

Supporting Information

Temperature-Controlled Thiation of α -Cyano- β -Alkynyl Carbon-yl Derivatives for De Novo Synthesis of 2-Aminothiophenes and Thieno[2,3-*c*]isothiazoles

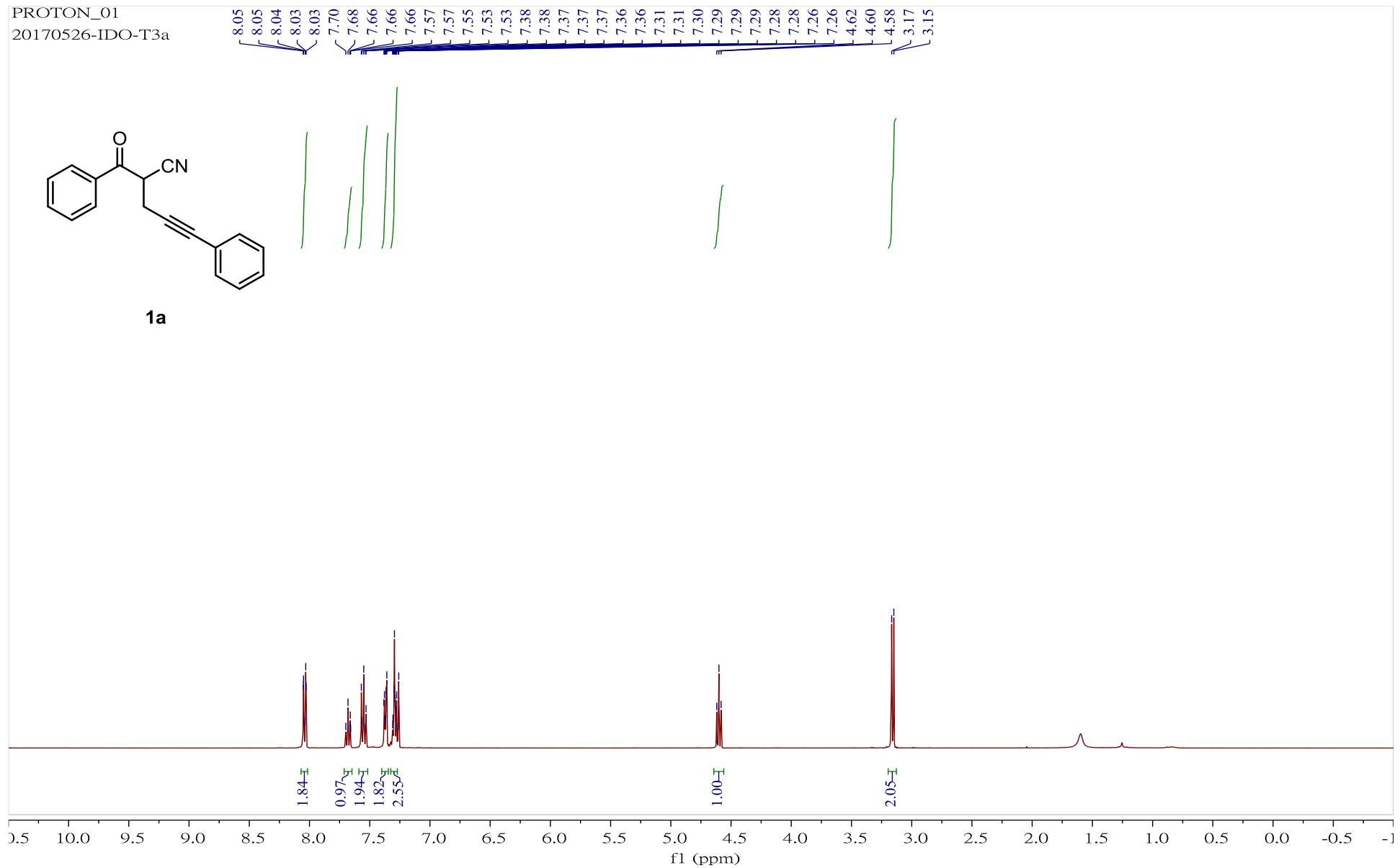
Tzu-Ting Kao[†], Bo-Kai Peng[‡], Min-Chieh Liang[‡], Chia-Jui Lee[†], I-Chia Chen[§], Kak-Shan Shia^{*†} and Yen-Ku Wu^{*‡}

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[‡] Department of Applied Chemistry, National Chiao Tung University, 1001 University Road, Hsinchu 30010, Taiwan

[§] Department of Cosmetic Applications and Management, Cardinal Tien Junior College of Healthcare and Management, New Taipei City 23143, Taiwan

PROTON_01
20170526-IDO-T3a



^1H NMR (400 MHz) spectrum of compound **1a** in CDCl_3

CARBON_01
20170526-IDO-T3a-13C

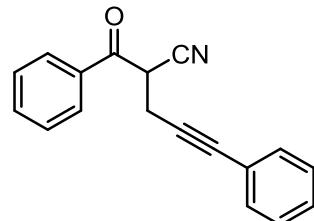
— 188.8

134.8
133.9
131.7
129.2
128.9
128.4
128.2
122.5
116.3

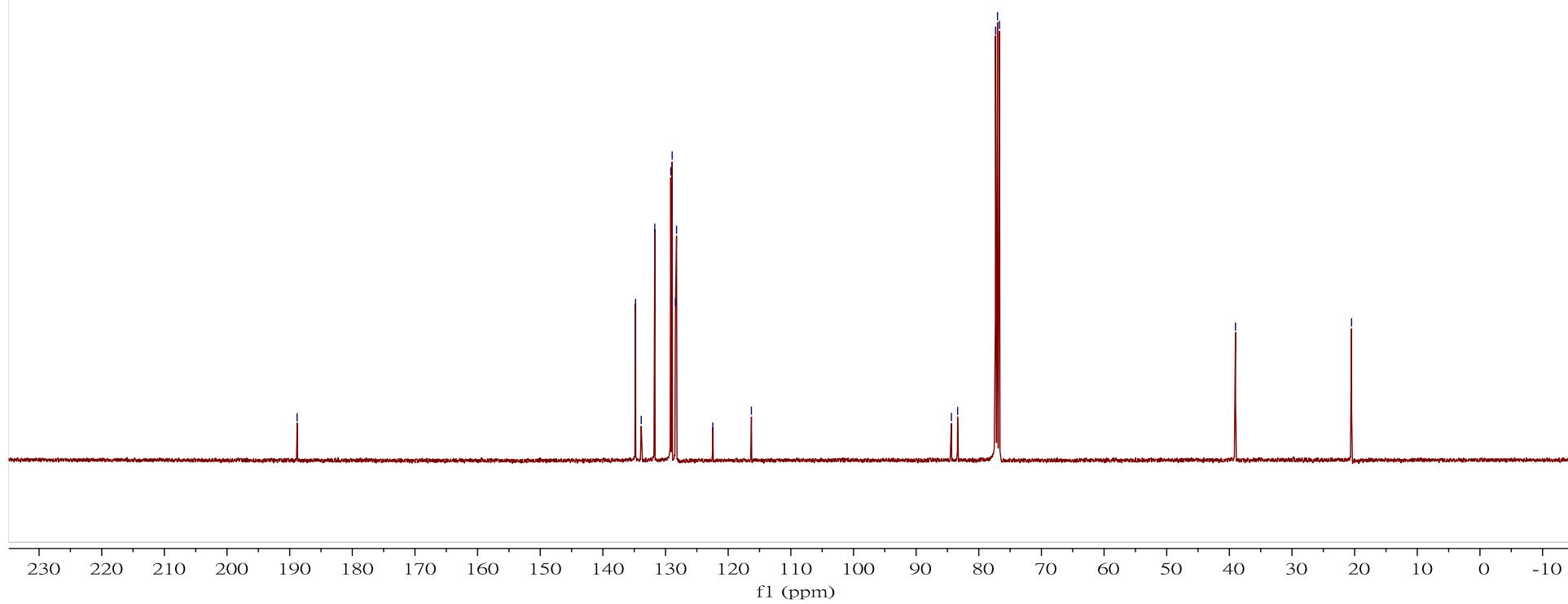
84.4
83.4
77.3
77.0
76.7

— 39.0

— 20.5

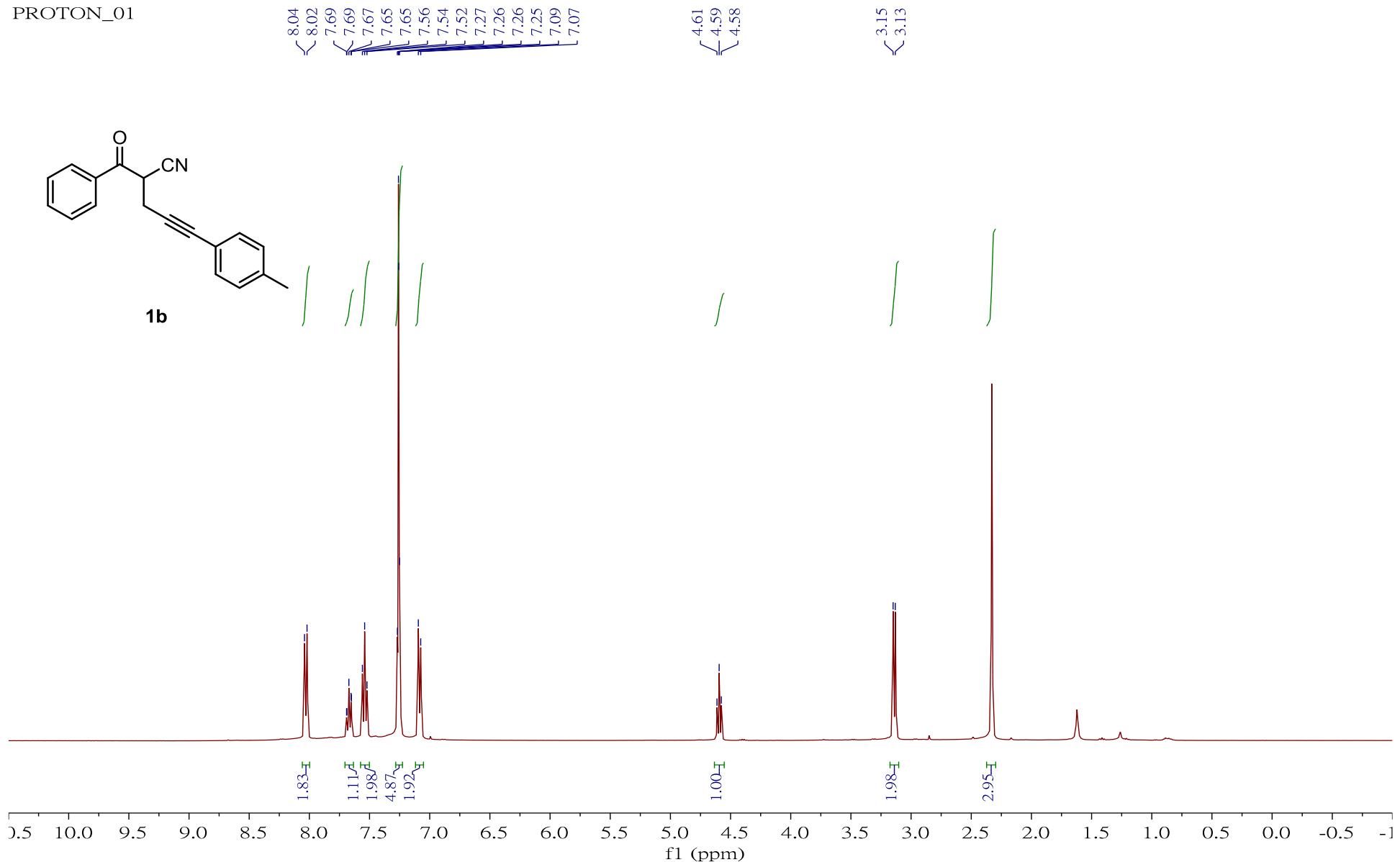


1a



^{13}C NMR (100 MHz) spectrum of compound **1a** in CDCl_3

PROTON_01



^1H NMR (400 MHz) spectrum of compound **1b** in CDCl_3

CARBON_01
1b carbon 1202

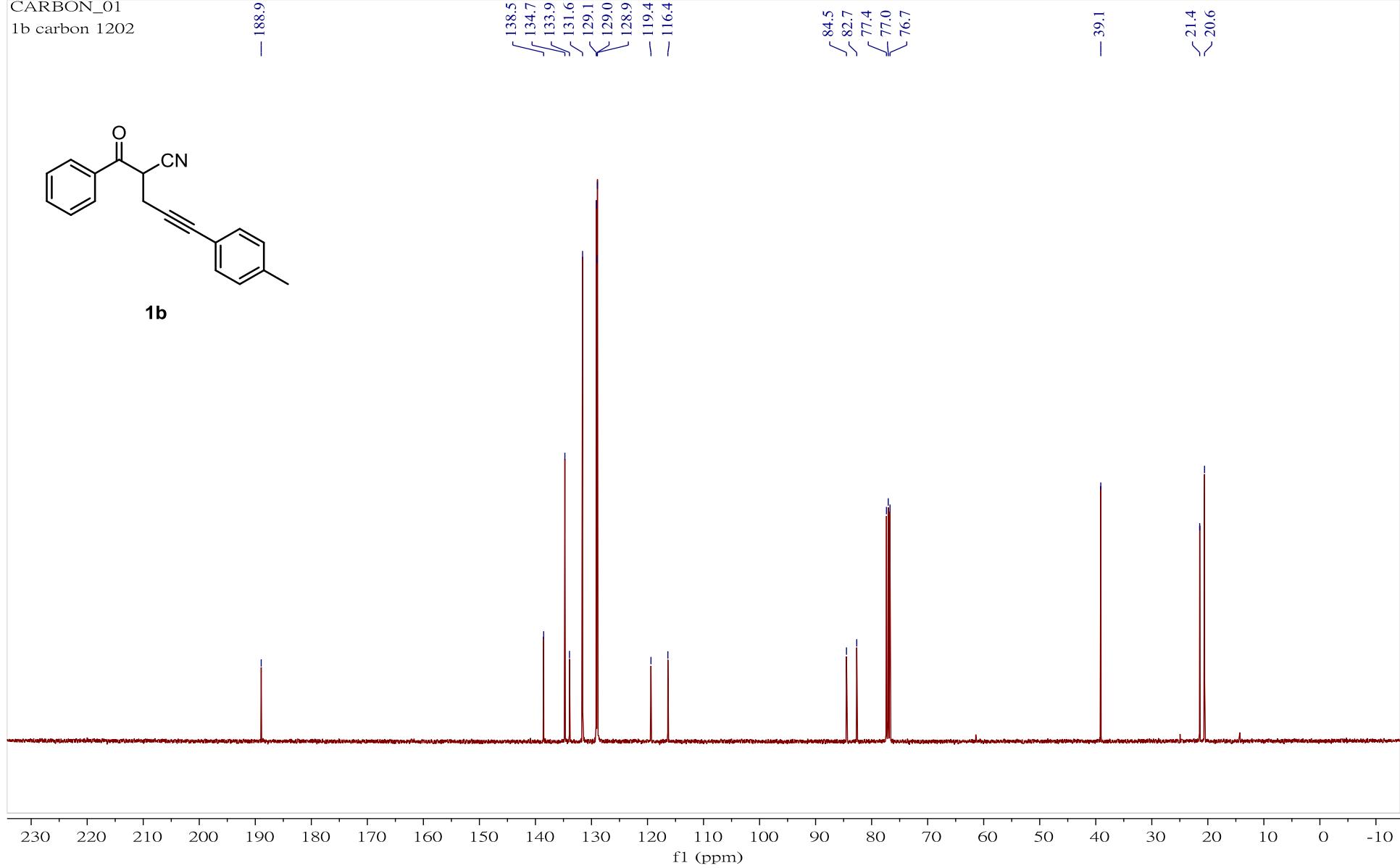
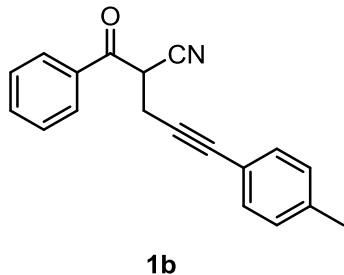
— 188.9

138.5
134.7
133.9
131.6
129.1
129.0
128.9
— 119.4
— 116.4

84.5
82.7
77.4
77.0
76.7

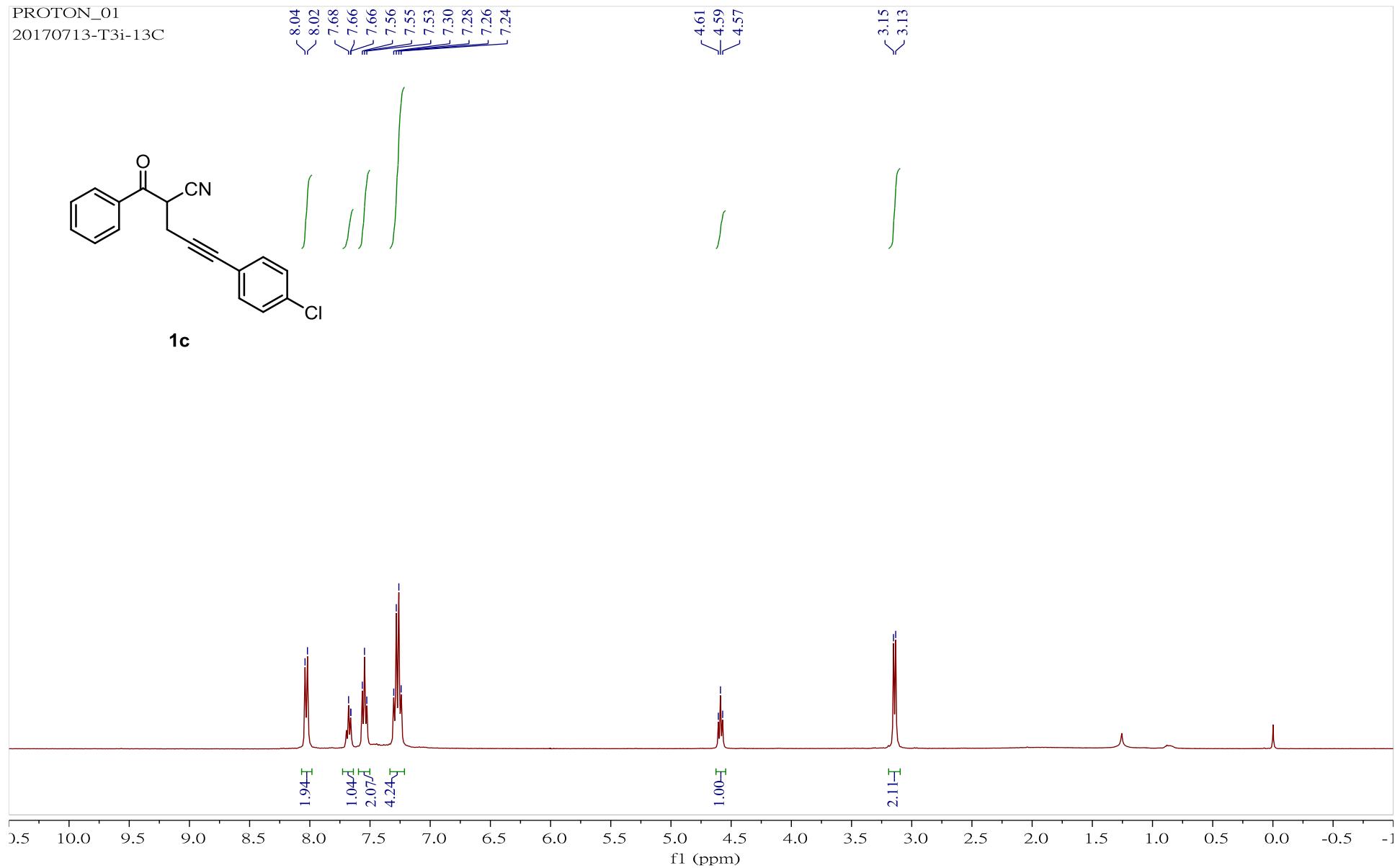
— 39.1

21.4
20.6



¹³C NMR (100 MHz) spectrum of compound **1b** in CDCl₃

PROTON_01
20170713-T3i-13C



^1H NMR (400 MHz) spectrum of compound **1c** in CDCl_3

CARBON_01
20170713-T3i-13C

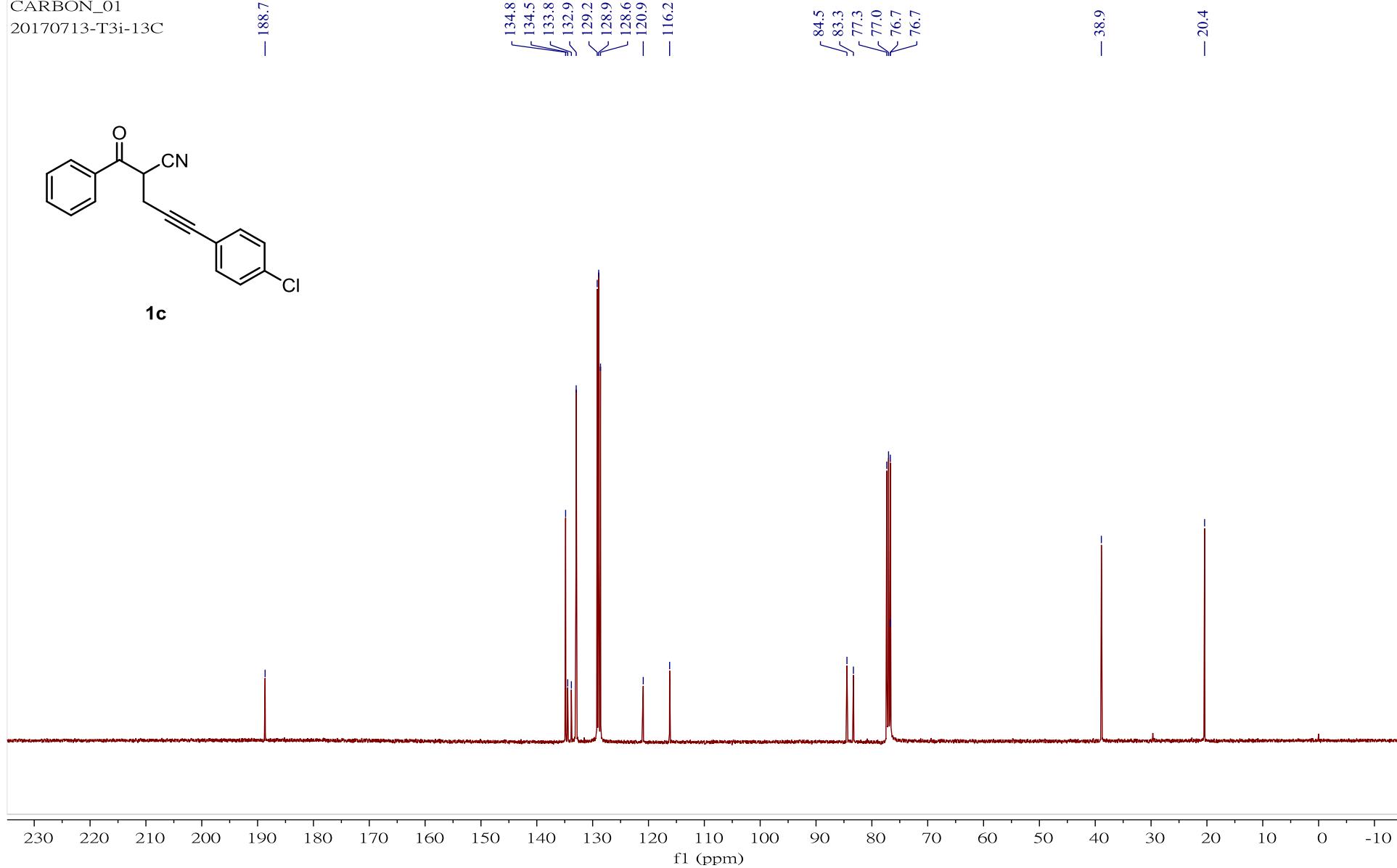
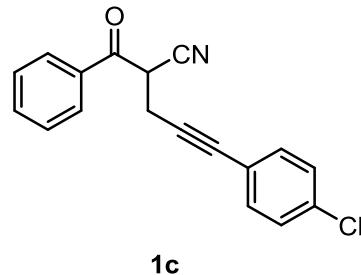
— 188.7

134.8
133.8
132.9
129.2
128.9
128.6
120.9
116.2

84.5
83.3
77.3
77.0
76.7
76.7

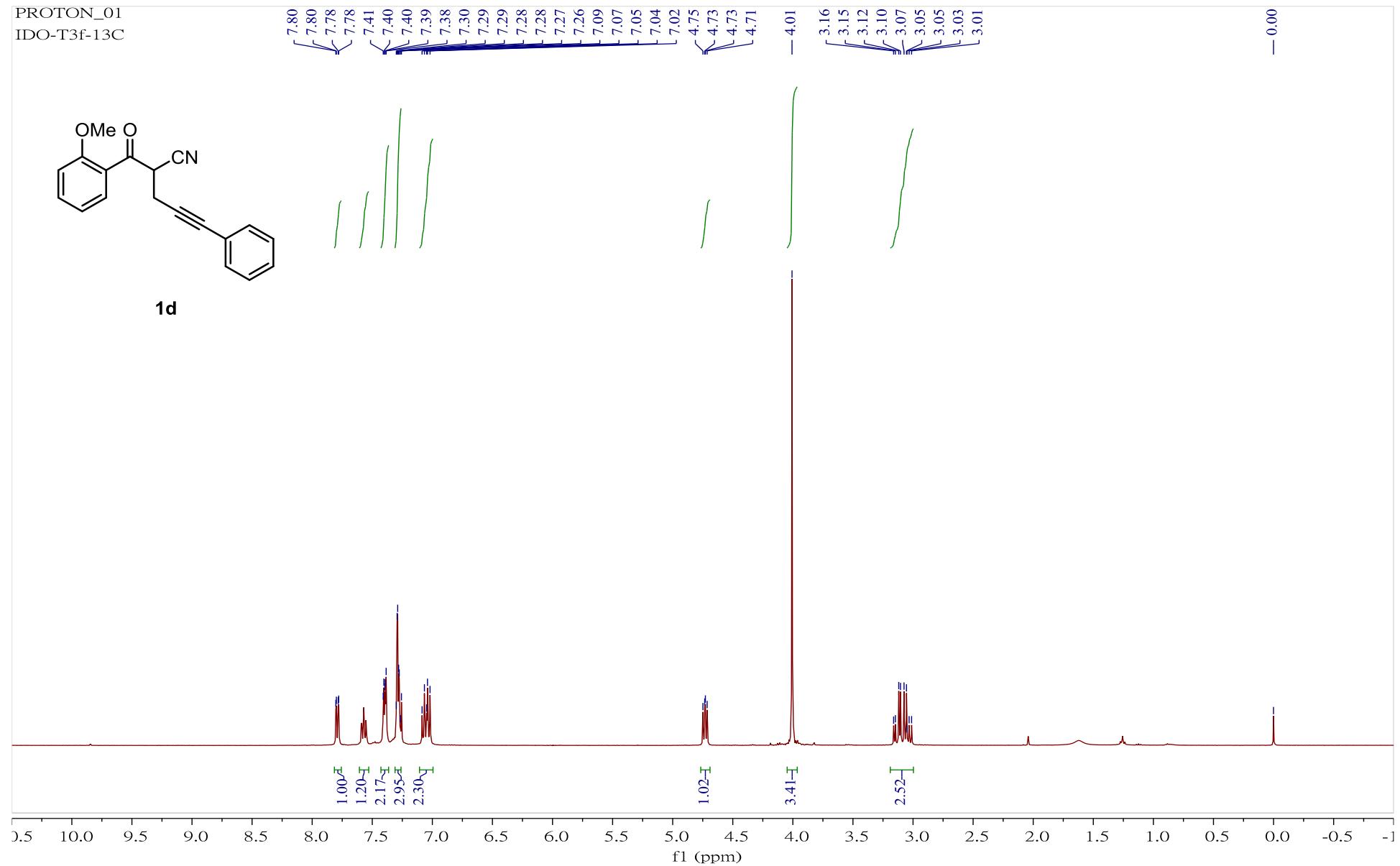
— 38.9

— 20.4



¹³C NMR (100 MHz) spectrum of compound **1c** in CDCl₃

PROTON_01
IDO-T3f-13C



^1H NMR (400 MHz) spectrum of compound **1d** in CDCl_3

CARBON_01
IDO-T3f-13C

— 190.4

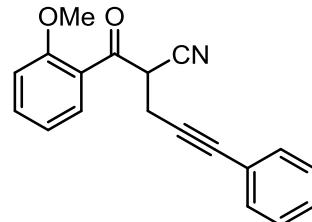
— 158.8

135.5
131.7
131.6
128.2
128.2
124.6
122.8
121.4
117.0
111.8

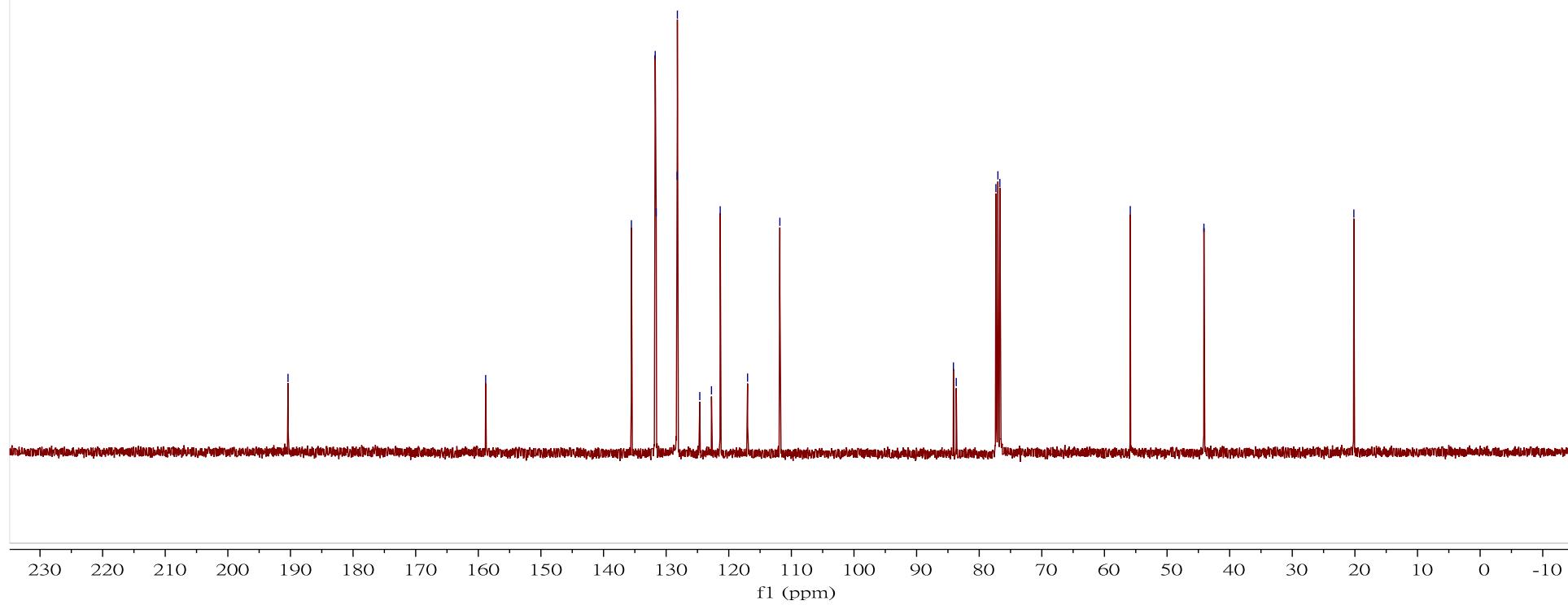
84.1
83.7
77.3
77.0
76.7

— 55.9
— 44.1

— 20.2

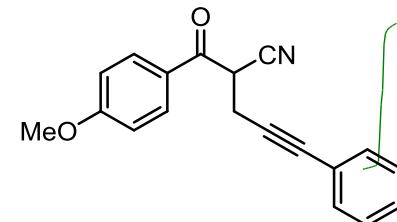


1d

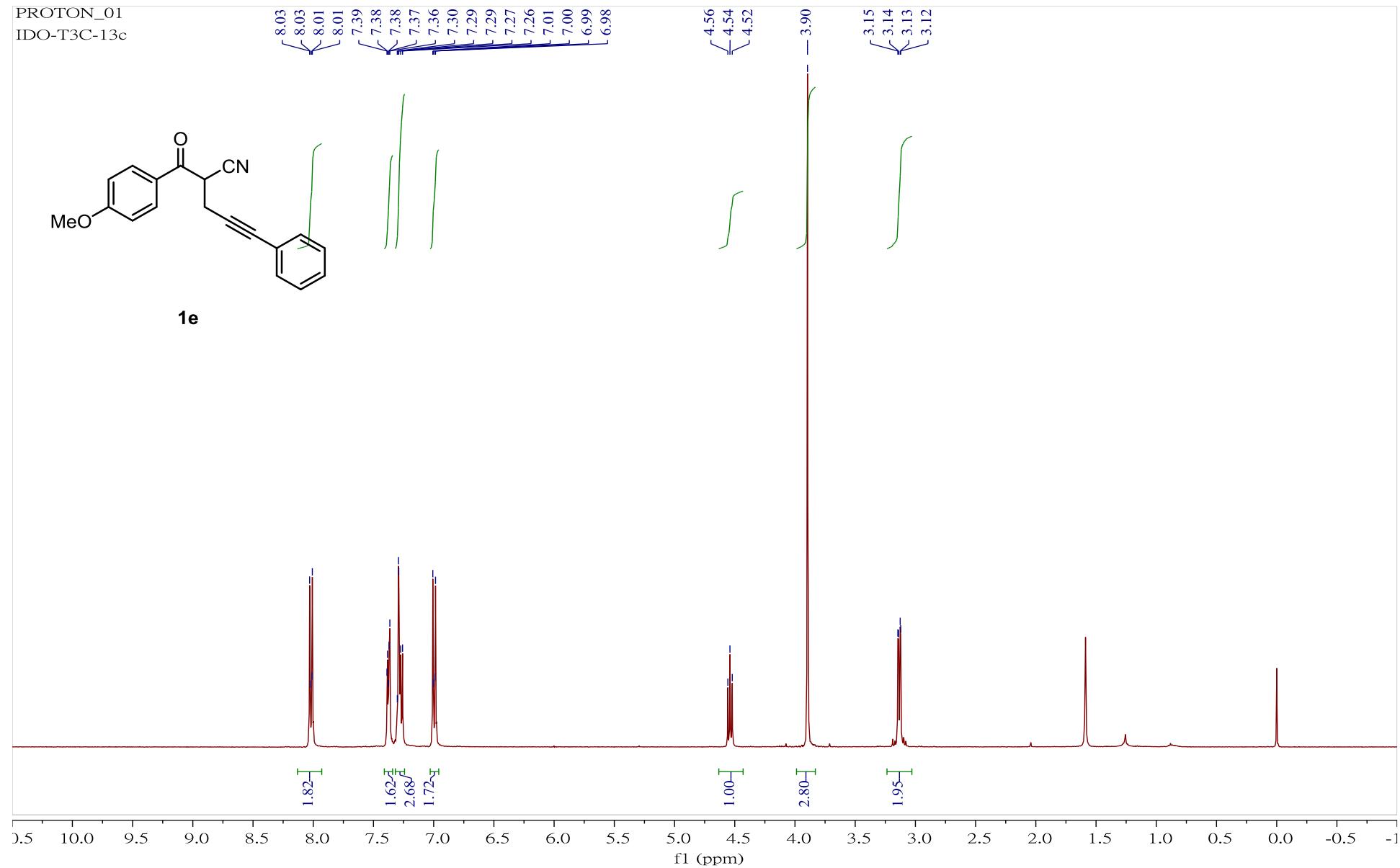


¹H NMR (400 MHz) spectrum of compound **1d** in CDCl_3

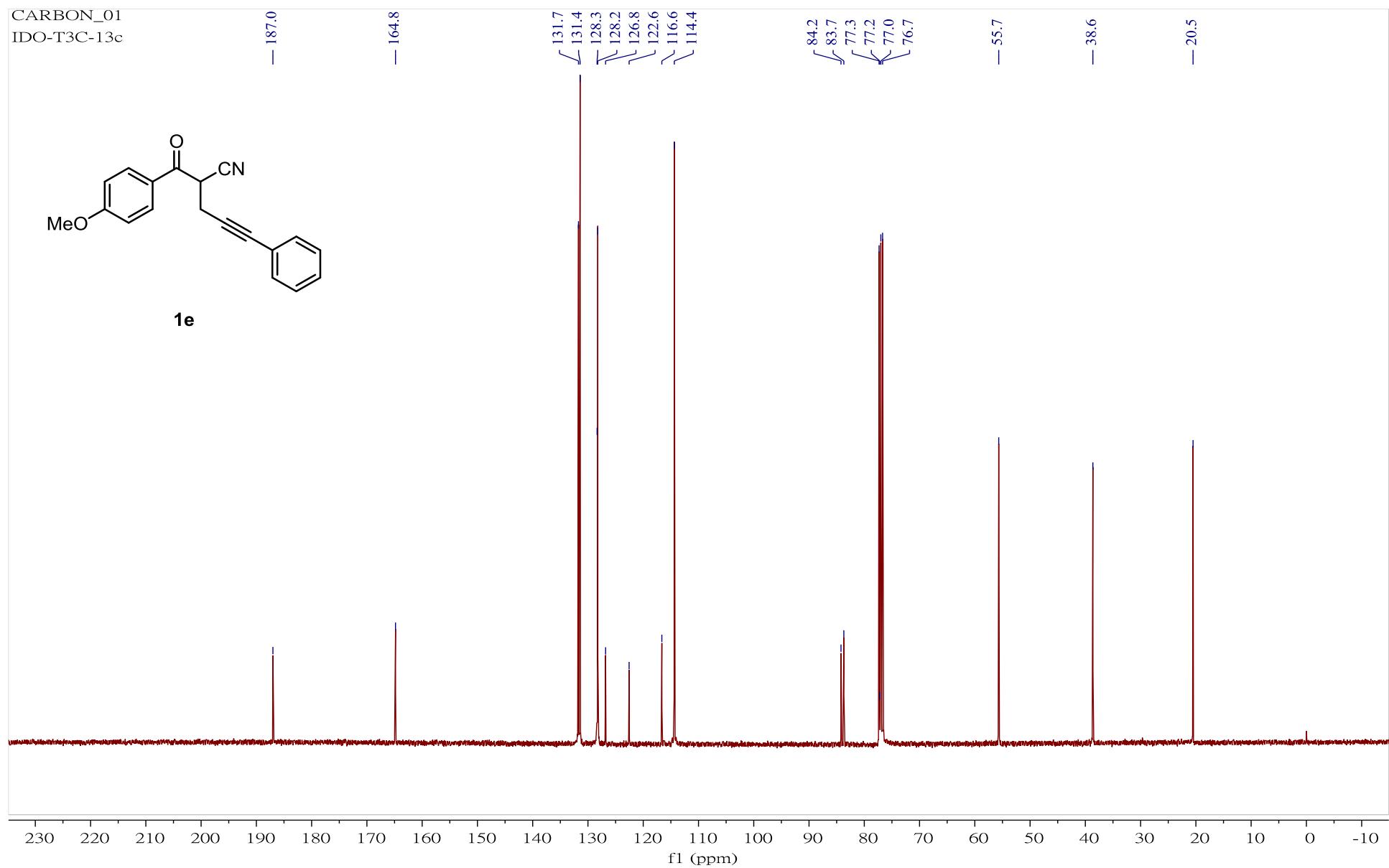
PROTON_01
IDO-T3C-13c



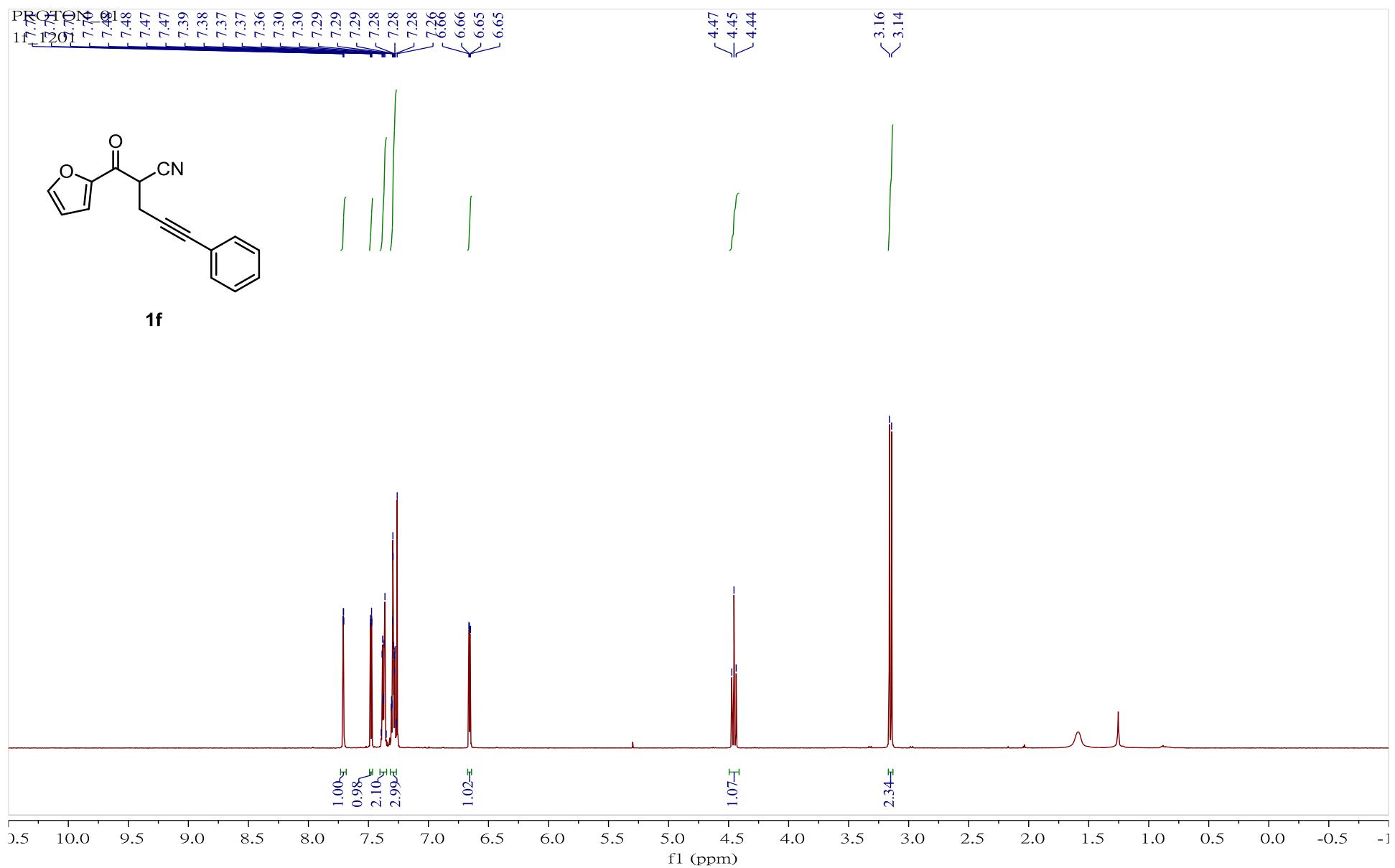
1e



¹H NMR (400 MHz) spectrum of compound **1e** in CDCl₃



^{13}C NMR (100 MHz) spectrum of compound **1e** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **1f** in CDCl_3

CARBON_01

1f carbon

— 177.3

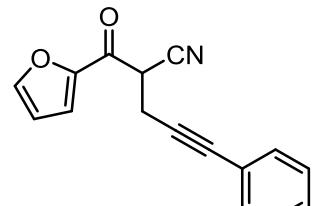
— 150.2
— 148.1

— 131.7
— 128.4
— 128.2
— 122.4
— 120.3
— 115.9
— 113.4

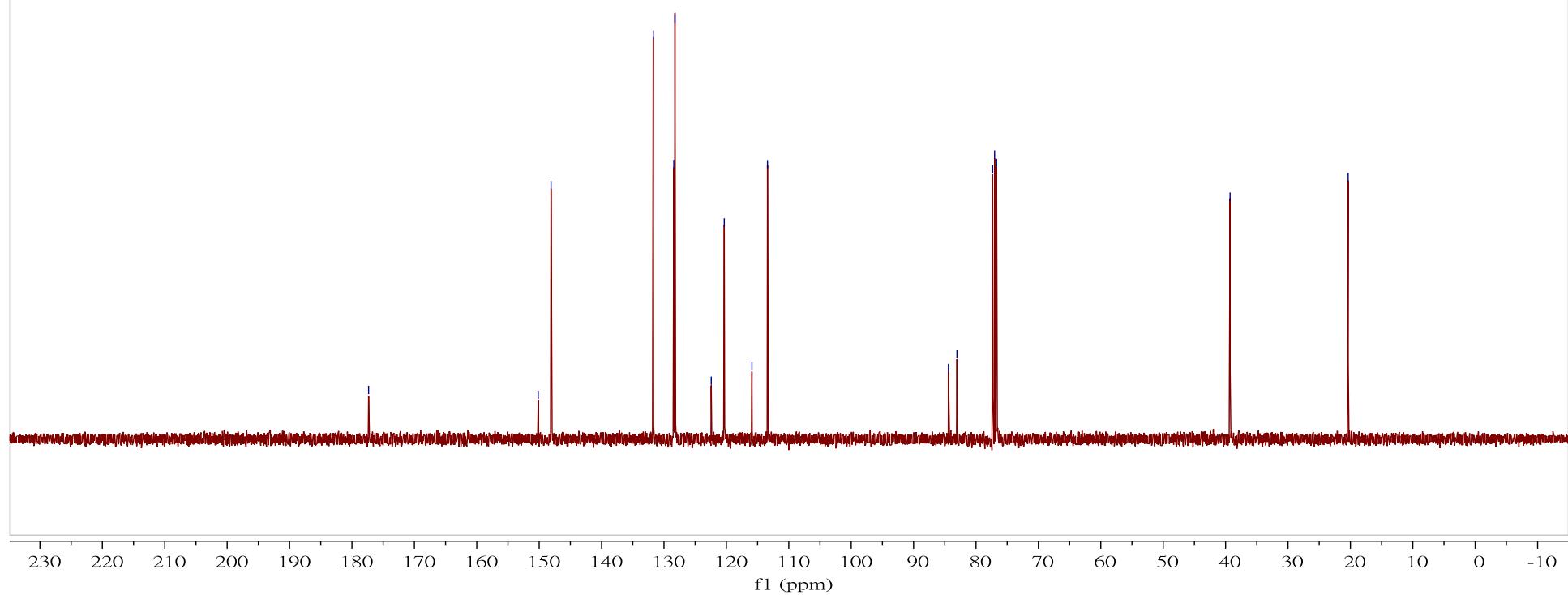
— 84.4
— 83.0
— 77.3
— 77.0
— 76.7

— 39.3

— 20.4



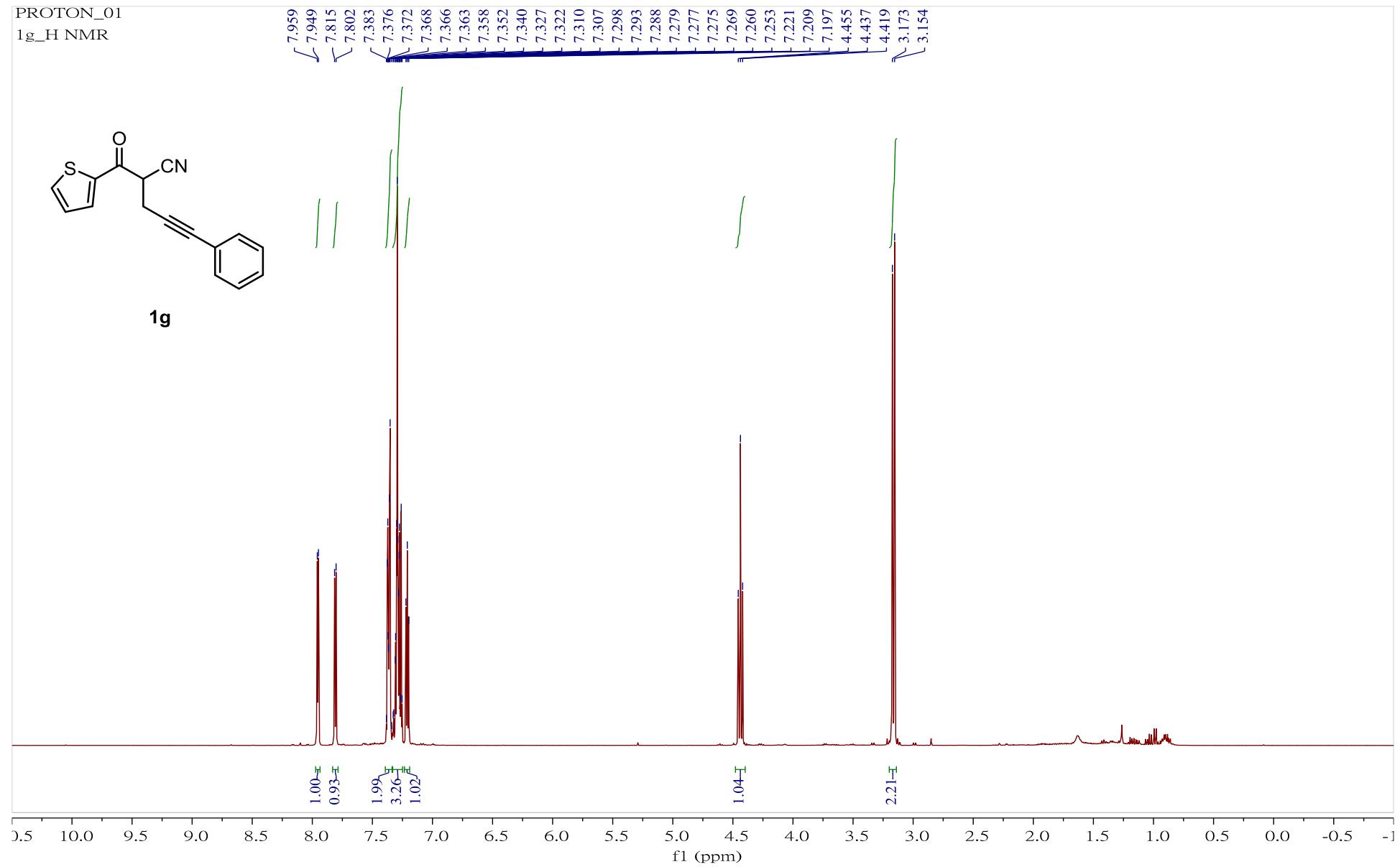
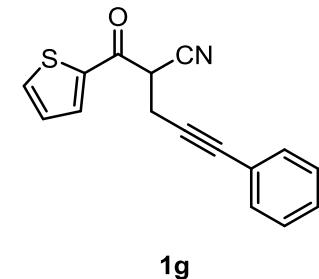
1f



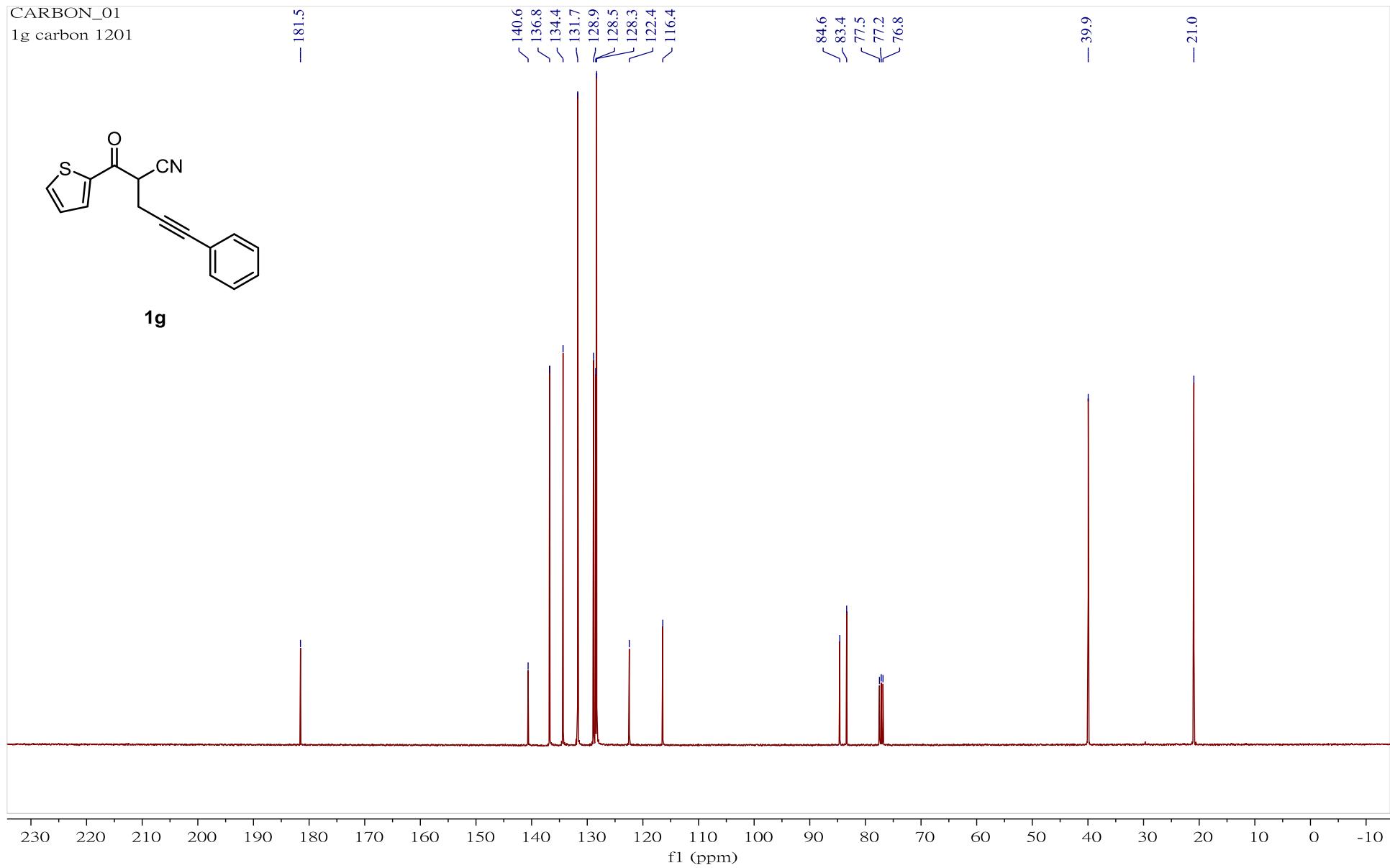
¹³C NMR (100 MHz) spectrum of compound **1f** in CDCl₃

