Supporting Information

Microwave-assisted synthesis of *ortho*-substituent diaryl *N*-(tert-butylsulfinyl) ketimines

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General Information

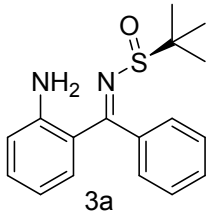
Microwave reactions were performed with a Biotage initiator (Model: Initiator EXP EU 355301) with a continuous focused microwave power delivery system in a pressure glass vessel (5 mL) sealed with a septum under magnetic stirring. The temperature of the reaction mixture was monitored using a calibrated infrared temperature control under the reaction vessel, and the pressure was controlled with a pressure sensor connected to the septum of the vessel. All glassware was dried in an oven at 100 °C and cooled to room temperature under nitrogen prior to use. All reactions were carried out under an nitrogen atmosphere. All the starting *ortho*-substituent diaryl ketones, (*R*)-t-BuSONH$_2$, and Ti(OEt)$_4$ (95%) are commercially available and were used as received. THF were distilled from sodium under nitrogen. Column chromatography was performed with silica gel of 200-300 mesh. Thin layer chromatography (TLC) was performed on precoated silica gel plates (0.25 mm); The detection was accomplished using a UV254 light. The HPLC analyses were performed using a UV detector, with 10% i-PrOH in hexane as the eluent and a flow rate of 1.0 mL/min. The retention times were 8.5 (S) and 9.9 (R) min for **3a** (OD-H column, 254 nm detector wavelength), 8.0 (S) and 9.4 (R) min for **3b** (OD-H column, 254 nm detector wavelength), and 9.2 (S) and 10.1 (R) min for **2h** (OD-H column, 5% i-PrOH in hexane as the eluent, 254 nm detector wavelength). Optical rotation measurements and HPLC analyses were performed at 20 °C.^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ operating at 400 MHz and 100 MHz. Proton chemical shifts are reported relative to the residual proton signals of the deuterated solvent $CDCl_3$ (7.26 ppm) or DMSO-d_6 (2.50 and 3.33 ppm) or TMS. Carbon chemical shifts were internally referenced to the deuterated solvent signals in $CDCl_3$ (77.00 ppm) or DMSO-d_6 (40.0 ppm). Data are represented as follows: chemical shift, multiplicity (bs = broad singlet, s = singlet, d = doublet, t = triplet, m = multiplet), coupling

constant in Hertz (Hz), and integration. Products were identified by comparison to spectral data reported in the literature. Mass spectra (both at low resolution and at high resolution) were recorded on a time-of-flight mass spectrometer with an ESI source. HPLC-MS were recorded on an Agilent 1200 LC/MSD Trap mass spectrometer. High-resolution mass spectra were recorded on a Shimadzu Liquid Chromatograph Mass Spectrometer (LCMS-IT-TOF).

Experimental Procedures and Characterization data of Compounds

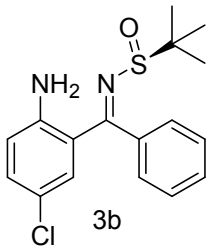
General procedure for synthesis of 3a-m

The corresponding diaryl ketone (1.0 mmol), (*R*)-t-BuSONH$_2$ (121 mg, 1.0 mmol), Ti(O^{i}Pr)$_4$ (0.84 mL, 4.0 mmol) and 1mL THF were mixed and stirred under nitrogen. The reaction vessel was placed into the microwave reactor and heated to 120 °C and 175W for 1 h (for the synthesis of **3a−g**) or 130 °C and 190W for 2.5 h (for the synthesis of **3h−m**) with air stream cooling. After cooling to room temperature, the mixture was diluted with ethyl acetate (10 mL) and poured into 10 mL of water while being rapidly stirred. The resulting suspension was filtered through a plug of Celite and the filter cake was washed with ethyl acetate. Sulfinyl ketimines **3a–m** were purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1 and 2:1), to give the expected imines in the yields indicated in **Table 3**.



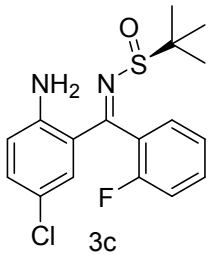
3a

3a: A yellow solid, yield 89%, $[\alpha]_D^{20}$ −122.5 (c 1.0, MeOH), mp 140.0-142.0 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49(s, 3H), 7.24-7.26 (m, 2H), 6.73-6.91 (m, 4H), 6.51 (s, 4H), 1.28 (s, 9H); MS (ESI) m/z: 301.2 $[M+H]^+$.



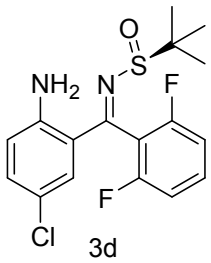
3b

3b: A yellow solid, yield 88%, $[\alpha]_D^{20}$ −123.5 (c 1.0, MeOH), mp 138.0-139.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50(s, 3H), 7.15-7.26 (m, 3H), 6.84 (s, 1H), 6.71 (d, *J* = 8.8 Hz, 1H), 1.27 (s, 9H); MS (ESI) m/z: 335.2 $[M+H]^+$.



3c

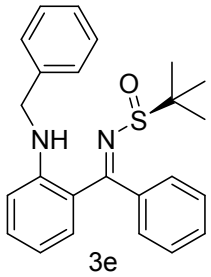
3c: A yellow solid, yield 86%, $[\alpha]_D^{20}$ −120.8 (c 1.0, MeOH), mp 136.0-138.0℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.53 (m, 1H), 7.15-7.30 (m, 4H), 6.84 (s, 1H), 6.71(d, *J* = 8.8 Hz, 1H), 1.27 (s, 9H); MS (ESI) m/z: 353.1 $[M+H]^+$.



3d

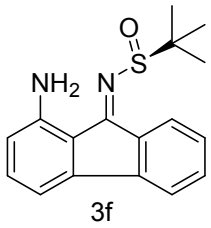
3d: a yellow solid, yield 73%, $[\alpha]_D^{20}$ −124.5 (c 1.0, MeOH), mp = 160.1 - 162.7℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.49 - 7.55 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.02 - 7.09 (m, 2H), 8.90 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.8, 148.8, 133.9, 132.0, 131.9, 131.8, 131.0, 120.8, 118.5, 117.8, 113.7, 111.6, 111.5, 56.7, 22.3; MS (ESI) *m/z*: 371.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{18}ClN_2F_2OS$ $[M + H]^+$ 371.0791, found

371.0793.



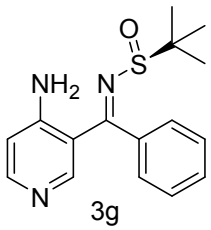
3e

3e: a yellow solid, yield 70%, $[\alpha]_D^{20}$ −95.5 (c 1.0, MeOH), mp = 142.5-144.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.84 (s, 1H), 7.28-7.48 (m, 12H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.47 (t, *J* = 7.0 Hz, 1H), 4.54 (s, 2H), 1.06 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 183.4, 151.2, 138.1, 137.3, 135.8, 134.2, 128.9, 128.7, 128.1, 127.9, 127.4, 117.2, 114.6, 111.6,55.2, 47.6, 22.1; MS (ESI) *m/z*: 391.2 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{24}H_{27}N_2OS$ $[M + H]^+$ 391.1839, found 391.1838.



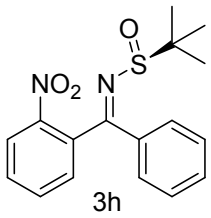
3f

3f: a yellow solid, yield 84%, $[\alpha]_D^{20}$ −135.8 (c 1.0, MeOH), mp =161.1-162.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.31 (d, *J* = 8.0Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 7.0 Hz, 1H), 6.55 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:175.0, 147.5, 143.7, 142.7, 134.5, 133.0, 132.4, 130.0, 128.2, 120.3, 117.1, 116.5, 109.3, 57.2, 22.3; MS (ESI) *m/z*: 299.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{18}N_2OS$ $[M + H]^+$ 299.1213, found 299.1212.



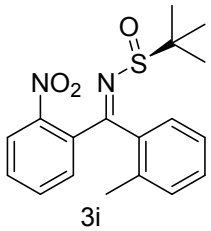
3g

3g: a yellow solid, yield 83%, $[\alpha]_D^{20}$ −98.6 (c 1.0, MeOH), mp = 112.6-113.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.11 (s, 1H), 7.97 (s, 1H), 7.50 (s, 1H), 7.49 (s, 1H), 7.28 (s, 1H), 6.61 (d, J = 7.0 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 182.5, 156.3, 154.9, 150.9, 135.7, 129.7, 128.5, 127.8, 114.6, 110.9, 55.7, 22.3; MS (ESI) *m/z*: 302.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{19}N_2OS$ $[M + H]^+$ 302.1322, found 302.1319.



3h

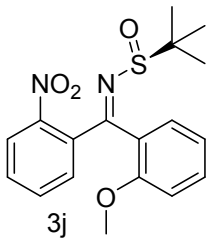
3h: a yellow solid, yield 41%, $[\alpha]_D^{20}$ −95.3 (c 1.0, MeOH), mp =143.6-146.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ:8.32 (t, J = 9.0 Hz, 1H), 7.77 (t, J = 8.0 Hz, 1H), 7.60 - 7.70 (m, 3H), 7.38 - 7.49 (m, 4H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.5, 147.3, 137.5, 133.8, 133.3, 132.3, 131.9, 130.9, 130.1, 129.8, 127.8, 59.2, 22.9; MS (ESI) *m/z*: 331.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_9N_2O_3S$ $[M + H]^+$ 331.1111, found 331.1110.



3i

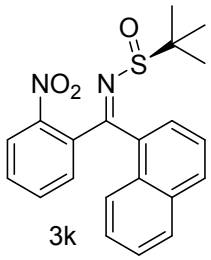
3i: a yellow solid, yield 38%, $[\alpha]_D^{20}$ −102.7 (c 1.0, MeOH), mp =167.5-168.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.76 (d, J = 2.0 Hz, 1H), 7.71 (d, J = 9.0 Hz, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.18

- 7.31 (m, 4H), 6.81 (d, J = 9.0 Hz, 1H), 2.31 (s, 3H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 200.6, 154.3, 138.8, 138.3, 135.5, 135.3, 131.1, 130.1, 127.3, 125.3, 121.2, 117.3, 116.7, 59.8, 23.5, 19.5; MS (ESI) *m/z*: 345.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{21}N_2O_3S$ $[M + H]^+$ 345.1267, found 345.1266.



3j

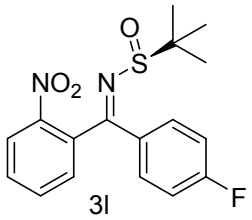
3j: a yellow solid, yield 42%, $[\alpha]_D^{20}$ −98.0 (c 1.0, MeOH), mp =174.0-174.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.82 (d, J = 2.0 Hz, 1H), 7.68 (d, J = 9.0 Hz, 1H), 7.47 (t, J = 8.0 Hz, 1H), 7.29 (d, J = 2.0 Hz, 2H), 7.05 (t, J = 8.0 Hz, 1H), 6.99 (d, J = 8.0, 1H), 6.78 (d, J = 8.0 Hz, 1H), 3.75 (s, 3H), 1.27(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.2, 156.3, 153.9, 138.7, 135.0, 131.9, 128.9, 128.8, 121.0, 120.8, 117.4, 116.6, 111.4, 59.6, 55.5, 23.5; MS (ESI) *m/z*: 361.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{21}N_2O_4S$ $[M + H]^+$ 361.1217, found 361.1216.



3k

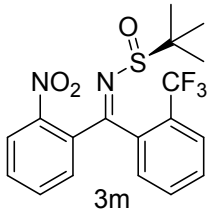
3k: a yellow solid, yield 44%, $[\alpha]_D^{20}$ −146.5 (c 1.0, MeOH), mp =171.5-172.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.71-7.76 (m, 2H), 7.88 (d, J = 8.0 Hz, 1H), 7.46-7.55 (m, 5H), 6.85 (d, J = 9.0 Hz, 1H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 199.9, 154.3, 138.6, 136.7, 135.4, 133.7, 130.9, 130.5, 128.6, 127.1, 126.4, 126.3,

125.1, 124.5, 121.2, 117.8, 116.8; MS (ESI) *m/z*: 381.1 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{21}H_{21}N_2O_3S$ $[M + H]^+$ 381.1267, found 381.1265.



3l

3l: a yellow solid, yield 30%, $[\alpha]_D^{20}$ −110.9 (c 1.0, MeOH), mp =161.3-162.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.27 (d, J = 8.0 Hz, 1H), 7.81 (dd, J_1 = 12.0 Hz, J_2 = 4.0 Hz, 3H), 7.72 (t, J = 8.0 Hz, 1H), 7.51 (d, J = 8.0 Hz, 1H), 7.15 (t, J = 8.0 Hz, 2H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 195.2, 163.3, 150.4, 136.3, 132.1, 130.5, 128.3, 127.9, 124.4, 121.8, 117.3, 59.8, 23.0; MS (ESI) *m/z*: 348.3 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{17}H_{18}FN_2O_3S$ $[M + H]^+$ 349.1017, found 349.1018.

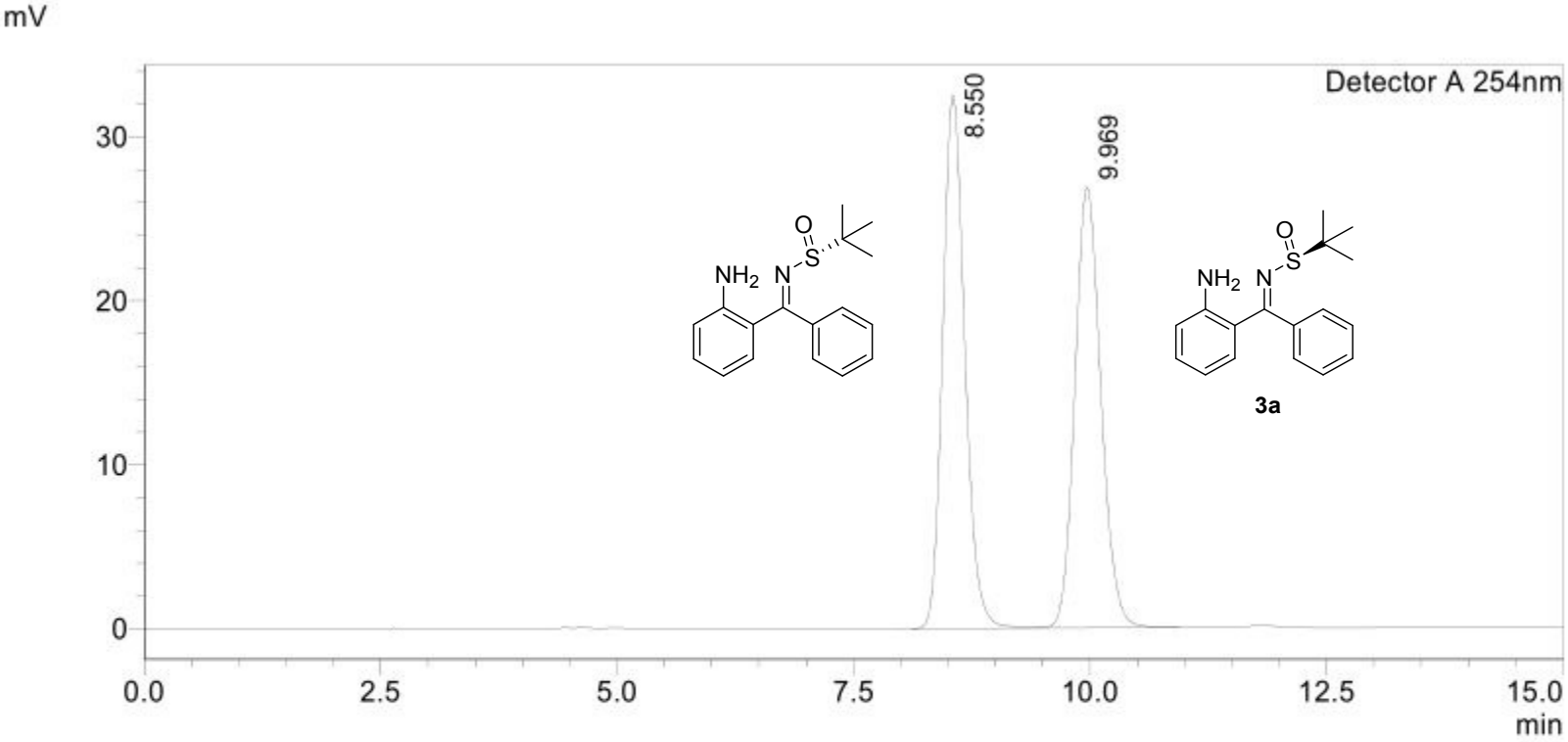


3m

3m: a yellow solid, yield 19%, $[\alpha]_D^{20}$ −95.2 (c 1.0, MeOH), mp =150.0-153.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 - 7.79 (d, 1H), 7.71 (d, J = 2.0 Hz, 1H), 7.64 (t, J = 4.0 Hz, 2H), 7.60 (d, J = 2.0 Hz, 1H), 7.36 (t, J = 6.0 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.2, 154.3, 138.3, 137.7, 135.6, 131.7, 129.9, 127.7, 126.8, 126.8, 121.3, 116.8, 116.5, 59.8, 23.4; MS (ESI) *m/z*: 399.0 $[M+H]^+$. HRMS (ESI-TOF) m/z: calcd for $C_{18}H_{18}F_3N_2O_3S$ $[M + H]^+$ 399.0985, found 399.0985.

