Supplementary Material (ESI) for Chemical Communications

Supporting Information

Copper-Mediated Methylthiolation of Aryl Halides with DMSO

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Experimental

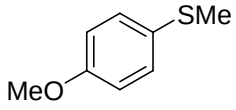
1. General experimental details

Chemicals were either purchased or purified by standard techniques without special instructions. ^{1}H NMR and ^{13}C NMR spectra were measured on a 500 MHz spectrometer (^{1}H 500 MHz, ^{13}C 125 MHz), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts (δ) are given in ppm relative to TMS, the coupling constants J are given in Hz.

General procedure for CuBr-catalyzed methylthiolation of aryl iodines with DMSO: Under air, a sealed tube was charged with aryl iodine (0.4 mmol), CuBr (5.8 mg, 10 mol %), ZnF_2 (0.8 mmol, 2 equiv.), and DMSO (2 mL). The reaction tube was kept stirring at 150 ^{o}C for 36 h. After the completion of the reaction, as monitored by TLC, brine was added (10 mL), and the reaction mixture was extracted with ethyl acetate (3×5 mL). The ethyl acetate extracts were concentrated in vacuo, and the residue was purified by flash column chromatography on silica gel to give the product.

2. Experimental characterization data for compounds

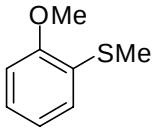
(4-methoxyphenyl)(methyl)sulfane (3a)[1]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.27 (d, J = 8.5 Hz, 2H), 6.85 (d, J = 9.0 Hz, 2H), 3.78 (s, 3H), 2.44 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ 158.2, 130.2, 128.8, 114.6, 55.4, 18.1.

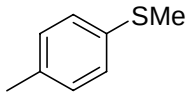
(2-methoxyphenyl)(methyl)sulfane (3b)[2]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.16-7.12 (m, 2H), 6.97-6.94 (m, 1H), 6.83 (d, J = 8.0 Hz, 1H), 3.88 (s, 3H), 2.42 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ 156.3, 126.8, 126.2, 125.9, 121.2, 110.1, 55.8, 14.7.

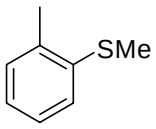
methyl(*p*-tolyl)sulfane (3c)[3]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.18 (d, J = 8.5 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H), 2.31 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ 135.1, 134.7, 129.6, 127.4, 20.9, 16.6.

methyl(*o*-tolyl)sulfane (3d)[4]



1H NMR ($CDCl_3$, 500 MHz): δ 7.22-7.12 (m, 3H), 7.07-7.03 (m, 1H), 2.45 (s, 3H), 2.33 (s, 3H).

^{13}C NMR ($CDCl_3$, 125 MHz): δ 137.7, 135.8, 129.8, 126.5, 124.6, 19.9, 15.3.

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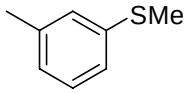
[1] Y. Jiang, Y. Qin, S. Xie, X. Zhang, J. Dong and D. Ma, *Org. Lett.,* 2009, **11**, 5250.

[2] J. P. Dunne, M. Bockmeyer, M. Tacke, J. P. Dunne, M. Bockmeyer and M. Tacke, *Eur. J. Inorg. Chem.,* 2003, 458.

[3] G. Hua and J. D. Woollins, *Tetrahedron Lett.,* 2007, **48**, 3677.

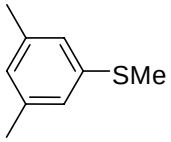
[4] T. Klis, J. Serwatowski, G. Wesela-Bauman and M. Zadrozna, *Tetrahedron Lett.,* 2010, **51**, 1685.

methyl(*m*-tolyl)sulfane (3e)[5]



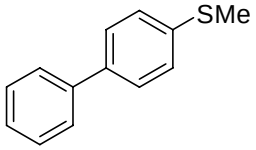
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.19-7.15 (m, 1H), 7.07-7.05 (m, 2H), 6.94 (d, J = 7.5 Hz, 1H), 2.47 (s, 3H), 2.32 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 138.6, 138.2, 128.7, 127.3, 125.9, 123.7, 21.4, 15.9.

(3,5-dimethylphenyl)(methyl)sulfane (3f)[6]



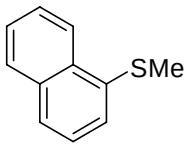
^{1}H NMR ($CDCl_3$, 500 MHz): δ 6.88 (s, 2H), 6.77 (s, 1H), 2.45 (s, 3H), 2.28 (s, 6H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 138.4, 137.9, 127.0, 124.3, 21.2, 15.8.

biphenyl-4-yl(methyl)sulfane (3g)[7]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.58-7.56 (m, 2H), 7.54-7.52 (m, 2H), 7.45-7.42 (m, 2H), 7.35-7.32 (m, 3H), 2.53 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 138.1, 137.6, 128.8, 127.5, 127.2, 126.9, 126.8, 15.9.

methyl(naphthalen-1-yl)sulfane (3h)[8]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.27 (d, J = 8.5 Hz, 1H), 7.82-7.80 (m, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.54-7.47 (m, 2H), 7.42-7.35 (m, 2H), 2.54 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 135.8, 133.7, 131.7, 128.6, 126.3, 126.2, 125.9, 125.7, 124.3, 123.7, 16.2.

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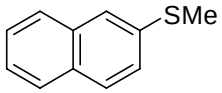
[5] M. G. Cabiddu, S. Cabiddu, E. Cadoni, S. D. Montis, C. Fattuoni and S. Melis, *Tetrahedron,* 2004, **60**, 3915.

[6] R. E. del Río, B. Wang, S. Achab and L. Bohé, *Org. Lett*., 2007, **9**, 2265.

[7] P. Nun, J. Martinez and F. Lamaty, *Synlett,* 2009, 1761.

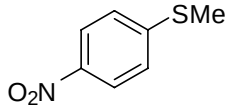
[8] L. C. Schmidt, J. E. Argüello and A. B. Peñéñory, *J. Org. Chem*., 2007, **72**, 2936.

methyl(naphthalen-2-yl)sulfane (3i)[9]



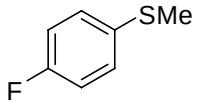
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.77 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.60-7.59 (m, 1H), 7.47-7.44 (m, 1H), 7.42-7.36 (m, 2H), 2.58 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 136.1, 133.9, 131.3, 128.2, 127.7, 126.8, 126.6, 125.7, 125.2, 123.4, 15.8.

methyl(4-nitrophenyl)sulfane (3j)[10]



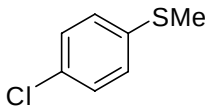
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.14 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.56 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 148.9, 144.8, 125.0, 123.9, 14.8.

(4-fluorophenyl)(methyl)sulfane (3k)[11]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.26-7.24 (m, 2H), 7.01-6.98 (m, 2H), 2.46 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 161.1 (d, *J* = 243.4 Hz), 133.3 (d, *J* = 3.2 Hz), 129.3 (d, *J* = 7.7 Hz), 115.9 (d, *J* = 21.9 Hz), 17.4.

(4-chlorophenyl)(methyl)sulfane (3l)[12]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.26-7.24 (m, 2H), 7.19-7.16 (m, 2H), 2.47 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 137.0, 130.9, 128.9, 127.9, 16.1.

methyl(3-(trifluoromethyl)phenyl)sulfane (3m)[13]

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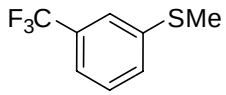
[9] J. S. Yadav, B. V. Subba Reddy, C. Srinivas and P. Srihari, *Synlett,* 2001, 854.

[10] S. C. Sousa and A. A. C. Fernandes, *Tetrahedron Lett.,* 2009, **50**, 6872.

[11] J. Ermert, T. Ludwig, R. Gail and H. H. Coenen, *J. Organometal. Chem.,* 2007, **692**, 4084.

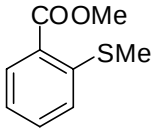
[12] R.Tang, P. Zhong and Q. Lin, *Synthesis,* 2007, 85.

[13] P. Hanson, R. A. A. J. Hendrickx and J. R. Lindsay Smith, *Org. Biomol. Chem.* 2008, **6**, 745.



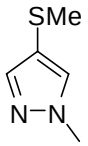
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.46 (s, 1H), 7.40-7.37 (m, 3H), 2.51 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 131.3 (q, J = 32.0 Hz), 129.4, 129.1, 123.9 (q, J = 270.9 Hz), 122.7 (q, J = 3.8 Hz), 121.6 (q, J = 3.7 Hz), 15.5.

methyl 2-(methylthio)benzoate (3n)[14]



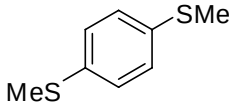
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.0 (d, J = 7.5 Hz, 1H), 7.49-7.46 (m, 1H), 7.28-7.26 (m, 1H), 7.17-7.14 (m, 1H), 3.92 (s, 3H), 2.46 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.9, 143.3, 132.5, 131.3, 126.8, 124.4, 123.4, 52.0, 15.6.

1-methyl-4-(methylthio)-1*H*-pyrazole (3o)



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.48 (s, 1H), 7.38 (s, 1H), 3.88 (s, 3H), 2.32 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 142.1, 132.4, 113.1, 39.1, 21.1.
IR (prism, cm^{-1}): 3055, 2950, 1669, 1519, 1436, 1266, 968.
HRMS (EI) Calcd for $C_5H_8N_2S$ (M^+) 128.0410, found 128.0408.

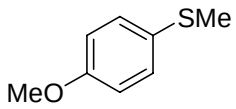
1,4-bis(methylthio)benzene (3p)[15]



^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.20 (s, 4H), 2.47 (s, 6H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 135.2, 127.7, 16.4.

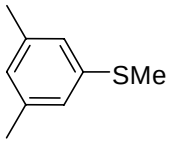
(4-methoxyphenyl)(methyl)sulfane (3a′)[1]

[14] S. C. A. Sousa and A. C. Fernandes, *Organometallics,* 2010, **29**, 1479.
[15] P. Gao, X. Feng, X. Yang, V. Enkelmann, M. Baumgarten and K. Müllen, *J. Org. Chem.,* 2008, **73**, 9207.



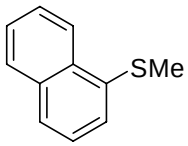
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.27 (d, J = 8.5 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 3.78 (s, 3H), 2.44 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 158.2, 130.2, 128.8, 114.6, 55.4, 18.1.

(3,5-dimethylphenyl)(methyl)sulfane (3f′)[6]



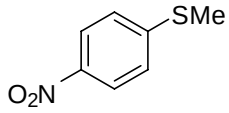
^{1}H NMR ($CDCl_3$, 500 MHz): δ 6.88 (s, 2H), 6.77 (s, 1H), 2.45 (s, 3H), 2.28 (s, 6H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 138.4, 137.9, 127.0, 124.3, 21.2, 15.8.

methyl(naphthalen-1-yl)sulfane (3h′)[8]



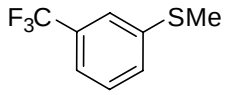
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.27 (d, J = 8.0 Hz, 1H), 7.83-7.81 (m, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.54-7.47 (m, 2H), 7.42-7.35 (m, 2H), 2.55 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 135.8, 133.7, 131.7, 128.6, 126.3, 126.2, 125.9, 125.7, 124.3, 123.7, 16.2.

methyl(4-nitrophenyl)sulfane (3j′)[10]



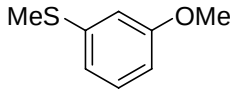
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.13 (d, J = 9.0 Hz, 2H), 7.29 (d, J = 9.0 Hz, 2H), 2.56 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 148.9, 144.7, 125.0, 123.9, 14.8.

methyl(3-(trifluoromethyl)phenyl)sulfane (3m′)[13]



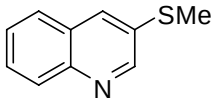
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.46 (s, 1H), 7.40-7.37 (m, 3H), 2.51 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 131.3 (q, J = 32.0 Hz), 129.4, 129.1, 123.9 (q, J = 270.9 Hz), 122.7 (q, J = 3.8 Hz), 121.6 (q, J = 3.7 Hz), 15.5.

(3-methoxyphenyl)(methyl)sulfane (3q)[16]



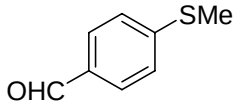
^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.20-7.17 (m, 1H), 6.84-6.79 (m, 2H), 6.68-6.66 (m, 1H), 3.78 (s, 3H), 2.47 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.9, 139.8, 129.6, 118.8, 112.1, 110.6, 55.2, 15.7.

3-(methylthio)quinoline (3r′)[17]



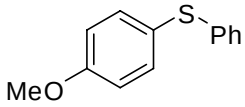
^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.79 (s, 1H), 8.05 (d, J = 8.5 Hz, 1H), 7.86 (s, 1H), 7.70 (d, J = 8.5 Hz, 1H), 7.64-7.61 (m, 1H), 7.52-7.50 (m, 1H), 2.58 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 149.9, 145.8, 132.7, 131.3, 129.3, 128.6, 128.3, 127.2, 126.7, 15.8.

4-(methylthio)benzaldehyde (3s′)[18]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 9.92 (s, 1H), 7.77 (d, J = 8.5 Hz, 1H), 7.32 (d, J = 8.5 Hz, 1H), 2.54 (s, 1H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 191.3, 147.9, 132.9, 130.0, 125.2, 14.7.

(4-methoxyphenyl)(phenyl)sulfane (5)[19]



^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.42-7.40 (m, 2H), 7.25-7.21 (m, 2H), 7.17-7.12 (m, 3H), 6.89 (d, J = 8.5 Hz, 2H), 3.82 (s, 3H).
^{13}C NMR ($CDCl_3$, 125 MHz): δ 159.8, 138.6, 135.4, 128.9, 128.2, 125.8, 124.3, 115.0, 55.4.

^{1}H NMR of **3**+**3′**: please see P59 in supporting information.

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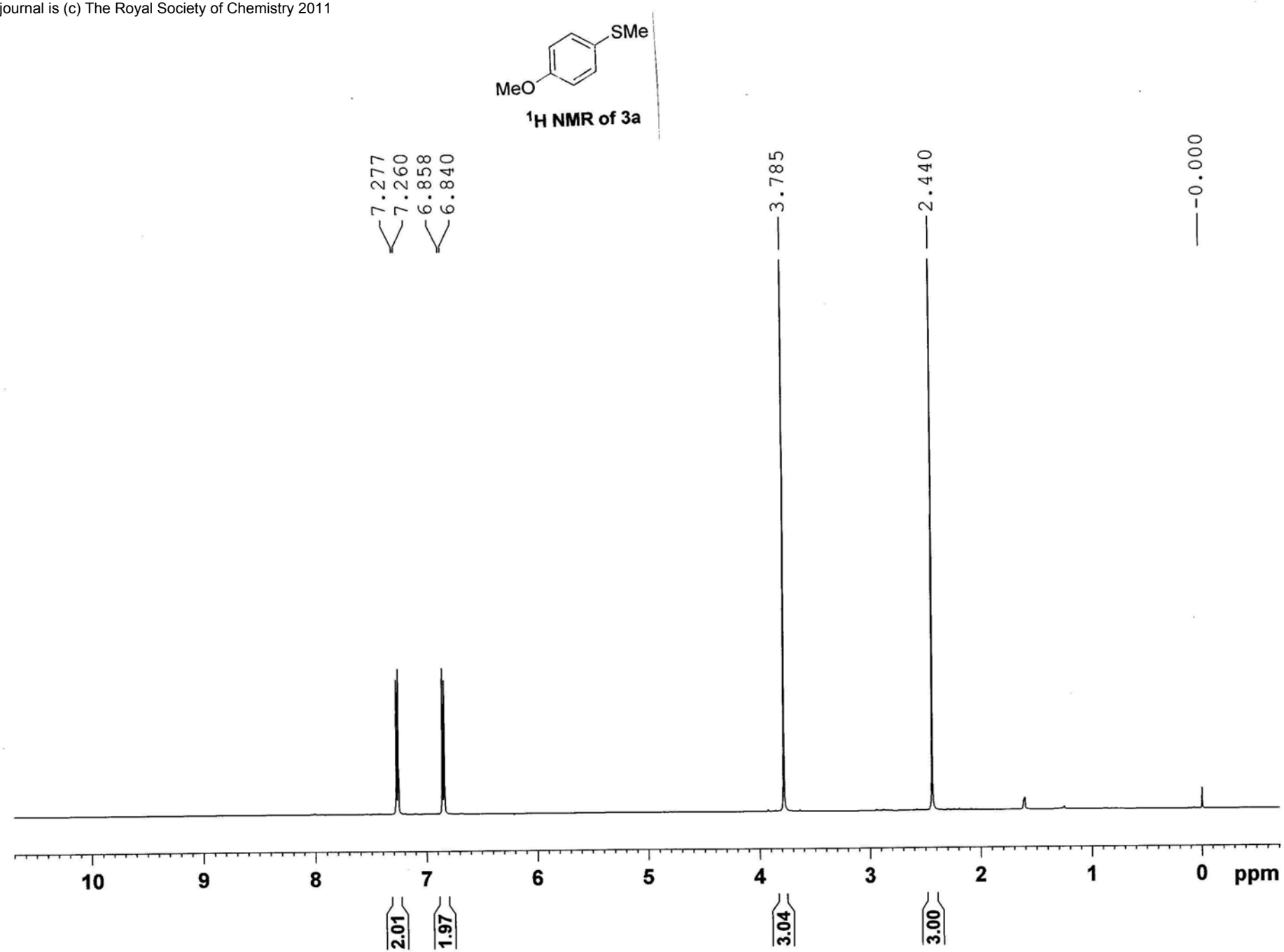
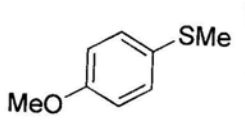
[16] C. Savarin, J. Srogl and L. S. Liebeskind, *Org. Lett.,* 2002, **4**, 4309.

[17] Y.-J. Cherng, *Tetrahedron,* 2002, **58**, 1125.

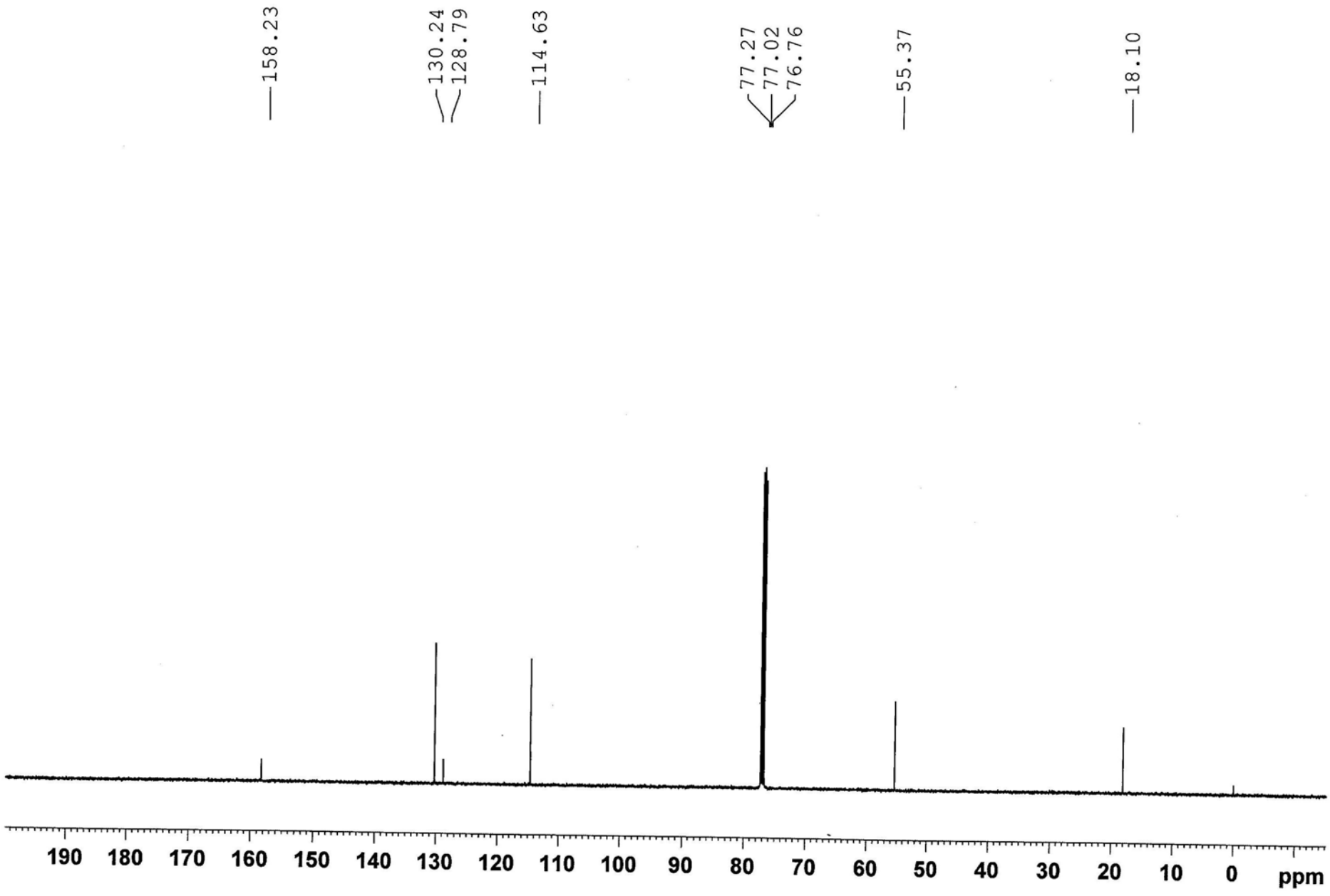
[18] W. Yin, C. Chu, Q. Lu, J. Tao, X. Liang and R. Liu, *Adv. Synth. Catal.,* 2010, **352**, 113.

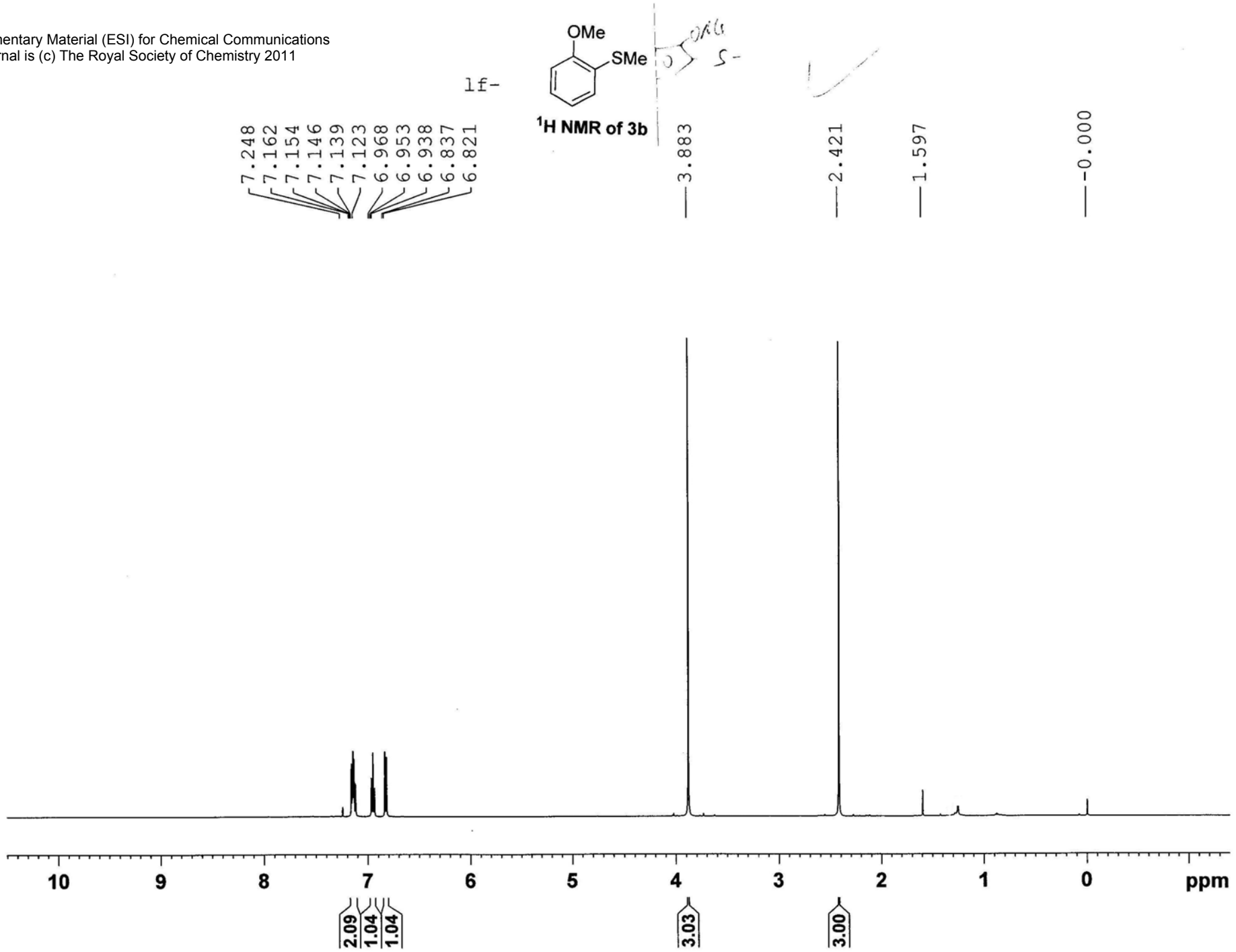
[19] T. Itoh and T. Mase, *Org. Lett.,* 2004, **6**, 4587.