PROTON_01

1g_H NMR



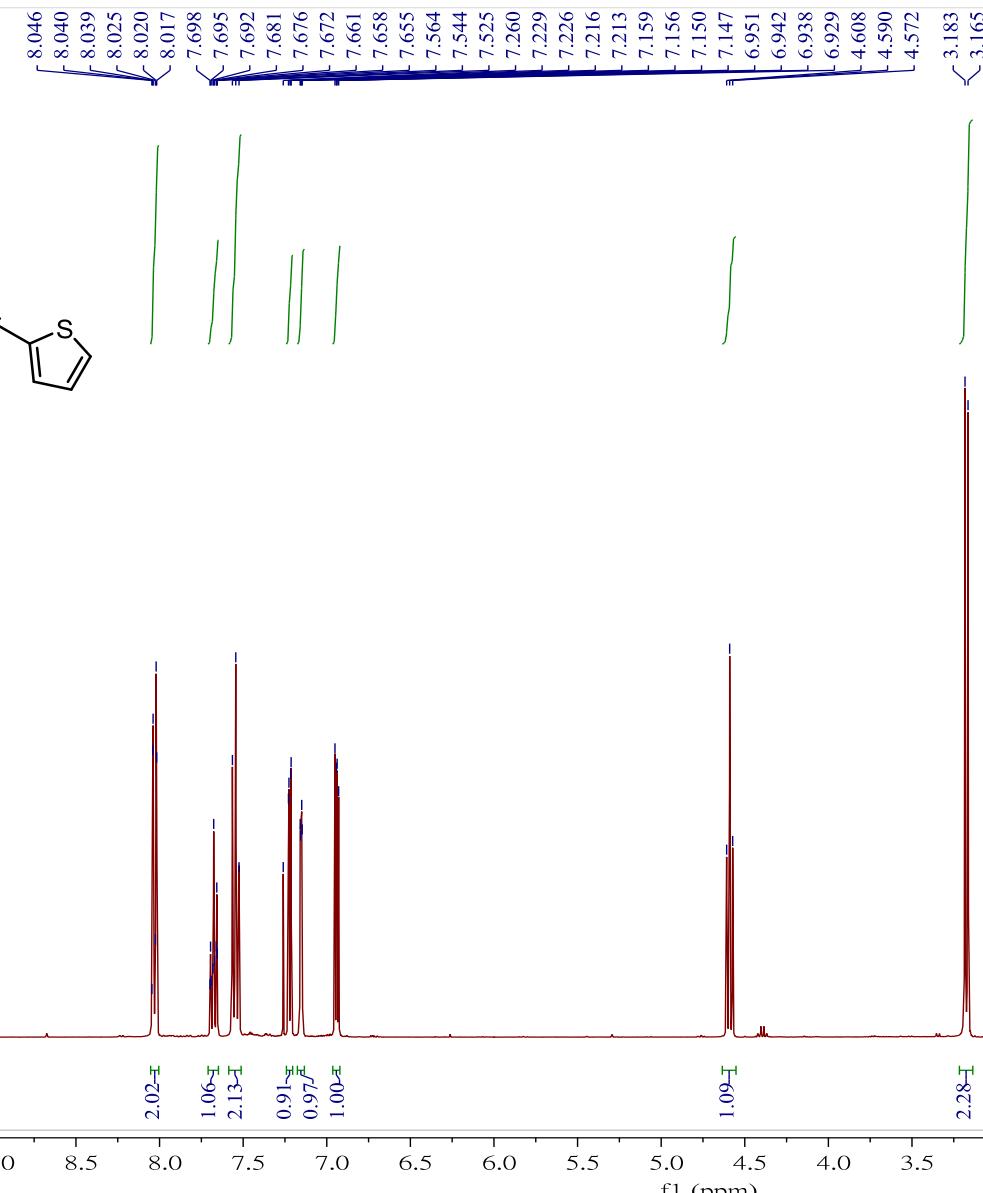
^{13}C NMR (100 MHz) spectrum of compound **1g** in CDCl_3

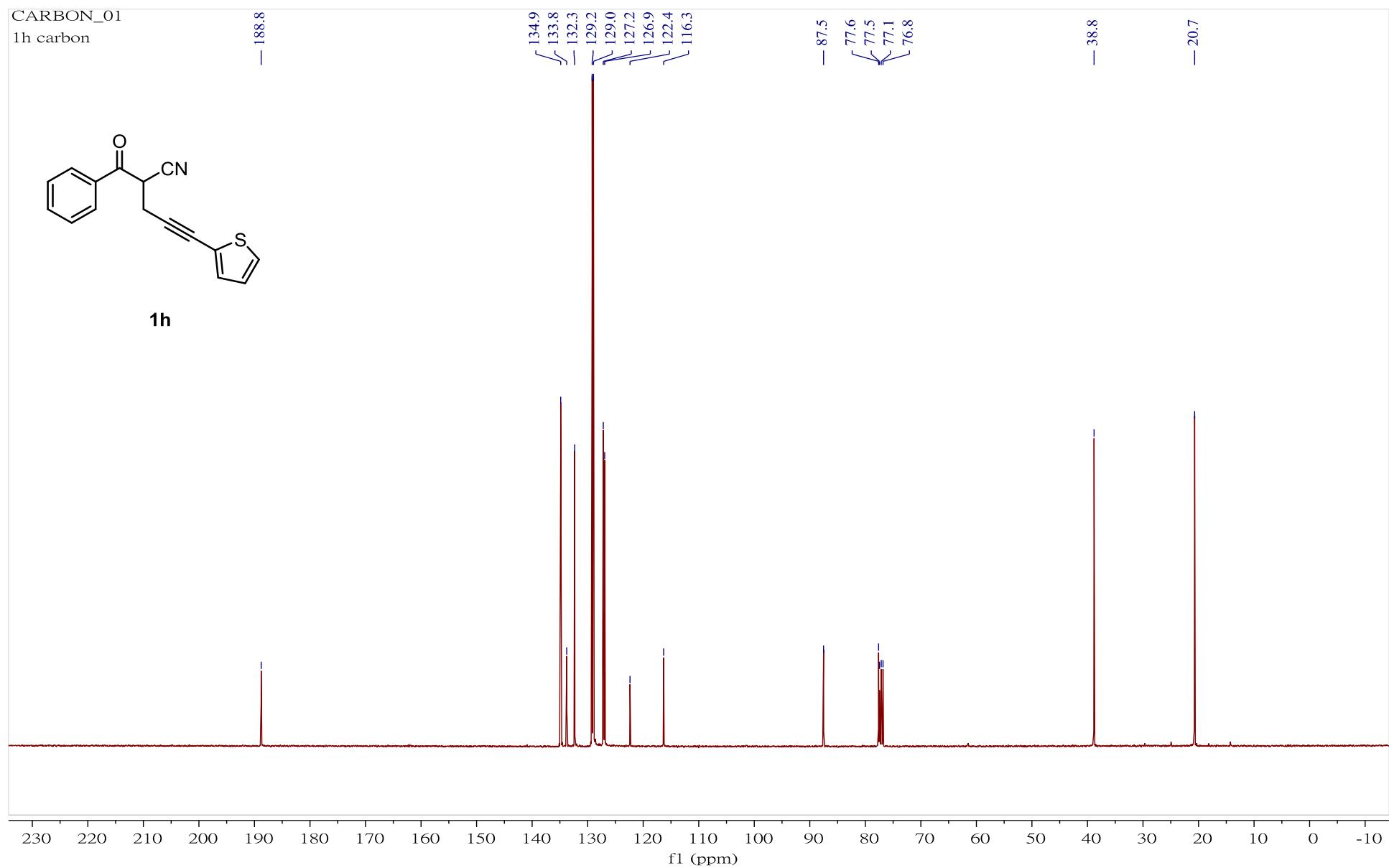


¹³C NMR (100 MHz) spectrum of compound **1g** in CDCl₃

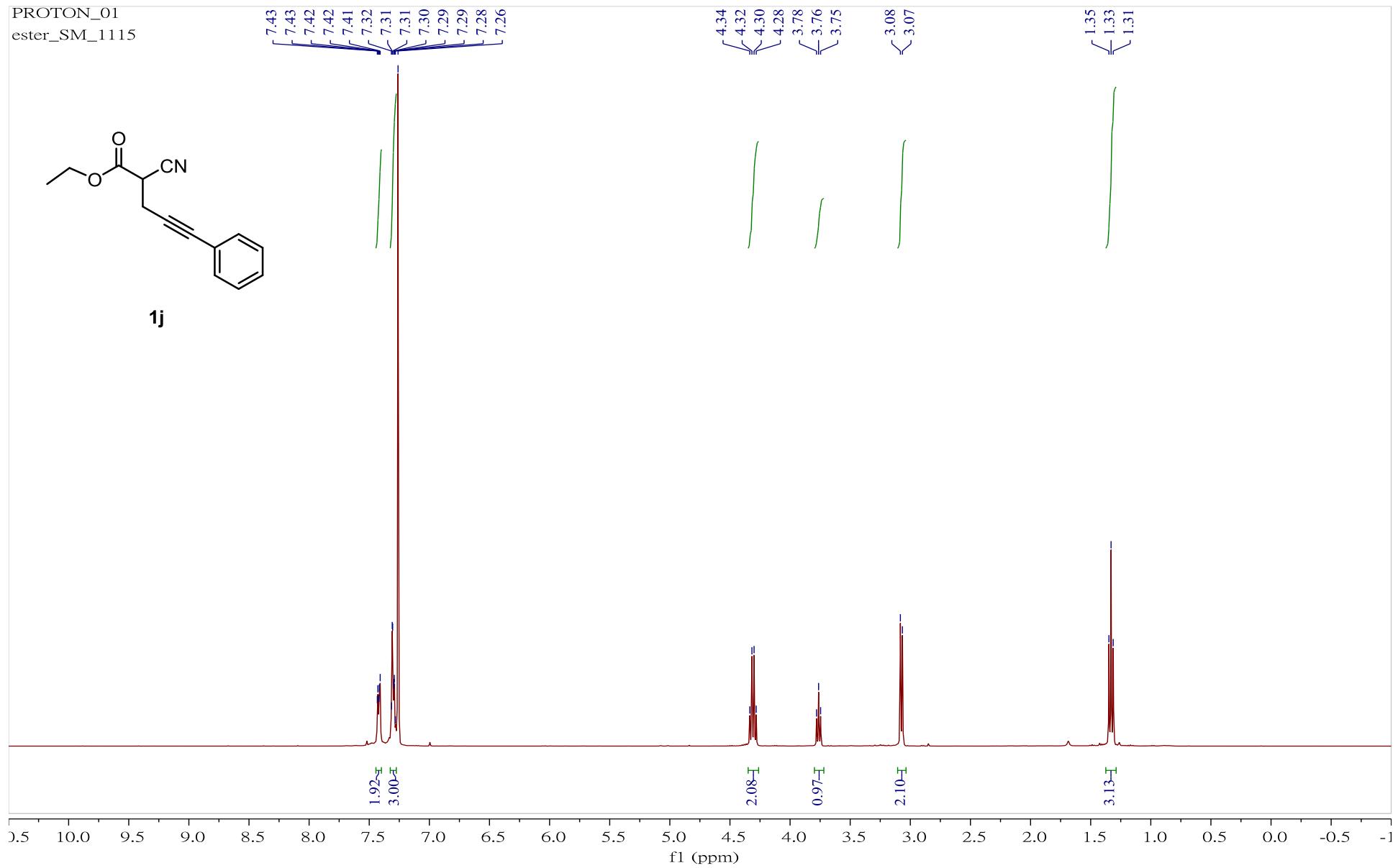
PROTON_01

1h_H_NMR

 ^{13}C NMR (100 MHz) spectrum of compound **1h** in CDCl_3

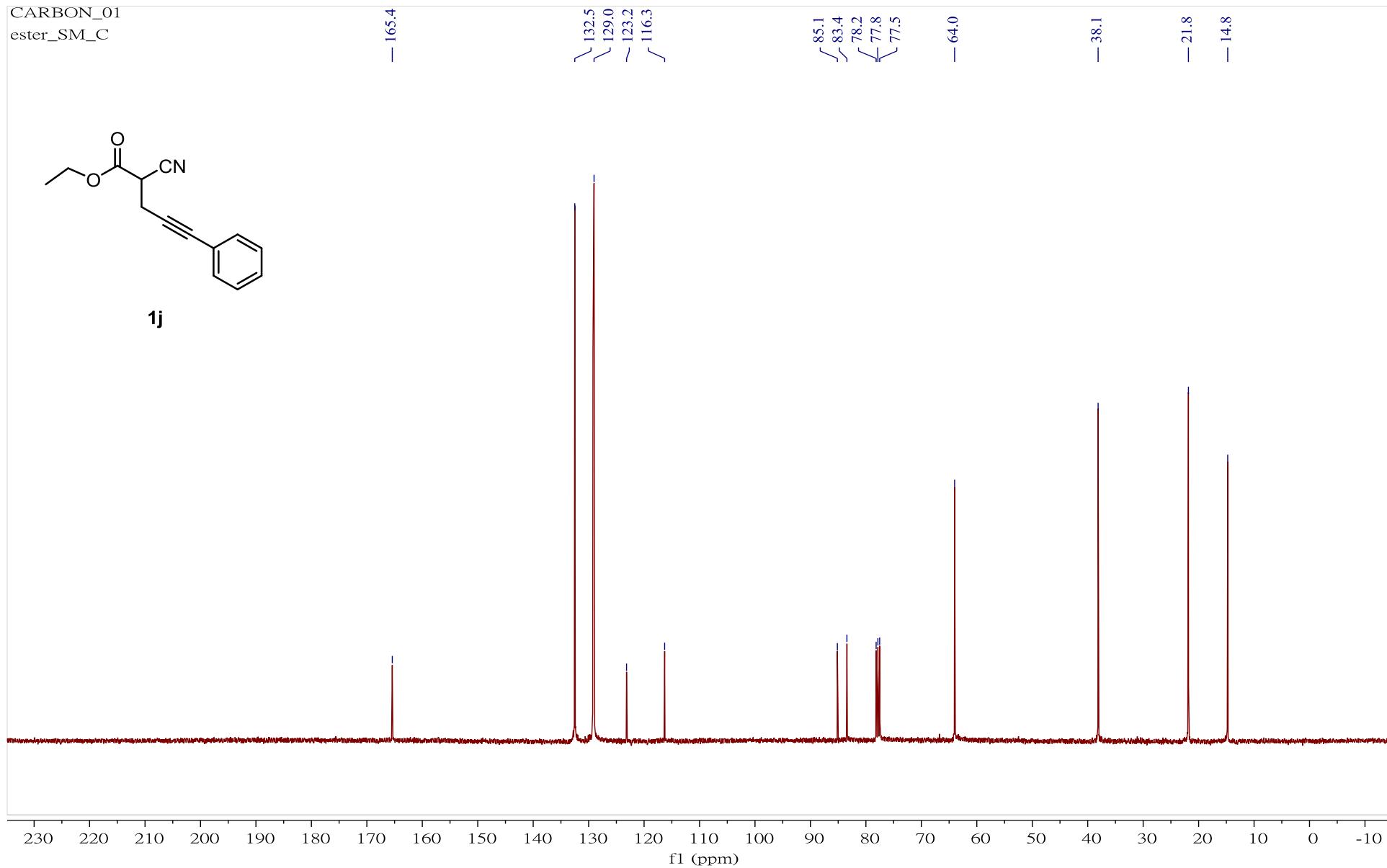


¹³C NMR (100 MHz) spectrum of compound **1h** in CDCl₃



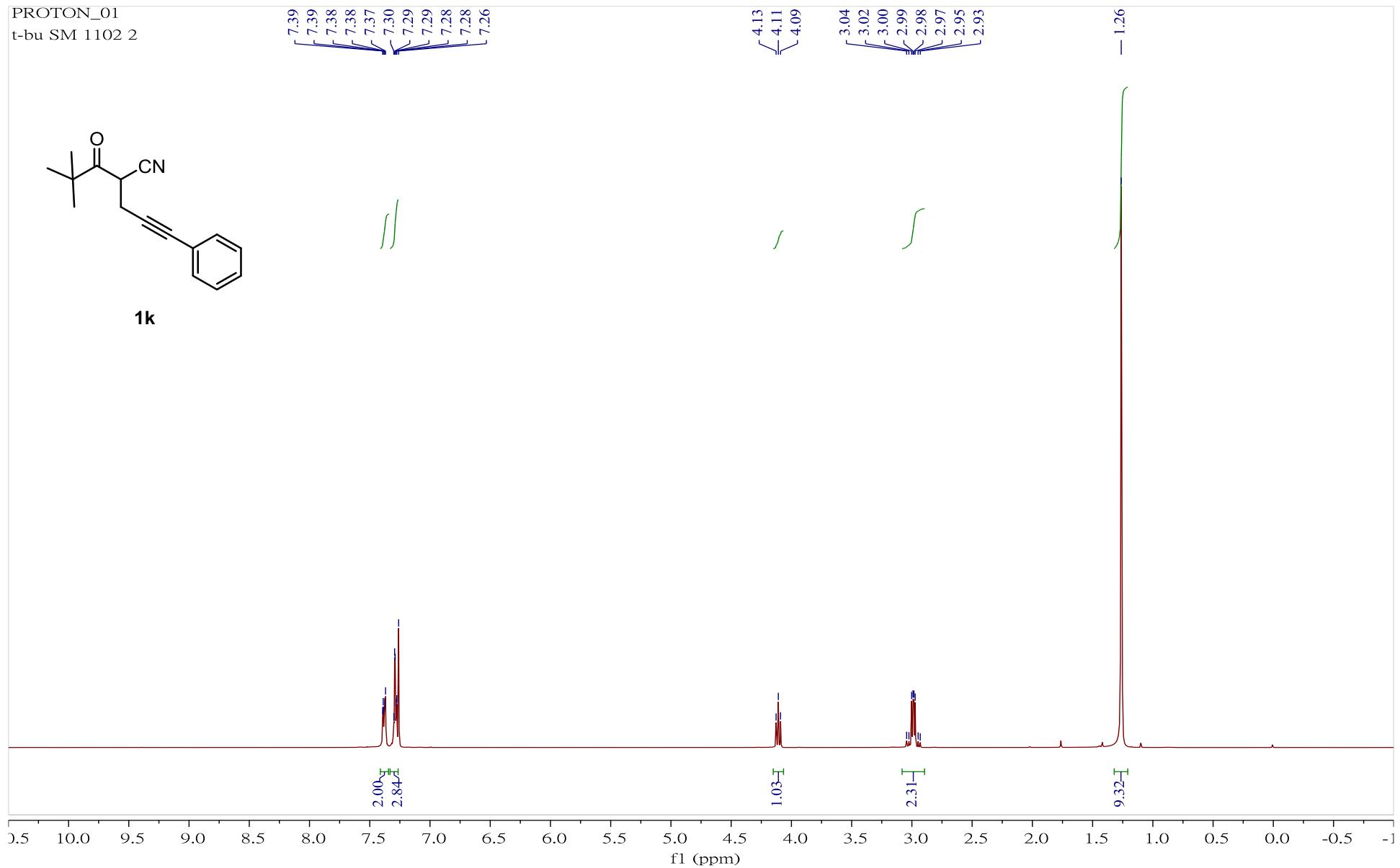
^1H NMR (400 MHz) spectrum of compound **1j** in CDCl_3

CARBON_01
ester_SM_C



¹³C NMR (100 MHz) spectrum of compound **1j** in CDCl₃

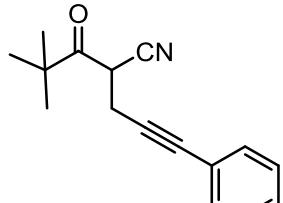
PROTON_01
t-bu SM 1102 2



^1H NMR (400 MHz) spectrum of compound **1k** in CDCl_3

CARBON_01
t-bu_SM_C_1106

— 203.9

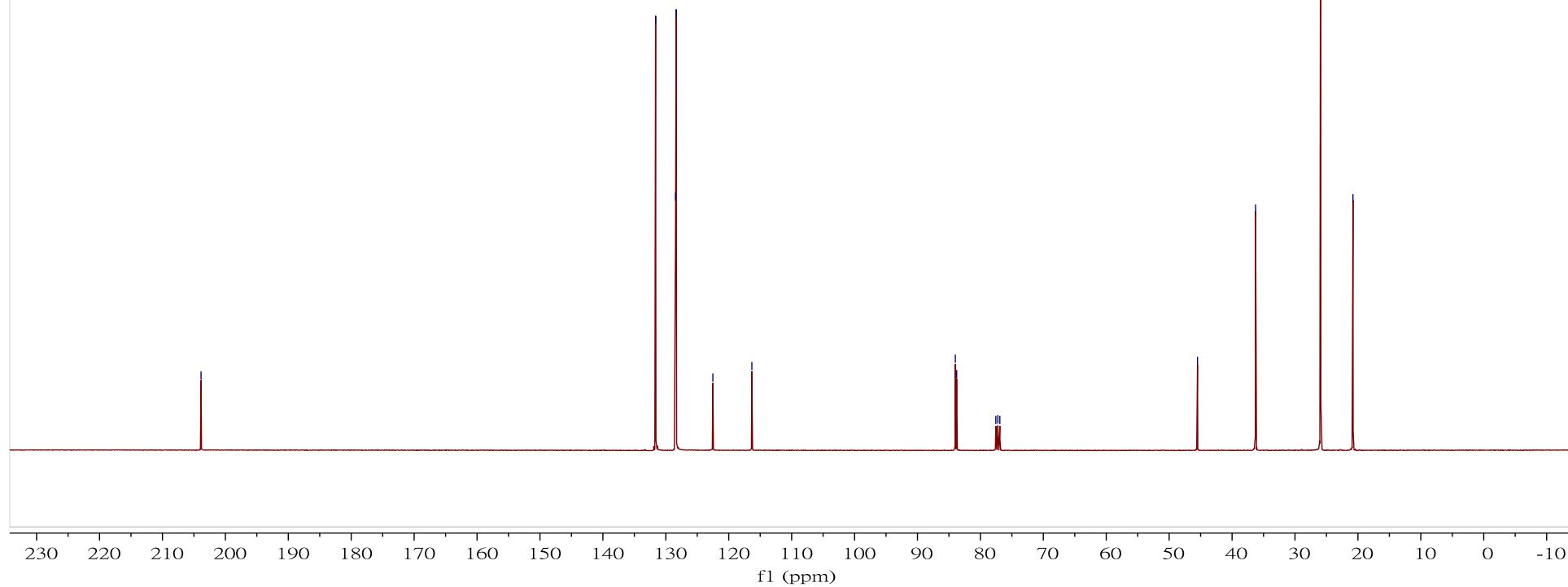


1k

~ 131.6
~ 128.5
~ 128.4
~ 122.5
~ 116.3

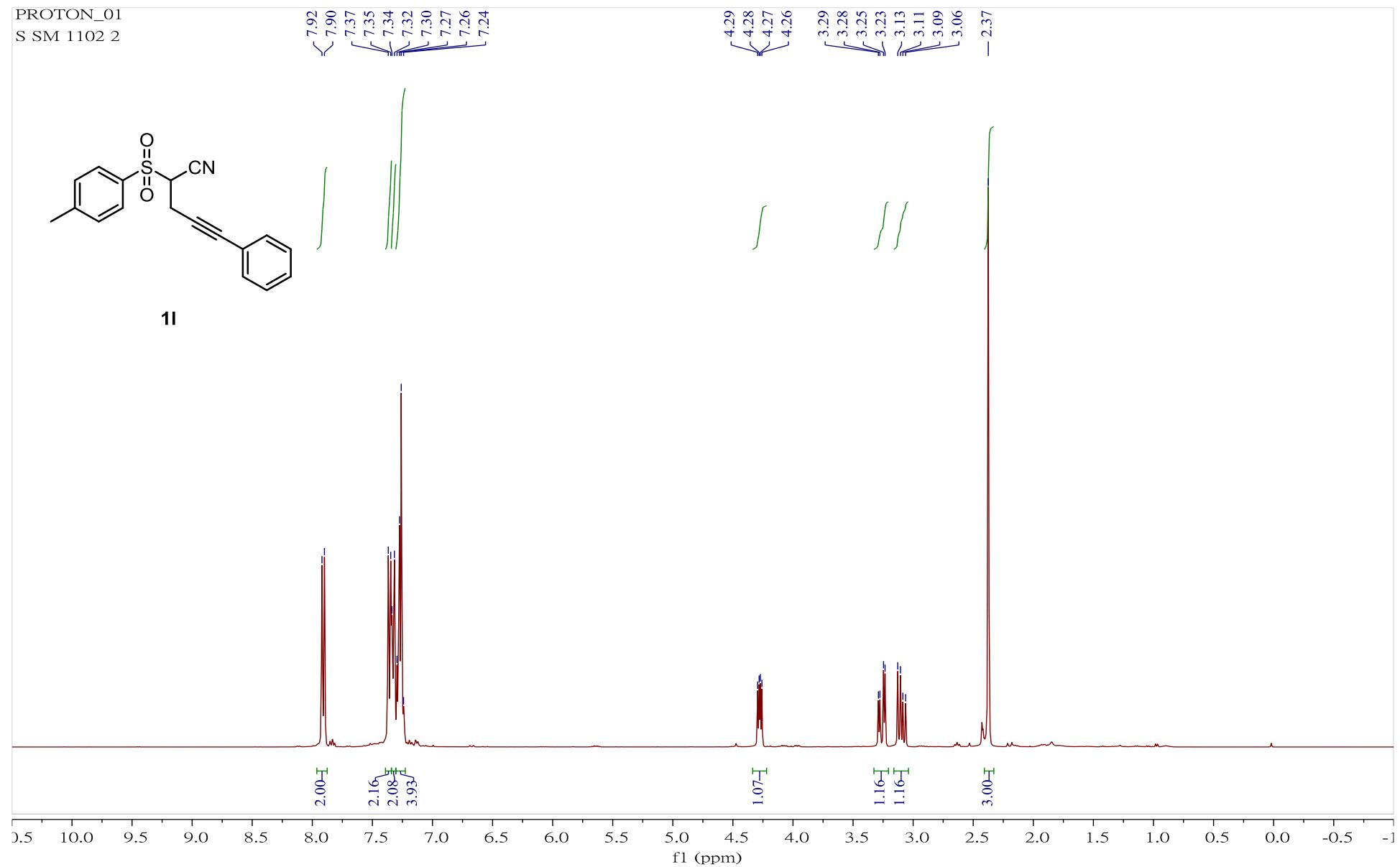
84.0
83.8
77.5
77.2
76.9

— 45.5
— 36.3
— 25.9
— 20.8



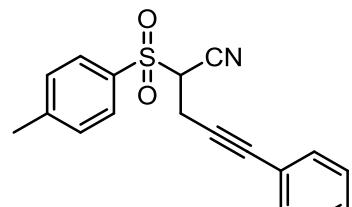
¹³C NMR (100 MHz) spectrum of compound **1k** in CDCl₃

PROTON_01
S SM 1102 2

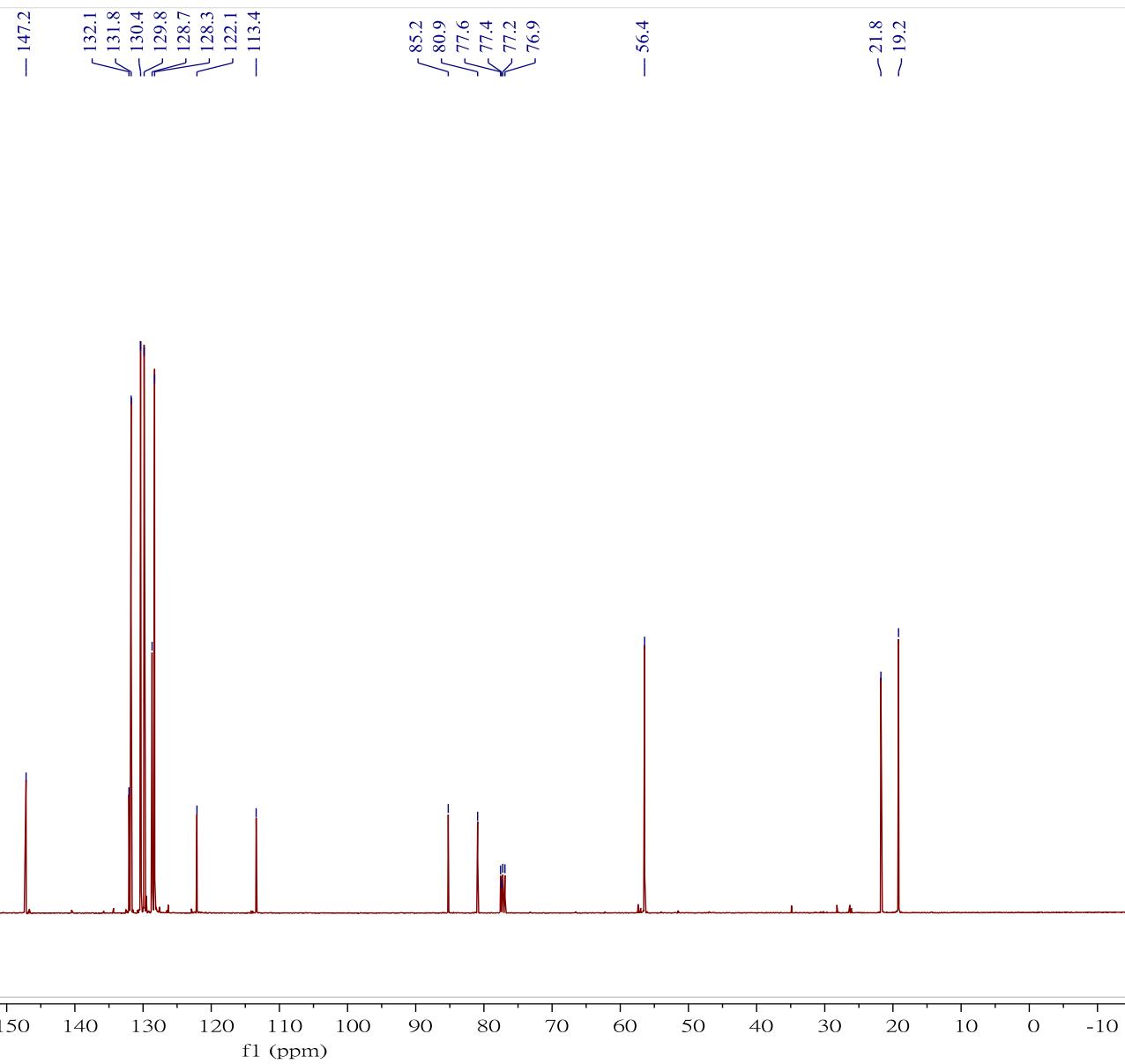


^1H NMR (400 MHz) spectrum of compound **1l** in CDCl_3

CARBON_01
S SM C 1106

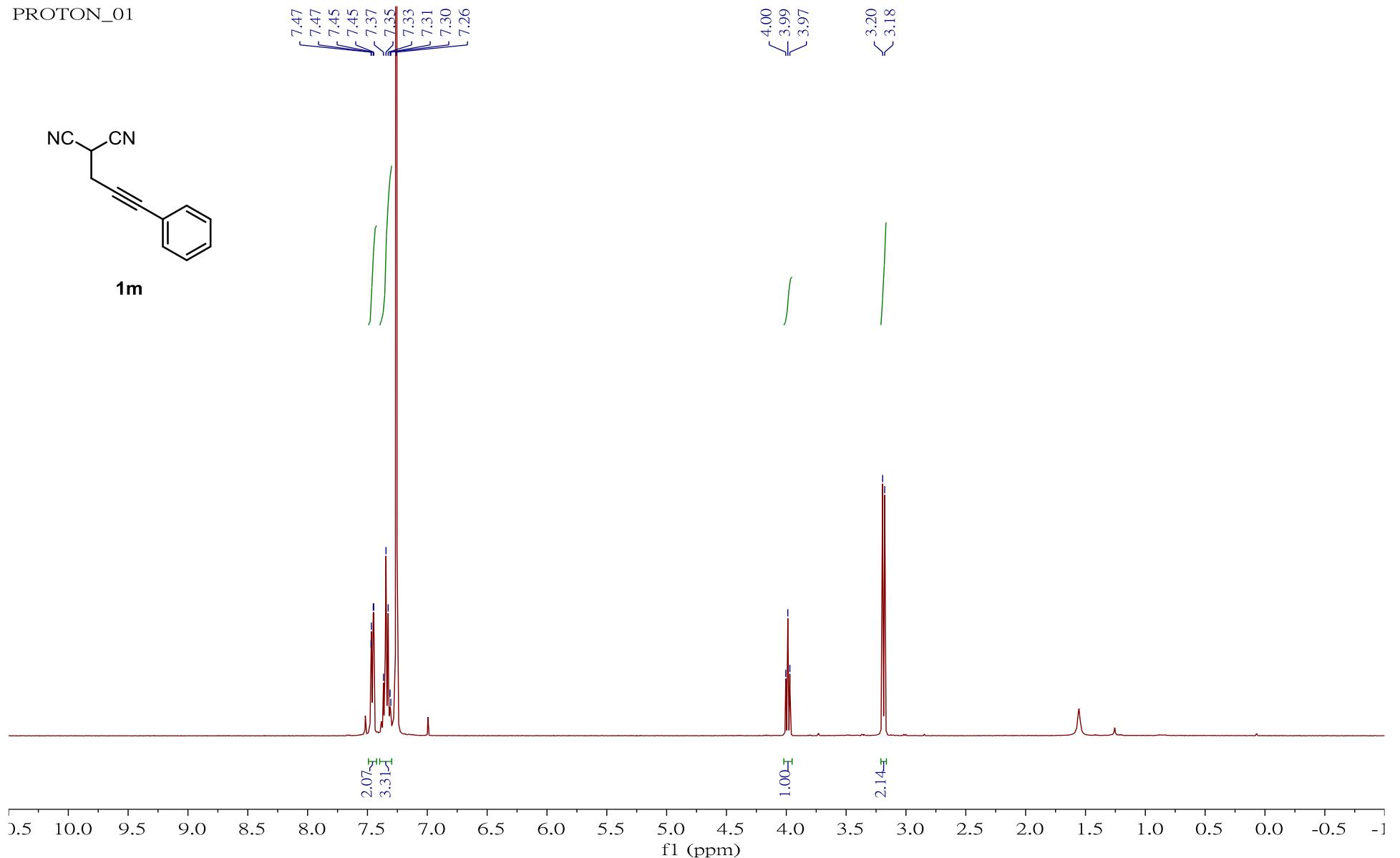


1l



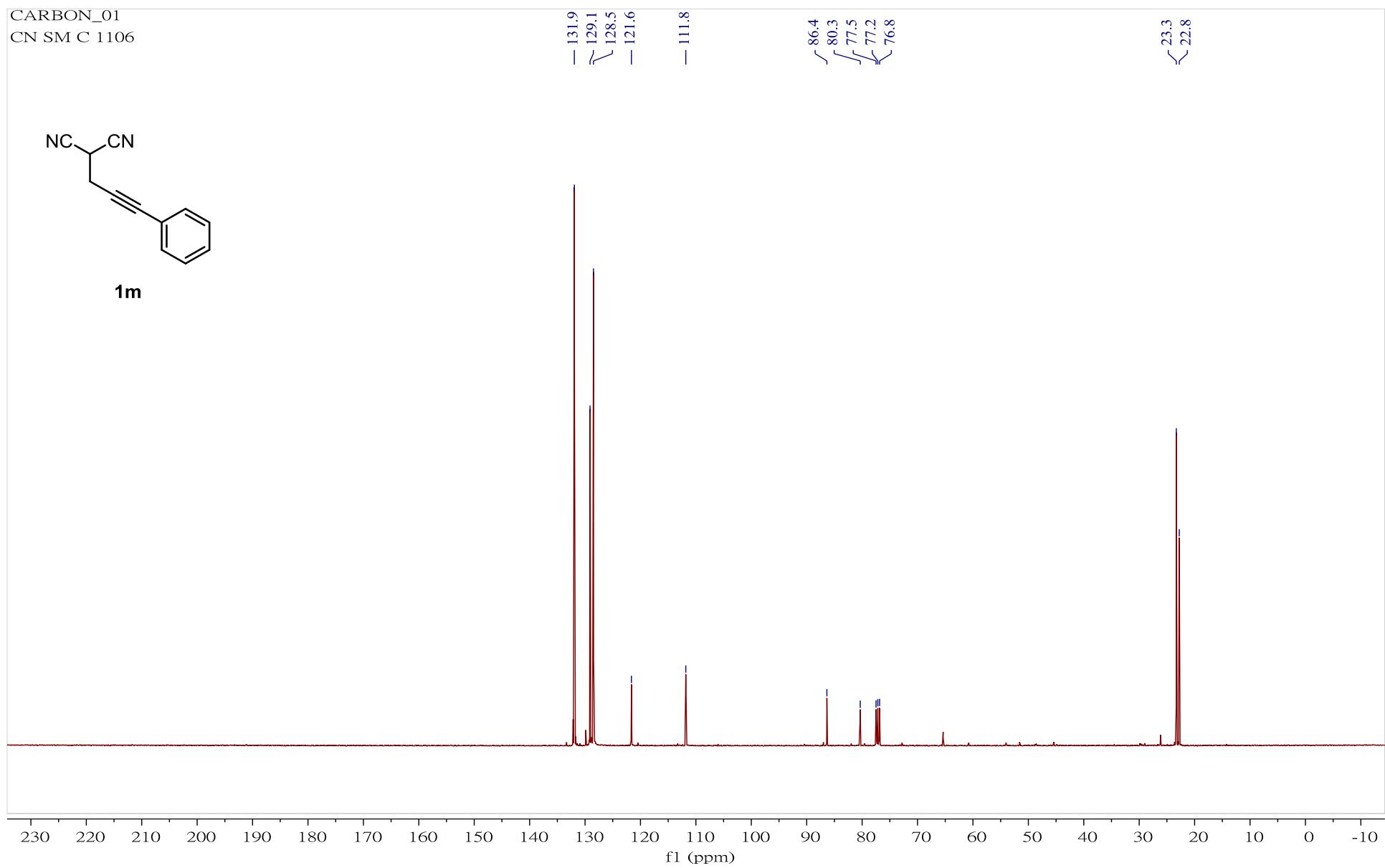
¹³C NMR (100 MHz) spectrum of compound **1l** in CDCl₃

PROTON_01

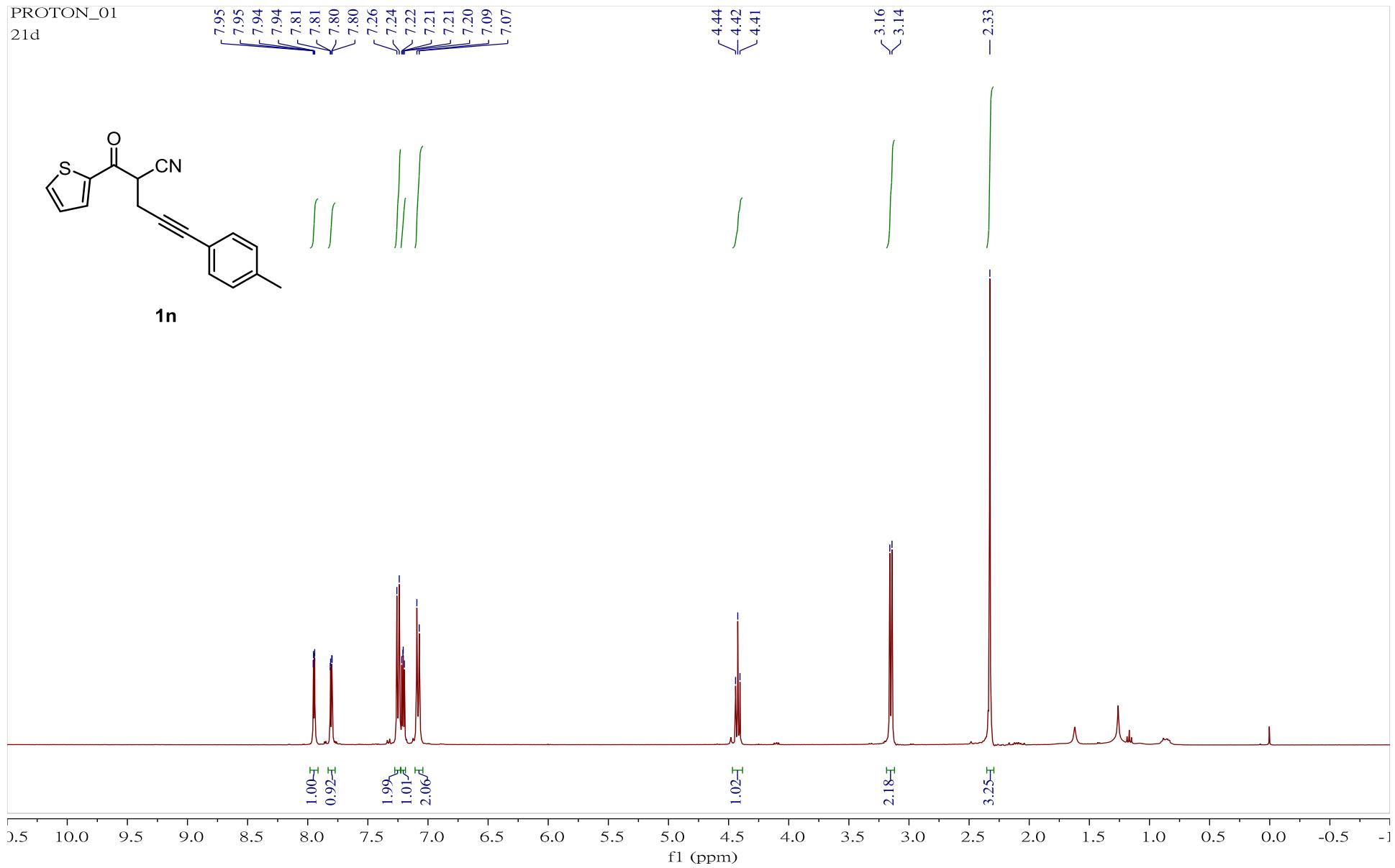


^1H NMR (400 MHz) spectrum of compound **1m** in CDCl_3

CARBON_01
CN SM C 1106



^{13}C NMR (100 MHz) spectrum of compound **1m** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **1n** in CDCl_3

CARBON_01
IDO-T3d-13C

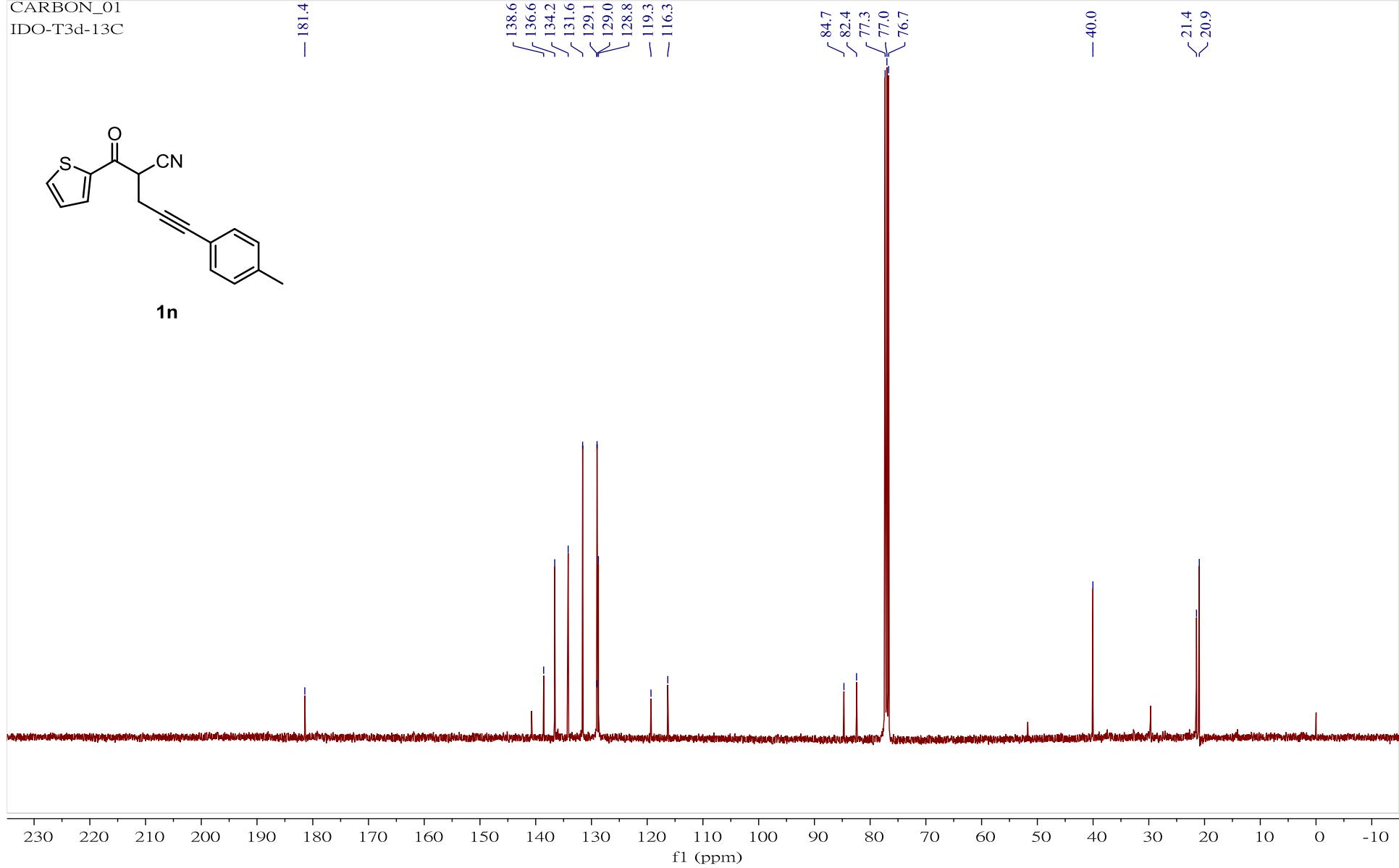
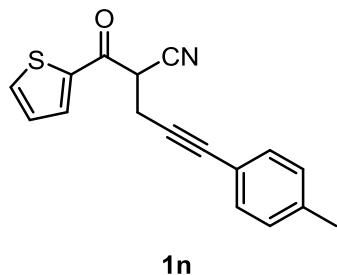
-181.4

138.6
136.6
134.2
131.6
129.1
129.0
128.8
119.3
116.3

84.7
82.4
77.3
77.0
76.7

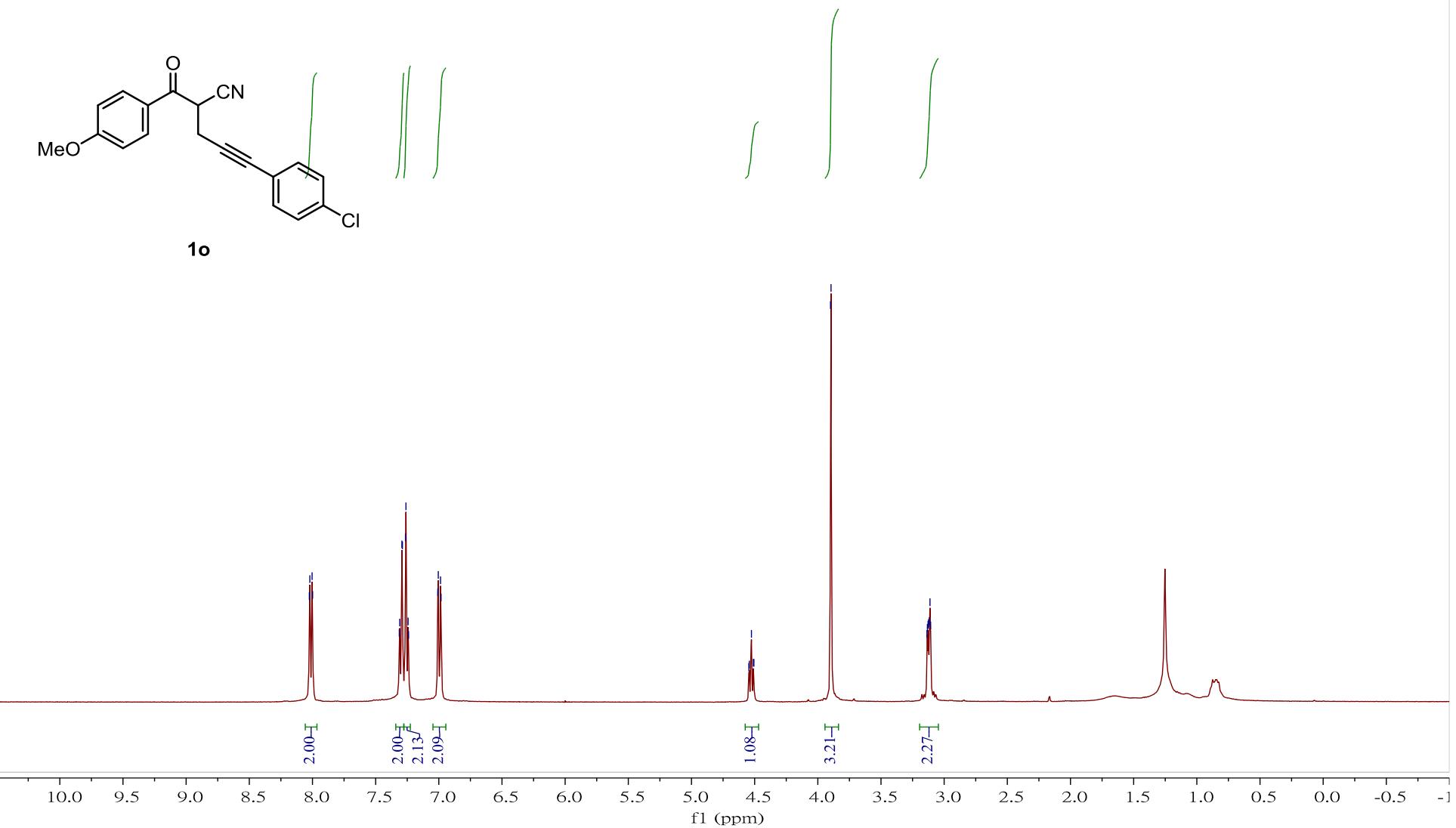
-40.0

21.4
20.9



¹³C NMR (100 MHz) spectrum of compound **1n** in CDCl₃

PROTON_01
OMe_C1_SM_1118 2



^1H NMR (400 MHz) spectrum of compound **1o** in CDCl_3

CARBON_01
OMe_Cl_SM_1118_C

— 187.4

— 165.4

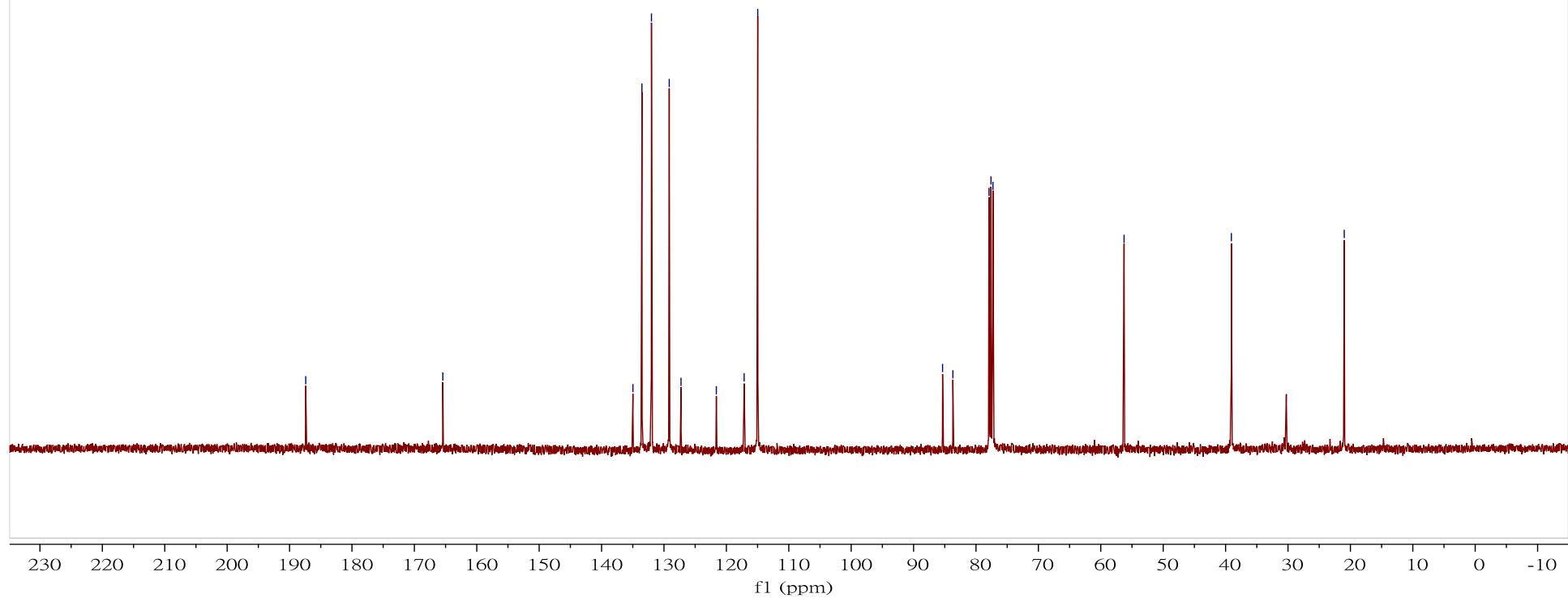
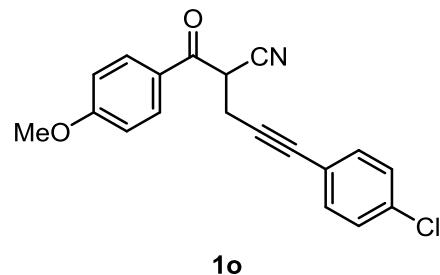
✓ 135.0
✓ 133.5
✓ 132.0
✓ 129.2
✓ 127.3
✓ 121.6
✓ 117.2
✓ 115.0