HPLC Analysis Report by Chiral Column (OD-H)

<Chromatogram>



<Peak Table>

Detector A 254nm

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HPLC Analysis Report by Chiral Column (OD-H)

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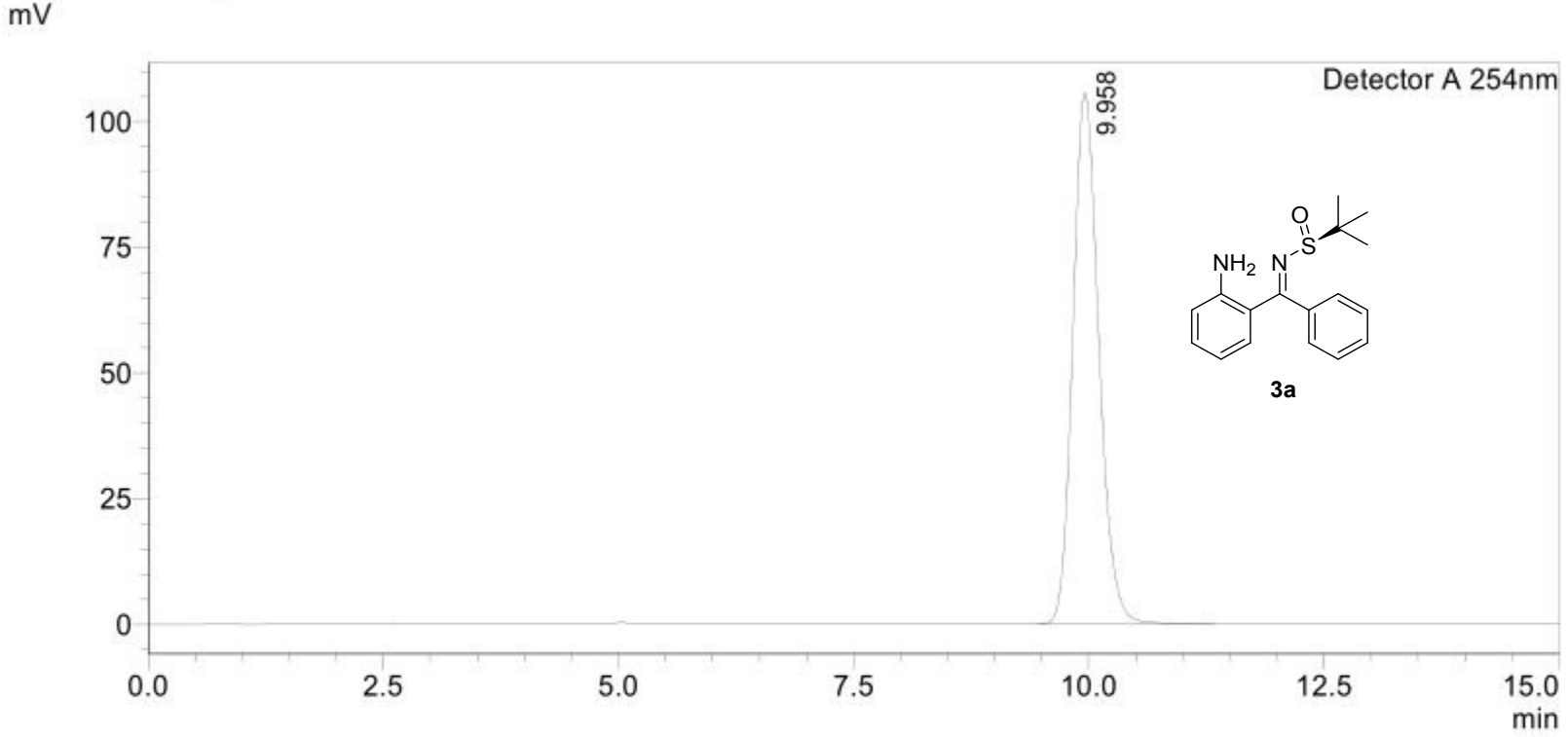

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
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HPLC Analysis Report by Chiral Column (OD-H)

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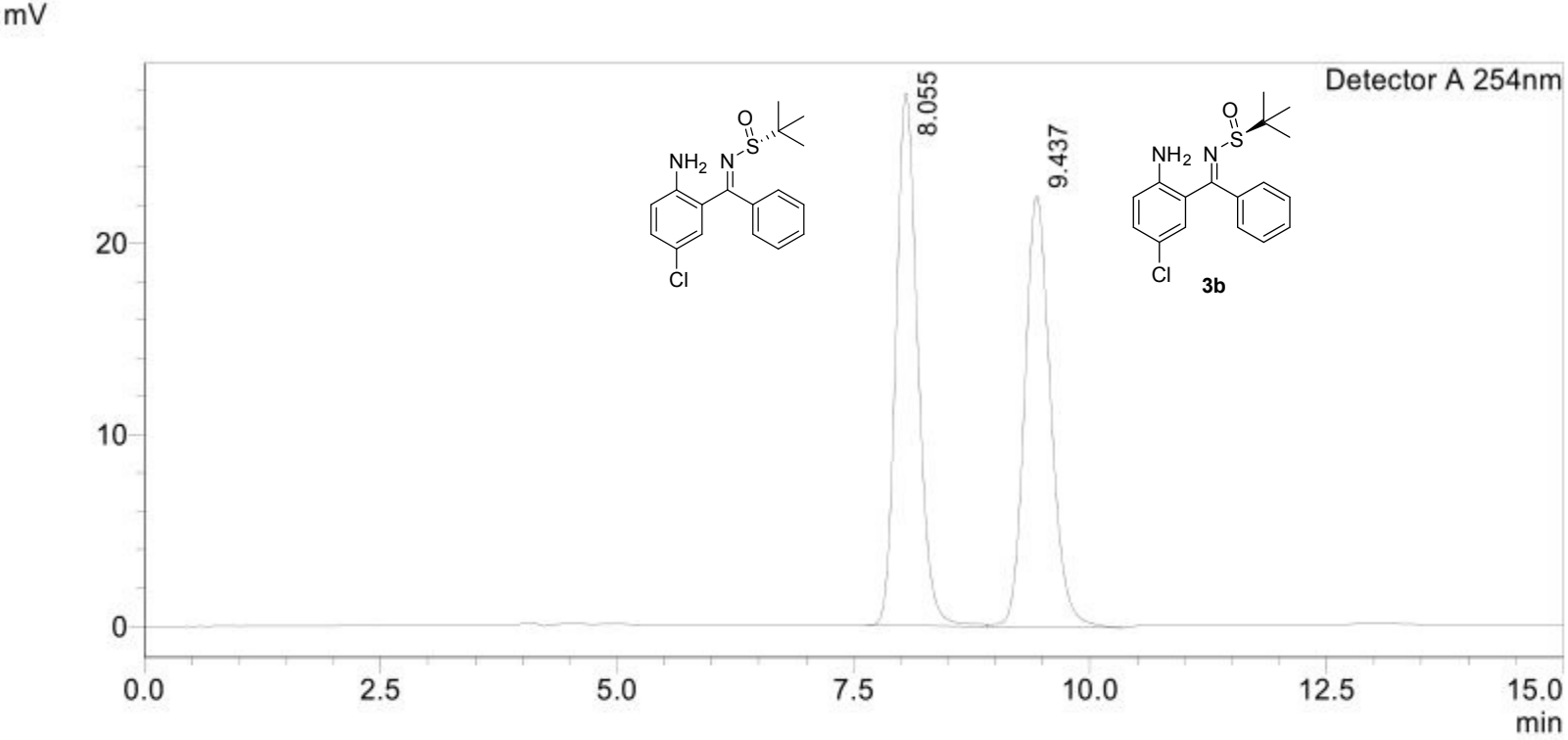

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.055	443766	27799	50.847			
2	9.437	428973	22503	49.153		V	
Total		872739	50302				

HPLC Analysis Report by Chiral Column (OD-H)

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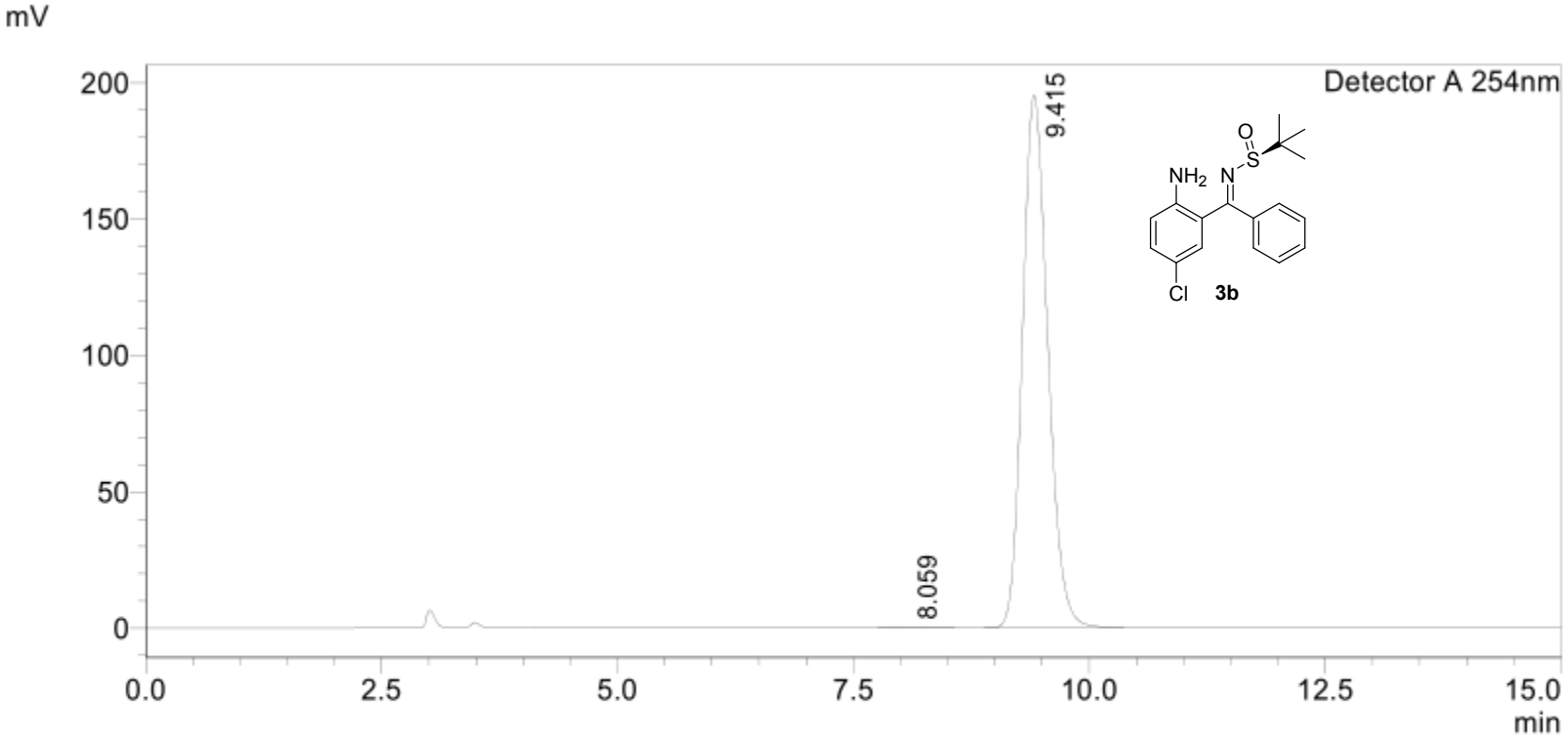

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.059	5824	350	0.160			
2	9.415	3640998	195491	99.840			
Total		3646822	195841				

HPLC Analysis Report by Chiral Column (OD-H)

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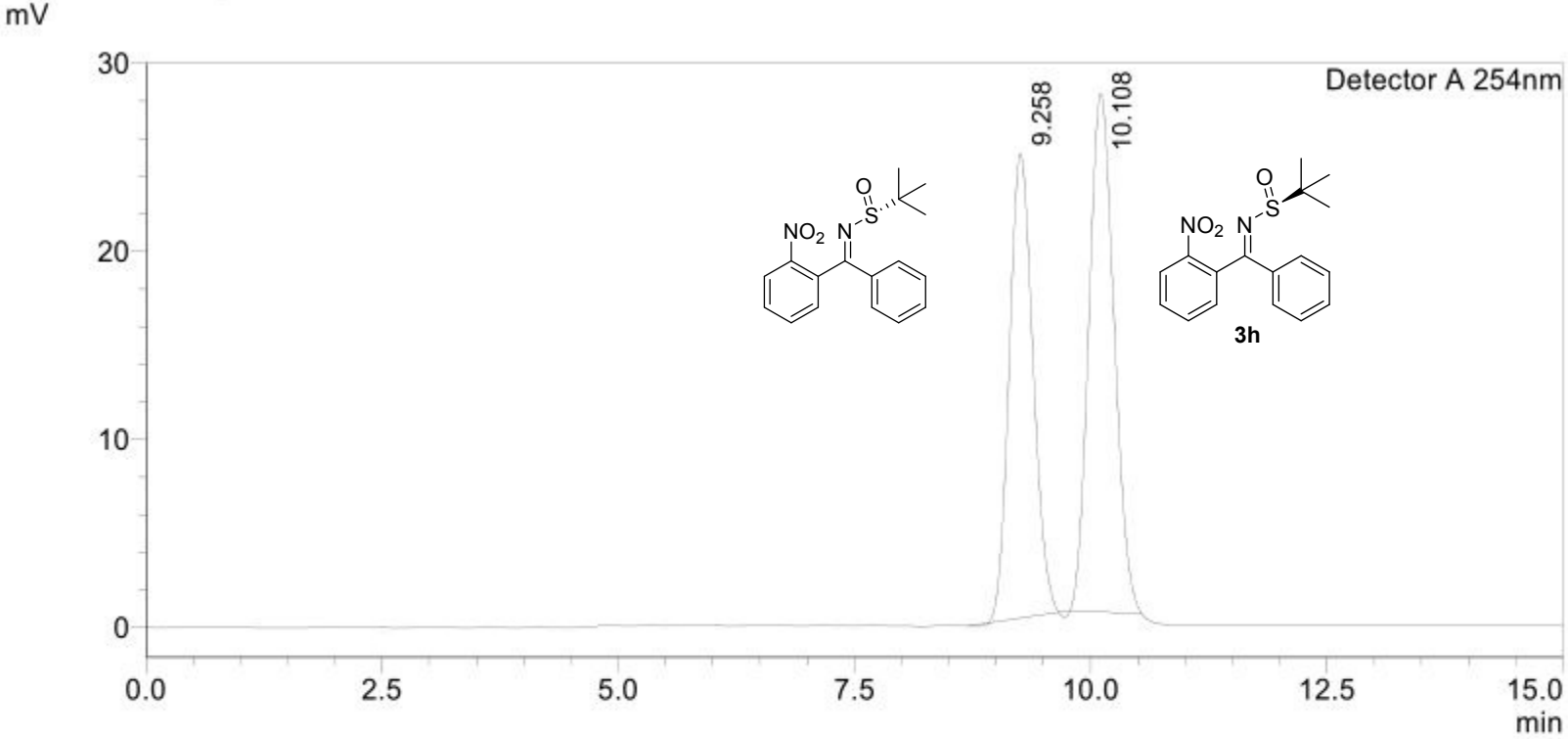