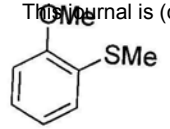

SMe
MeO
¹H NMR of 3a
7.277
7.260
6.858
6.840
3.785
2.440
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.97
3.04
3.00


SMe
MeO

^{13}C NMR of 3a

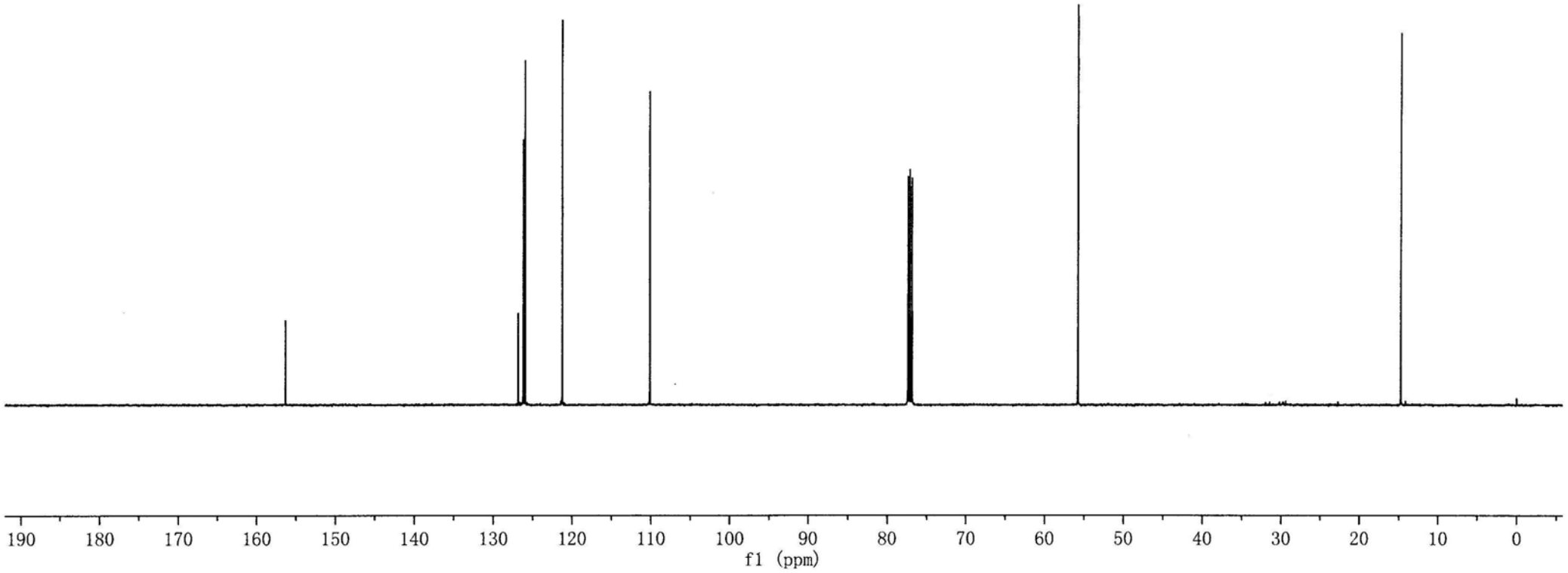

158.23
130.24
128.79
114.63
77.27
77.02
76.76
55.37
18.10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

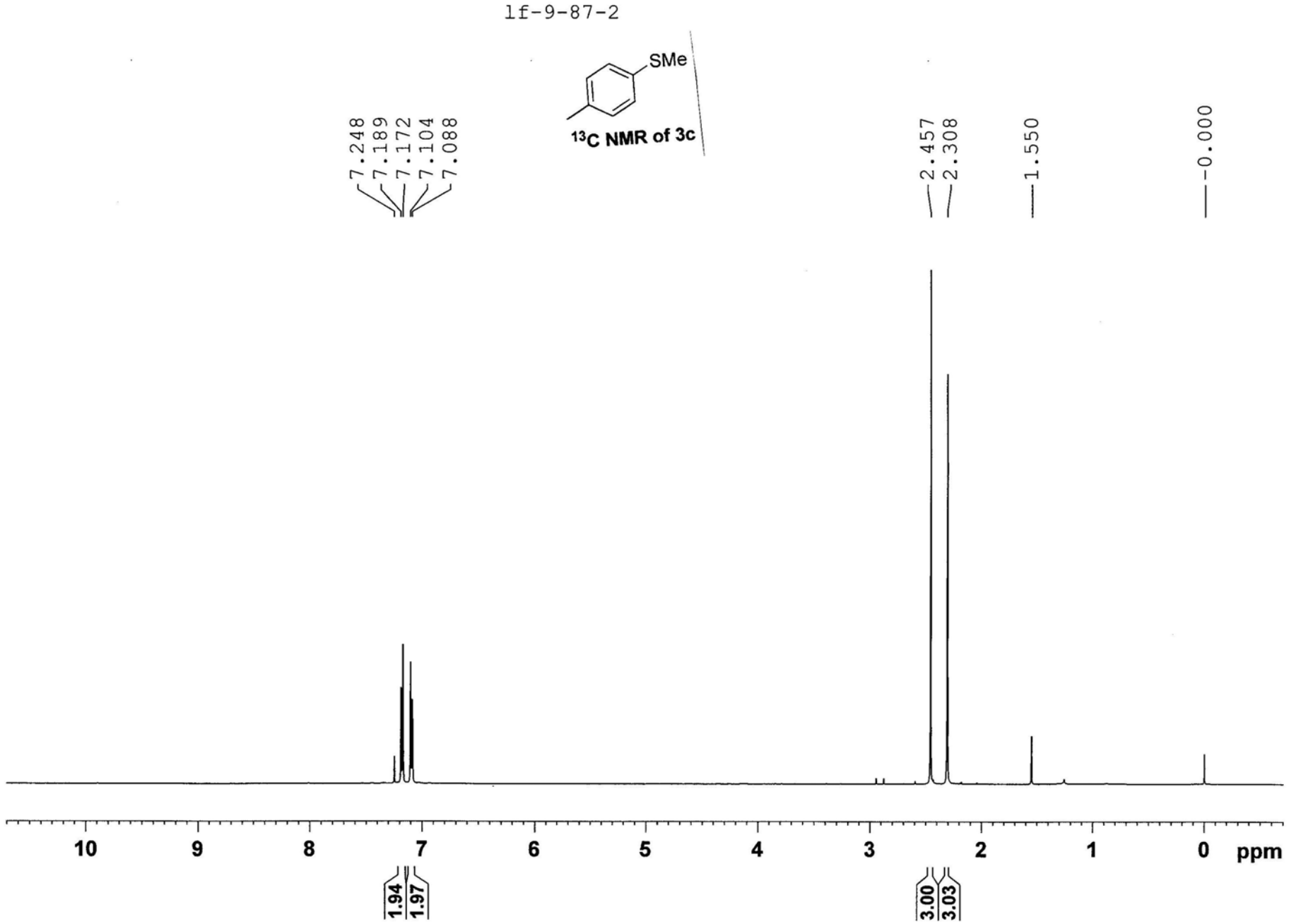

lf-
OMe
SMe
^{1}H NMR of 3b
7.248
7.162
7.154
7.146
7.139
7.123
6.968
6.953
6.938
6.837
6.821
3.883
2.421
1.597
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
2.09
1.04
1.04
3.03
3.00

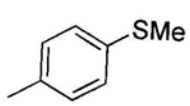


^{13}C NMR of 3b

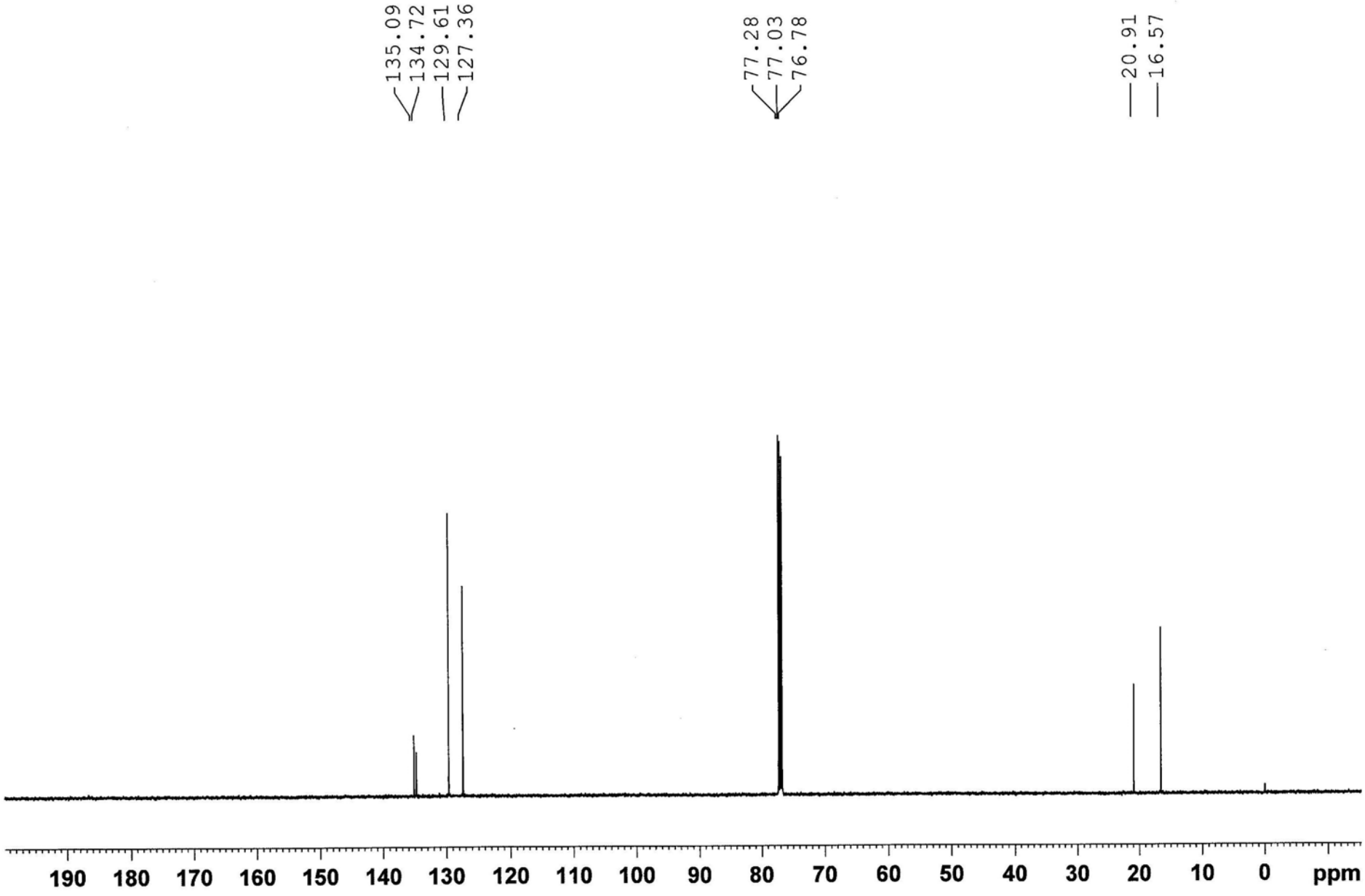
156.323
126.851
126.215
125.958
121.214
110.109
77.371
77.117
76.863
55.785
14.767

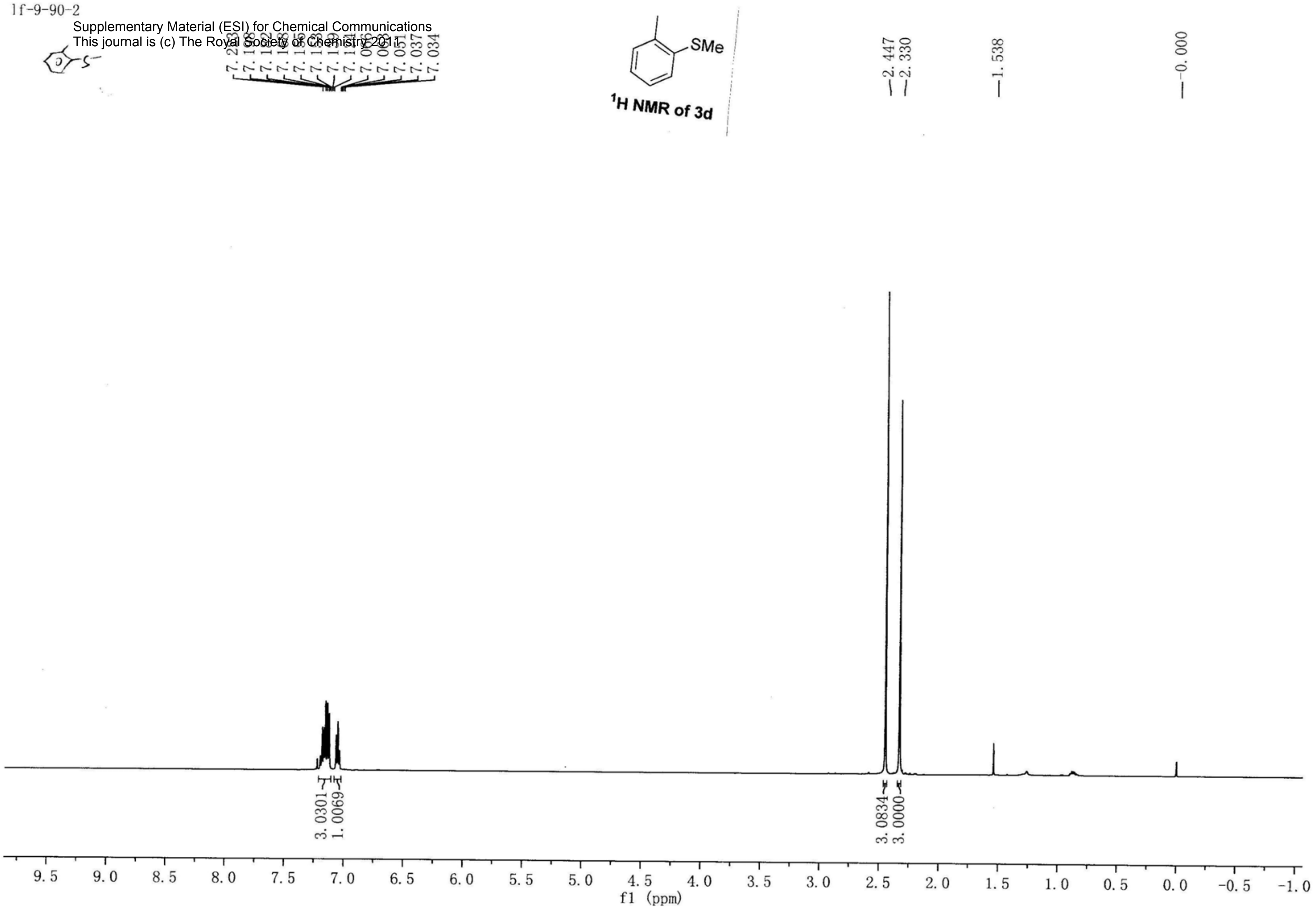


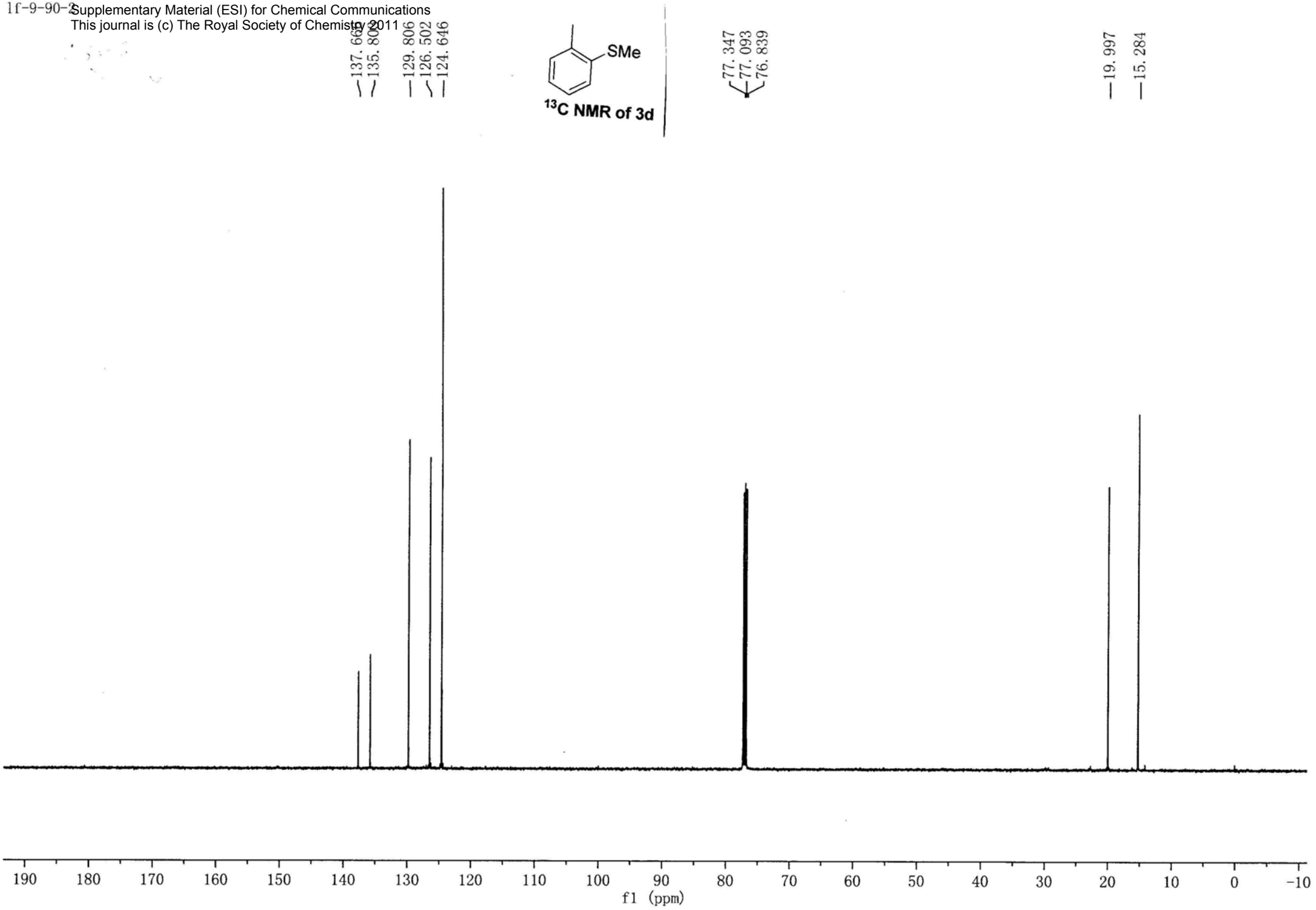

lf-9-87-2
SMe
13C NMR of 3c
7.248
7.189
7.172
7.104
7.088
2.457
2.308
1.550
-0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.94
1.97
3.00
3.03


SMe

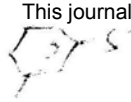
^{1}H NMR of 3c


135.09
134.72
129.61
127.36
77.28
77.03
76.78
20.91
16.57
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

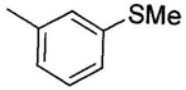




^{13}C NMR of 3d



7.244
7.186
7.171
7.155
7.078
7.061
7.051
6.951
6.936

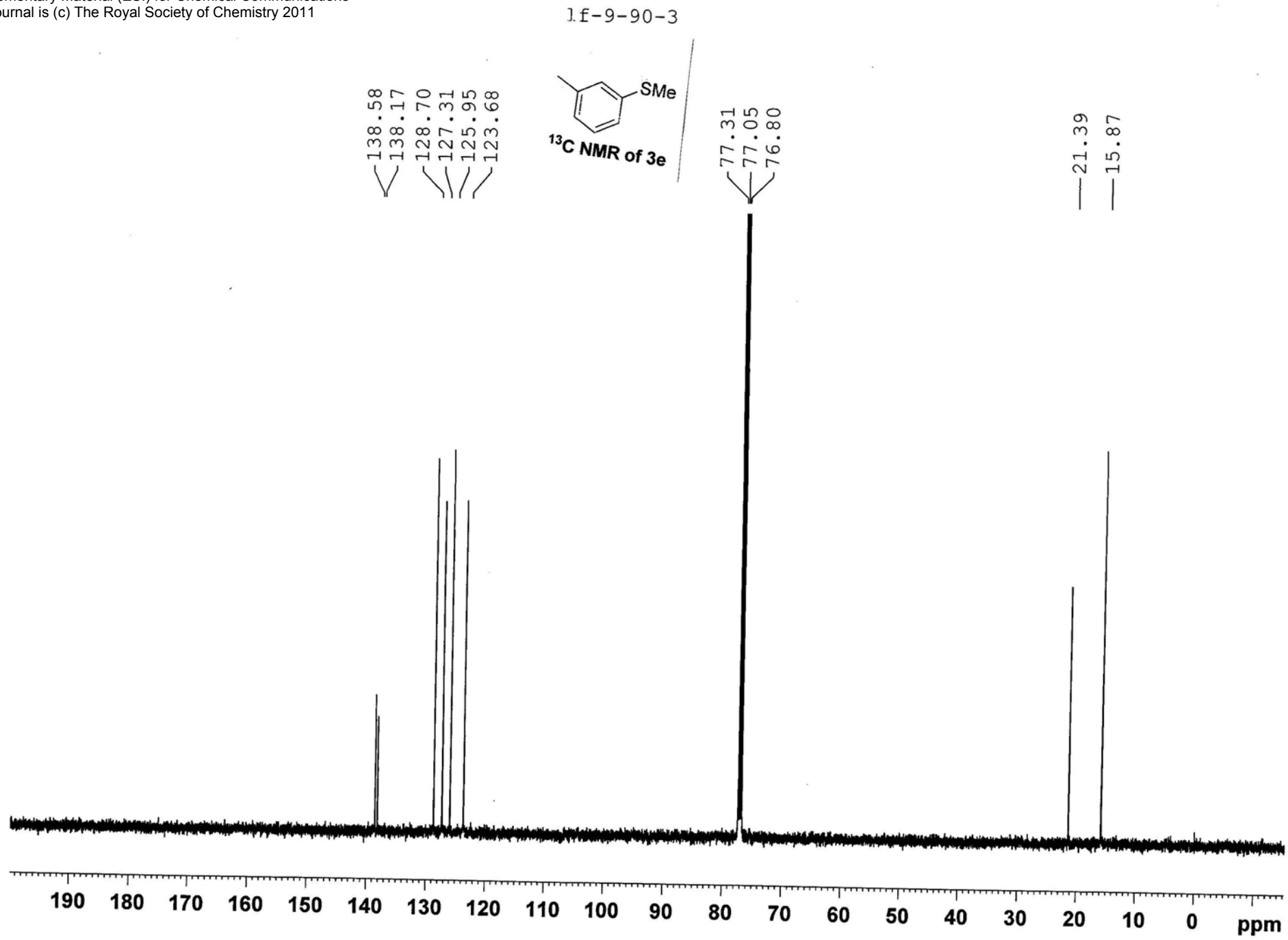


^{1}H NMR of 3e

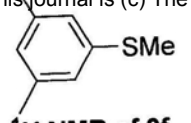
2.467
2.322
1.554
0.000

1.0041
1.9672
0.9916
3.0476
3.0000

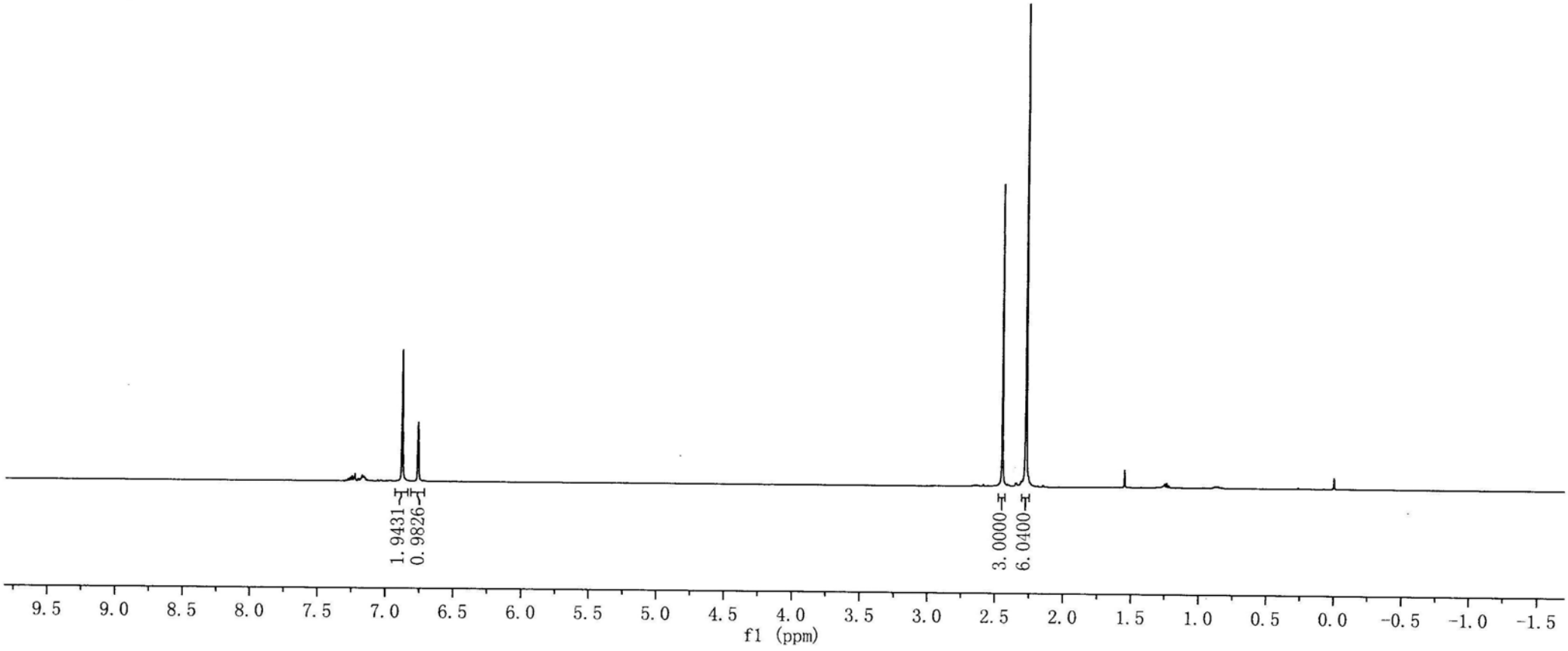
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

