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Supplementary Information

Ligand-free Suzuki–Miyaura cross-coupling with low Pd content: Rapid development by fluorescence-based high-throughput screening method

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Table S1. Metal oxide catalysts numbering and Pd content.

Catalyst number	Metal oxide	Catalyst number	Metal oxide
3a	MgO	**3m**	Pd/MgO (712 ppm)[a]
3b	Al_2O_3	**3n**	Pd/Al_2O_3 (752 ppm)[a]
3c	CaO+$CaCO_3$	**3o**	Pd/(CaO+$CaCO_3$) (1378 ppm)[a]
3d	Cr_2O_3	**3p**	Pd/Cr_2O_3[b]
3e	Mn_2O_3	**3q**	Pd/Mn_2O_3 (1613 ppm)[a]
3f	Fe_2O_3	**3r**	Pd/Fe_2O_3 (1356 ppm)[a]
3g	Co_3O_4	**3s**	Pd/Co_3O_4 (1174 ppm)[a]
3h	NiO	**3t**	Pd/NiO (1735 ppm)[a]
3i	CuO	**3u**	Pd/CuO (1347 ppm)[a]
3j	ZnO	**3v**	Pd/ZnO (111 ppm)[a]
3k	$SrCO_3$	**3w**	Pd/$SrCO_3$ (676 ppm)[a]
3l	ZrO_2	**3x**	Pd/ZrO_2[b]

[a]Pd content of metal oxides measured by ICP-OES. [b]Could not be measured due to insoluble metal oxides

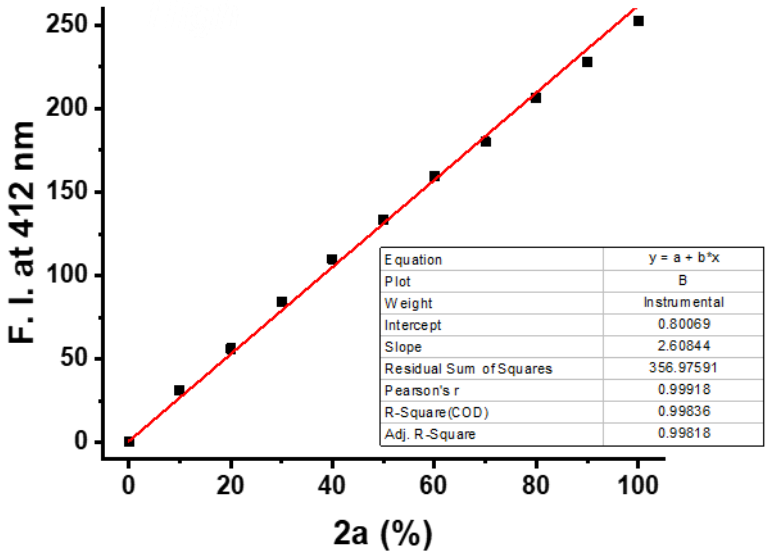
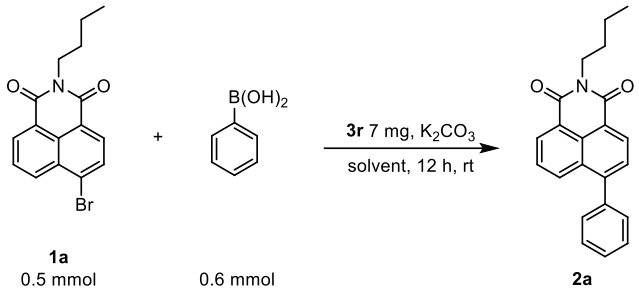


Figure S1. Plot of fluorescence intensity at 412 nm versus various percent of **2a** in toluene (λ_{ex} = 370 nm, [**1a**+**2a**] = 10 μM) and the standard curve (red line). The equation of the standrad curve is in the table. The fluorescence yield was calculated by following equation. Yield of **2a** = ((F_{412}–0.80069)/2.60844).

Table S2. Solvent screening[a]



entry	catalyst	solvent	fluorescence yield (%)[b]
1	**3r** 7 mg	EtOH	42
2	**3r** 7 mg	ACN	1
3	**3r** 7 mg	ACN/H_2O (3:1)	7
4	**3r** 7 mg	DMF	1
5	**3r** 7 mg	ACN/H_2O (3:1)	0
6	**3r** 7 mg	1,4 Dioxane	46
7	**3r** 7 mg	1,4 Dioxane/H_2O (3:1)	1
8	**3r** 7 mg	Toluene	2
9	**3r** 7 mg	H_2O	2

[a]Reaction conditions: **1a** (0.5 mmol), phenylboronic acid (0.6 mmol), K_2CO_3 (2 equiv), **3r** 7 mg, and 5 mL of solvent at room temperature. [b]Fluorescence yield calculated by standard curve.