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Detector A 254nm

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1	9.258	431754	24702	45.823		M	
2	10.108	510465	27573	54.177		M	
Total		942219	52275				

HPLC Analysis Report by Chiral Column (OD-H)

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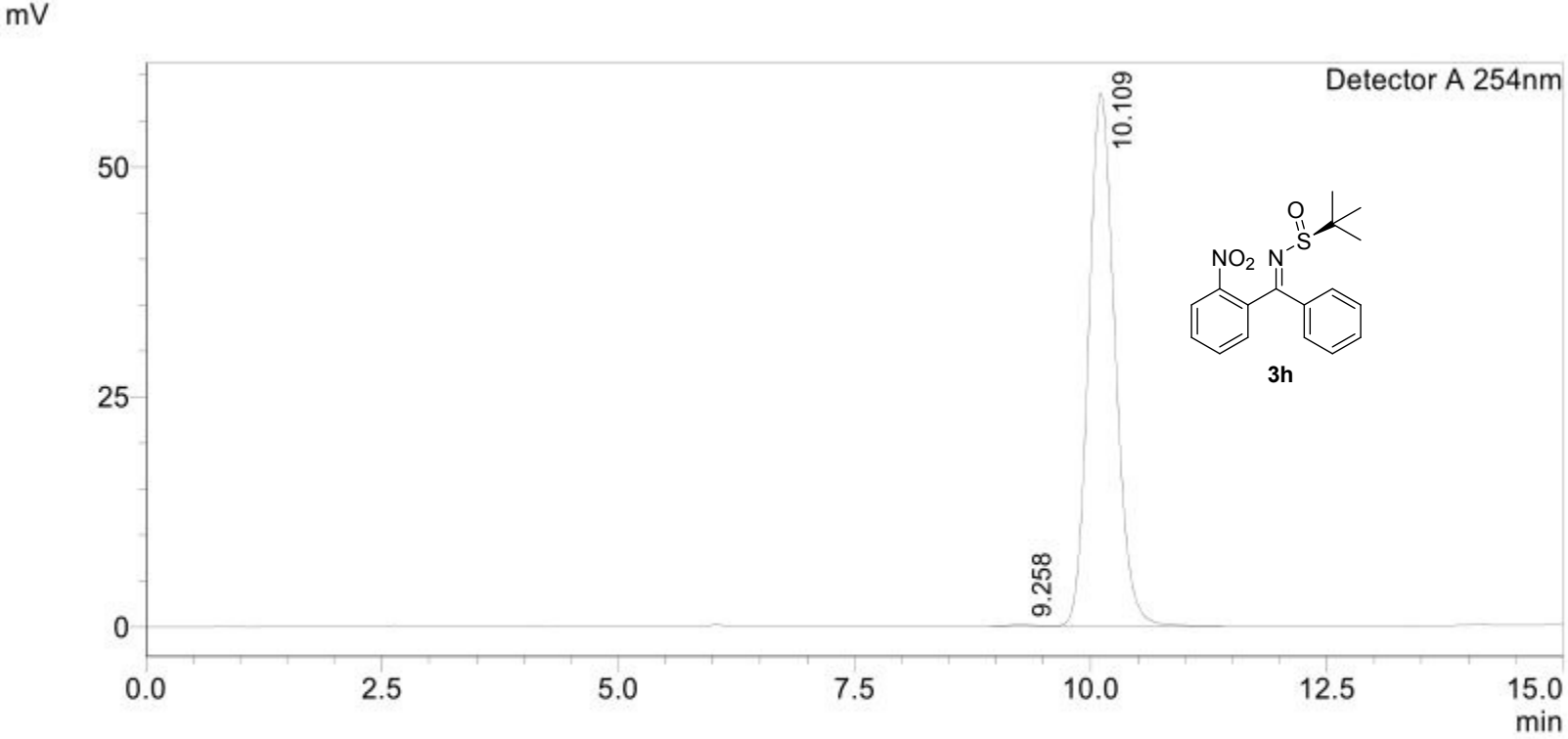

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.258	2448	131	0.217			
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Total		1126834	58068				

Copies of ^{1}H NMR and ^{13}C NMR Spectra

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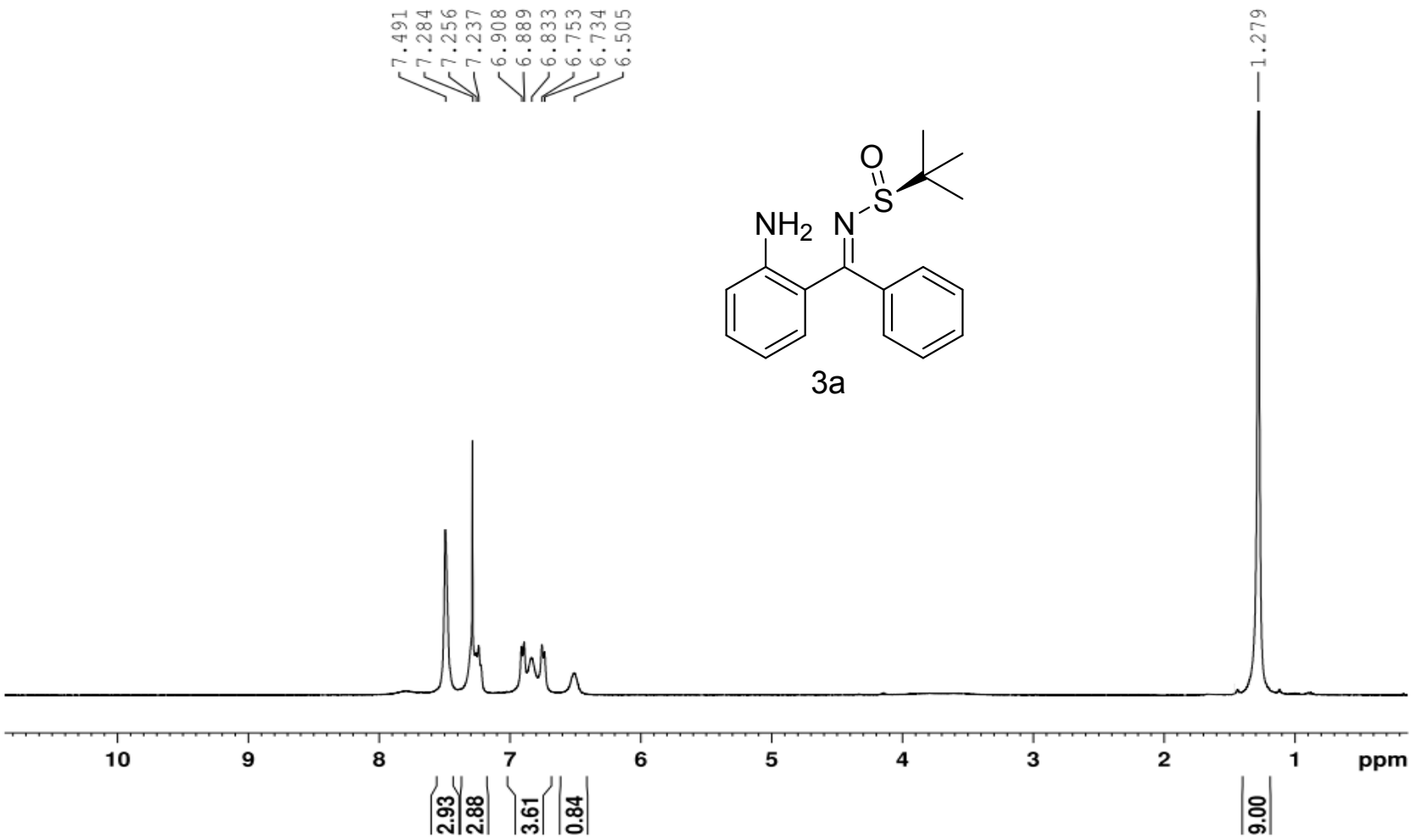
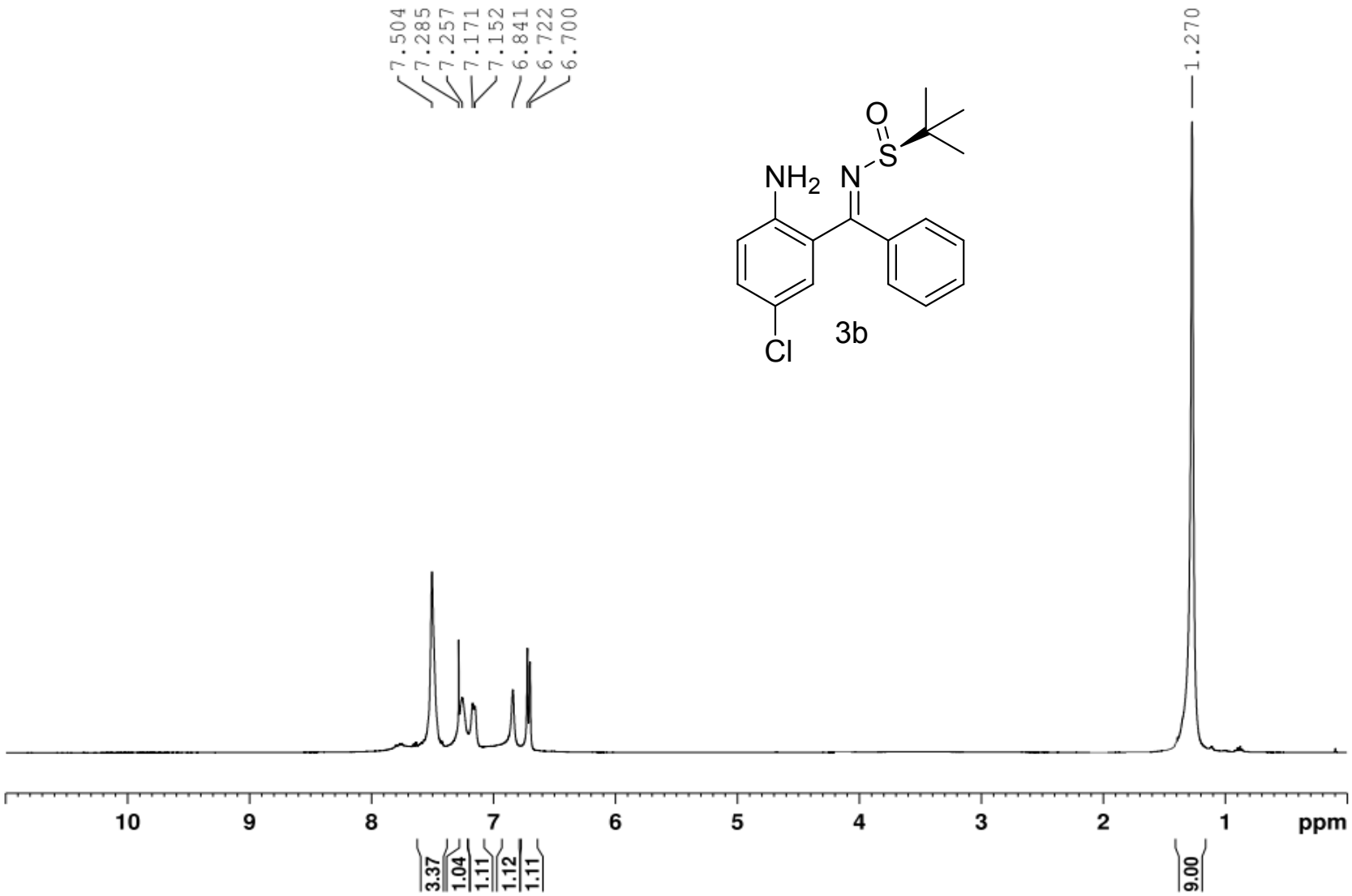


^{1}H NMR: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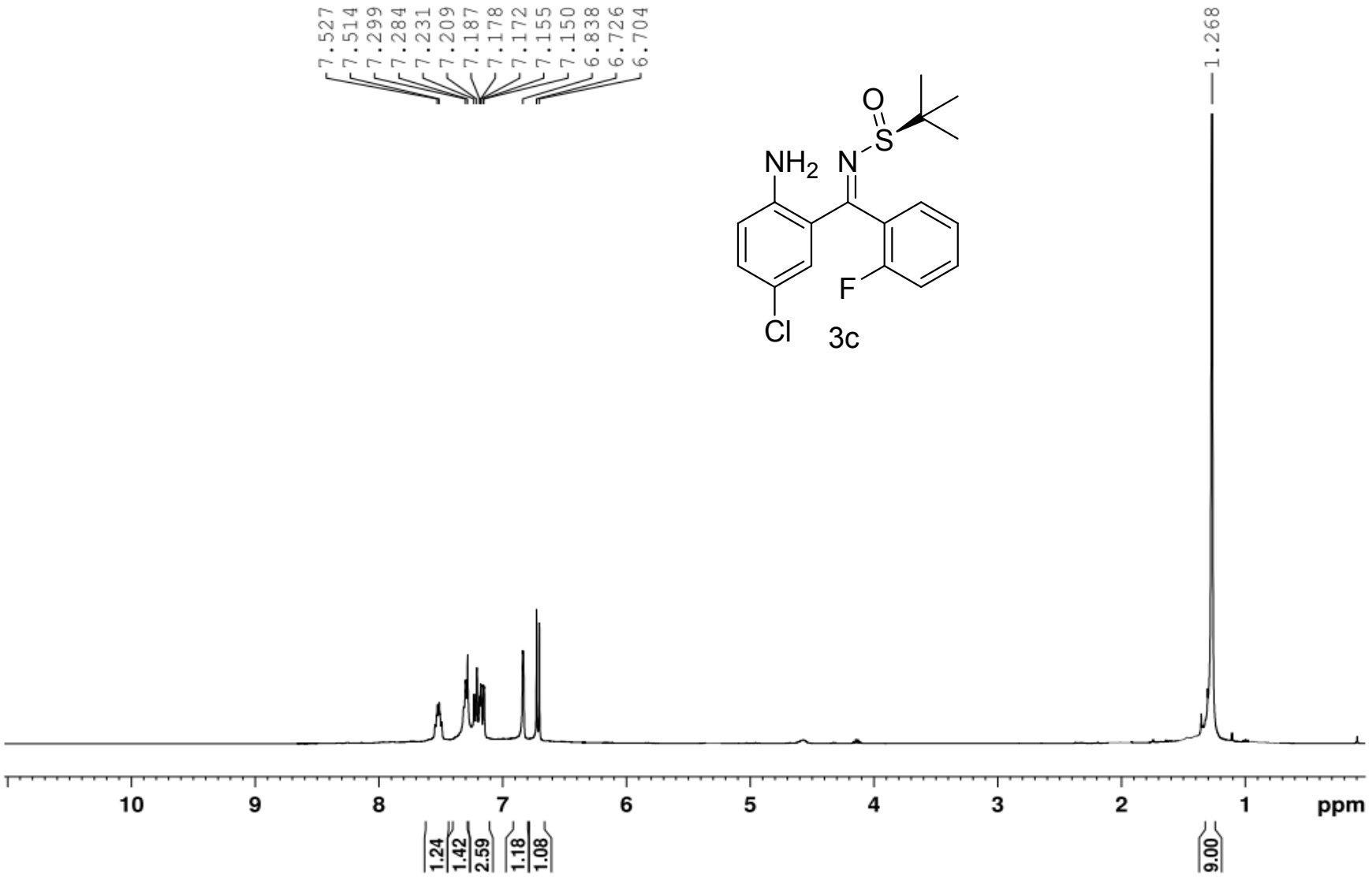
7.171
7.152
6.841
6.722
6.700
1.270
O
S
NH2
N
Cl
3b
10
9
8
7
6
5
4
3
2
1
ppm
3.37
1.04
1.11
1.12
1.11
9.00