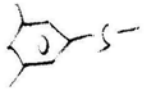

lf-9-90-3
138.58
138.17
128.70
127.31
125.95
123.68
SMe
13C NMR of 3e
77.31
77.05
76.80
21.39
15.87
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Supplementary Material (ESI) for Chemical Communications

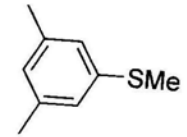


^{1}H NMR of 3f

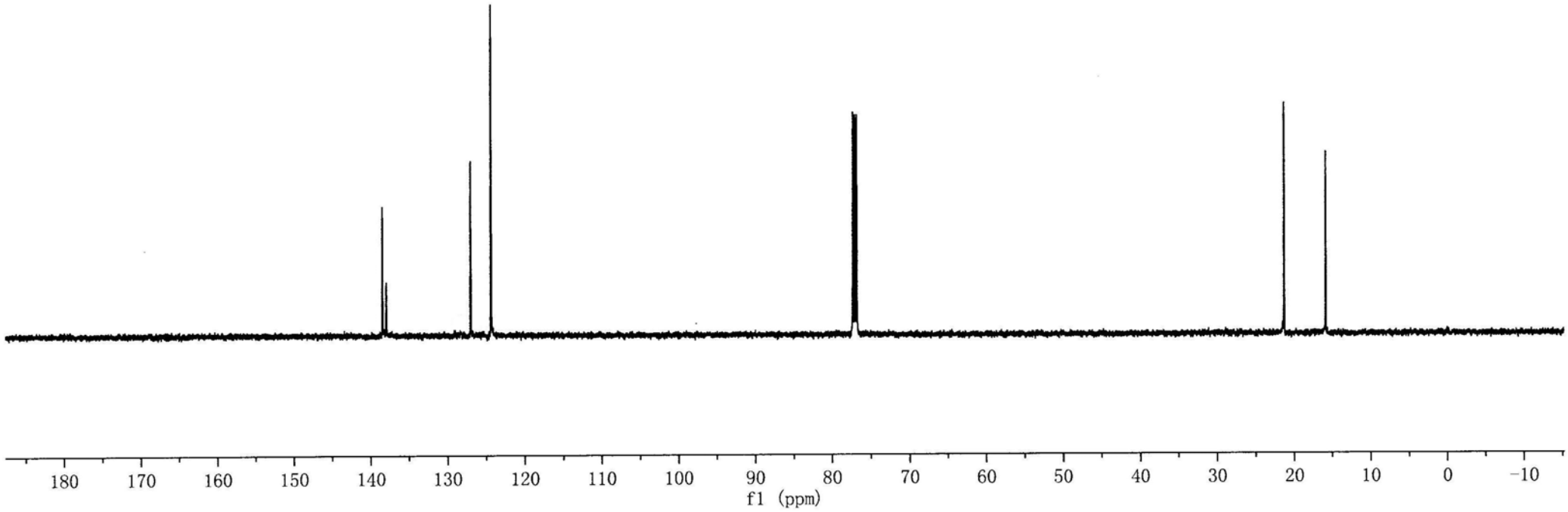


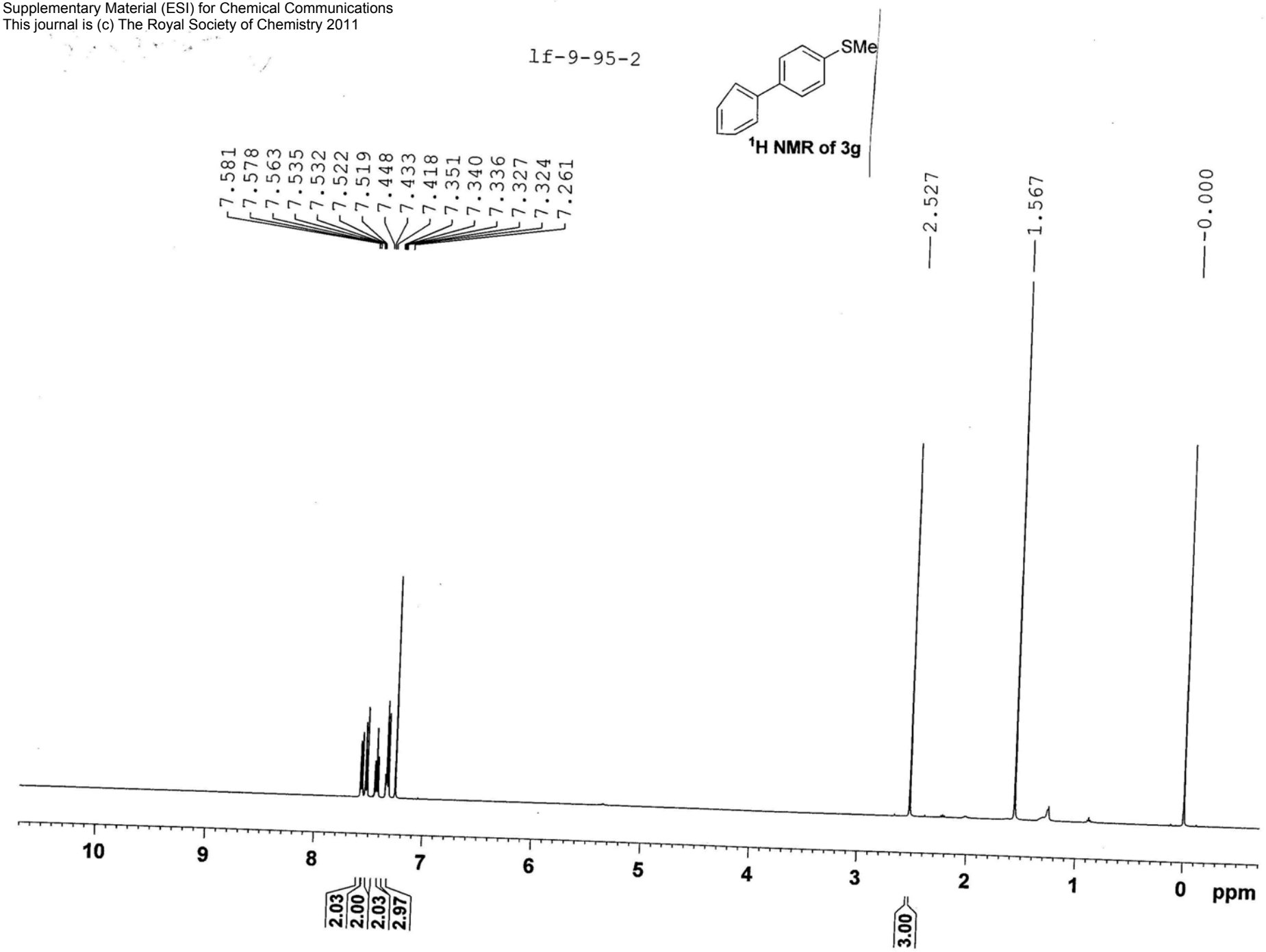


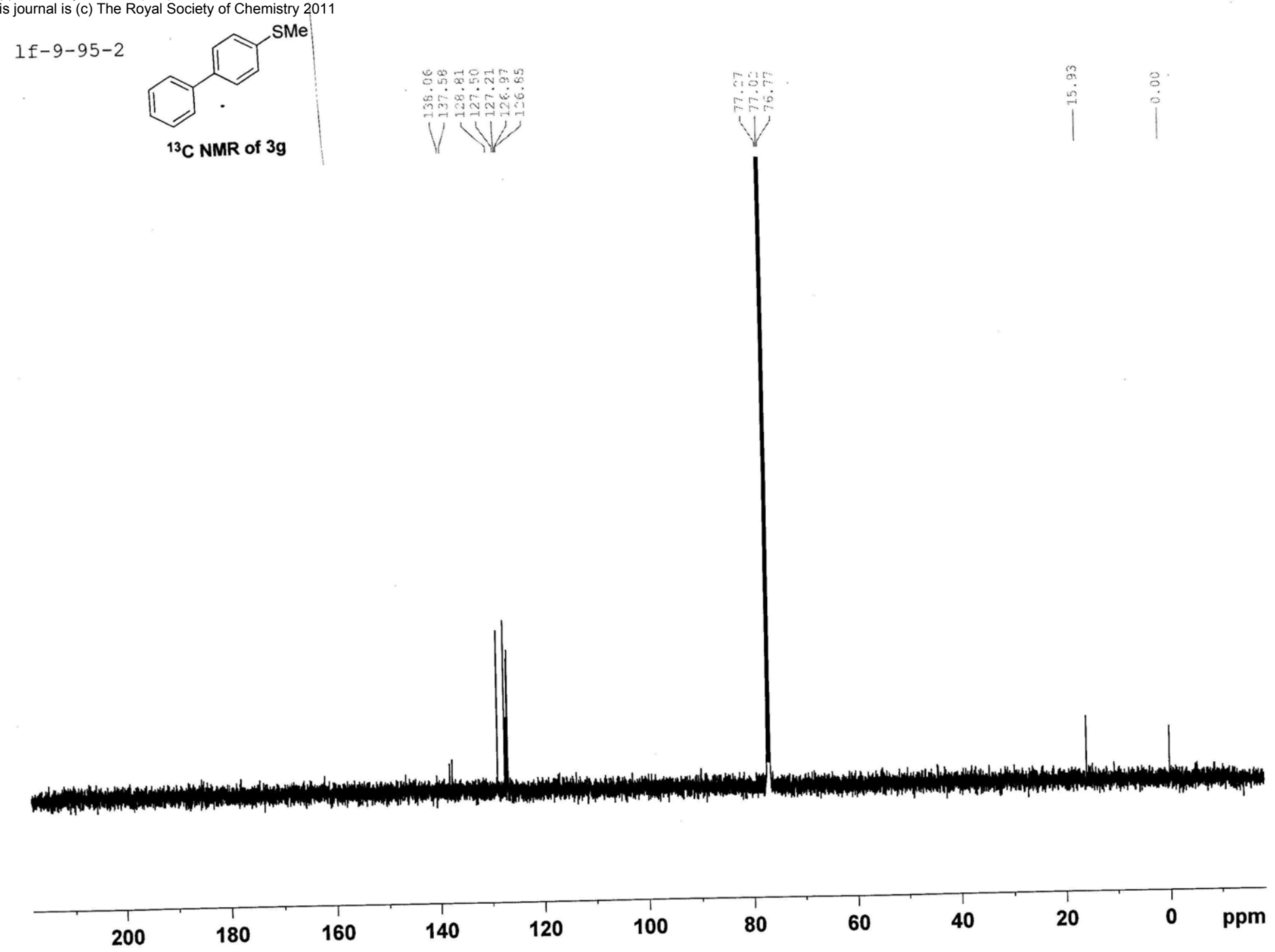
138.459
137.947
127.014
124.375
77.327
77.074
76.821
21.289
15.867

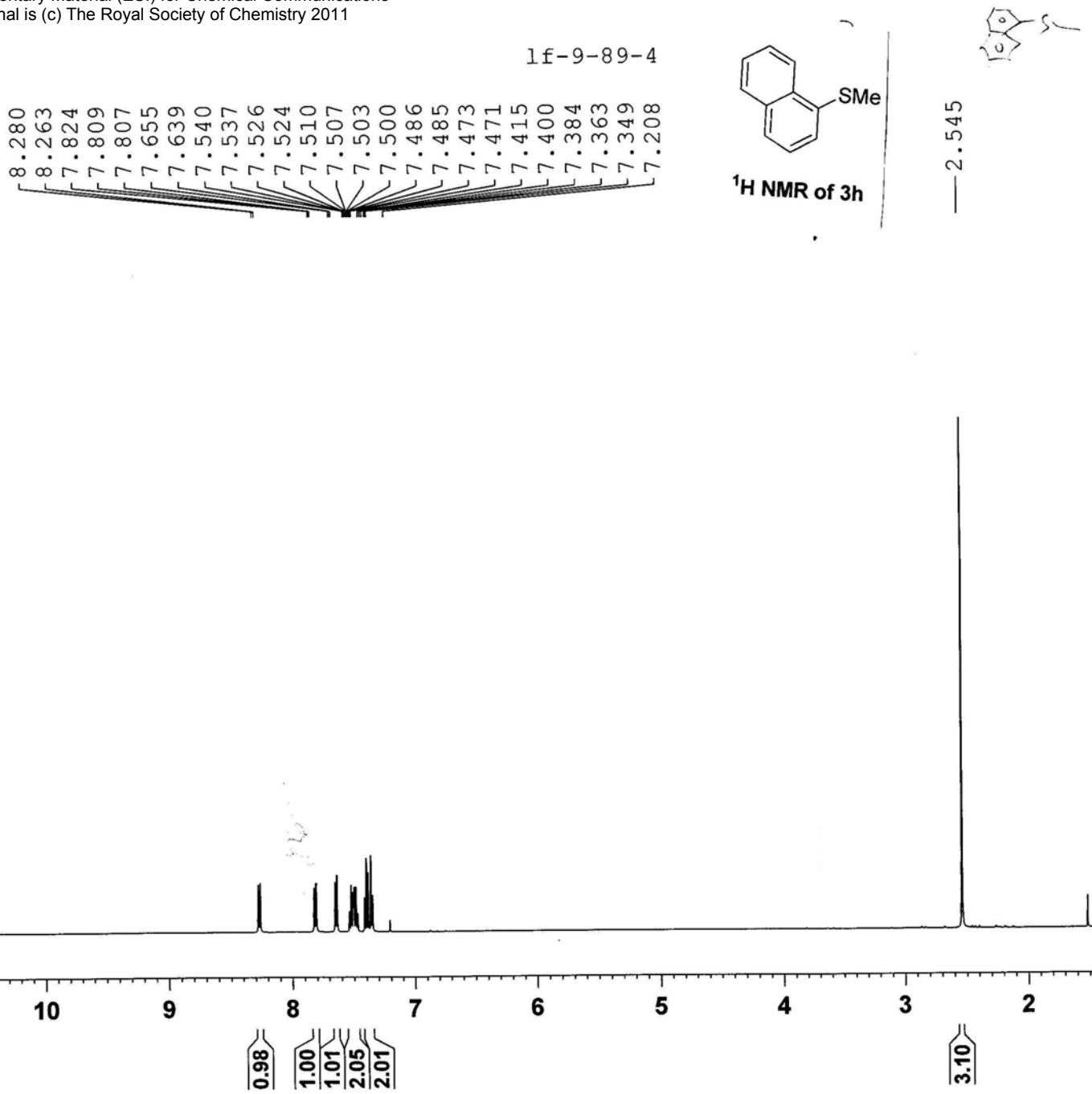


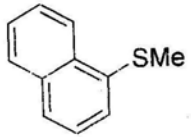
^{13}C NMR of 3f



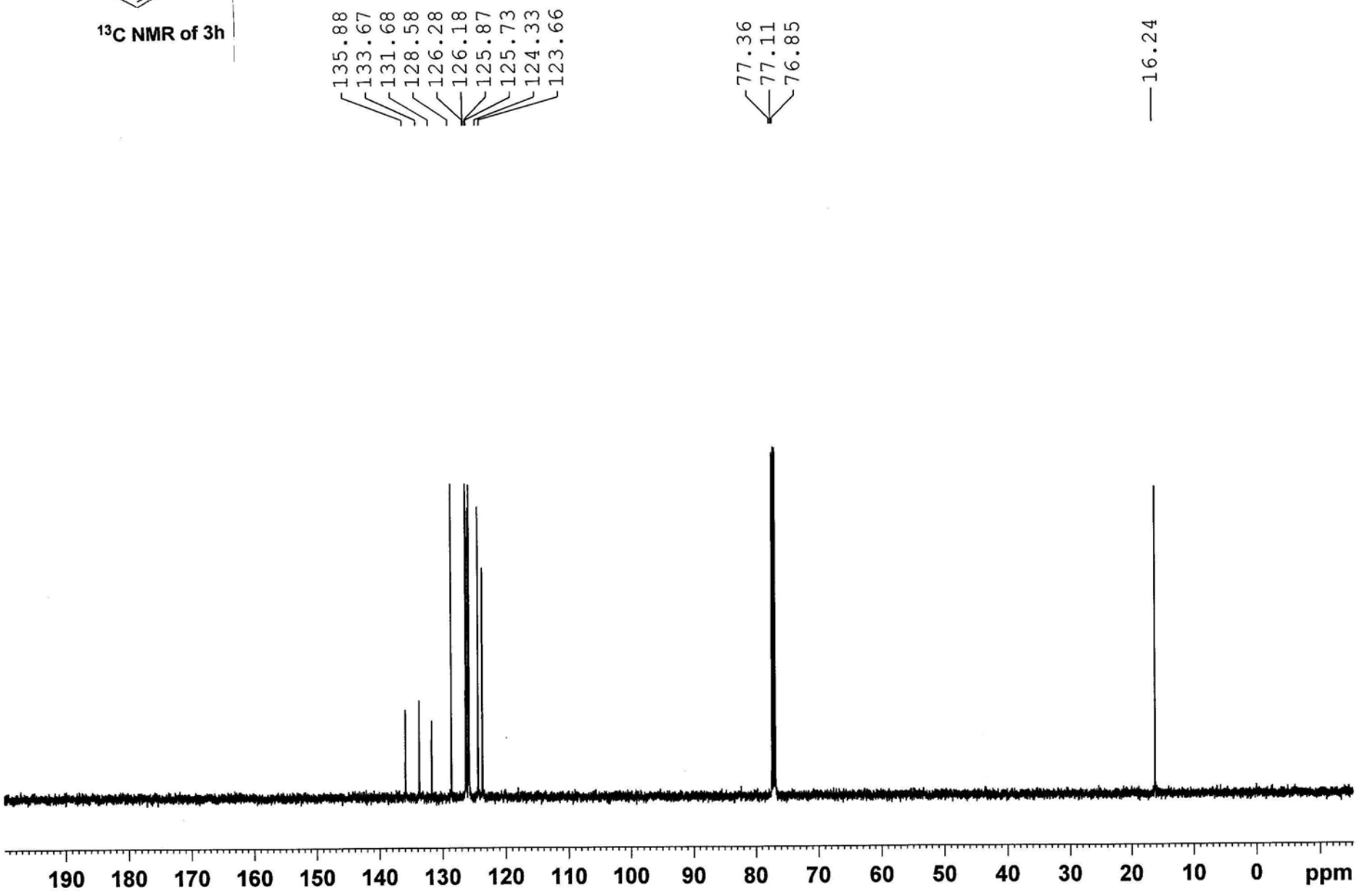

lf-9-95-2
SMe
^{1}H NMR of 3g
7.581
7.578
7.563
7.535
7.532
7.522
7.519
7.448
7.433
7.418
7.351
7.340
7.336
7.327
7.324
7.261
2.527
1.567
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.00
2.03
2.97
3.00

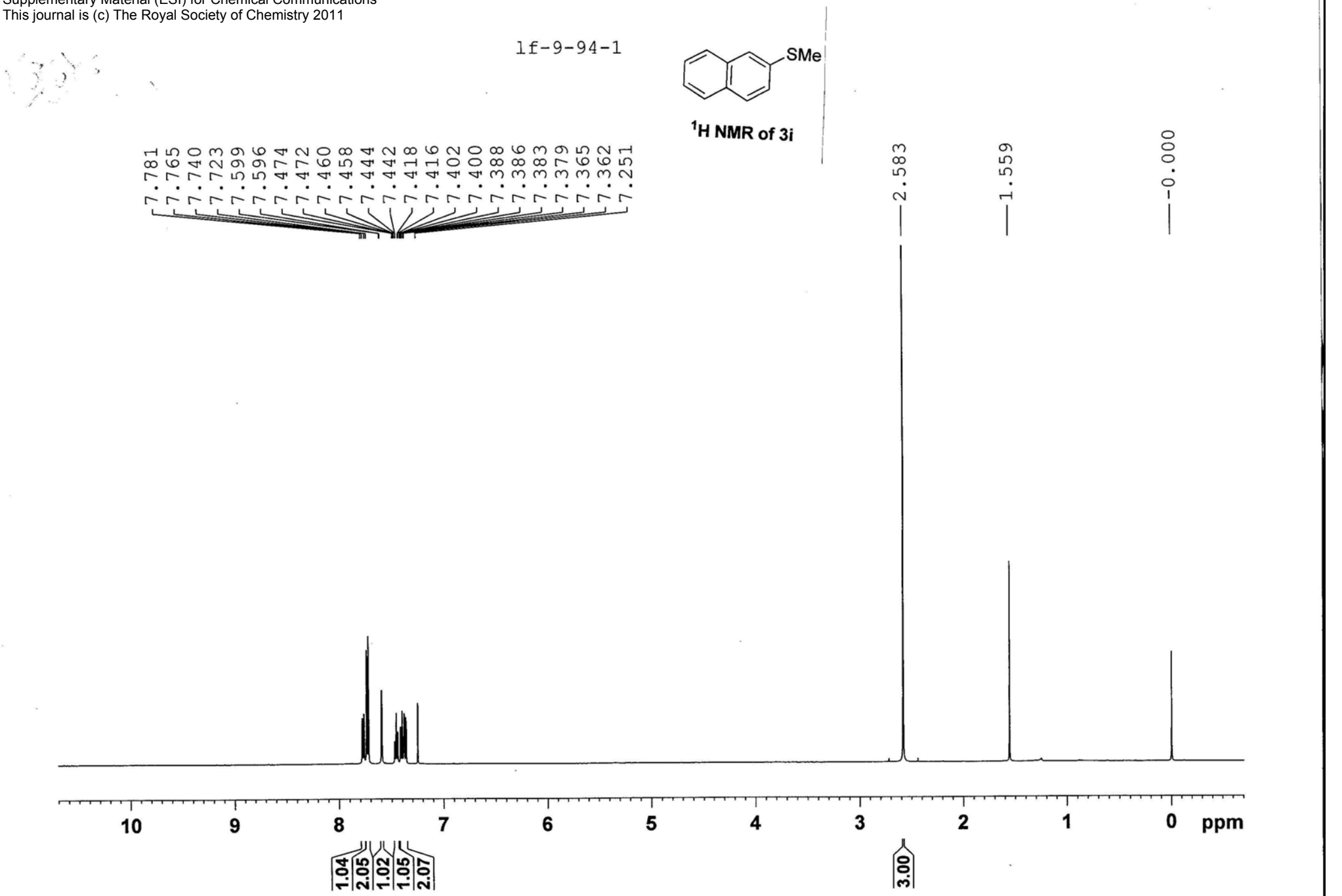

1f-9-95-2
SMe
^{13}C NMR of 3g
136.06
137.58
128.81
127.50
127.21
126.97
126.65
77.27
77.02
76.77
15.93
0.00
200
180
160
140
120
100
80
60
40
20
0
ppm


lf-9-89-4
8.280
8.263
7.824
7.809
7.807
7.655
7.639
7.540
7.537
7.526
7.524
7.510
7.507
7.503
7.500
7.486
7.485
7.473
7.471
7.415
7.400
7.384
7.363
7.349
7.208
SMe
2.545
¹H NMR of 3h
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.00
1.01
2.05
2.01
3.10


SMe

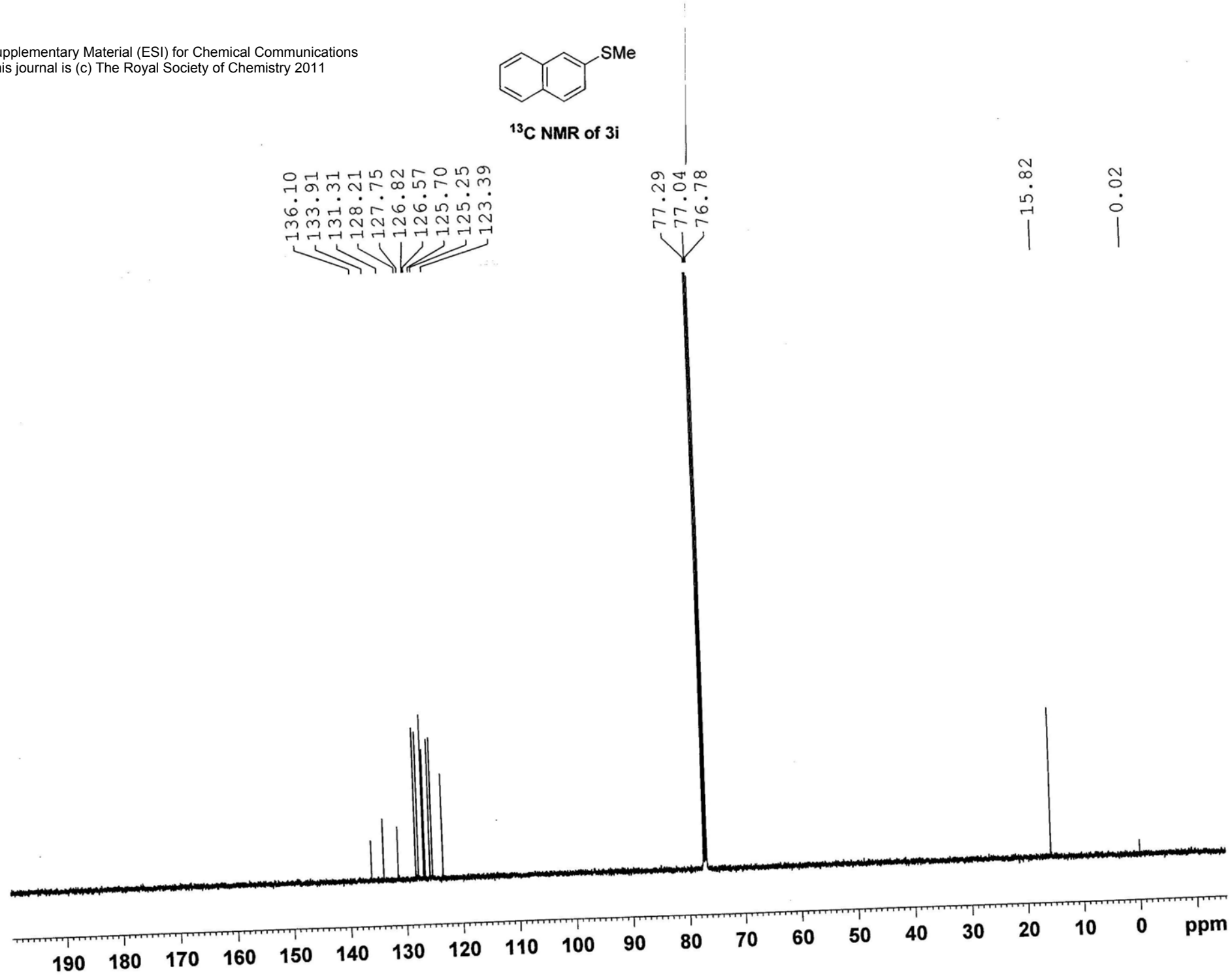
^{13}C NMR of 3h


lf-9-89-4
135.88
133.67
131.68
128.58
126.28
126.18
125.87
125.73
124.33
123.66
77.36
77.11
76.85
16.24
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