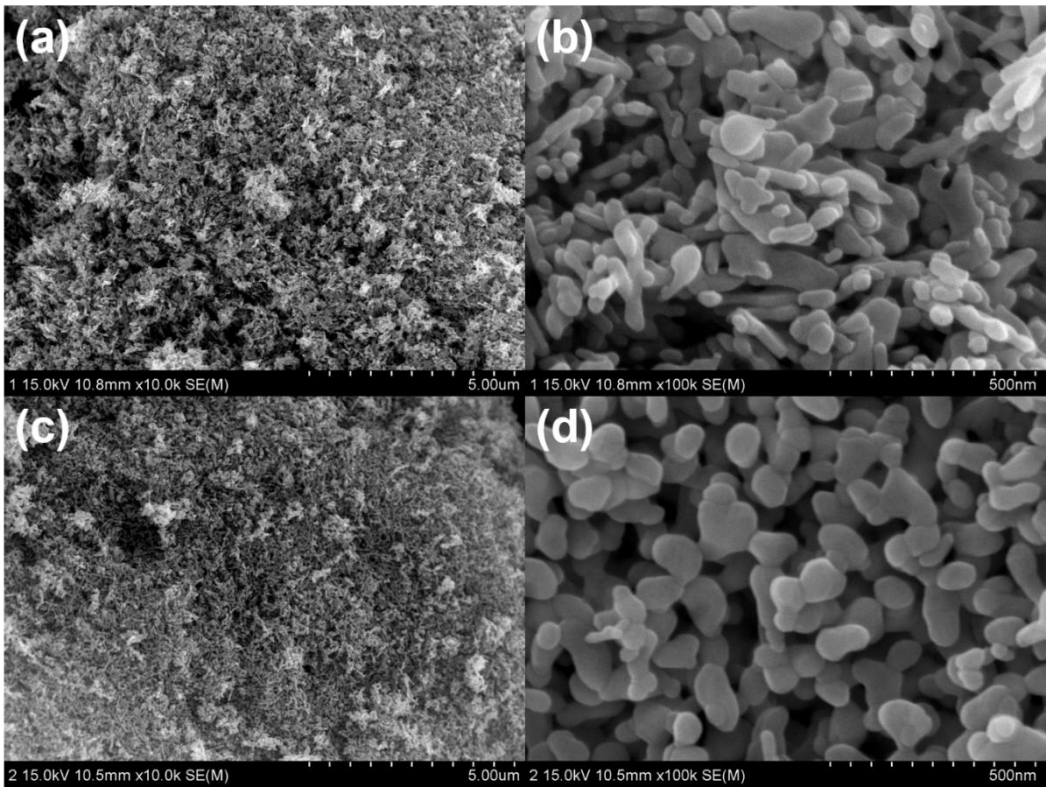


Figure S2. SEM image of Pd/Fe_2O_3 (a) and (b). SEM image of Fe_2O_3 (c) and (d).

Characterization of biaryl compounds

[1,1'-biphenyl]-4-carbonitrile (**2b**). Obtained as a white solid (0.0872 g, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.66 (m, 4H), 7.60–7.57 (m, 2H), 7.50–7.40 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 139.3, 132.7, 129.2, 128.8, 127.8, 127.3, 119.0, 111.0. The NMR data were consistent with reported data.[1]

4-Nitro-1,1'-biphenyl (**2c**). Obtained as a white solid (0.0878 g, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (dt, *J* = 9.1, 2.3 Hz, 2H), 7.73 (dt, *J* = 9.2, 2.2 Hz, 2H), 7.62 (dt, *J* = 6.5, 1.5 Hz, 2H), 7.51–7.42 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 147.2, 138.8, 129.3, 129.0, 127.9, 127.5, 124.2. The NMR data were consistent with reported data.[1]

[1,1'-Biphenyl]-2-carbaldehyde (2d). Obtained as a yellowish solid (0.0884 g, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.03 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.64 (td, *J* = 7.6, 1.4 Hz, 1H), 7.52–7.44 (m, 5H), 7.38 (td, *J* = 3.9, 1.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 146.1, 137.8, 133.8, 133.7, 130.9, 130.2, 128.5, 128.2, 127.9, 127.7. The NMR data were consistent with reported data.[2]

Methyl [1,1'-biphenyl]-4-carboxylate (2e). Obtained as a white solid (0.1045 g, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 2H), 7.66–7.61 (m, 4H), 7.48–7.44 (m, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 145.7, 140.1, 130.2, 129.0, 128.2, 127.4, 127.1, 52.2. The NMR data were consistent with reported data.[3]

2-Chloro-5-nitro-1,1'-biphenyl (2f). Obtained as a white solid (0.1157 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 2.7 Hz, 1H), 8.14 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.51–7.43 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 142.0, 139.7, 137.3, 131.1, 129.3, 128.8, 128.6, 126.1, 123.3. The NMR data were consistent with reported data.[4]

4-Fluoro-1,1'-biphenyl (2g). Obtained as a white solid (0.0774 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56–7.52 (m, 4H), 7.45–7.41 (m, 2H), 7.36–7.32 (m, 1H), 7.15–7.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (d, *J* = 245.4 Hz), 140.3, 137.4 (d, *J* = 2.9 Hz), 128.9, 128.8 (d, *J* = 7.7 Hz), 127.4, 127.1, 115.7 (d, *J* = 21.1 Hz). The NMR data were consistent with reported data.[1]

4-Methoxy-1,1'-biphenyl (2h). Obtained as a white solid (0.0735 g, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56–7.51 (m, 4H), 7.43–7.39 (m, 2H), 7.32–7.27 (m, 1H), 6.97 (dt, *J* = 9.5, 2.6 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 140.9, 133.9, 128.8, 128.3, 126.8, 126.8, 114.3, 55.4. The NMR data were consistent with

reported data.[1]

[1,1'-Biphenyl]-4-ol (2i). Obtained as a white solid (0.0551 g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.47 (dt, *J* = 9.3, 2.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.32–7.27 (m, 1H), 6.90 (dt, *J* = 9.2, 2.6 Hz, 2H), 4.76 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 140.8, 134.1, 128.8, 128.5, 126.8, 115.7. The NMR data were consistent with reported data.[3]