^{1}H NMR: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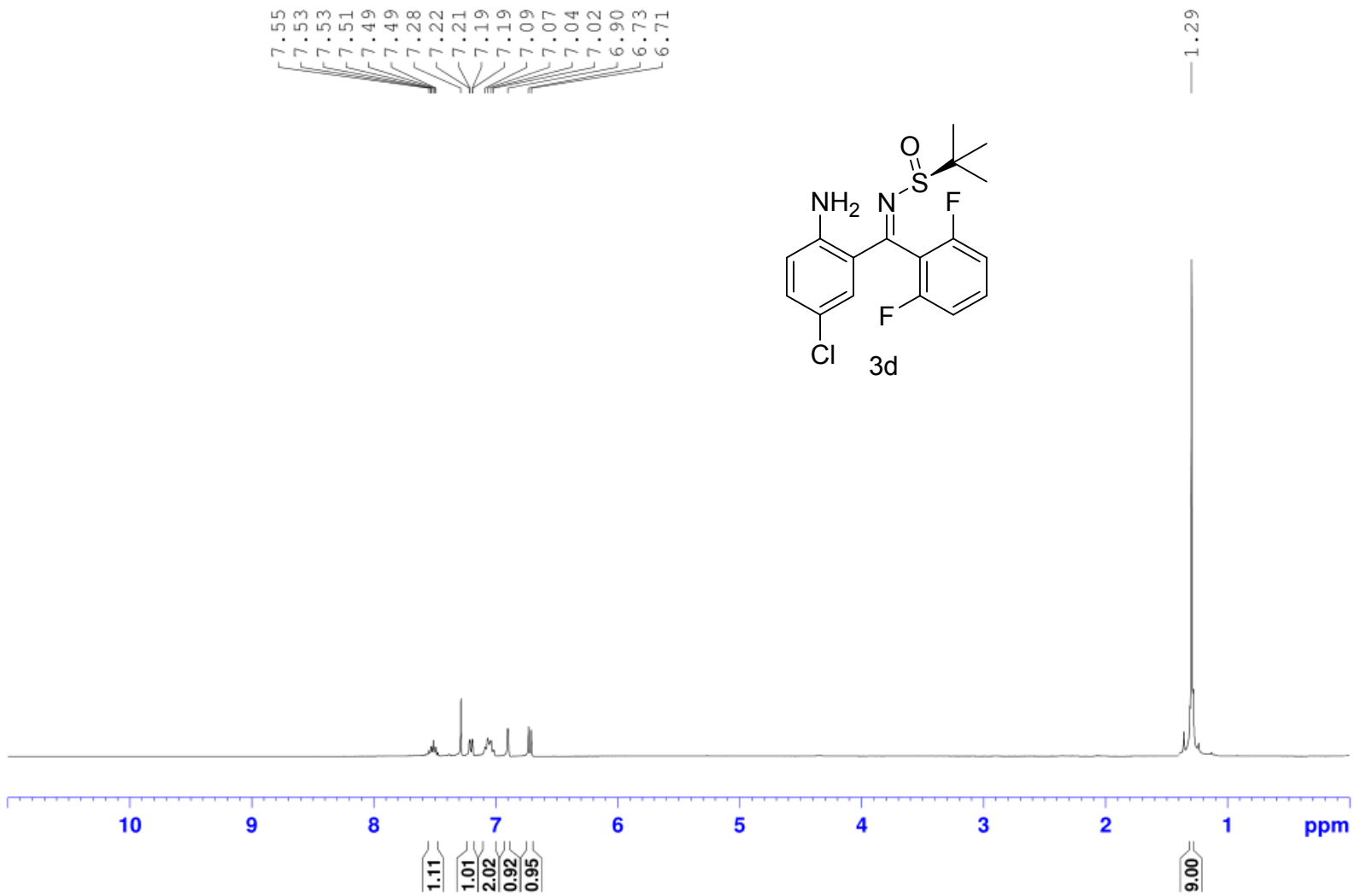
7.514
7.299
7.284
7.231
7.209
7.187
7.178
7.172
7.155
7.150
6.838
6.726
6.704
1.268
O
S
NH2
N
F
Cl
3c
10
9
8
7
6
5
4
3
2
1
ppm
1.24
1.42
2.59
1.18
1.08
9.00

^{1}H NMR: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7.53
7.53
7.51
7.49
7.49
7.28
7.22
7.21
7.19
7.19
7.09
7.07
7.04
7.02
6.90
6.73
6.71
1.29
O
S
NH2
N
F
F
Cl
3d
10
9
8
7
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3
2
1
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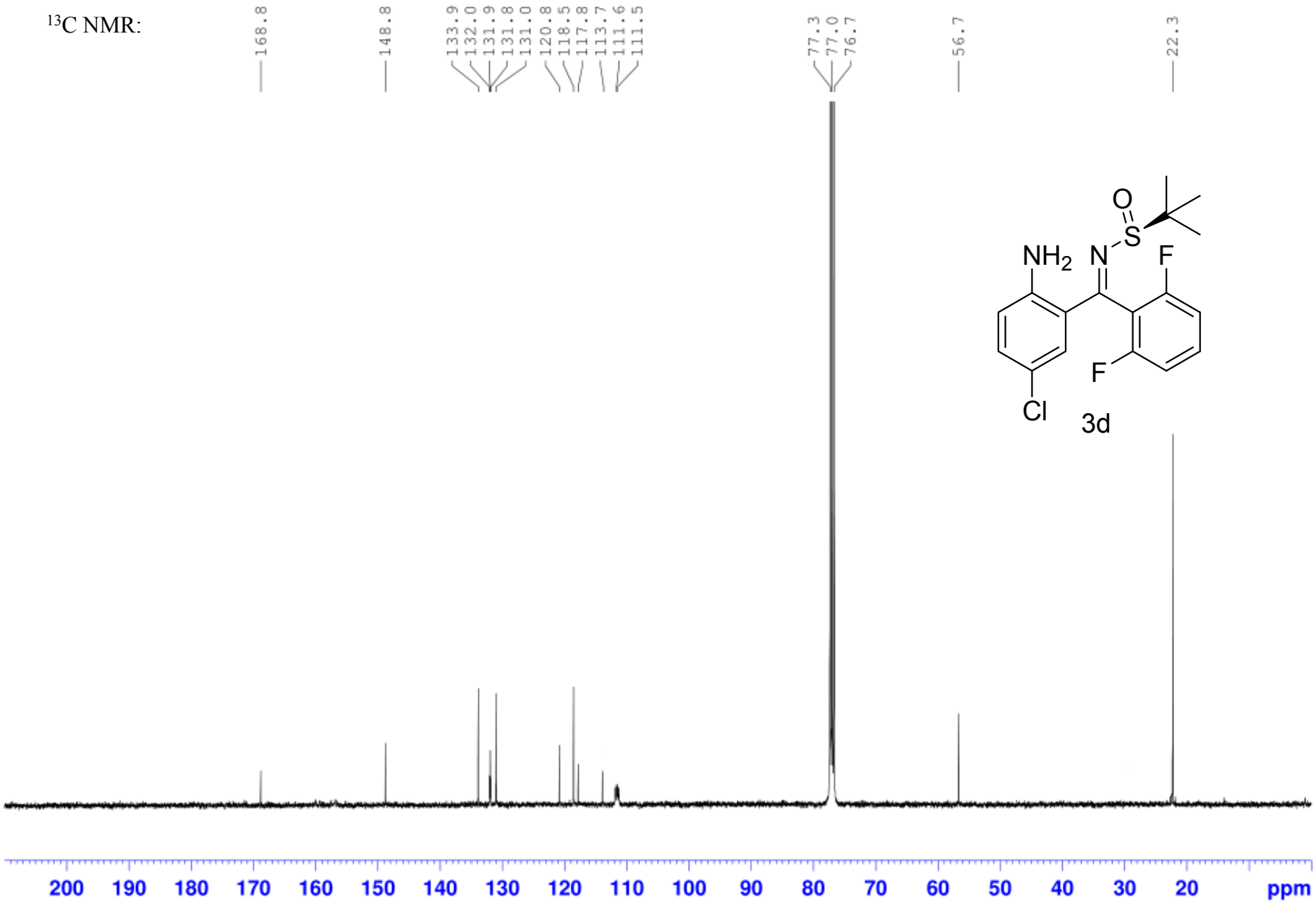
1.01
2.02
0.92
0.95
9.00

^{13}C NMR: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148.8
133.9
132.0
131.9
131.8
131.0
120.8
118.5
117.8
113.7
111.6
111.5
77.3
77.0
76.7
56.7
22.3
O
S
NH2
N
F
F
Cl
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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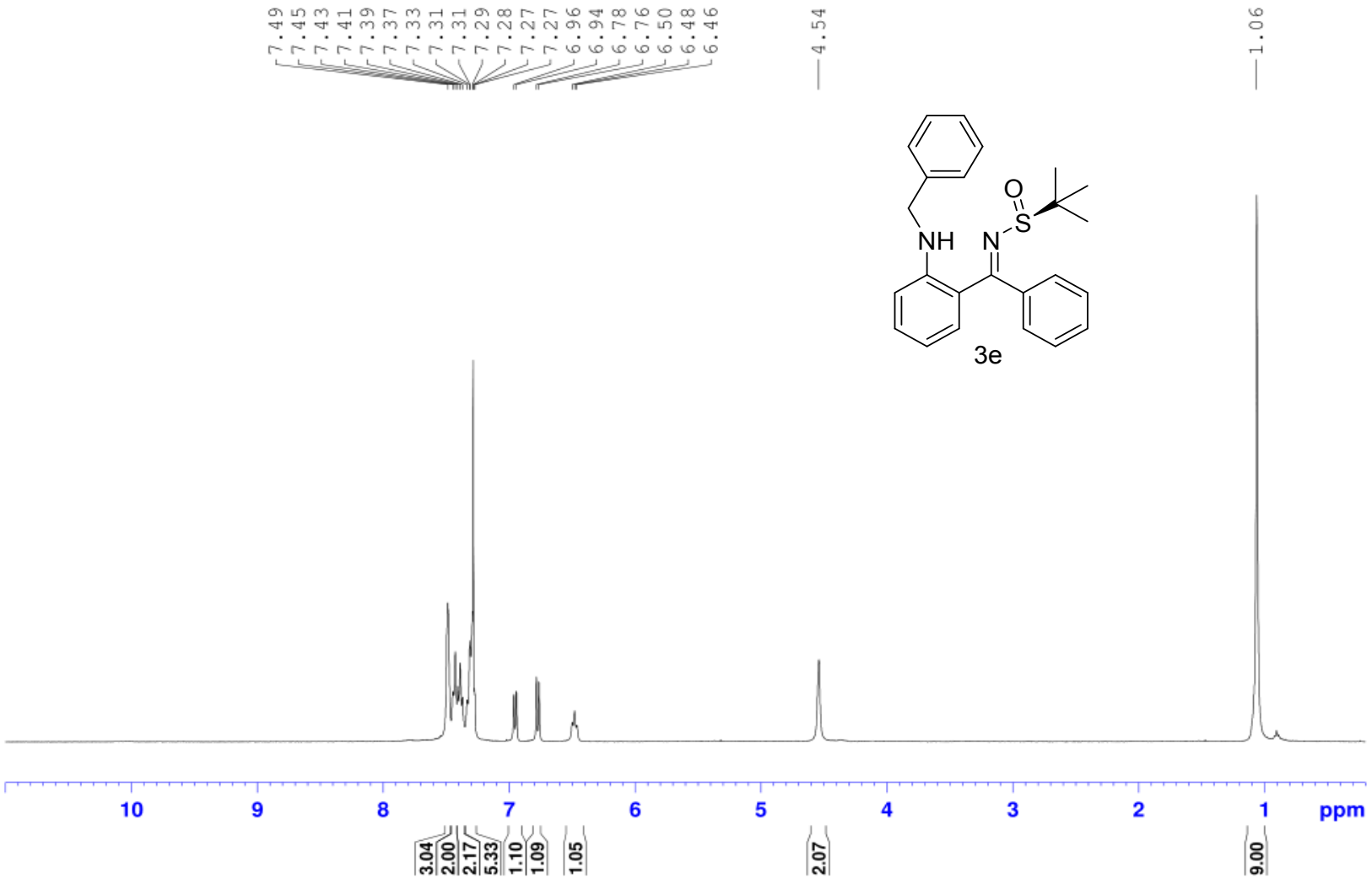
50
40
30
20
ppm

^{1}H NMR: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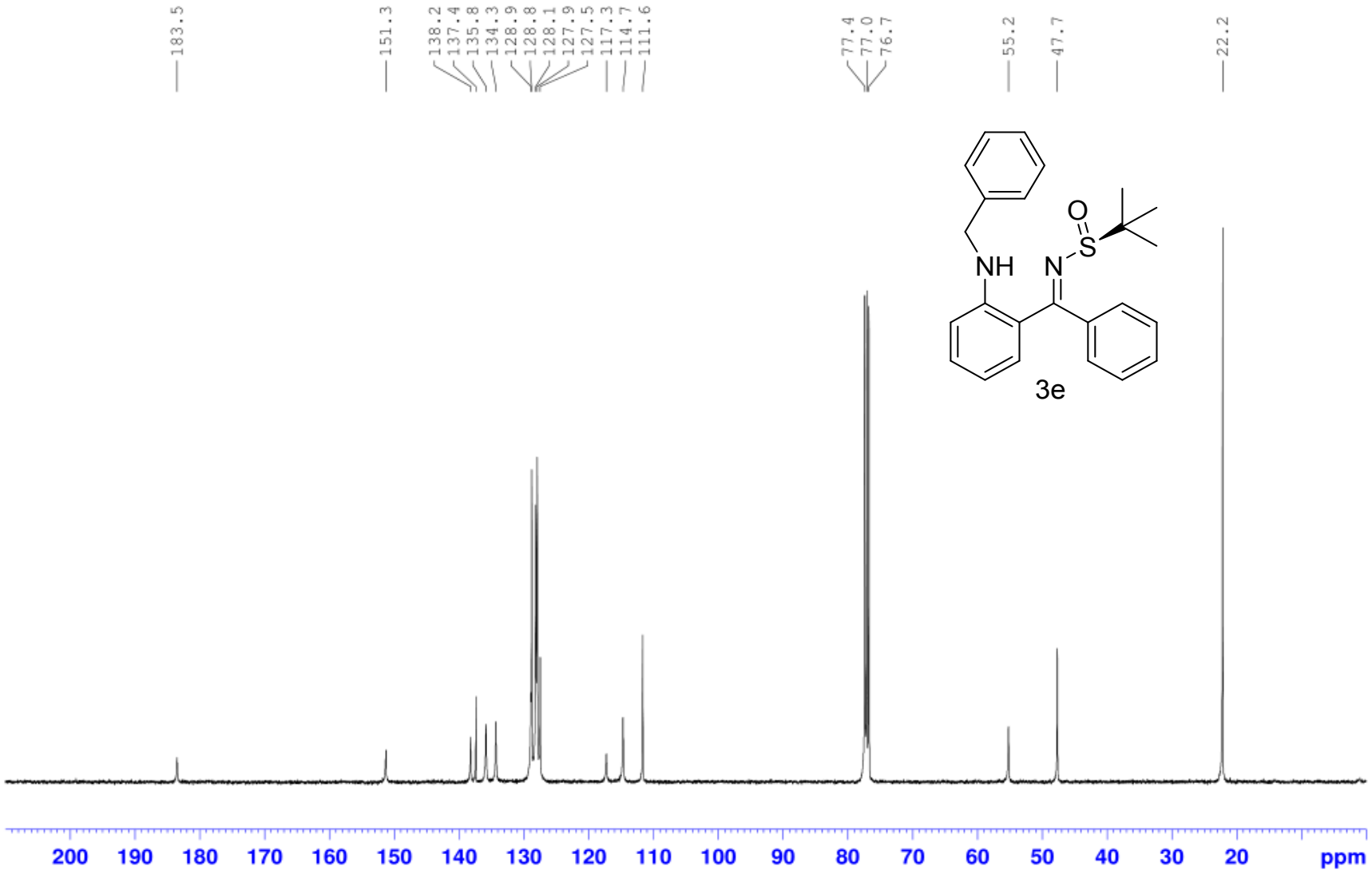
7.45
7.43
7.41
7.39
7.37
7.33
7.31
7.31
7.29
7.28
7.27
7.27
6.96
6.94
6.78
6.76
6.50
6.48
6.46
4.54
1.06
NH
N
O
S
3e
10
9
8
7
6
5
4
3
2
1
ppm
3.04
2.00
2.17
5.33
1.10
1.09
1.05
2.07
9.00