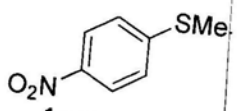

lf-9-94-1
SMe
^{1}H NMR of 3*i*
7.781
7.765
7.740
7.723
7.599
7.596
7.474
7.472
7.460
7.458
7.444
7.442
7.418
7.416
7.402
7.400
7.388
7.386
7.383
7.379
7.365
7.362
7.251
2.583
1.559
-0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
2.05
1.02
1.05
2.07
3.00

SMe

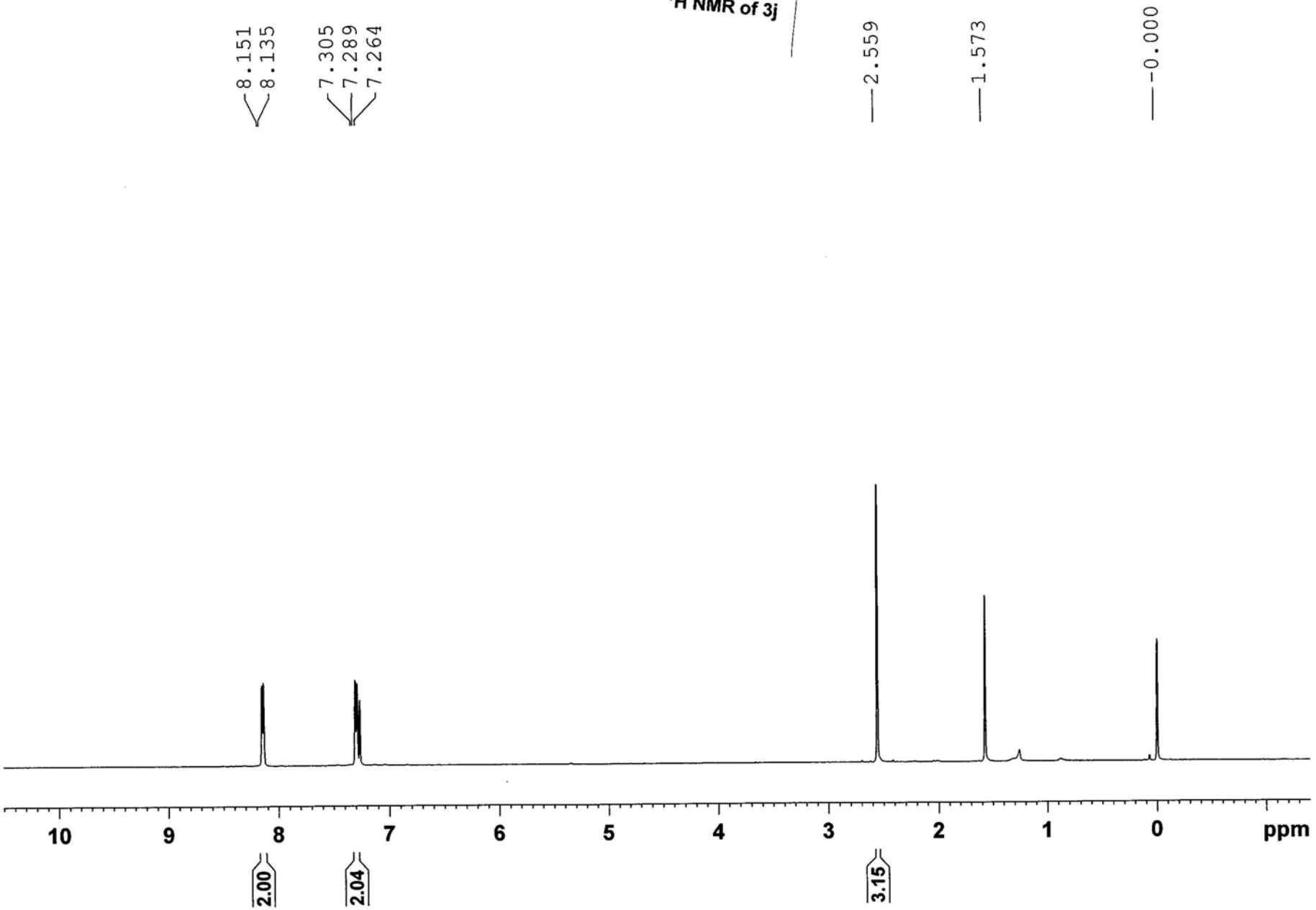
^{13}C NMR of 3i

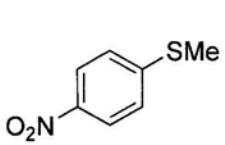

136.10
133.91
131.31
128.21
127.75
126.82
126.57
125.70
125.25
123.39
77.29
77.04
76.78
15.82
0.02
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

lf-9-89-5

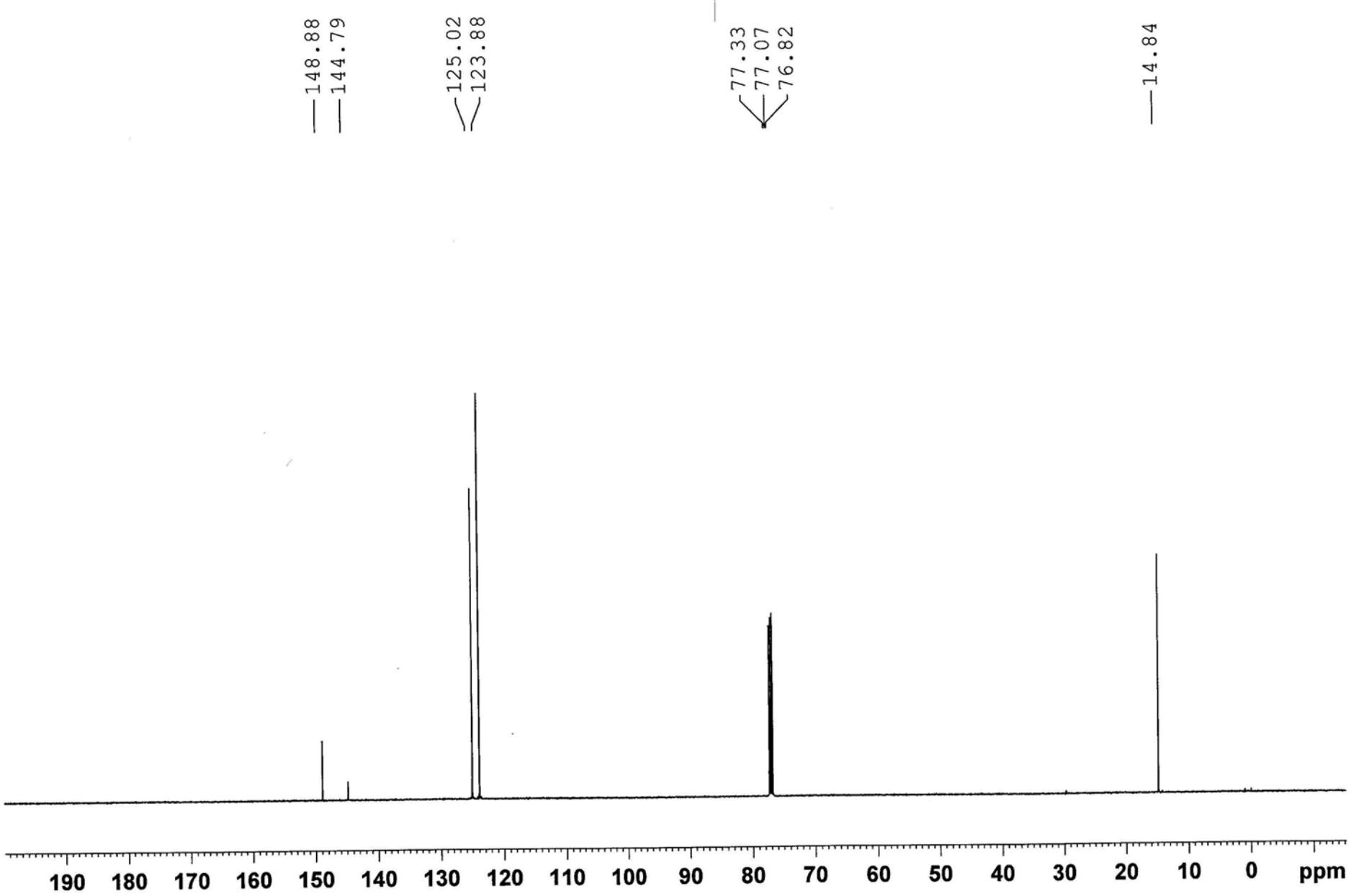


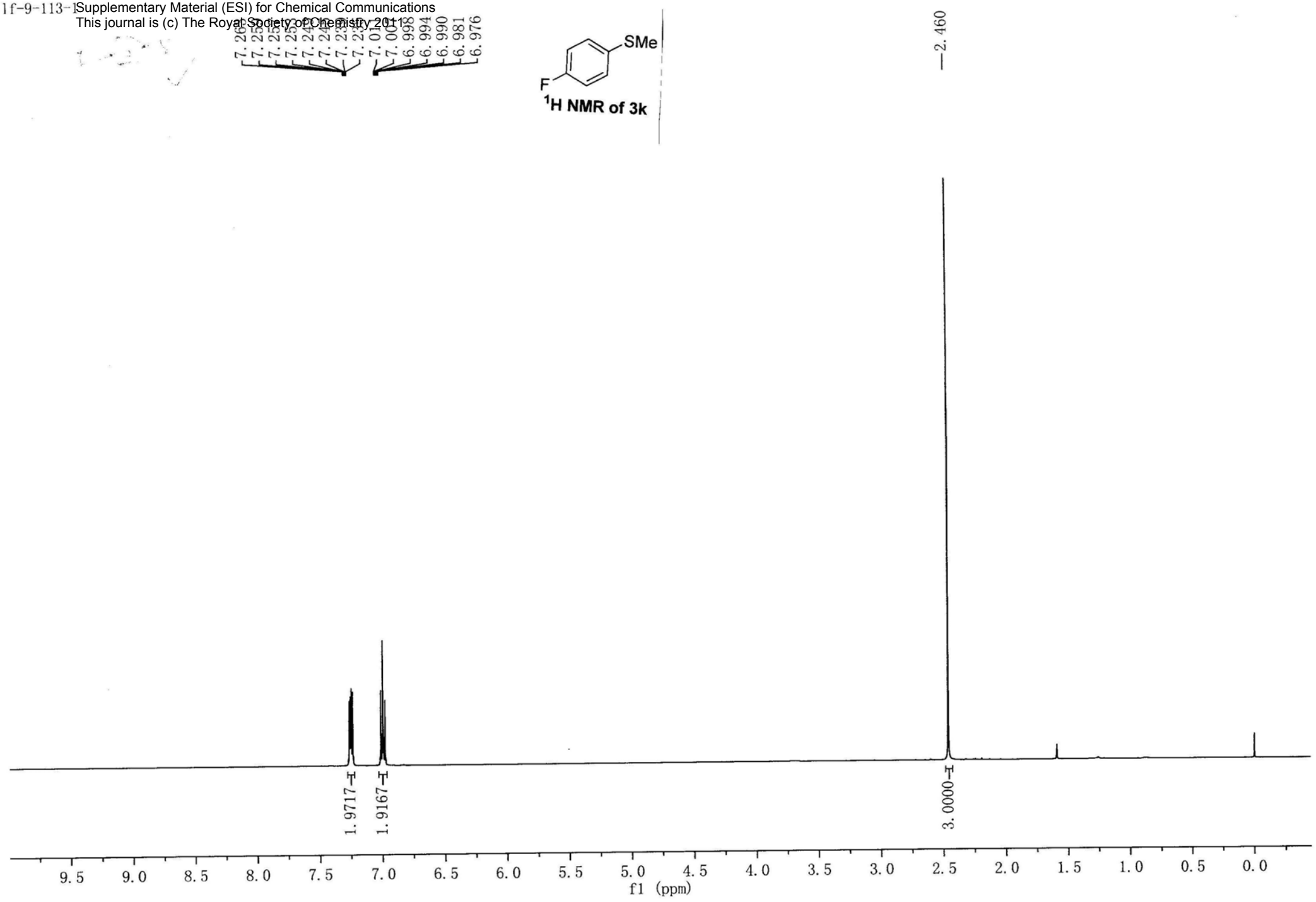
^{1}H NMR of 3j



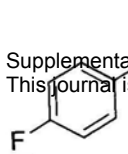

SMe
O_2N

^{13}C NMR of 3j

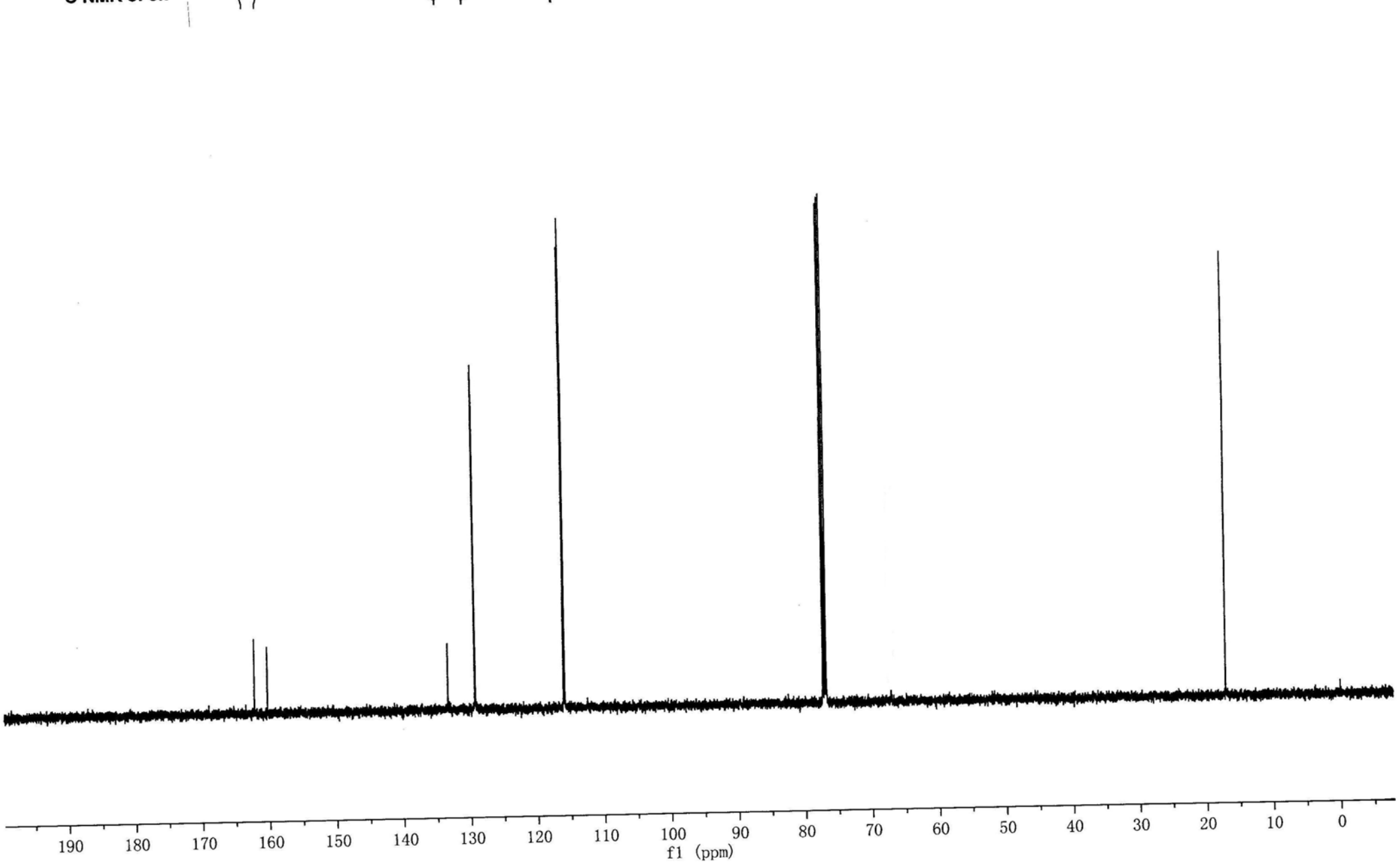

148.88
144.79
125.02
123.88
77.33
77.07
76.82
14.84
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



