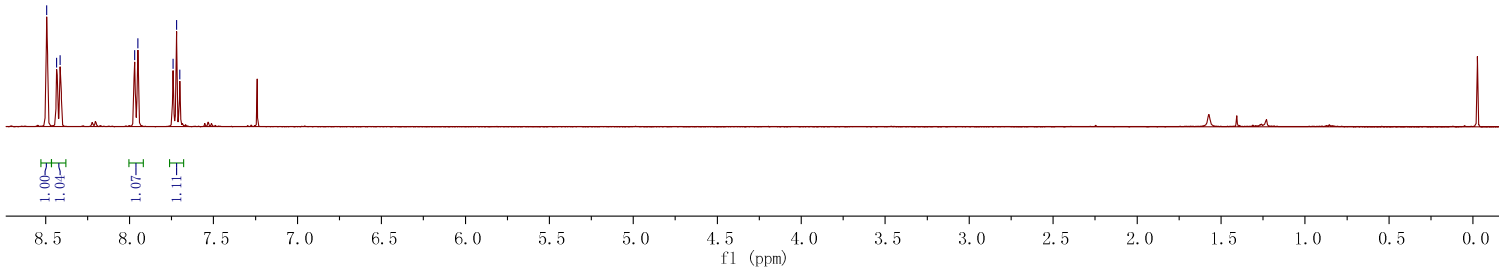
O2N
CF3
2g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2.0
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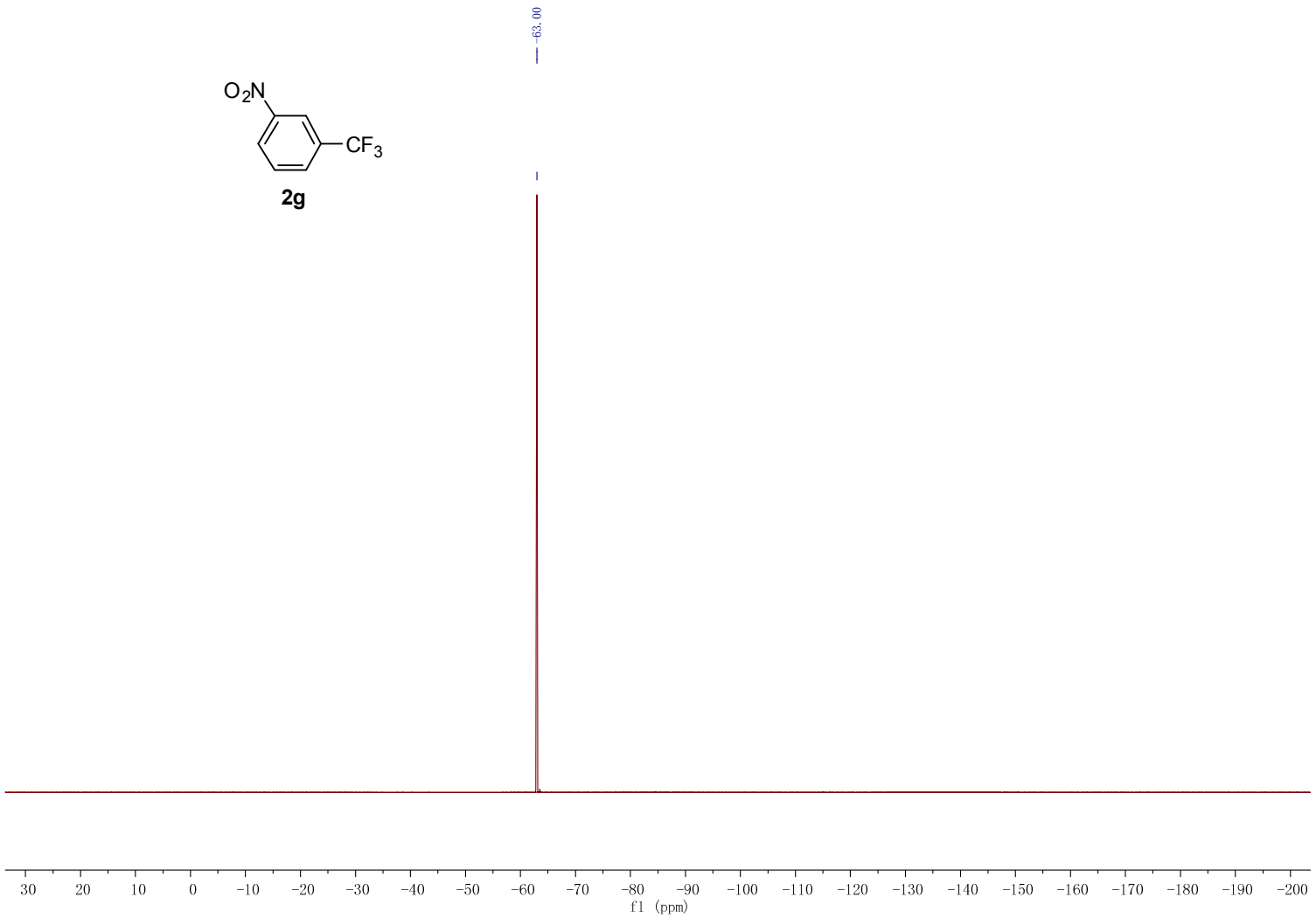
f1 (ppm)