***N*,*N*-Dimethyl-[1,1'-biphenyl]-4-amine (2j)**. Obtained as a yellowish solid (0.0975 g, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 1.2 Hz, 1H), 7.55 (d, *J* = 1.2 Hz, 1H), 7.51 (dt, *J* = 9.5, 2.6 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.26 (tt, *J* = 7.5, 1.4 Hz, 1H), 6.81 (dt, *J* = 9.5, 2.6 Hz, 2H), 3.00 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 141.3, 129.4, 128.7, 127.8, 126.4, 126.1, 112.9, 40.7. The NMR data were consistent with reported data.[5]

2-Methoxy-6-(4-nitrophenyl)naphthalene (2k). Obtained as a yellowish solid (0.1368 g, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (dt, *J* = 9.4, 2.3 Hz, 2H), 8.01 (d, *J* = 1.5 Hz, 1H), 7.85–7.80 (m, 4H), 7.70 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.21 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.17 (d, *J* = 2.4 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 147.7, 146.9, 134.7, 133.8, 130.1, 129.0, 127.9, 127.8, 126.7, 125.5, 124.3, 119.9, 105.7, 55.5. The NMR data were consistent with reported data.[6]

1-(4-(Pyren-1-yl)phenyl)ethan-1-one (2l). Obtained as a white solid (0.1395 g, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19–7.79 (m, 10H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 2H), 2.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.0, 146.3, 136.4, 136.0, 131.5, 131.1, 130.9, 128.6, 128.4, 128.0, 127.9, 127.5, 127.4, 126.3, 125.5, 125.2, 125.0, 124.9, 124.8, 26.9. The NMR data were consistent with reported data.[7]

4'-Fluoro-2'-methyl-[1,1'-biphenyl]-4-carbonitrile (2m). Obtained as a white solid (0.1017 g, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dt, *J* = 8.2, 1.8 Hz, 2H), 7.39 (dt, *J* = 8.3, 1.8 Hz, 2H), 7.14 (dd, *J* = 8.2, 5.8 Hz, 1H), 7.01–6.93 (m, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8 (d, *J* = 247.3 Hz), 145.9, 137.7 (d, *J* = 7.7 Hz), 136.1 (d, *J* = 2.9 Hz), 132.1, 131.1 (d, *J* = 8.6 Hz), 130.2, 118.9, 117.3 (d. *J* = 21.1 Hz), 113.1 (d, *J* = 22.0 Hz), 111.0, 20.6. HRMS-EI (m/z): $[M]^+$ cald for $C_{14}H_{10}FN^+$: 211.0792; found: 211.0795.