^{13}C NMR: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151.3
138.2
137.4
135.8
134.3
128.9
128.8
128.1
127.9
127.5
117.3
114.7
111.6
77.4
77.0
76.7
55.2
47.7
22.2
NH
N
O
S
3e
200
190
180
170
160
150
140
130
120
110
100
90
80
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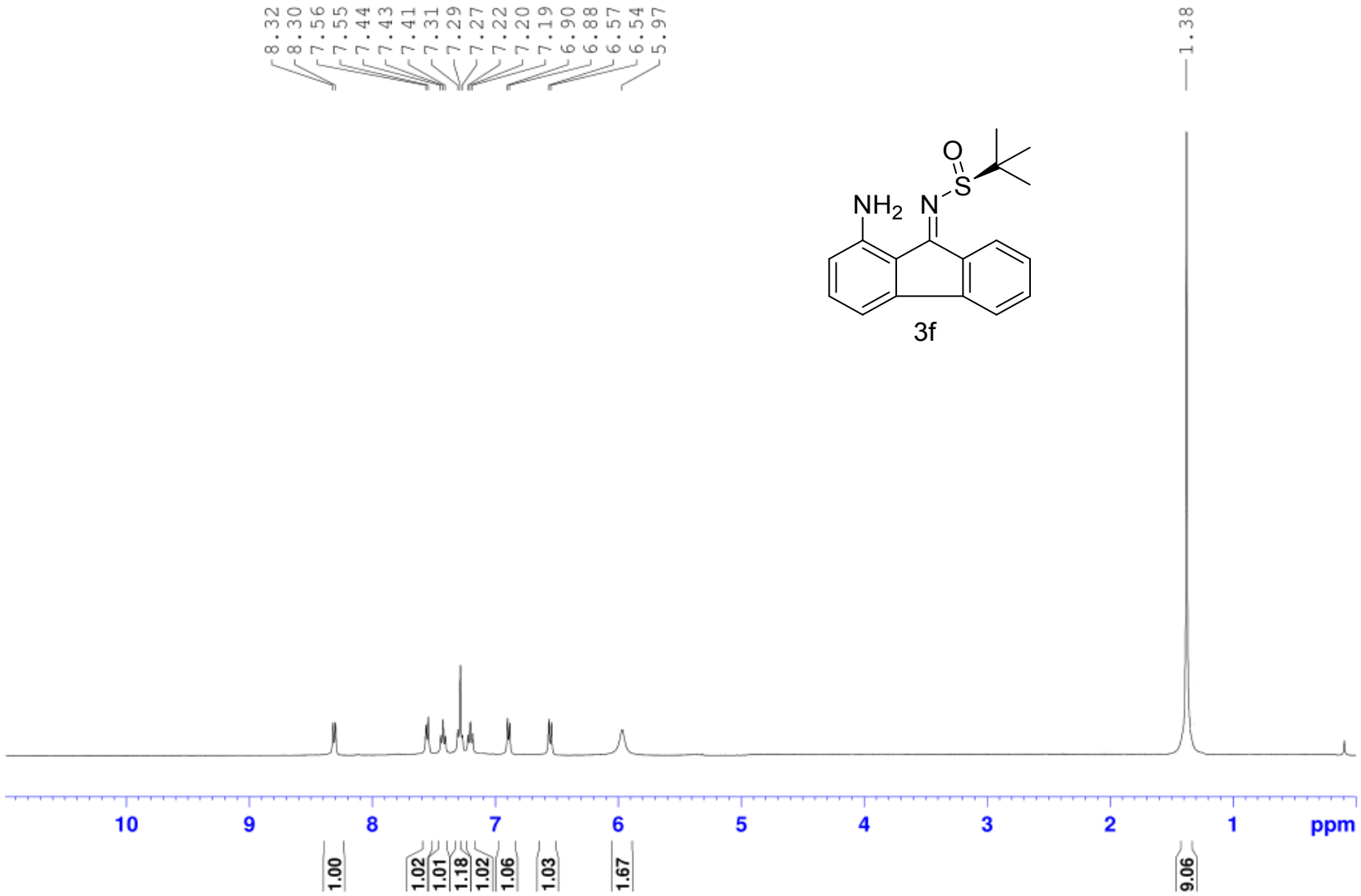
60
50
40
30
20
ppm

^{1}H NMR: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8.30
7.56
7.55
7.44
7.43
7.41
7.31
7.29
7.27
7.22
7.20
7.19
6.90
6.88
6.57
6.54
5.97
1.38
O
S
NH2
N
3f
10
9
8
7
6
5
4
3
2
1
ppm
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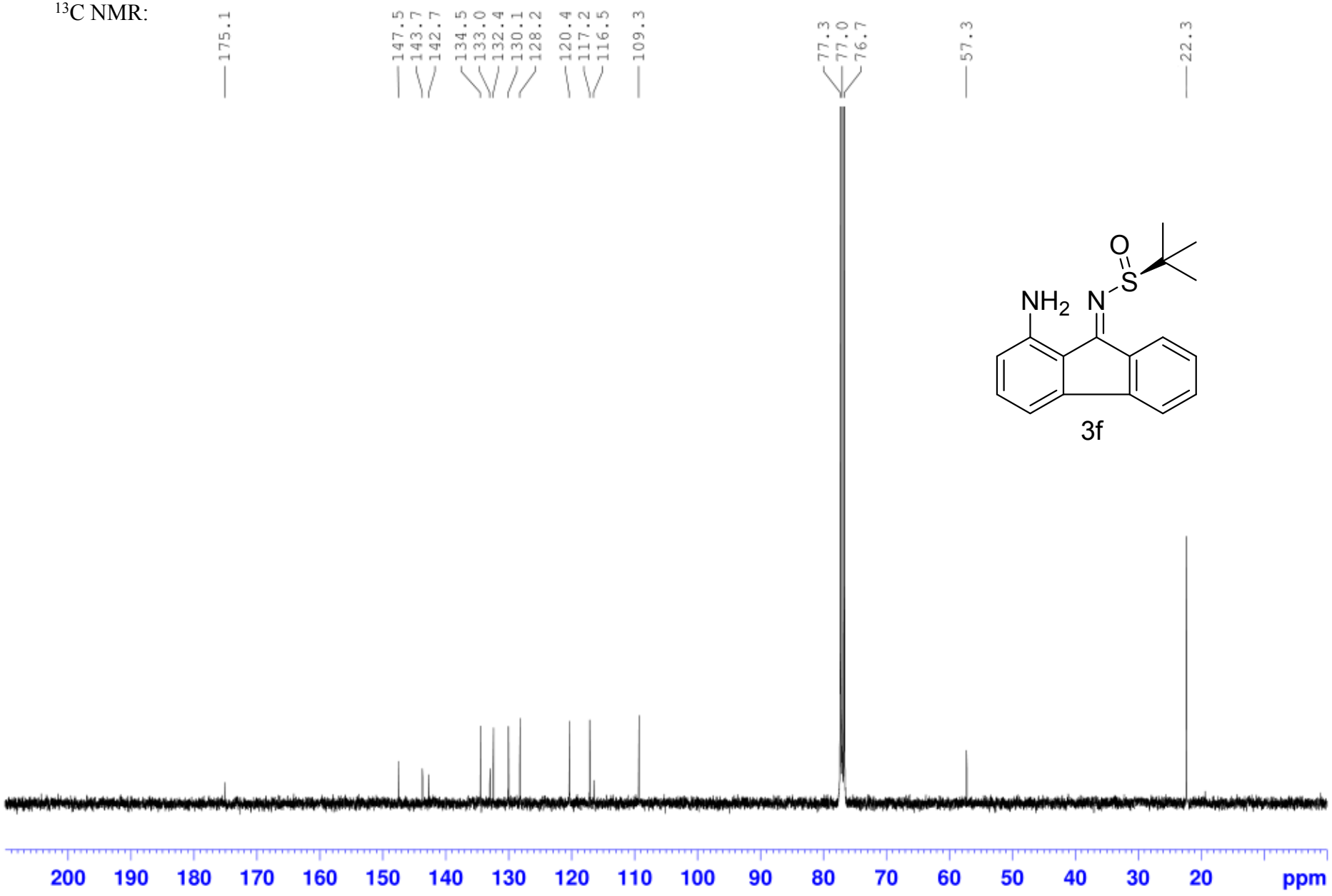
1.02
1.01
1.18
1.02
1.06
1.03
1.67
9.06

^{13}C NMR: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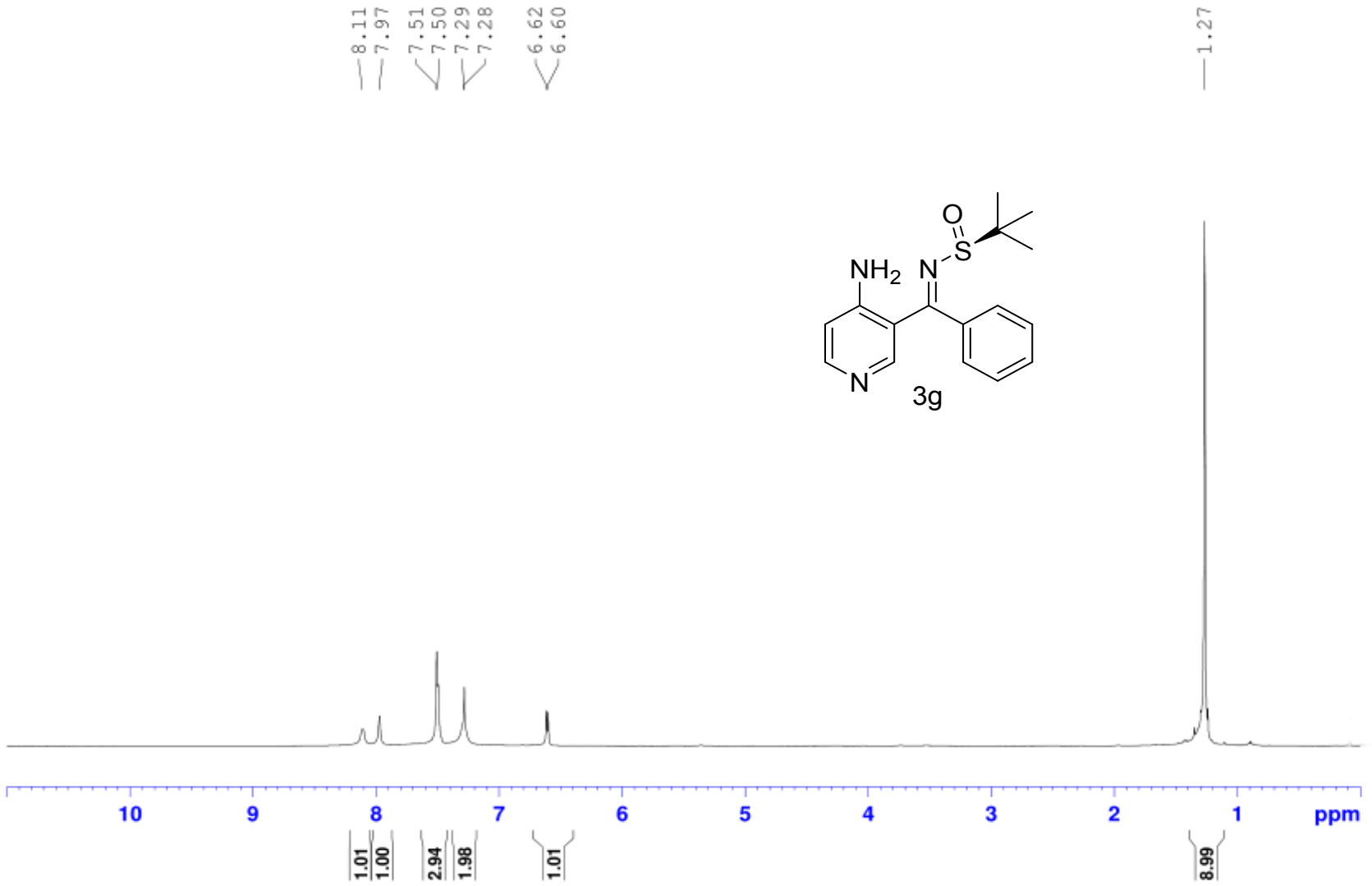
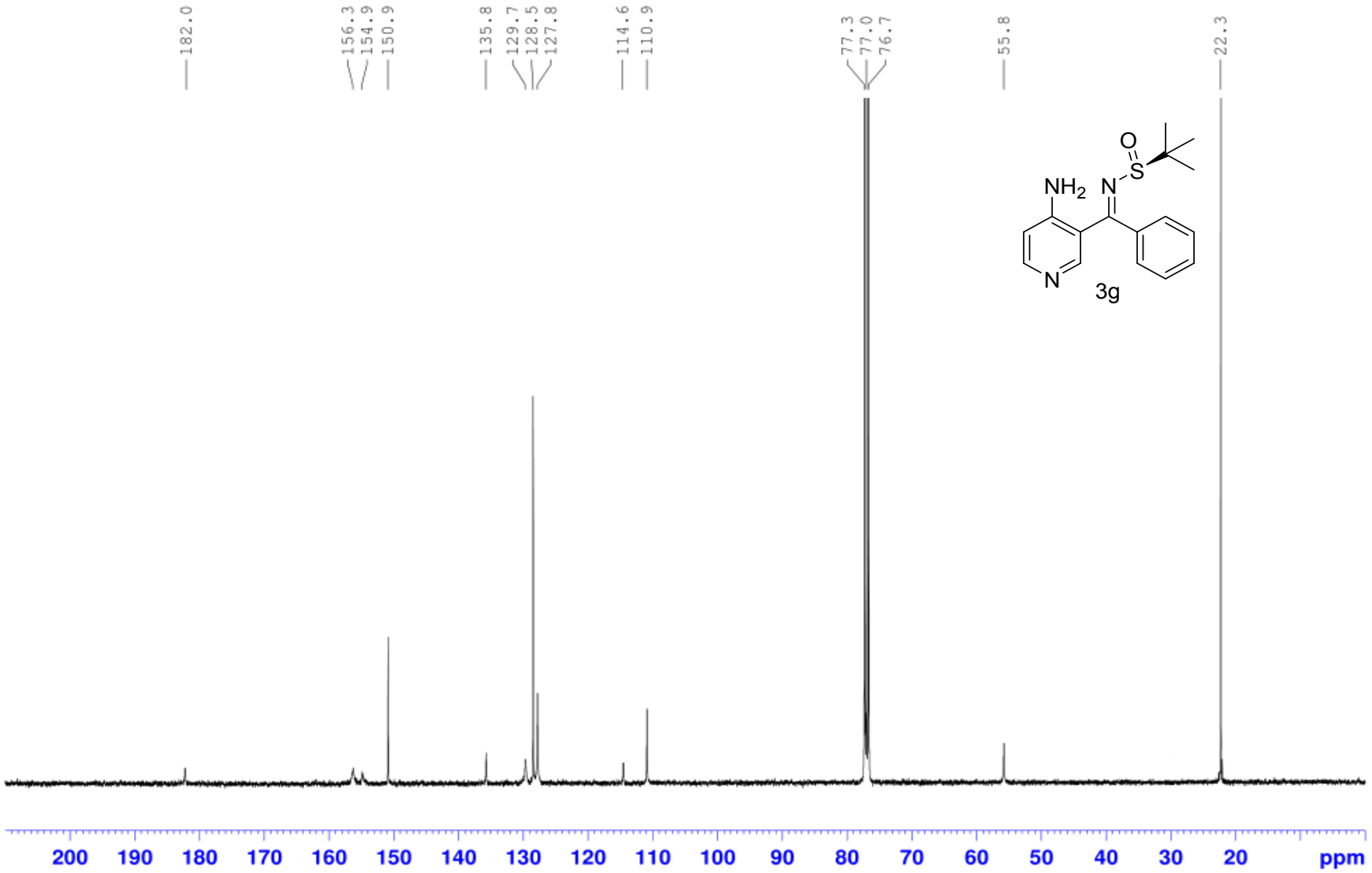
147.5
143.7
142.7
134.5
133.0
132.4
130.1
128.2
120.4
117.2
116.5
109.3
77.3
77.0
76.7
57.3
22.3
O
S
NH2
N
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