O2N
CF3
2g
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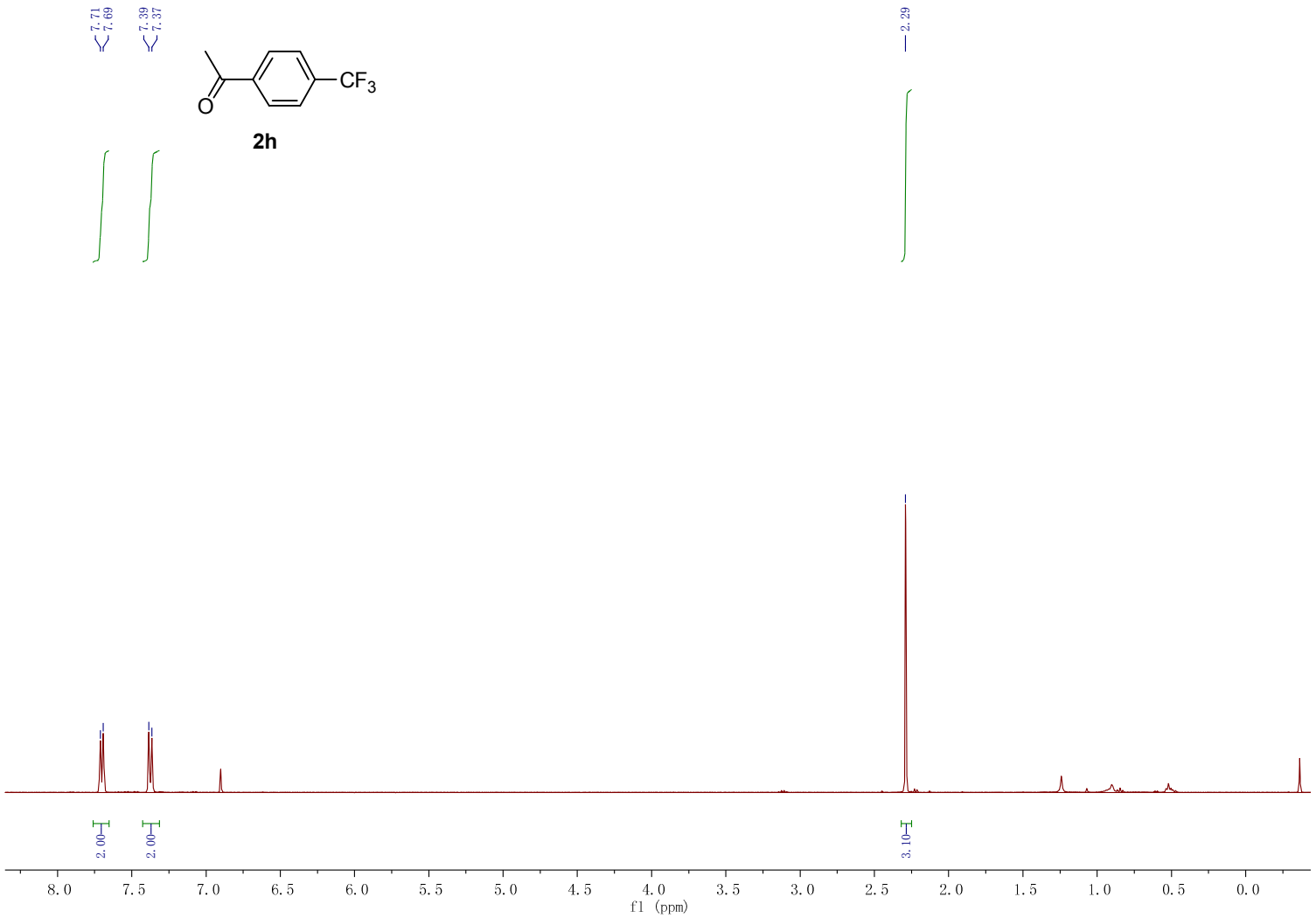
f1 (ppm)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6.5
6.0
5.5
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3.0
2.5
2.0
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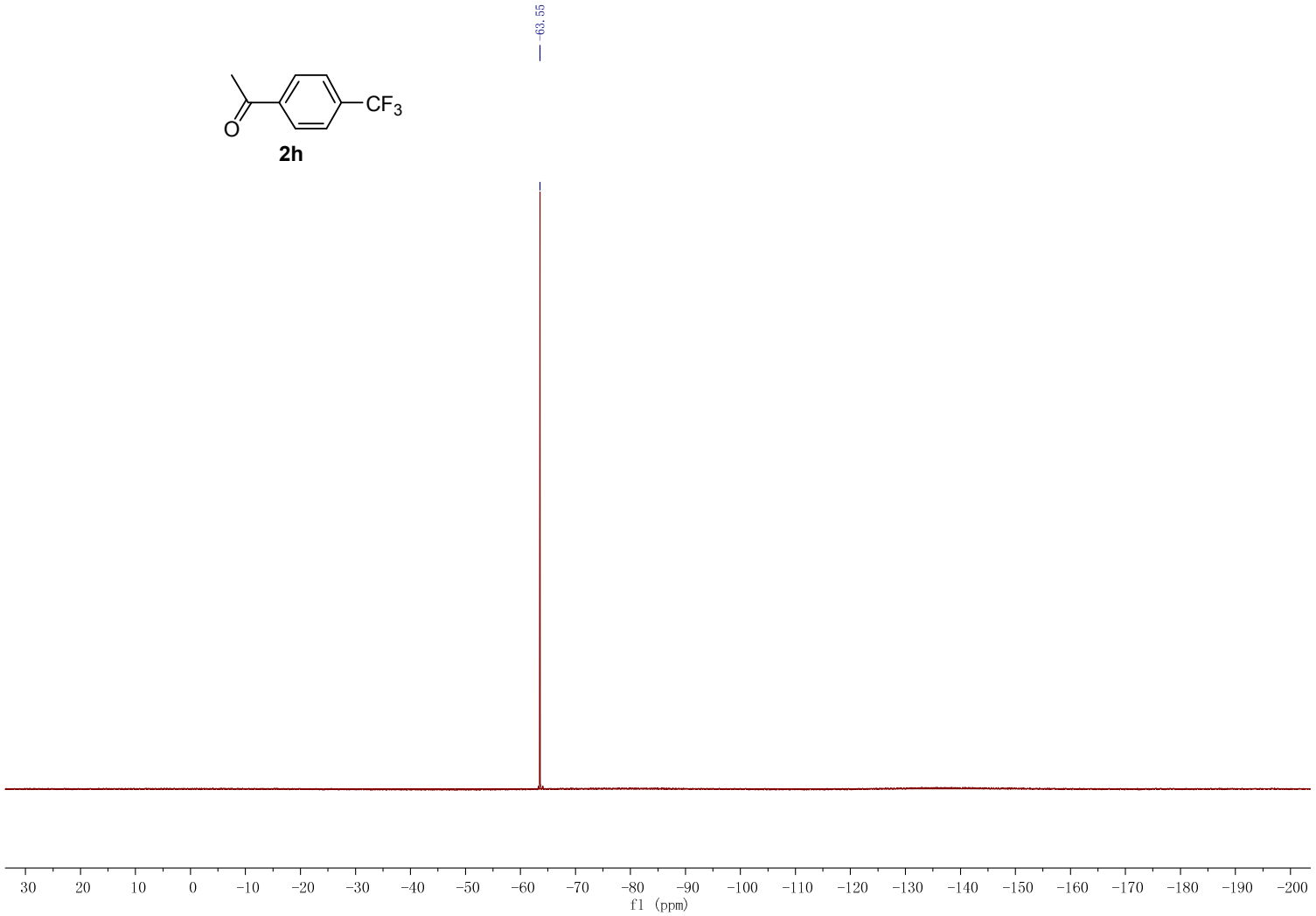
f1 (ppm)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O
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2h
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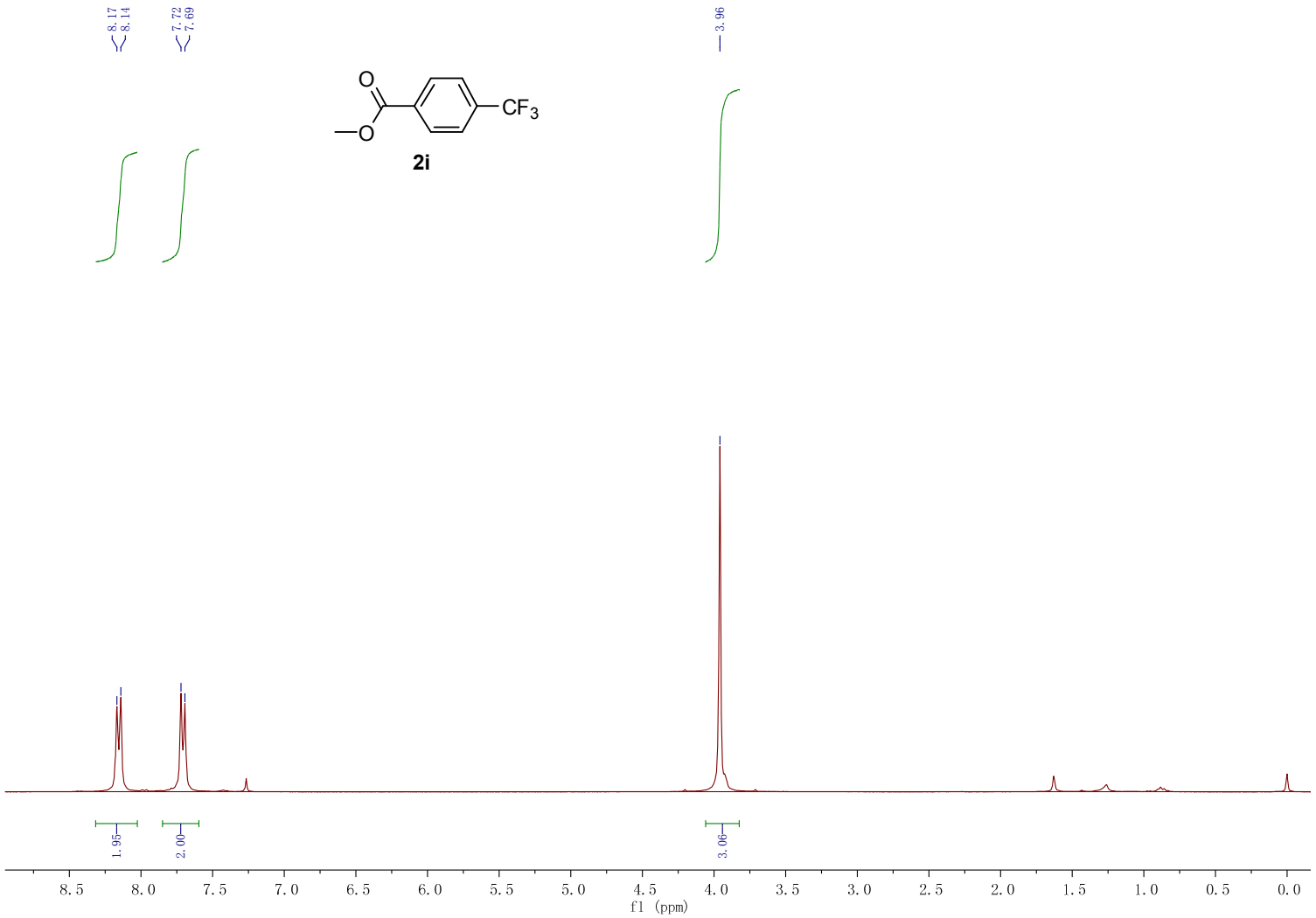
f1 (ppm)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O
CF3
2i
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7.5
7.0
6.5
6.0
5.5