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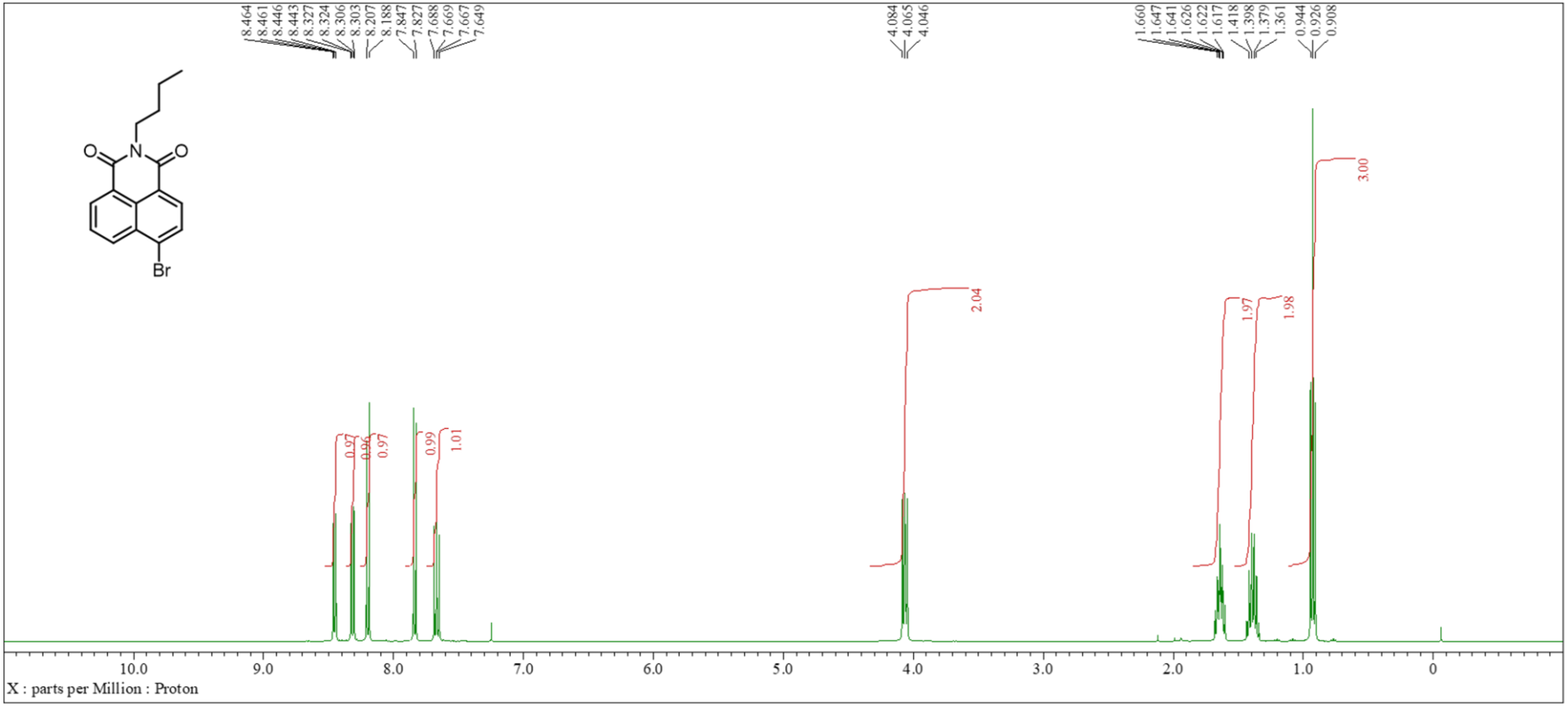
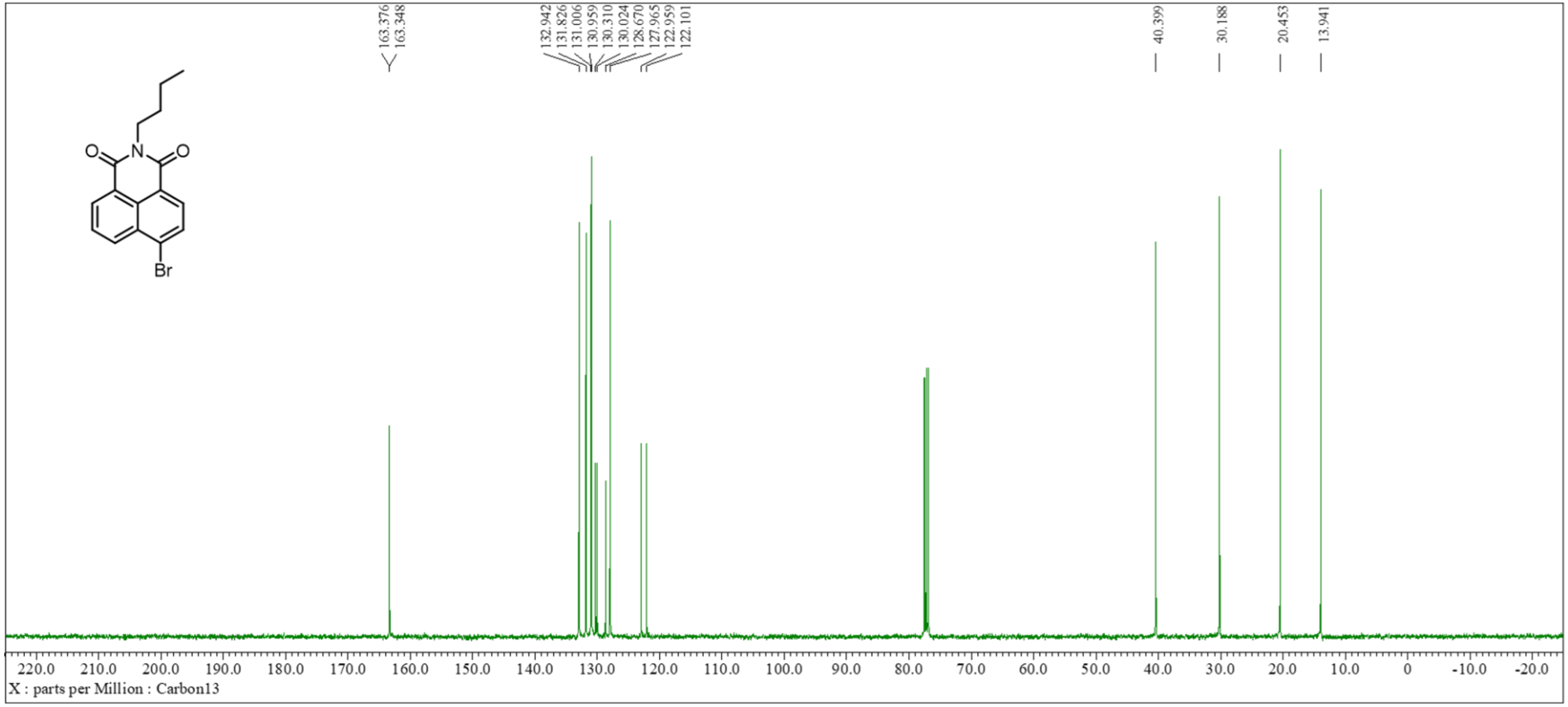