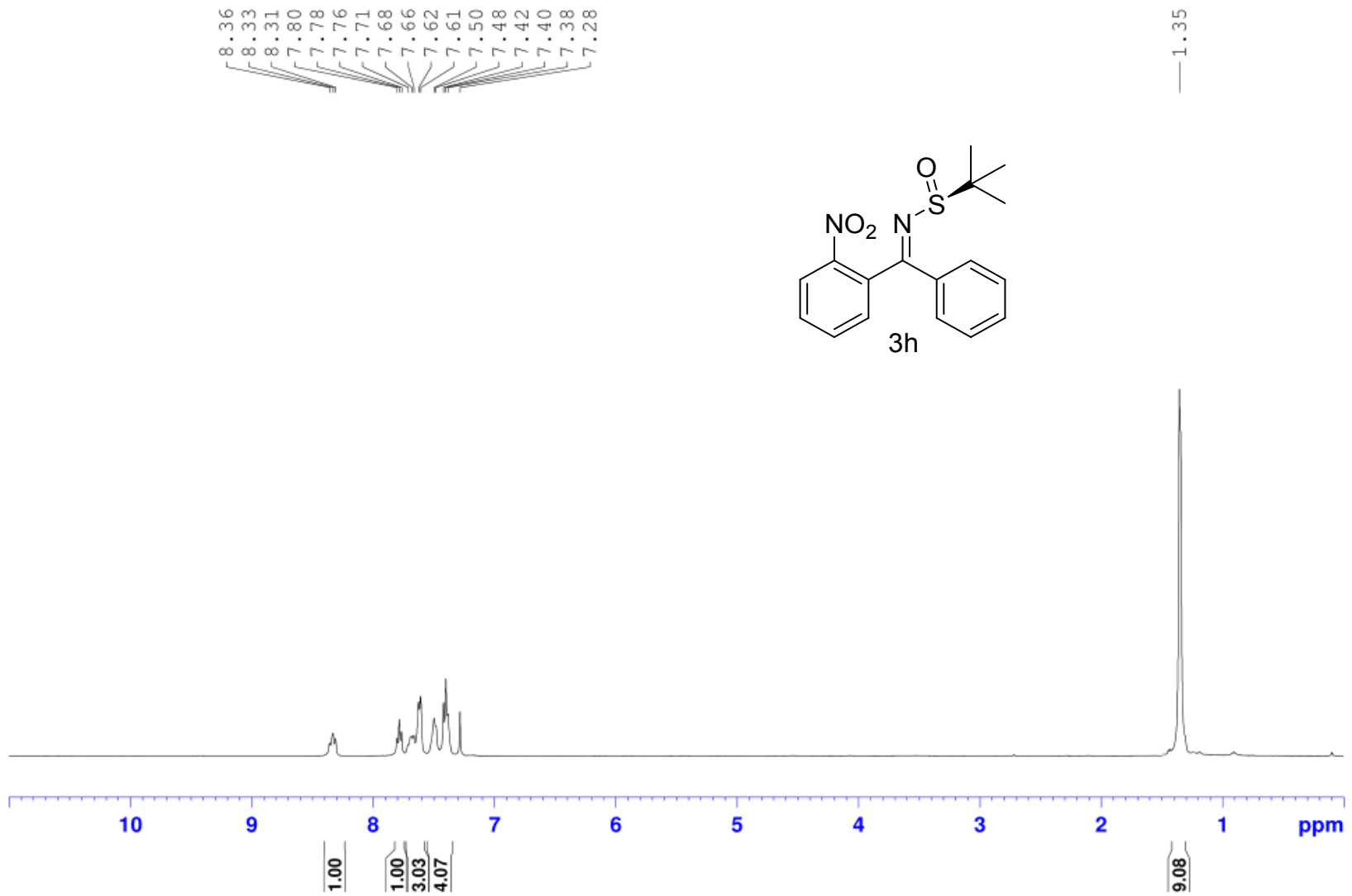
^{1}H NMR:


8.11
7.97
7.51
7.50
7.29
7.28
6.62
6.60
1.27
O
S
NH2
N
N
3g
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.00
2.94
1.98
1.01
8.99

^{13}C NMR:


182.0
156.3
154.9
150.9
135.8
129.7
128.5
127.8
114.6
110.9
77.3
77.0
76.7
55.8
22.3
NH2
N
O
S
N
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

^{1}H NMR:


8.36
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8.31
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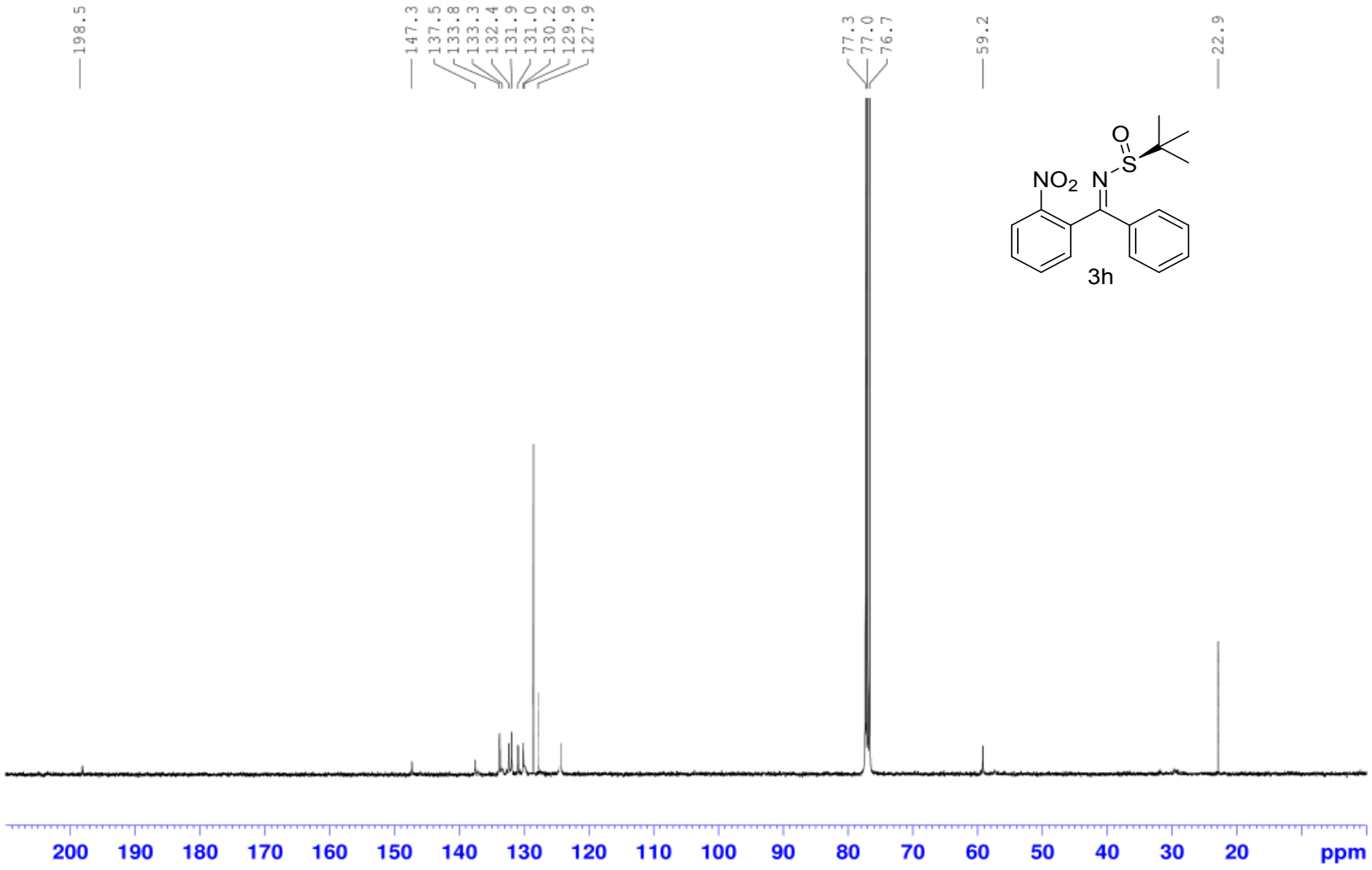
7.78
7.76
7.71
7.68
7.66
7.62
7.61
7.50
7.48
7.42
7.40
7.38
7.28
1.35
O
S
NO2
N
3h
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
3.03
4.07
9.08

^{13}C NMR: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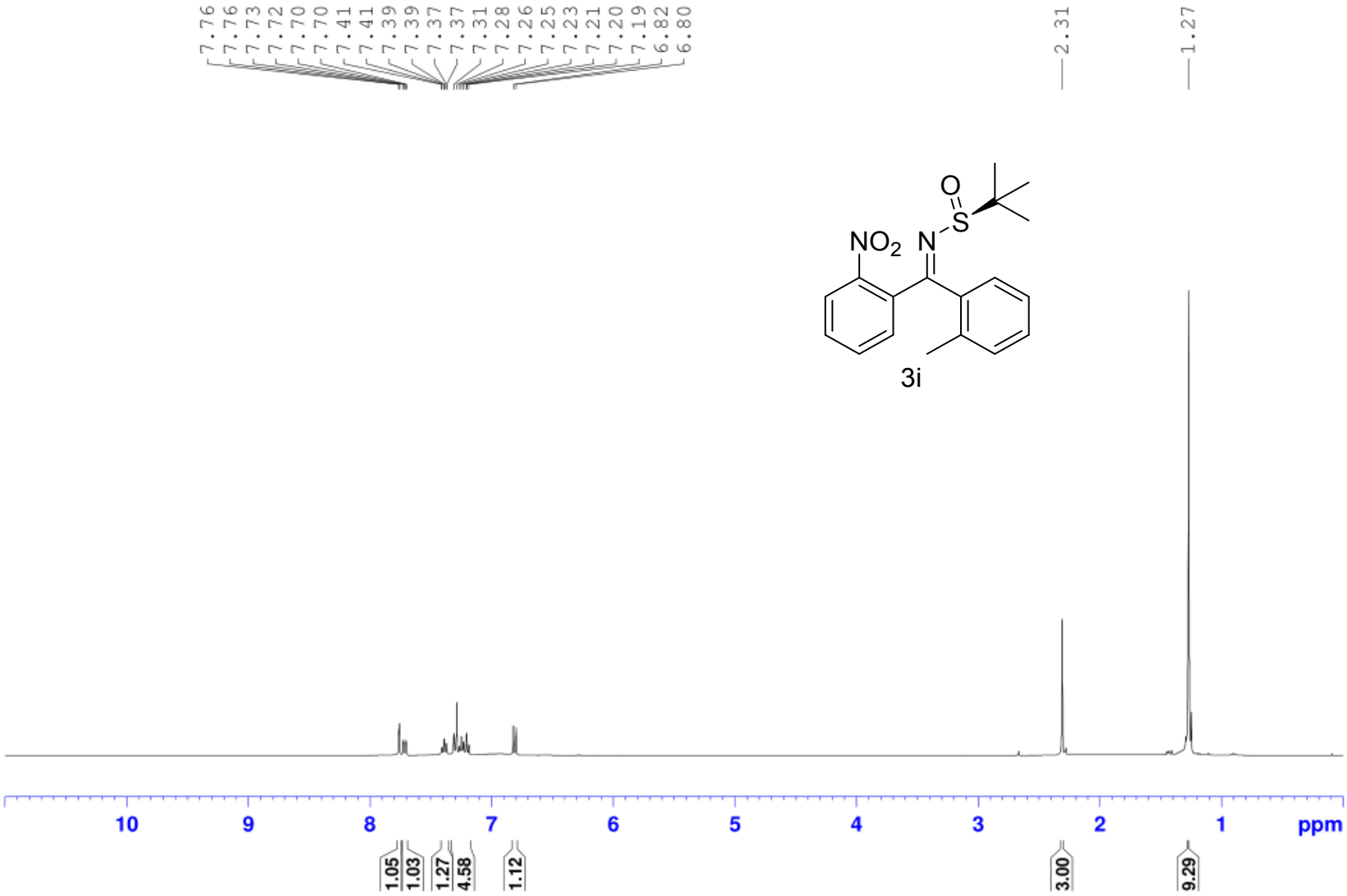
137.5
133.8
133.3
132.4
131.9
131.0
130.2
129.9
127.9
77.3
77.0
76.7
59.2
22.9
NO2
N
O
S
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

^{1}H NMR: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7.70
7.41
7.41
7.39
7.39
7.37
7.37
7.31
7.28
7.26
7.25
7.23
7.21
7.20
7.19
6.82
6.80
2.31
1.27
O
S
NO2
N
3i
10
9
8
7
6
5
4
3
2
1
ppm
1.05
1.03
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1.12
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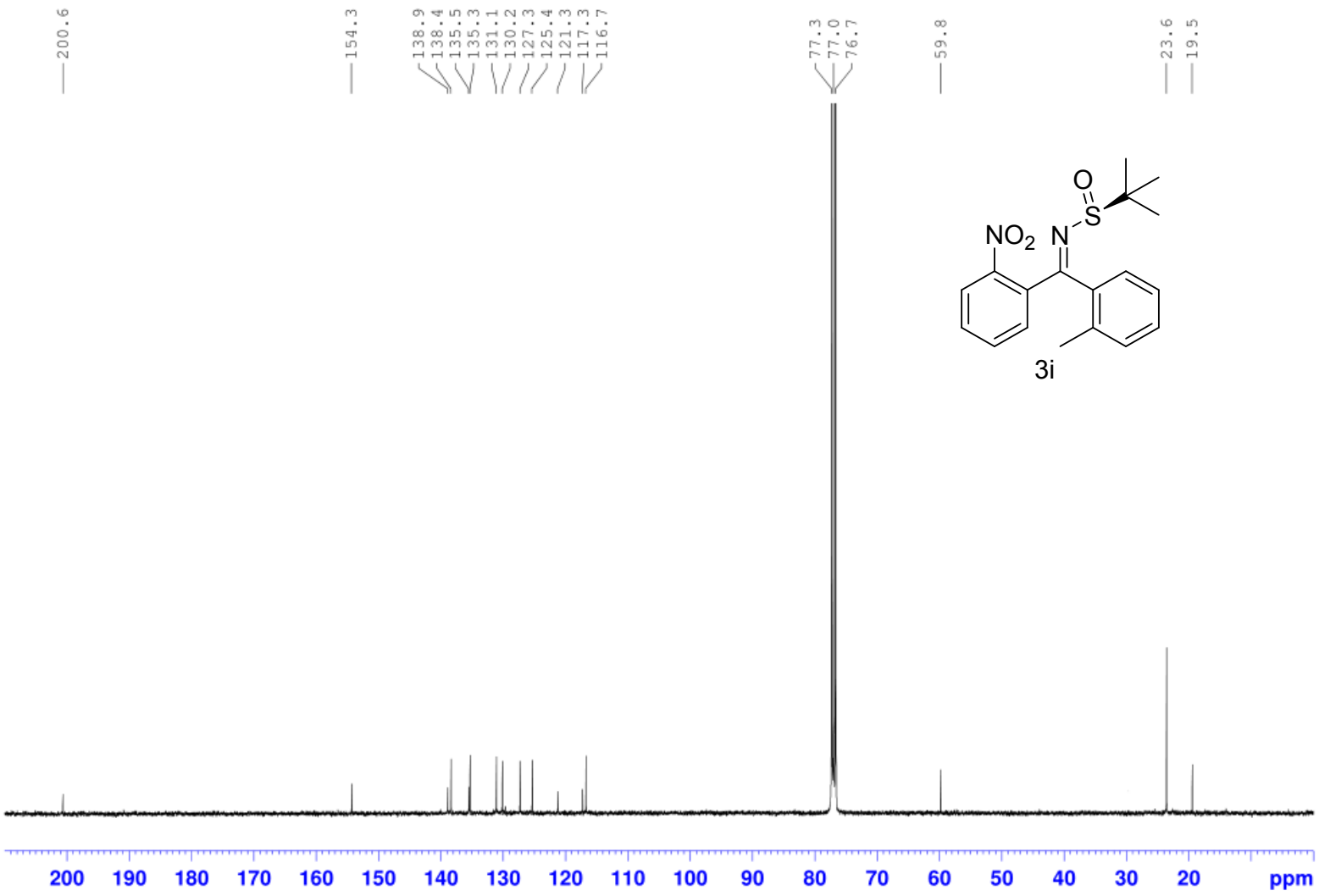
9.29