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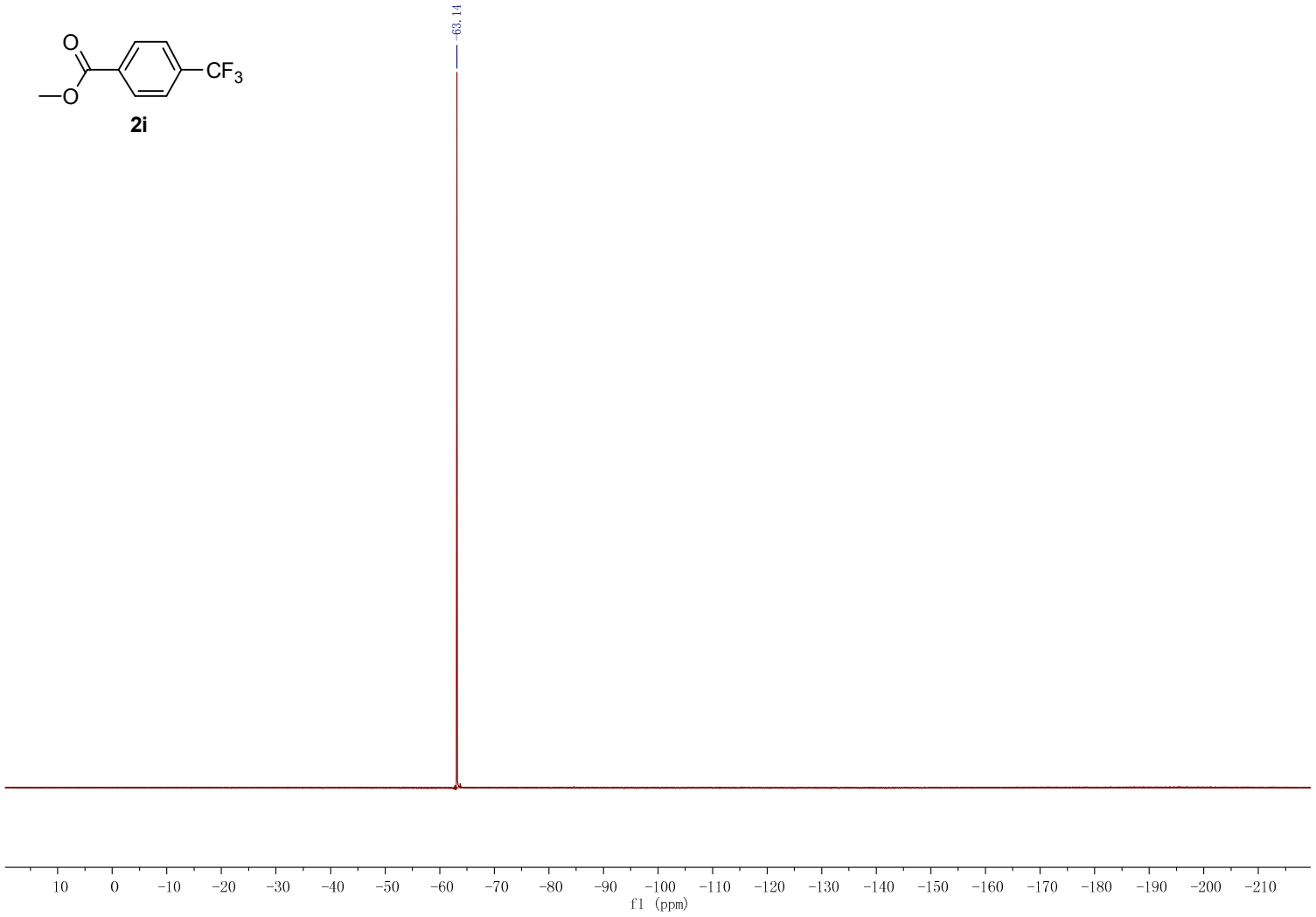
f1 (ppm)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O
CF3
2i
-63.14
10
0
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-20
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-60
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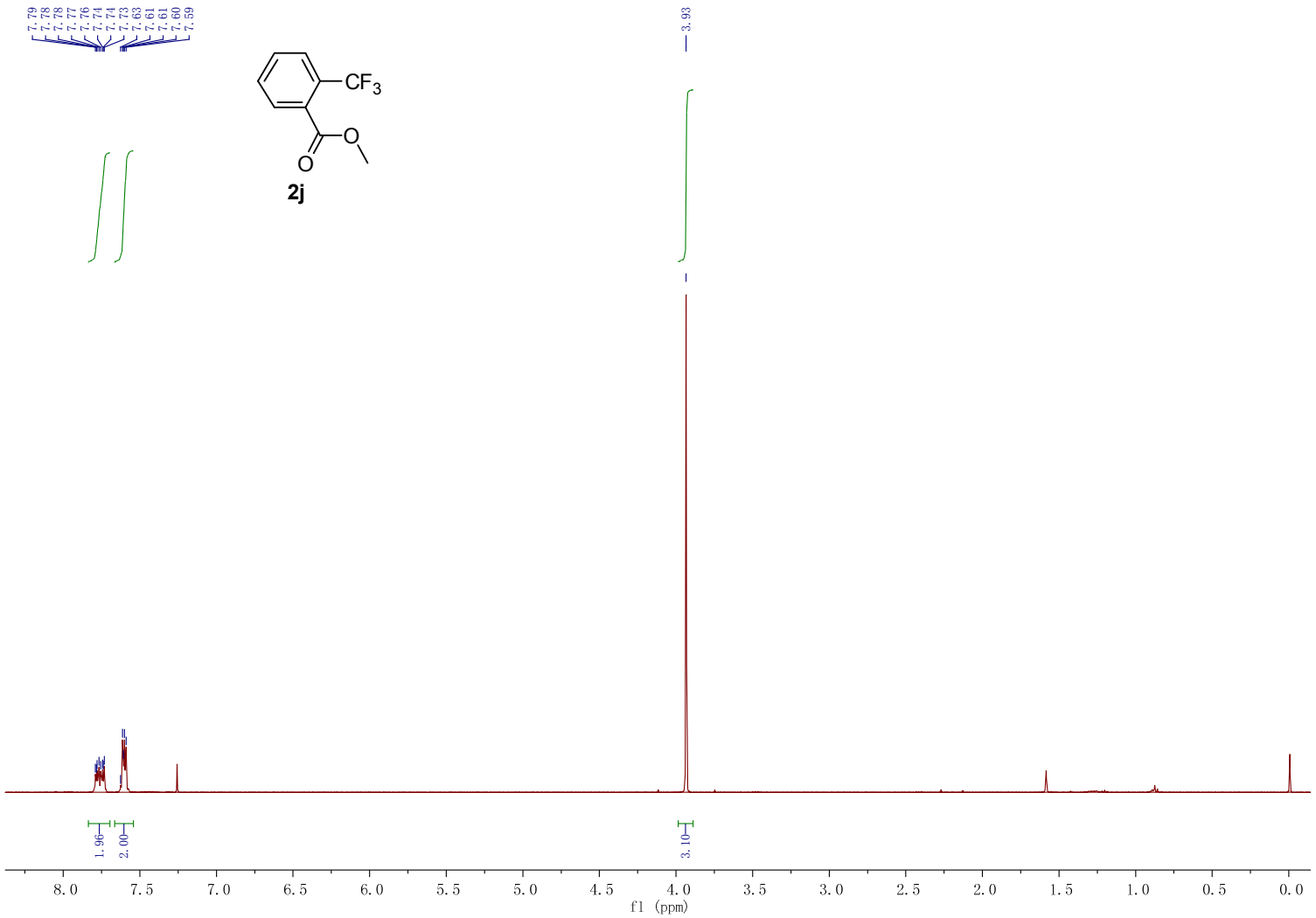
-170
-180
-190
-200
-210
f1 (ppm)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7.73
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7.61
7.60
7.59
3.93
CF3
O
O
2j
1.96
2.00
3.10
8.0
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6.0
5.5
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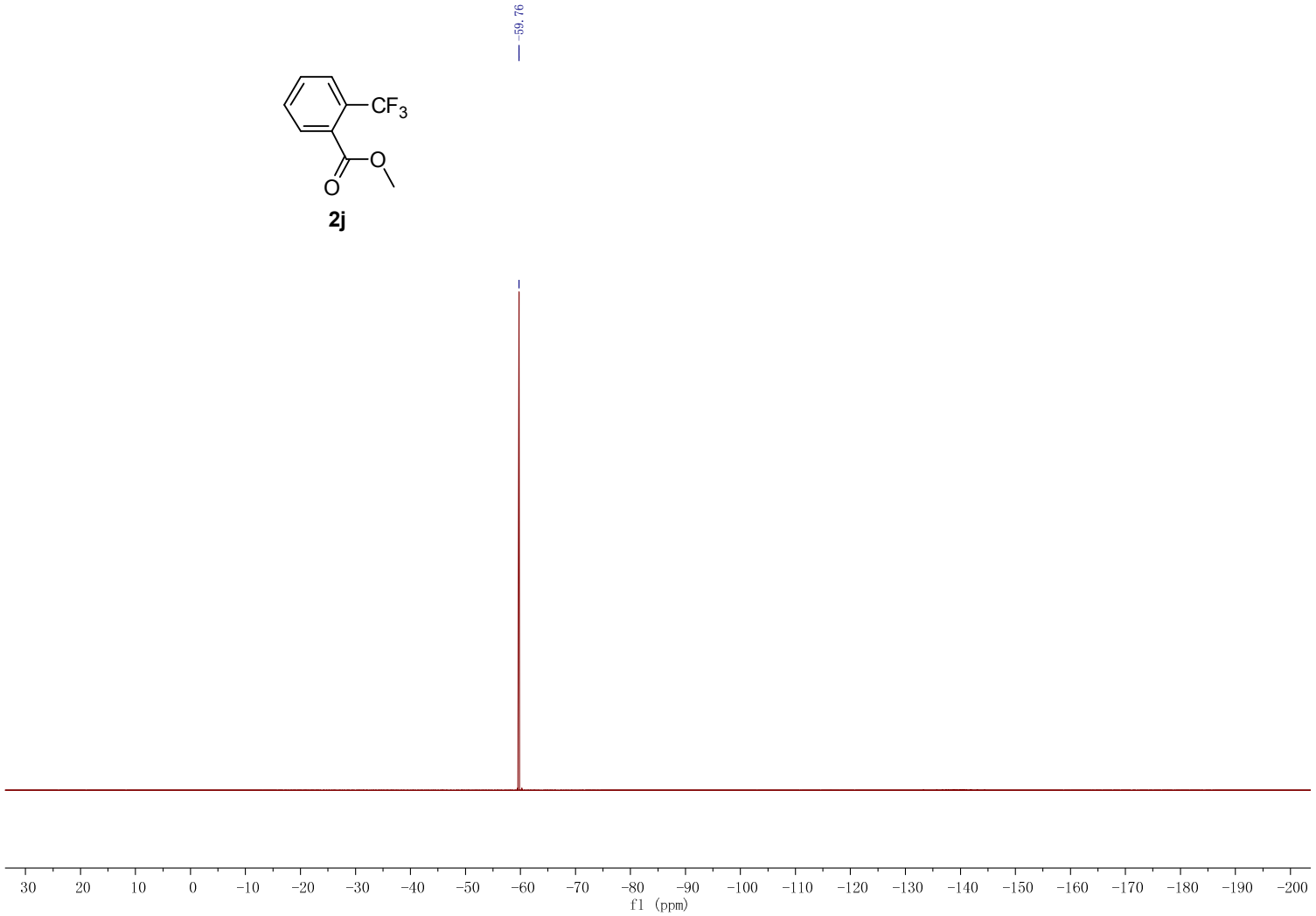
f1 (ppm)