^{1}H NMR of **1a**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40.399
30.188
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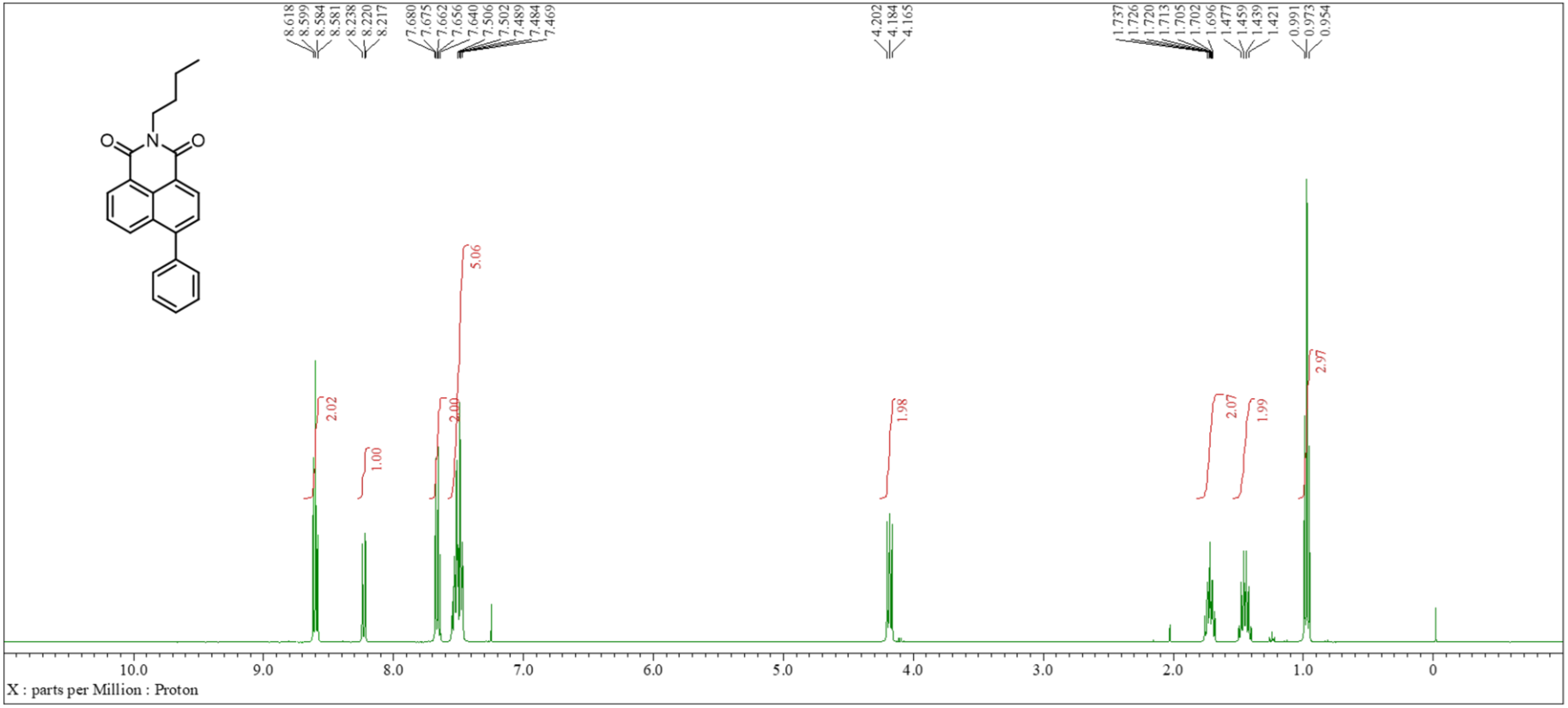
13.941
O
N
O
Br
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

^{13}C NMR of **1a**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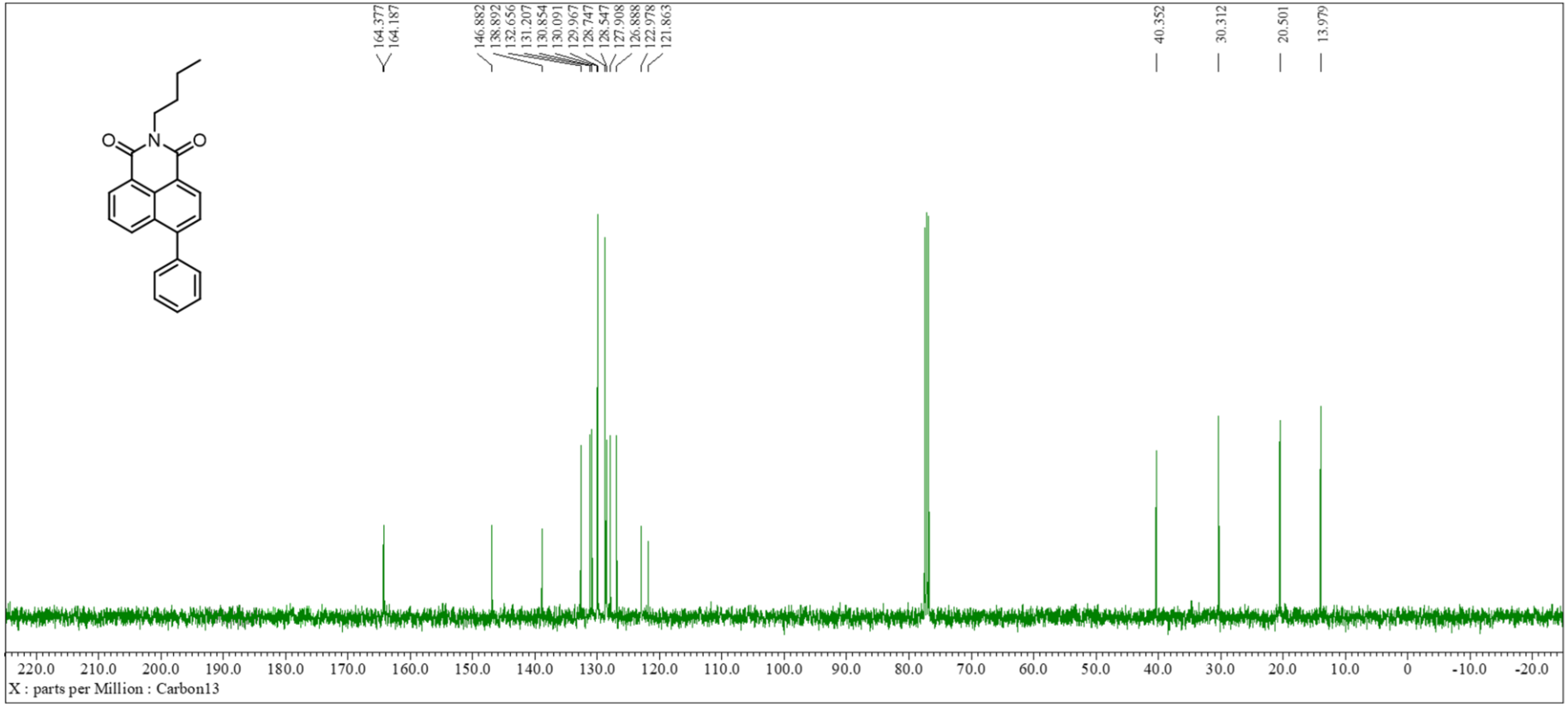
X : parts per Million : Proton