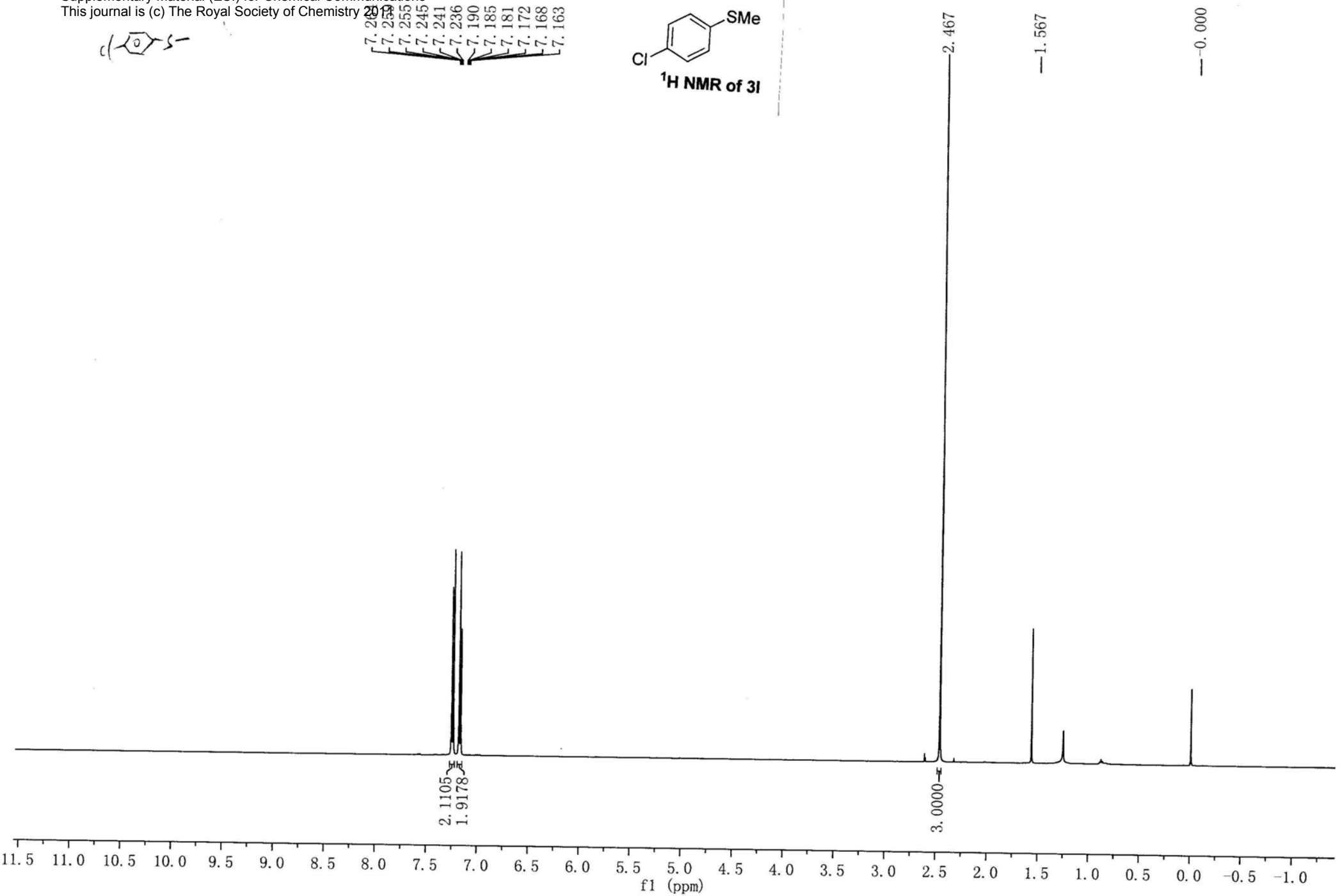
^{1}H NMR of 3k

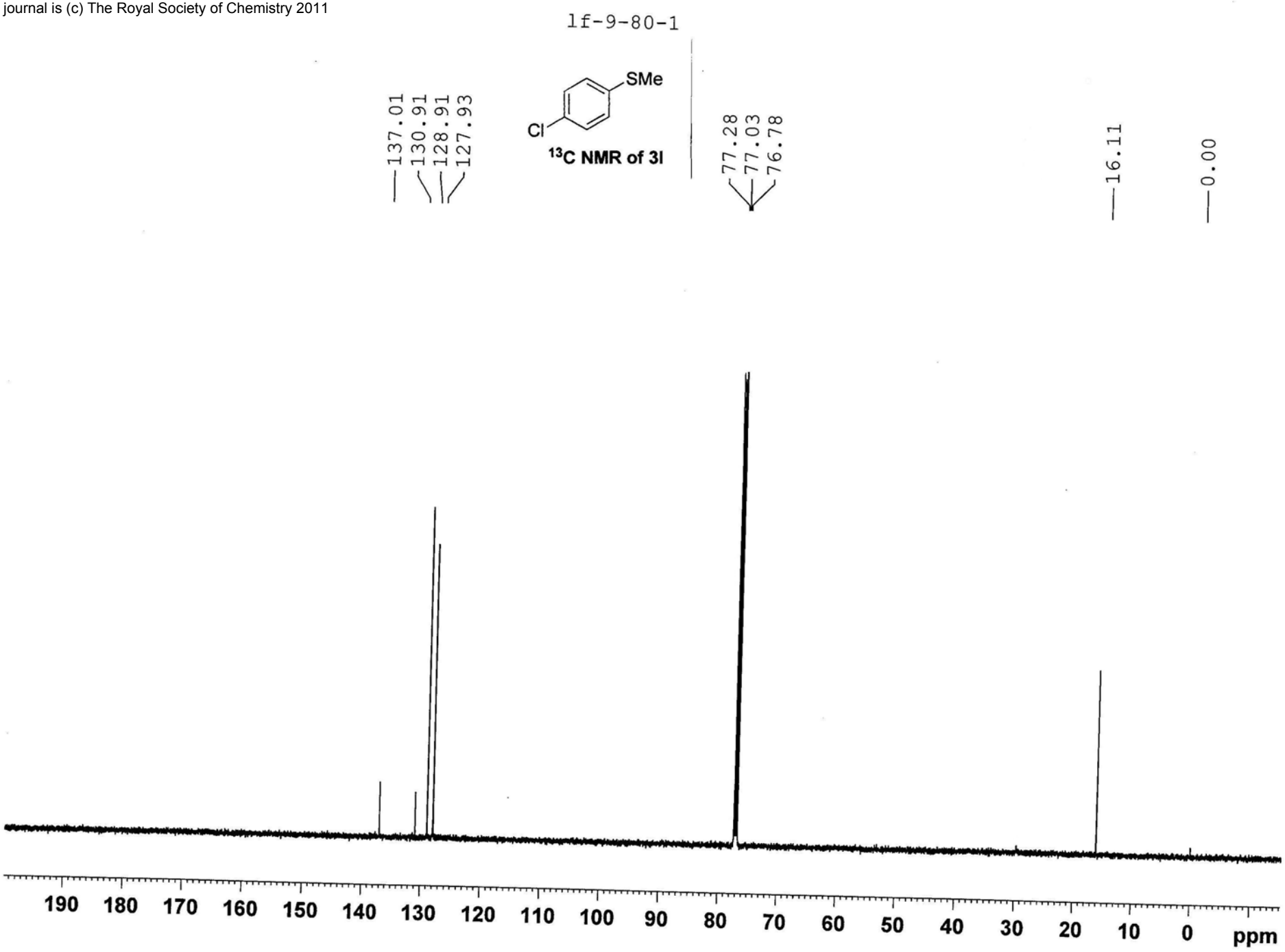


^{13}C NMR of 3k

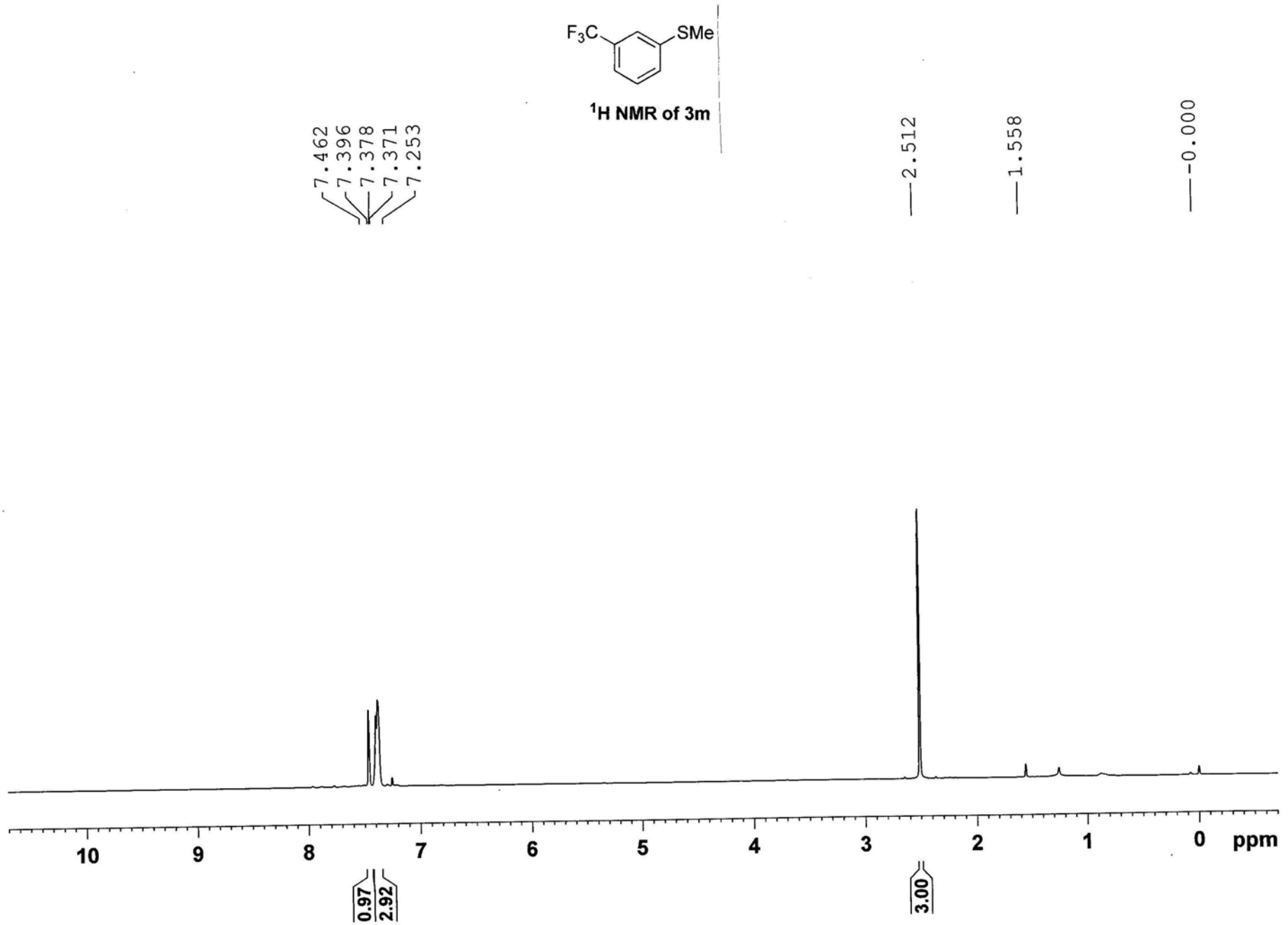


Supplementary Material (ESI) for Chemical Communications

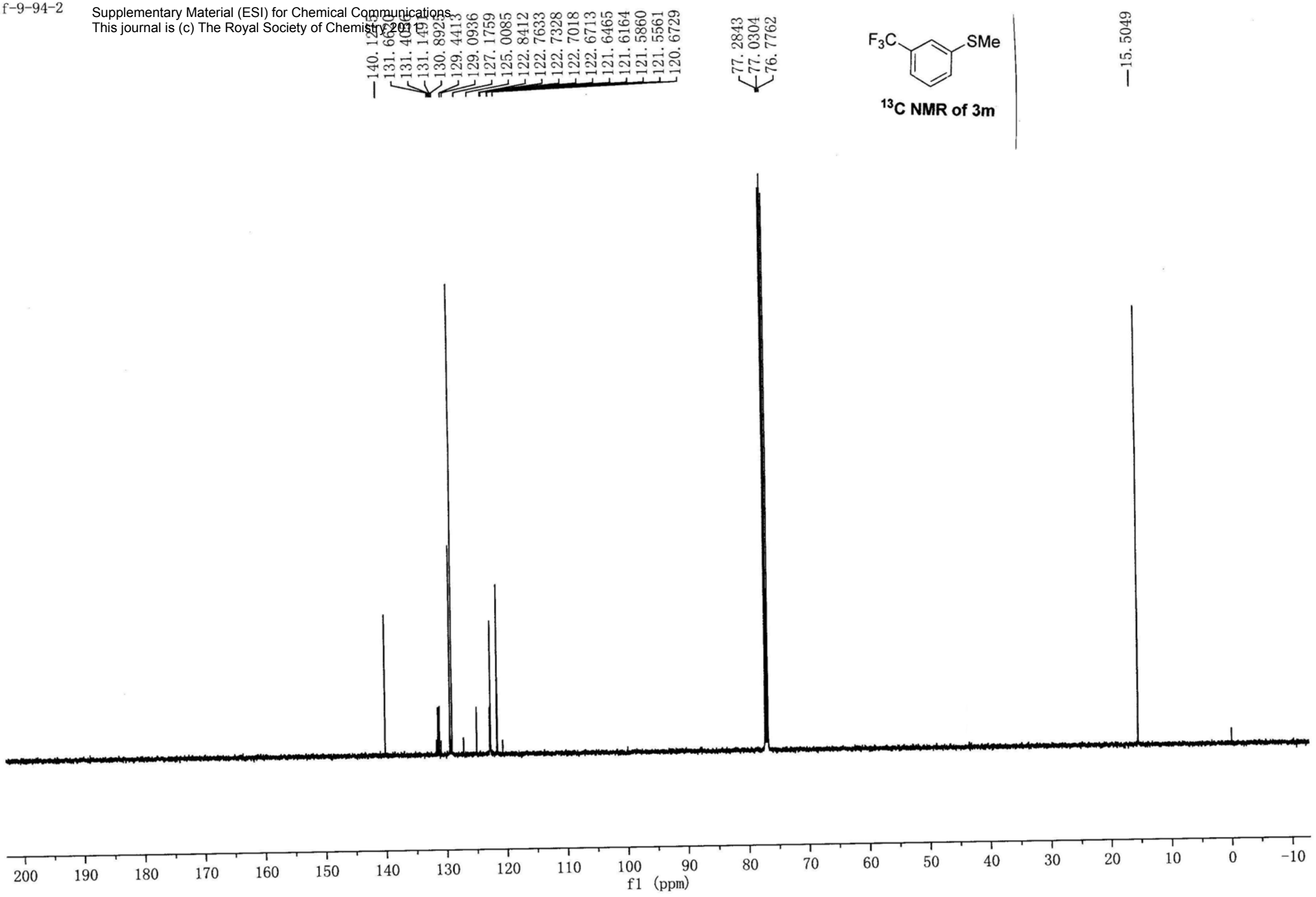


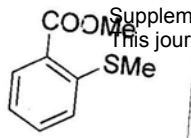

lf-9-80-1
SMe
Cl
137.01
130.91
128.91
127.93
77.28
77.03
76.78
16.11
0.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR of 3l

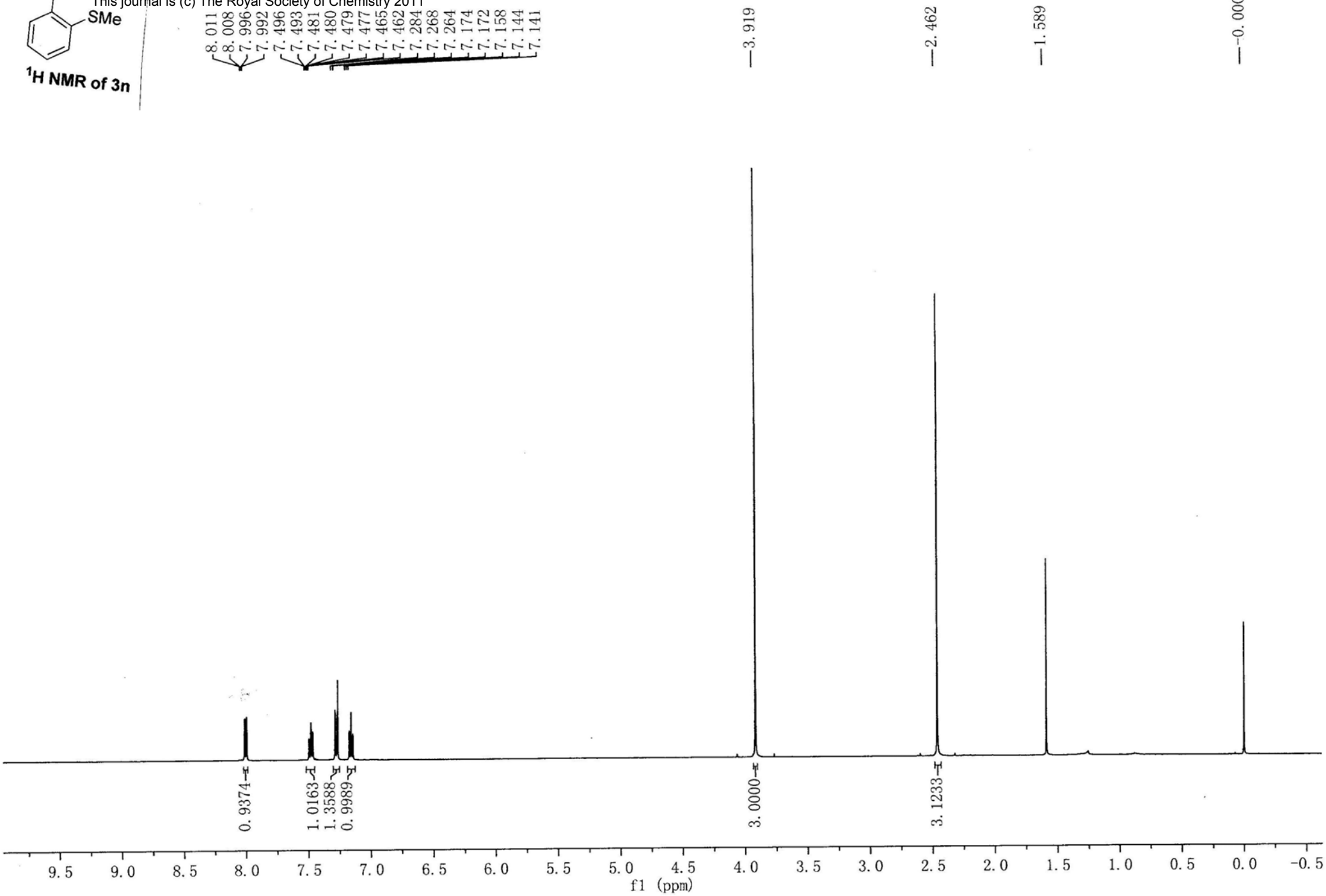

F3C
SMe
1H NMR of 3m
7.462
7.396
7.378
7.371
7.253
2.512
1.558
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.92
3.00

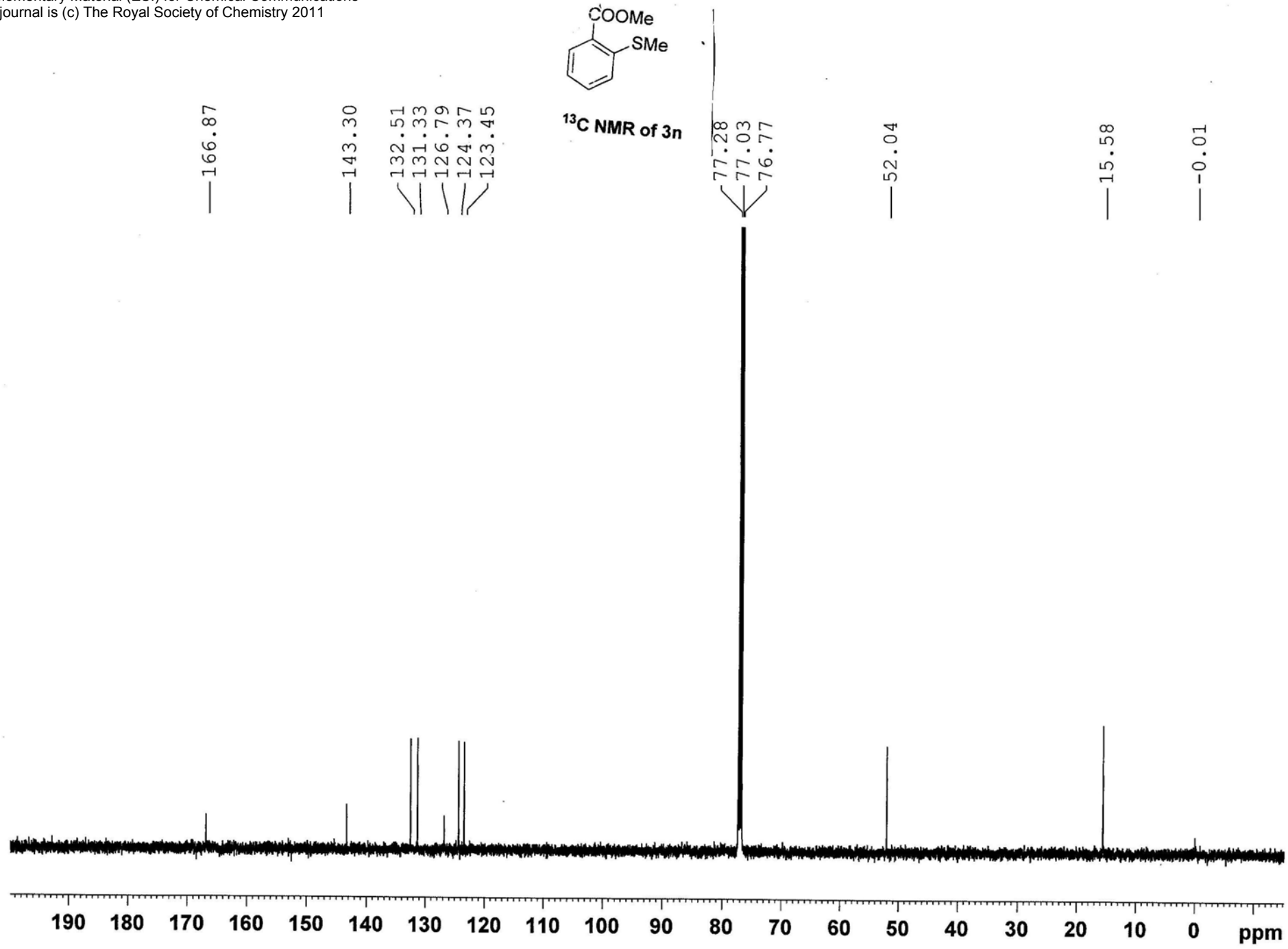
Supplementary Material (ESI) for Chemical Communications