-59.76
CF3
O
O
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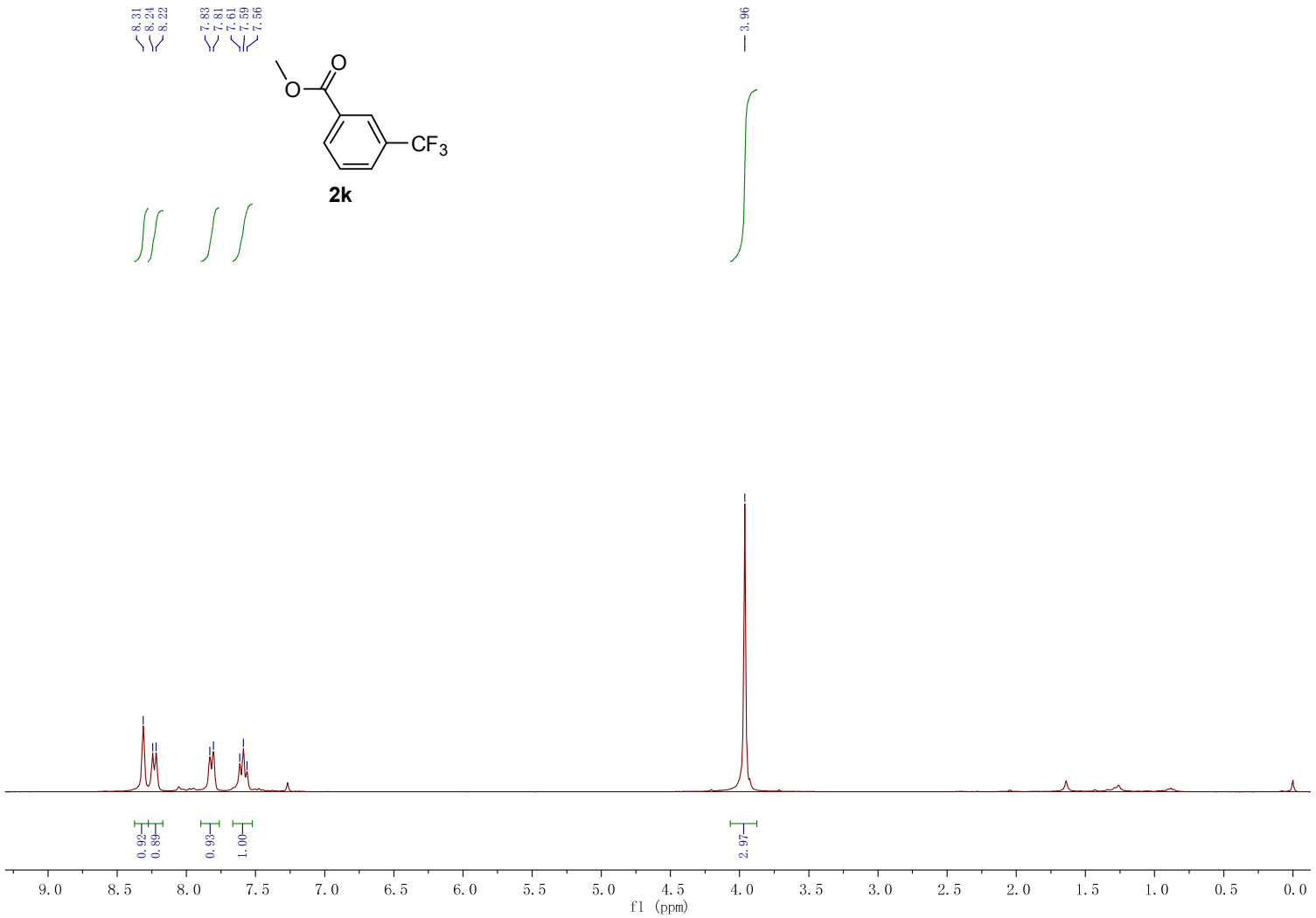
f1 (ppm)