^{13}C NMR: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154.3
138.9
138.4
135.5
135.3
131.1
130.2
127.3
125.4
121.3
117.3
116.7
77.3
77.0
76.7
59.8
23.6
19.5
O
S
NO2
N
3i
200
190
180
170
160
150
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130
120
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100
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50
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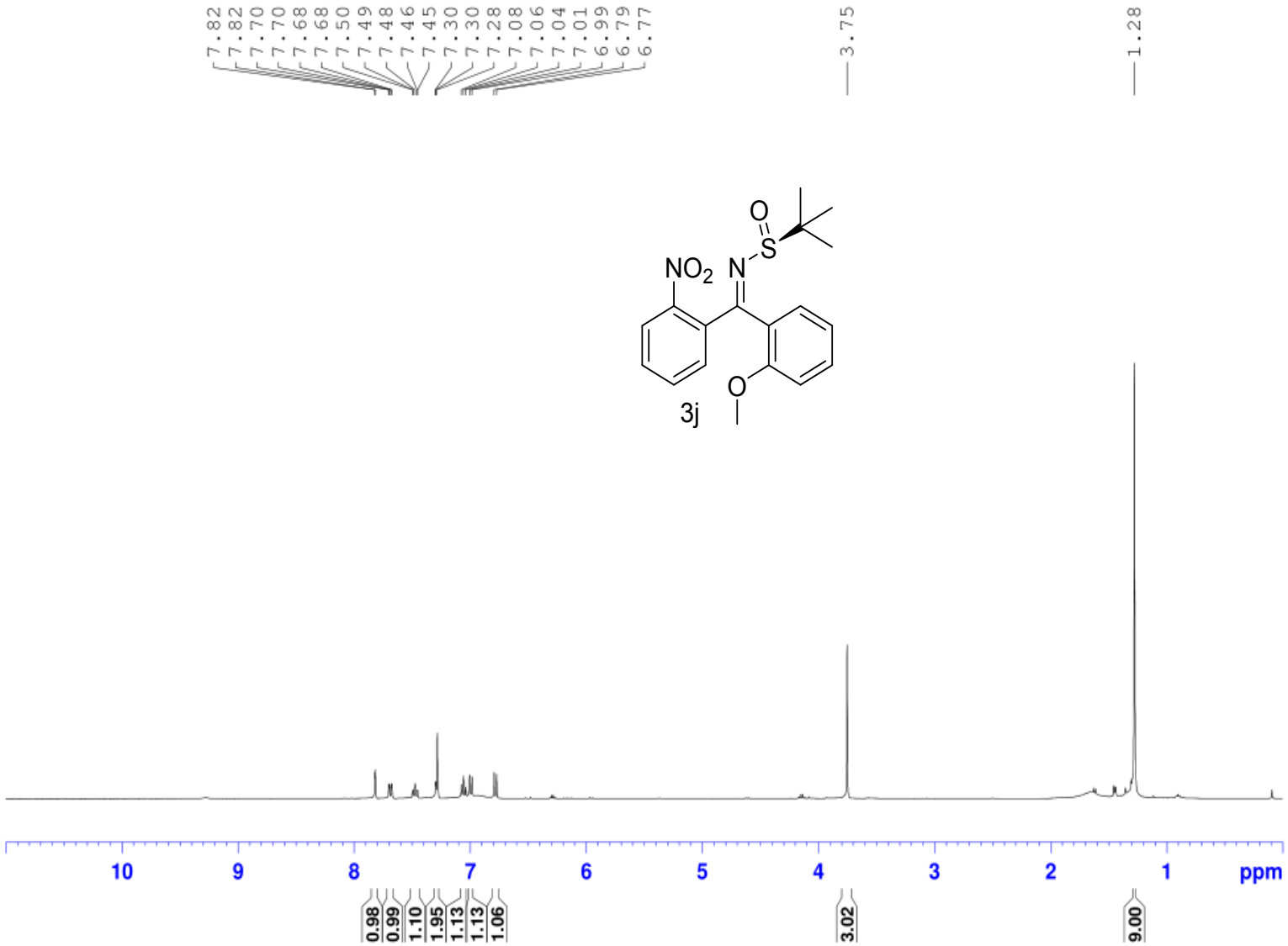
30
20
ppm

^{1}H NMR: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7.68
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7.49
7.48
7.46
7.45
7.30
7.30
7.28
7.08
7.06
7.04
7.01
6.99
6.79
6.77
3.75
1.28
O
S
NO2
N
O
3j
10
9
8
7
6
5
4
3
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ppm
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1.95
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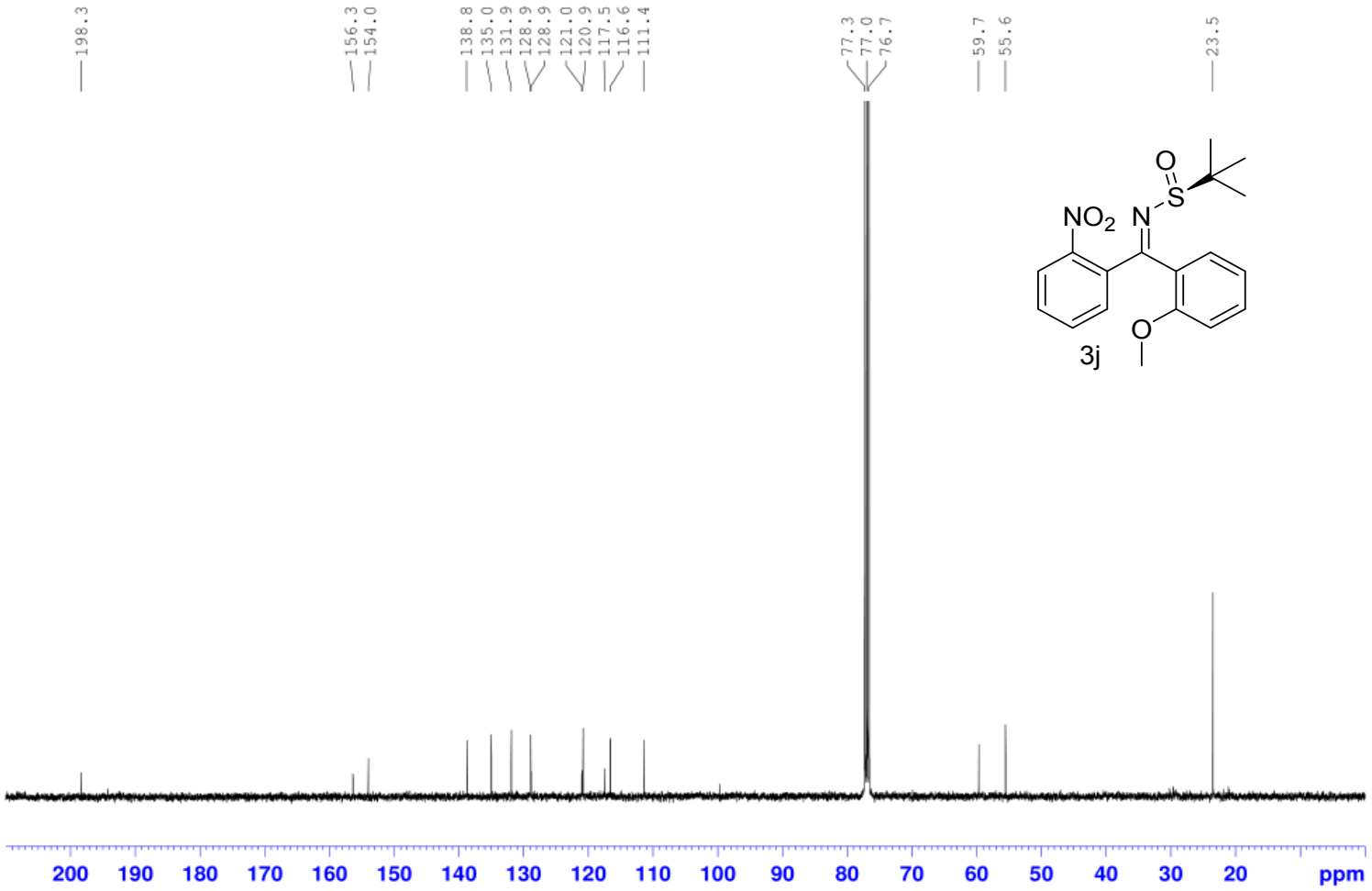
1.13
1.06
3.02
9.00

^{13}C NMR: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154.0
138.8
135.0
131.9
128.9
128.9
121.0
120.9
117.5
116.6
111.4
77.3
77.0
76.7
59.7
55.6
23.5
O
S
N
NO2
O
3j
200
190
180
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150
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120
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100
90
80
70
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50
40
30
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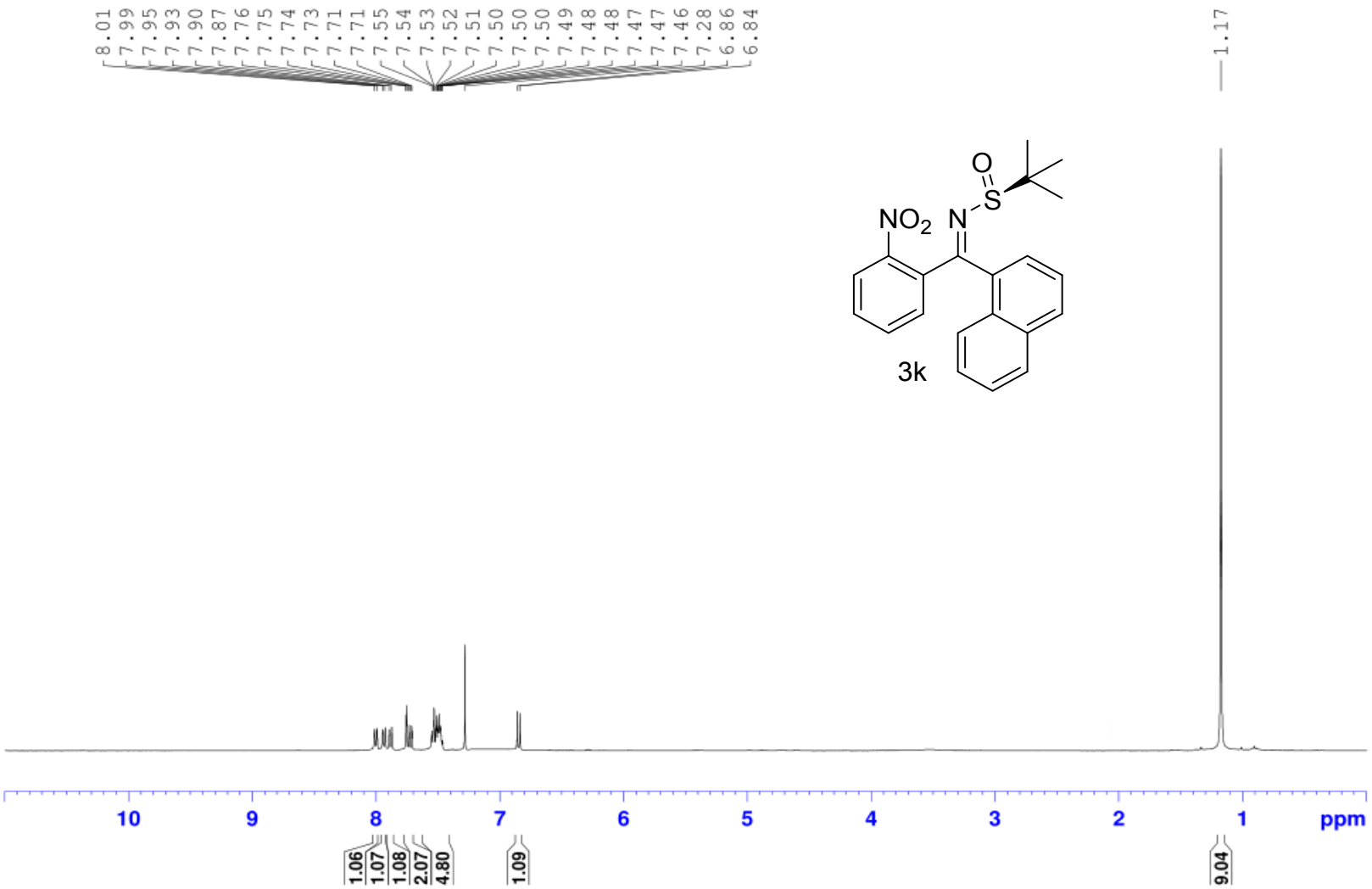
ppm

^{1}H NMR: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7.73
7.71
7.71
7.55
7.54
7.53
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.28
6.86
6.84
1.17
O
S
N
NO2
3k
10
9
8
7
6
5
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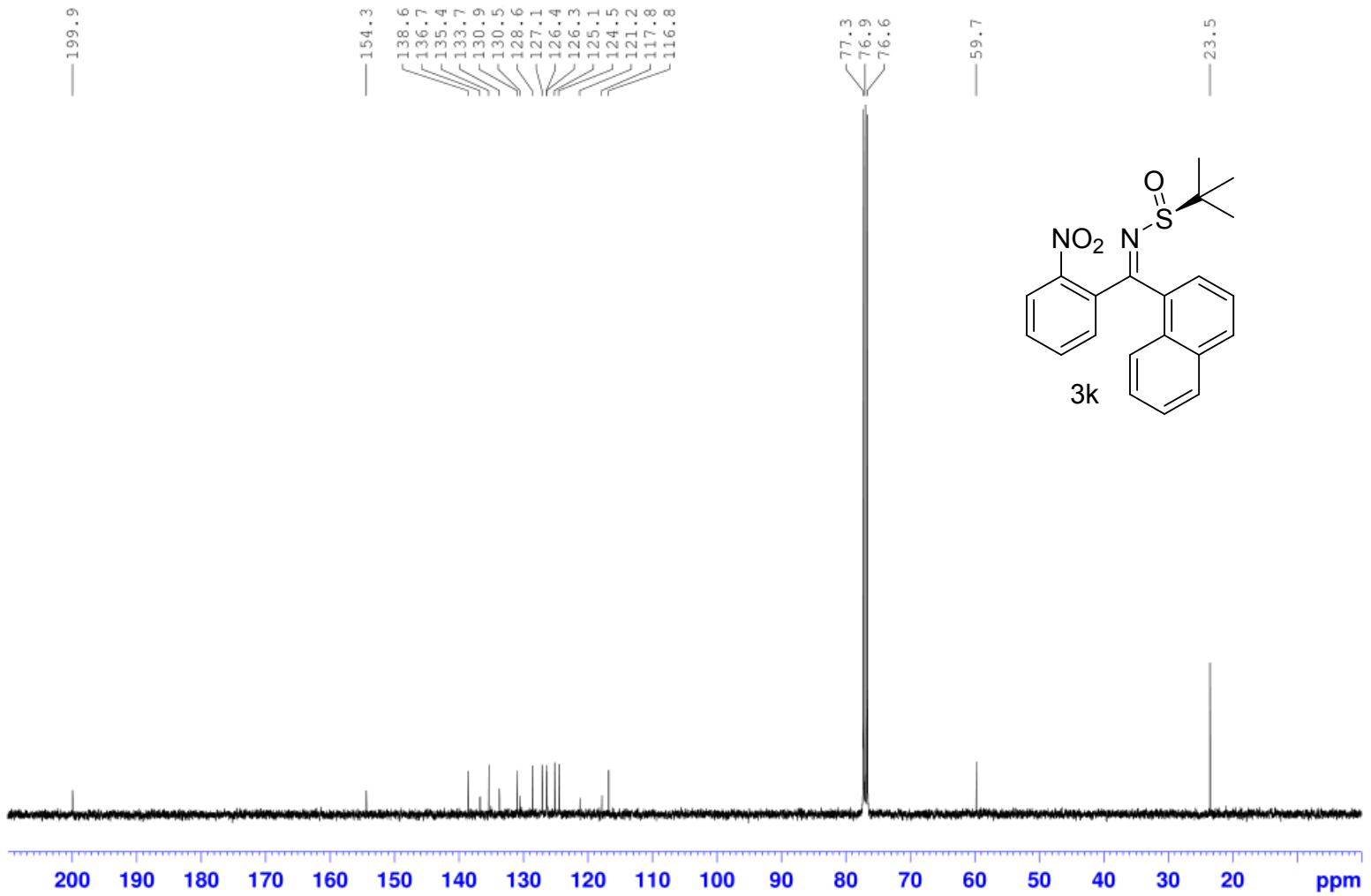
ppm
1.06
1.07
1.08
2.07
4.80
1.09
9.04