✓ 85.4
✓ 83.7
✓ 77.9
✓ 77.6
✓ 77.3

— 56.3

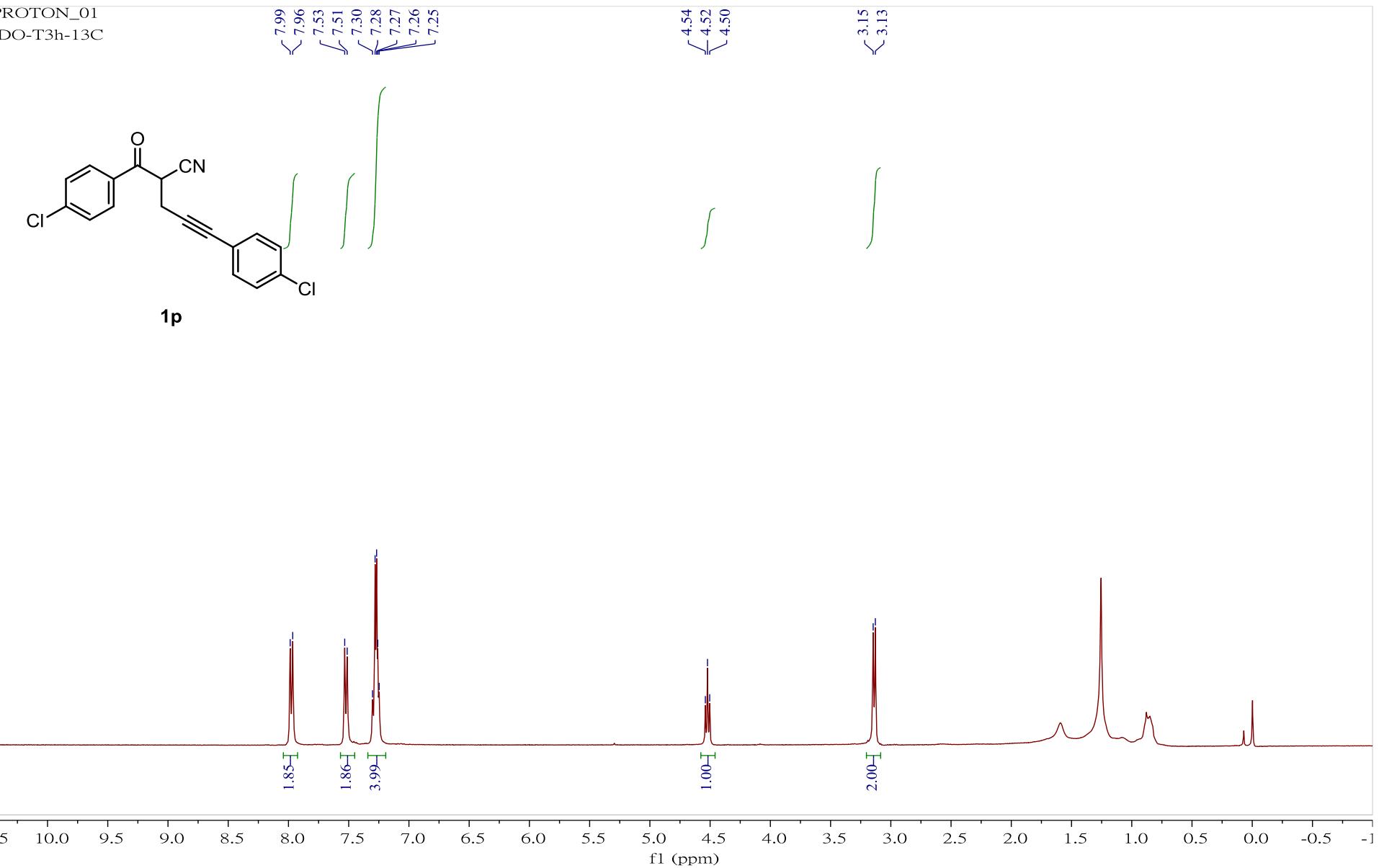
— 39.1

— 21.0



¹³C NMR (100 MHz) spectrum of compound **1o** in CDCl₃

PROTON_01
IDO-T3h-13C



^1H NMR (400 MHz) spectrum of compound **1p** in CDCl_3

CARBON_01
IDO-T3h-13C

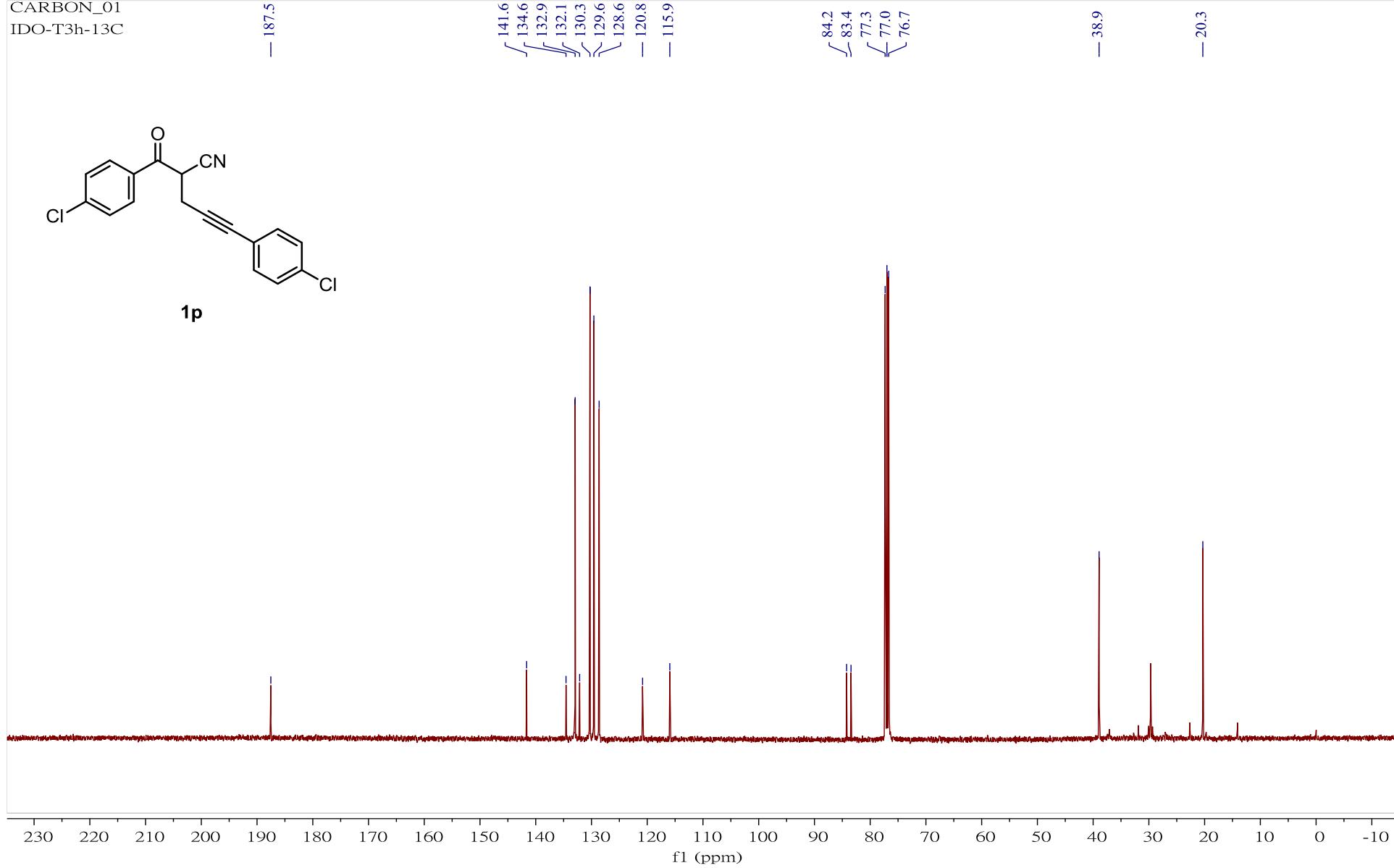
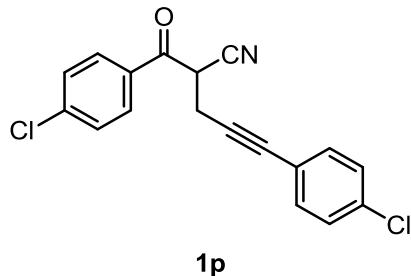
— 187.5

141.6
134.6
132.9
132.1
130.3
129.6
128.6
— 120.8
— 115.9

84.2
83.4
77.3
77.0
76.7

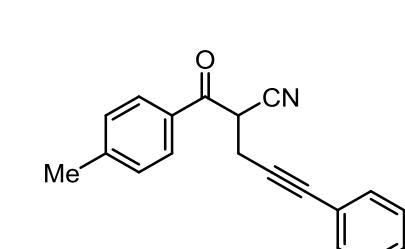
— 38.9

— 20.3

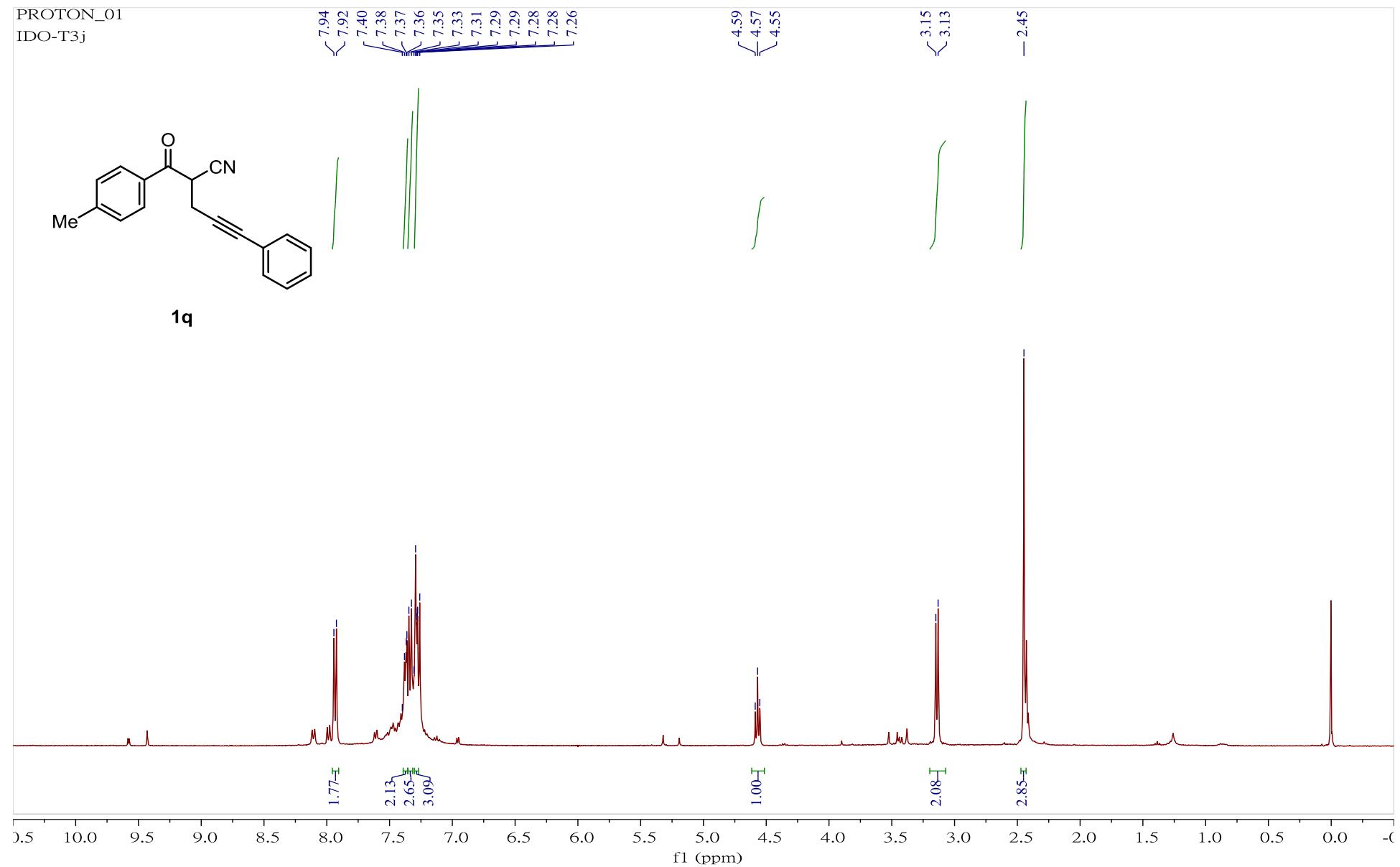


¹³C NMR (100 MHz) spectrum of compound **1p** in CDCl₃

PROTON_01
IDO-T3j

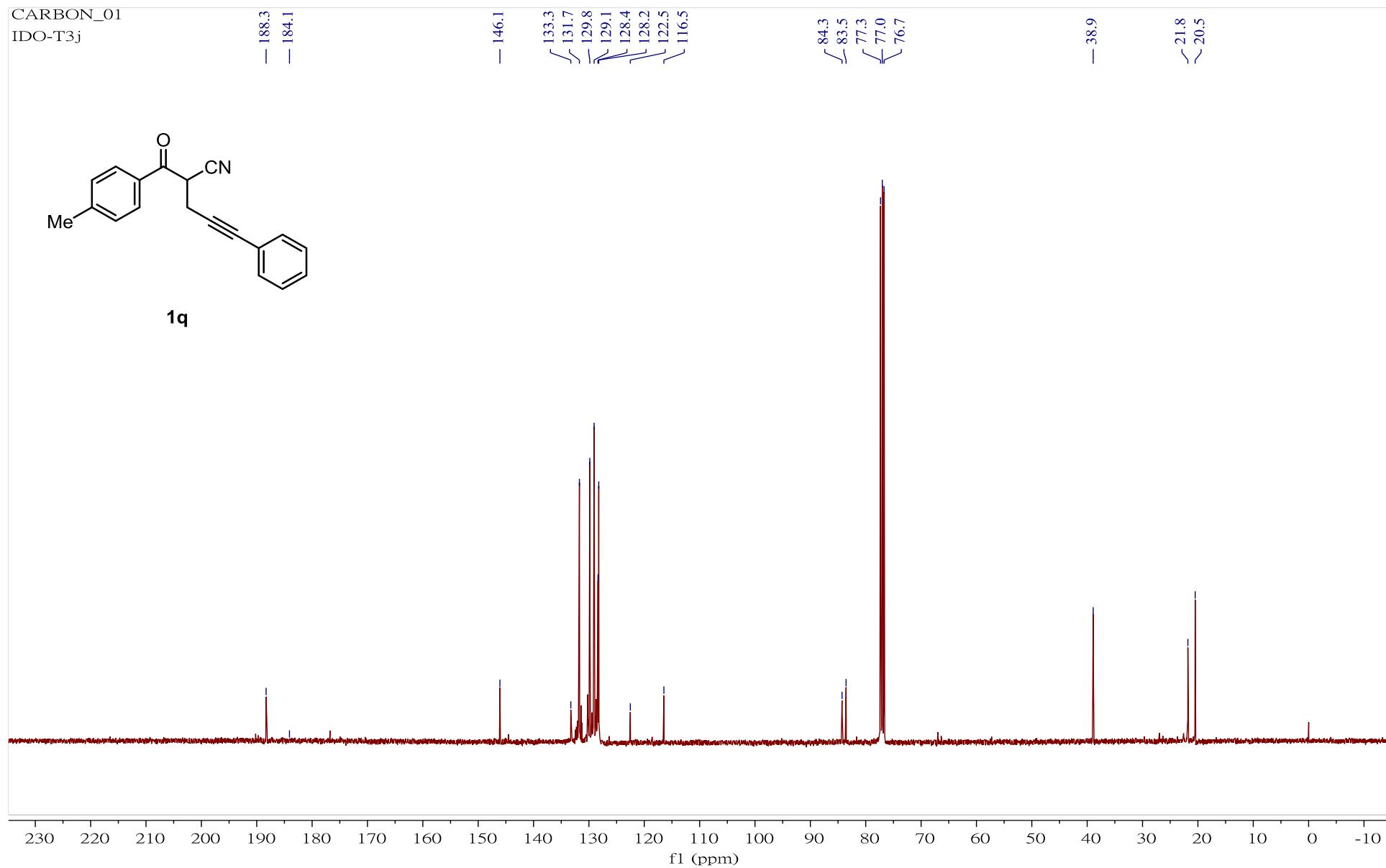


1q



¹H NMR (400 MHz) spectrum of compound **1q** in CDCl₃

CARBON_01
IDO-T3j



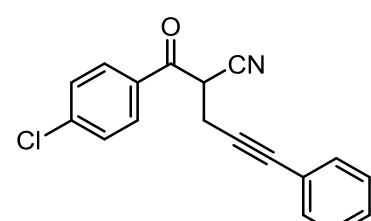
^{13}C NMR (100 MHz) spectrum of compound **1q** in CDCl_3

PROTON_01
IDO-T3h-13C

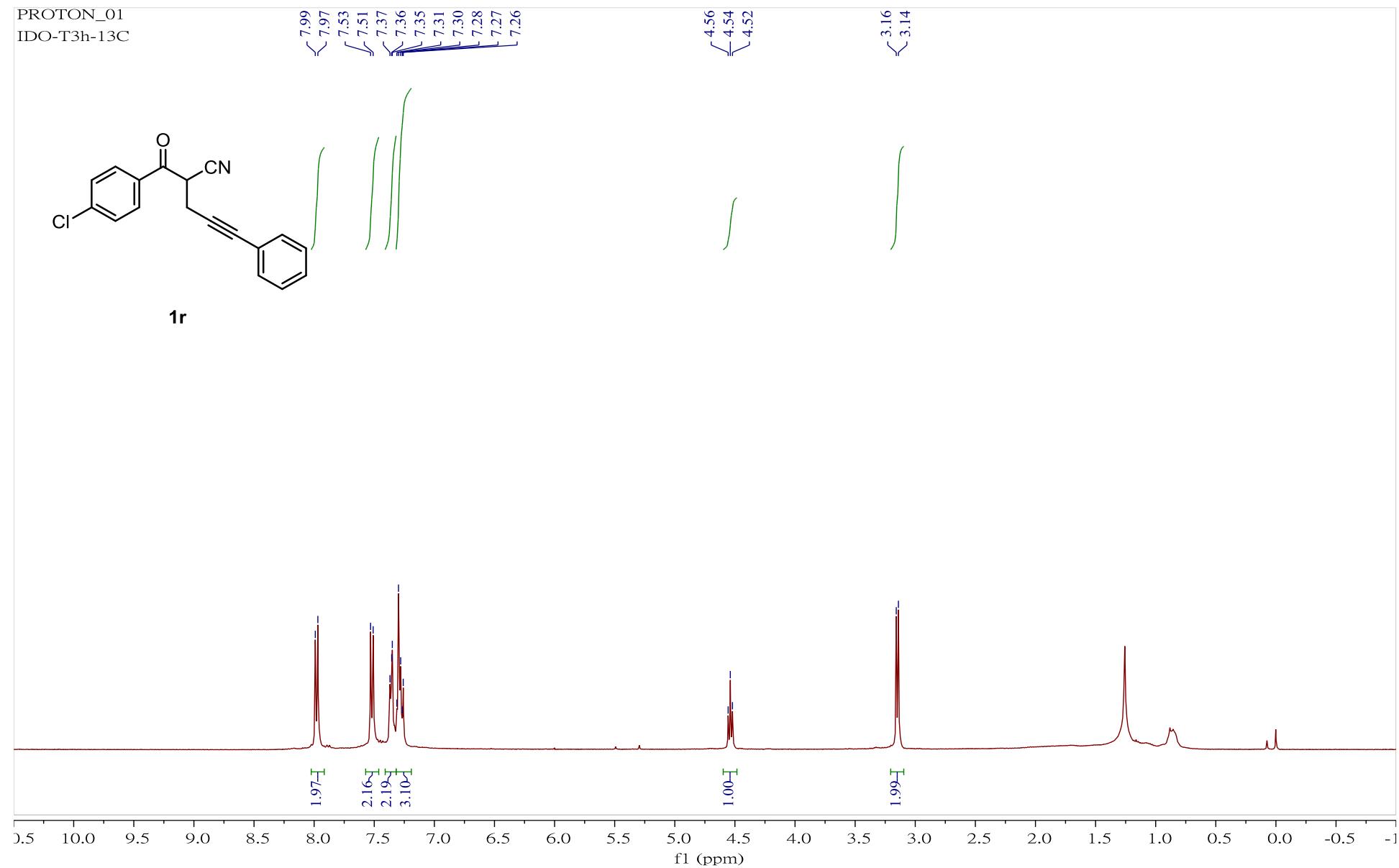
7.99
7.97
7.53
7.51
7.37
7.36
7.35
7.31
7.30
7.28
7.27
7.26

4.56
4.54
4.52

3.16
3.14



1r



^1H NMR (400 MHz) spectrum of compound **1r** in CDCl_3

CARBON_01
IDO-T3h-13C

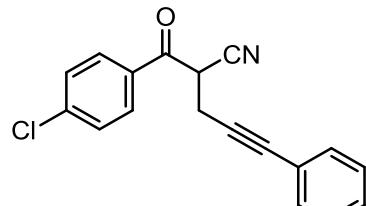
— 187.7

— 141.5
132.2
131.7
130.3
129.5
128.5
128.3
122.3
116.1

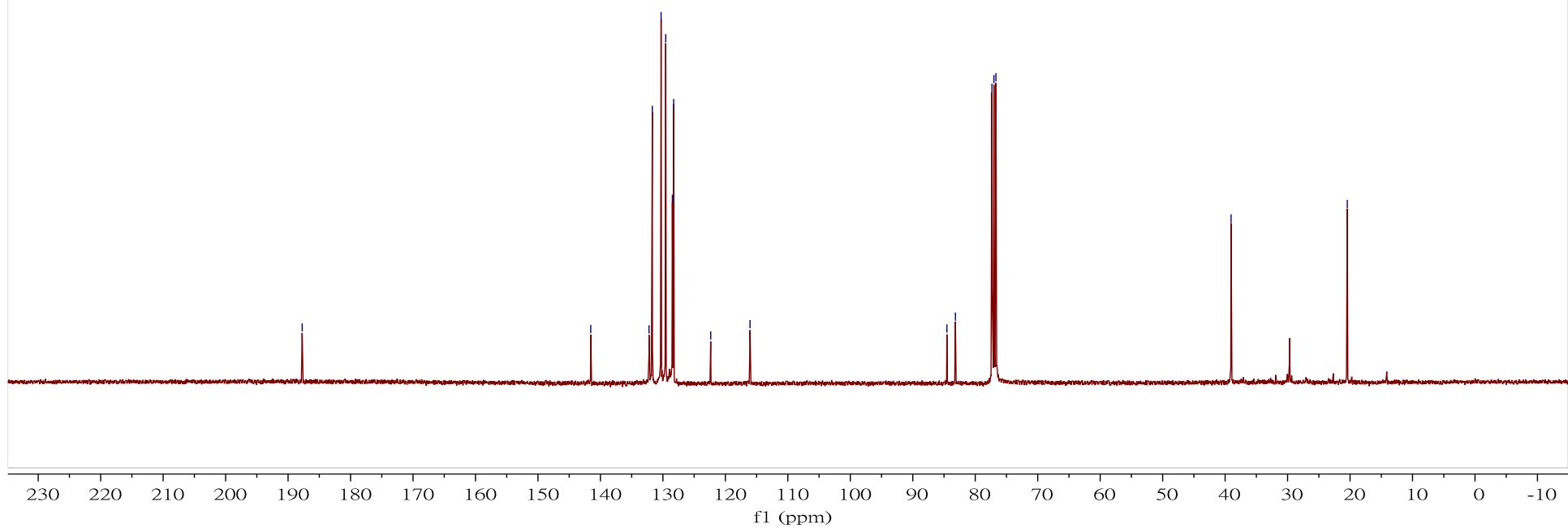
— 84.5
83.2
77.3
77.0
76.7

— 39.0

— 20.4



1r



¹³C NMR (100 MHz) spectrum of compound **1r** in CDCl₃

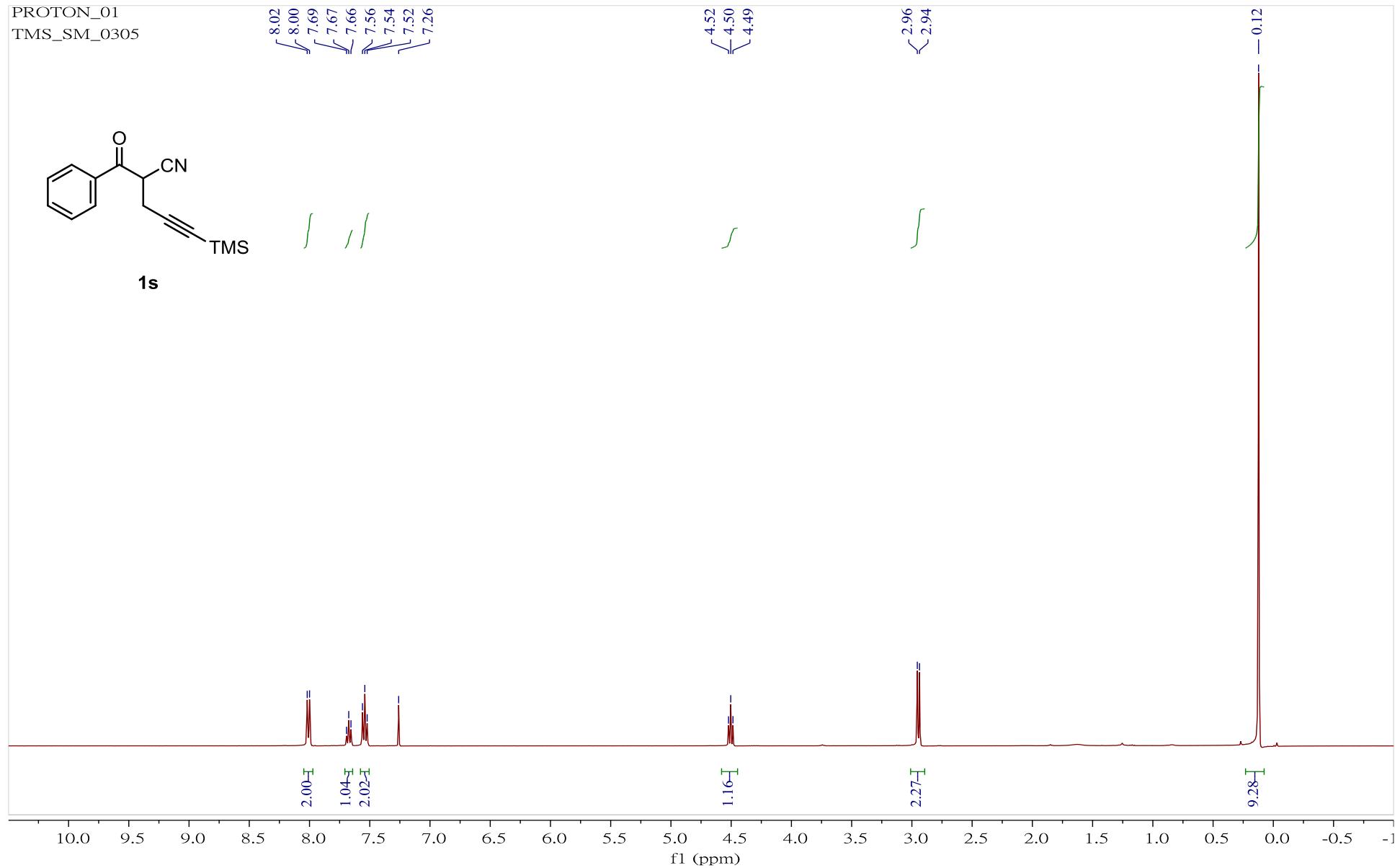
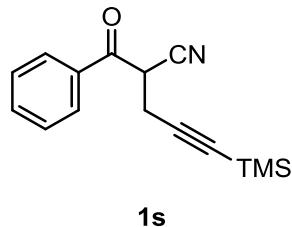
PROTON_01
TMS_SM_0305

8.02
7.69
7.67
7.66
7.56
7.54
7.52
7.26

4.52
4.50
4.49

2.96
2.94

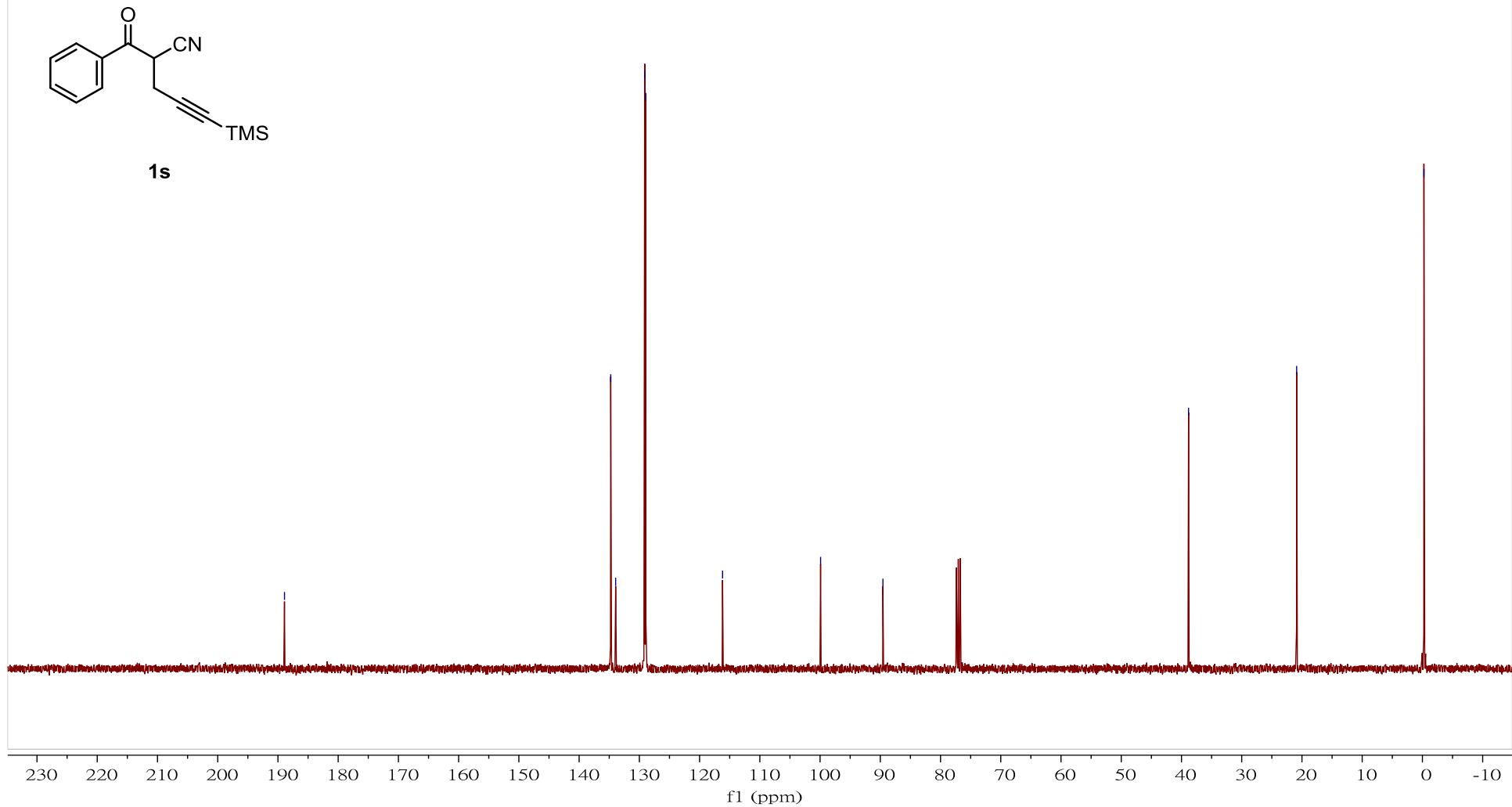
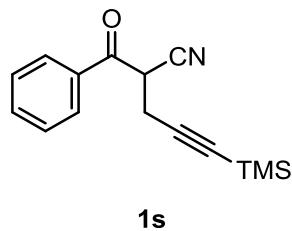
0.12



^1H NMR (400 MHz) spectrum of compound **1s** in CDCl_3

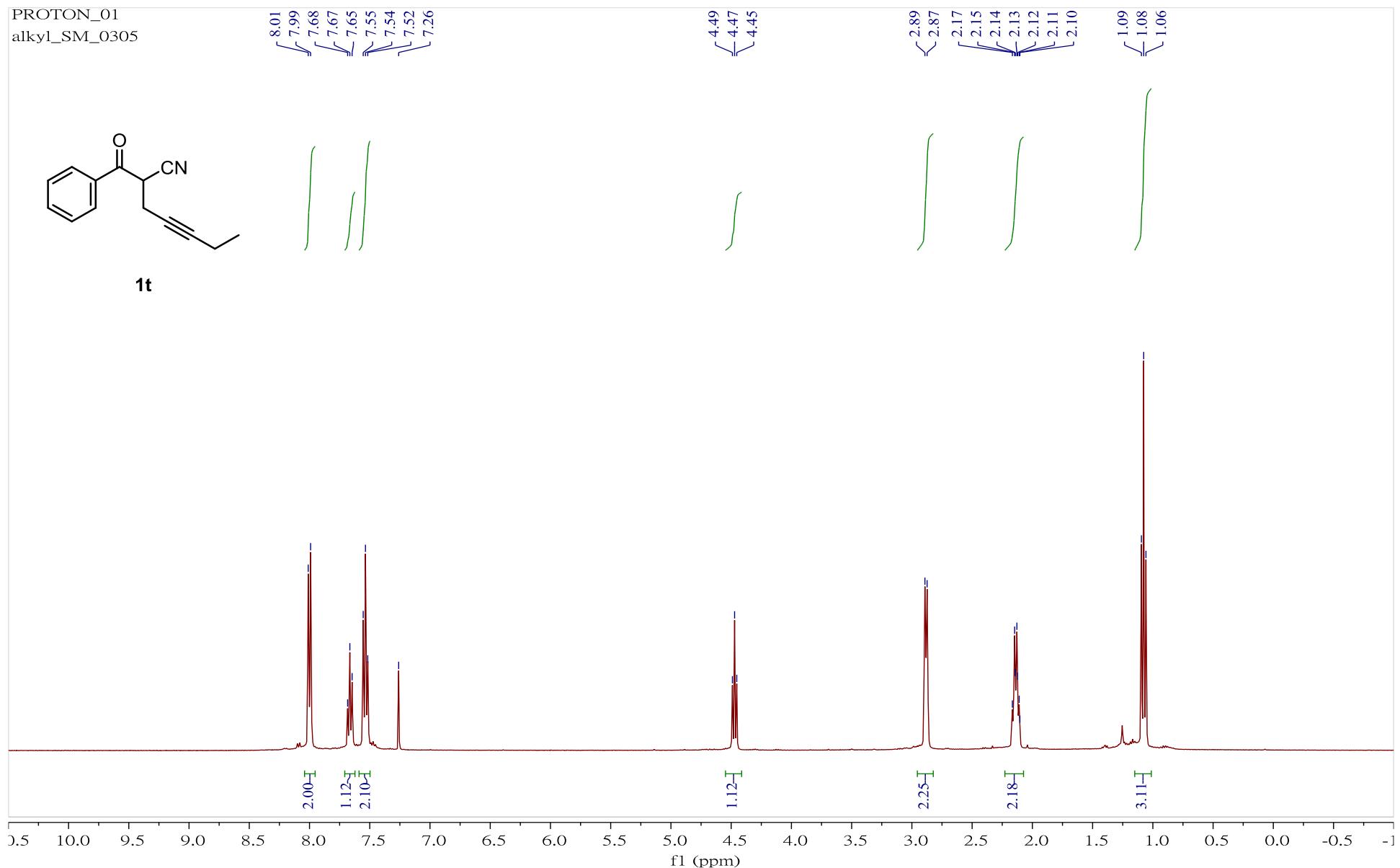
CARBON_01
TMS_SM C_0302

—188.9 —
—134.8 —
—133.9 —
—129.1 —
—128.9 —
—116.2 —
—99.9 —
—89.6 —
—38.8 —
—20.9 —
—0.2 —



¹³C NMR (100 MHz) spectrum of compound **1s** in CDCl₃

PROTON_01
alkyl_SM_0305



^1H NMR (400 MHz) spectrum of compound **1t** in CDCl_3

CARBON_01
alkyl SM 2

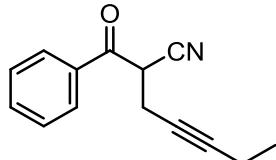
— 189.3

— 134.7
— 133.9
— 129.1
— 128.9

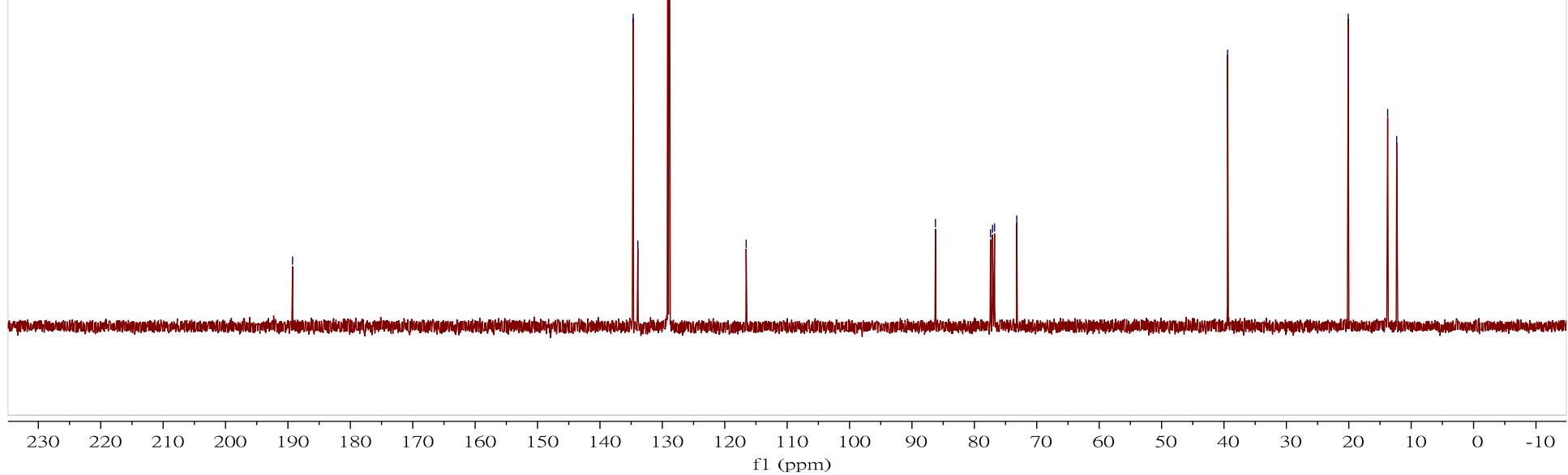
— 116.6

— 86.2
— 77.4
— 77.1
— 76.8
— 73.2

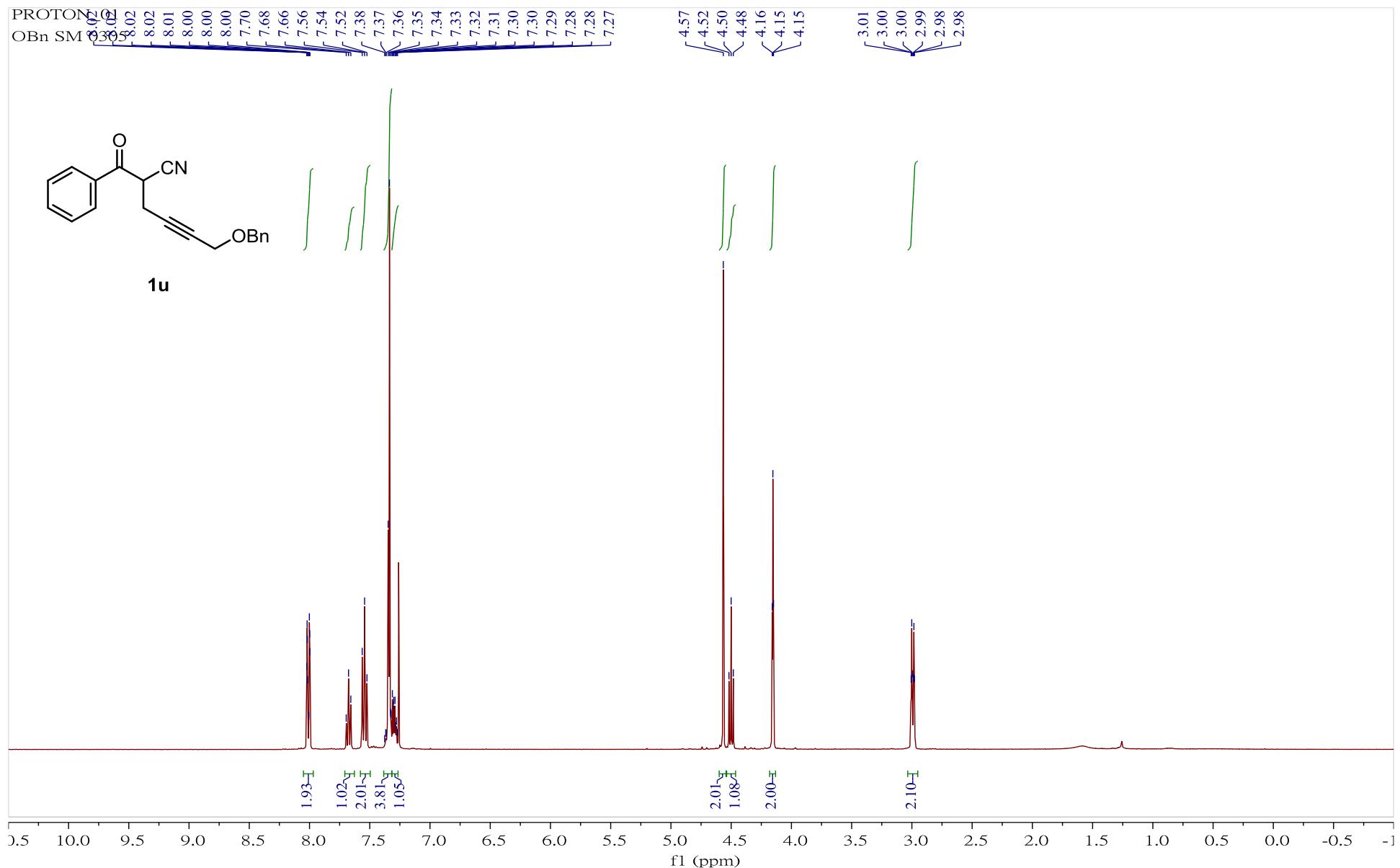
— 39.4
— 20.1
— 13.8
— 12.3



1t



¹³C NMR (100 MHz) spectrum of compound **1t** in CDCl₃



CARBON_01
OBn_SM_C

— 188.7

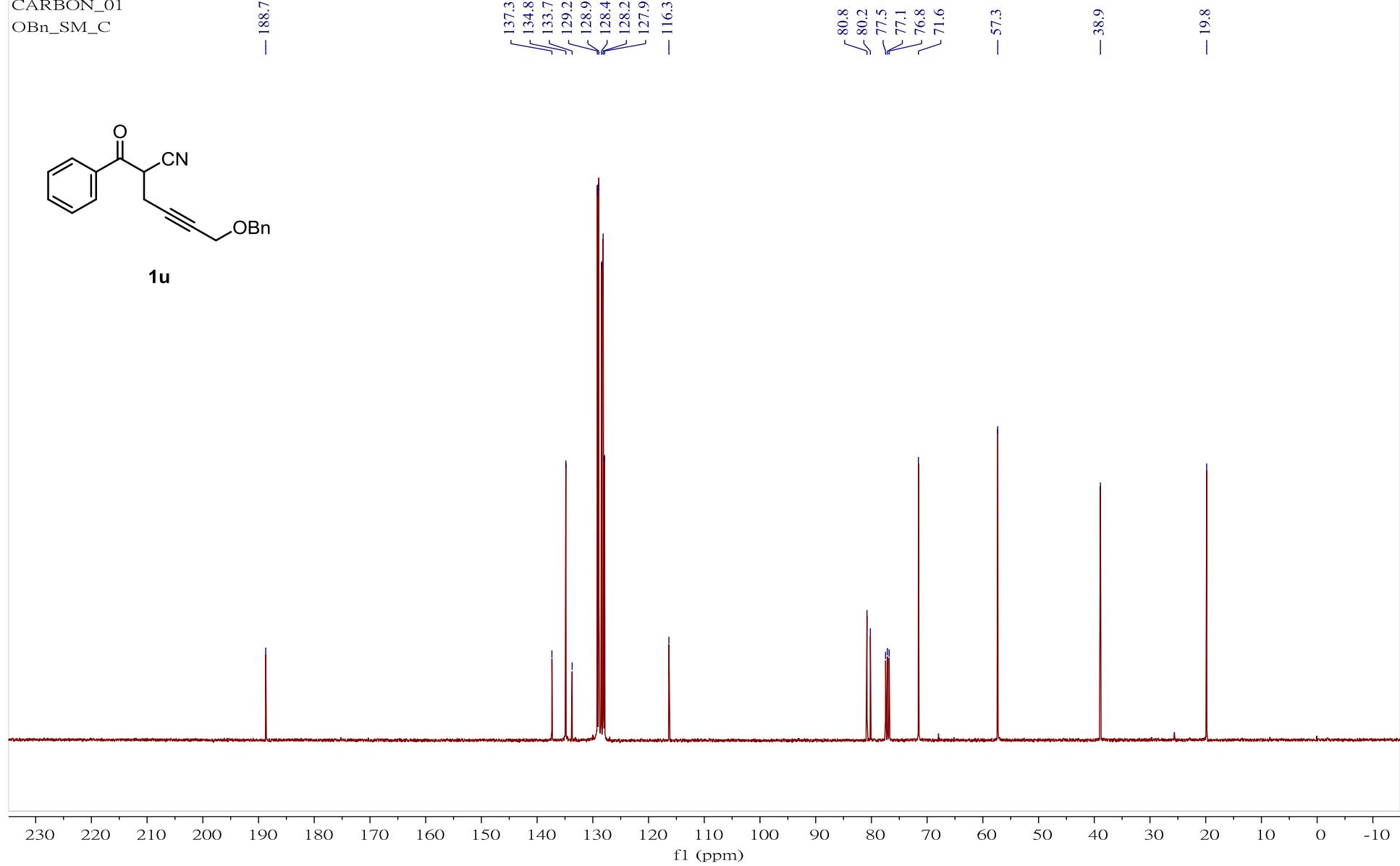
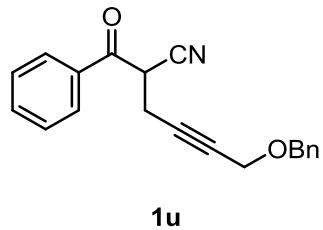
137.3
134.8
133.7
129.2
128.9
128.4
128.2
127.9
— 116.3

80.8
80.2
77.5
77.1
76.8
71.6

— 57.3

— 38.9

— 19.8



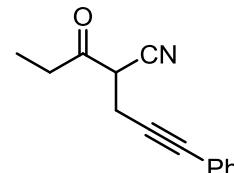
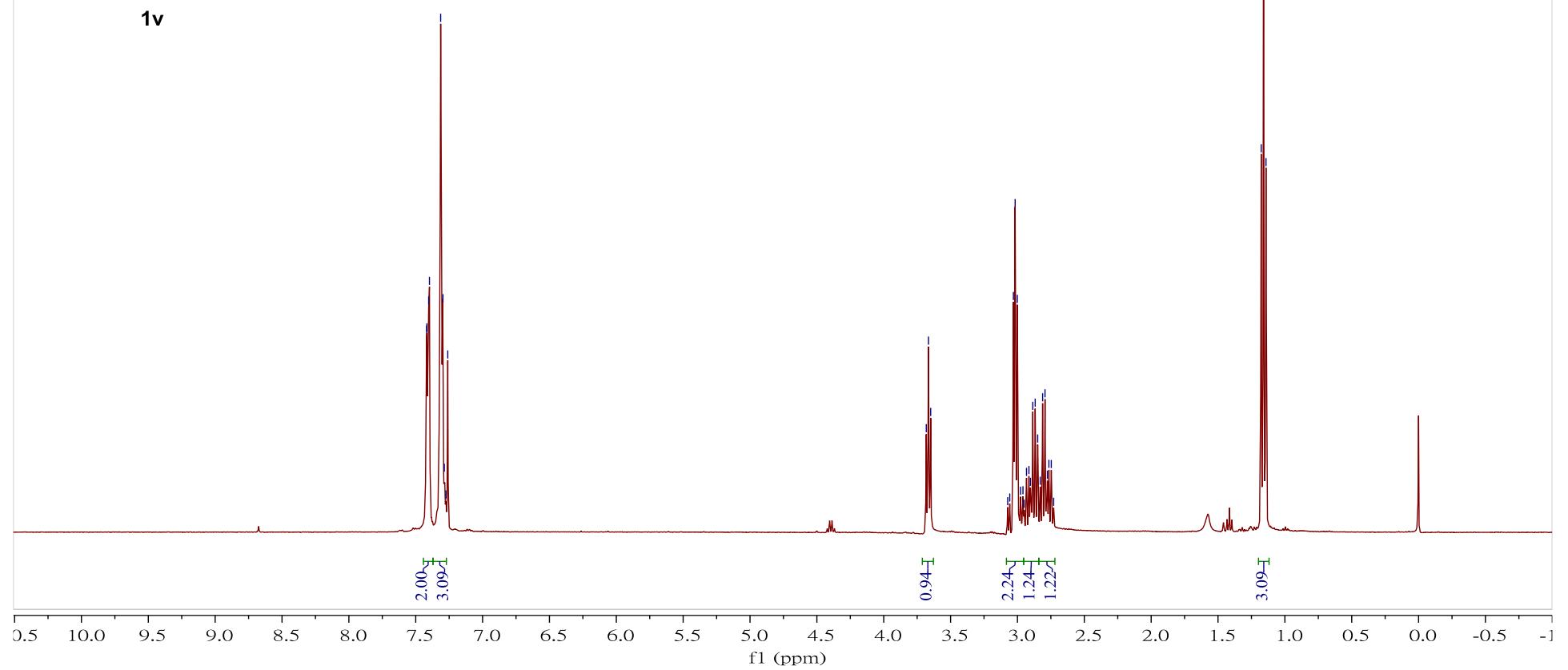
¹³C NMR (100 MHz) spectrum of compound **1u** in CDCl₃

PROTON_01

ethyl SM

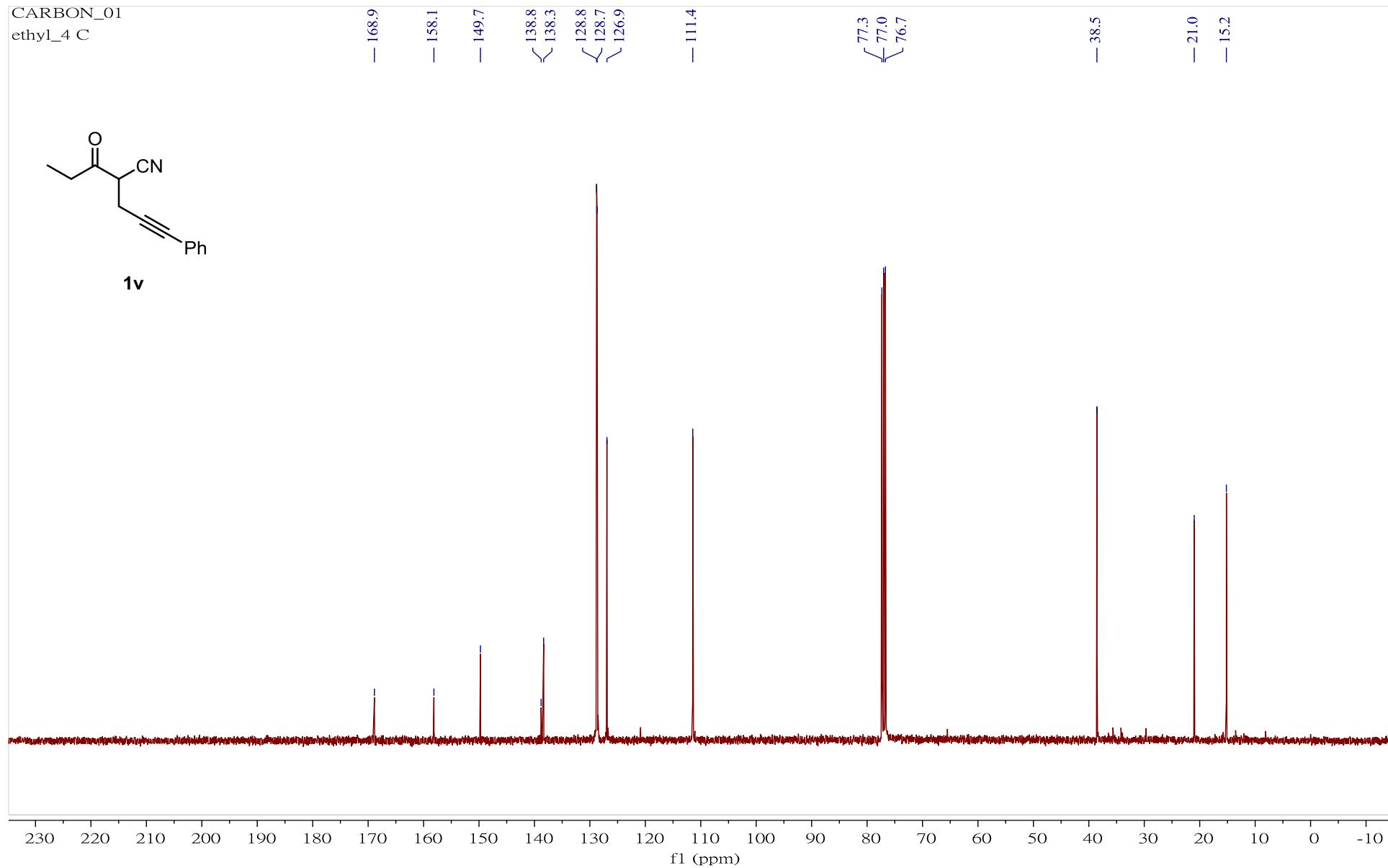
7.42
7.42
7.40
7.40
7.31
7.30
7.29
7.27
7.26

3.68
3.67
3.65
3.07
3.06
3.03
3.02
3.00
2.98
2.96
2.95
2.93
2.91
2.90
2.89
2.87
2.85
2.83
2.81
2.79
2.78
2.76
2.75
2.73
2.73
1.18
1.16
1.14