2j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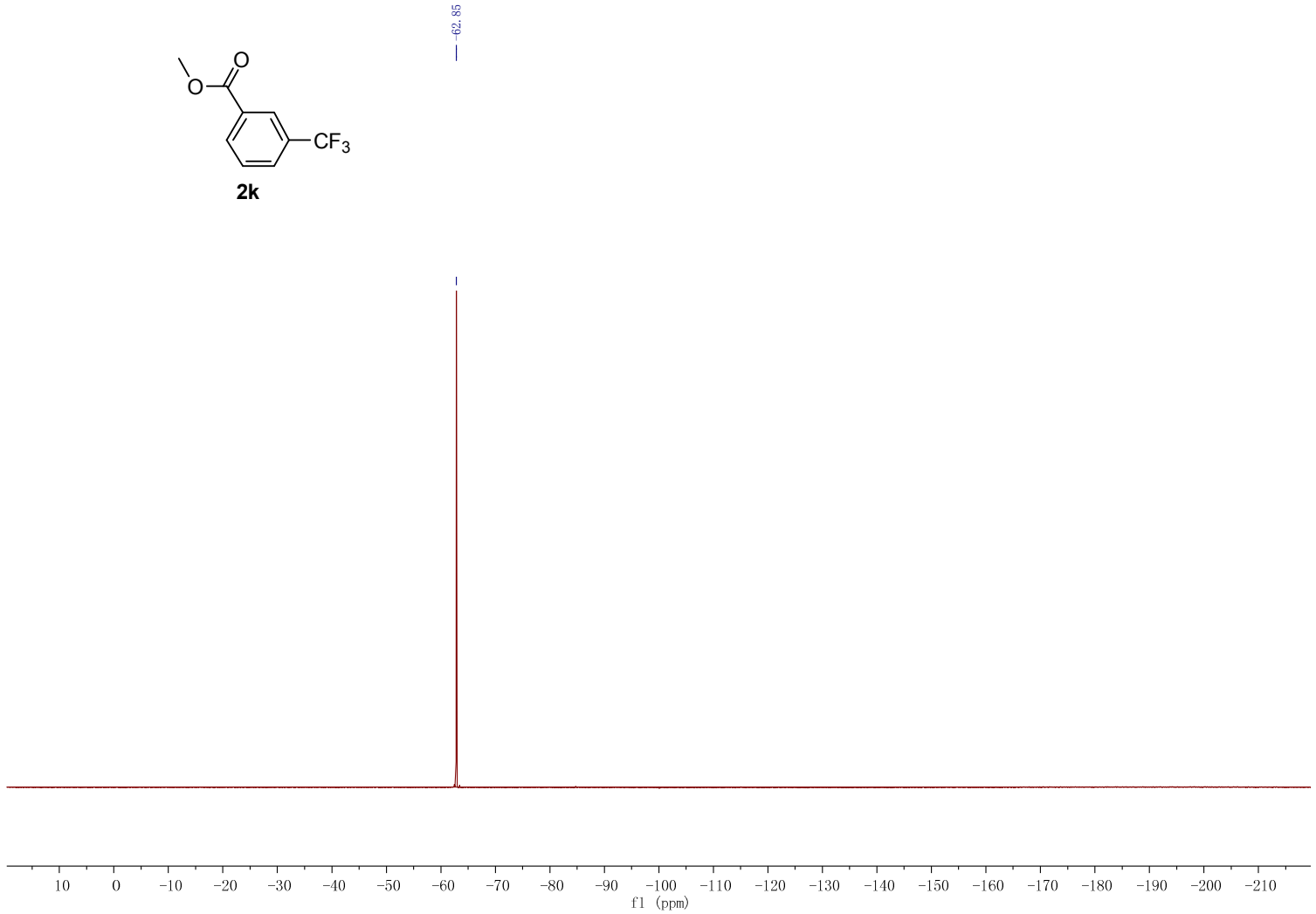
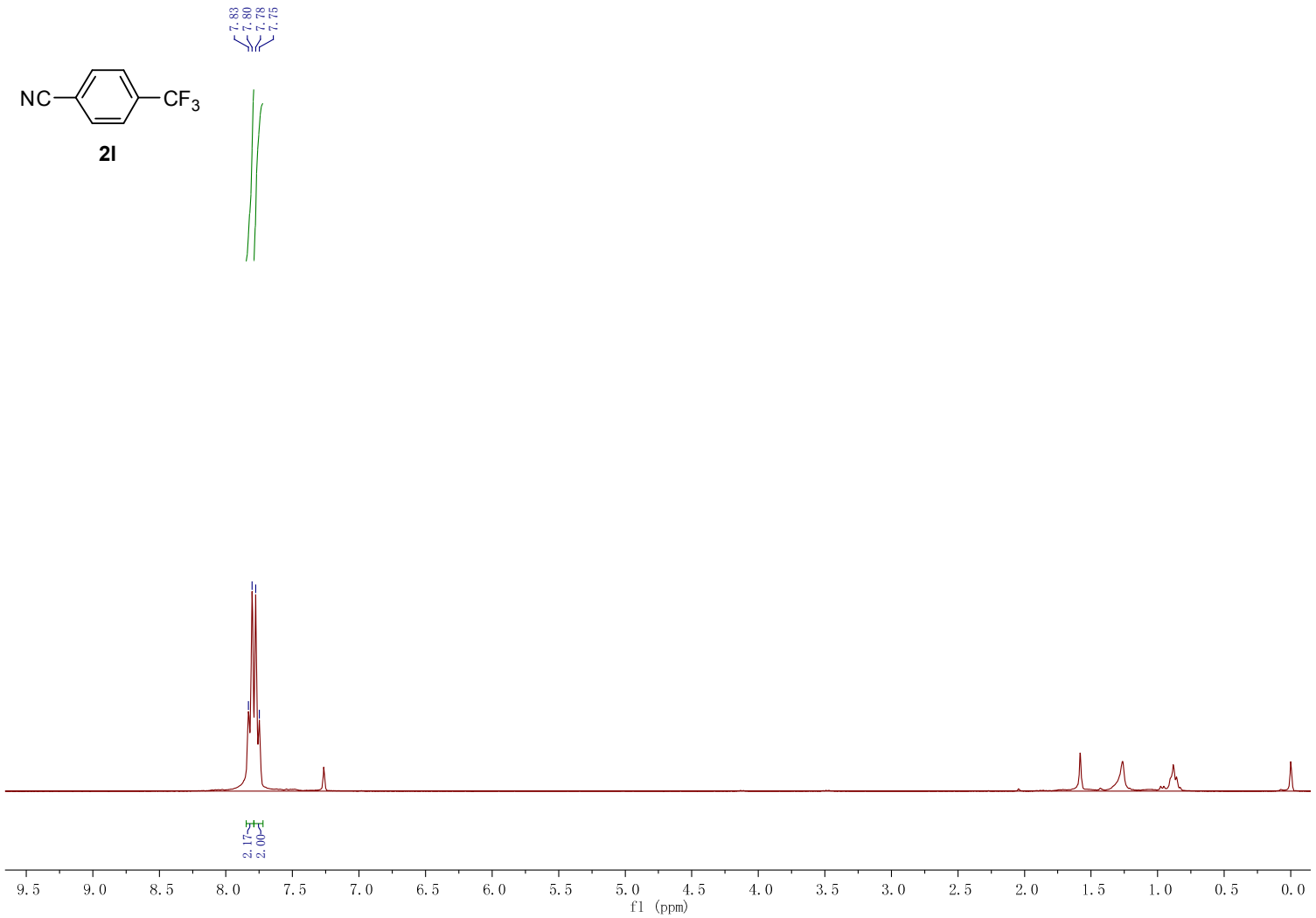
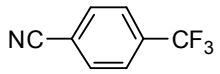
7.83
7.81
7.61
7.59
7.56
3.96
O
O
CF3
2k
0.92
0.89
0.93
1.00
2.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
O
CF3
2k
-62.85
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