^{1}H NMR of **2a**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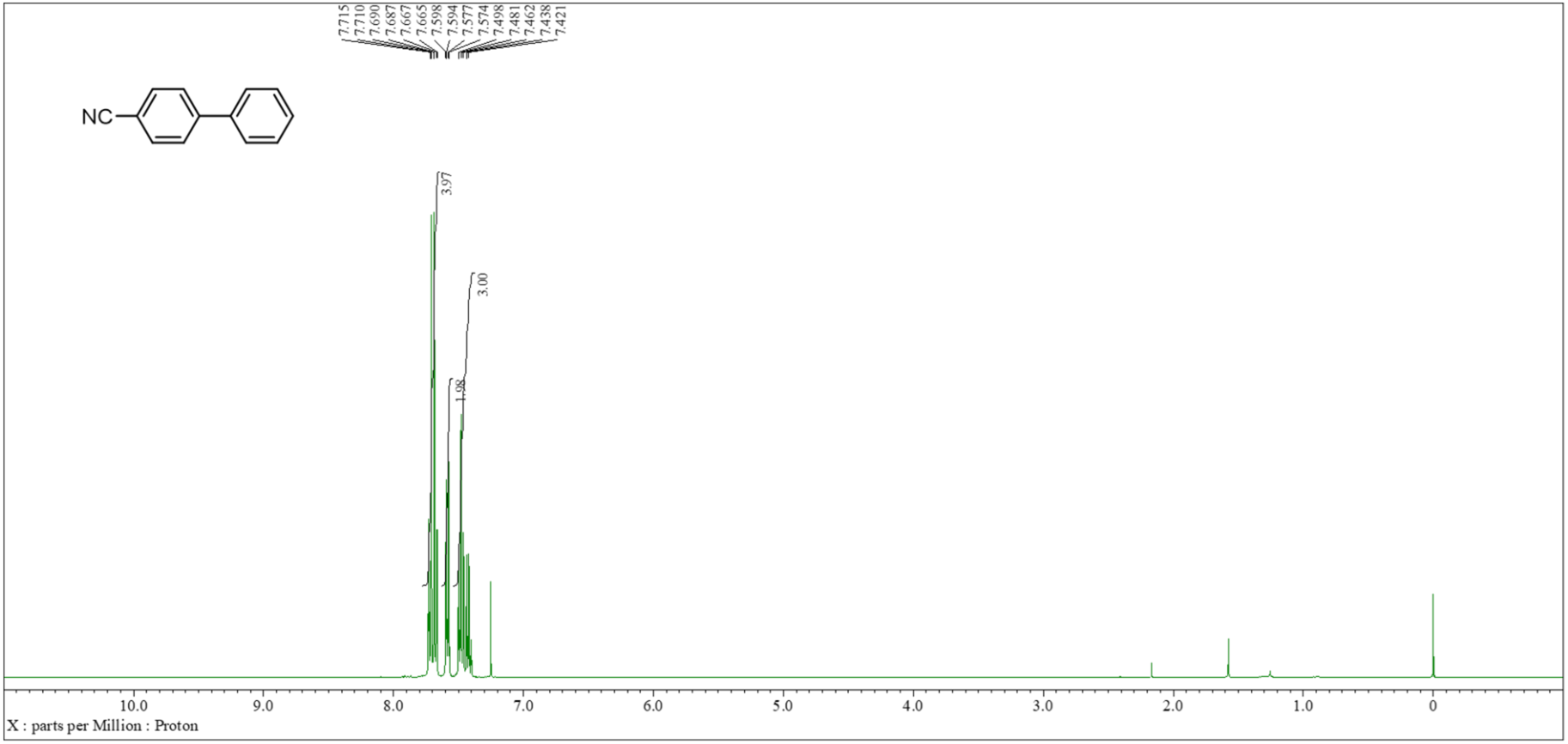
^{13}C NMR of **2a**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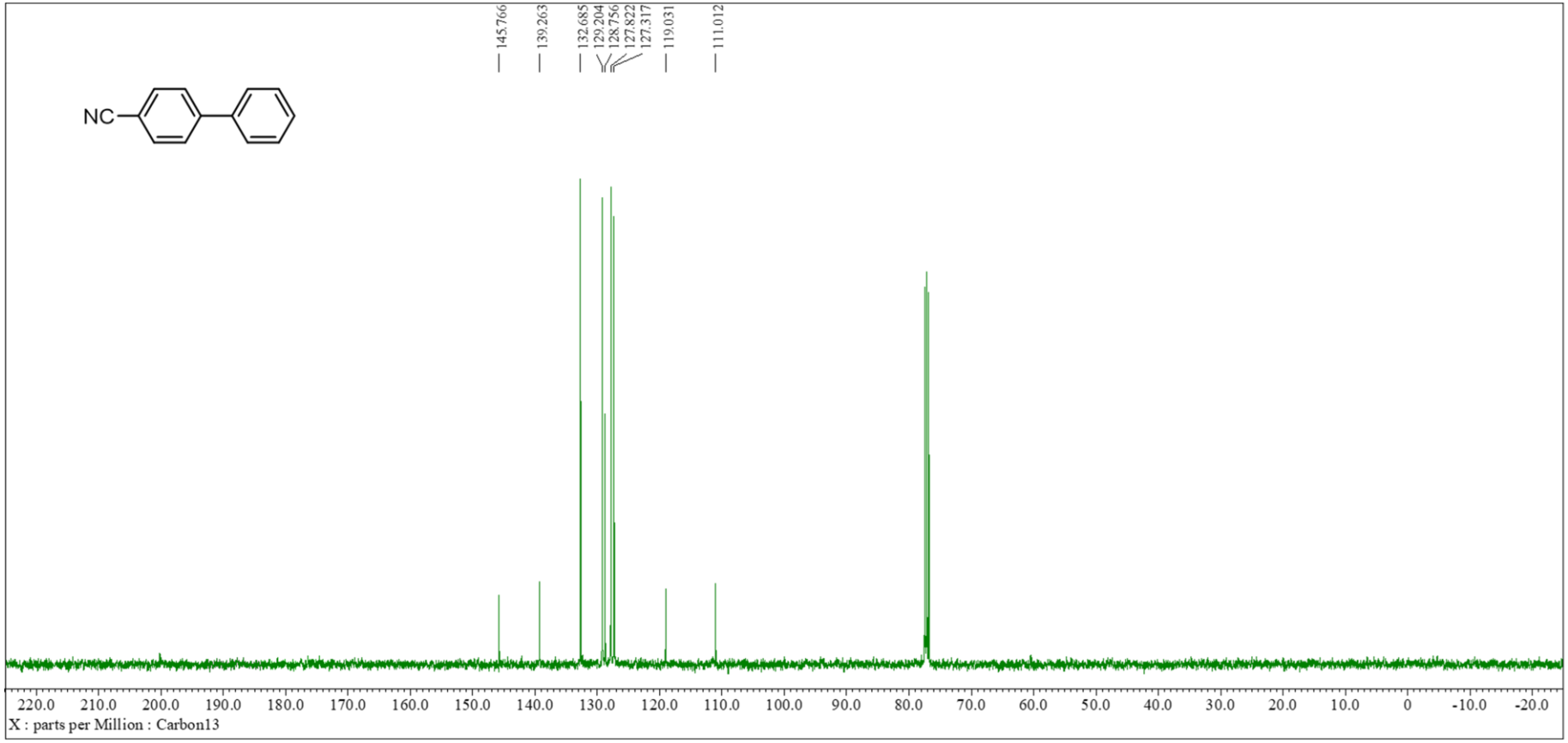