**1v**

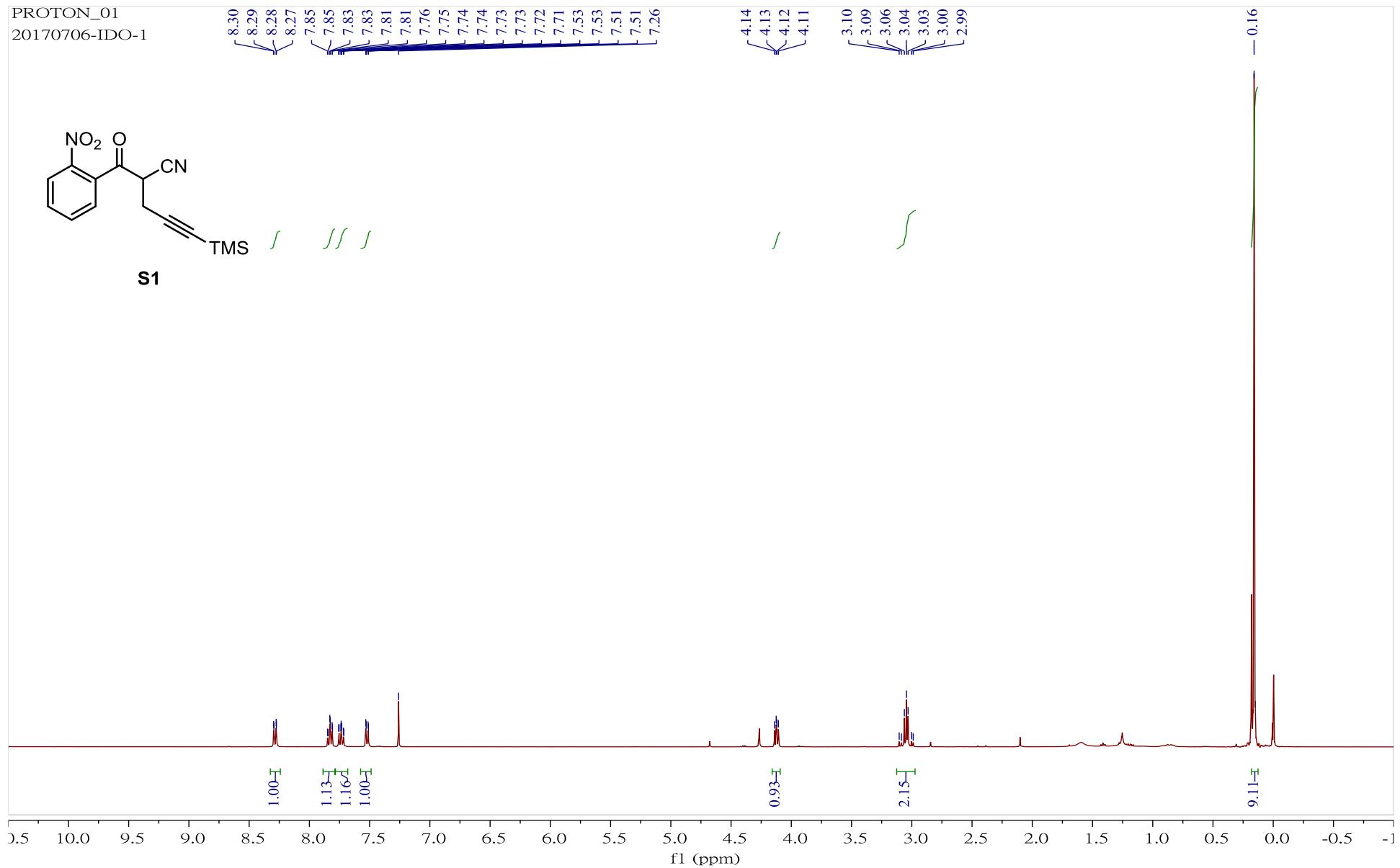
^1H NMR (400 MHz) spectrum of compound **1v** in CDCl_3

CARBON_01
ethyl_4 C



¹³C NMR (100 MHz) spectrum of compound **1v** in CDCl₃

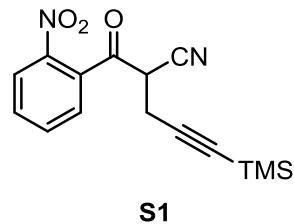
PROTON_01
20170706-IDO-1



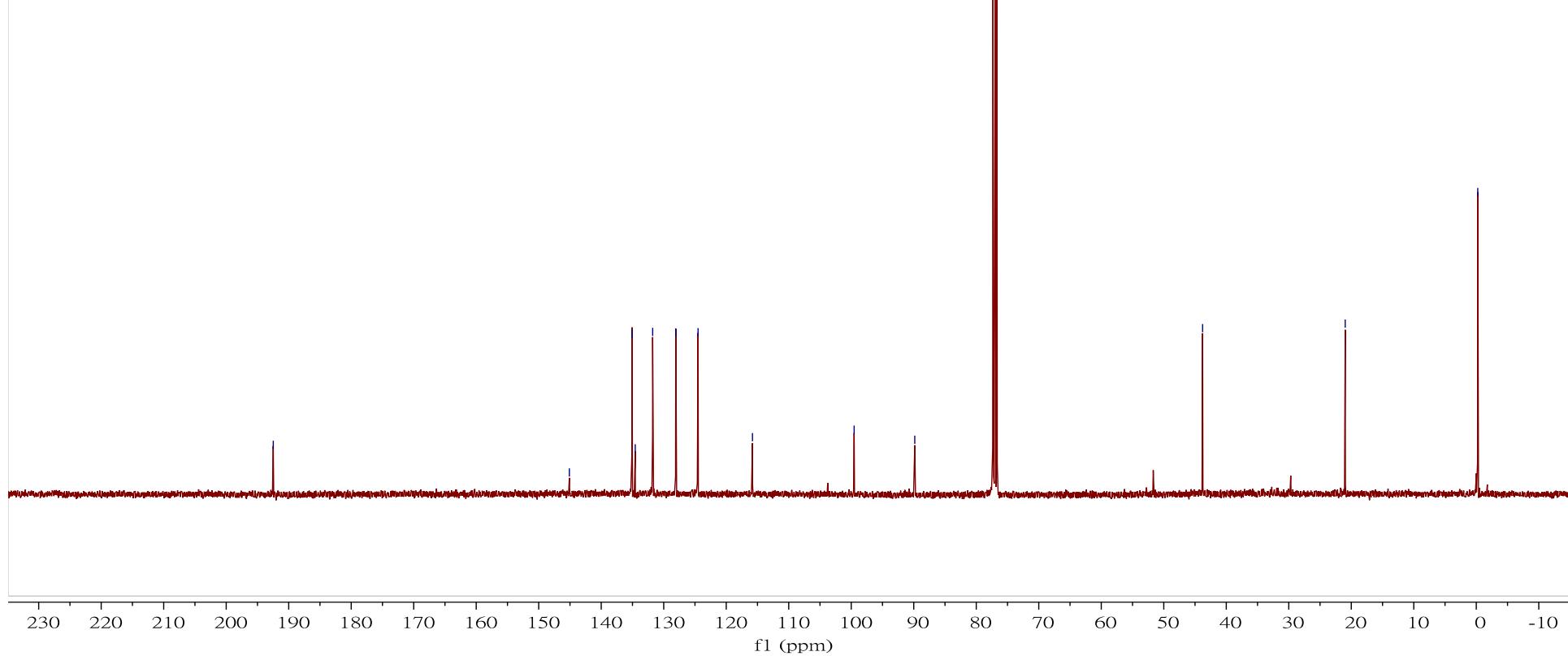
^1H NMR (400 MHz) spectrum of compound **S1** in CDCl_3

CARBON_01
20170706-IDO-1

— 192.5 — 145.1 — 135.1
— 134.6 — 131.8 — 128.1 — 124.5 — 115.8 — 99.5 — 89.8 — 77.3
— 77.0 — 76.7 — 43.8 — 21.0 — -0.2

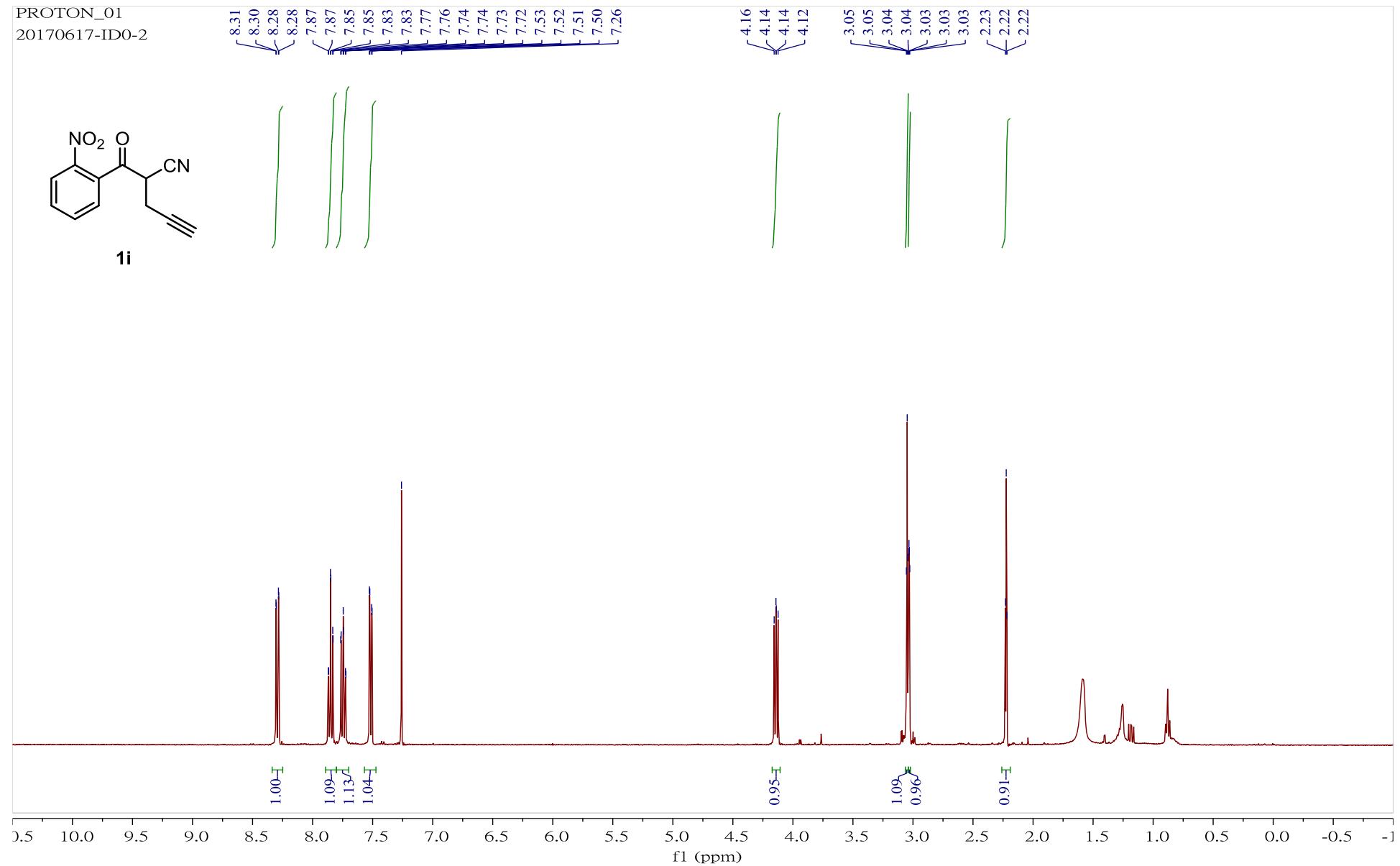
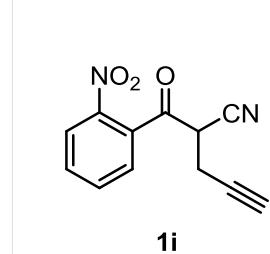


S1



^{13}C NMR (100 MHz) spectrum of compound **S1** in CDCl_3

PROTON_01
20170617-ID0-2



^1H NMR (400 MHz) spectrum of compound **1i** in CDCl_3

CARBON_01
20170617-ID0-2

— 192.1

— 145.0

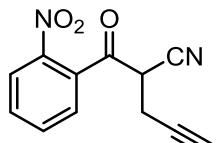
— 135.2
— 134.3
— 131.9
— 128.0
— 124.6

— 115.7

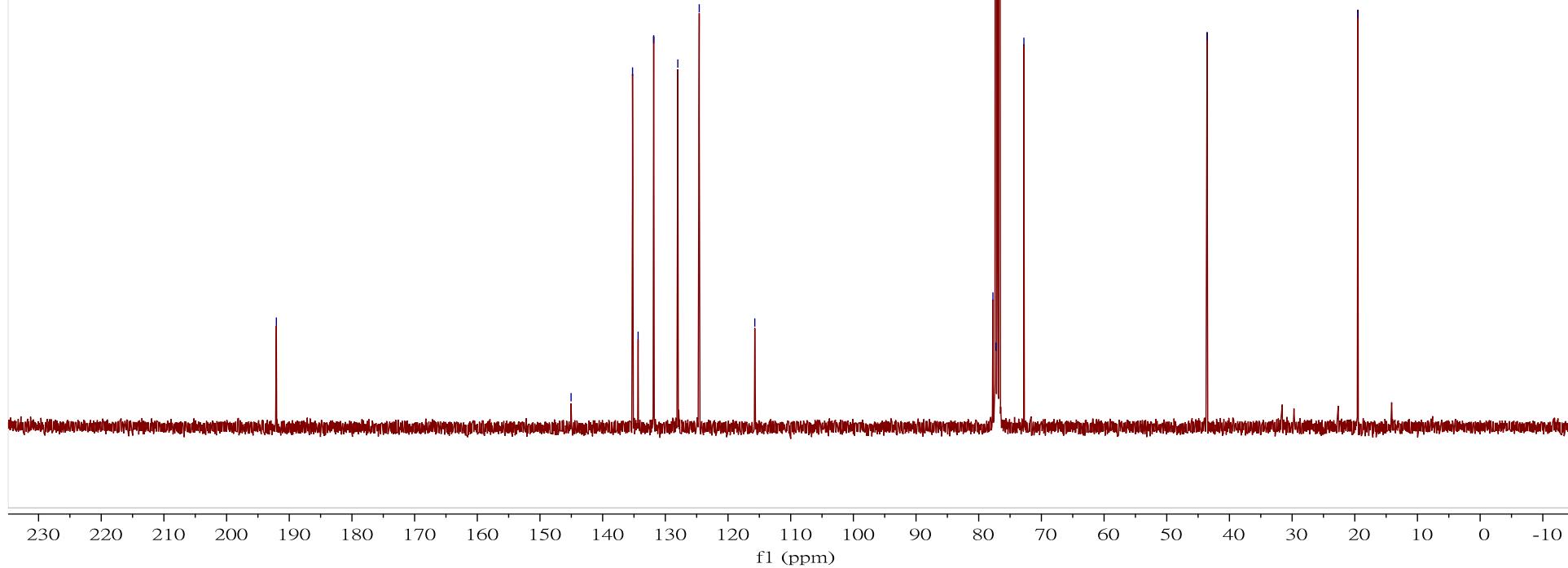
— 77.7
— 77.3
— 77.2
— 77.0
— 76.7
— 72.8

— 43.6

— 19.5

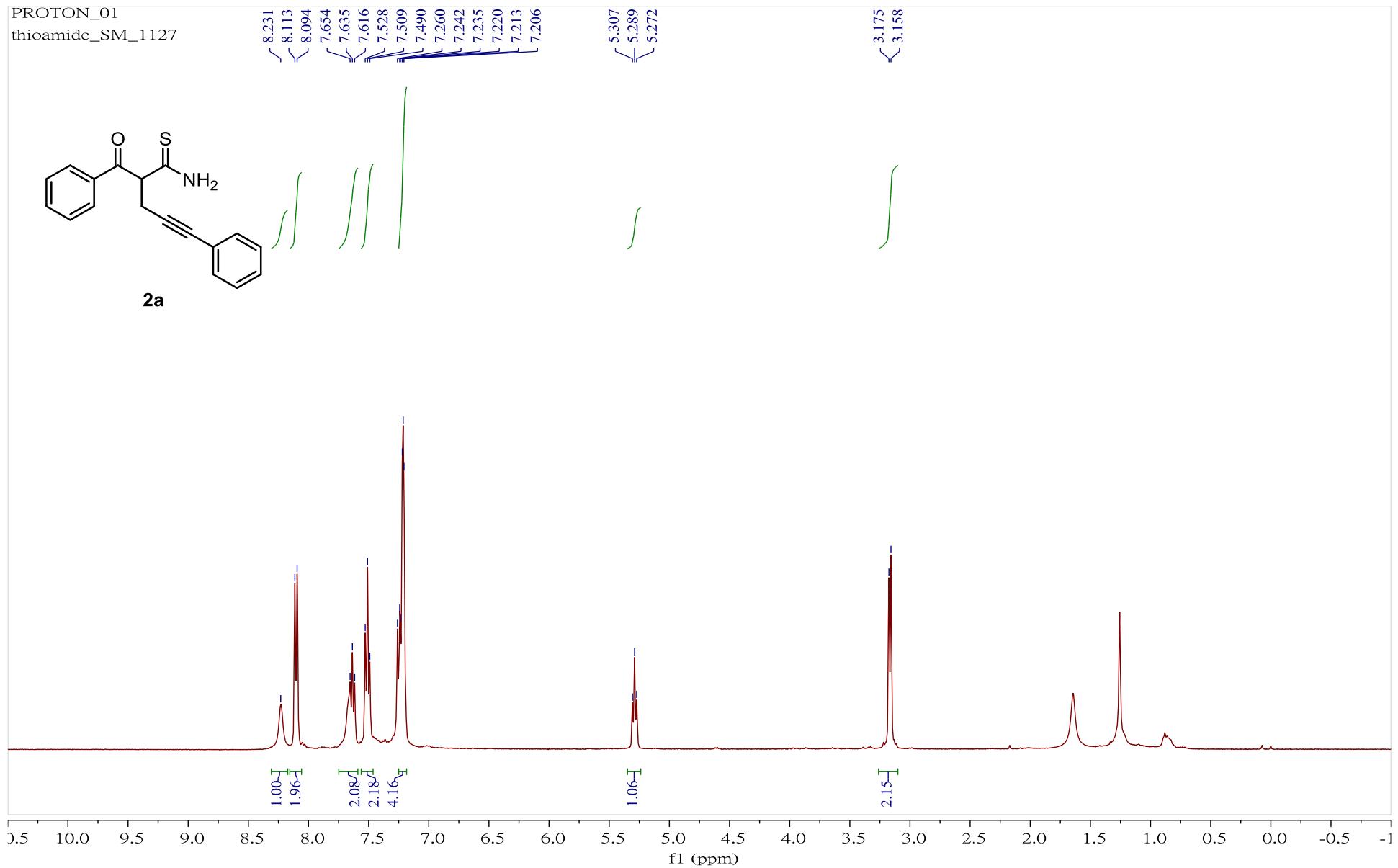


1i

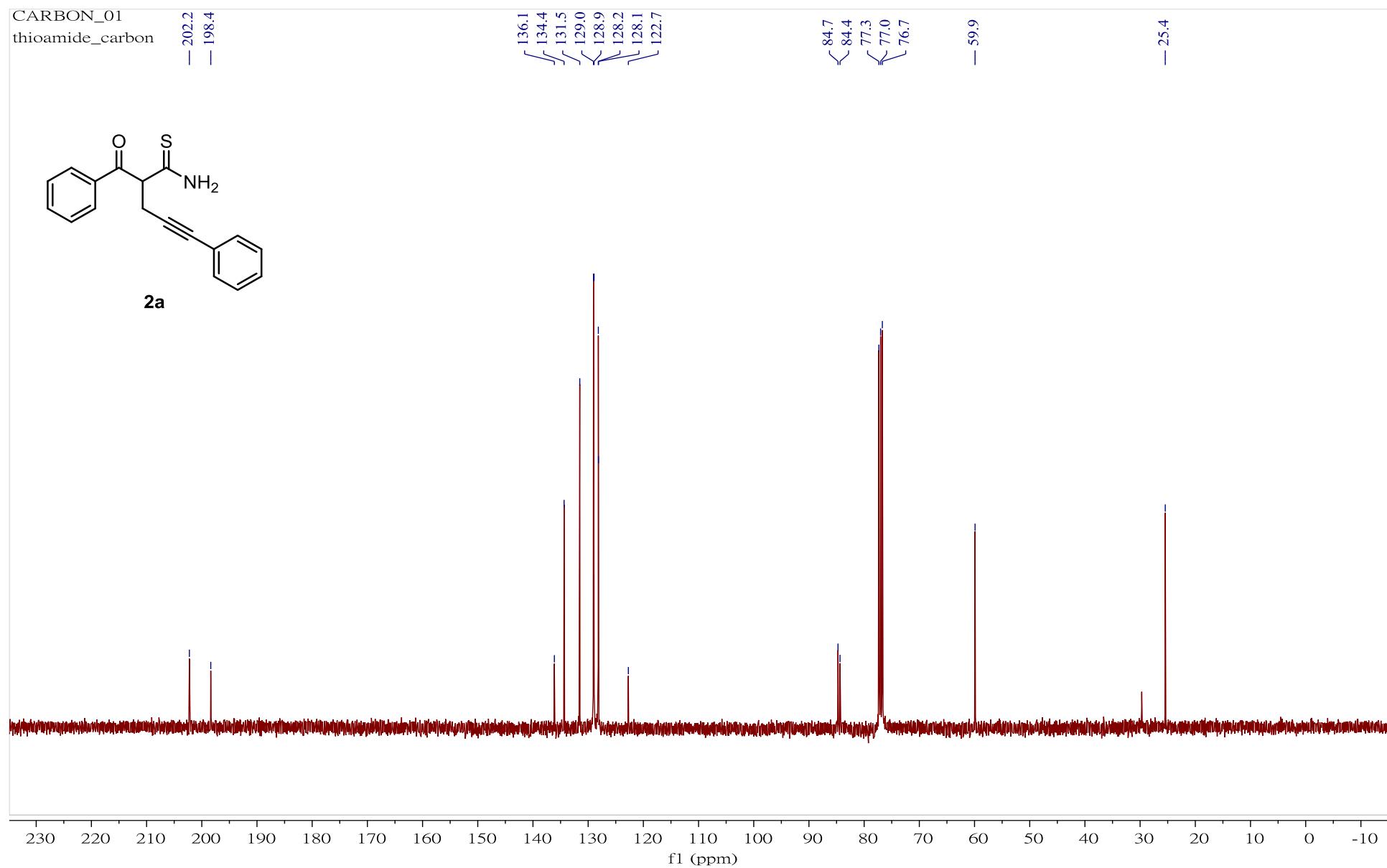


^{13}C NMR (100 MHz) spectrum of compound **1i** in CDCl_3

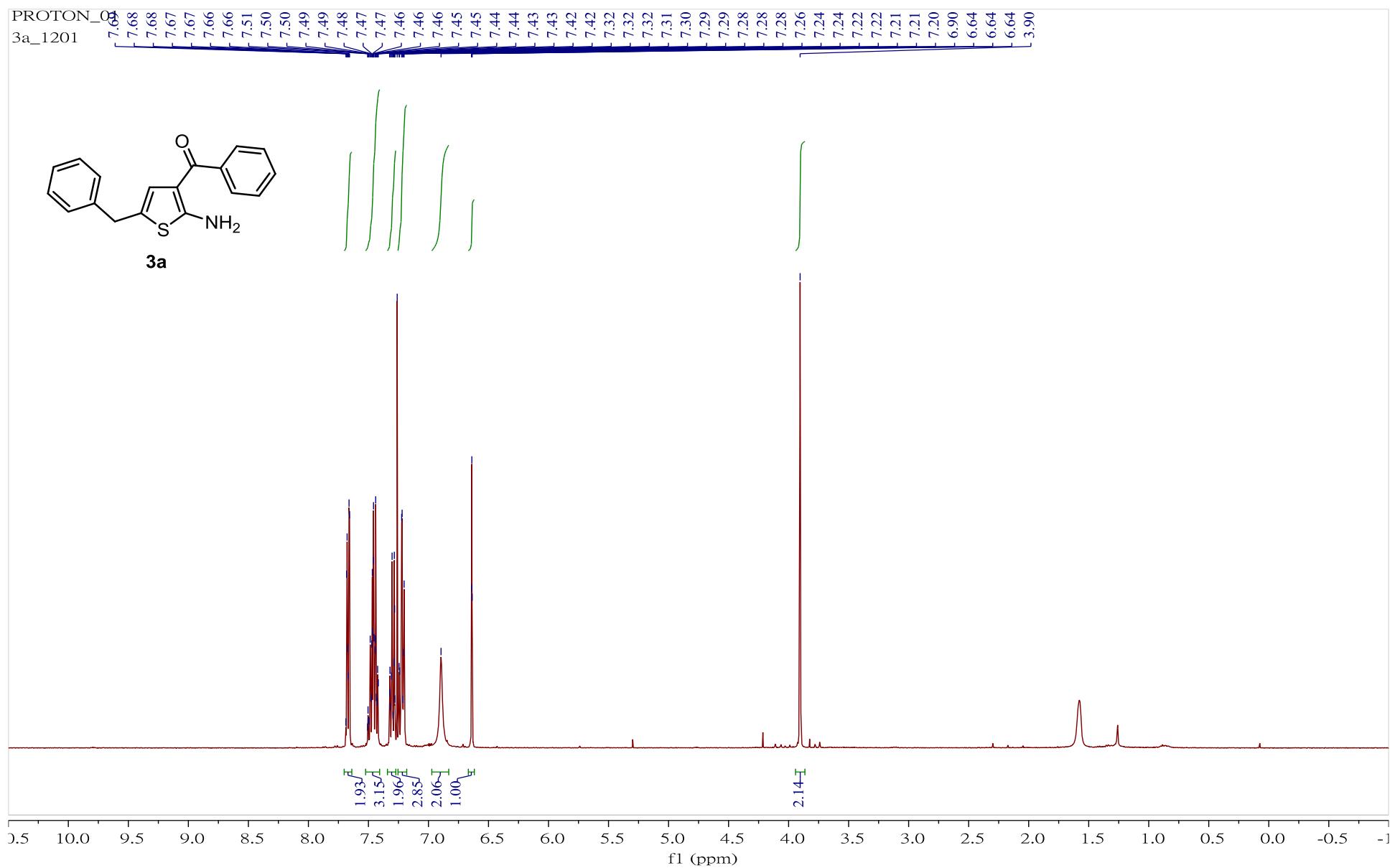
PROTON_01
thioamide_SM_1127



^1H NMR (400 MHz) spectrum of compound **2a** in CDCl_3



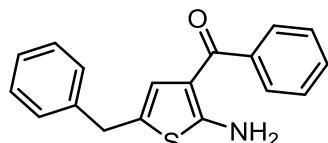
¹³C NMR (100 MHz) spectrum of compound **2a** in CDCl₃



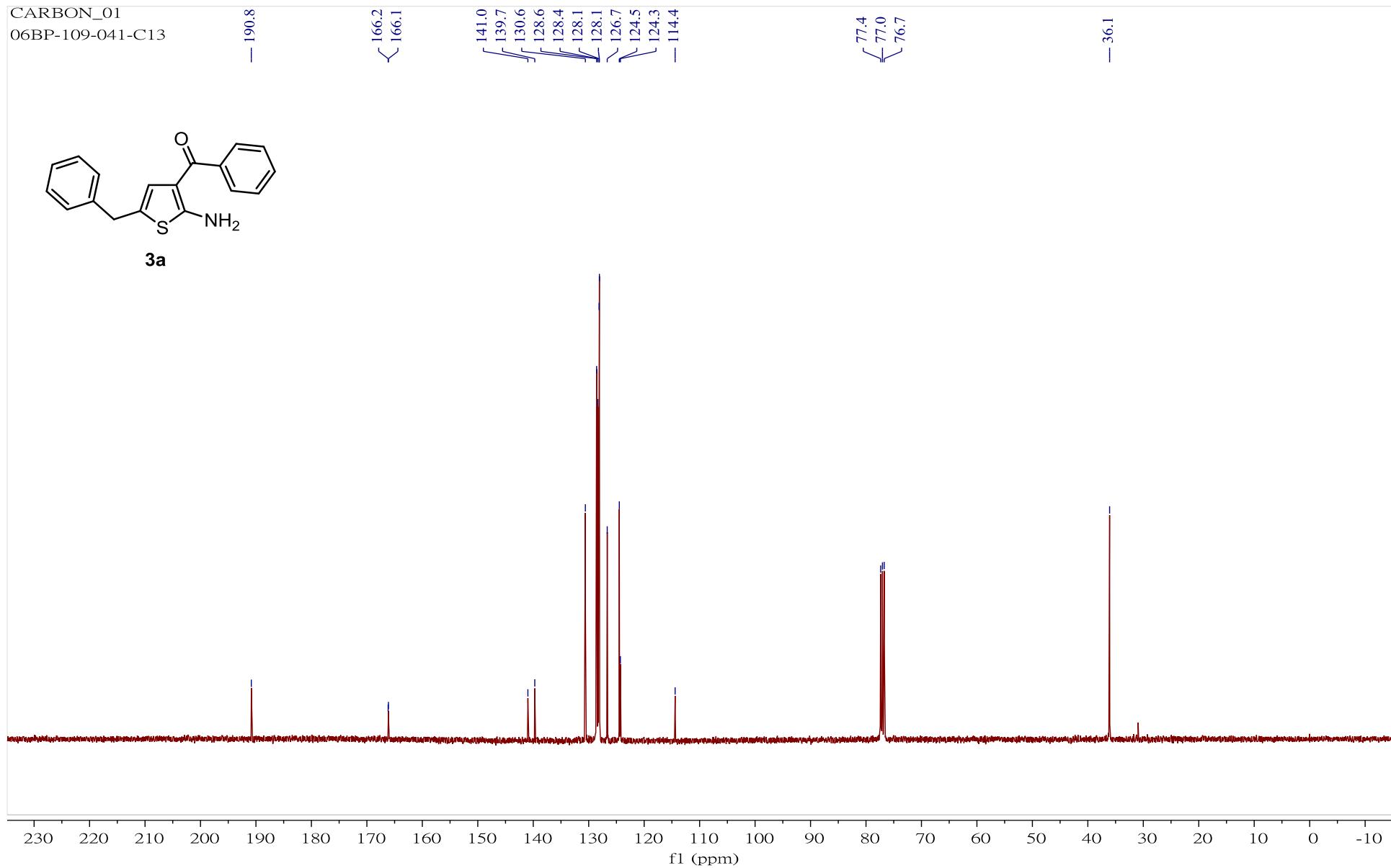
^1H NMR (400 MHz) spectrum of compound **3a** in CDCl_3

CARBON_01
06BP-109-041-C13

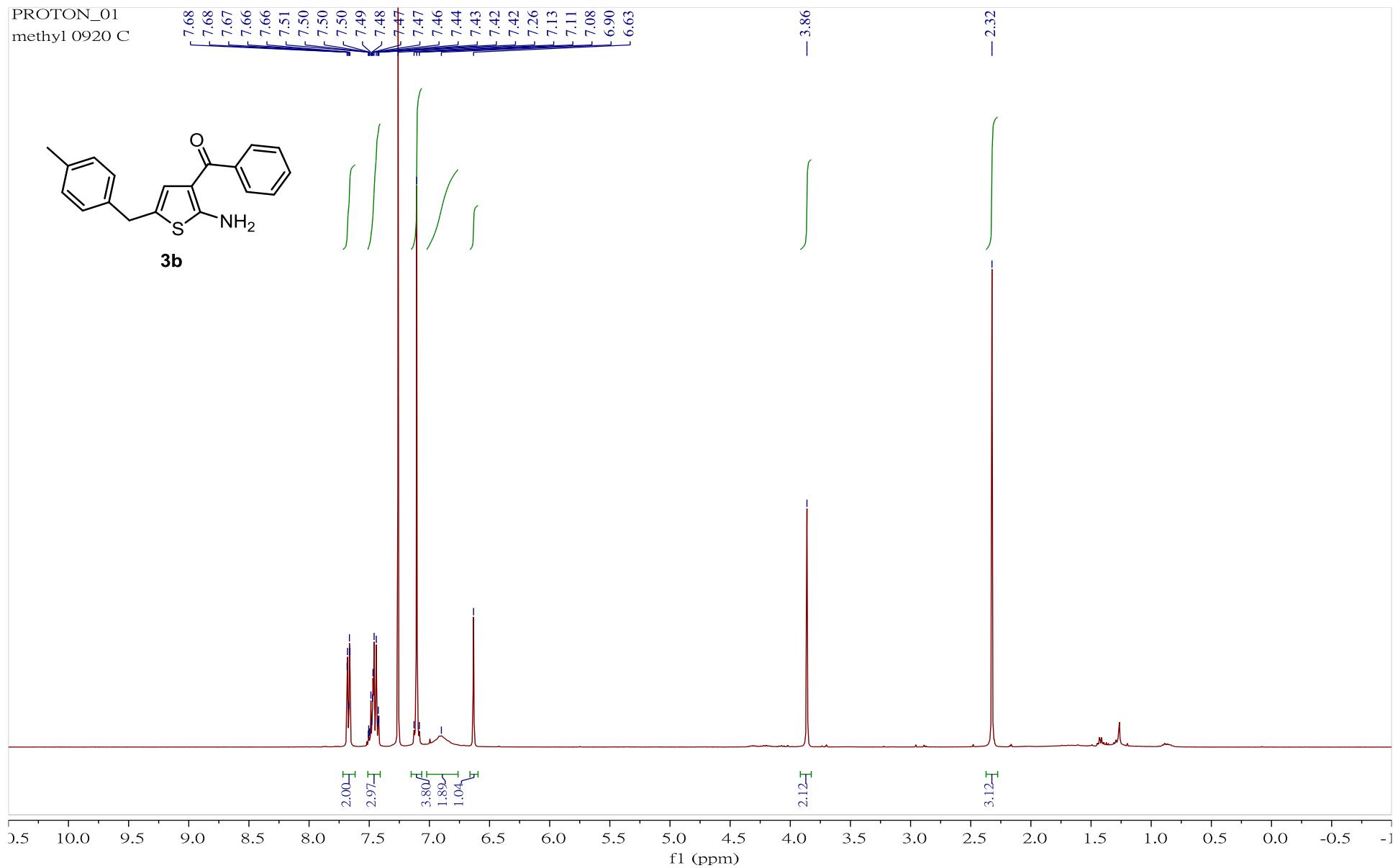
— 190.8 166.2 166.1 141.0
139.7 130.6 128.6 128.4
128.1 128.1 126.7 124.5
124.3 114.4 77.4 77.0
76.7 — 36.1



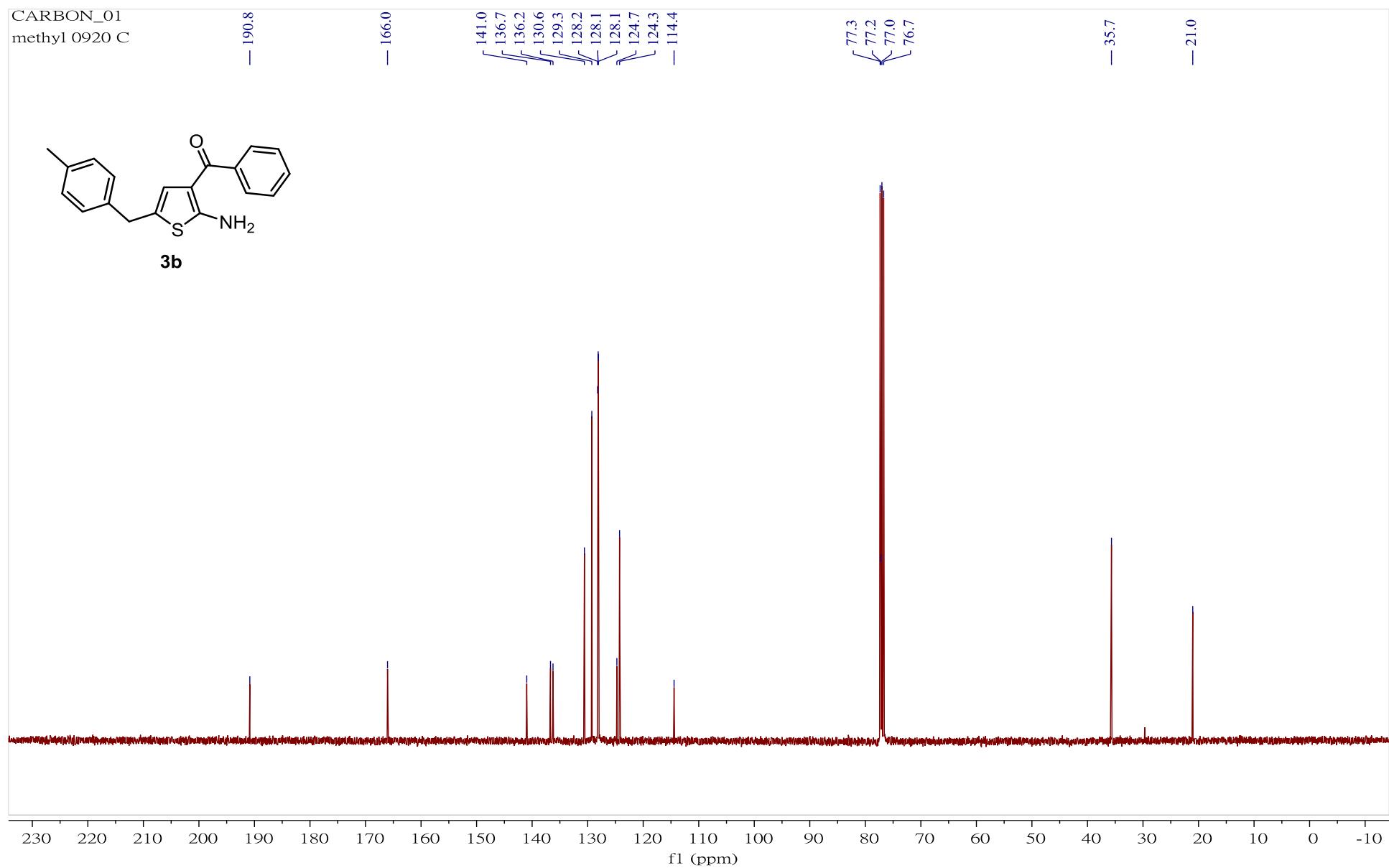
3a



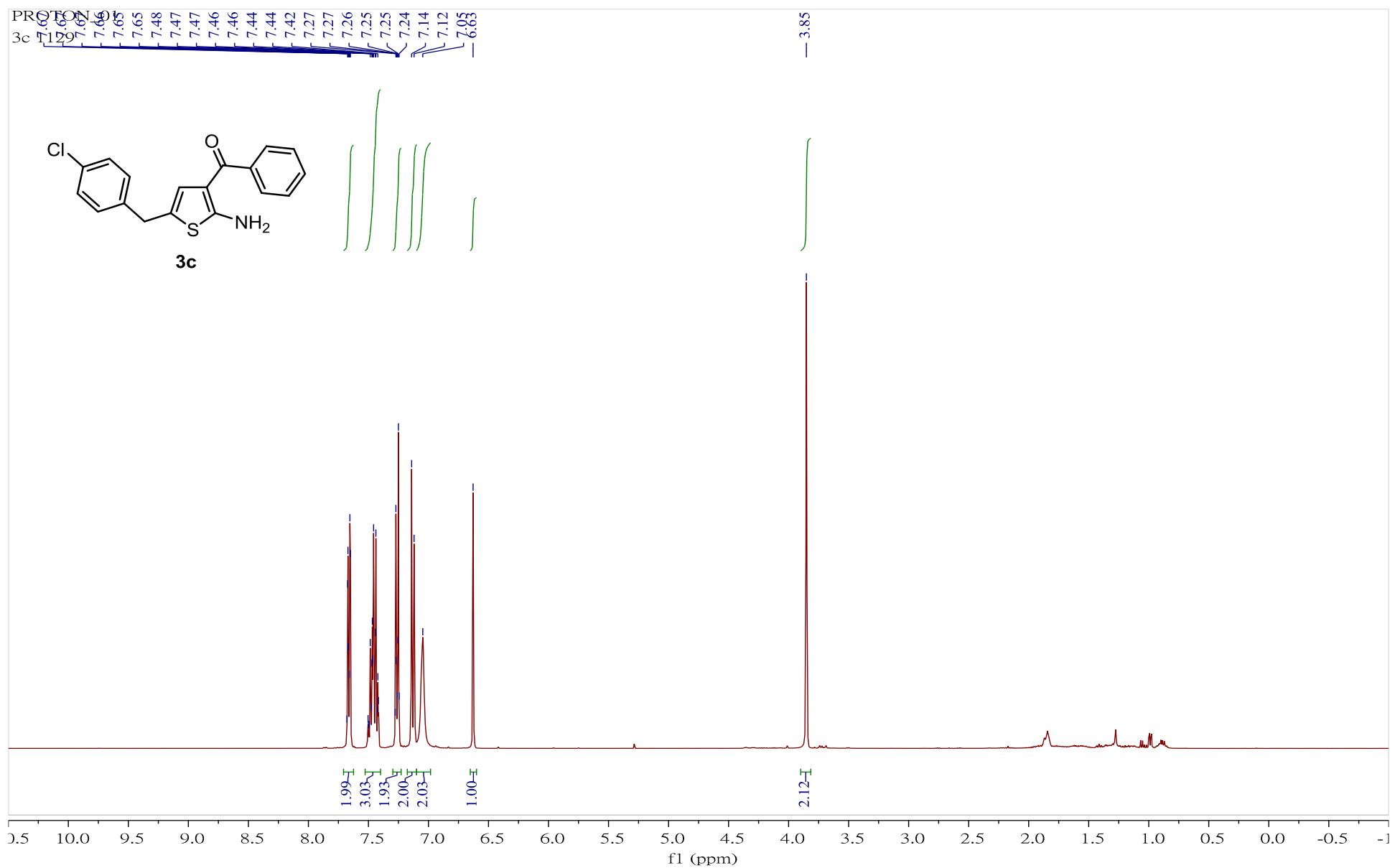
^{13}C NMR (100 MHz) spectrum of compound **3a** in CDCl_3



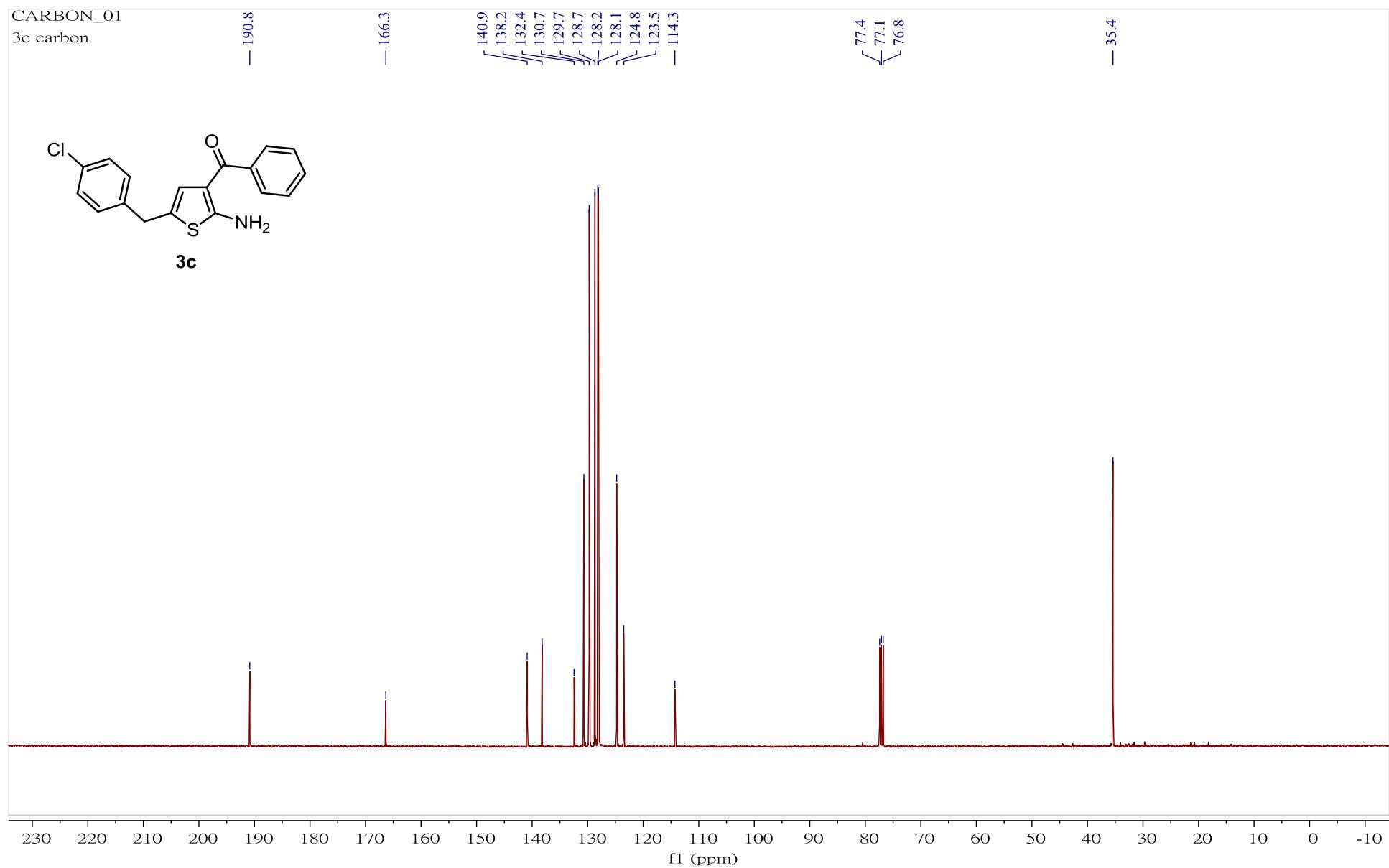
^1H NMR (400 MHz) spectrum of compound **3b** in CDCl_3



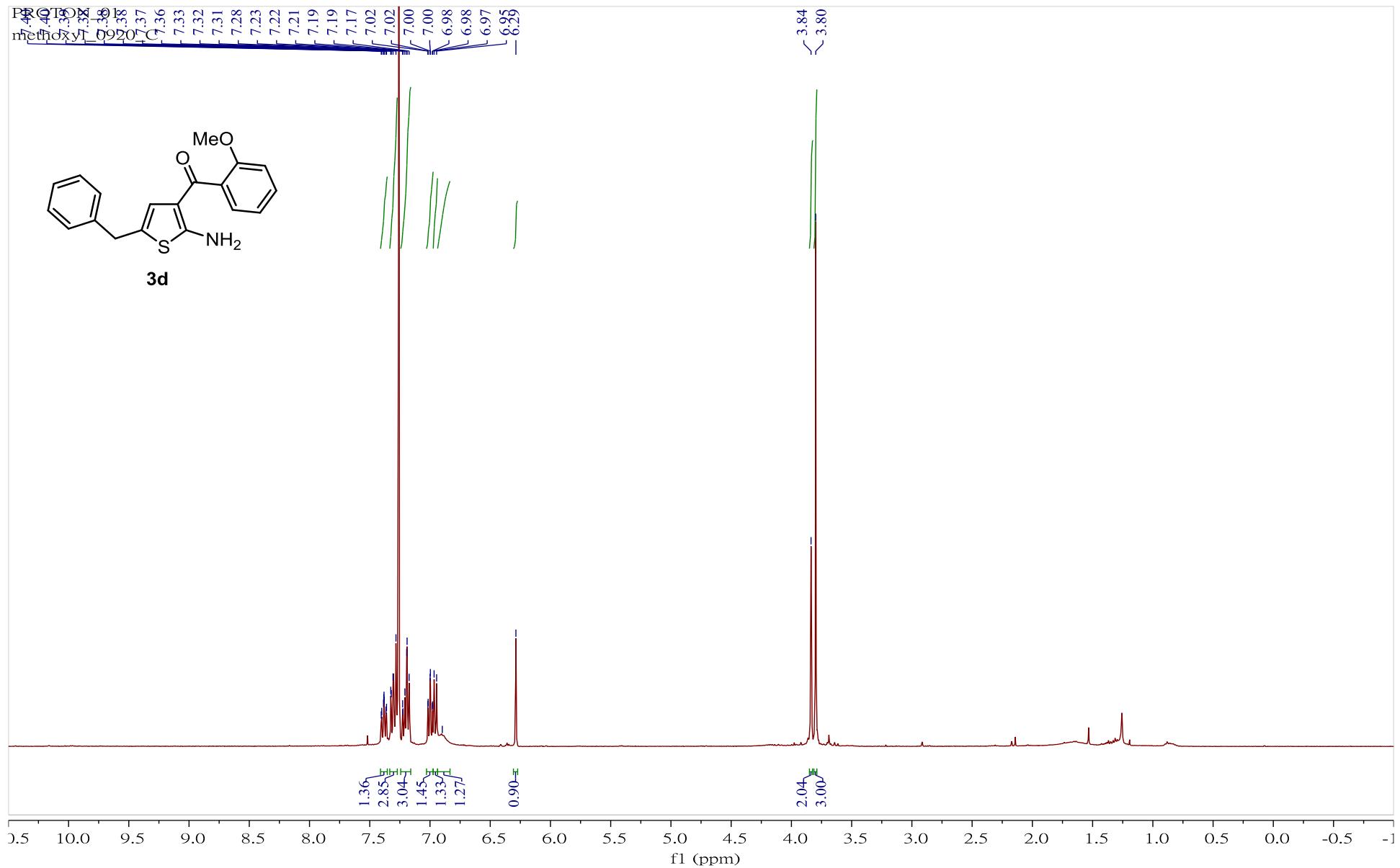
¹³C NMR (100 MHz) spectrum of compound **3b** in CDCl₃