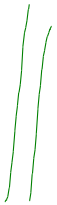

7.83
7.80
7.78
7.75
NC
CF3
2l
2.17
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

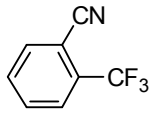

NC
CF3

2l

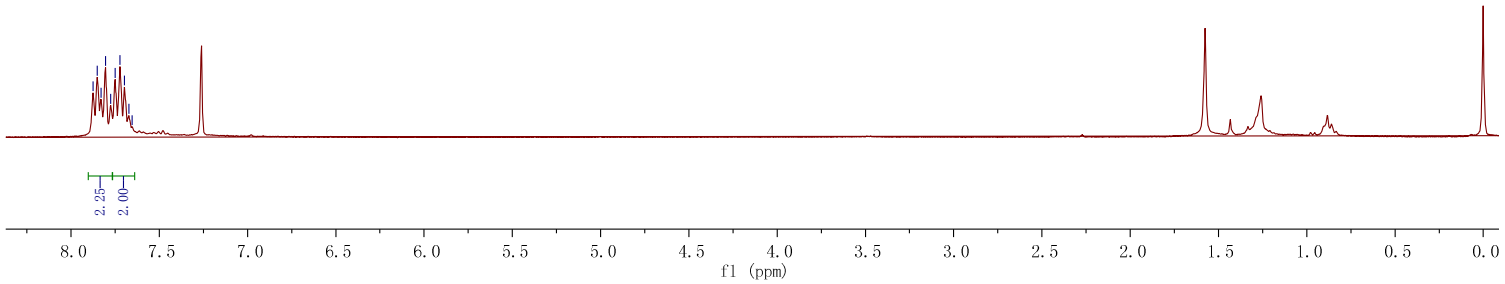
-63.54
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