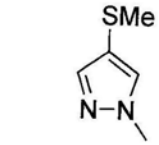


^{1}H NMR of 3n

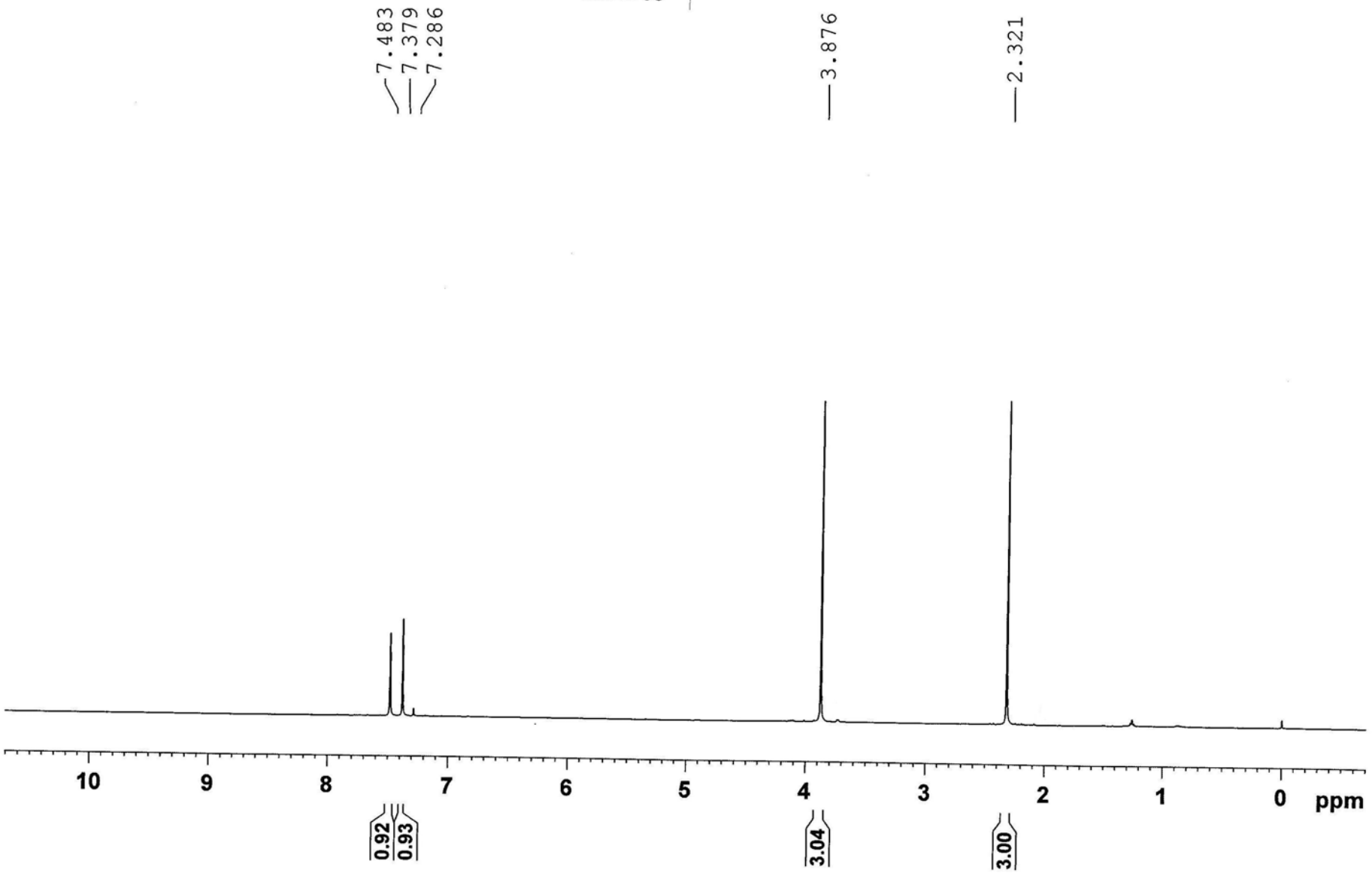




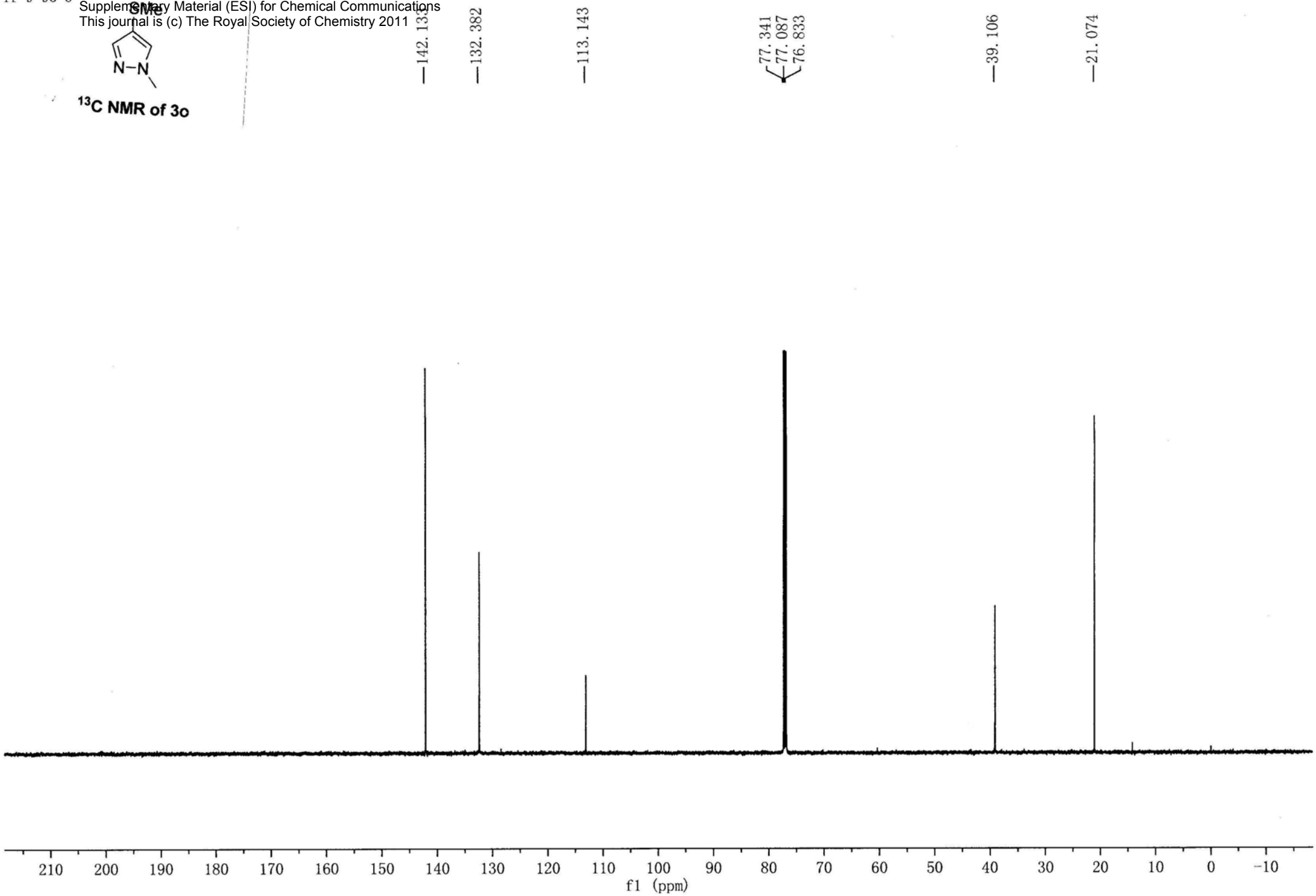
^{13}C NMR of 3n

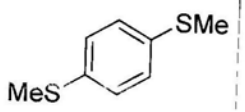

SMe
N–N

^{1}H NMR of 3o

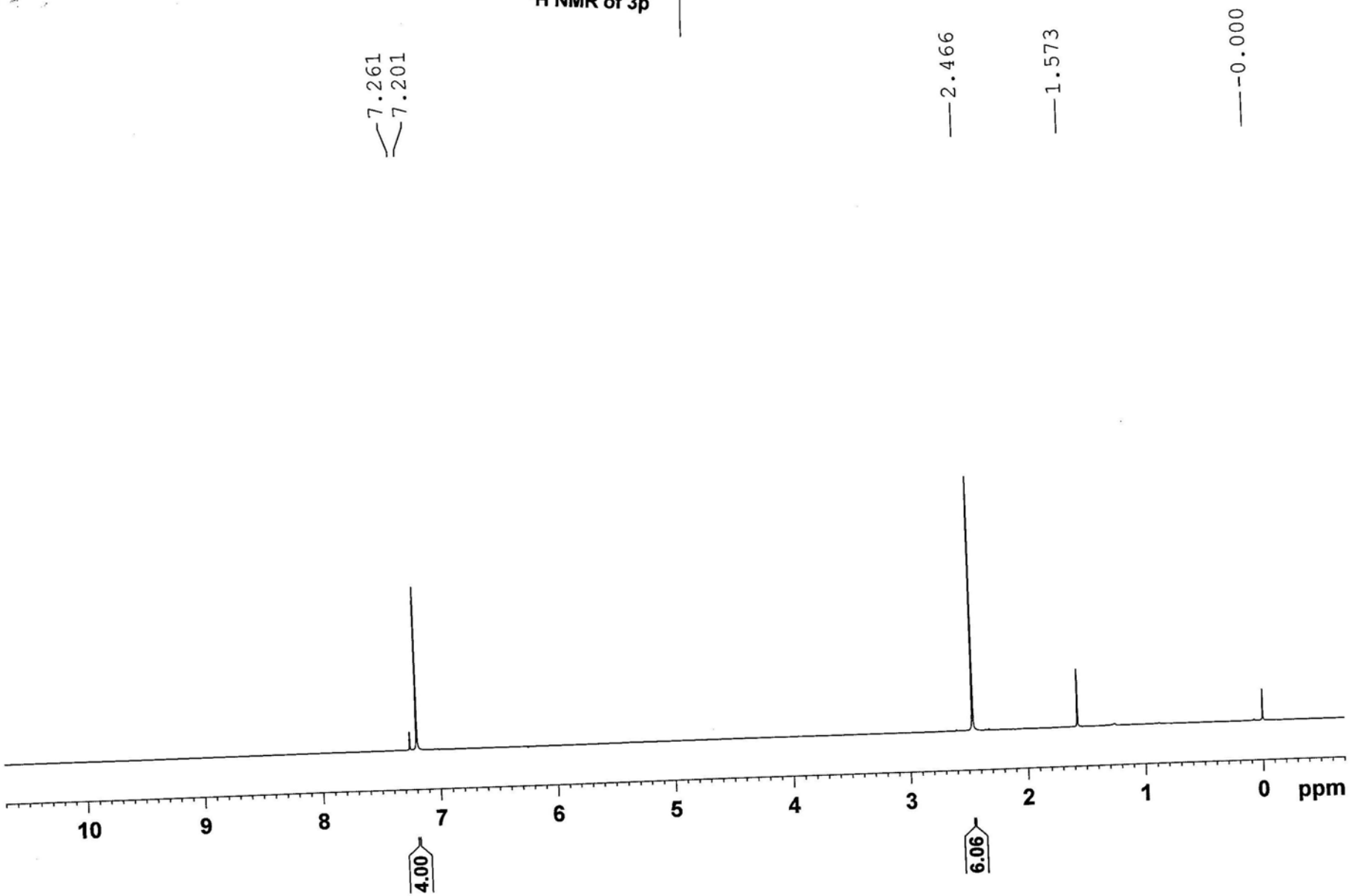

7.483
7.379
7.286
3.876
2.321
10
9
8
7
6
5
4
3
2
1
0
ppm
0.92
0.93
3.04
3.00

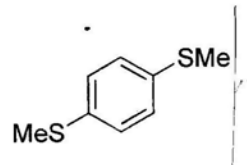
^{13}C NMR of 3o



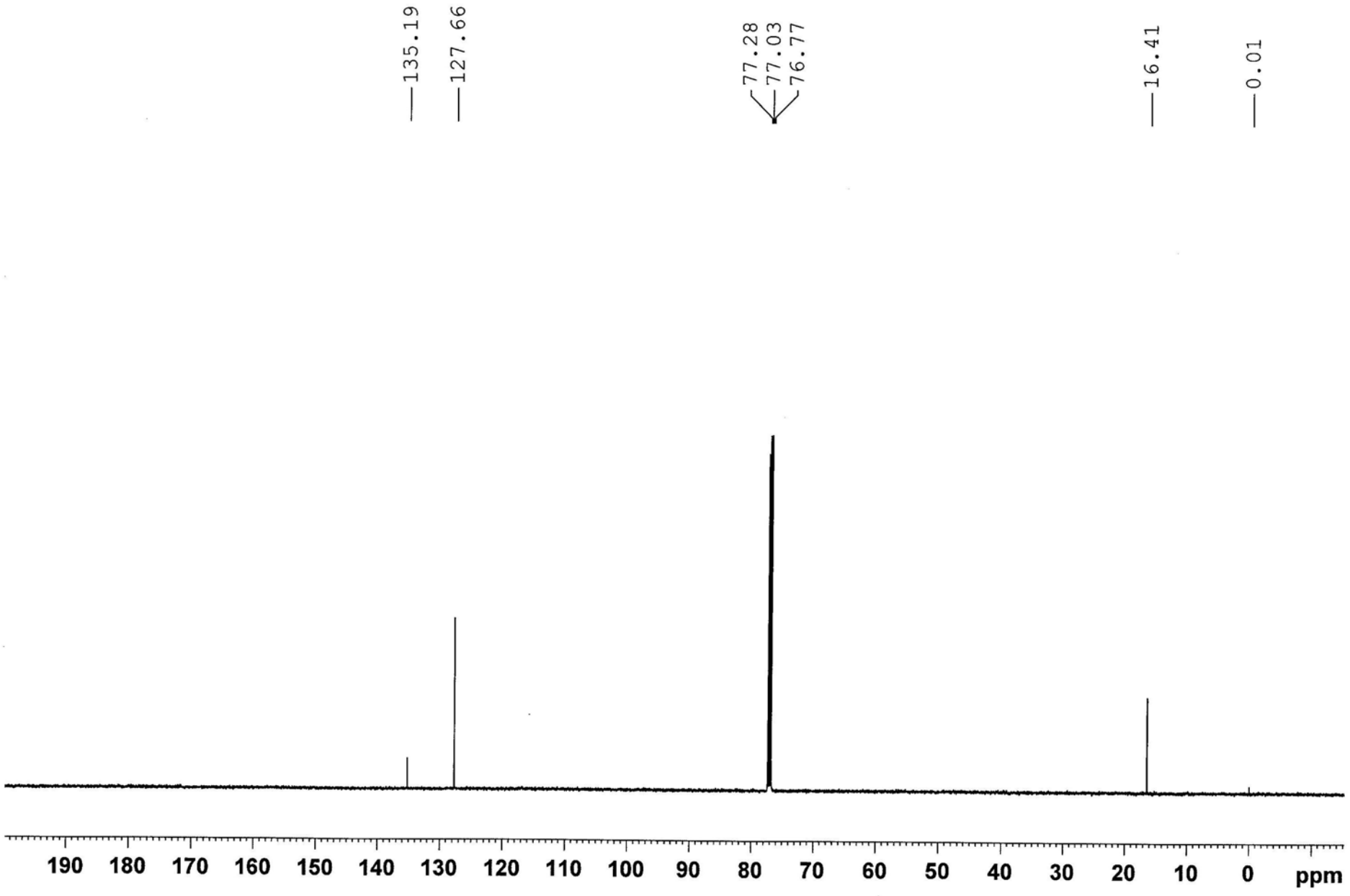


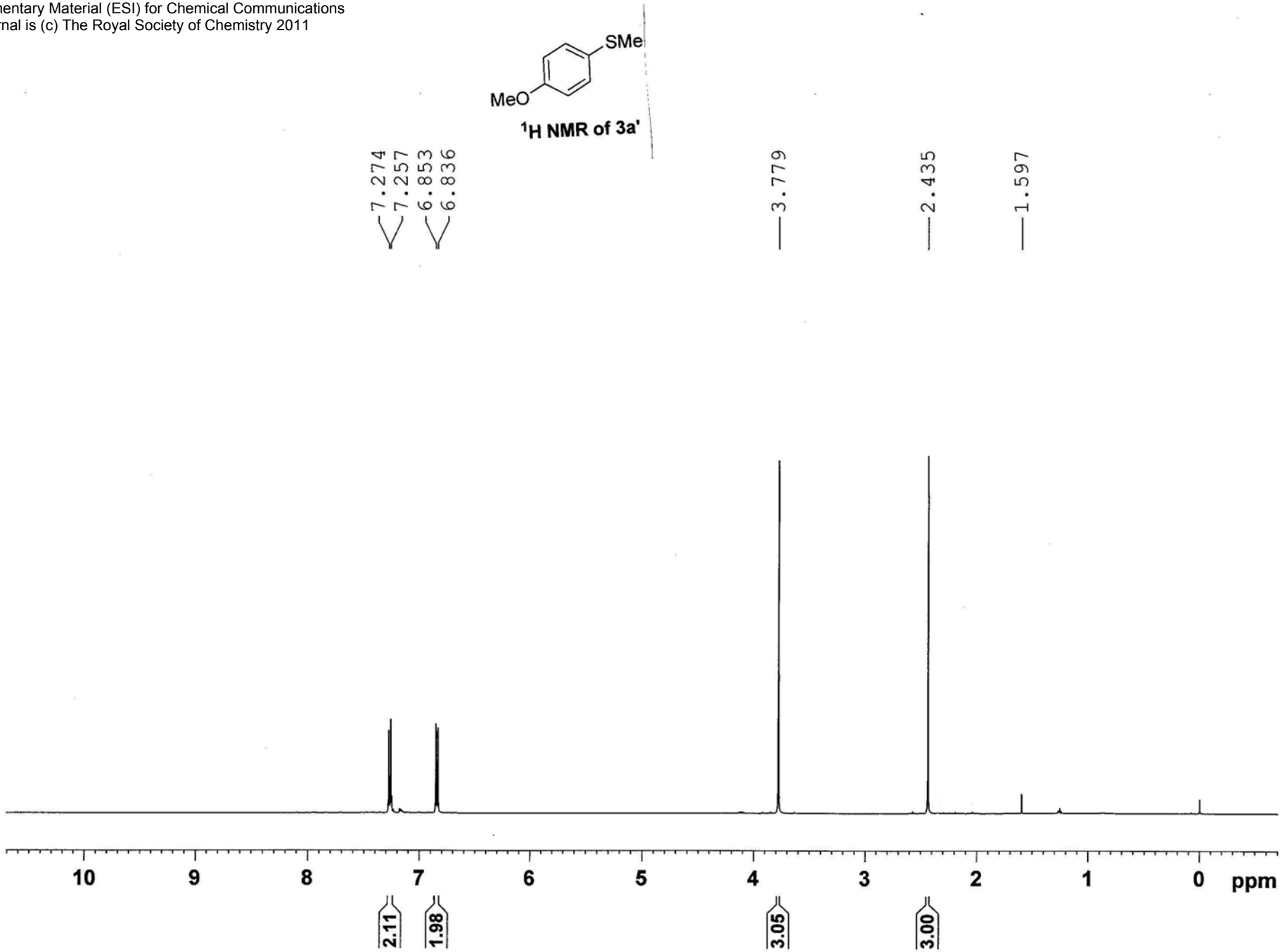
^{1}H NMR of 3p

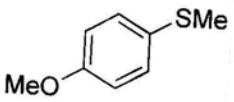



SMe
MeS

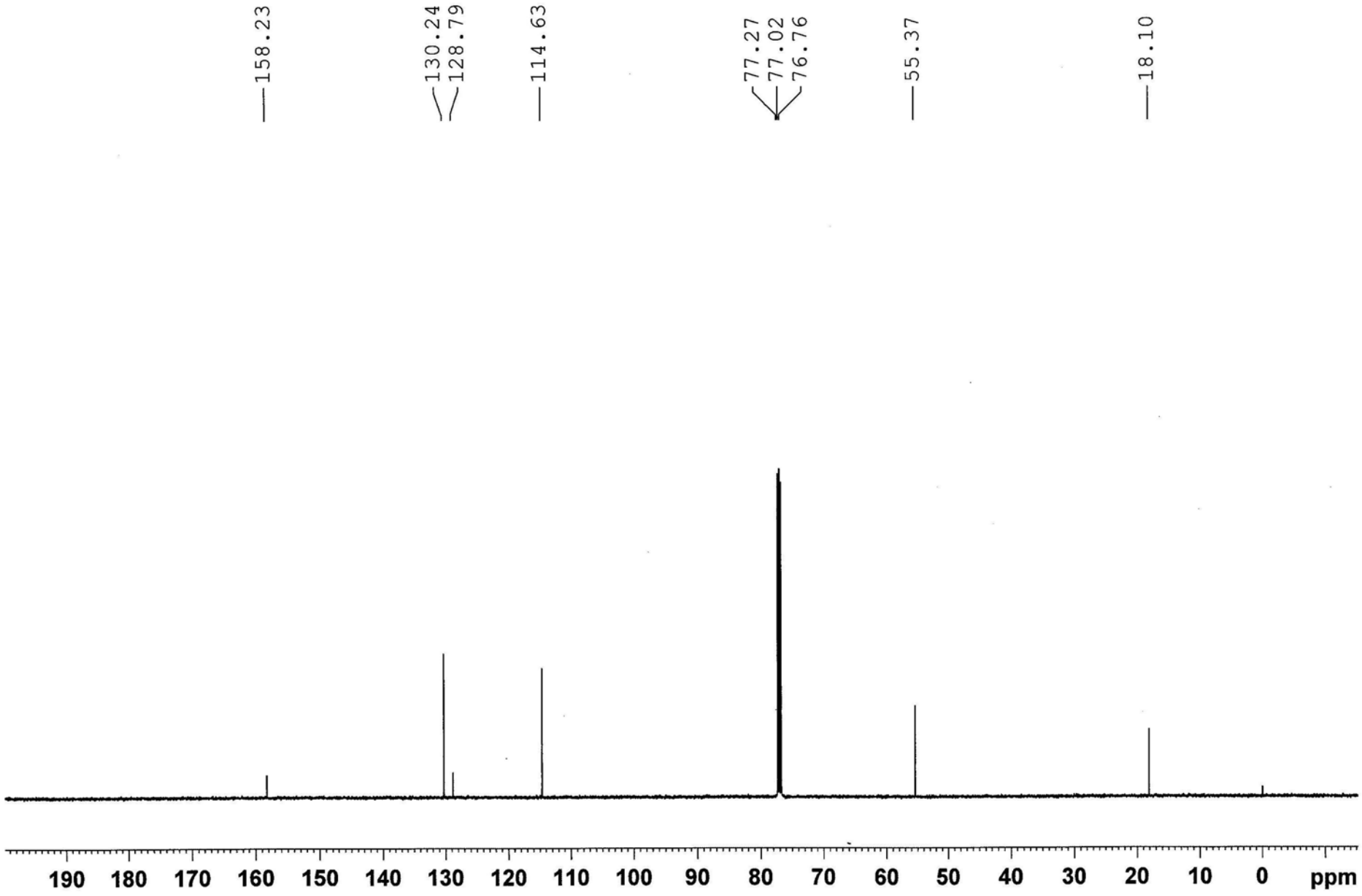
^{13}C NMR of 3p

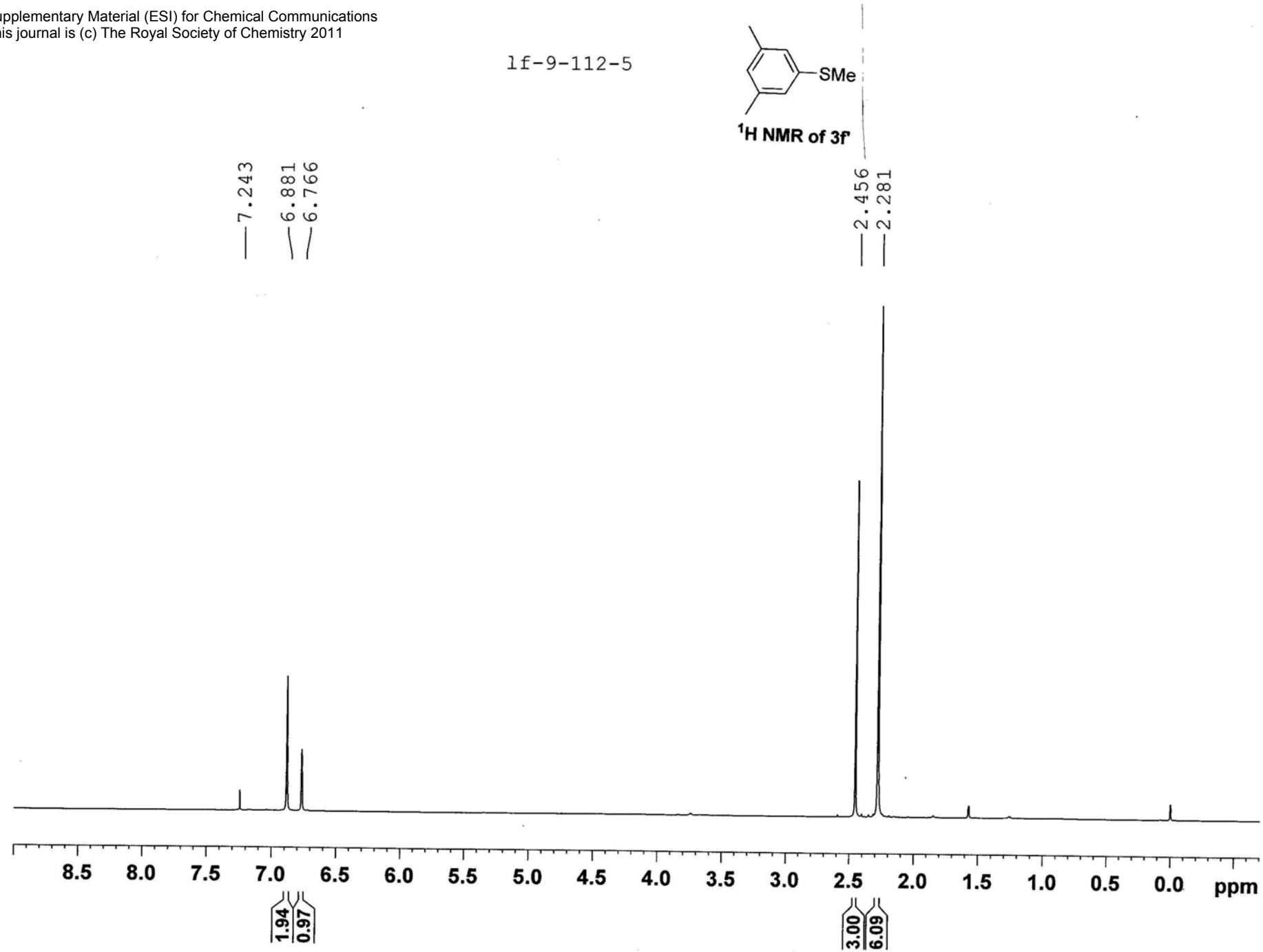

135.19
127.66
77.28
77.03
76.77
16.41
0.01
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


SMe
MeO
¹H NMR of 3a'
7.274
7.257
6.853
6.836
3.779
2.435
1.597
10
9
8
7
6
5
4
3
2
1
0
ppm
2.11
1.98
3.05
3.00

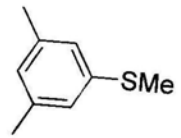

SMe
MeO

^{13}C NMR of 3a'

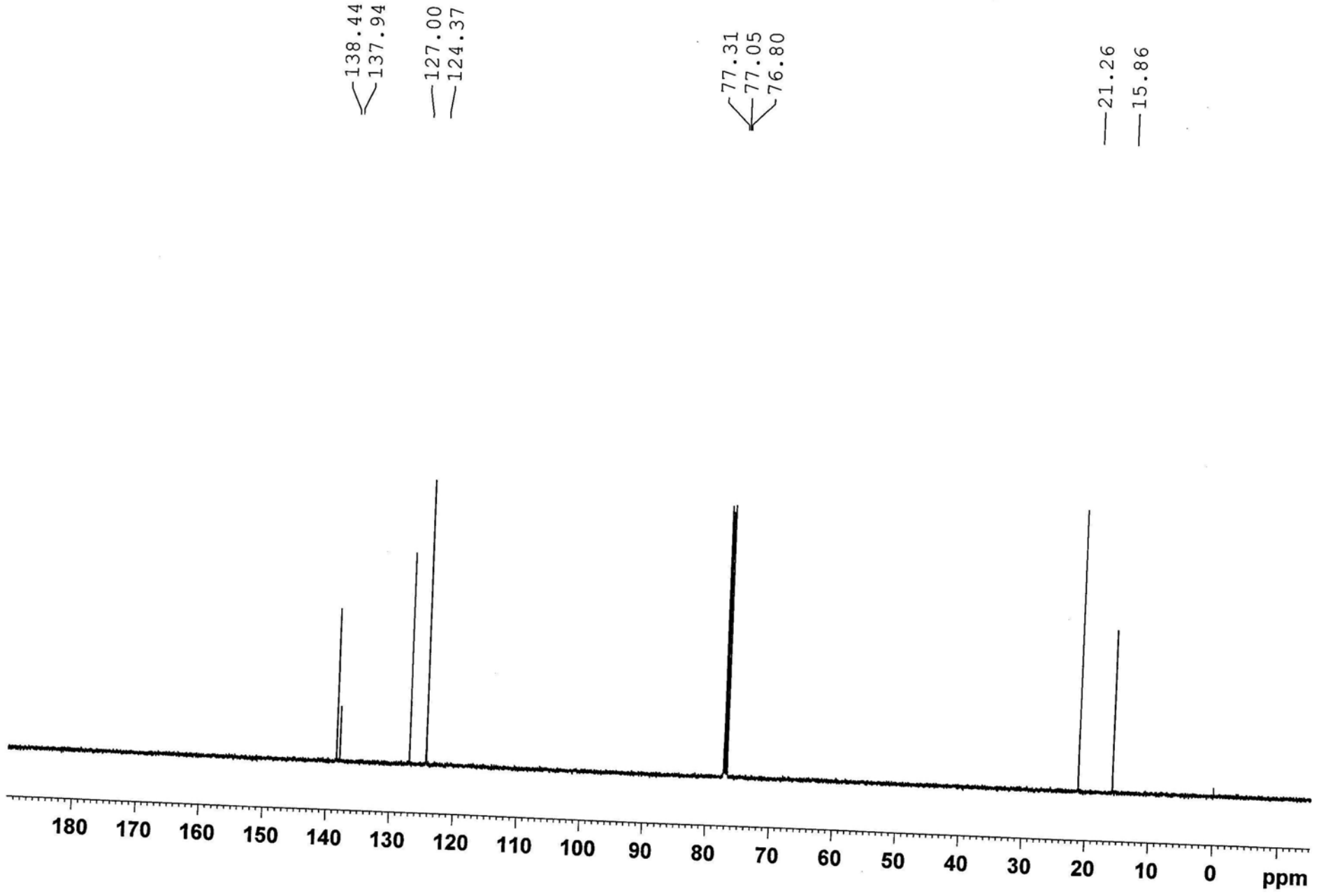

158.23
130.24
128.79
114.63
77.27
77.02
76.76
55.37
18.10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

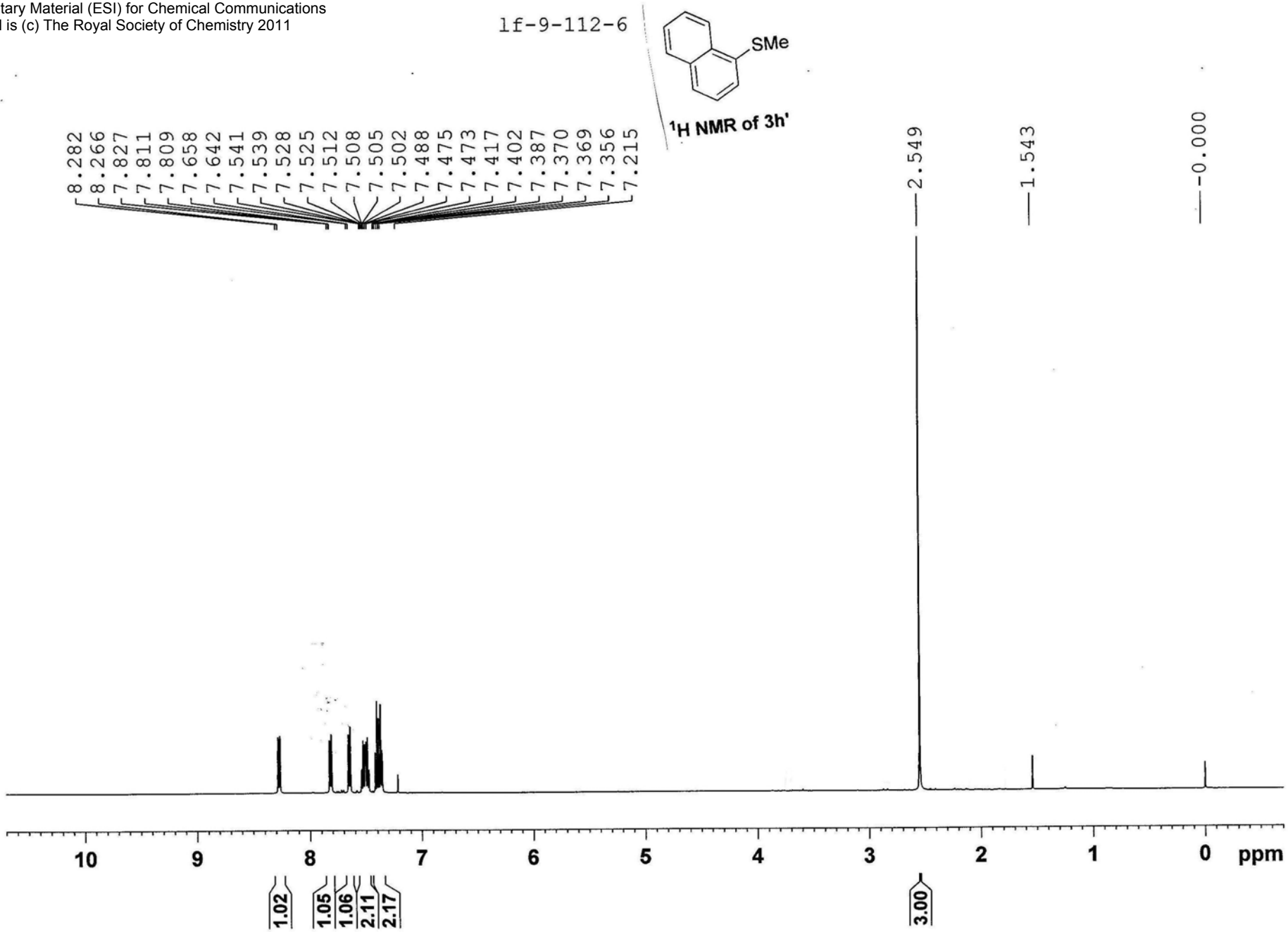

lf-9-112-5
SMe
1H NMR of 3f
7.243
6.881
6.766
2.456
2.281
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.94
0.97
3.00
6.09

lf-9-112-5

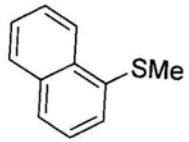


^{13}C NMR of 3f'




lf-9-112-6
SMe
^{1}H NMR of 3h'
8.282
8.266
7.827
7.811
7.809
7.658
7.642
7.541
7.539
7.528
7.525
7.512
7.508
7.505
7.502
7.488
7.475
7.473
7.417
7.402
7.387
7.370
7.369
7.356
7.215
2.549
1.543
-0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.05
1.06
2.11
2.17
3.00

lf-9-112-6

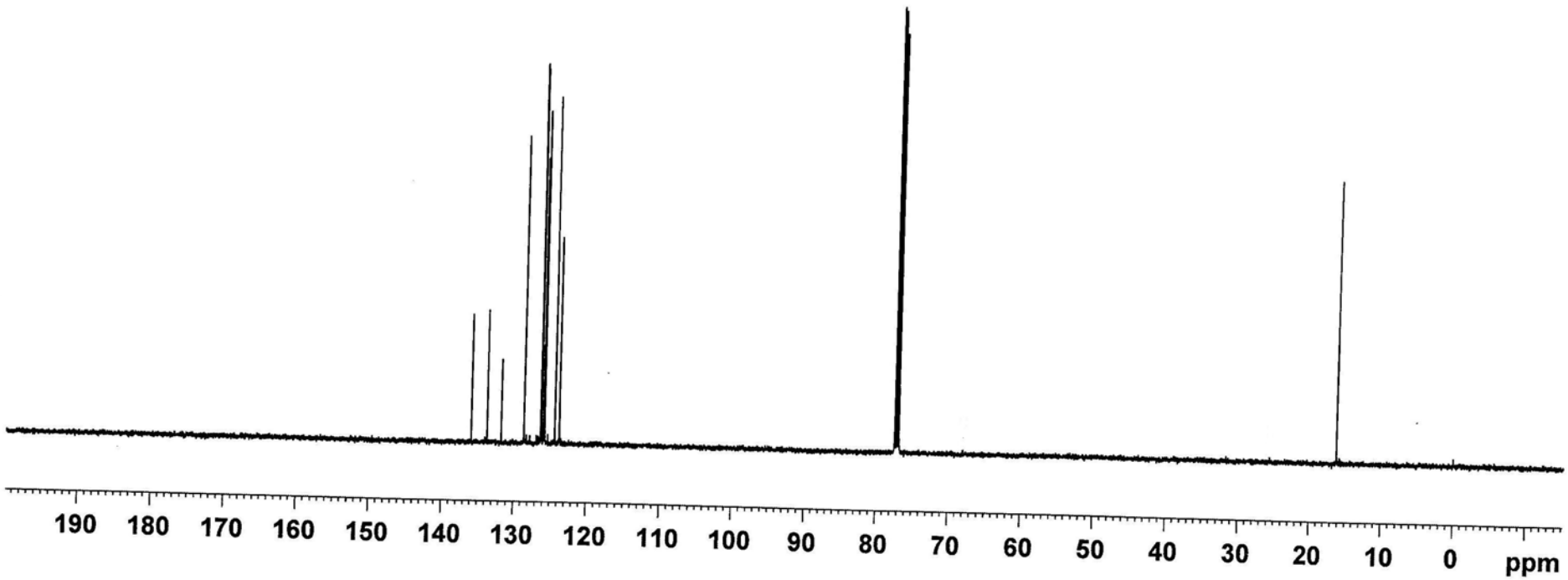


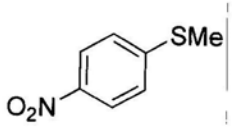
^{13}C NMR of 3h'