^1H NMR (400 MHz) spectrum of compound **3c** in CDCl_3

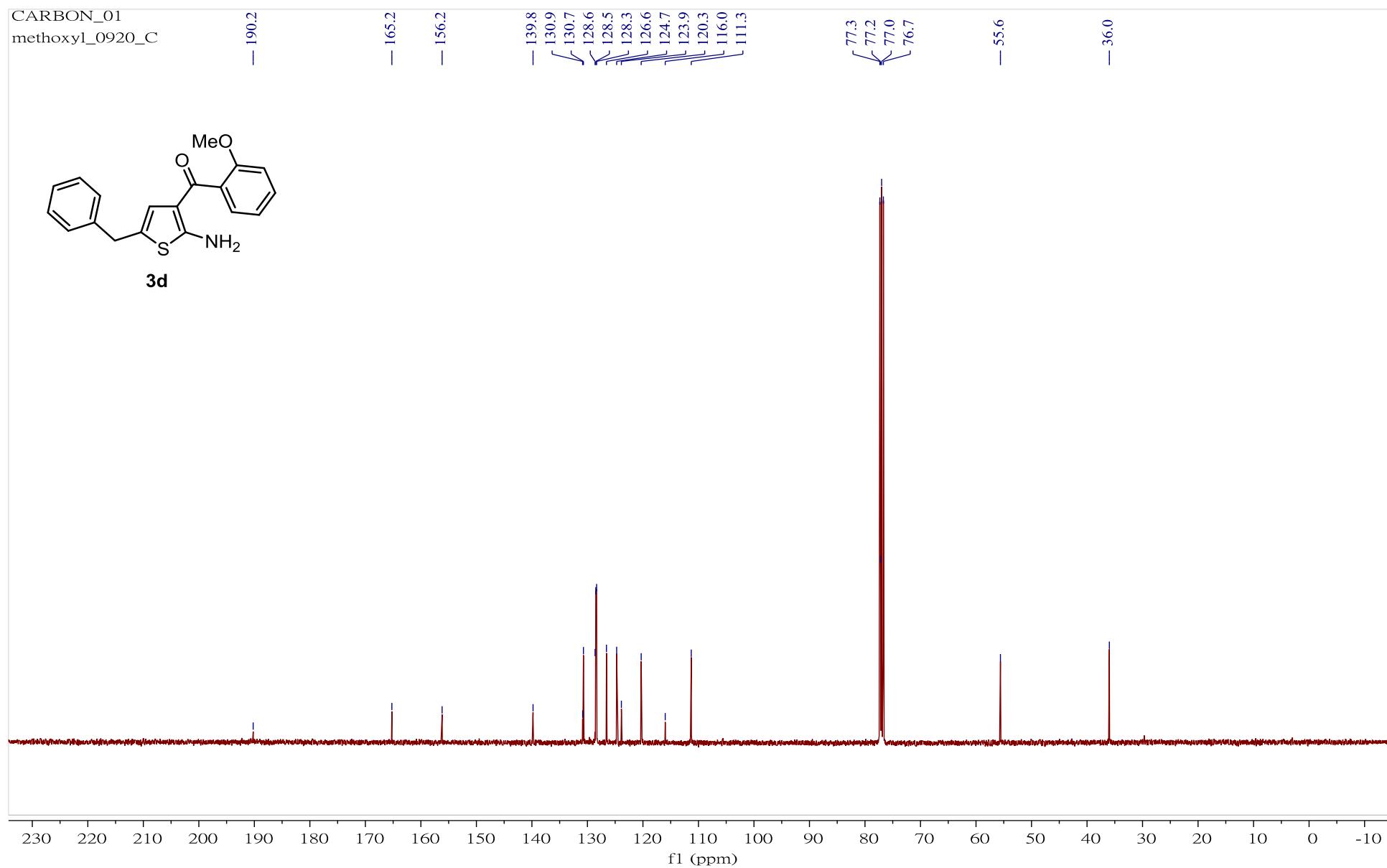


^{13}C NMR (100 MHz) spectrum of compound **3c** in CDCl_3

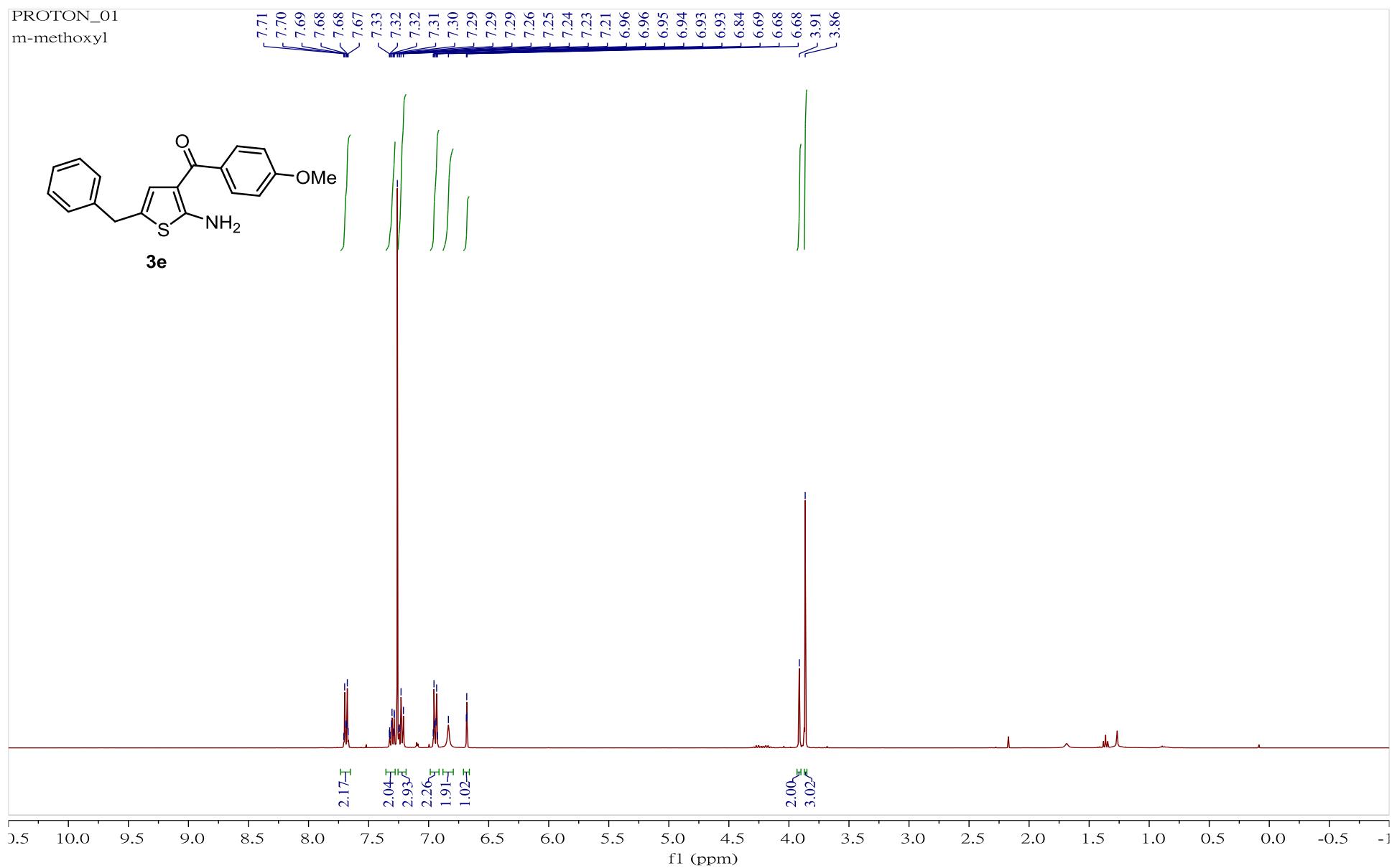


¹H NMR (400 MHz) spectrum of compound **3d** in CDCl₃

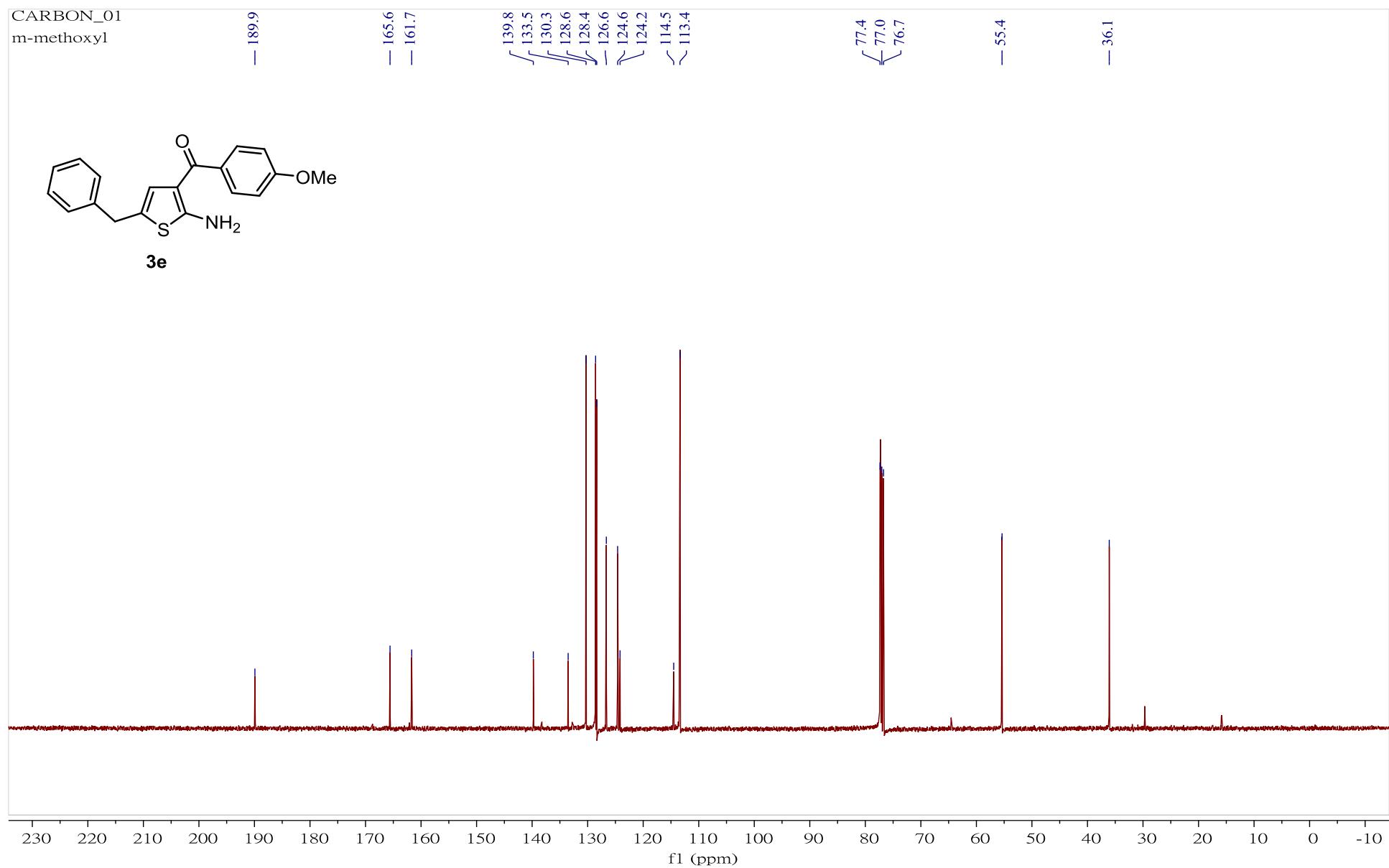
CARBON_01
methoxyl_0920_C



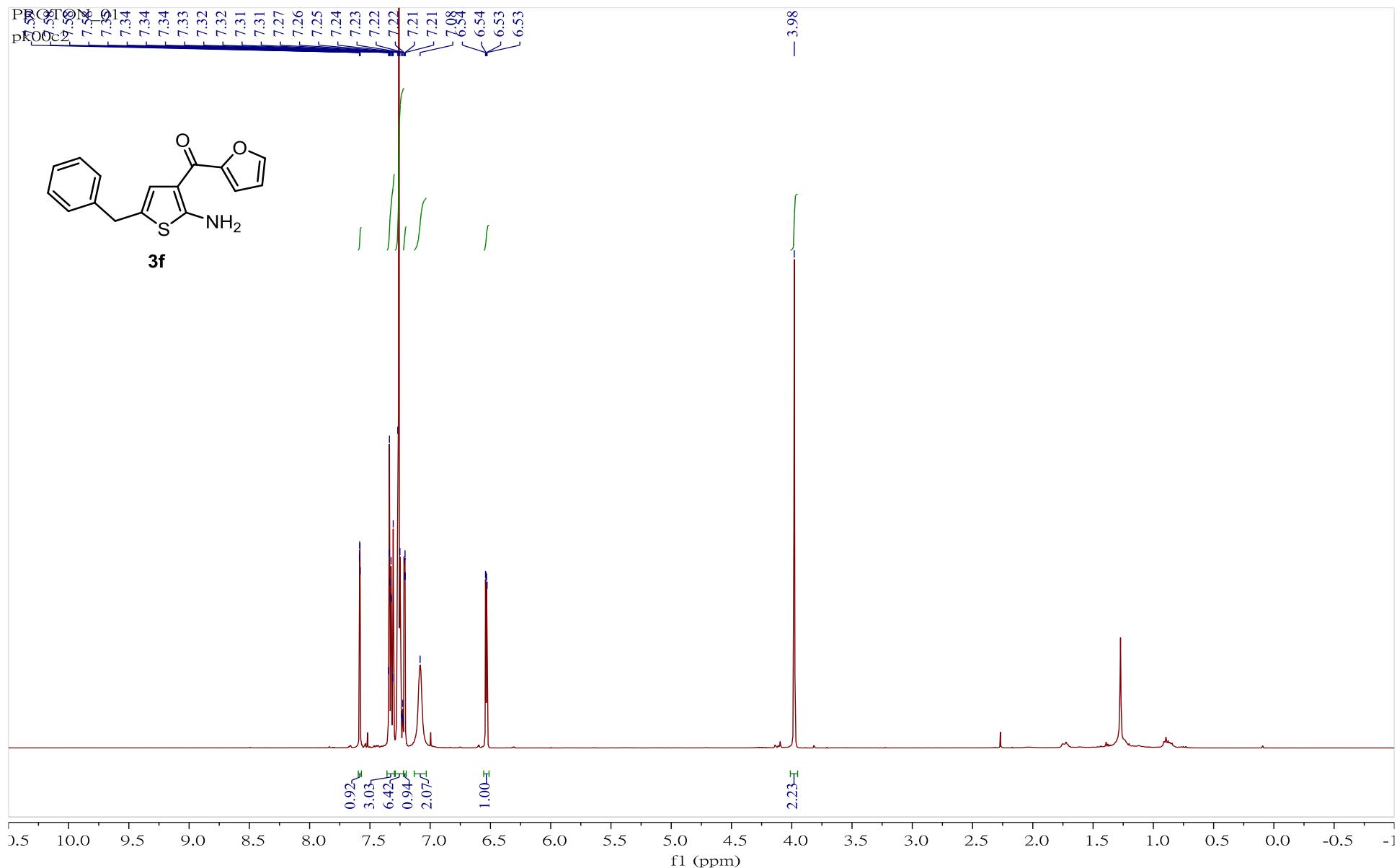
^{13}C NMR (100 MHz) spectrum of compound **3d** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **3e** in CDCl_3

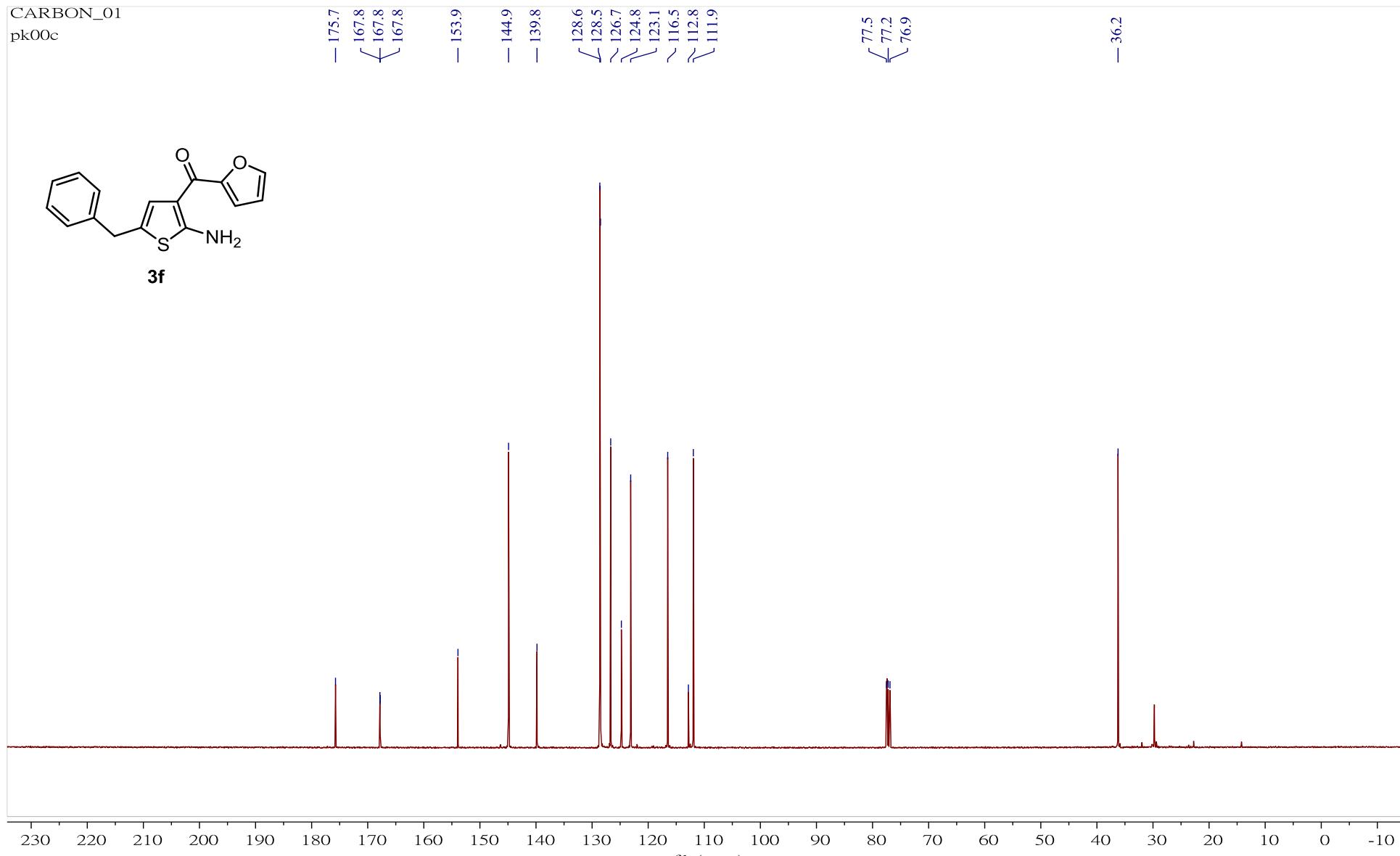


^{13}C NMR (100 MHz) spectrum of compound **3e** in CDCl_3

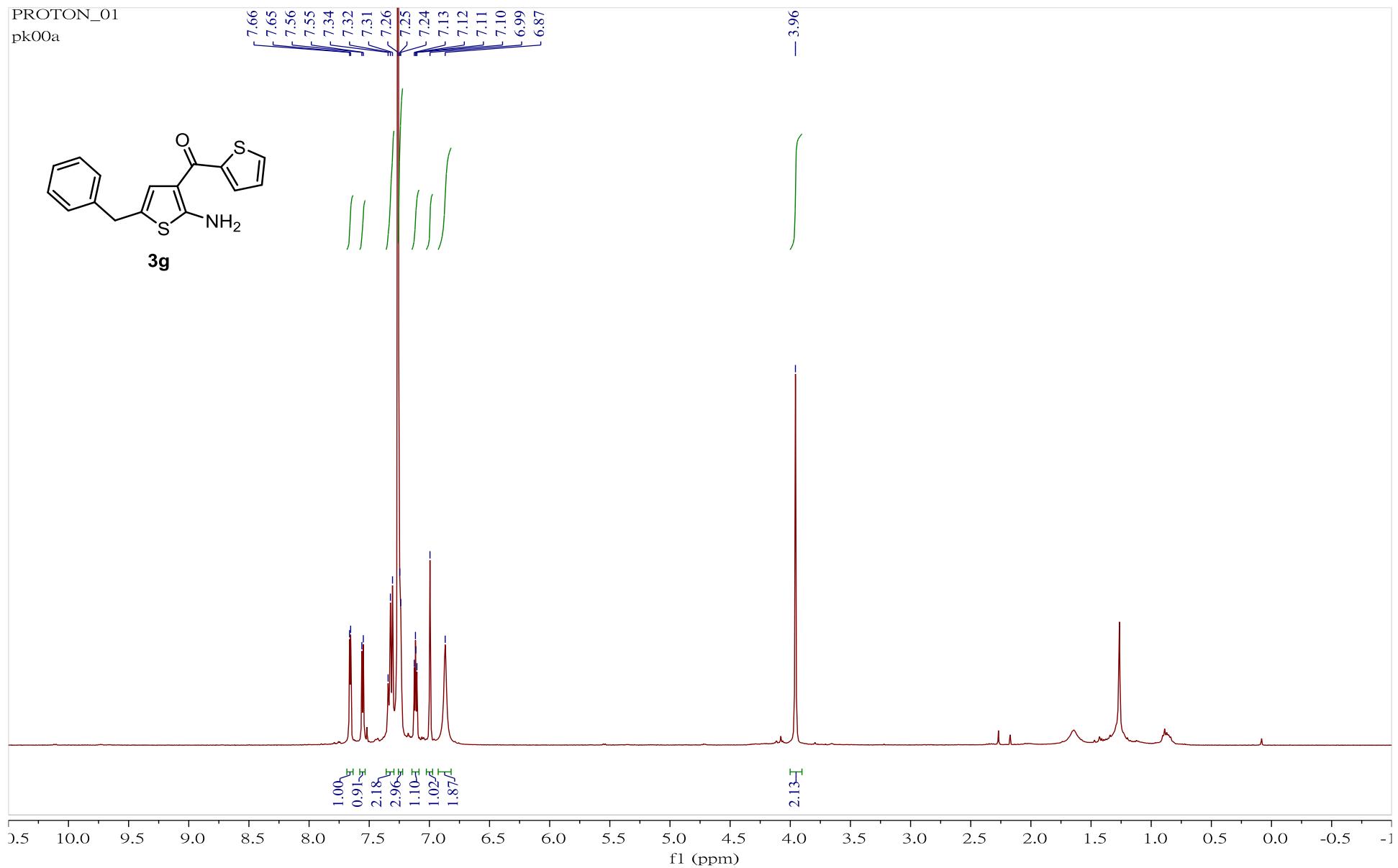


¹H NMR (400 MHz) spectrum of compound **3f** in CDCl₃

CARBON_01
pk00c



^{13}C NMR (100 MHz) spectrum of compound **3f** in CDCl_3



^1H NMR (400 MHz) spectrum of compound **3g** in CDCl_3

CARBON_01
pk00a

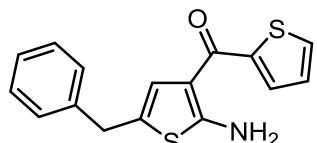
— 181.0

— 166.2

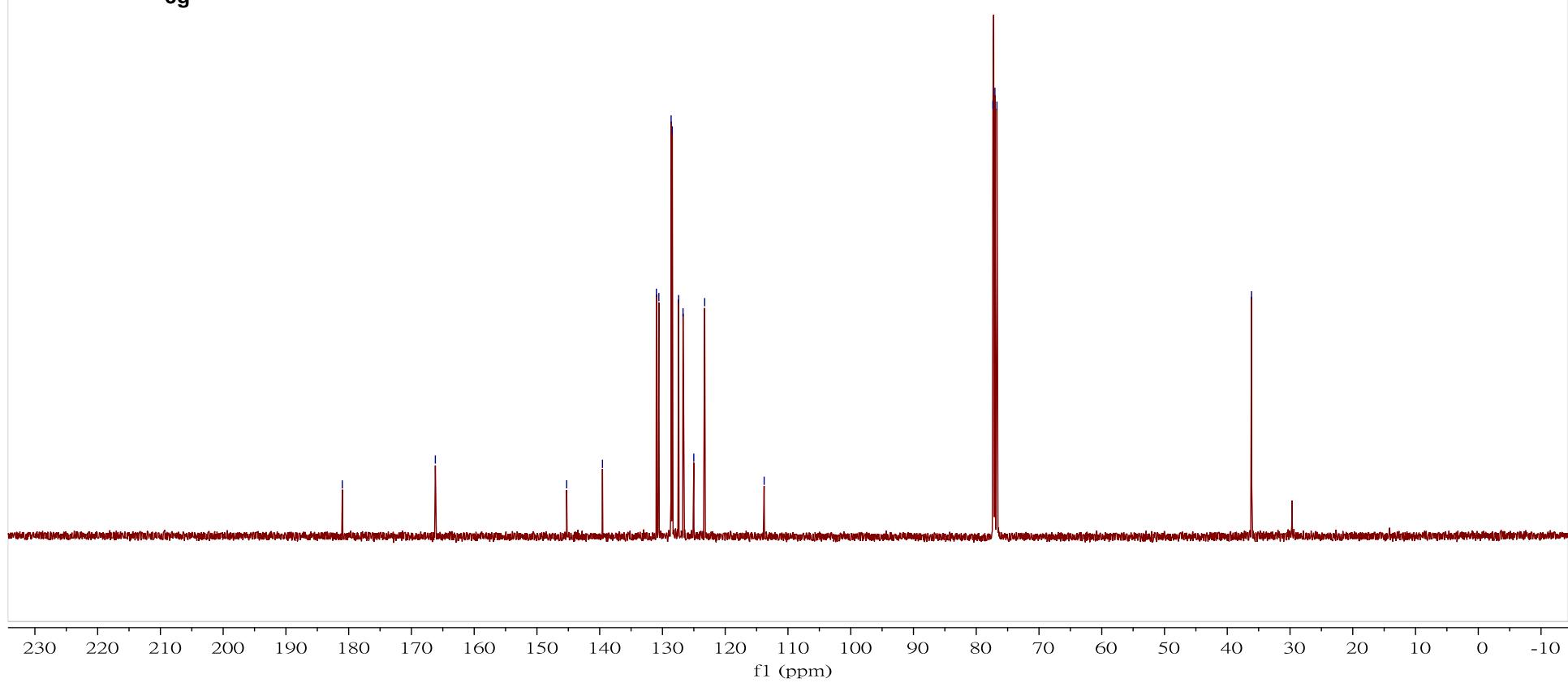
145.3
139.6
131.0
130.6
128.6
128.4
127.4
126.7
125.0
123.3
— 113.8

77.3
77.0
76.7

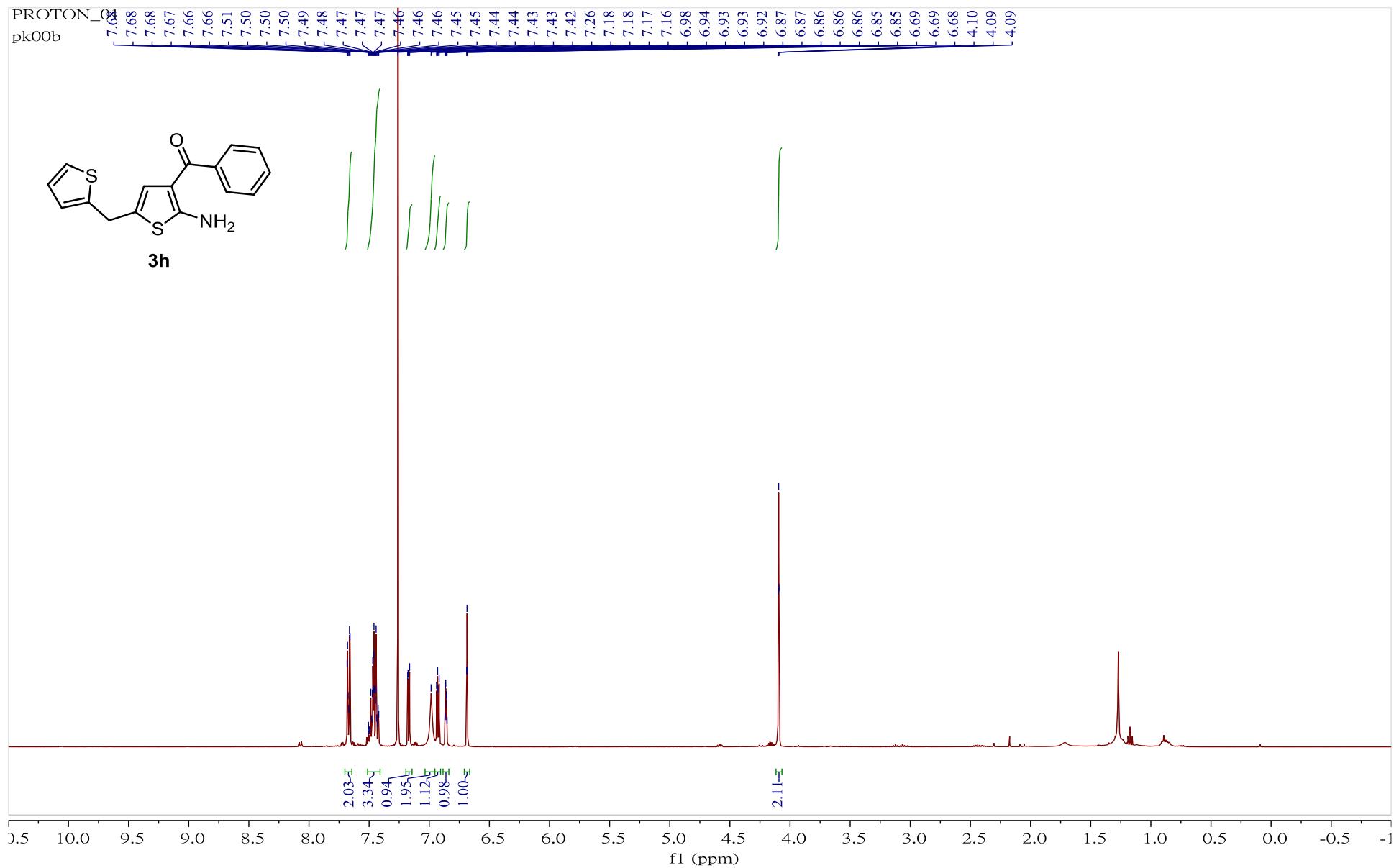
— 36.1



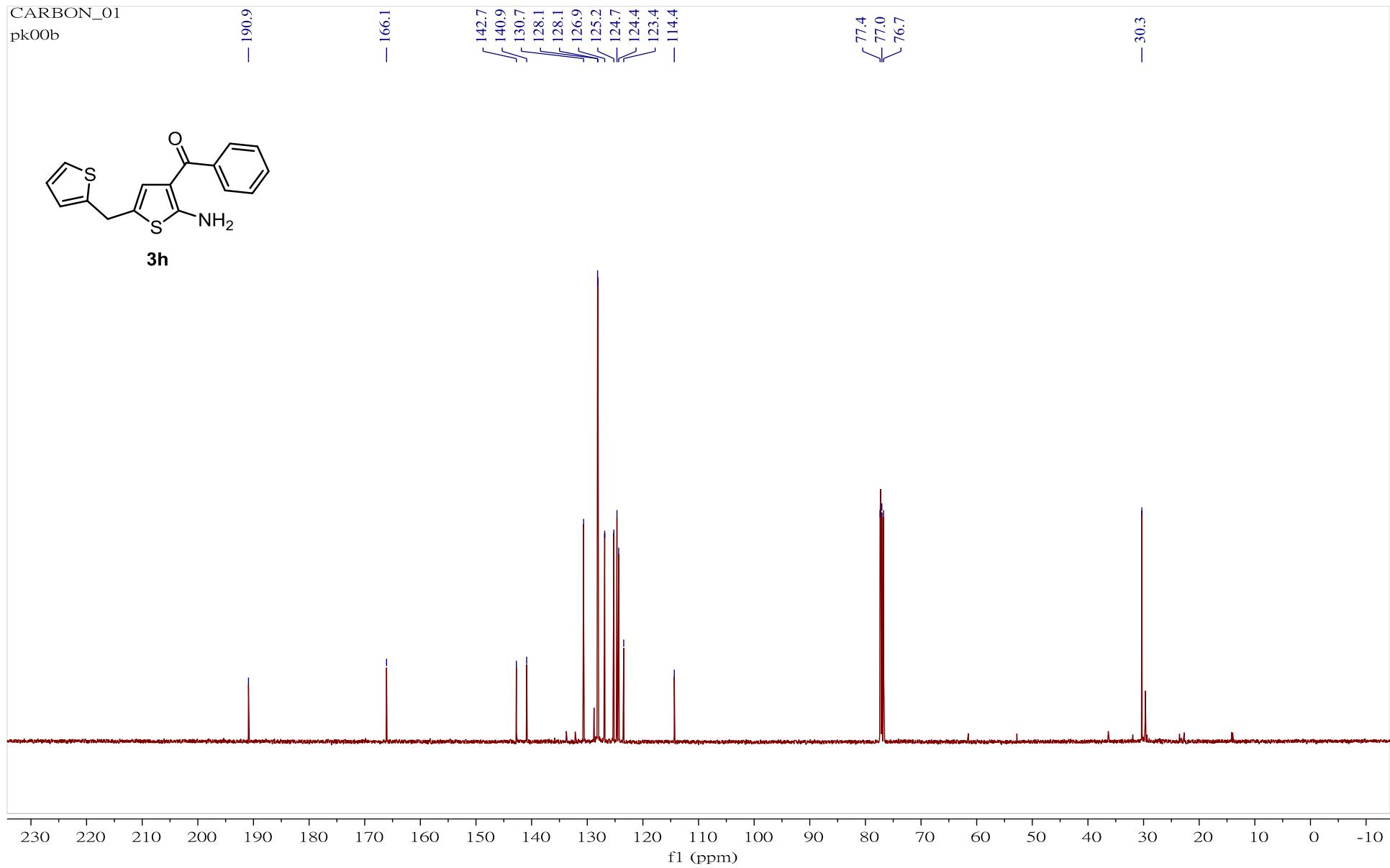
3g



¹³C NMR (100 MHz) spectrum of compound **3g** in CDCl₃

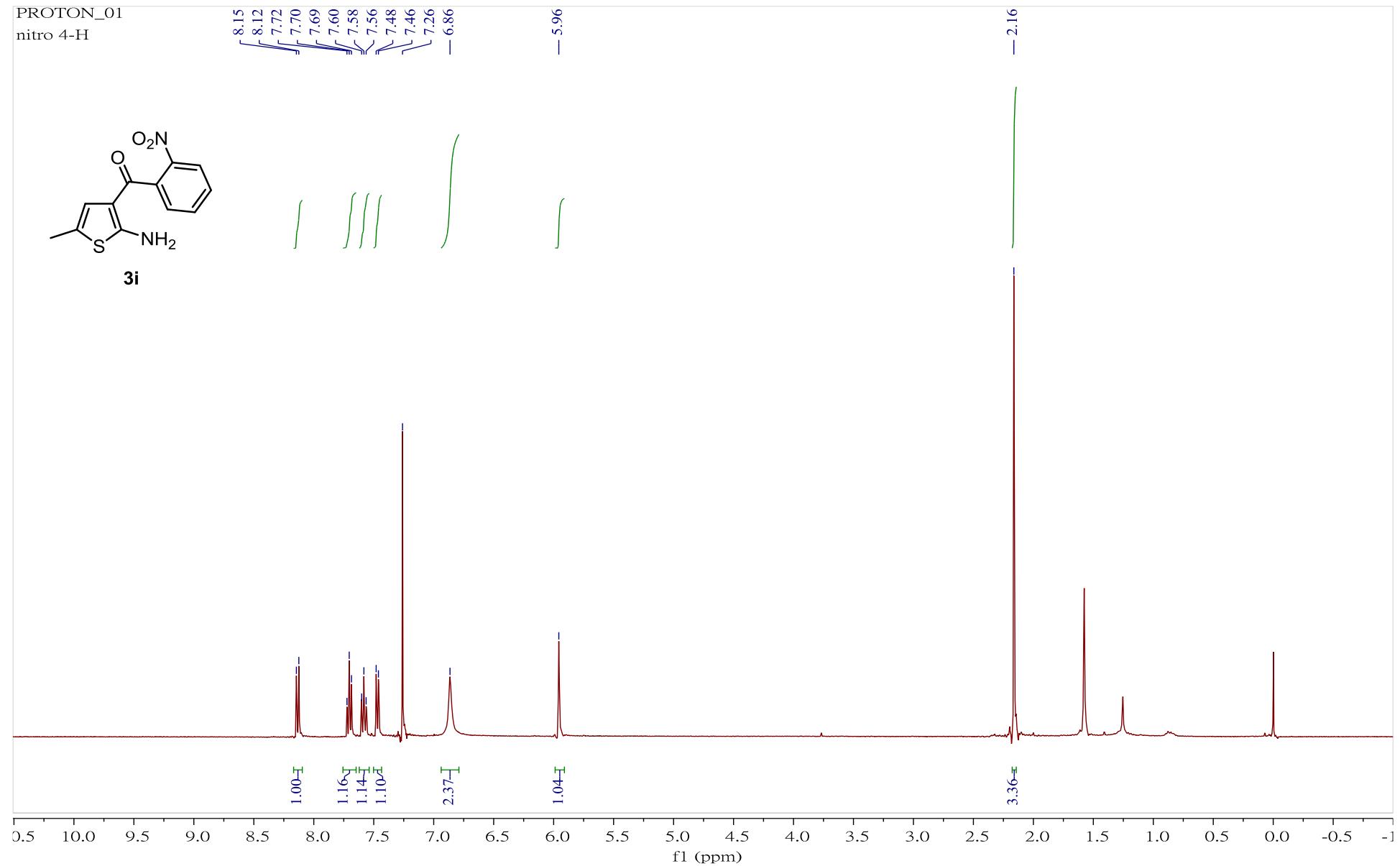
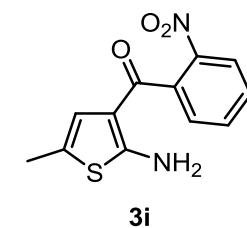


^1H NMR (400 MHz) spectrum of compound **3h** in CDCl_3



¹³C NMR (100 MHz) spectrum of compound **3h** in CDCl₃

PROTON_01
nitro 4-H



¹H NMR (400 MHz) spectrum of compound **3i** in CDCl₃

CARBON_01

20170701-20170701-IDO-3-13C

— 186.7

— 165.7

— 146.2

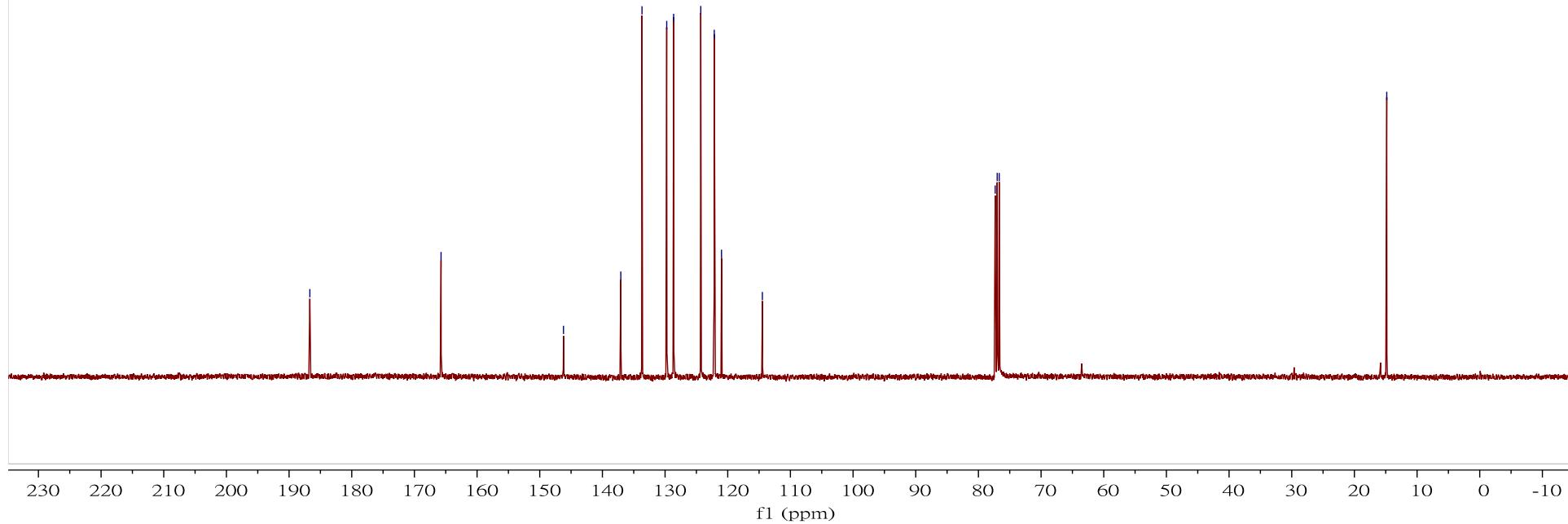
— 137.1
— 133.7
— 129.7
— 128.6
— 124.3
— 122.2
— 121.0
— 114.5

— 77.3
— 77.0
— 76.7

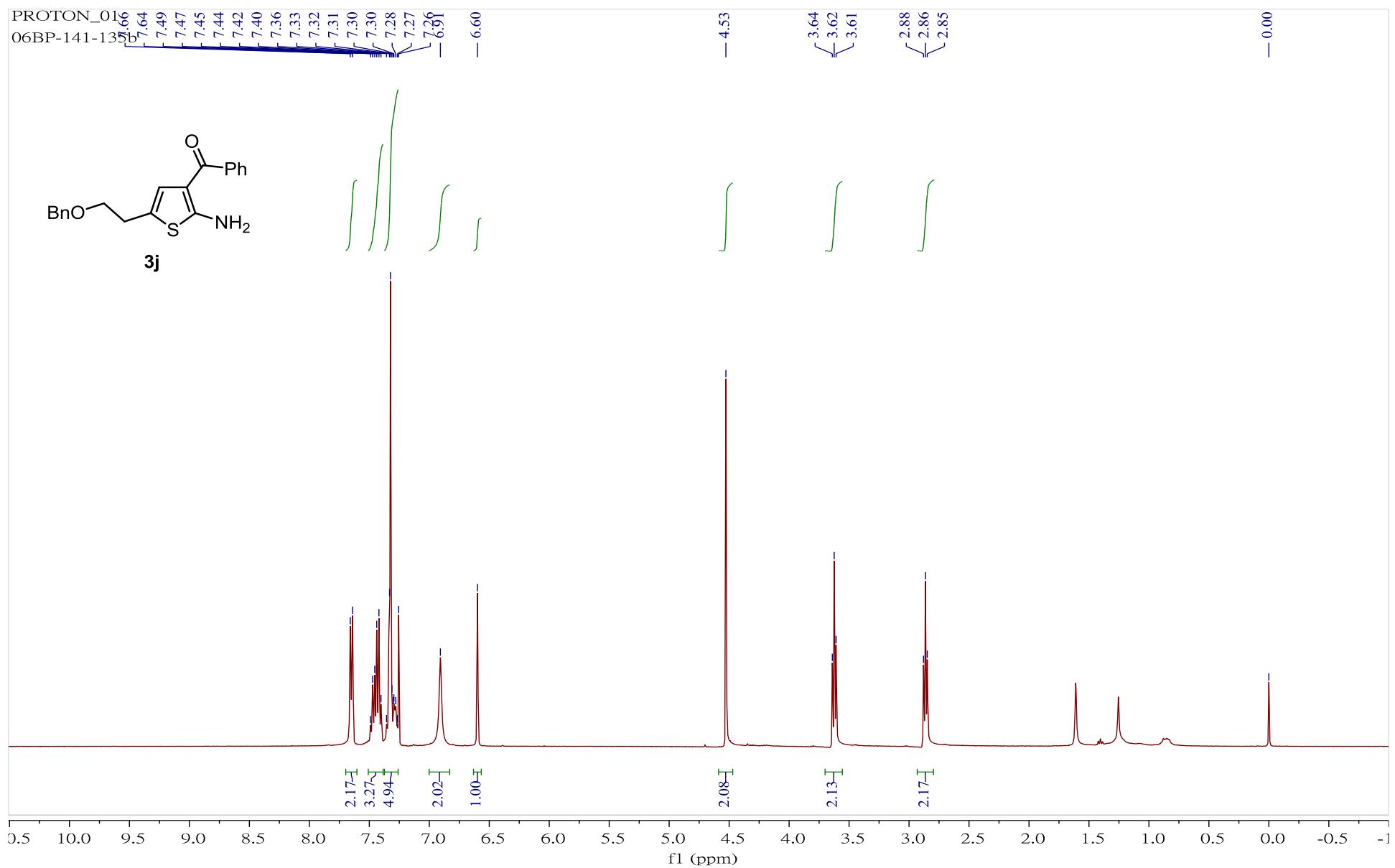
— 14.8



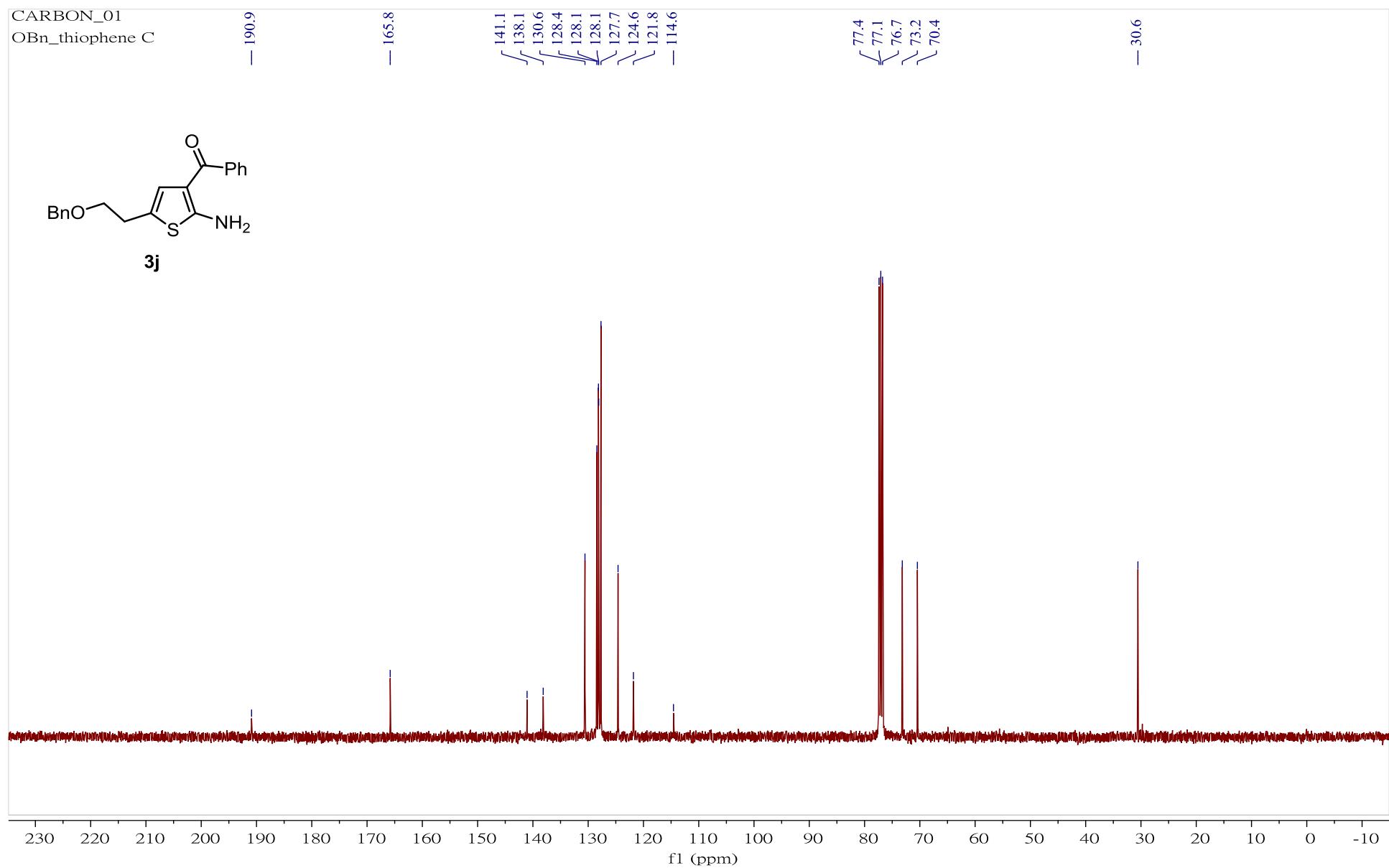
3i



^{13}C NMR (100 MHz) spectrum of compound **3i** in CDCl_3



¹H NMR (400 MHz) spectrum of compound **3j** in CDCl₃



¹³C NMR (100 MHz) spectrum of compound **3j** in CDCl₃

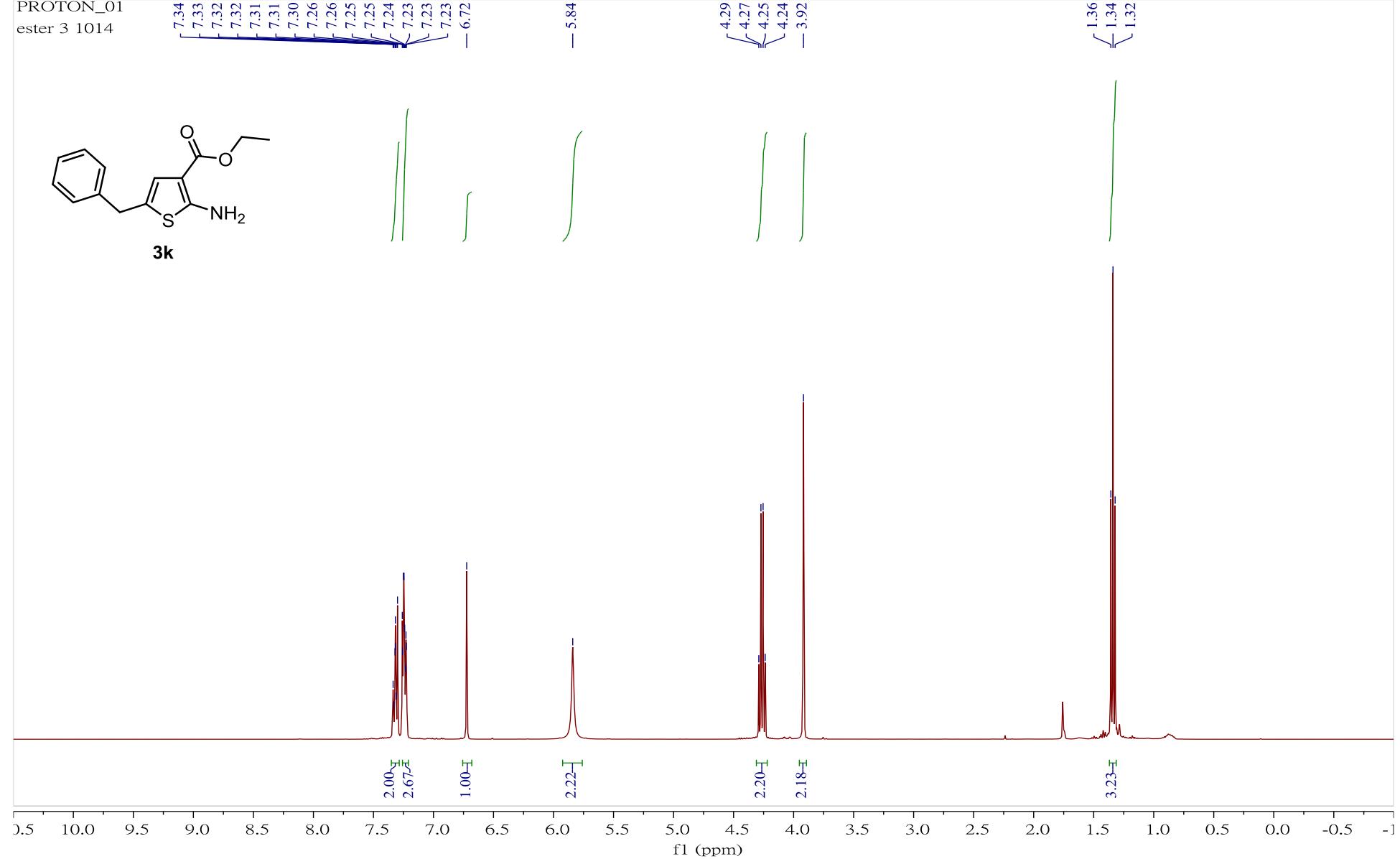
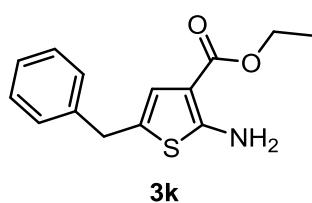
PROTON_01
ester 3 1014

7.34
7.33
7.32
7.32
7.31
7.31
7.30
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.23
— 6.72

— 5.84

4.29
4.27
4.25
4.24
— 3.92

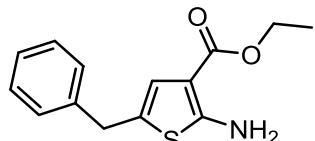
1.36
1.34
1.32



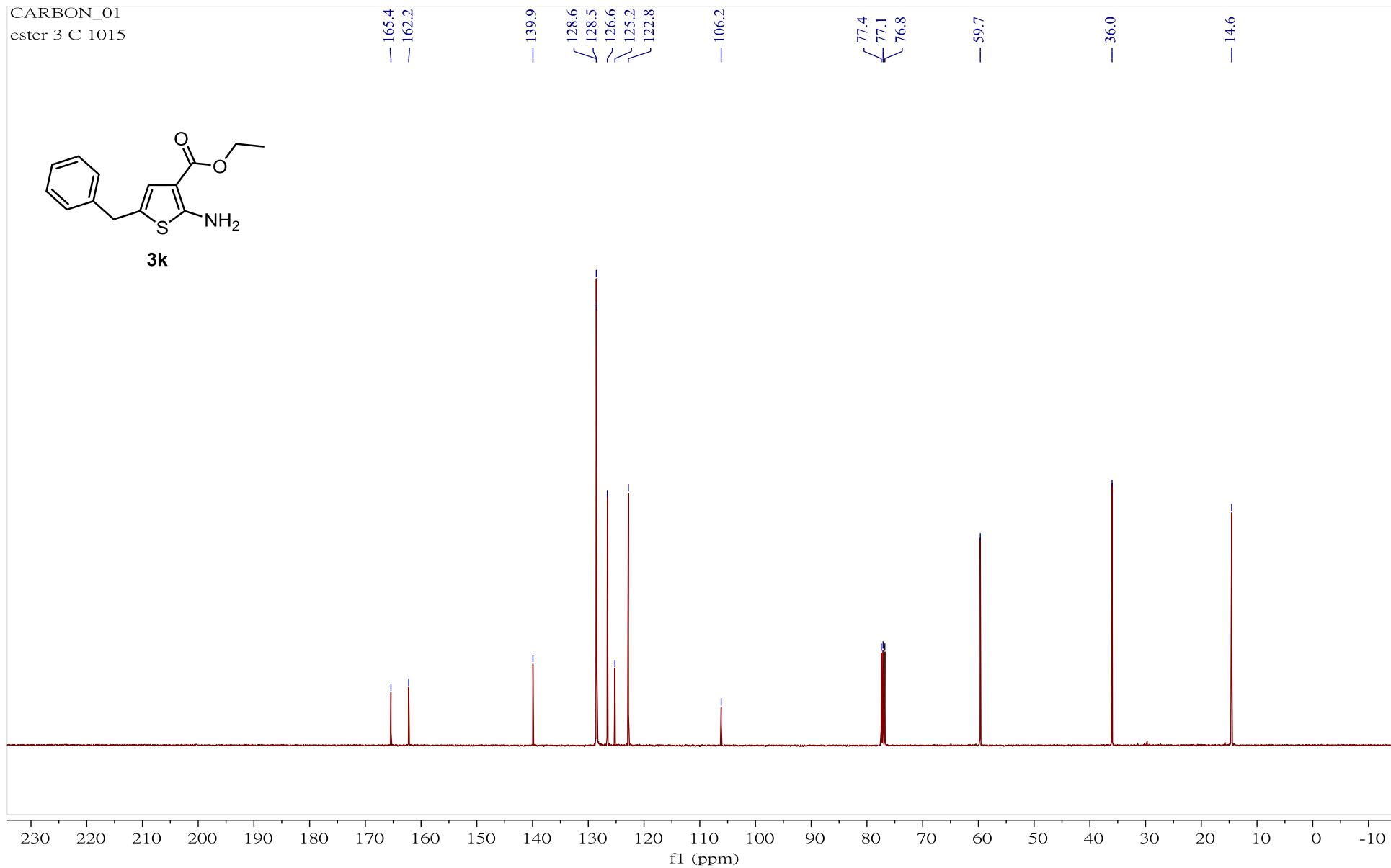
^1H NMR (400 MHz) spectrum of compound **3k** in CDCl_3

CARBON_01
ester 3 C 1015

— 165.4
— 162.2
— 139.9
— 128.6
— 128.5
— 126.6
— 125.2
— 122.8
— 106.2
— 59.7
— 36.0
— 14.6