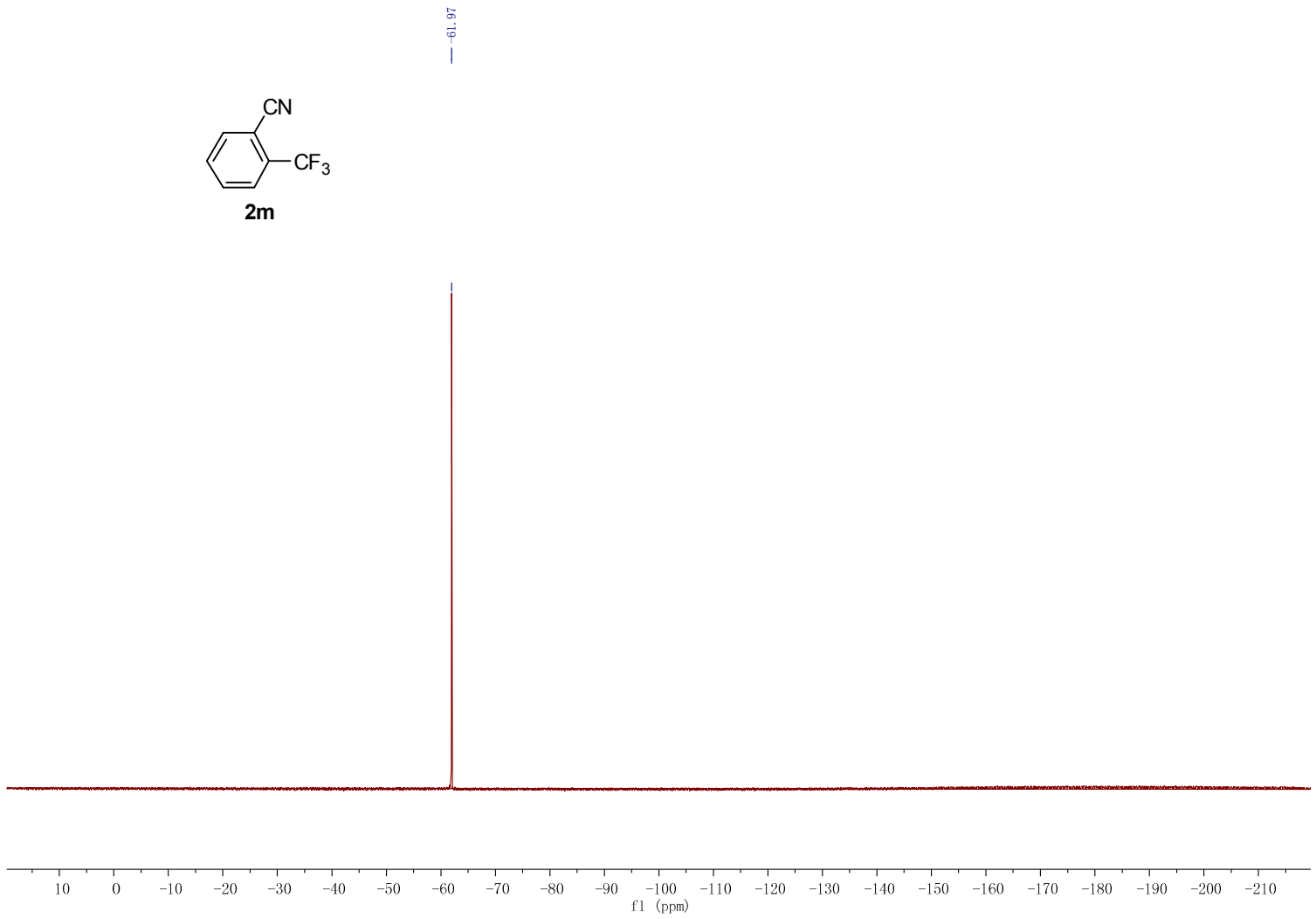

7.88
7.85
7.83
7.80
7.77
7.75
7.72
7.70
7.67
7.65

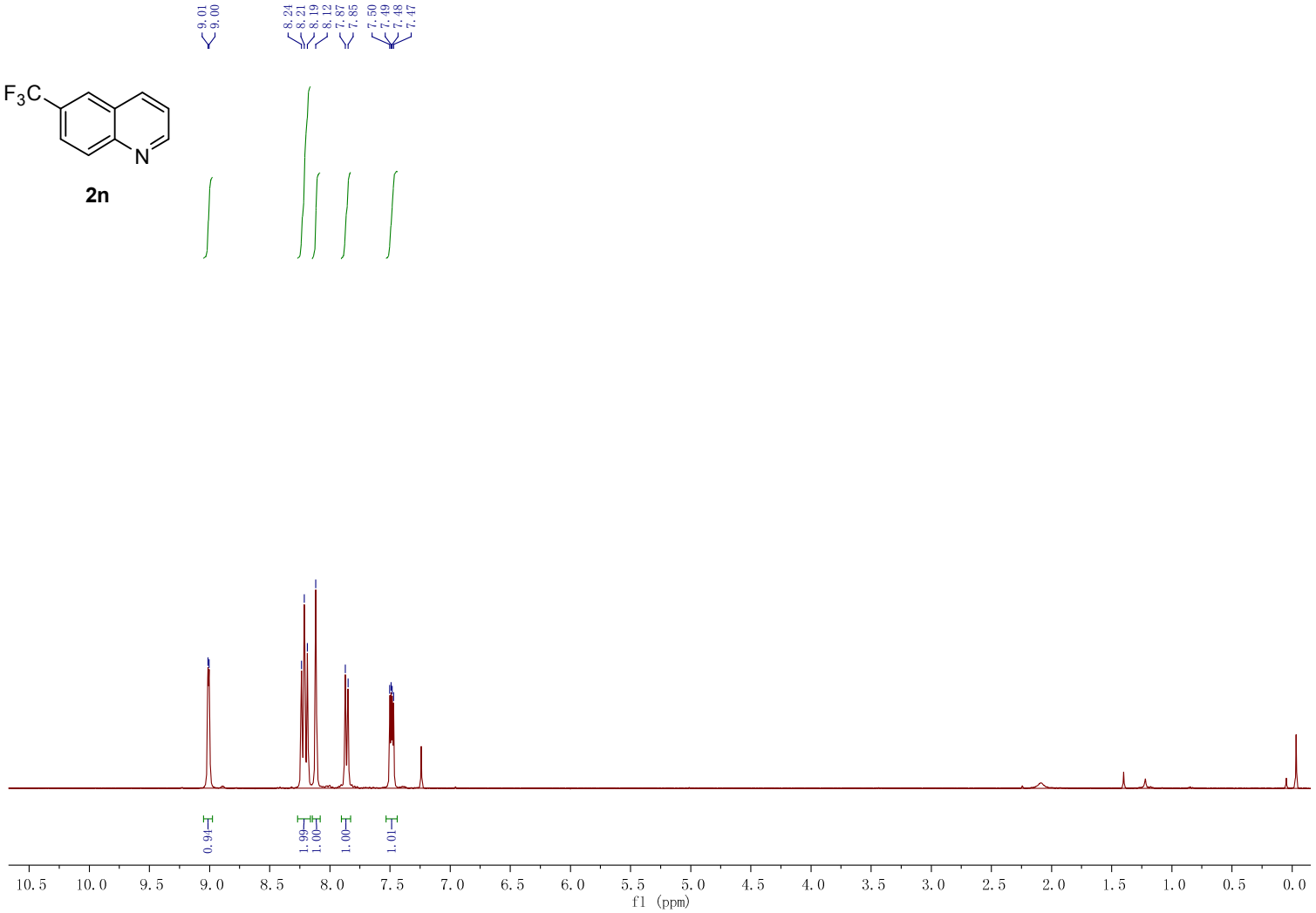


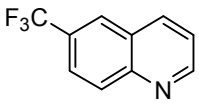

CN
CF3

2m


2.25
2.00
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)

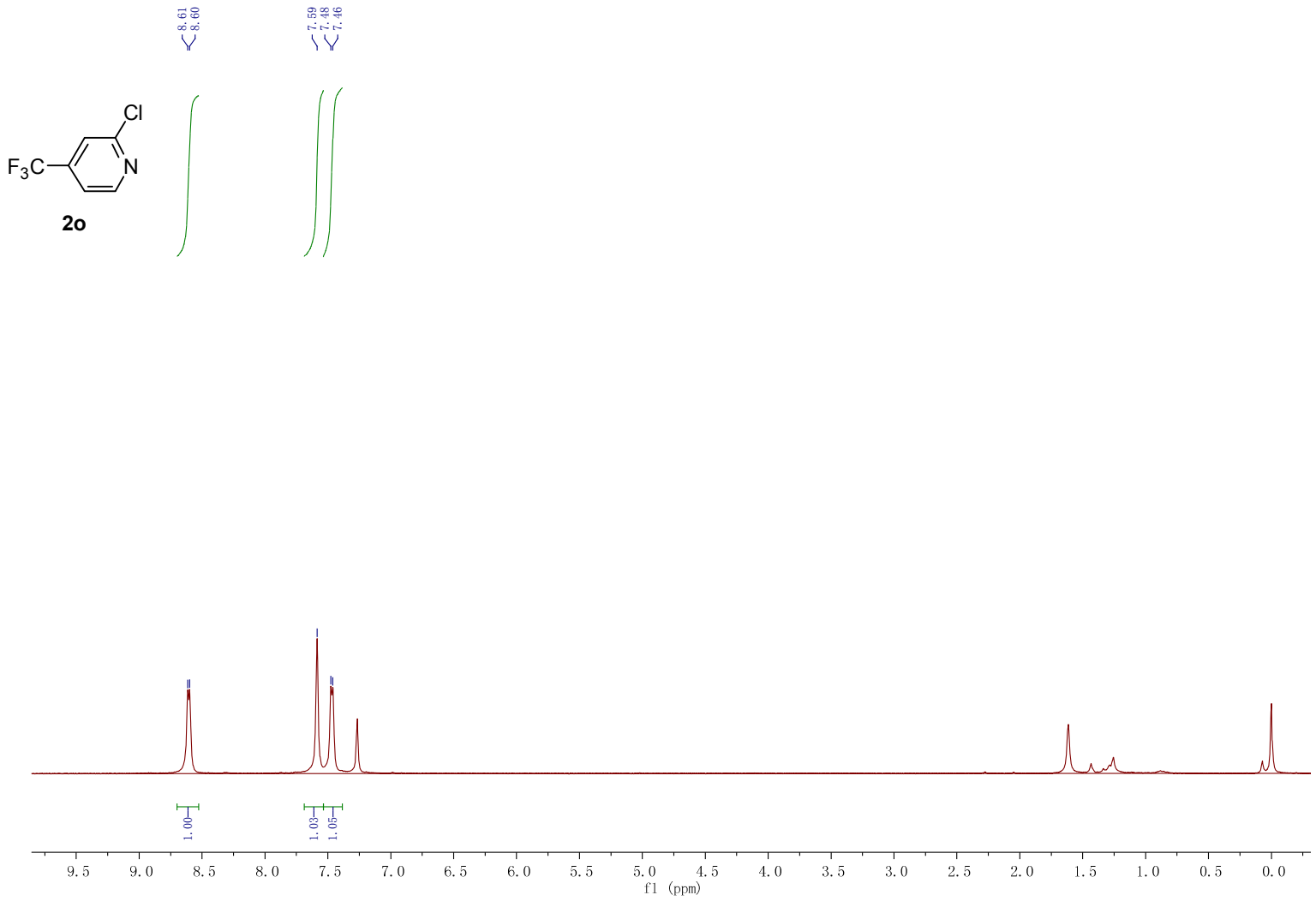

-61.97
CN
CF3
2m
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

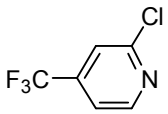

9.01
9.00
8.24
8.21
8.19
8.12
7.87
7.85
7.50
7.49
7.48
7.47
F3C
N
2n
0.94
1.99
1.00
1.00
1.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