^{13}C NMR: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136.7
135.4
133.7
130.9
130.5
128.6
127.1
126.4
126.3
125.1
124.5
121.2
117.8
116.8
77.3
76.9
76.6
59.7
23.5
O
S
NO2
N
3k
200
190
180
170
160
150
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120
110
100
90
80
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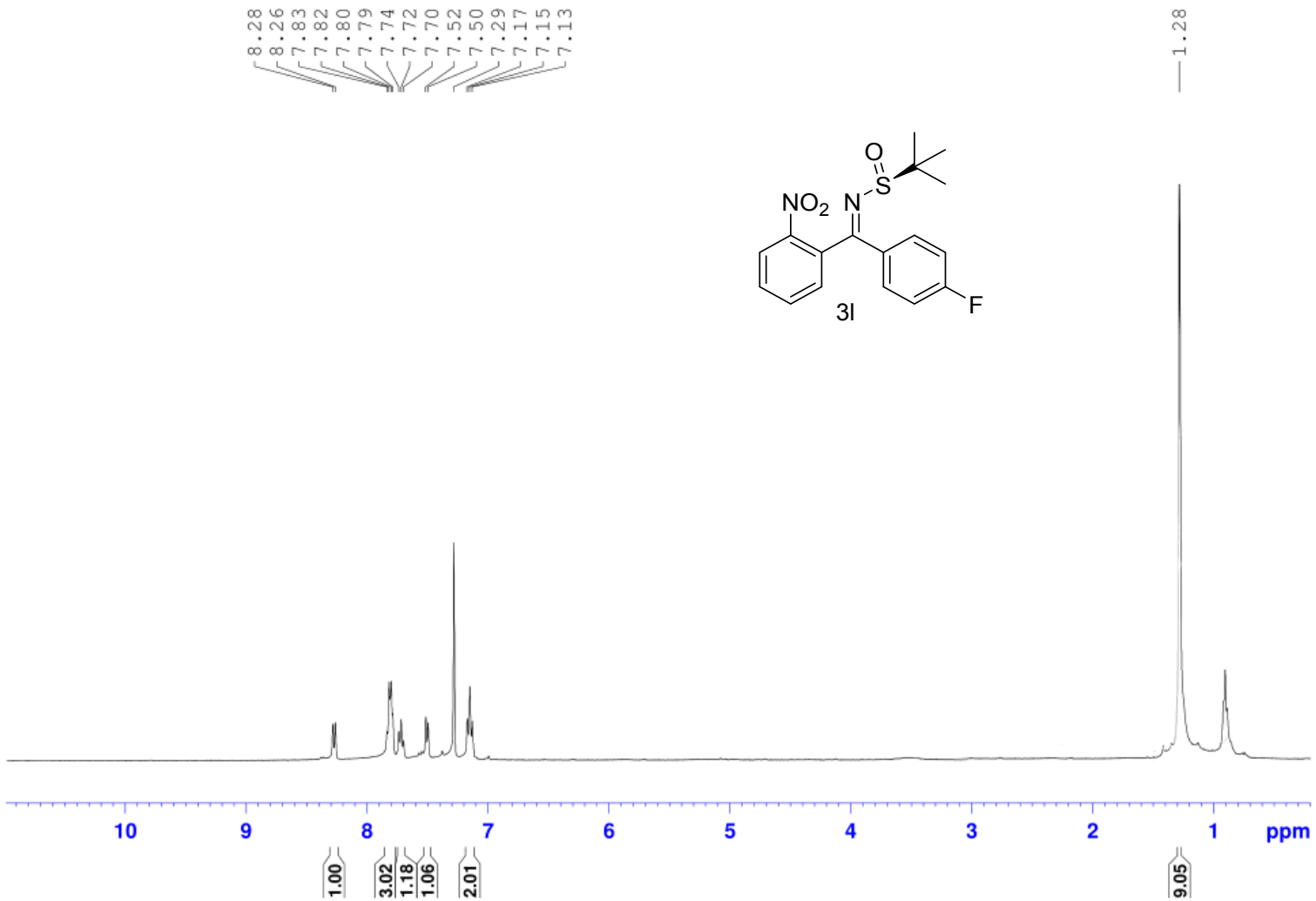
50
40
30
20
ppm

^{1}H NMR: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7.72
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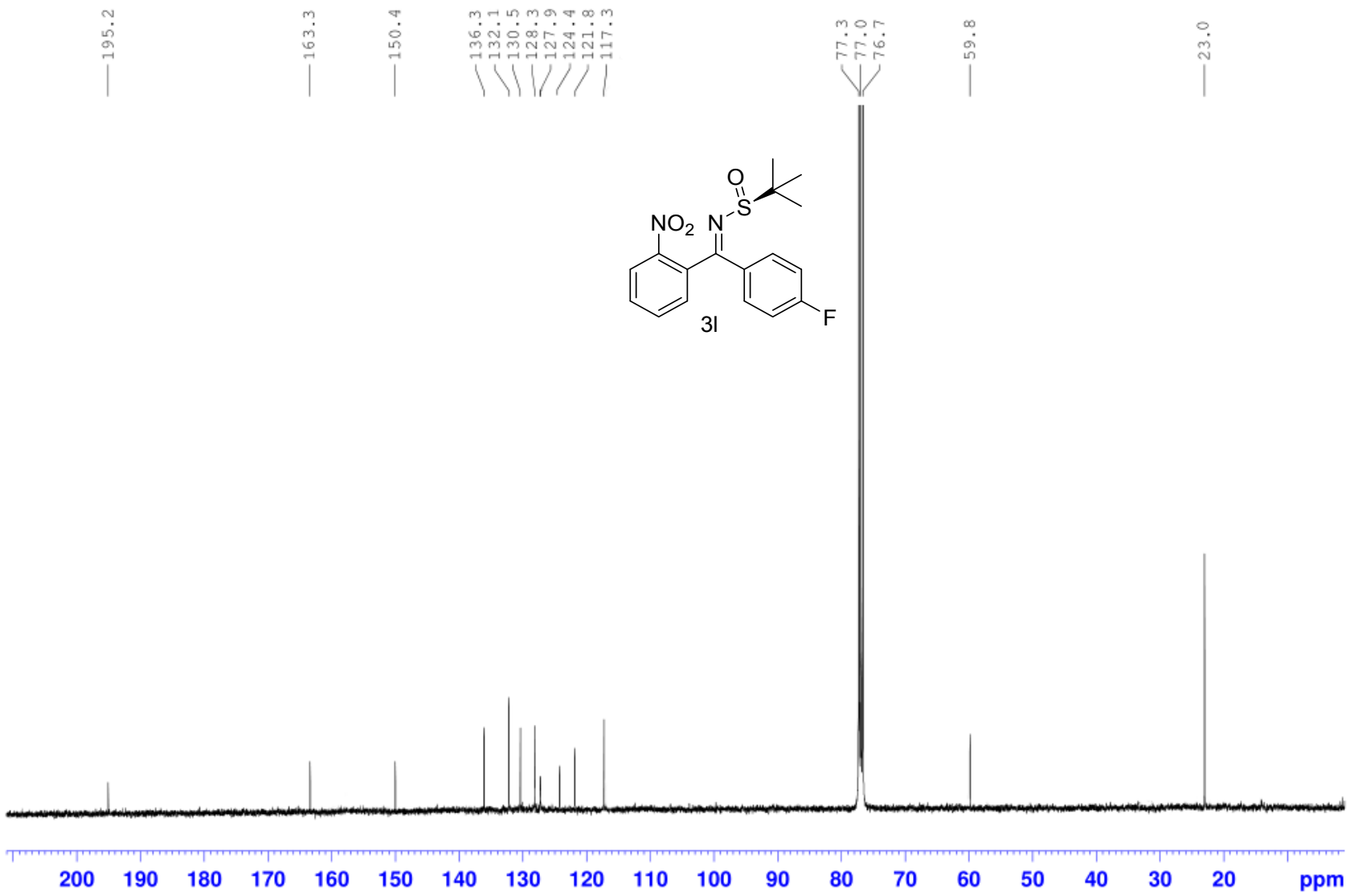
7.52
7.50
7.29
7.17
7.15
7.13
1.28
O
S
NO2
N
F
3l
10
9
8
7
6
5
4
3
2
1
ppm
1.00
3.02
1.18
1.06
2.01
9.05

^{13}C NMR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130.5
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127.9
124.4
121.8
117.3
77.3
77.0
76.7
59.8
23.0
O
S
N
NO2
F
3l
200
190
180
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120
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100
90
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50
40
30
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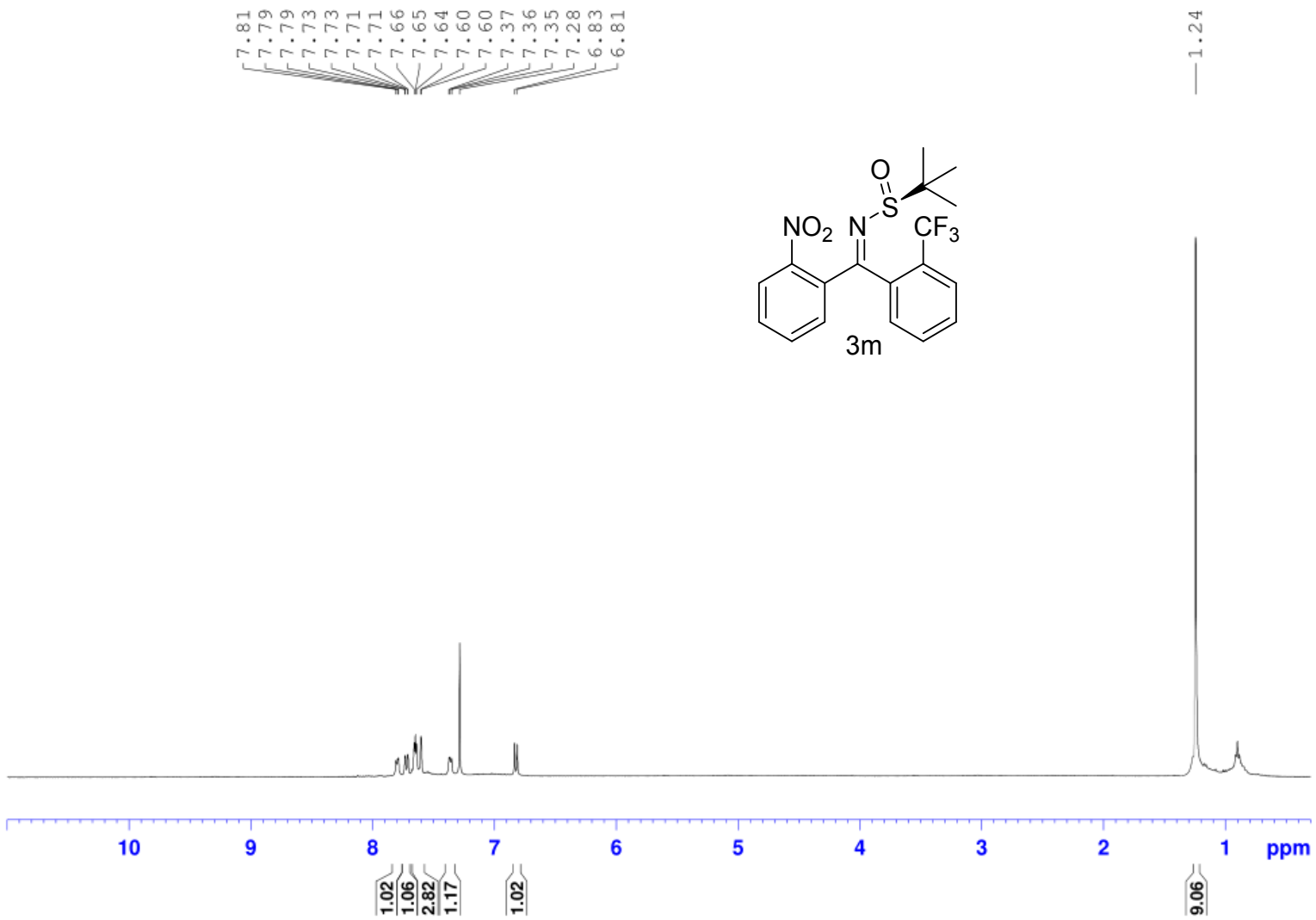
ppm

^{1}H NMR: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7.64
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7.60
7.37
7.36
7.35
7.28
6.83
6.81
1.24
O
S
NO2
N
CF3
3m
10
9
8
7
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5
4
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2
1
ppm
1.02
1.06
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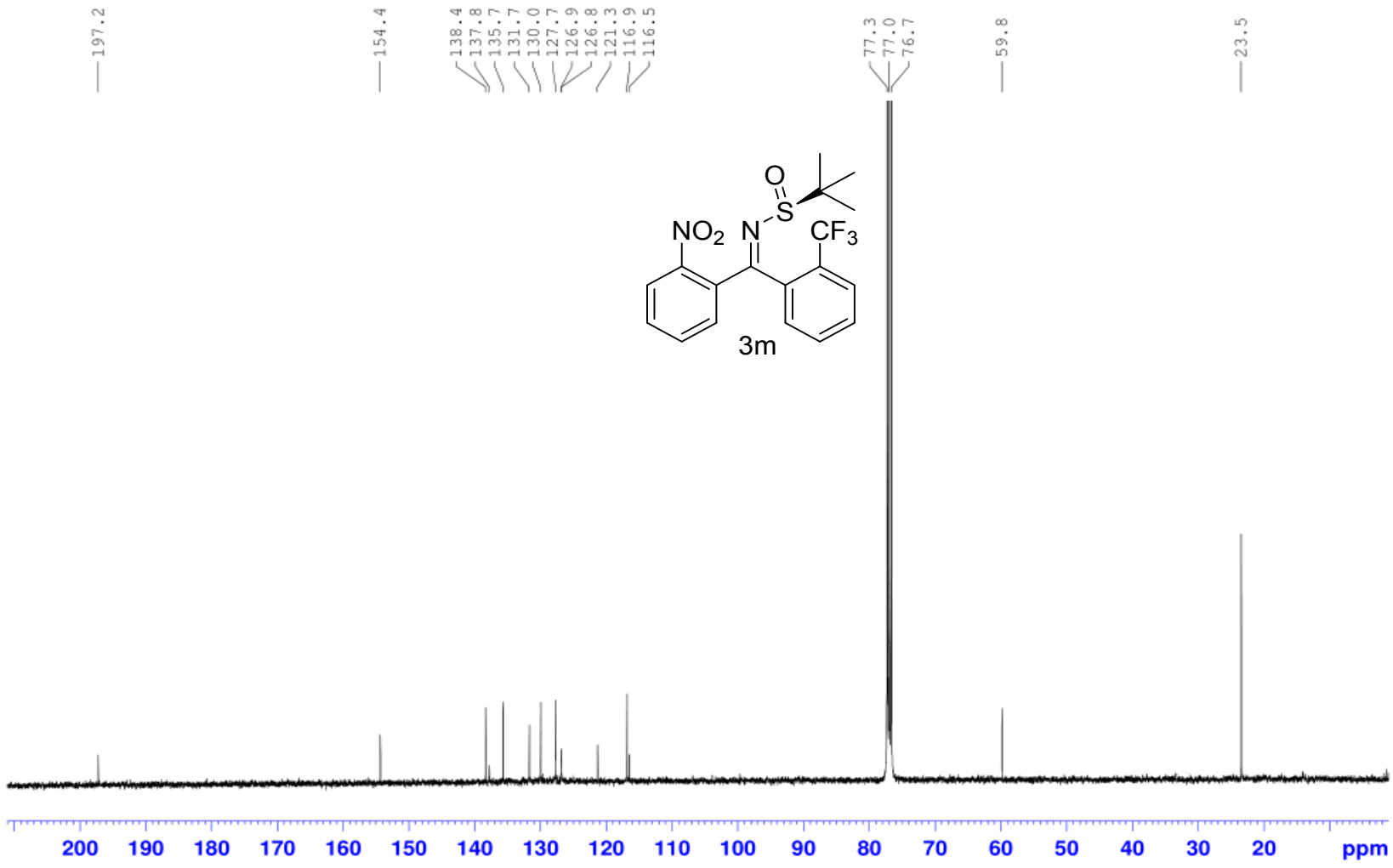
1.17
1.02
9.06

^{13}C NMR: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138.4
137.8
135.7
131.7
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127.7
126.9
126.8
121.3
116.9
116.5
77.3
77.0
76.7
59.8
23.5
O
S
NO2
N
CF3
3m
200
190
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170
160
150
140
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120
110
100
90
80
70
60
50
40
30
20
ppm