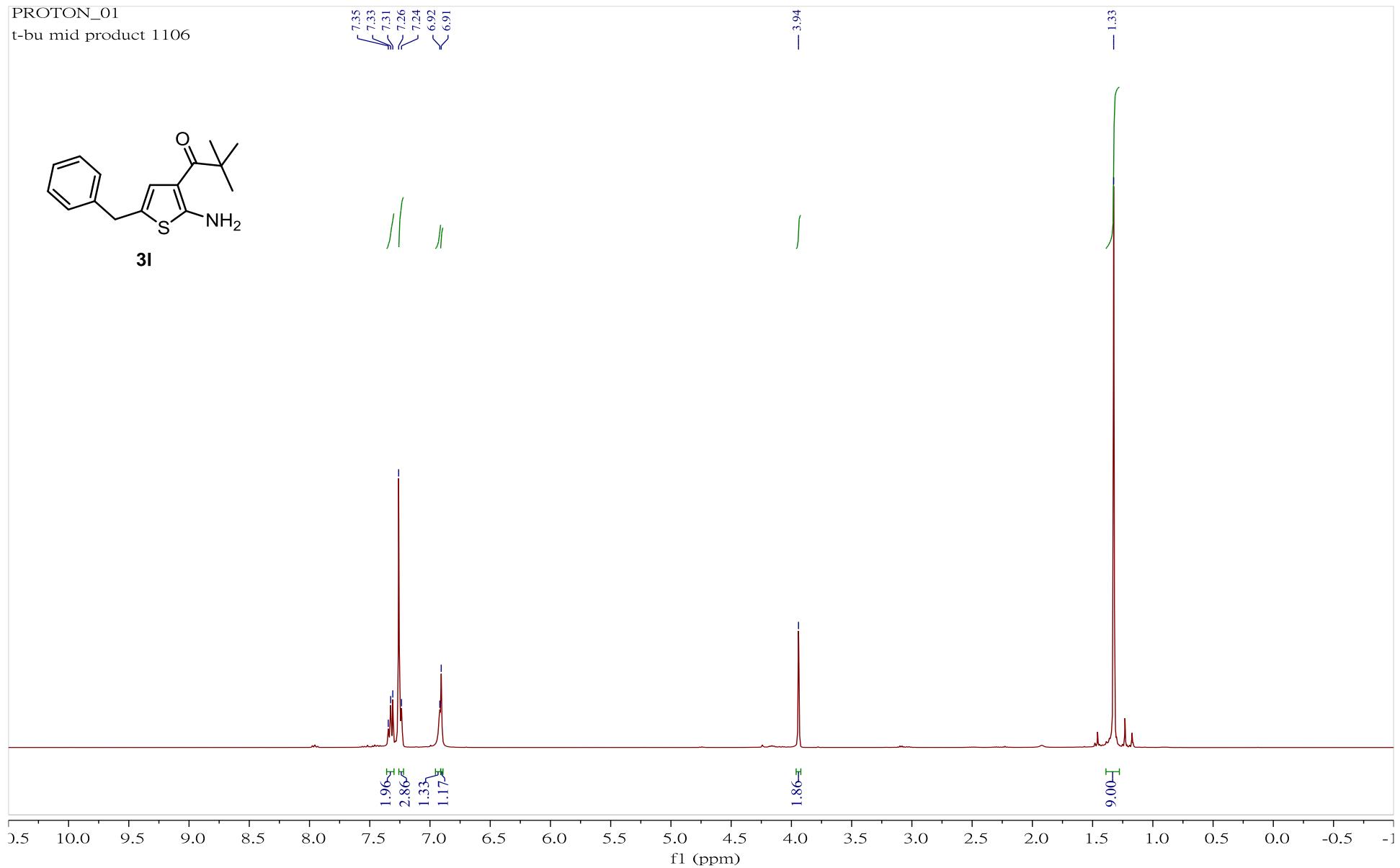


3k



¹³C NMR (100 MHz) spectrum of compound **3k** in CDCl_3

PROTON_01
t-bu mid product 1106



^1H NMR (400 MHz) spectrum of compound **3l** in CDCl_3

CARBON_01
t-bu product C

— 201.9

— 166.3

— 139.8

— 128.6
— 128.4
— 126.7
— 123.3
— 123.2

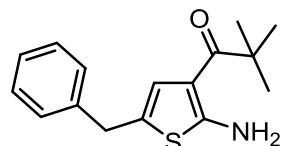
— 112.1

— 77.4
— 77.1
— 76.8

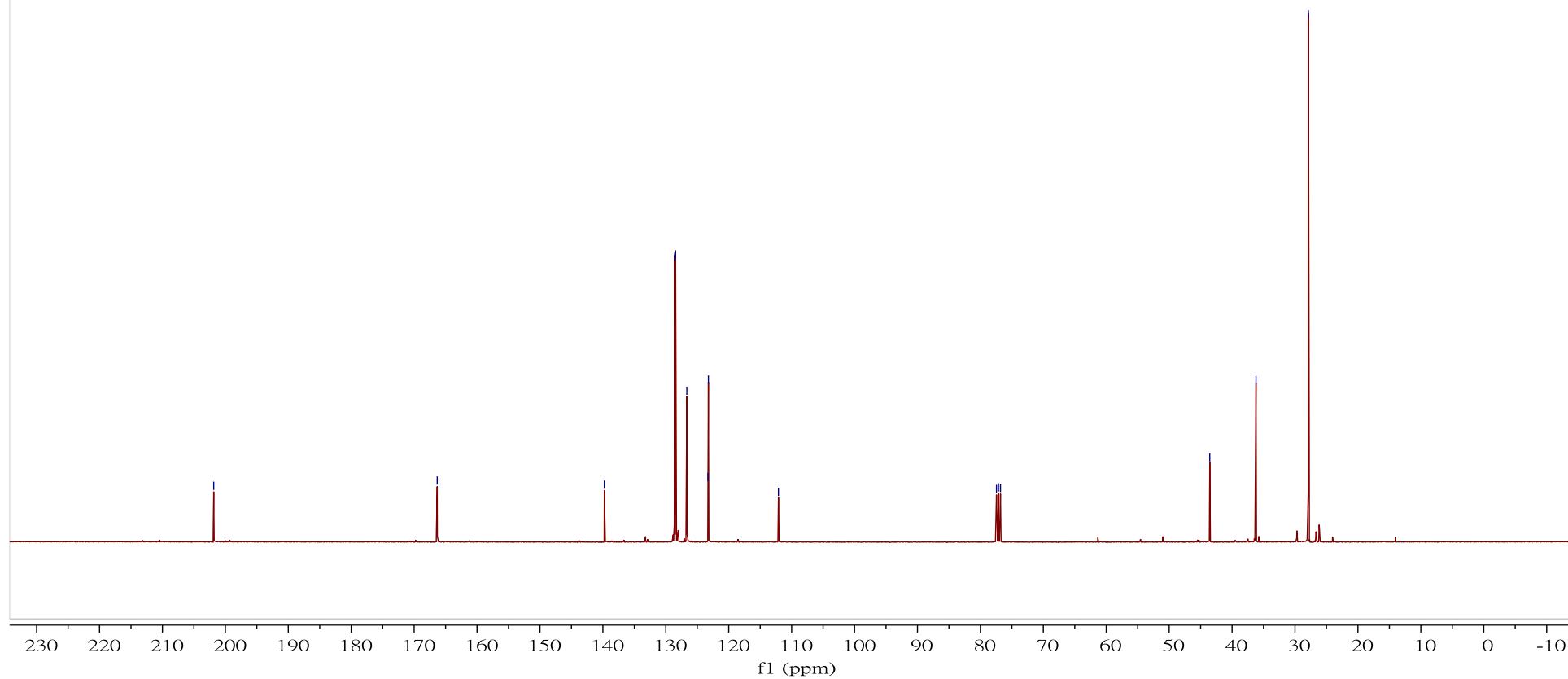
— 43.5

— 36.2

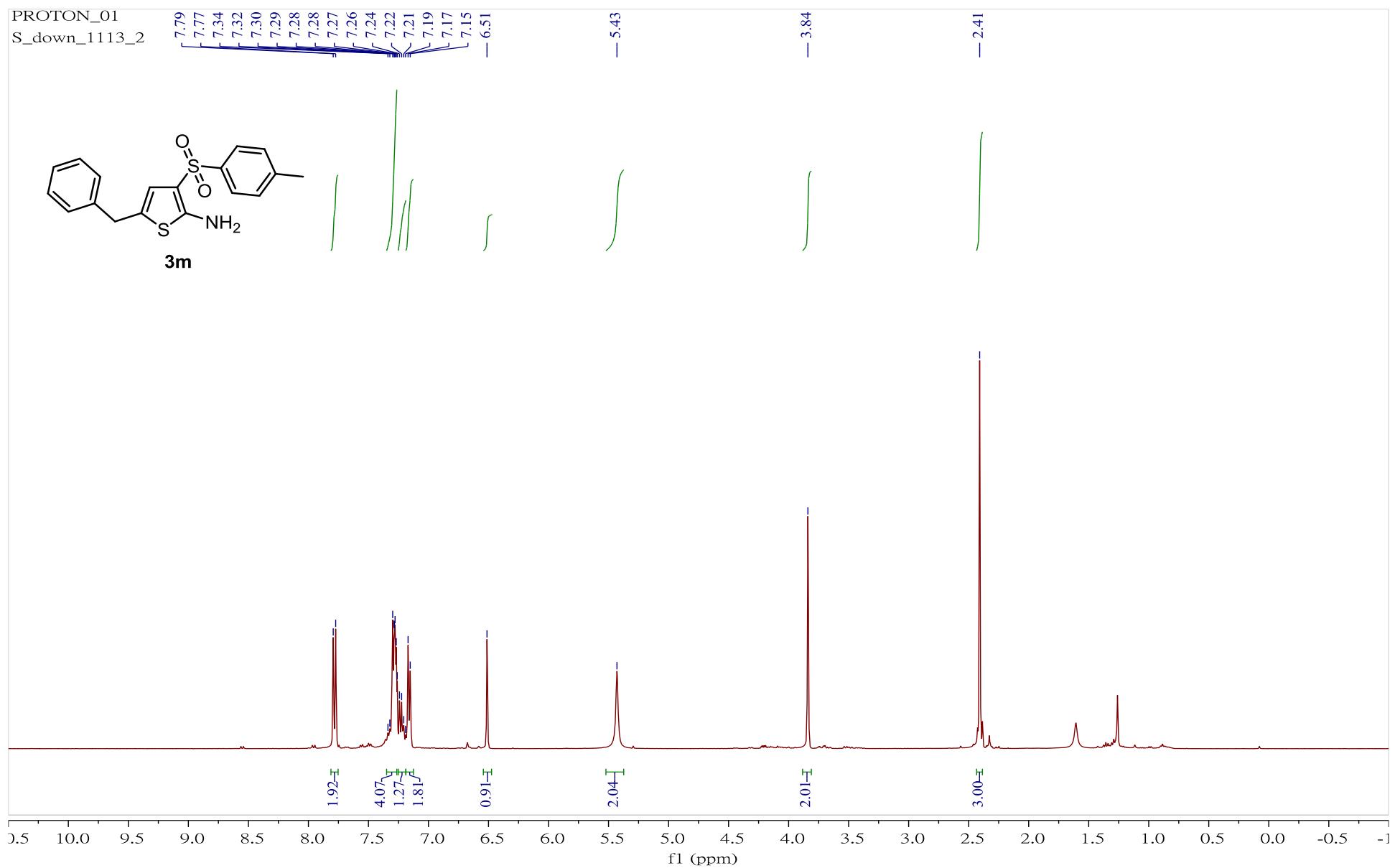
— 27.9



3l



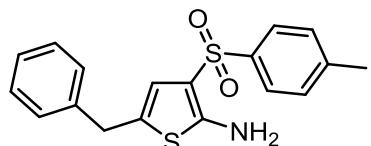
^{13}C NMR (100 MHz) spectrum of compound **3l** in CDCl_3



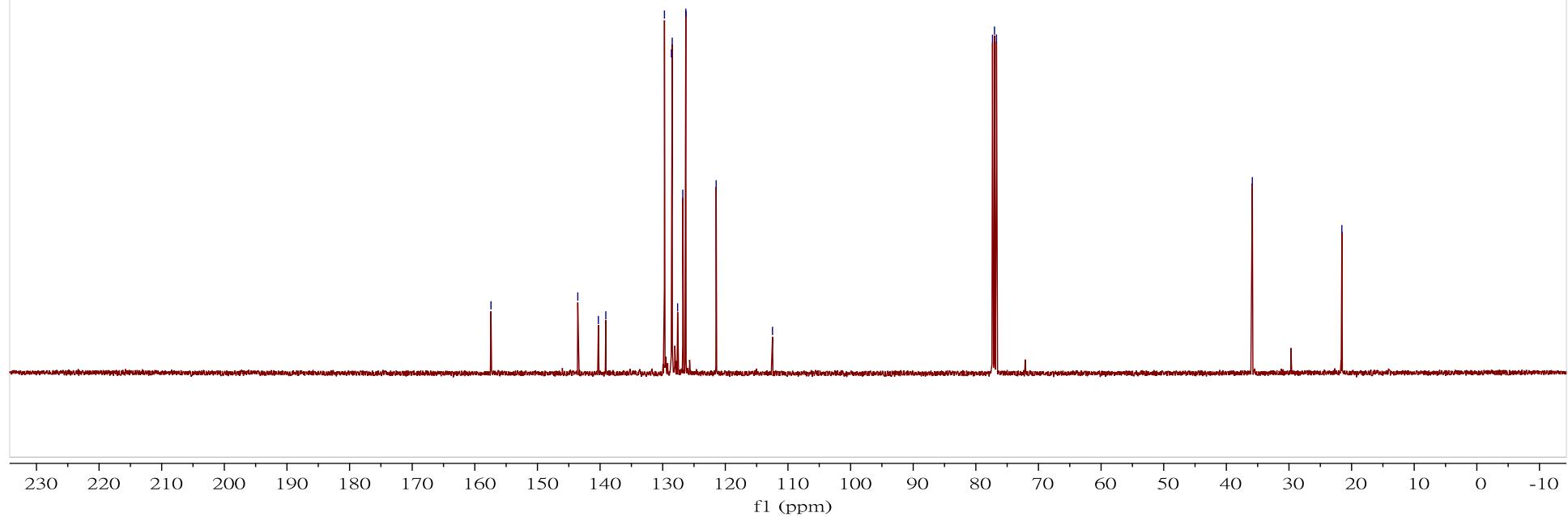
^1H NMR (400 MHz) spectrum of compound **3m** in CDCl_3

CARBON_01
S_down_1113_2

— 157.4
143.6
140.3
139.1
129.7
128.6
128.5
127.6
126.8
126.3
121.5
— 112.5
— 35.8
77.3
77.0
76.7
— 21.6

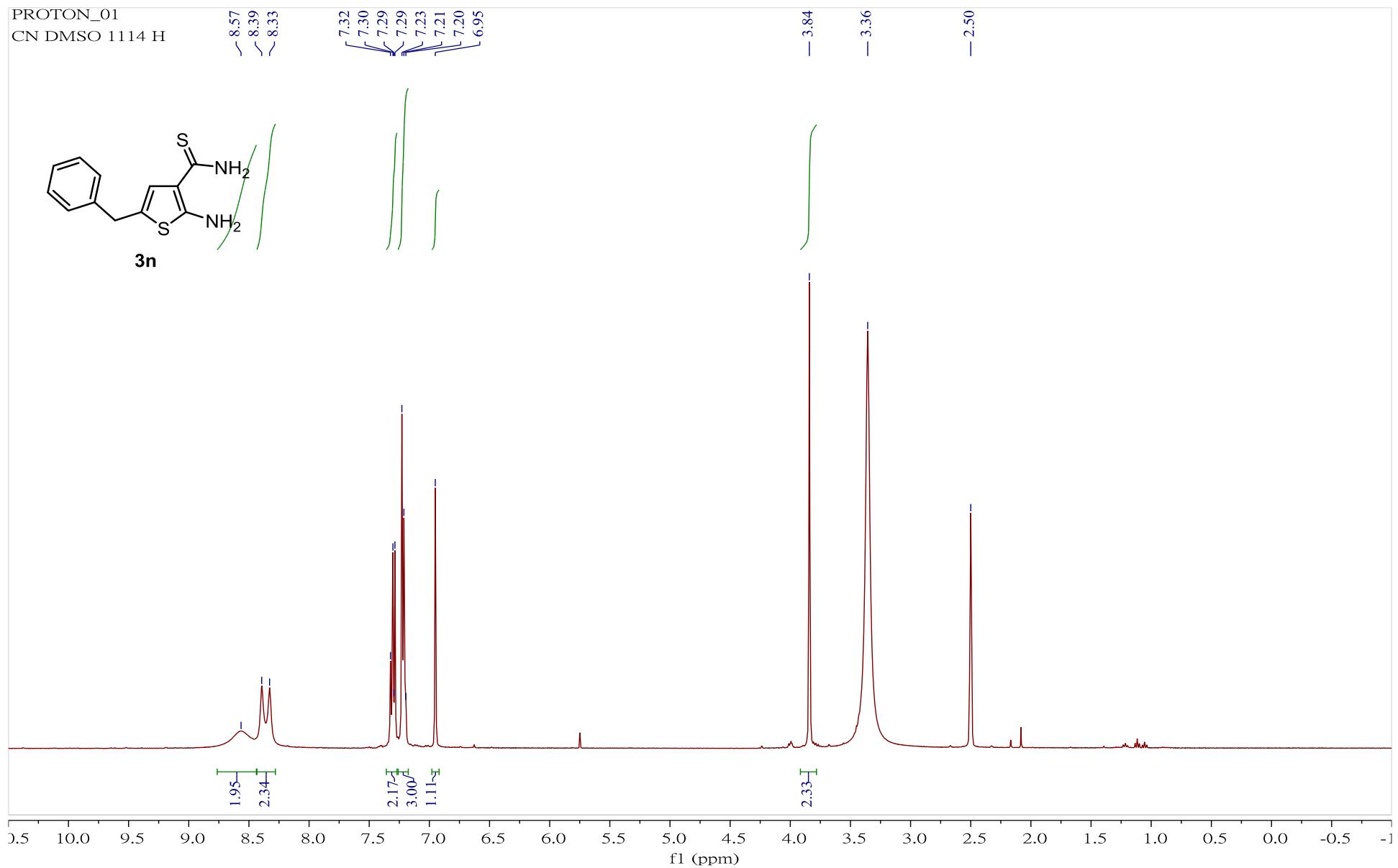


3m



^{13}C NMR (100 MHz) spectrum of compound **3m** in CDCl_3

PROTON_01
CN DMSO 1114 H



^1H NMR (400 MHz) spectrum of compound **3n** in DMSO-d^6

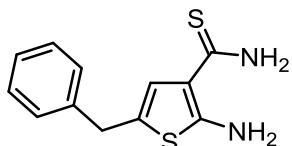
CARBON_01
CN product 1113

— 189.1

— 164.8

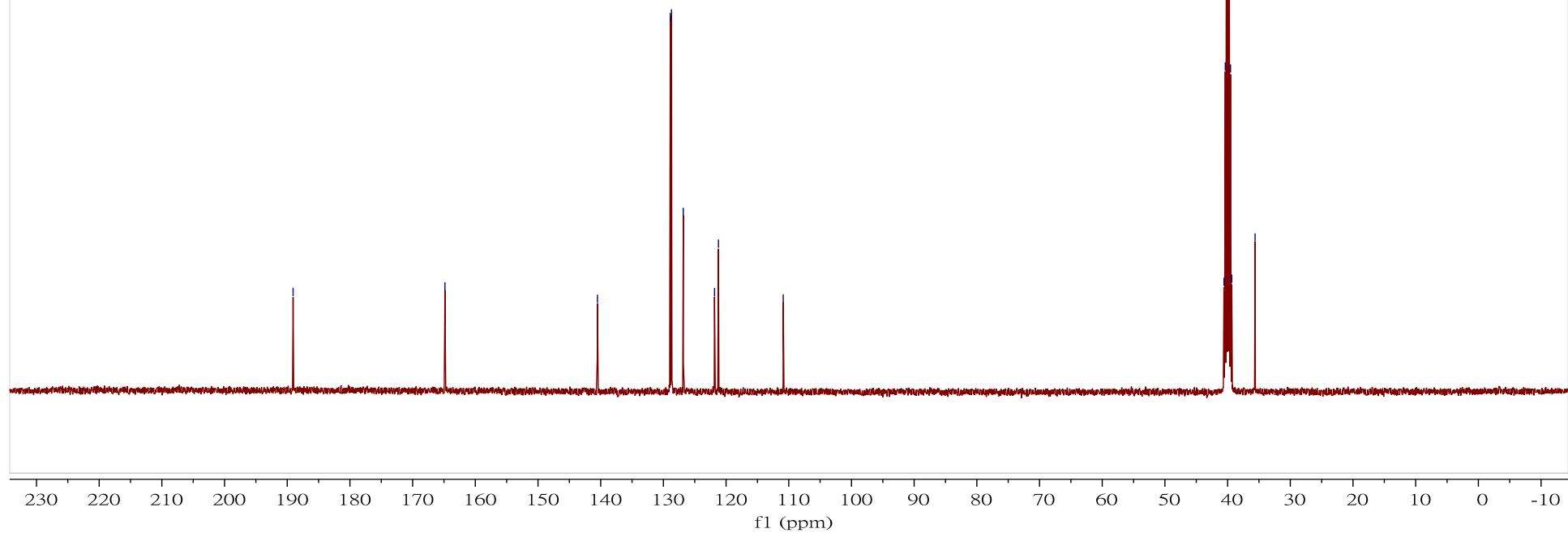
— 140.5

— 110.9

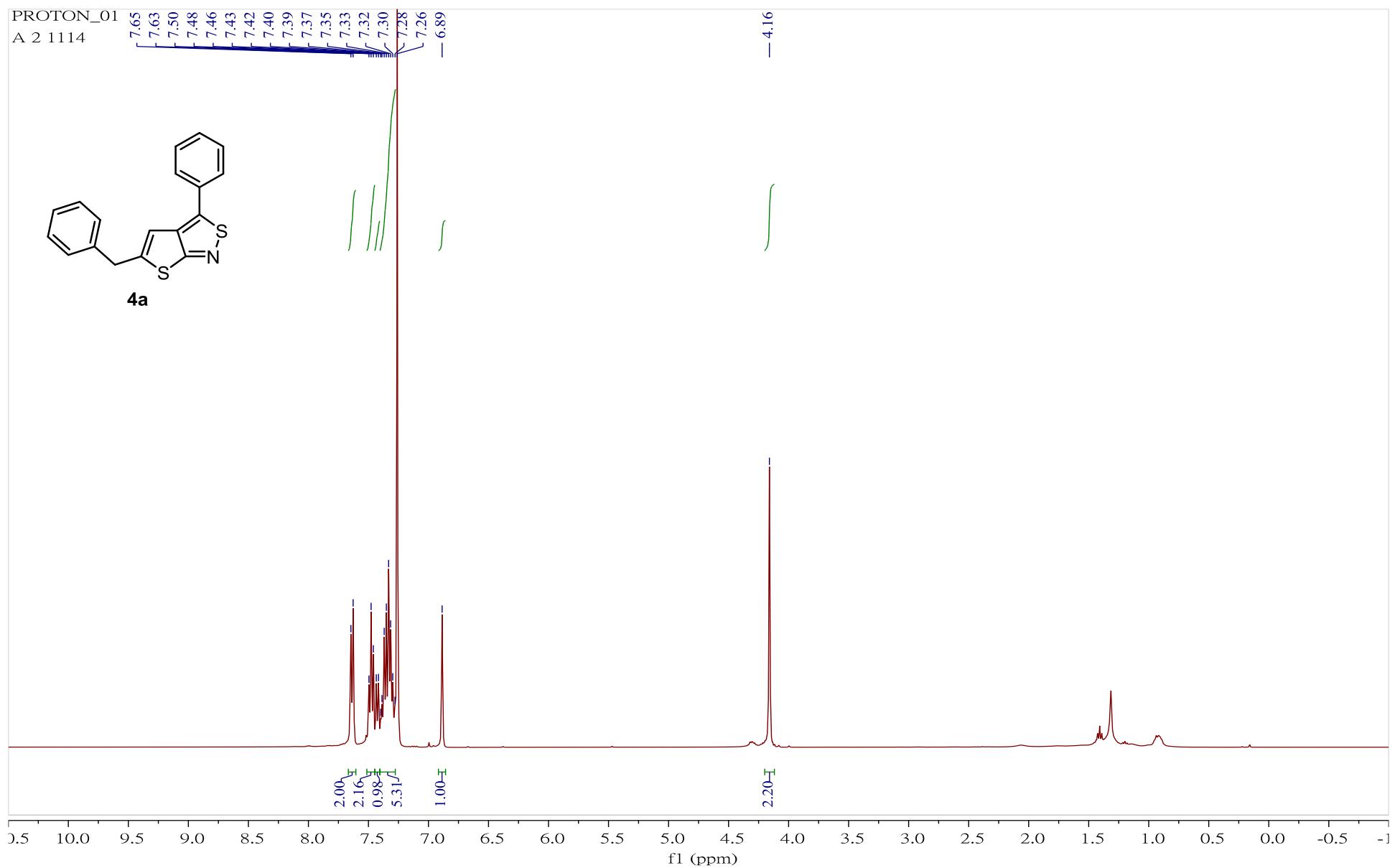


3n

— 40.6
— 40.4
— 40.2
— 40.0
— 39.7
— 39.5
— 39.3
— 35.6

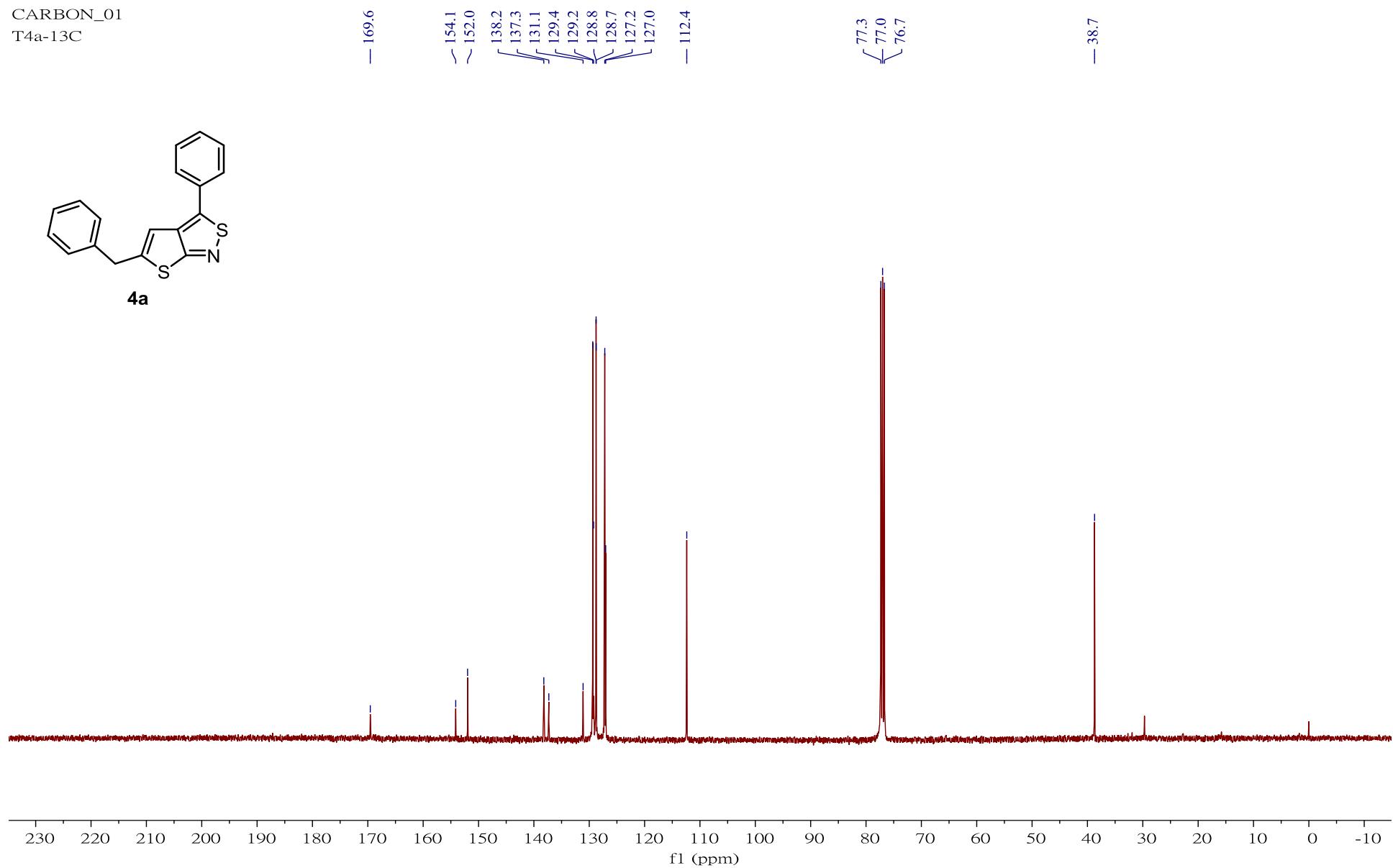


^{13}C NMR (100 MHz) spectrum of compound **3n** in DMSO-d^6

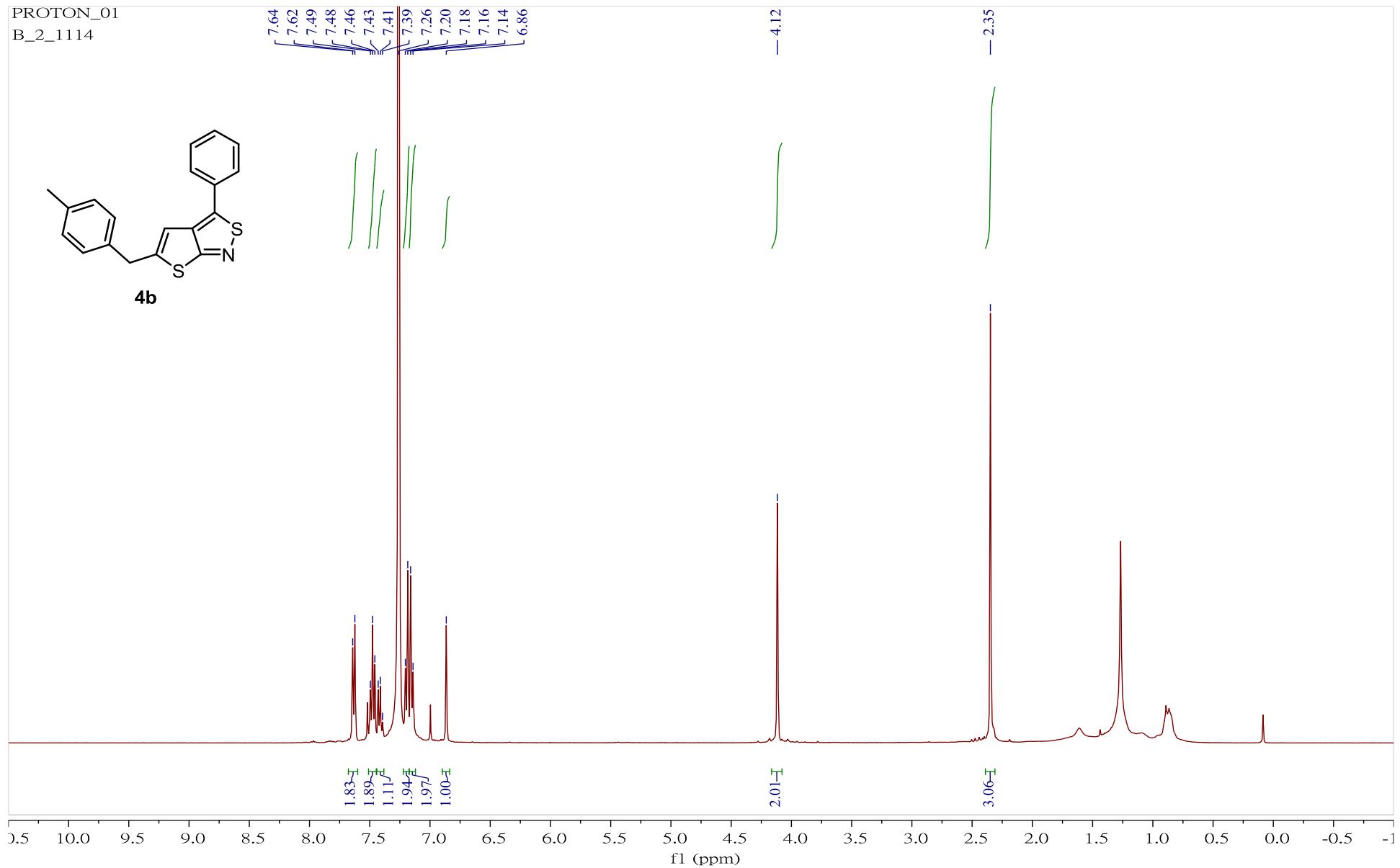


^1H NMR (400 MHz) spectrum of compound **4a** in CDCl_3

CARBON_01
T4a-13C

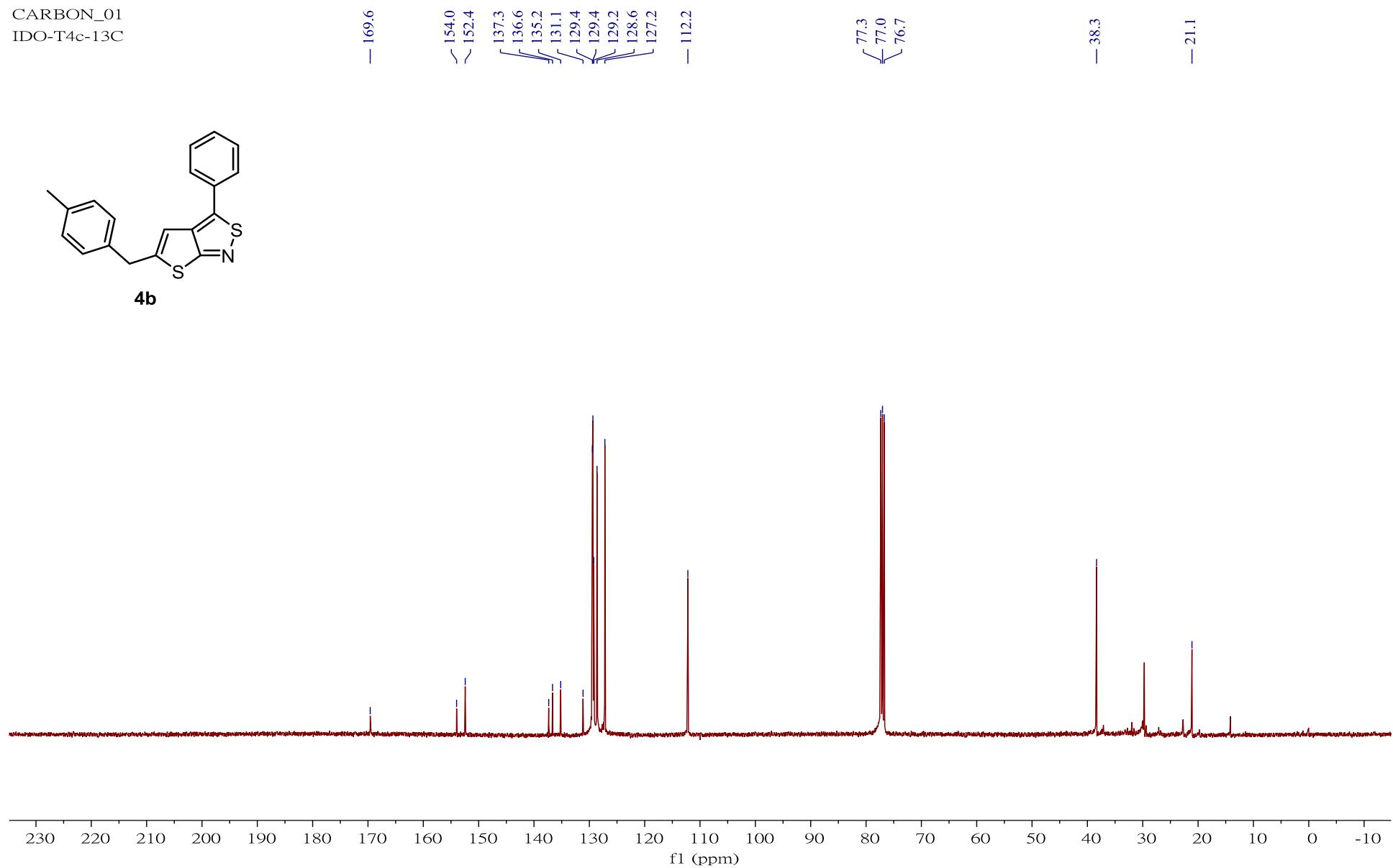


^{13}C NMR (100 MHz) spectrum of compound **4a** in CDCl_3



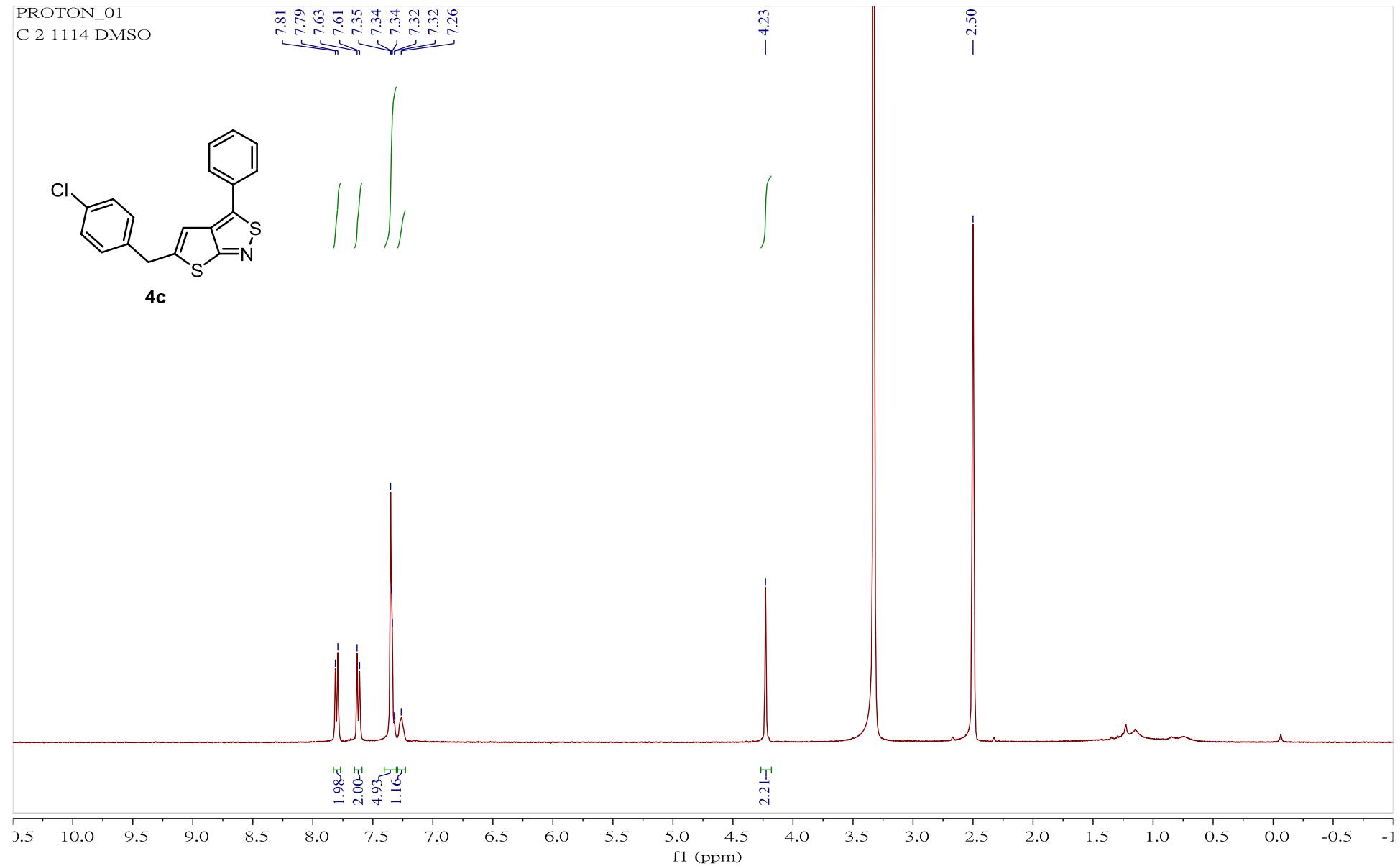
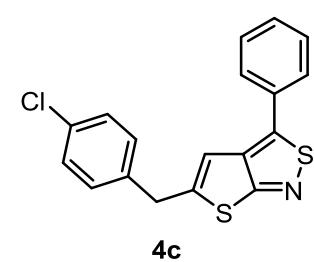
^1H NMR (400 MHz) spectrum of compound **4b** in CDCl_3

CARBON_01
IDO-T4c-13C



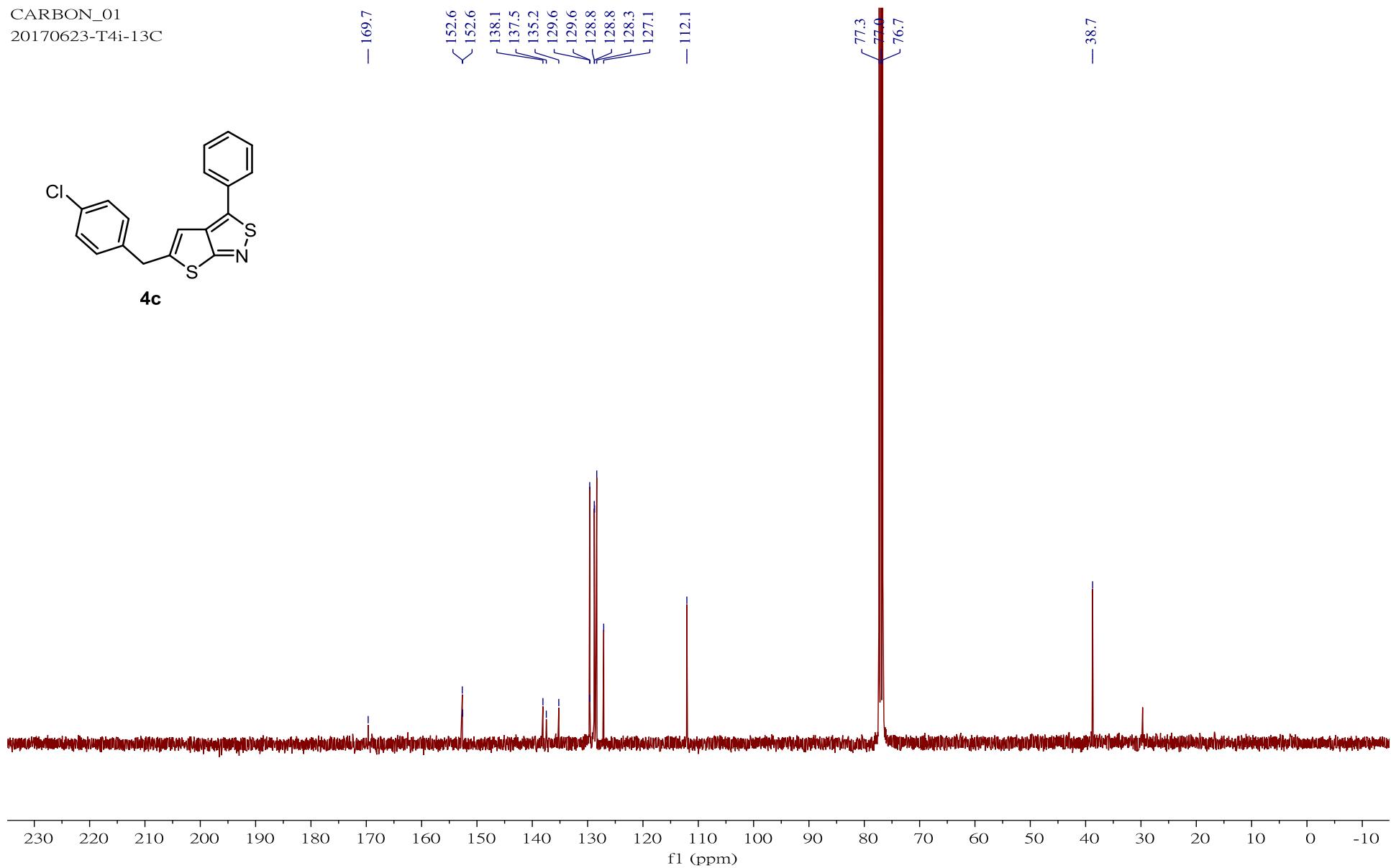
^{13}C NMR (100 MHz) spectrum of compound **4b** in CDCl_3

PROTON_01
C 2 1114 DMSO



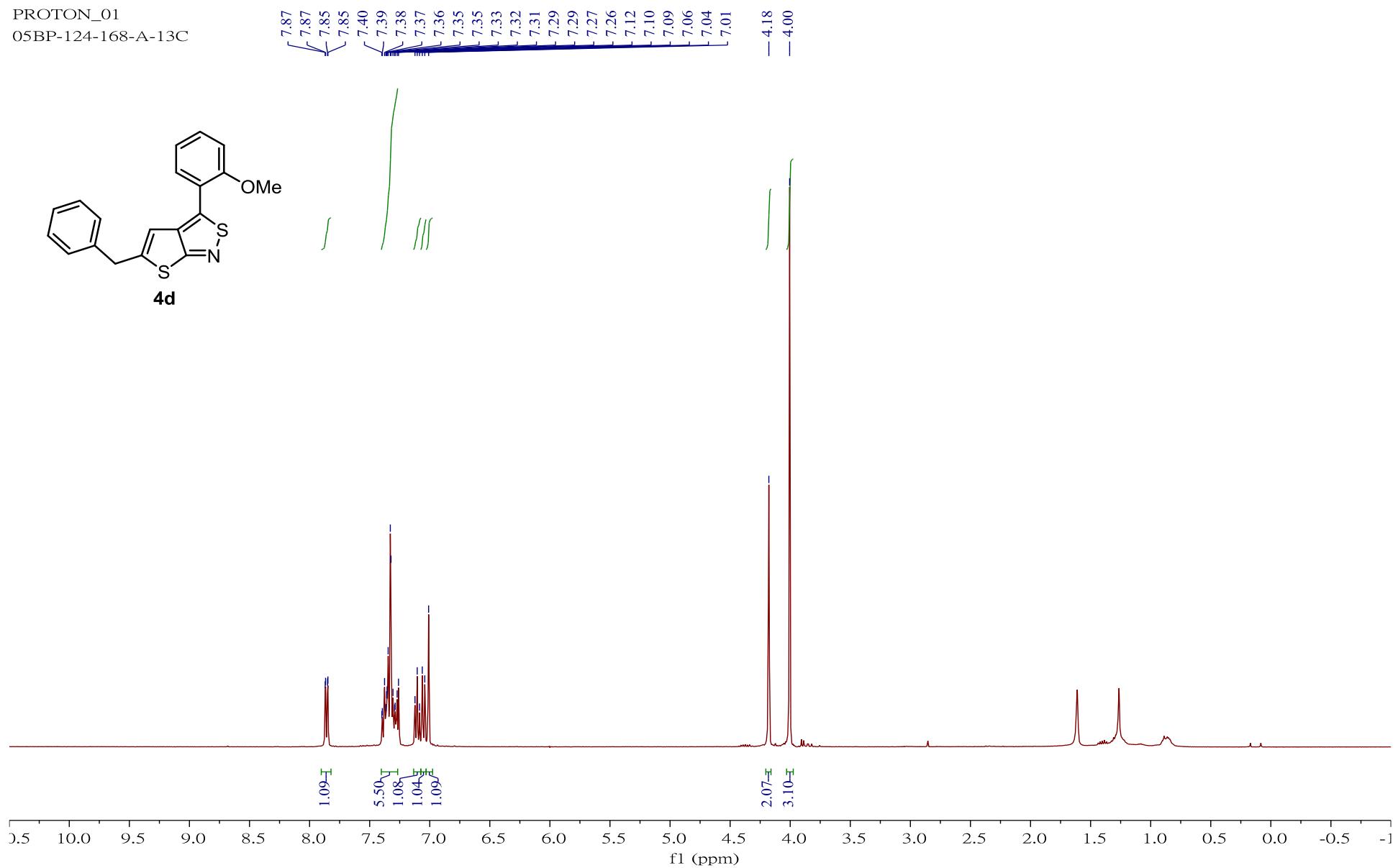
^1H NMR (400 MHz) spectrum of compound **4c** in $\text{DMSO}-\text{d}^6$

CARBON_01
20170623-T4i-13C



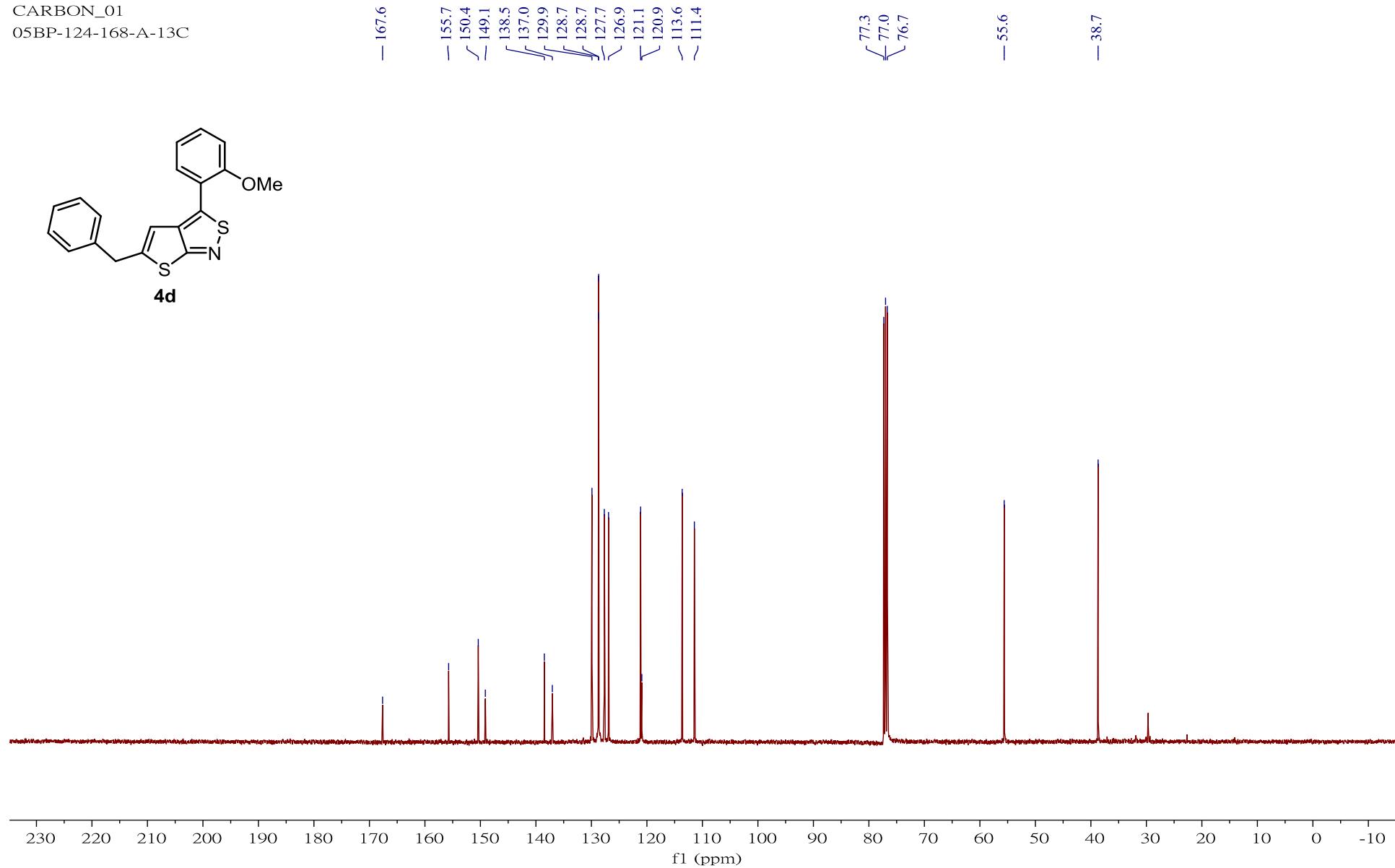
^{13}C NMR (100 MHz) spectrum of compound **4c** in CDCl_3

PROTON_01
05BP-124-168-A-13C



^1H NMR (400 MHz) spectrum of compound **4d** in CDCl_3

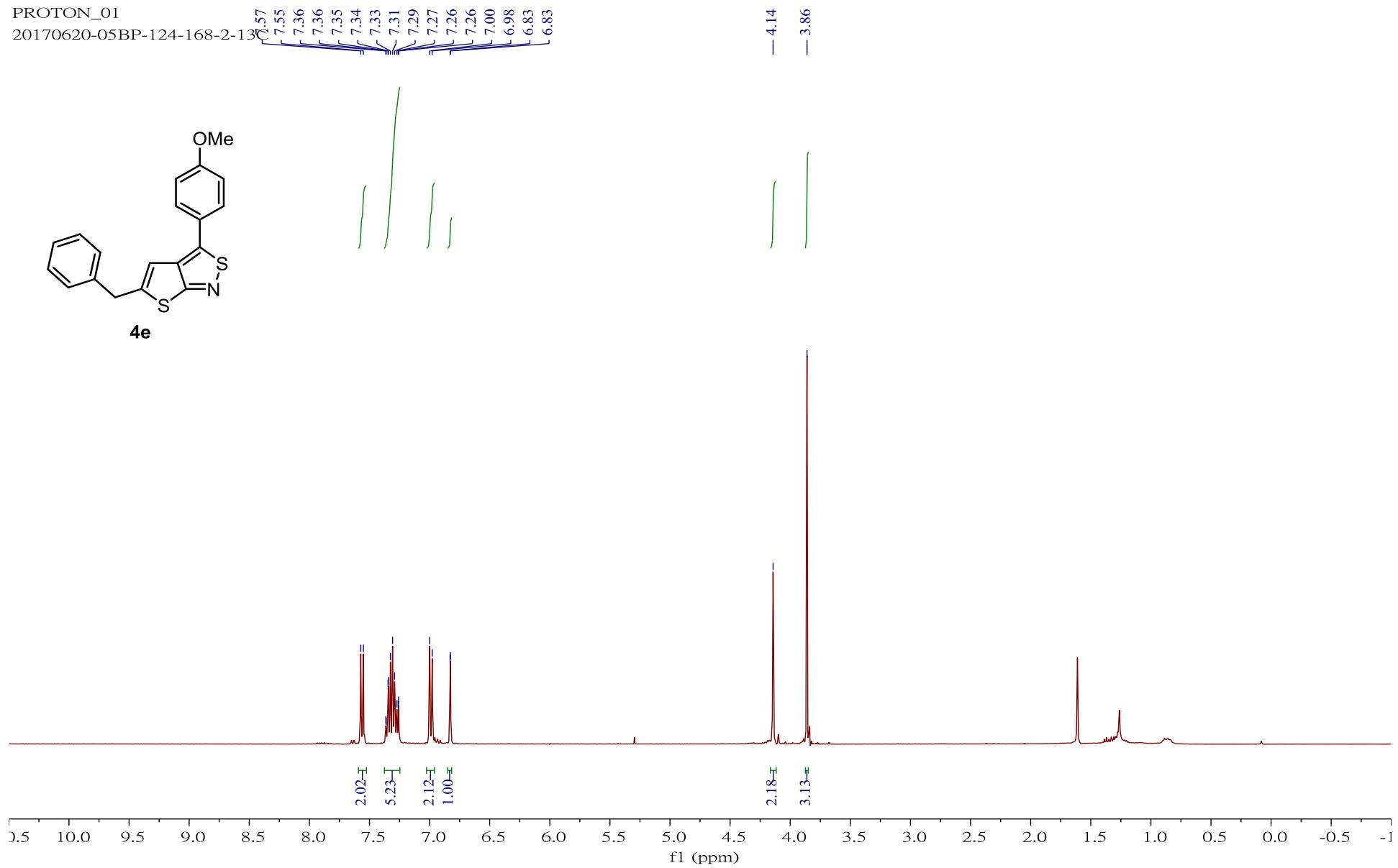
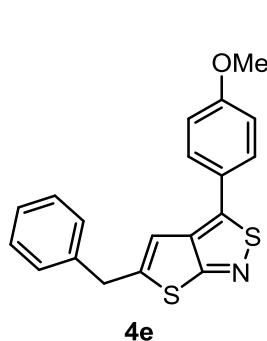
CARBON_01
05BP-124-168-A-13C