^{1}H NMR of **2b**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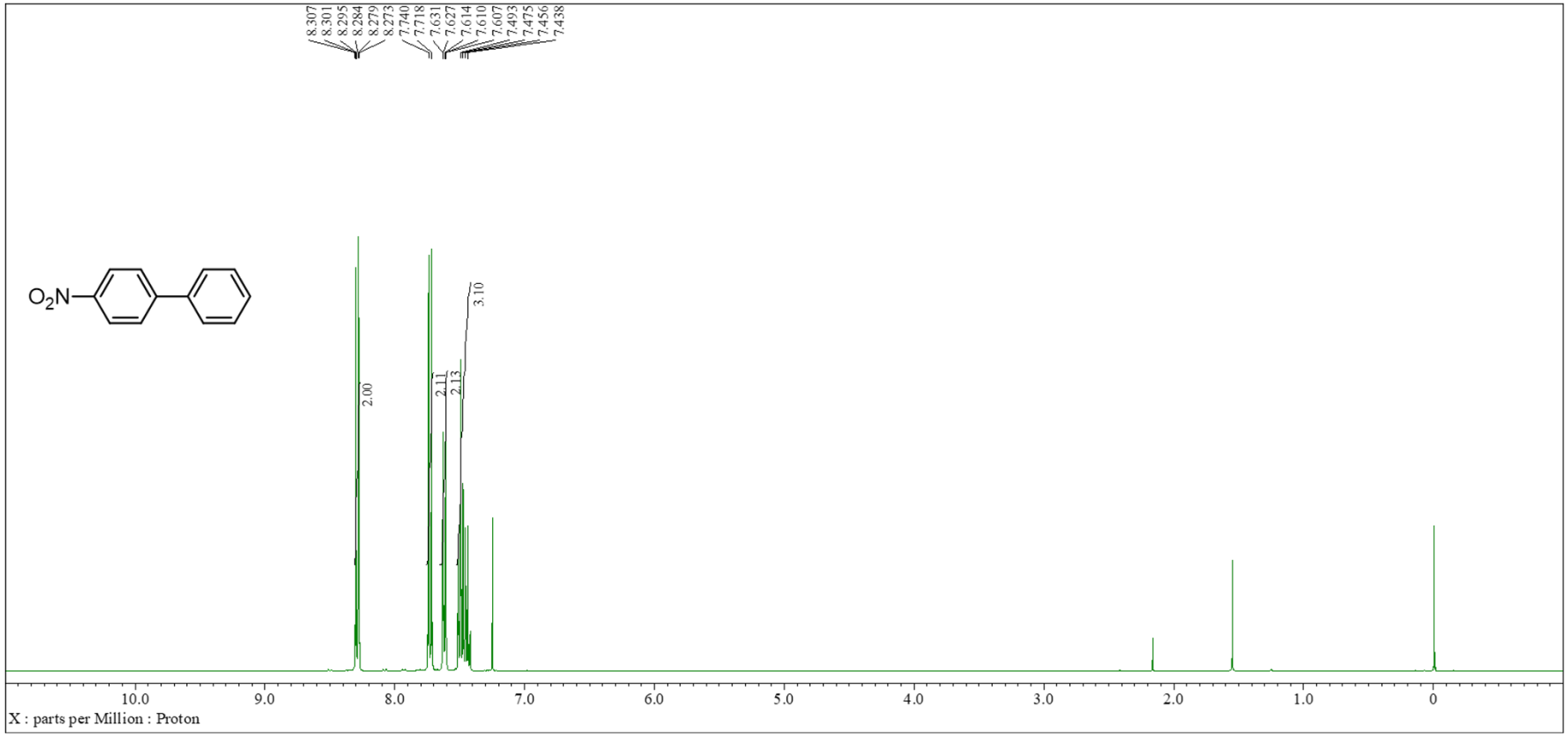
^{13}C NMR of **2b**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3.10