135.87
133.67
131.71
128.57
126.26
126.17
125.88
125.72
124.33
123.70

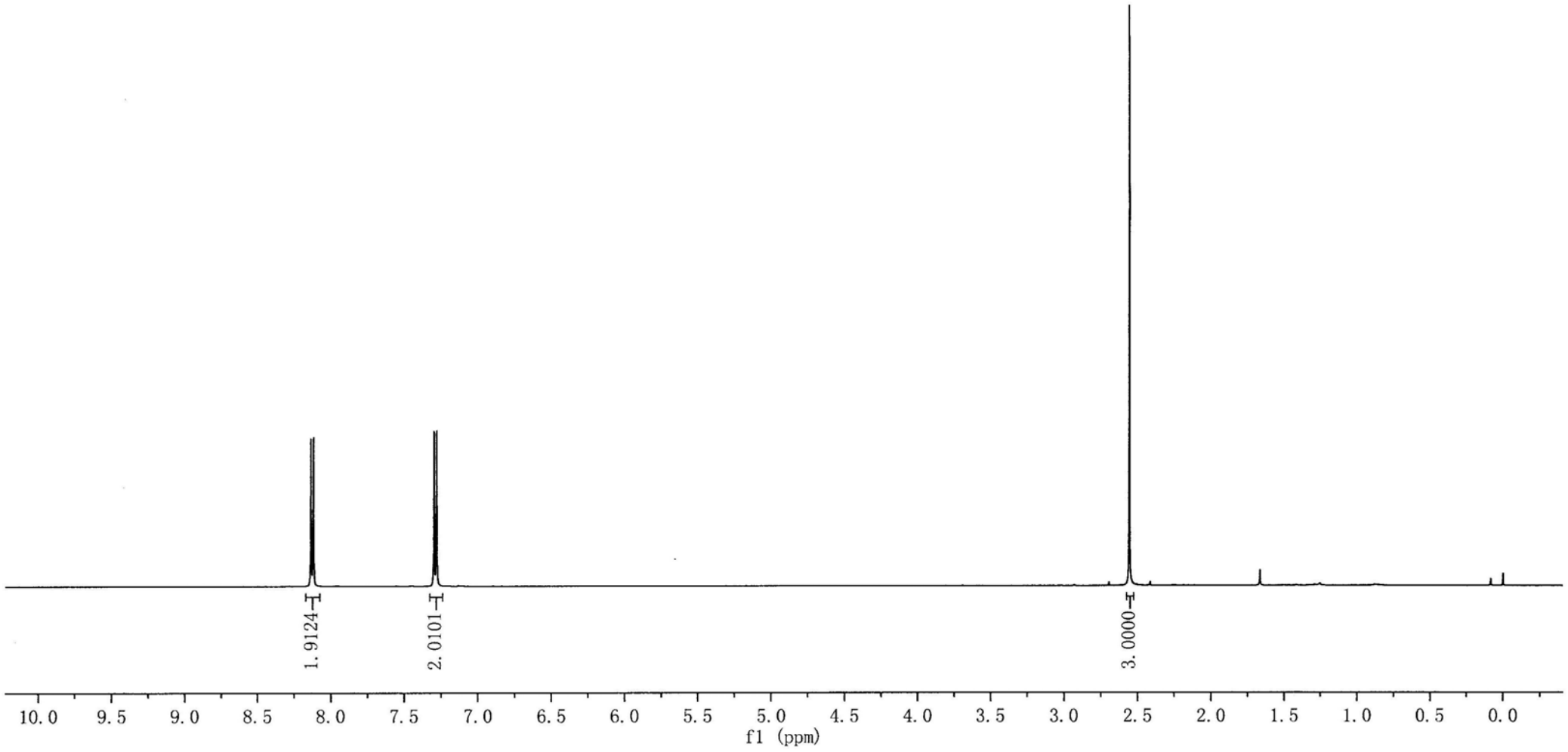
77.34
77.09
76.83

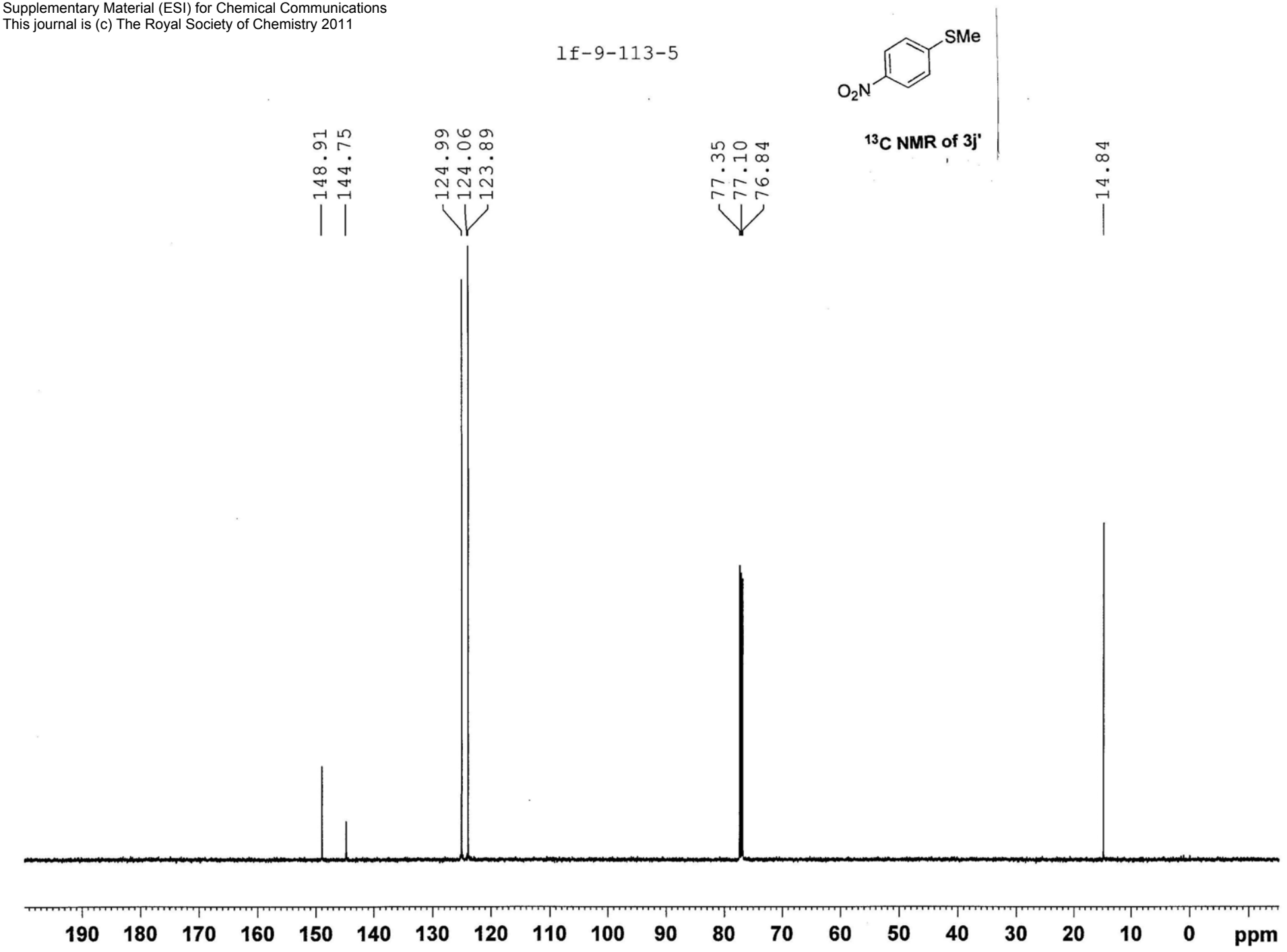
16.25

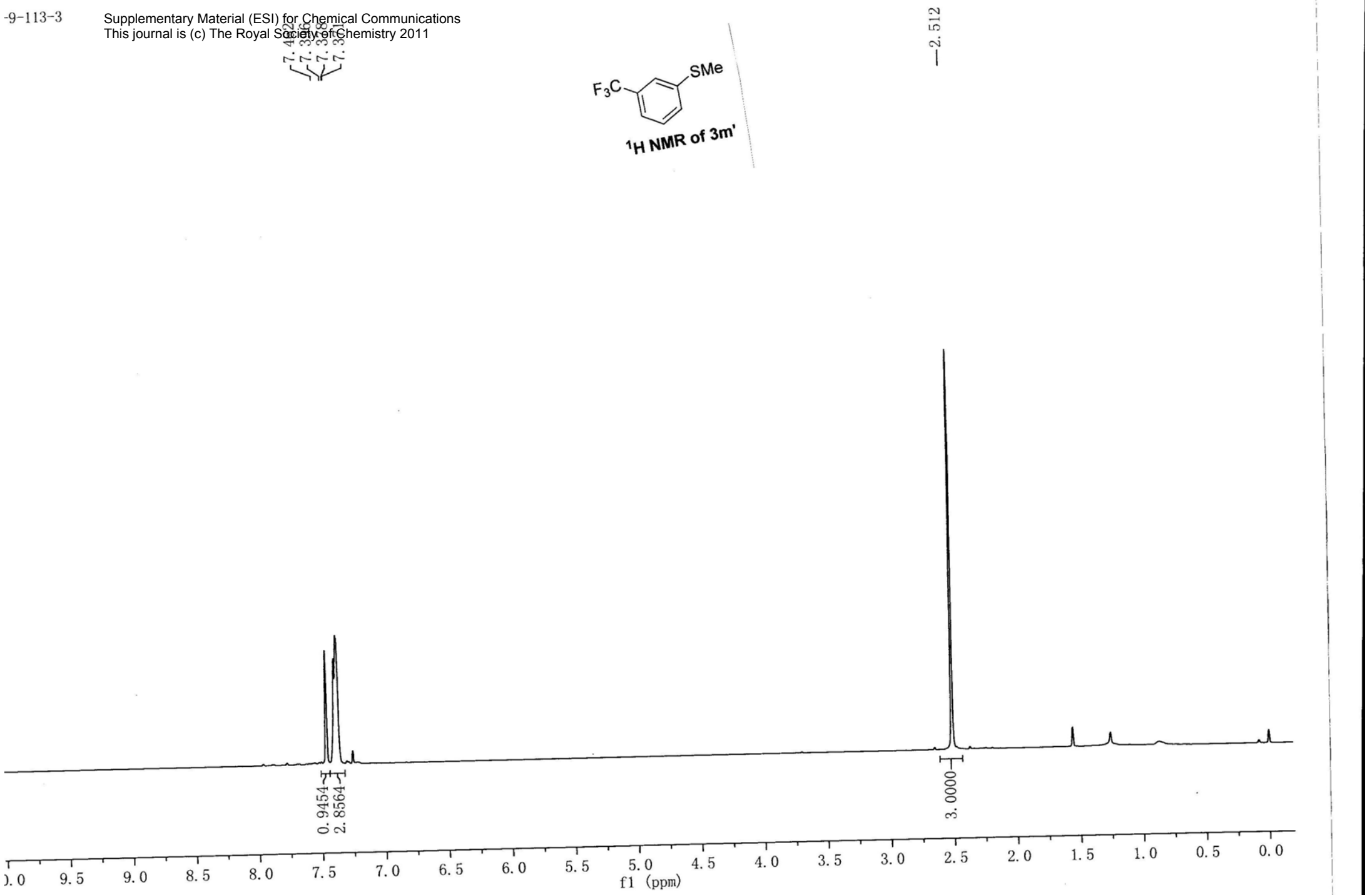




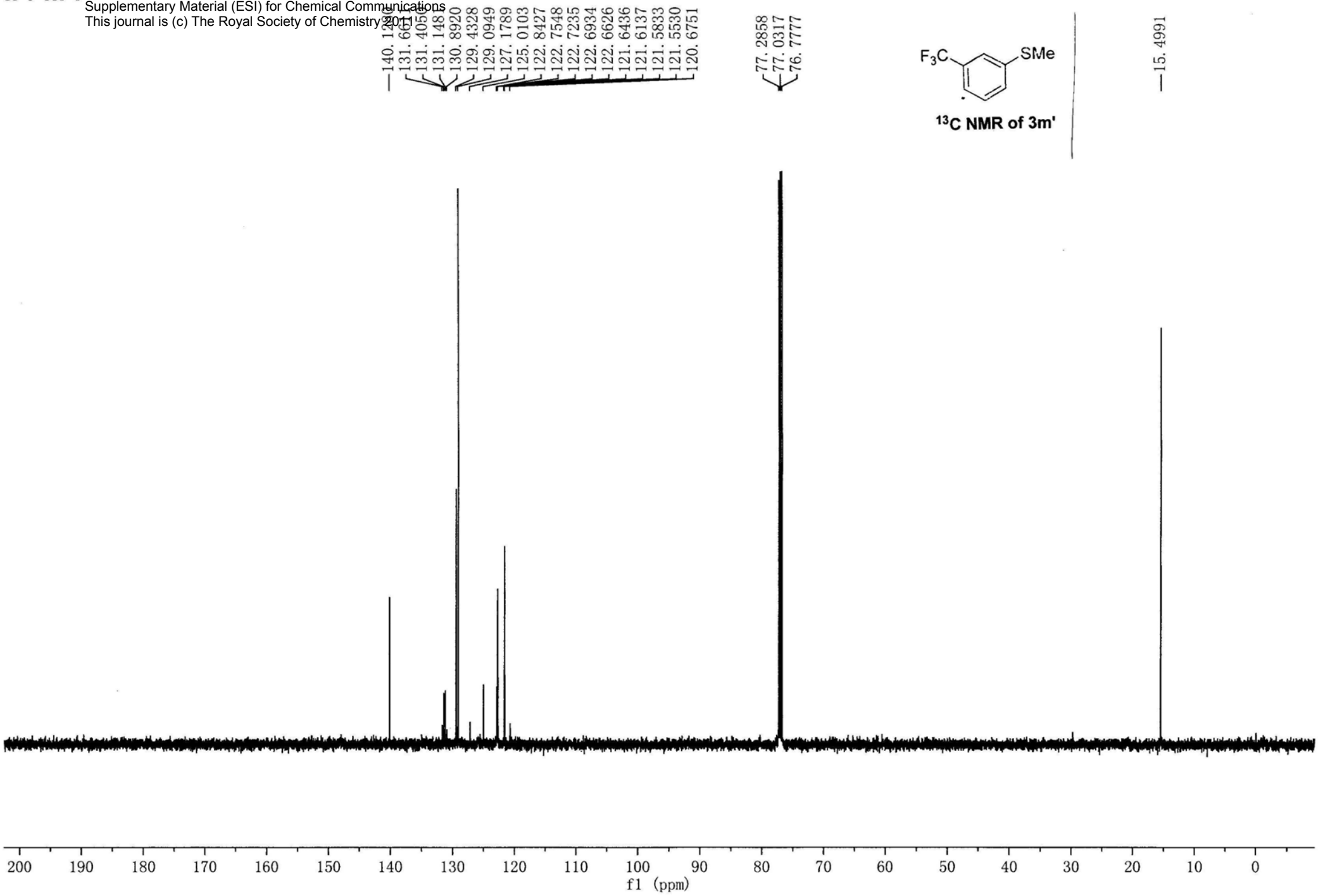
^{1}H NMR of 3j'




lf-9-113-5
SMe
O_2N
^{13}C NMR of 3j'
148.91
144.75
124.99
124.06
123.89
77.35
77.10
76.84
14.84
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

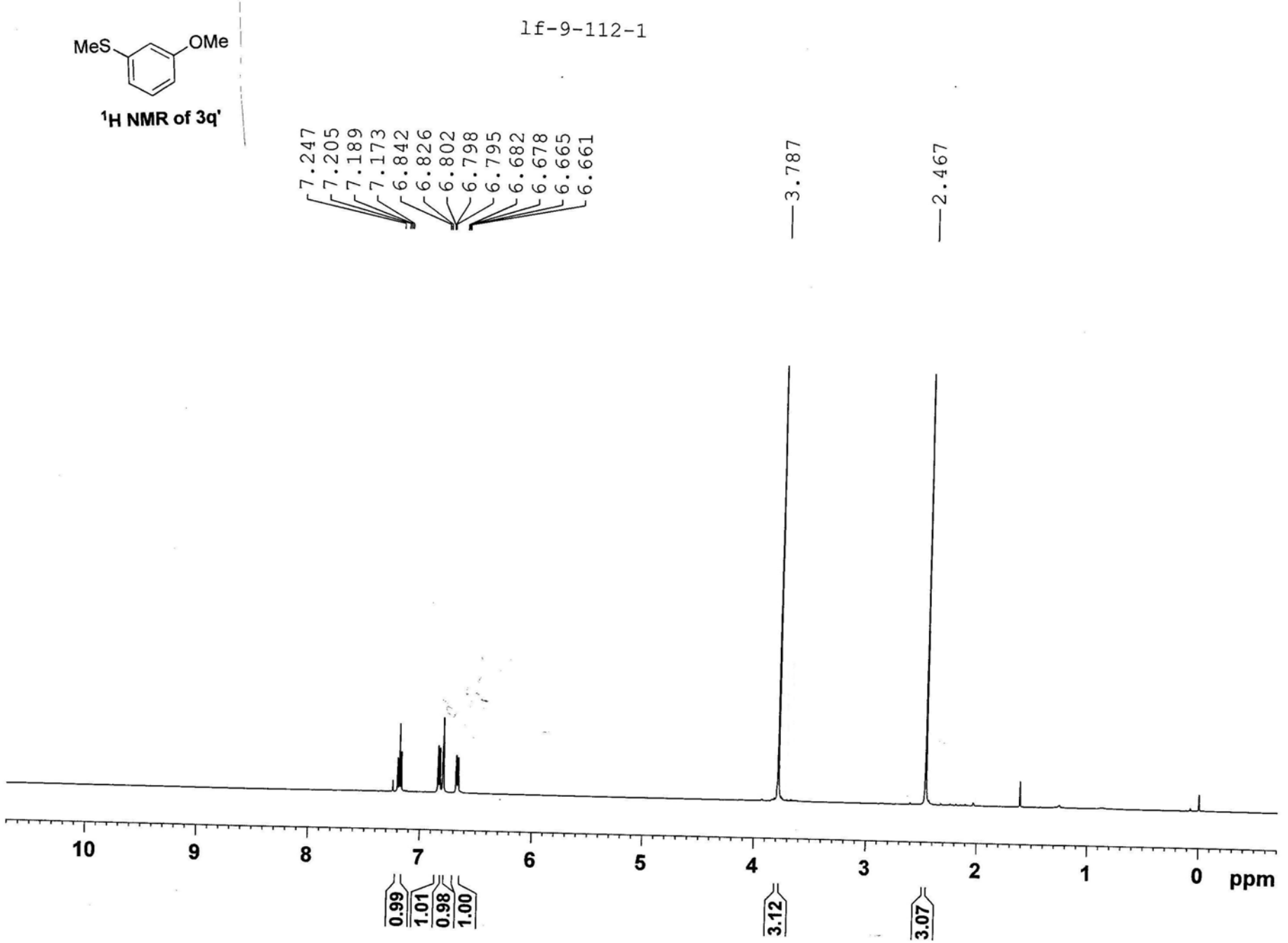


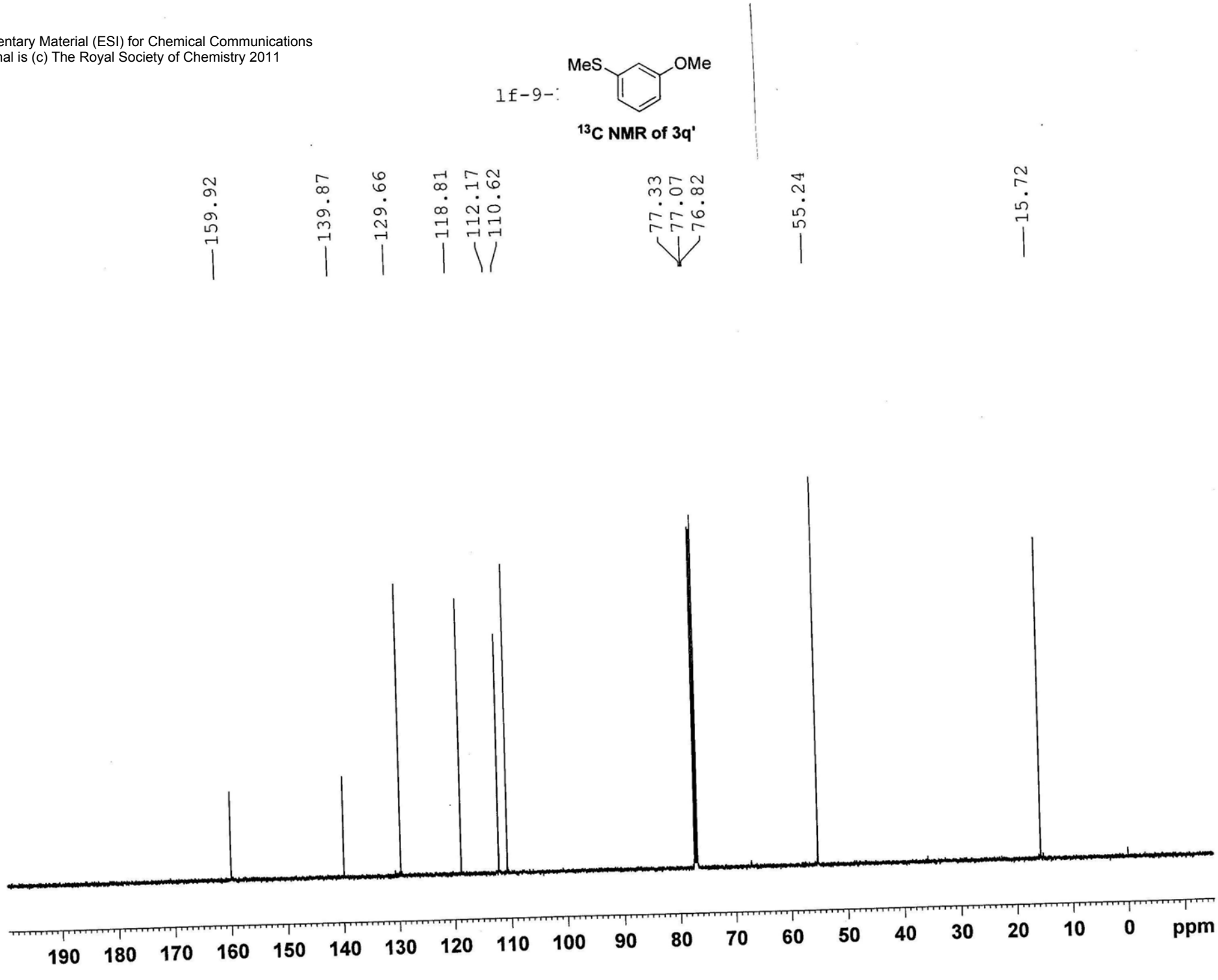
^{1}H NMR of 3m'