^{13}C NMR (100 MHz) spectrum of compound **4d** in CDCl_3

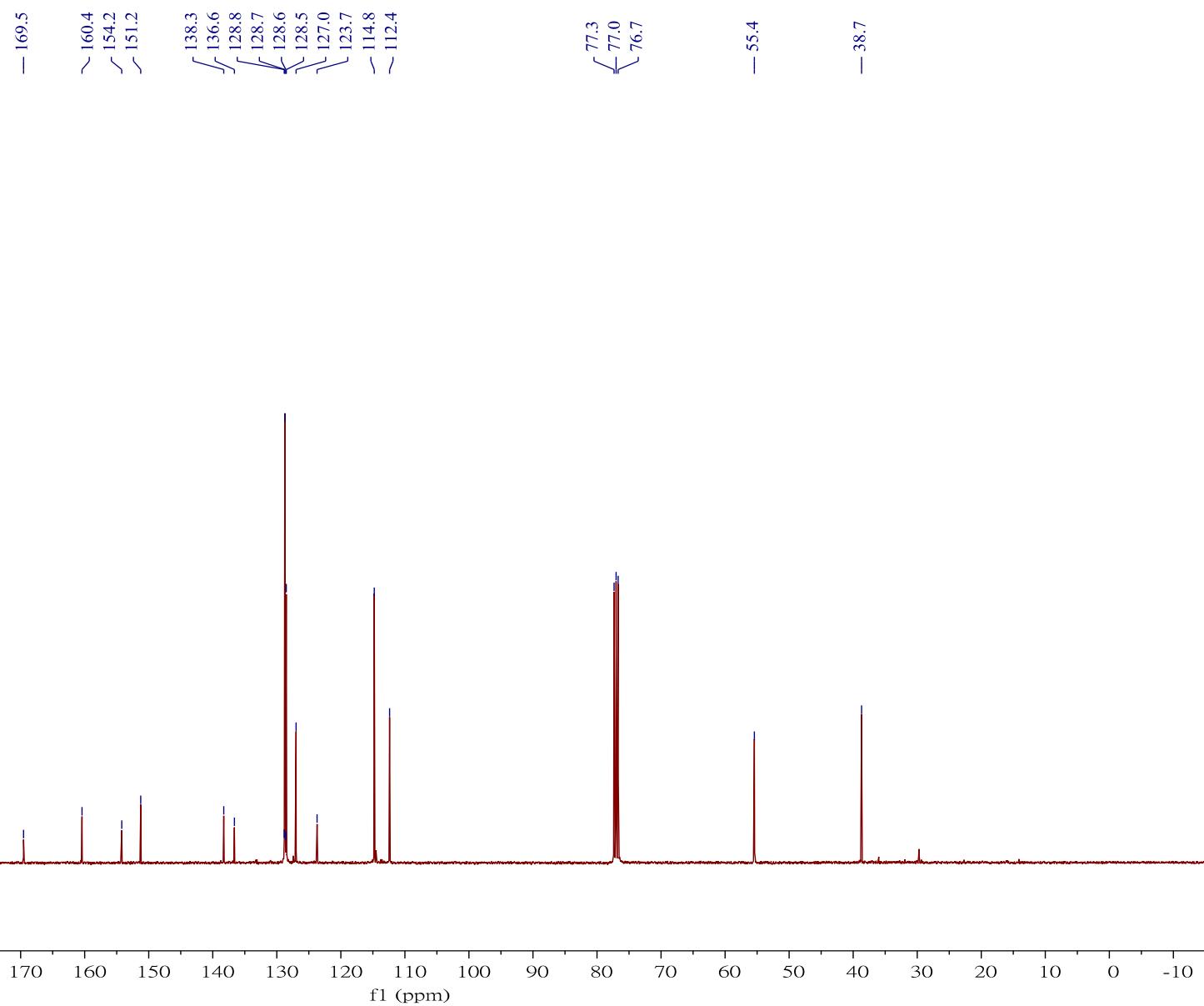
PROTON_01

20170620-05BP-124-168-2-13C



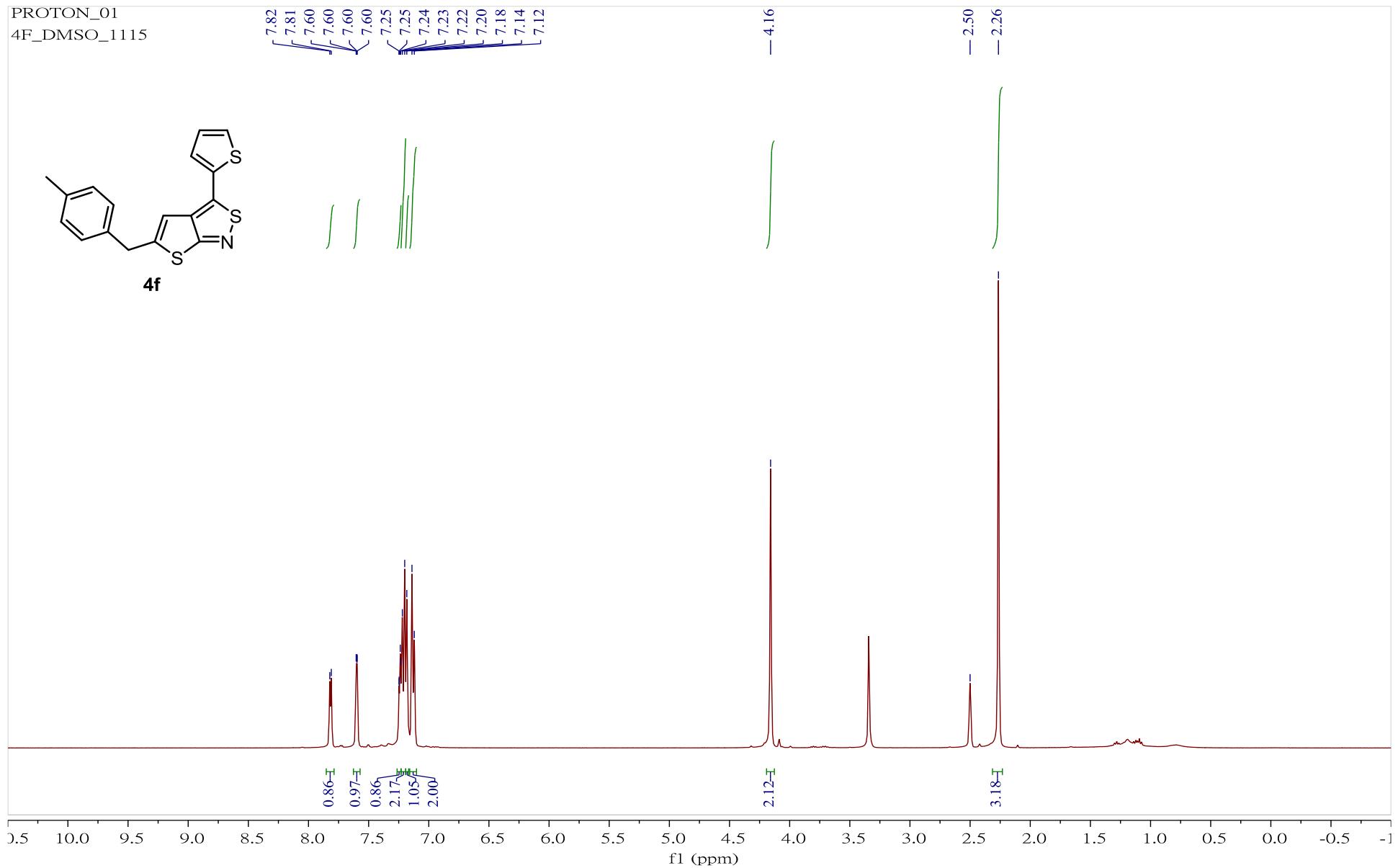
¹H NMR (400 MHz) spectrum of compound **4e** in CDCl₃

CARBON_01
20170620-05BP-124-168-2-13C



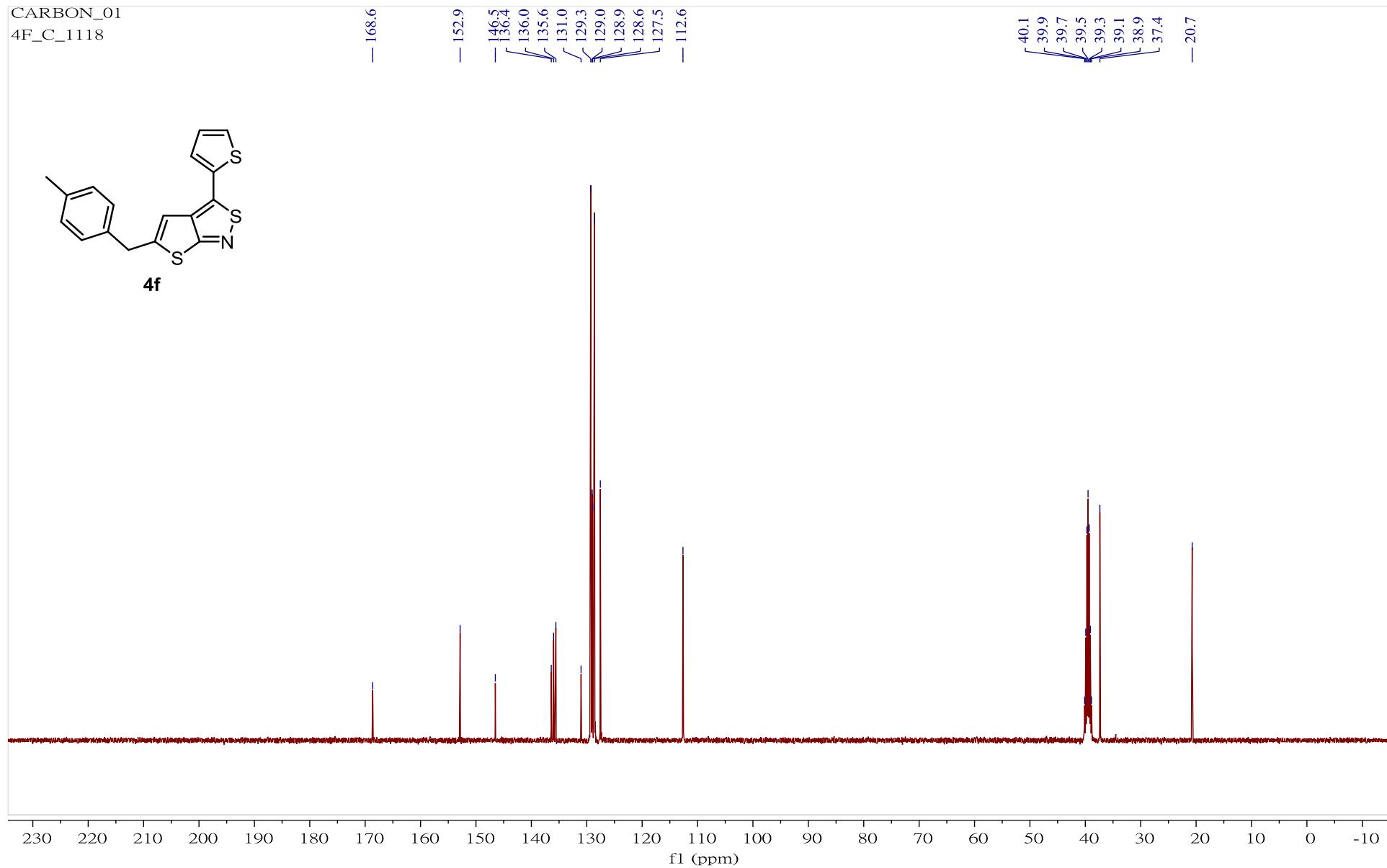
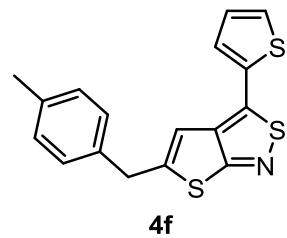
^{13}C NMR (100 MHz) spectrum of compound **4e** in CDCl_3

PROTON_01
4F_DMSO_1115

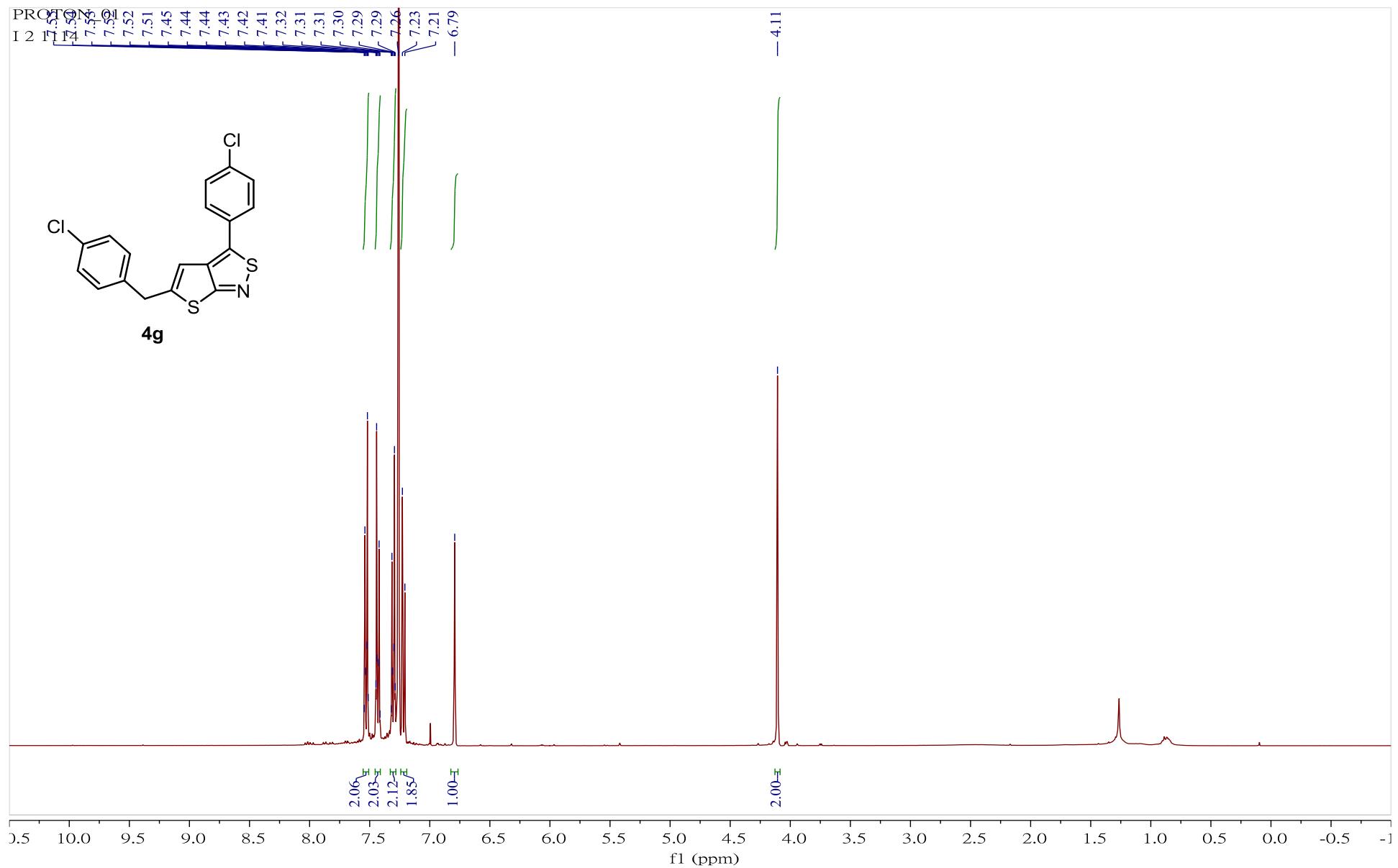


^1H NMR (400 MHz) spectrum of compound **4f** in DMSO-d^6

CARBON_01
4F_C_1118

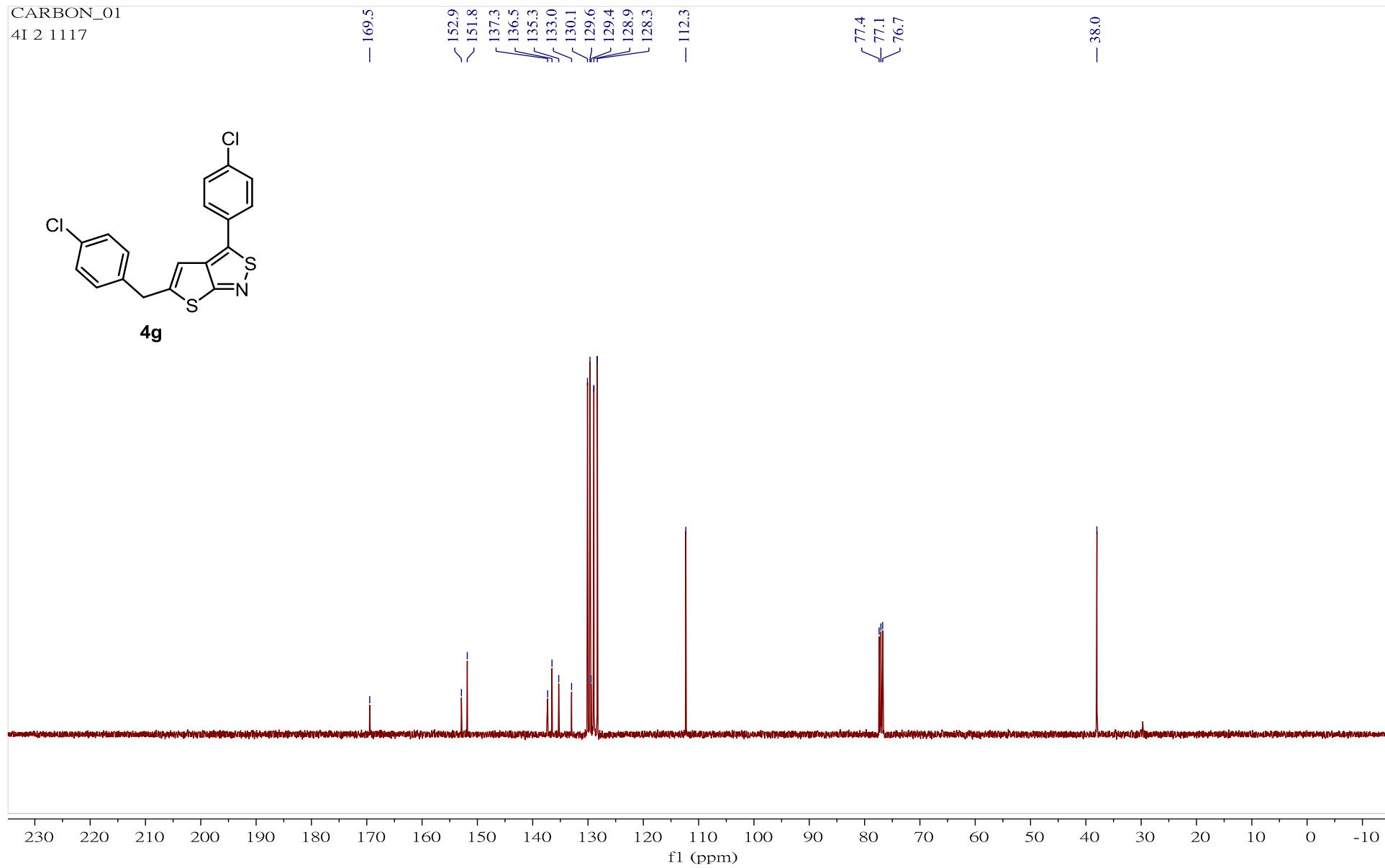


^{13}C NMR (100 MHz) spectrum of compound **4f** in DMSO-d^6



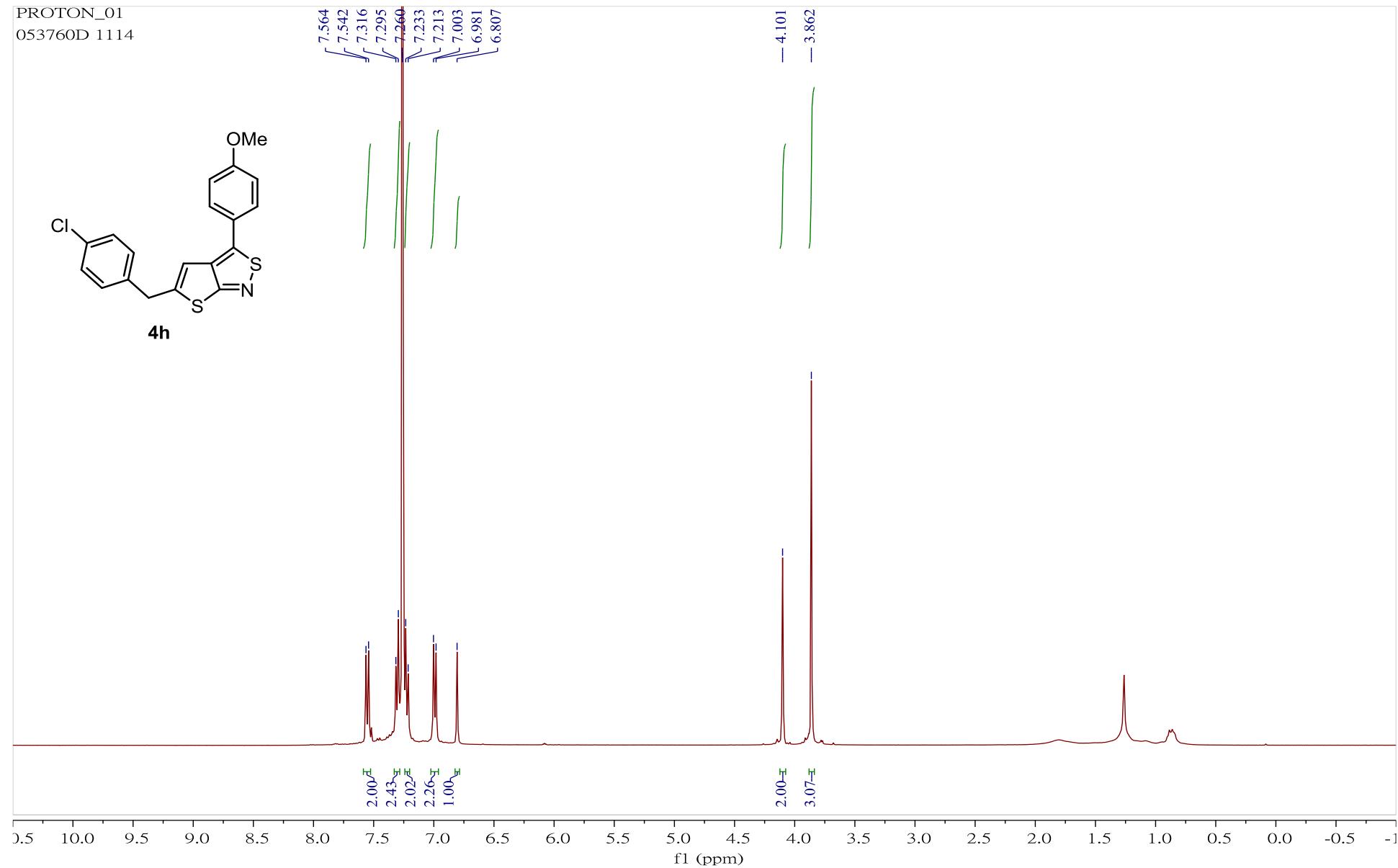
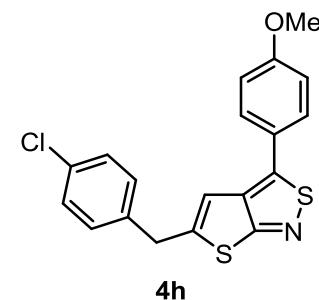
^1H NMR (400 MHz) spectrum of compound **4g** in CDCl_3

CARBON_01
4I 2 1117



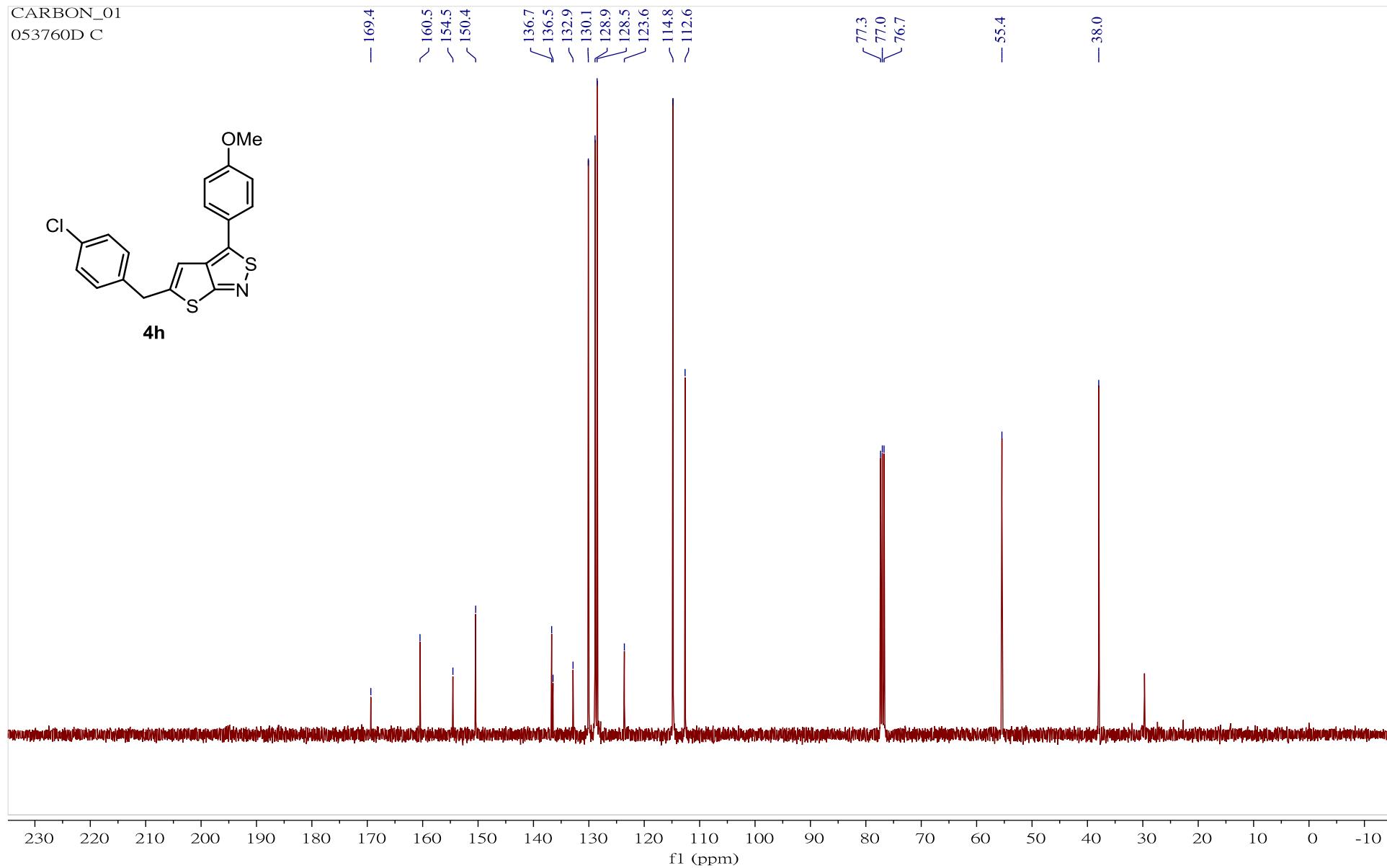
^{13}C NMR (100 MHz) spectrum of compound **4g** in CDCl_3

PROTON_01
053760D 1114



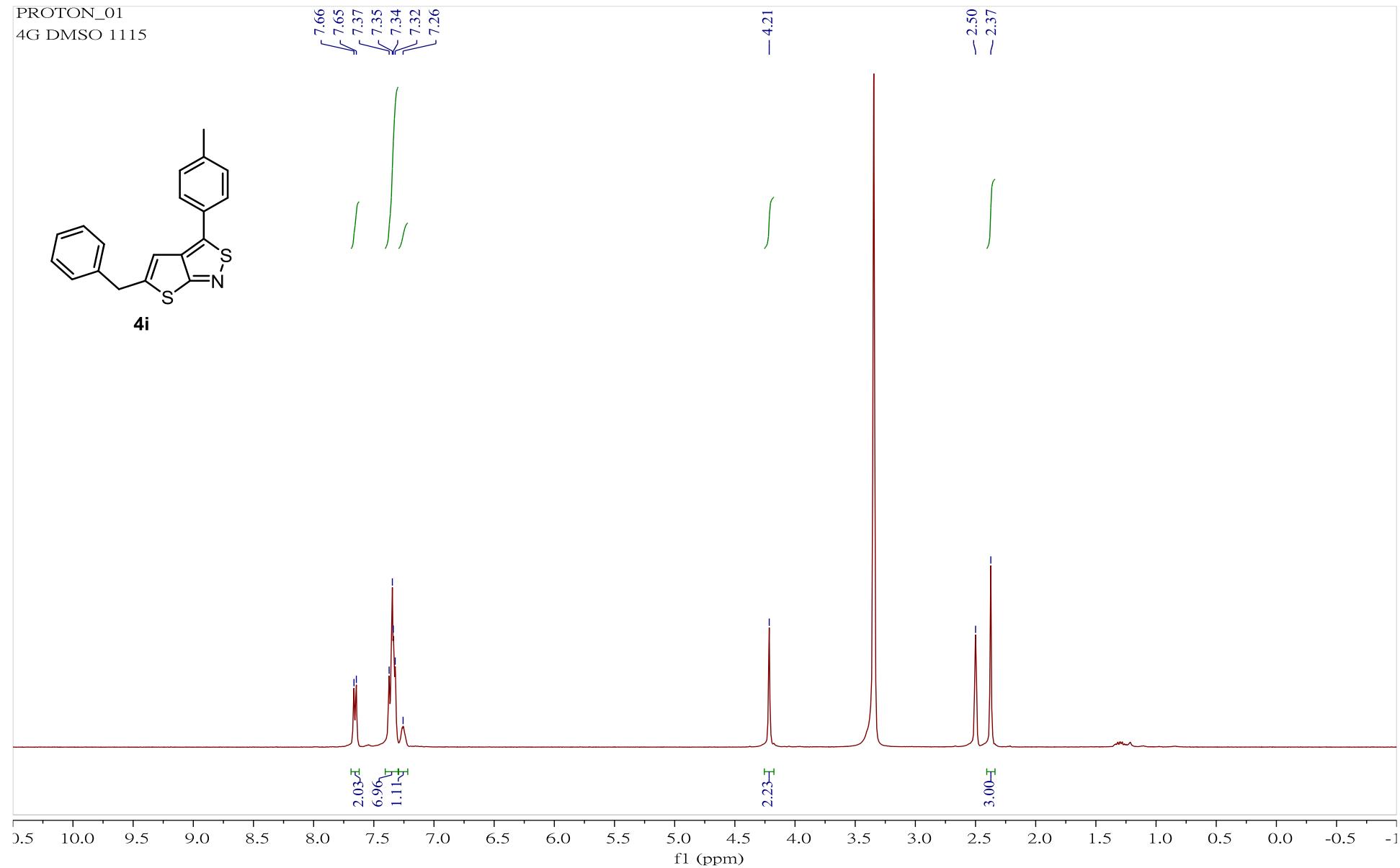
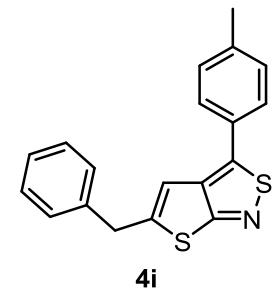
^1H NMR (400 MHz) spectrum of compound **4h** in CDCl_3

CARBON_01
053760D C



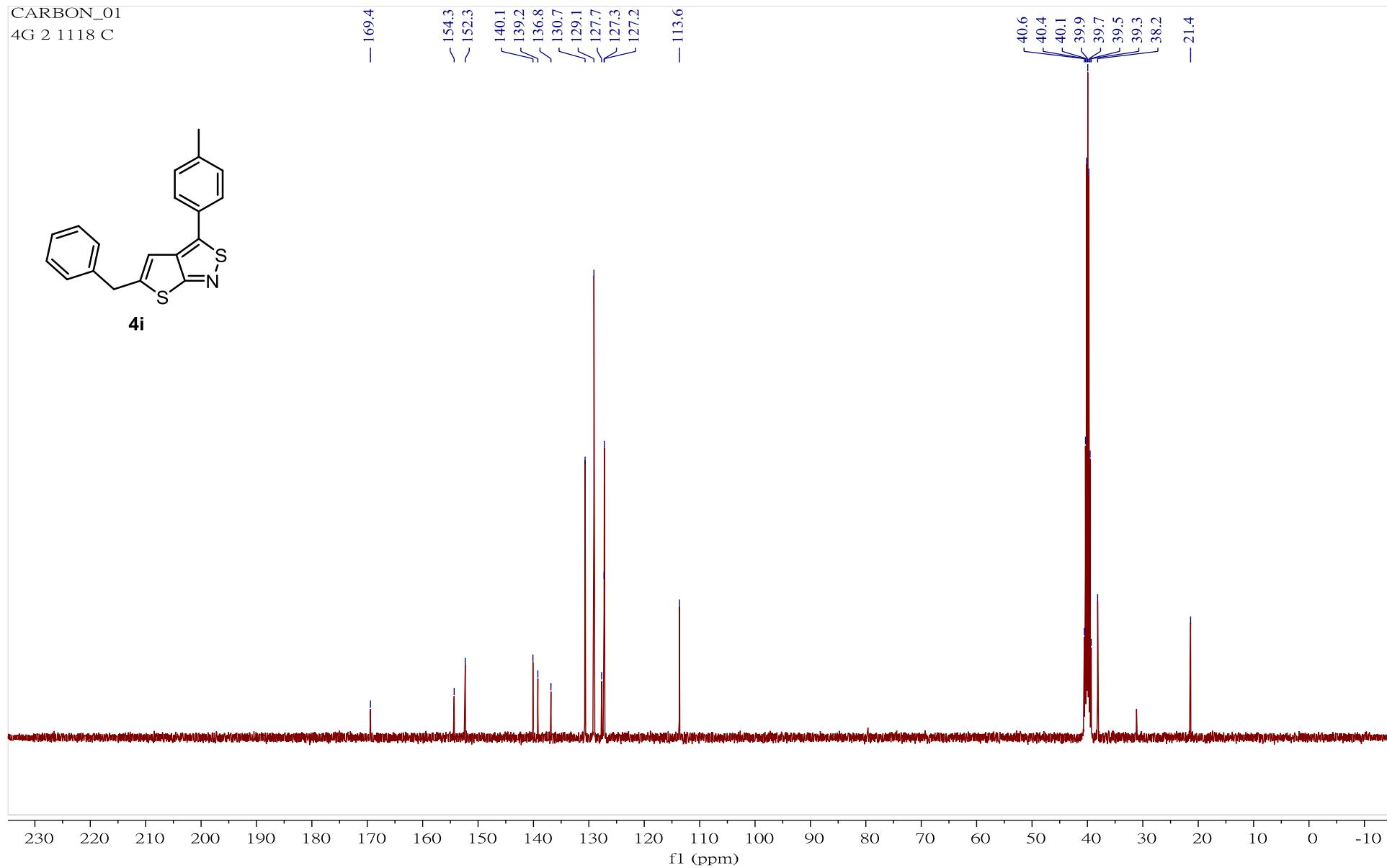
^{13}C NMR (100 MHz) spectrum of compound **4h** in CDCl_3

PROTON_01
4G DMSO 1115

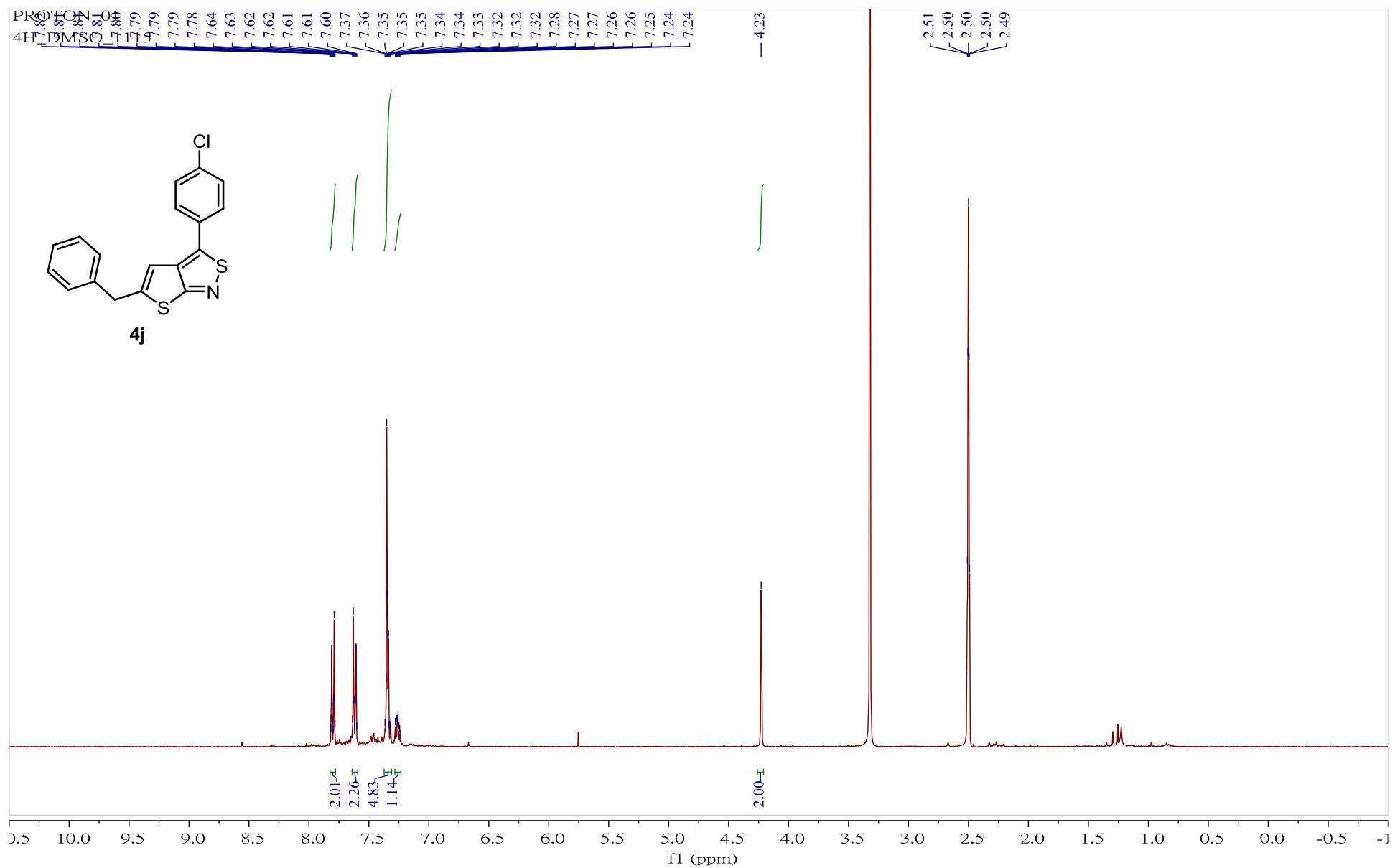


^1H NMR (400 MHz) spectrum of compound **4i** in DMSO-d^6

CARBON_01
4G 2 1118 C

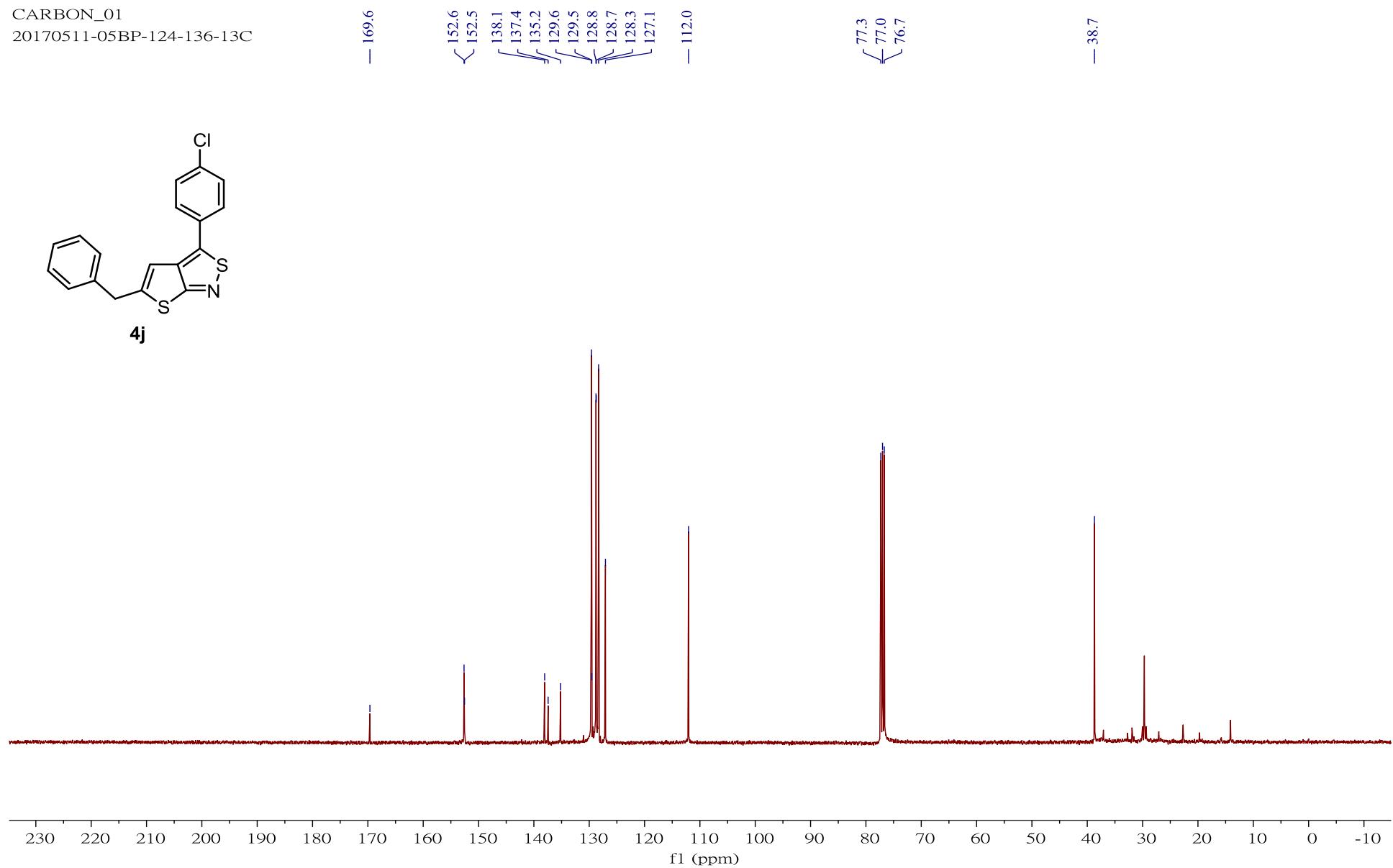


^{13}C NMR (100 MHz) spectrum of compound **4i** in DMSO-d^6

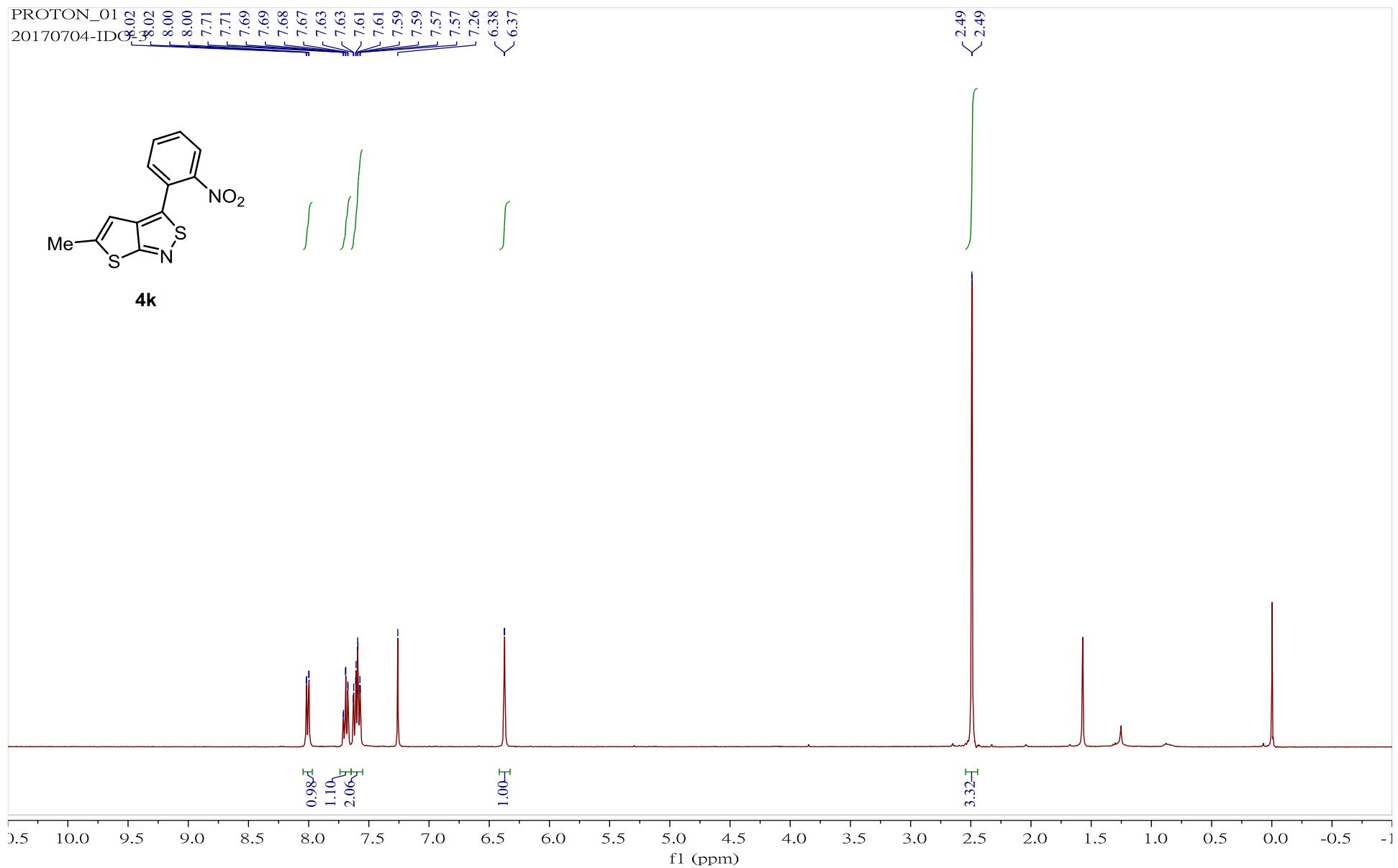


¹H NMR (400 MHz) spectrum of compound **4j** in DMSO-d⁶

CARBON_01
20170511-05BP-124-136-13C



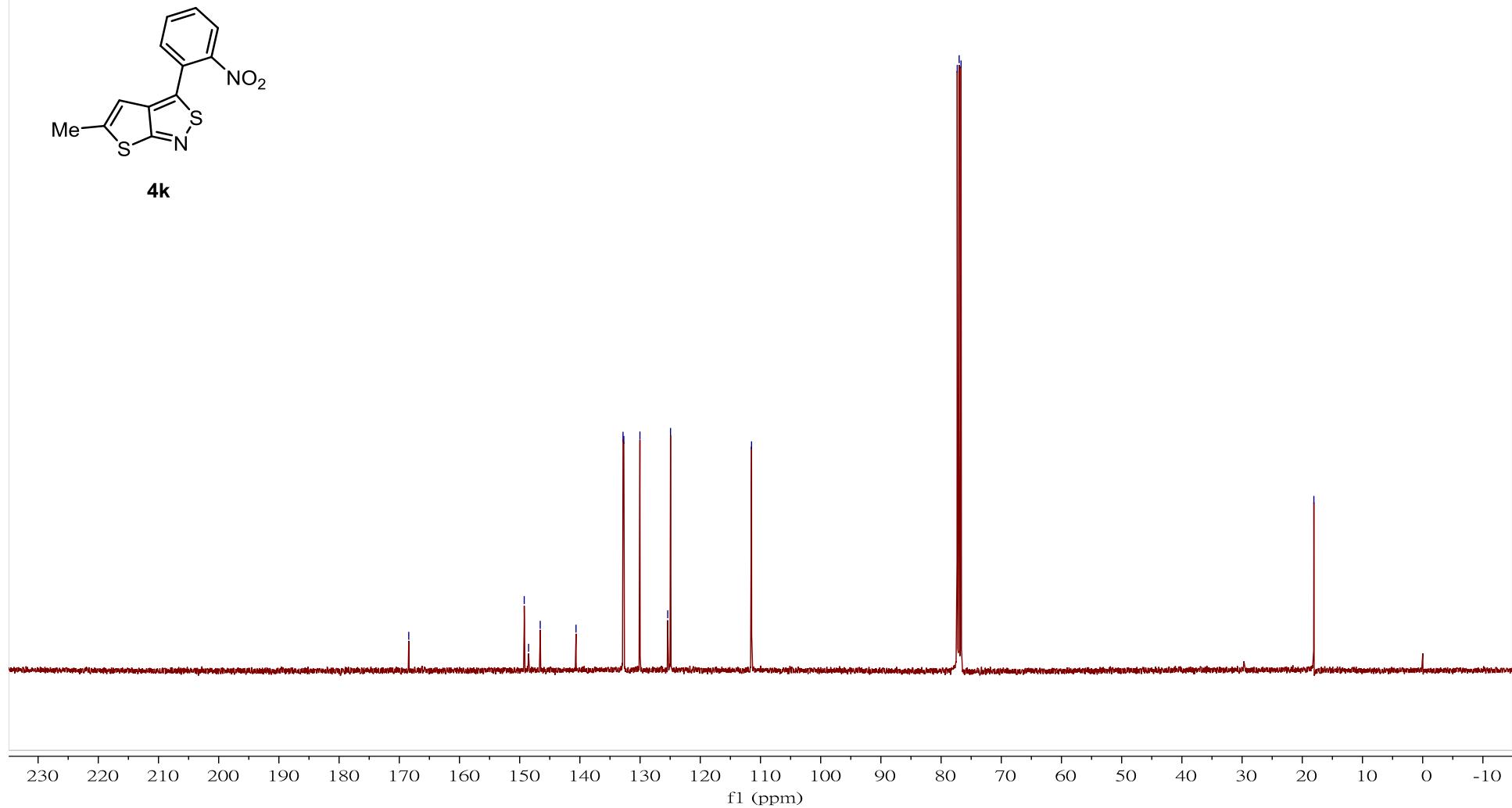
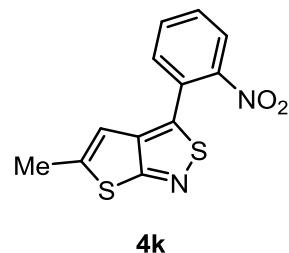
^{13}C NMR (100 MHz) spectrum of compound **4j** in CDCl_3



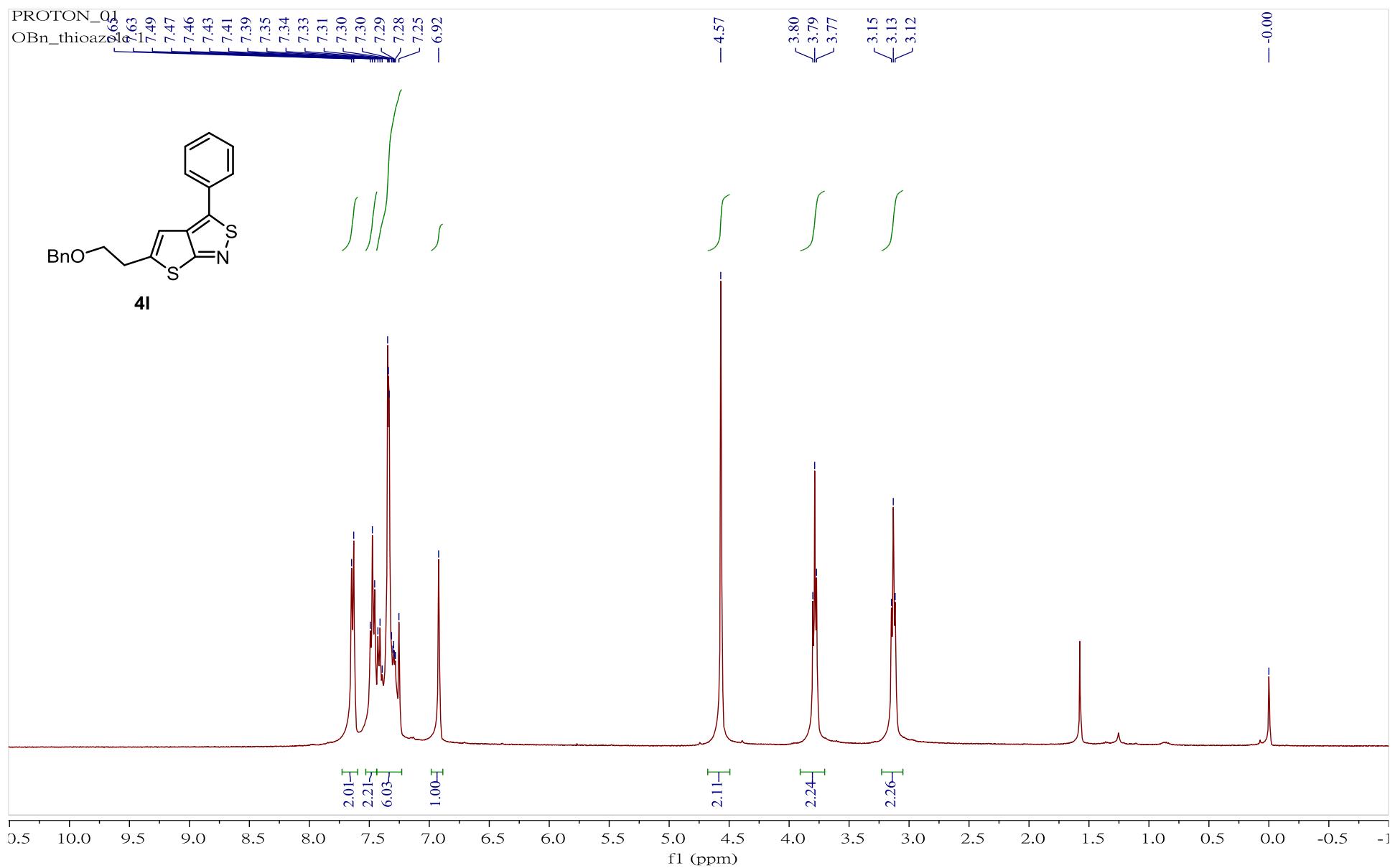
^1H NMR (400 MHz) spectrum of compound **4k** in CDCl_3

CARBON_01
20170704-IDO-3

— 168.4 —
— 149.2 —
— 148.5 —
— 146.6 —
— ~ 140.6 —
— < 132.8 —
— < 132.7 —
— ~ 130.0 —
— 125.4 —
— 124.9 —
— 111.5 —
— 77.3 —
— 77.0 —
— 76.7 —
— 18.1 —



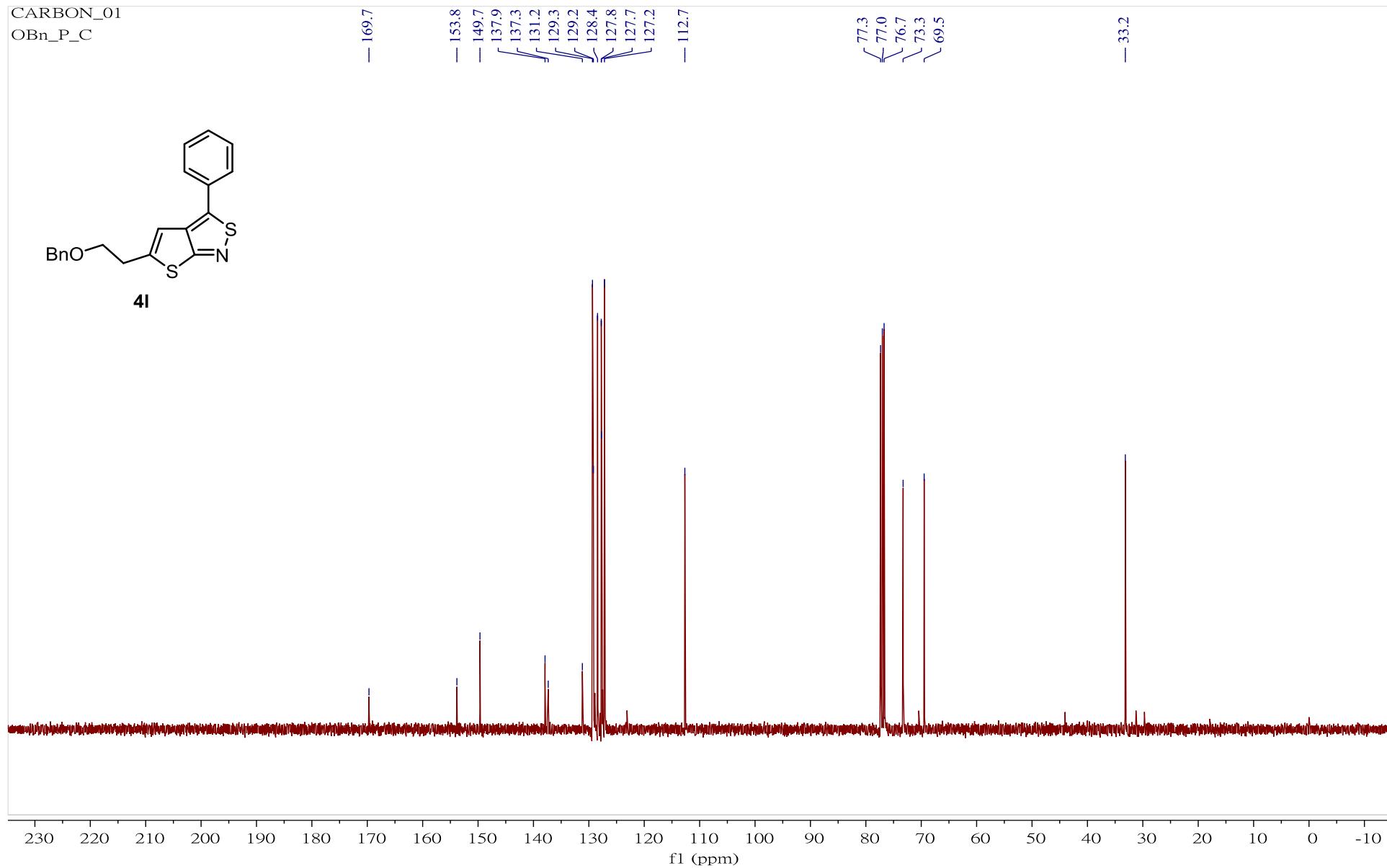
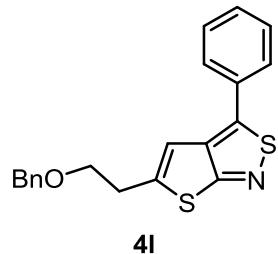
^{13}C NMR (100 MHz) spectrum of compound **4k** in CDCl_3