F3C
N

2n

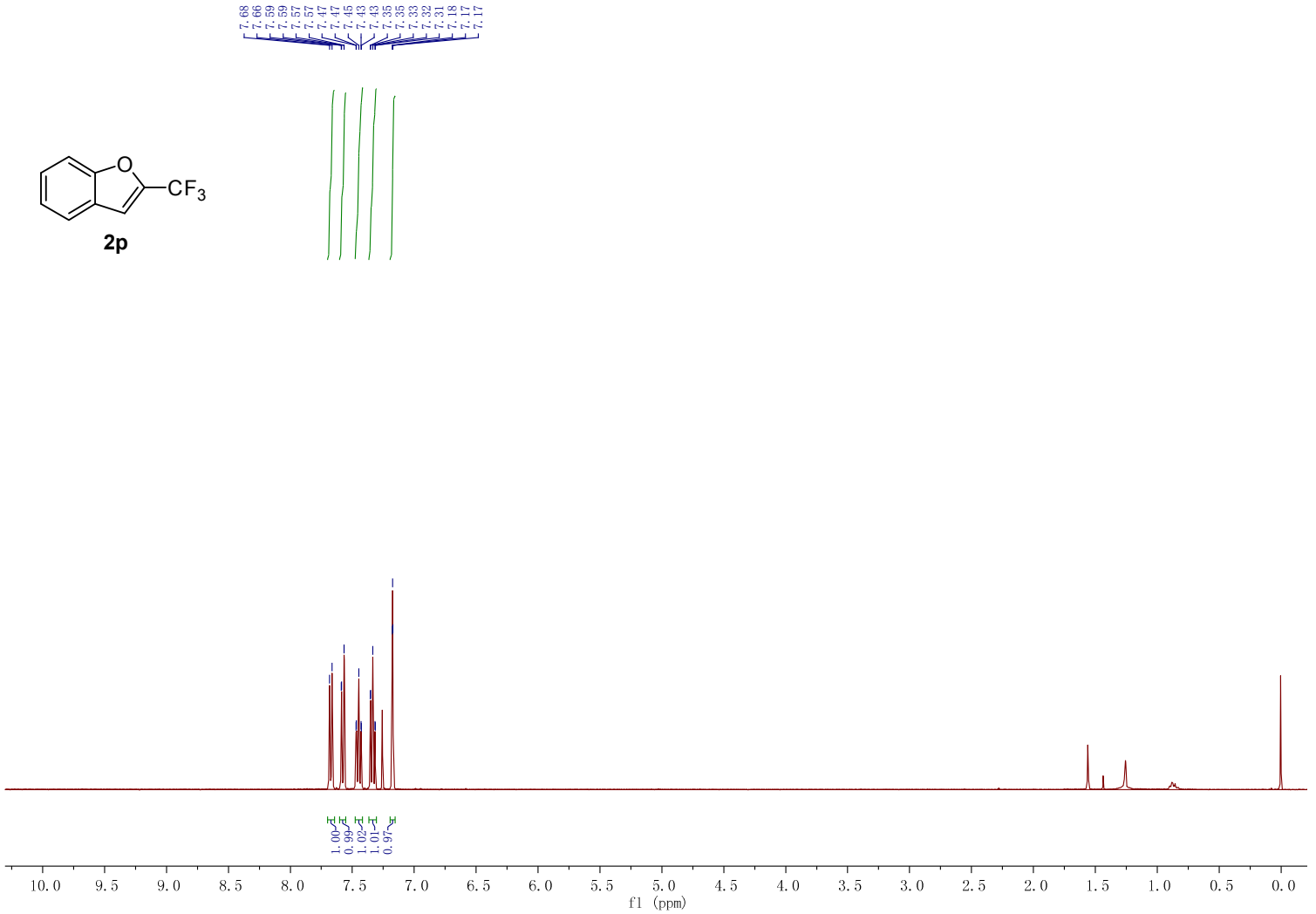
-62.40
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

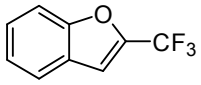

8.61
8.60
7.59
7.48
7.46
Cl
F3C
N
2o
1.00
1.03
1.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Cl
F3C
N

2o

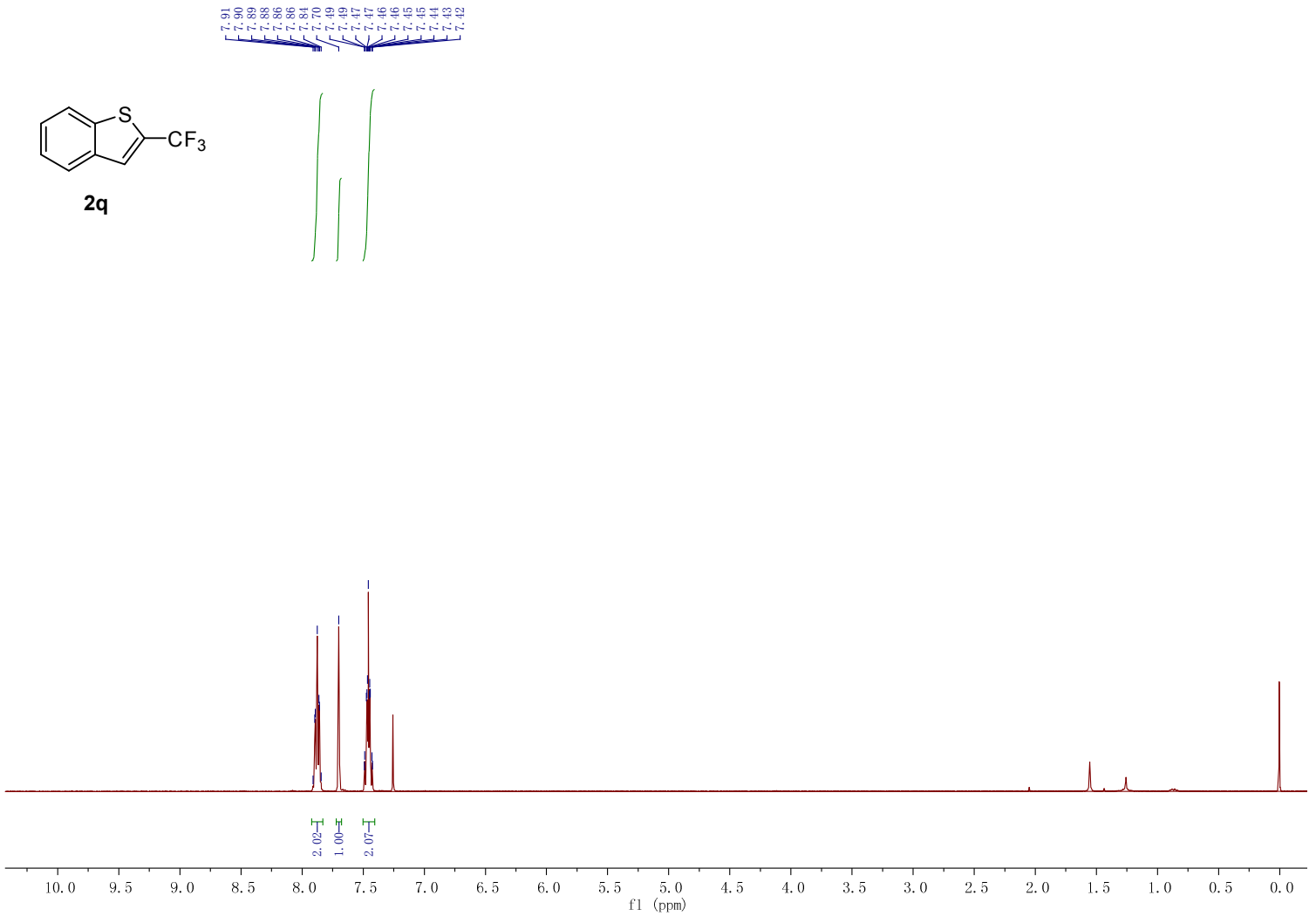
-64.80
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

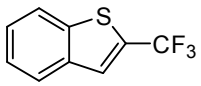

7.68
7.66
7.59
7.59
7.57
7.57
7.47
7.47
7.45
7.43
7.43
7.35
7.33
7.32
7.31
7.18
7.17
7.17
O
CF3
2p
1.00
0.99
1.02
1.01
0.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
CF3

2p

-64.85
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.91
7.90
7.89
7.88
7.86
7.86
7.84
7.70
7.49
7.49
7.47
7.47
7.46
7.46
7.45
7.45
7.44
7.43
7.42
S
CF3
2q
2.02
1.00
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


S
CF3

2q

-56.31
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)