MeS
OMe

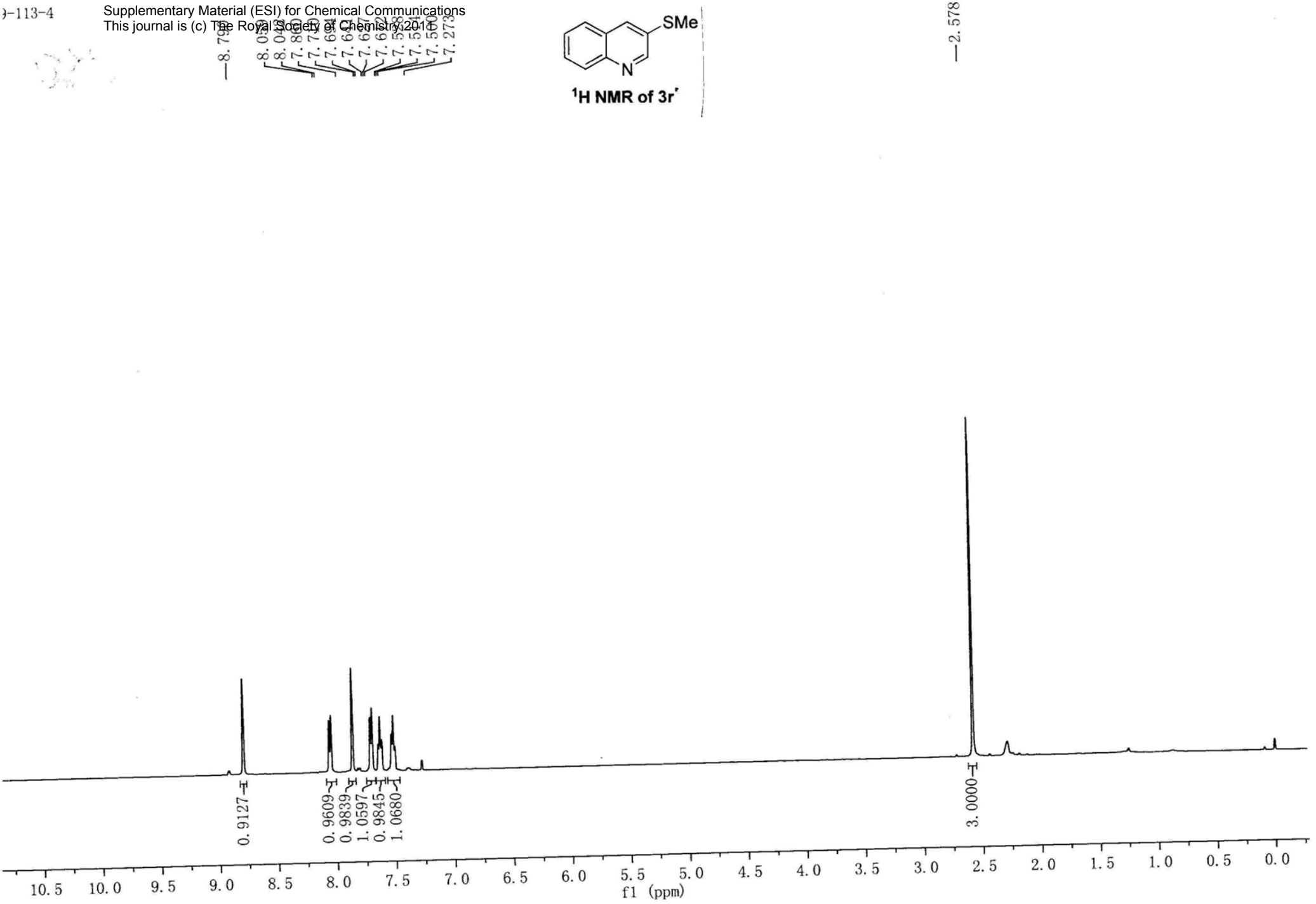
^{1}H NMR of 3q'


lf-9-112-1
7.247
7.205
7.189
7.173
6.842
6.826
6.802
6.798
6.795
6.682
6.678
6.665
6.661
3.787
2.467
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.01
0.98
1.00
3.12
3.07


MeS
OMe
1f-9-1
13C NMR of 3q'
159.92
139.87
129.66
118.81
112.17
110.62
77.33
77.07
76.82
55.24
15.72
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Supplementary Material (ESI) for Chemical Communications

^{1}H NMR of 3r'



Supplementary Material (ESI) for Chemical Communications
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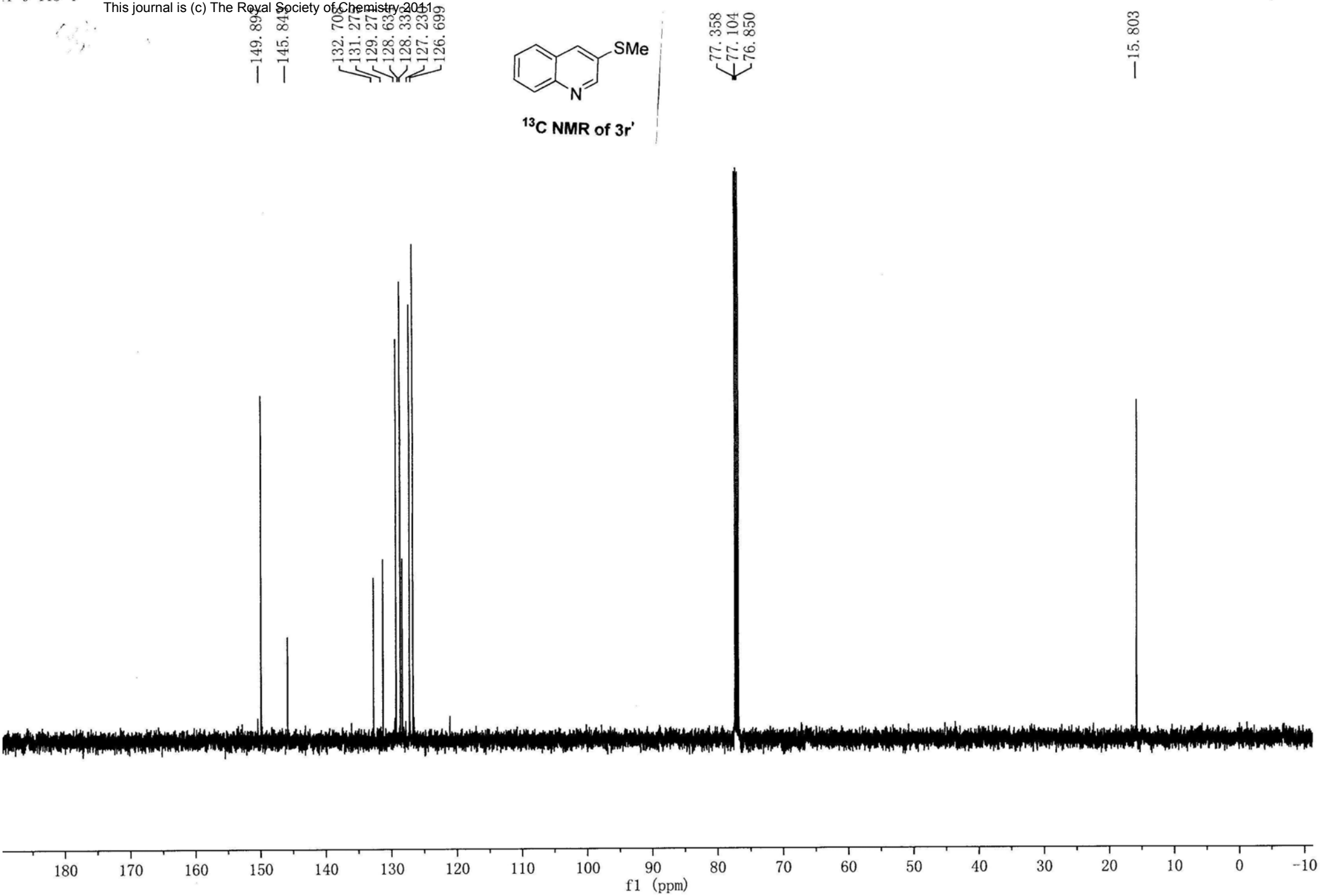
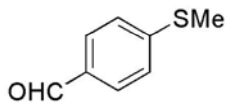
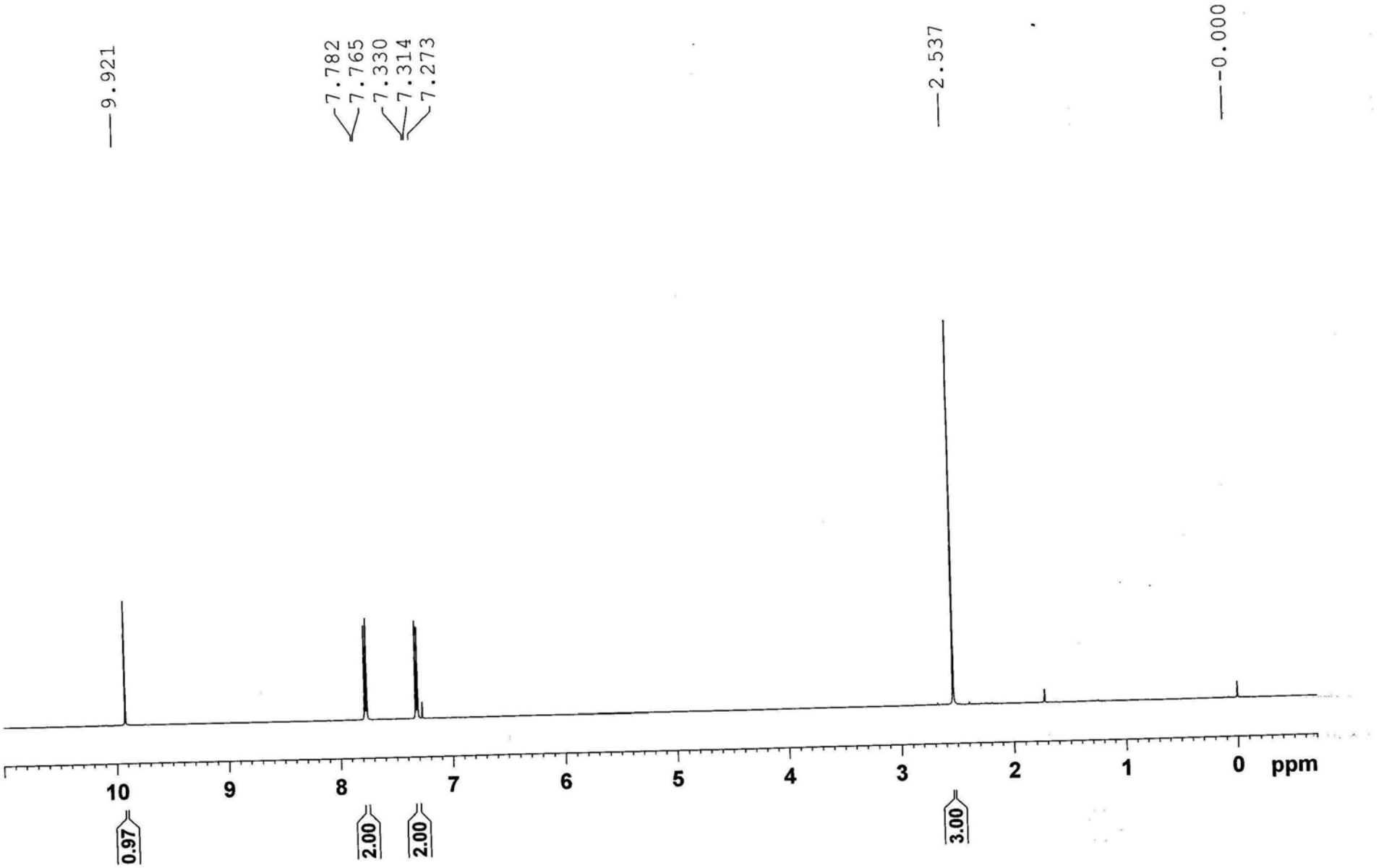
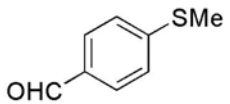


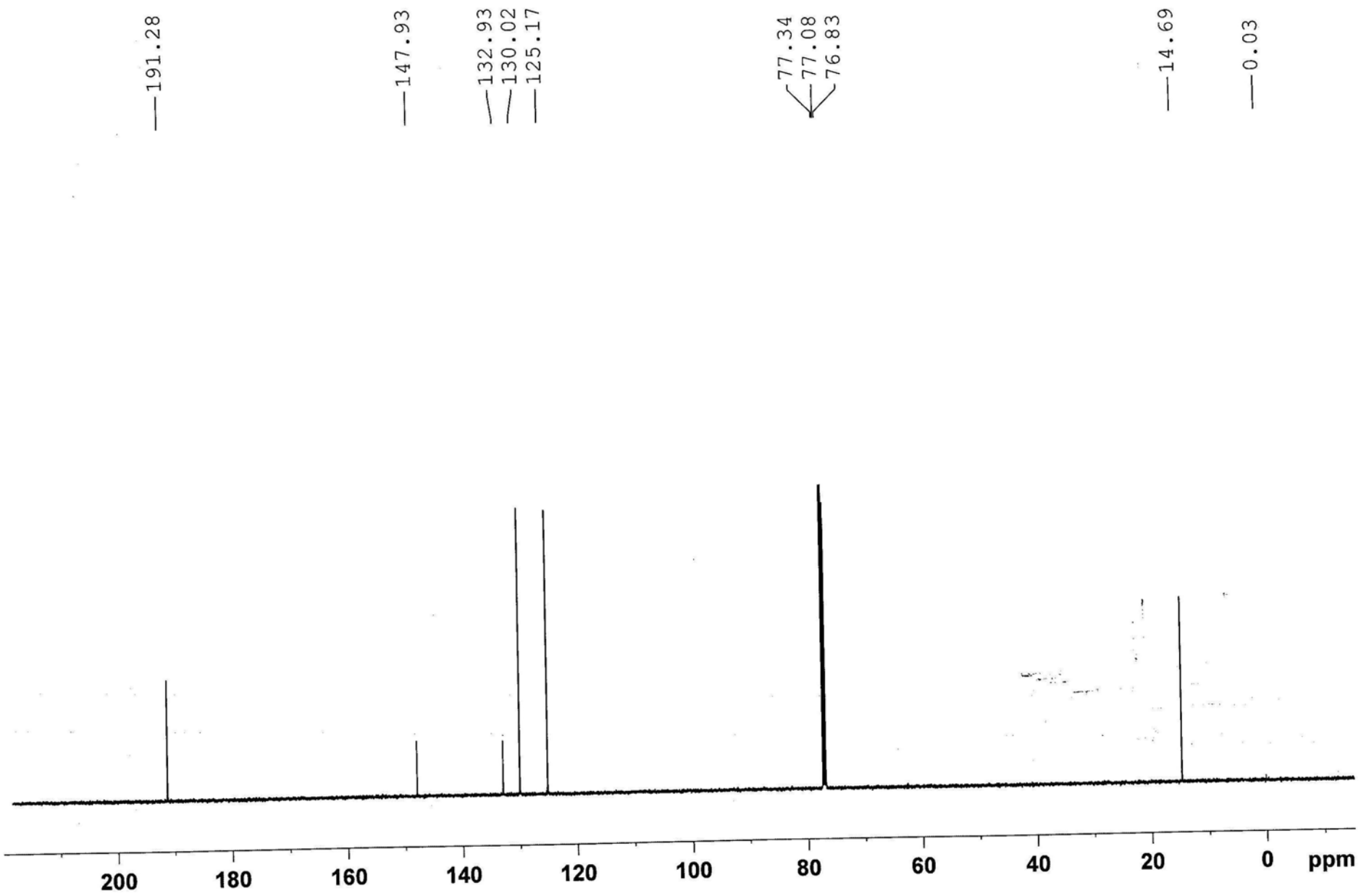

SMe
OHC

^{1}H NMR of 3s'

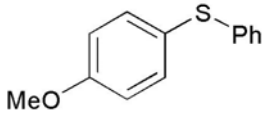

9.921
7.782
7.765
7.330
7.314
7.273
2.537
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.00
2.00
3.00


SMe
OHC

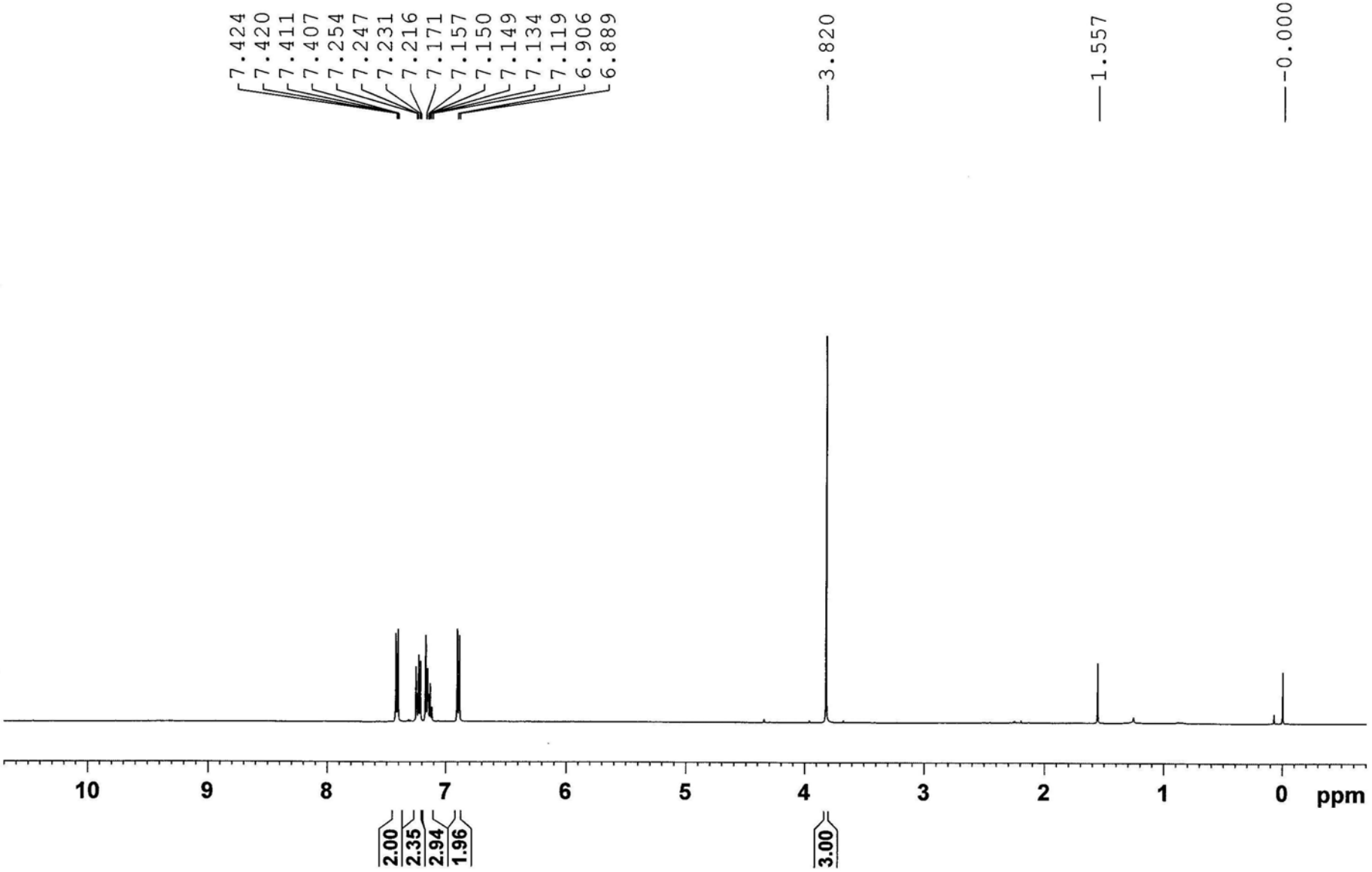
^{13}C NMR of 3s'

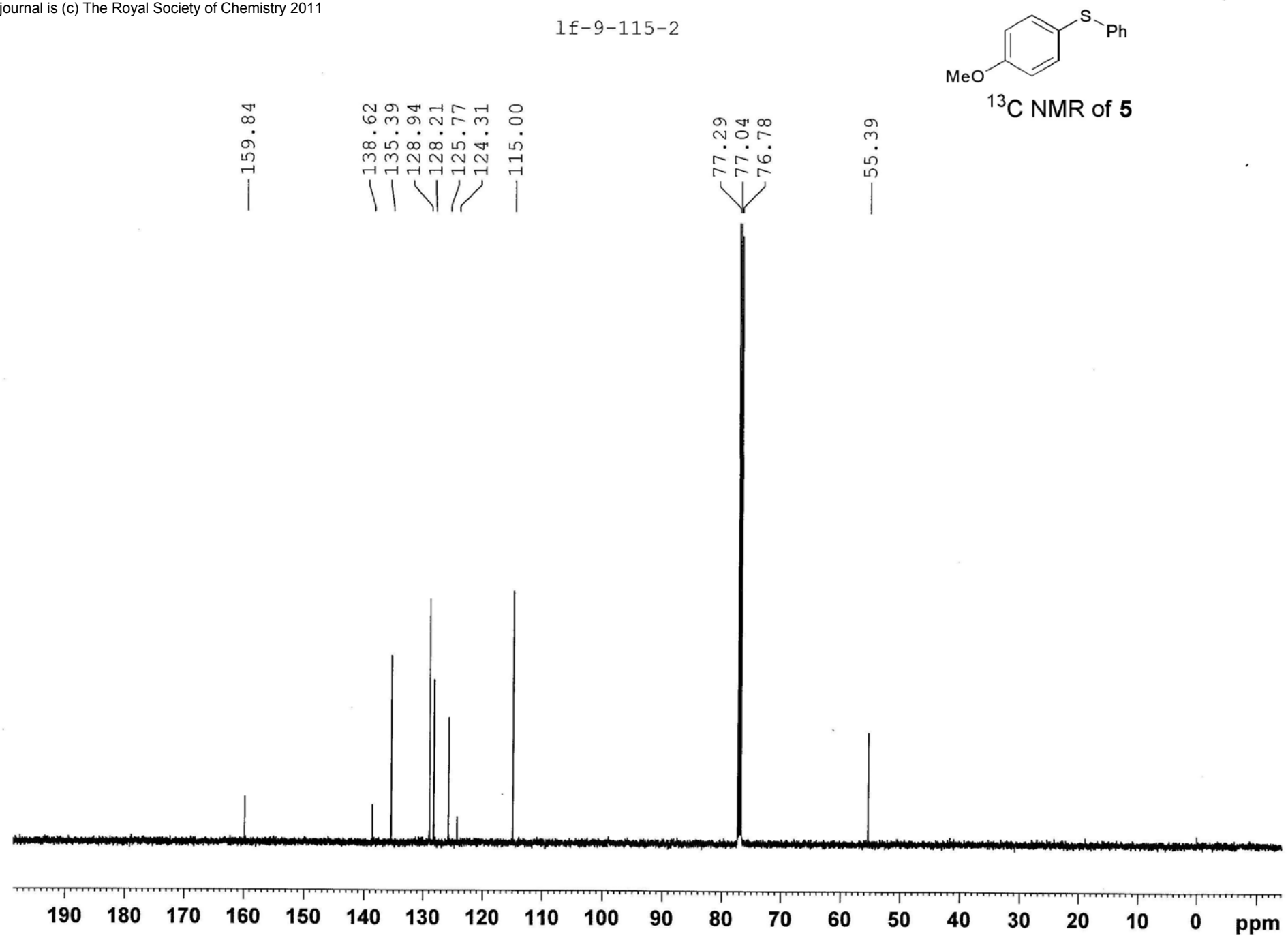

191.28
147.93
132.93
130.02
125.17
77.34
77.08
76.83
14.69
0.03
200
180
160
140
120
100
80
60
40
20
0
ppm

lf-9-115-2



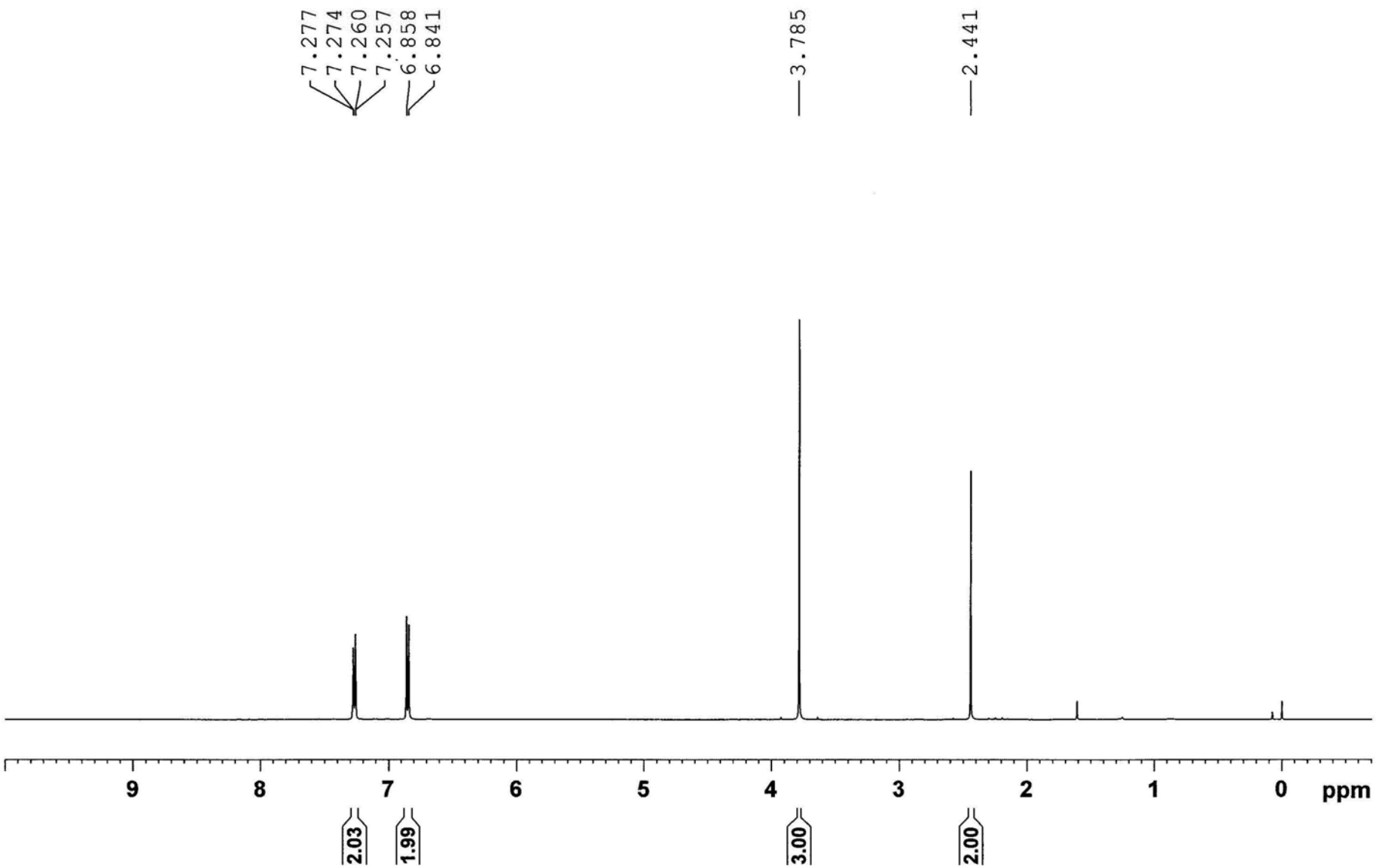
^{1}H NMR of **5**




1f-9-115-2
S
Ph
MeO
159.84
138.62
135.39
128.94
128.21
125.77
124.31
115.00
77.29
77.04
76.78
55.39
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C NMR of **5**

HNMR of 3+3'


7.277
7.274
7.260
7.257
6.858
6.841
3.785
2.441
9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.99
3.00
2.00