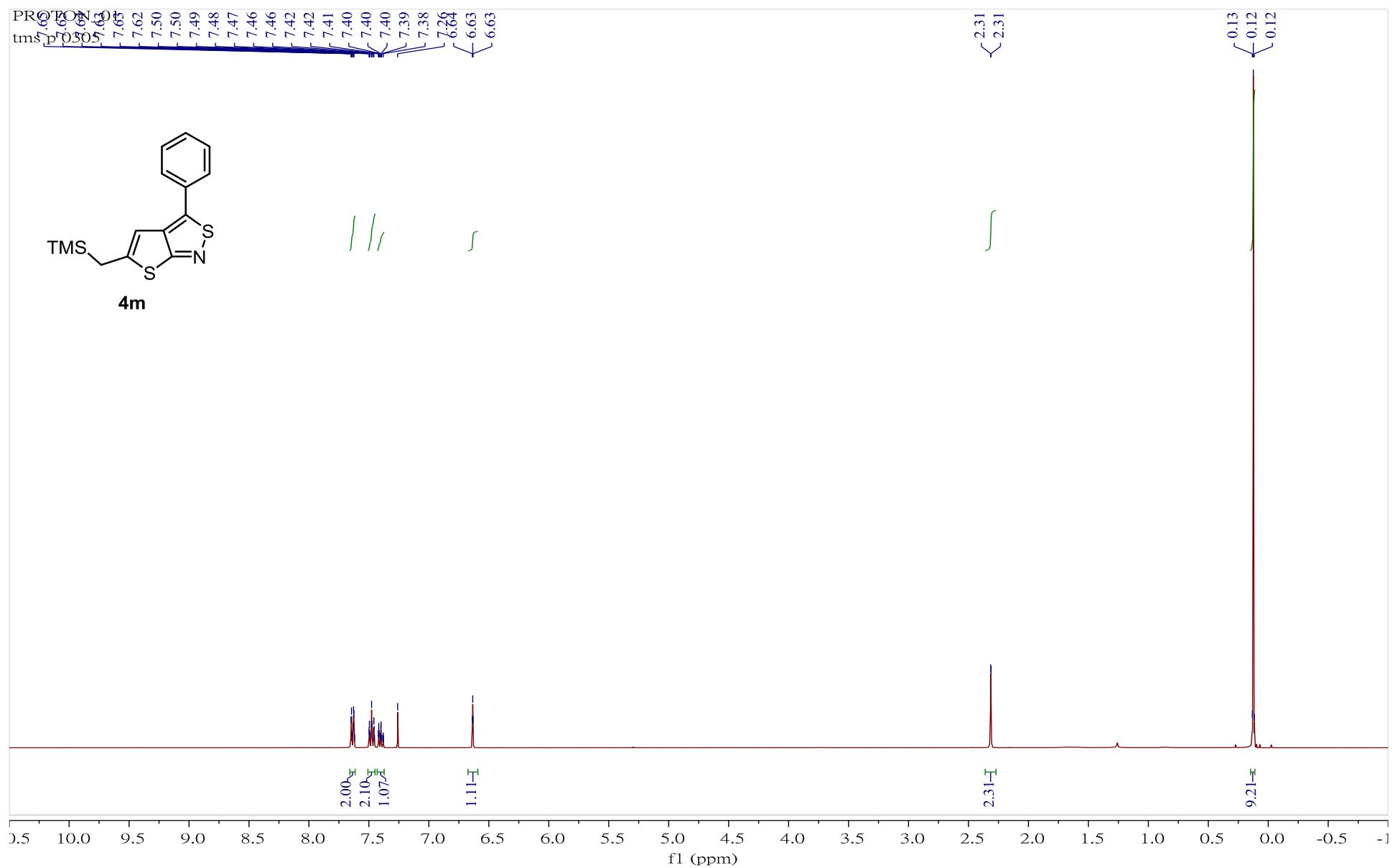
¹H NMR (400 MHz) spectrum of compound **4l** in DMSO-d⁶

CARBON_01
OBn_P_C

— 169.7 — 153.8 — 149.7 — 137.9 — 137.3 — 131.2 — 129.3 — 129.2 — 128.4 — 127.8 — 127.7 — 127.2 — 112.7 — 33.2

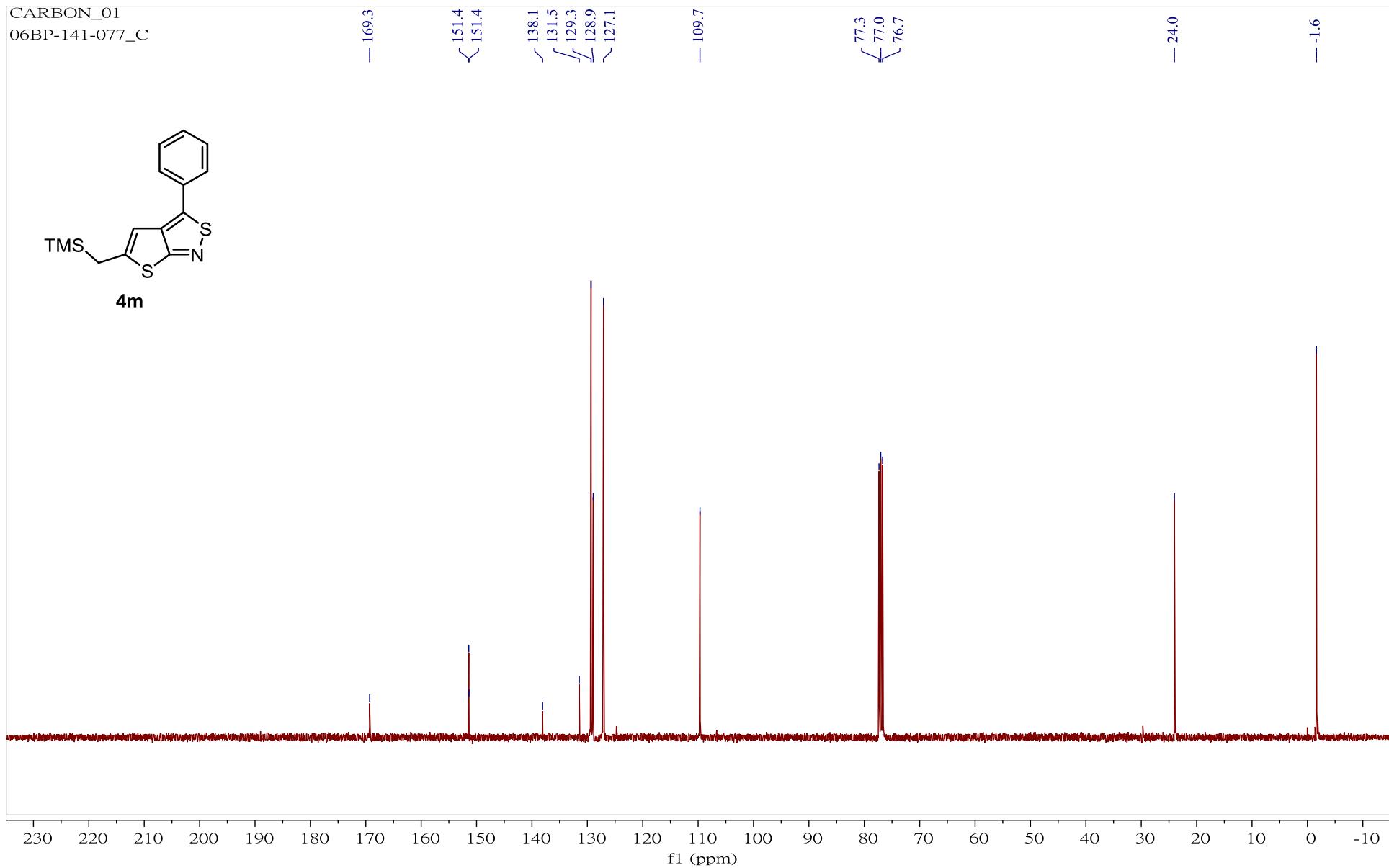


^{13}C NMR (100 MHz) spectrum of compound **4l** in DMSO-d^6

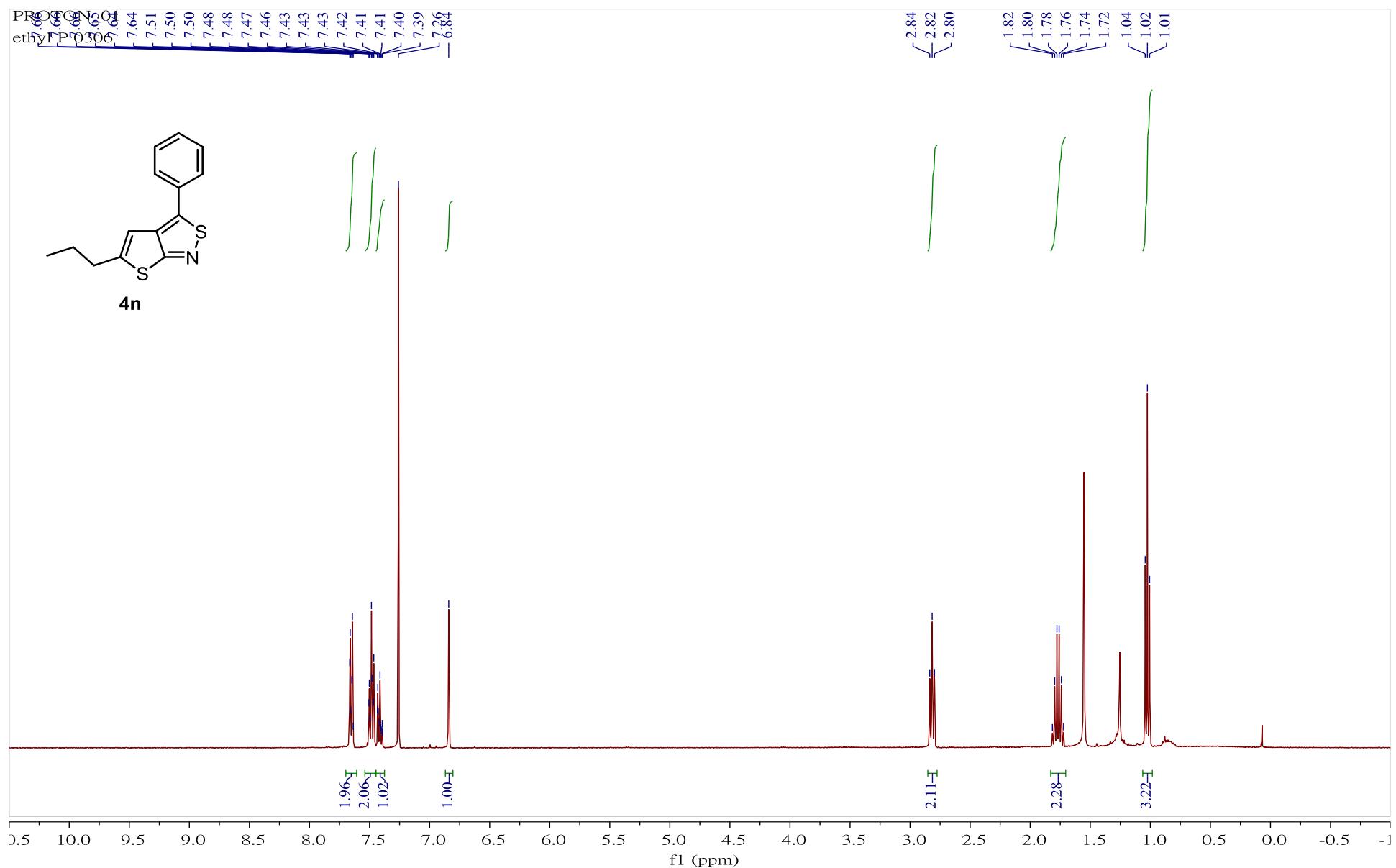


¹H NMR (400 MHz) spectrum of compound **4m** in CDCl₃

CARBON_01
06BP-141-077_C

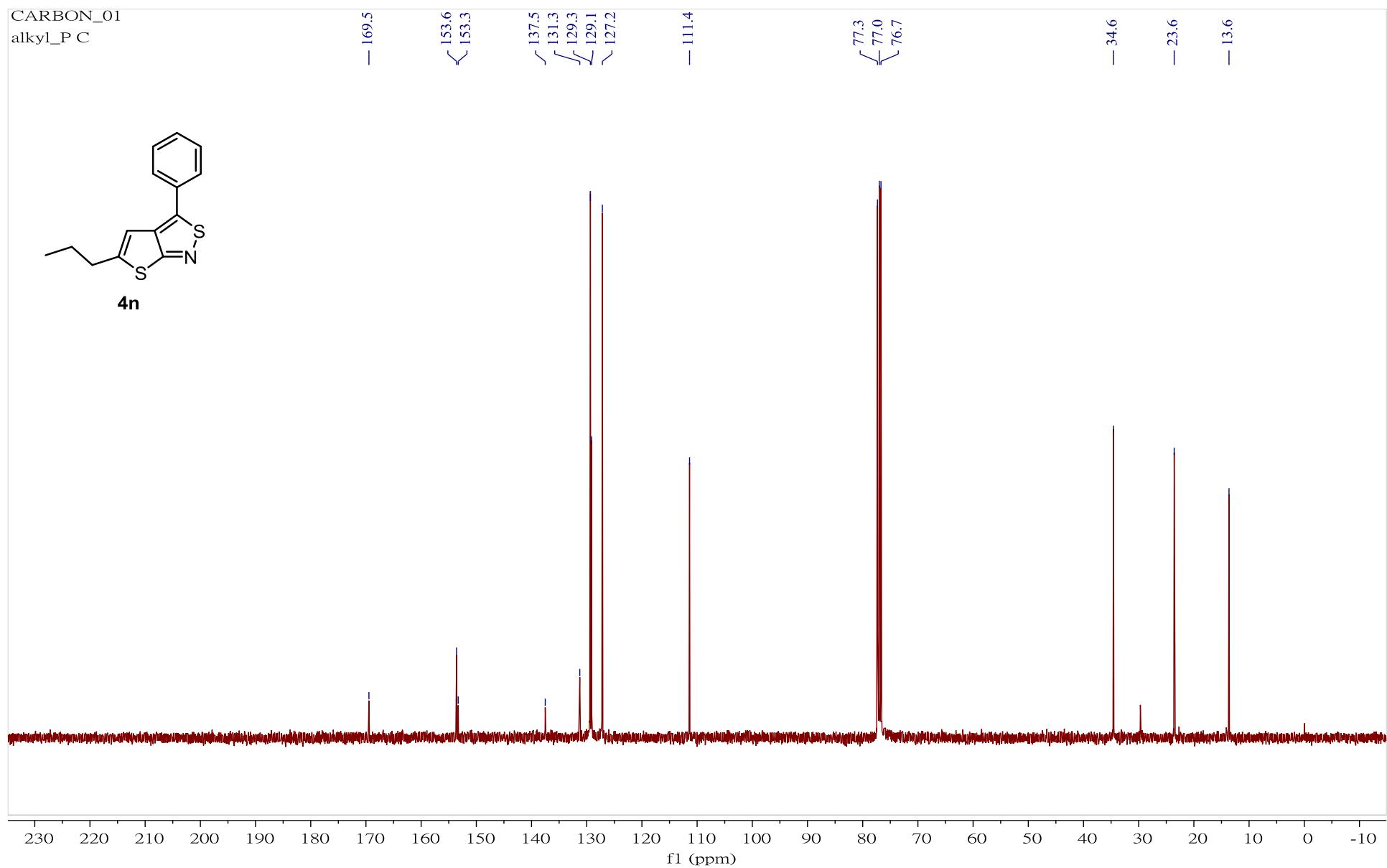


^{13}C NMR (100 MHz) spectrum of compound **4m** in CDCl_3

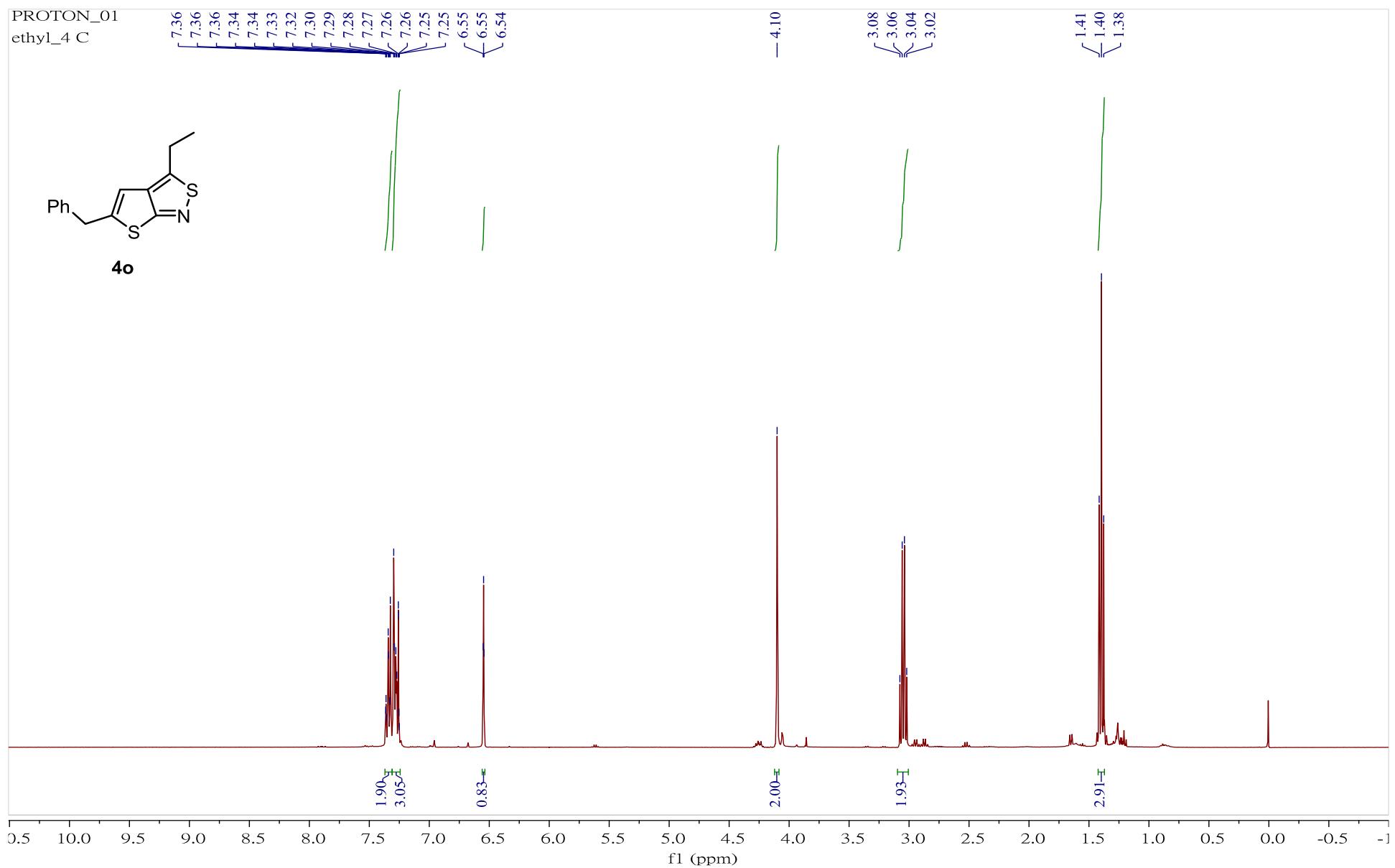


^1H NMR (400 MHz) spectrum of compound **4n** in CDCl_3

CARBON_01
alkyl_P C

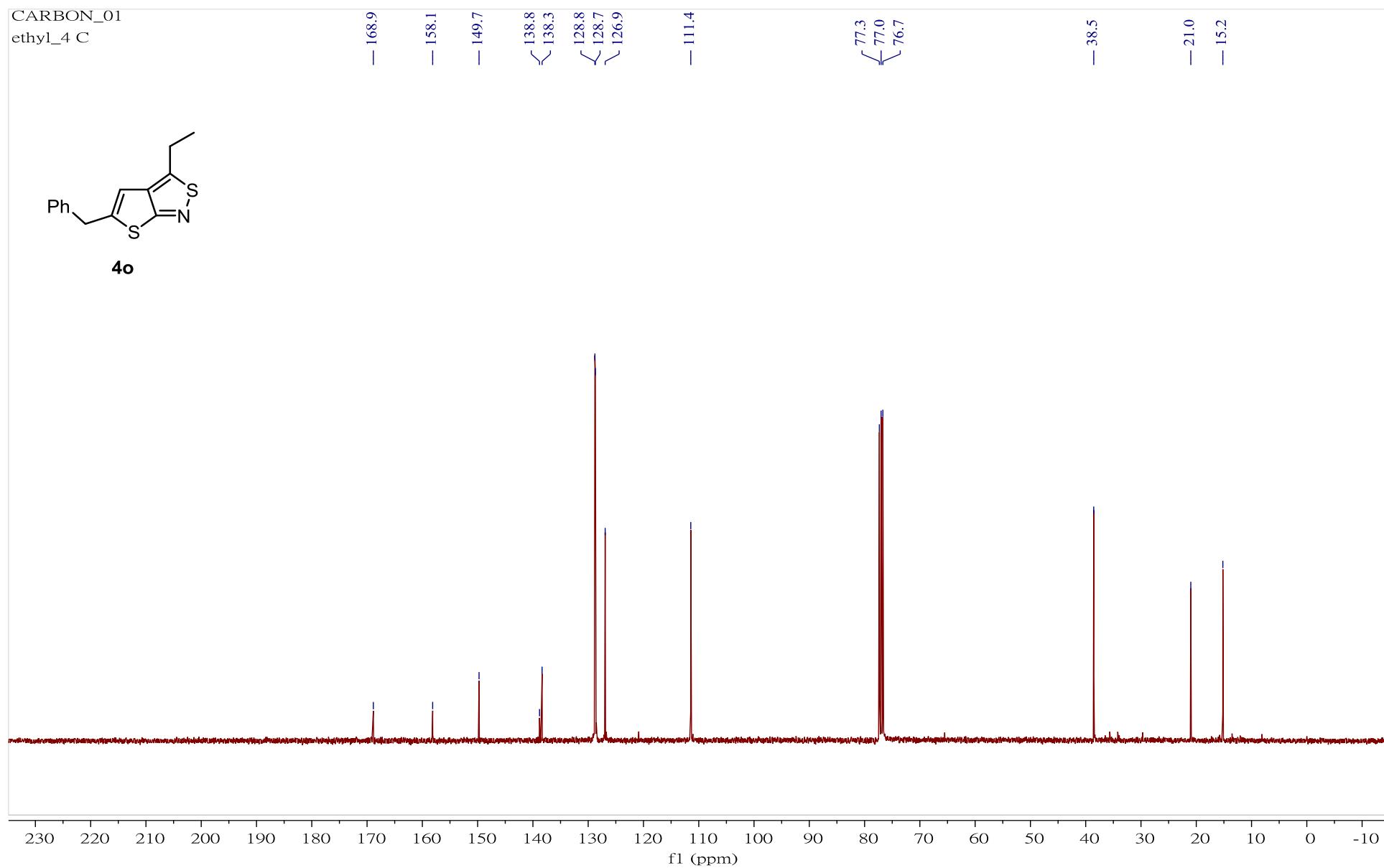


¹³C NMR (100 MHz) spectrum of compound **4n** in CDCl₃



^1H NMR (400 MHz) spectrum of compound **4o** in CDCl_3

CARBON_01
ethyl_4 C

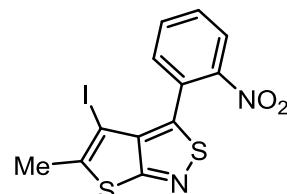


¹³C NMR (100 MHz) spectrum of compound **4o** in CDCl₃

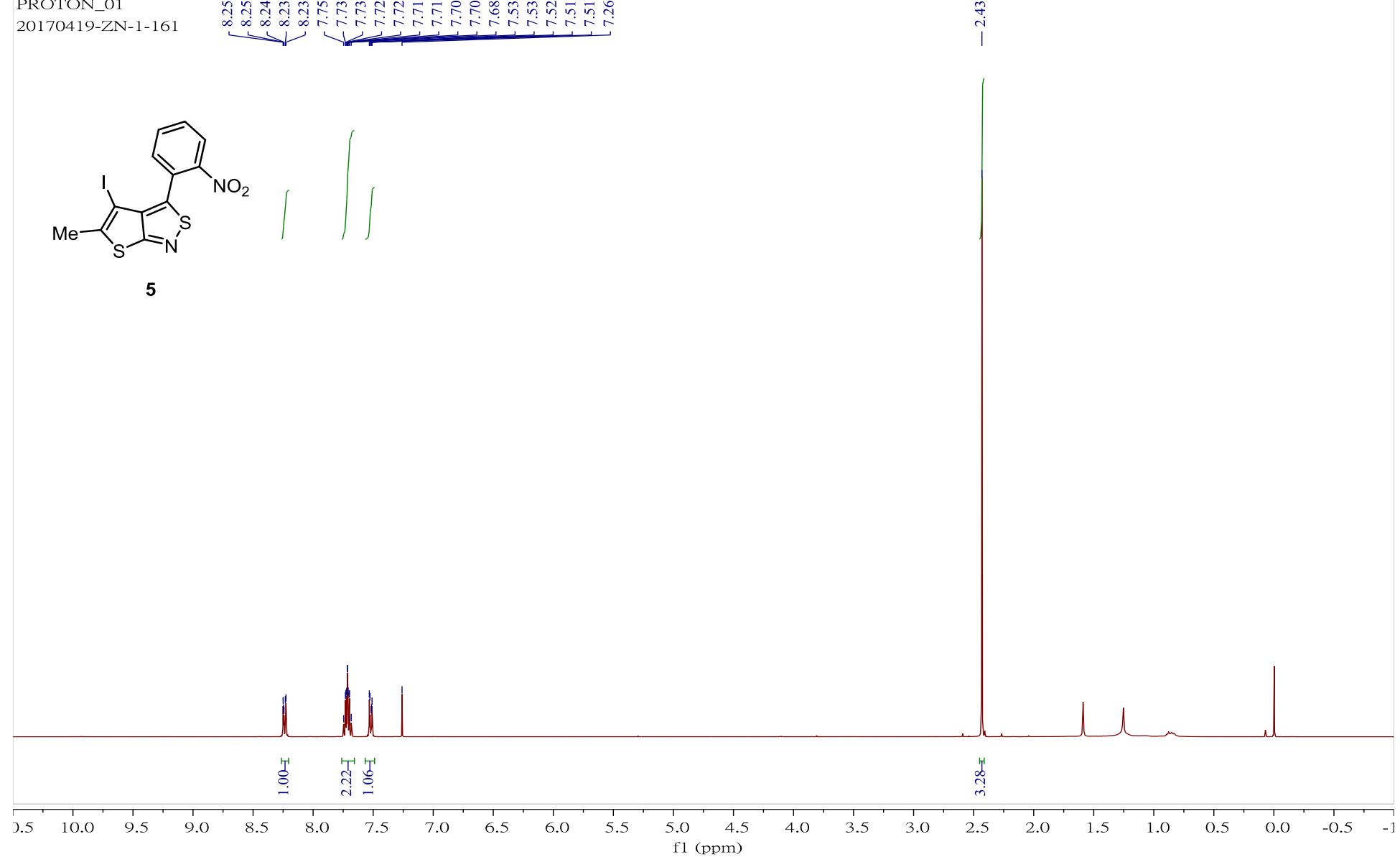
PROTON_01
20170419-ZN-1-161

8.25
8.25
8.24
8.23
8.23
7.75
7.73
7.73
7.72
7.72
7.71
7.71
7.70
7.70
7.68
7.68
7.53
7.53
7.52
7.52
7.51
7.51
7.26

-2.43



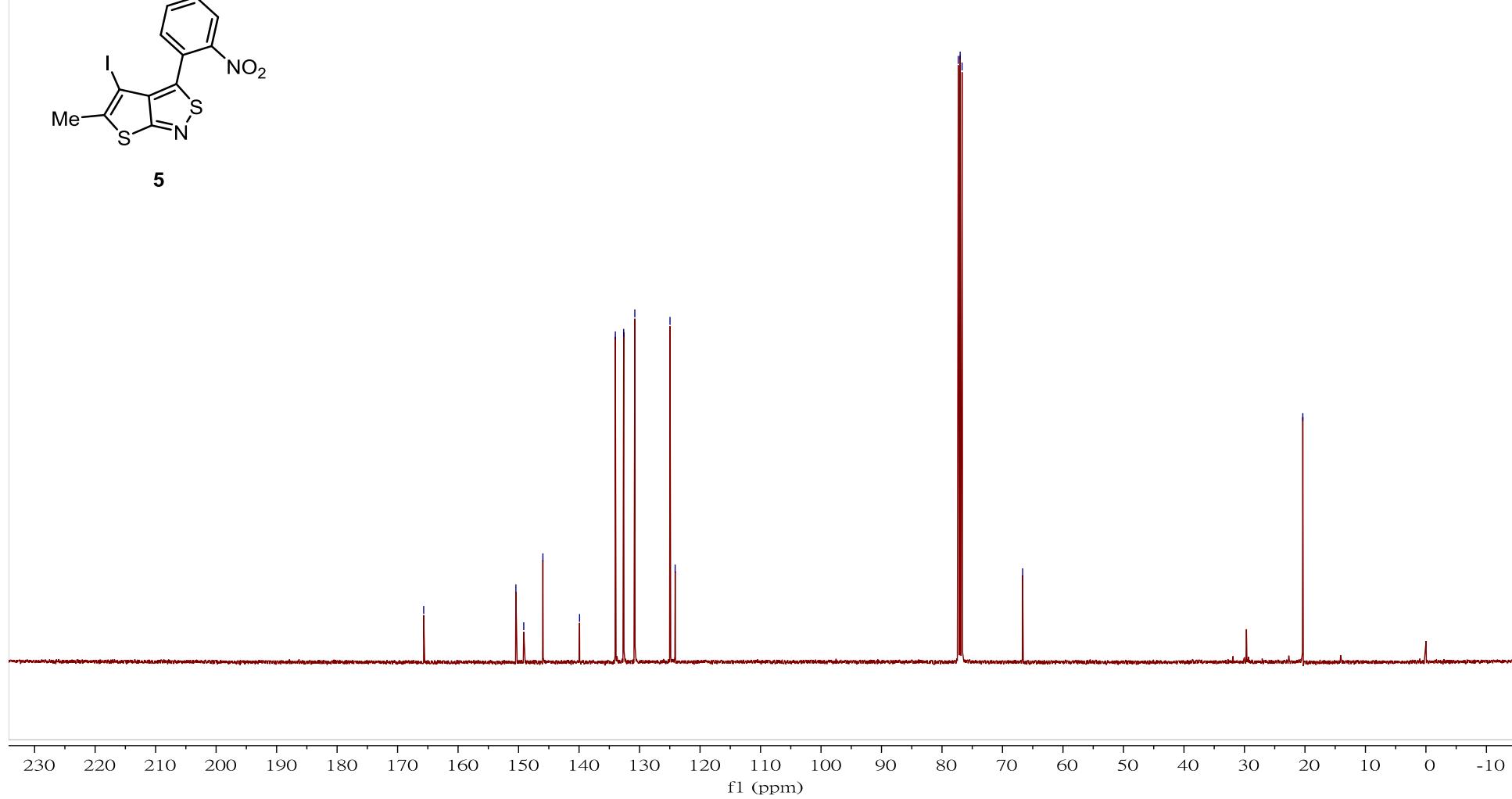
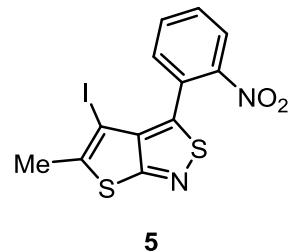
5



^1H NMR (400 MHz) spectrum of compound **5** in CDCl_3

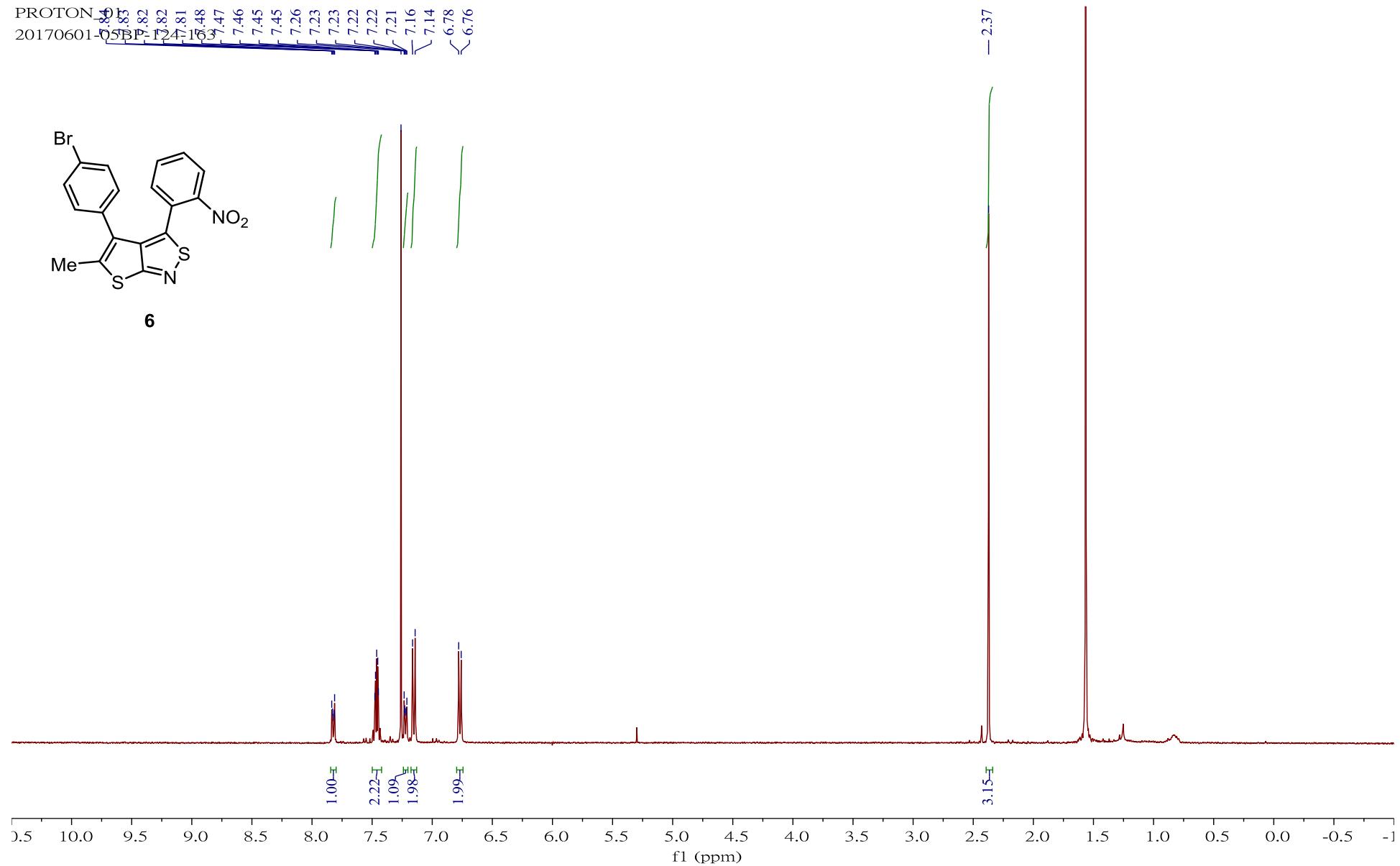
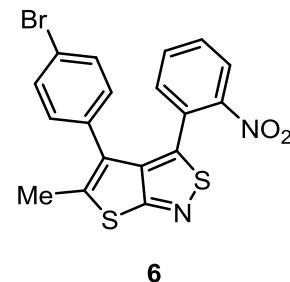
CARBON_01
20170419-ZN-1-161

— 165.7
— 150.4
— 149.1
— 146.0
— 139.9
— 134.0
— 132.6
— 130.8
— 125.0
— 124.1
— 77.3
— 77.0
— 76.7
— 66.7
— 20.4



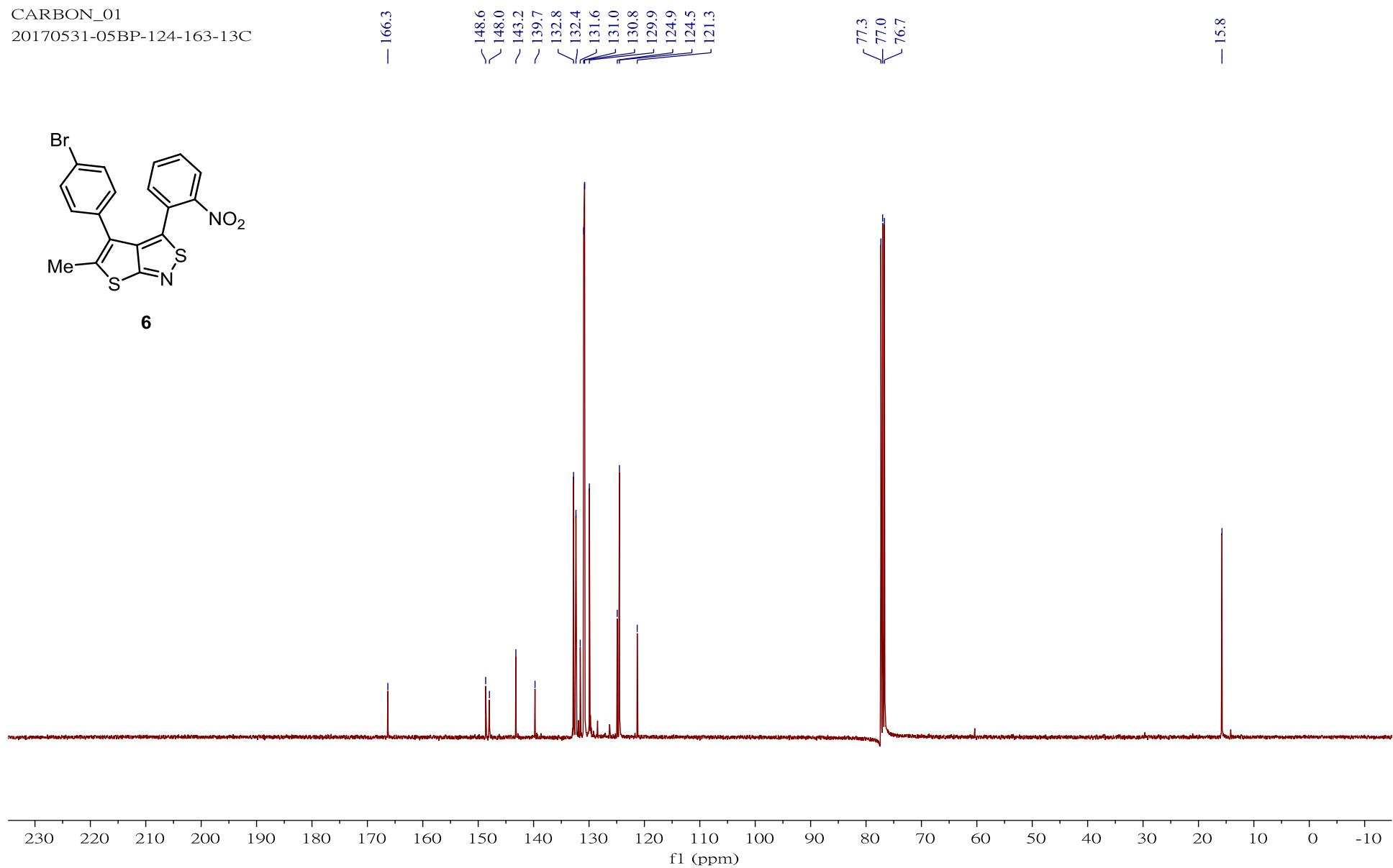
^{13}C NMR (100 MHz) spectrum of compound **5** in CDCl_3

PROTON
20170601-05BP-124-163



^1H NMR (400 MHz) spectrum of compound **6** in CDCl_3

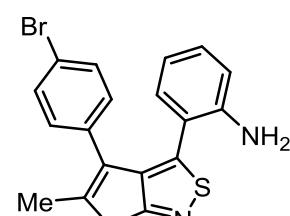
CARBON_01
20170531-05BP-124-163-13C



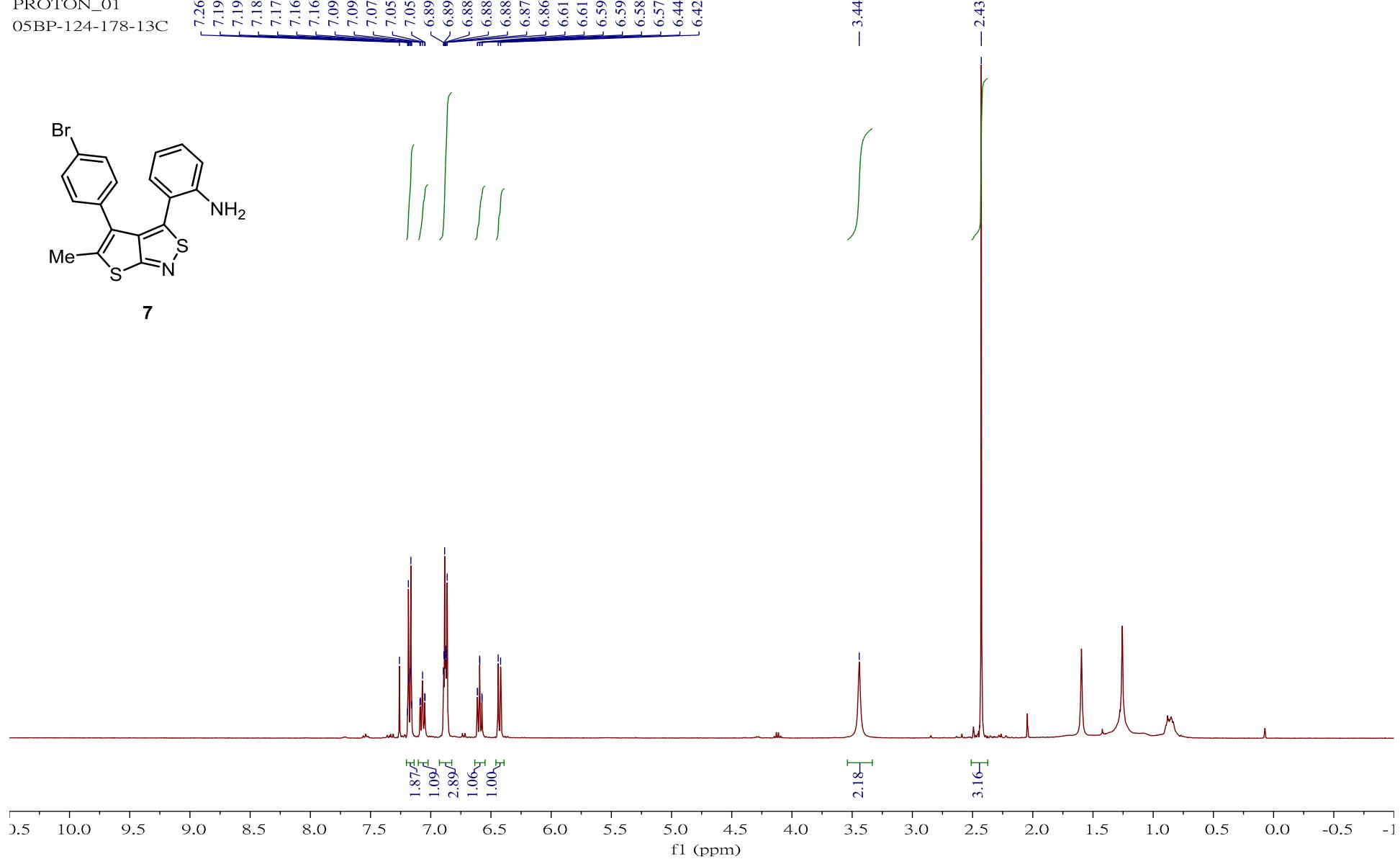
¹³C NMR (100 MHz) spectrum of compound 6 in CDCl₃

PROTON_01
05BP-124-178-13C

7.26 [7.19
7.19 [7.18
7.18 [7.17
7.17 [7.16
7.16 [7.16
7.09 [7.09
7.09 [7.09
7.07 [7.05
7.05 [7.05
6.89 [6.89
6.89 [6.88
6.88 [6.88
6.87 [6.87
6.86 [6.86
6.61 [6.61
6.61 [6.61
6.59 [6.59
6.58 [6.58
6.57 [6.57
6.44 [6.44
6.42 [6.42

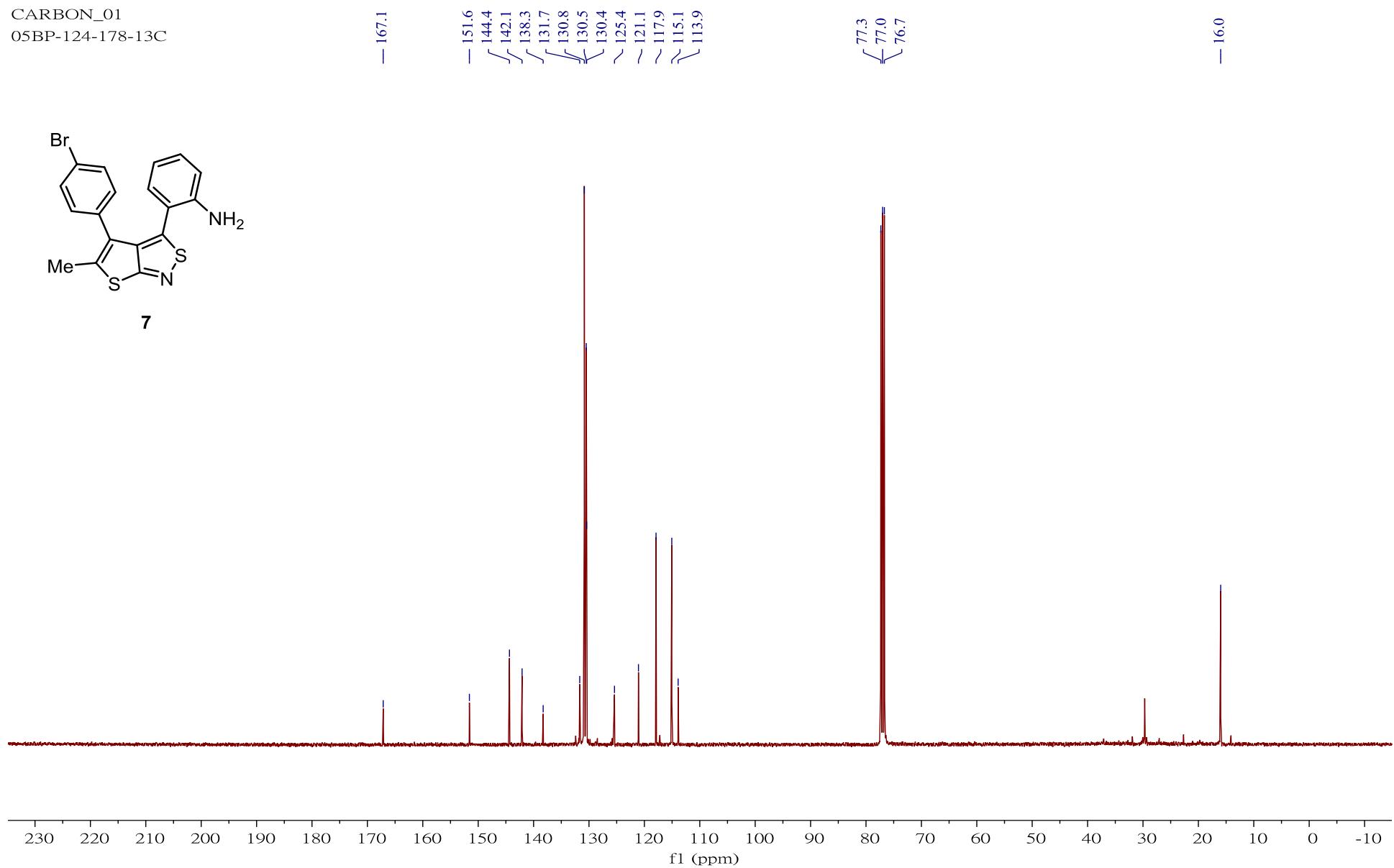


7

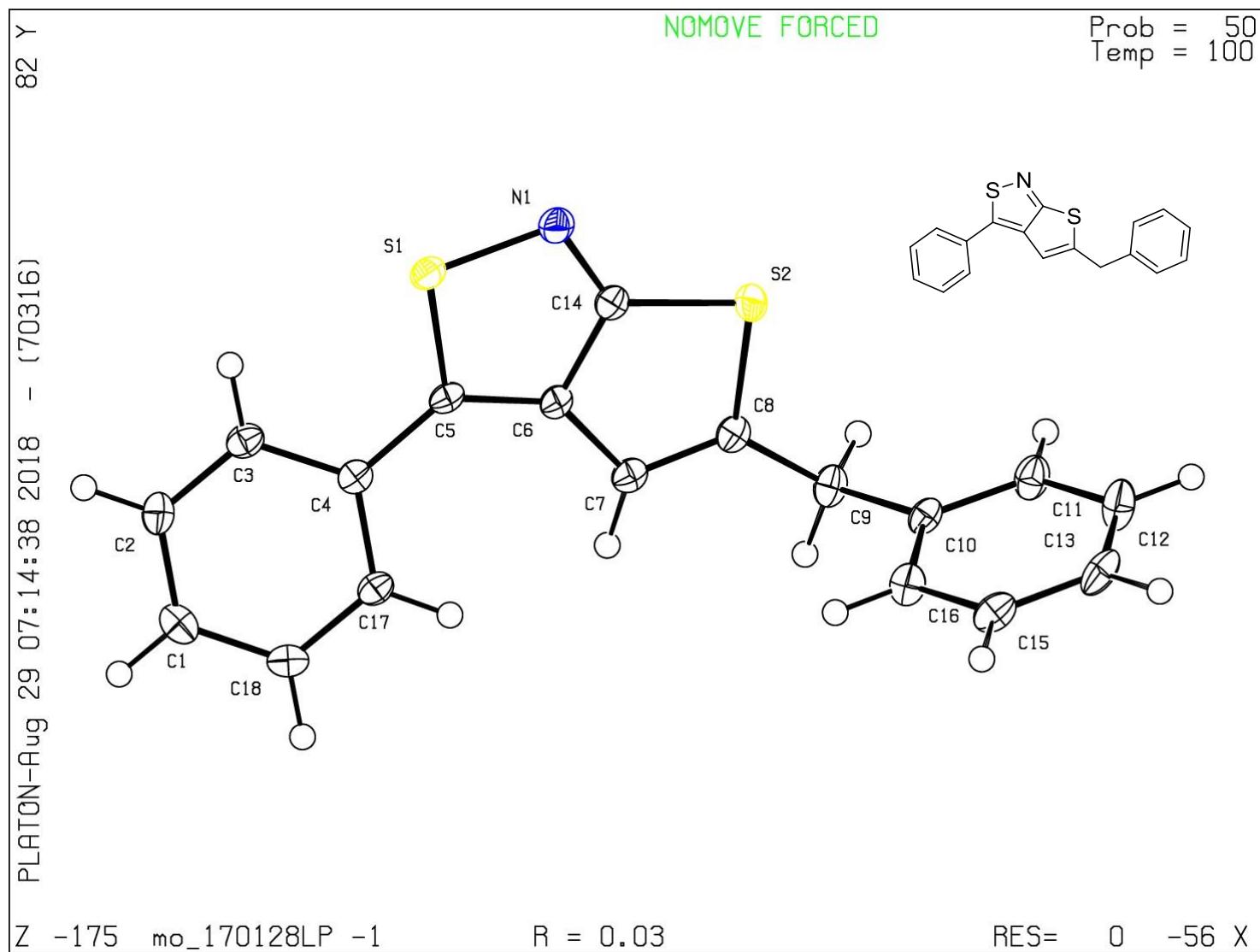


^1H NMR (400 MHz) spectrum of compound 7 in CDCl_3

CARBON_01
05BP-124-178-13C



^{13}C NMR (100 MHz) spectrum of compound 7 in CDCl_3



The ORTEP diagram of **4a** (thermal ellipsoids are shown at 50% probability).

- Sample Preparation: A crystalline solid was obtained via slow evaporation of compound **4a** in CH₂Cl₂: hexane= 1: 4 at room temperature.
 - Crystal data and structure refinement for compound **4a** (CCDC: 1532241)
-

Bond precision: C-C = 0.0021 Å Wavelength=0.71073

Cell: a=8.4886(9) b=8.9588(10) c=10.1158(11)
 alpha=86.119(3) beta=83.374(2) gamma=71.079(3)

Temperature: 100 K

	Calculated	Reported	Volume
	722.48(14)	722.48(14)	
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C18 H13 N S2	?	
Sum formula	C18 H13 N S2	C18 H13 N S2	
Mr	307.41	307.41	
Dx, g cm-3	1.413	1.413	
Z	2	2	
Mu (mm-1)	0.360	0.360	
F000	320.0	320.0	
F000'	320.59		
h, k, lmax	10,11,12	10,11,12	
Nref	2997	2971	
Tmin, Tmax	0.907, 0.924	0.845, 0.948	
Tmin'	0.907		

Correction method= # Reported T Limits: Tmin=0.845 Tmax=0.948
 AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta (max)= 26.475

R(reflections)= 0.0316(2539) wR2(reflections)= 0.0871(2971)

S = 1.053 Npar= 190