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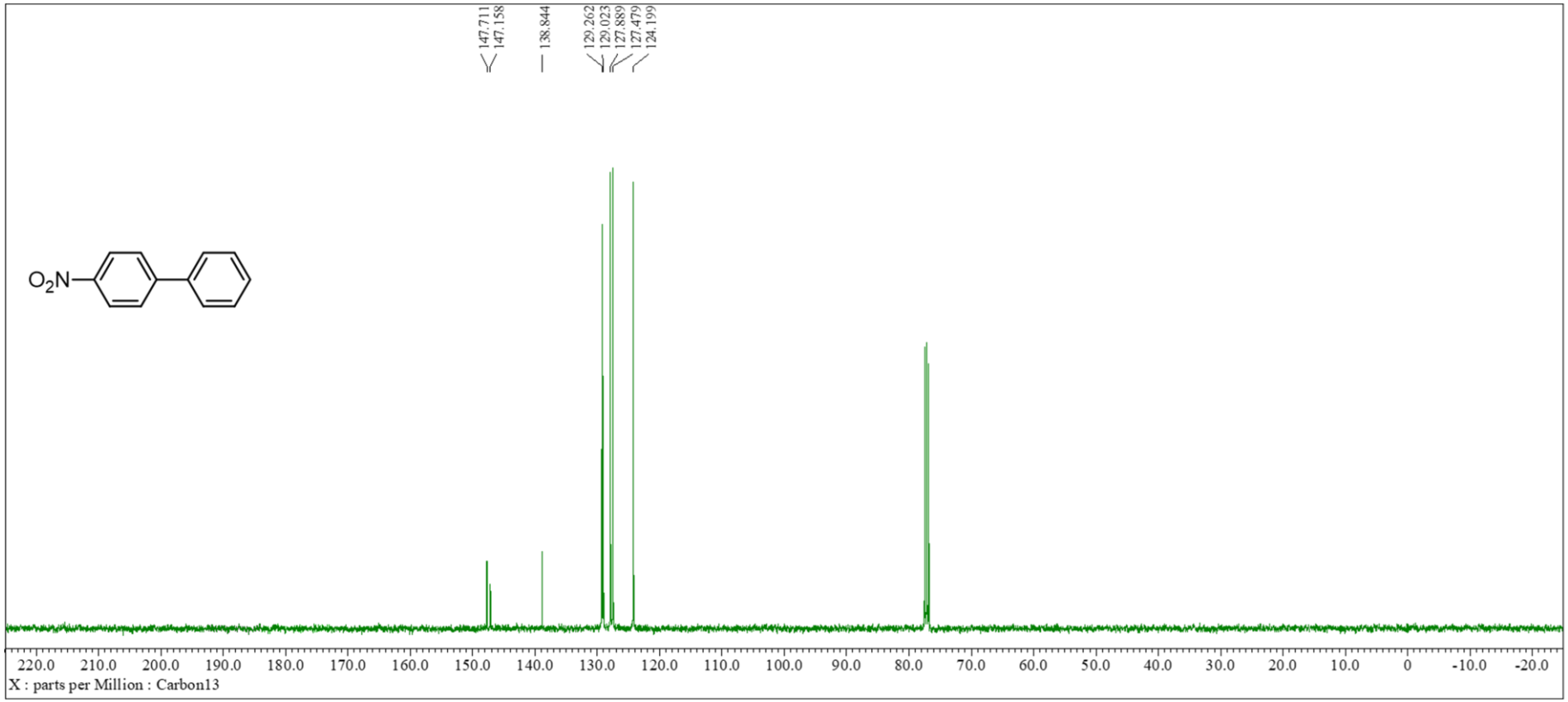
X : parts per Million : Proton

^{1}H NMR of **2c**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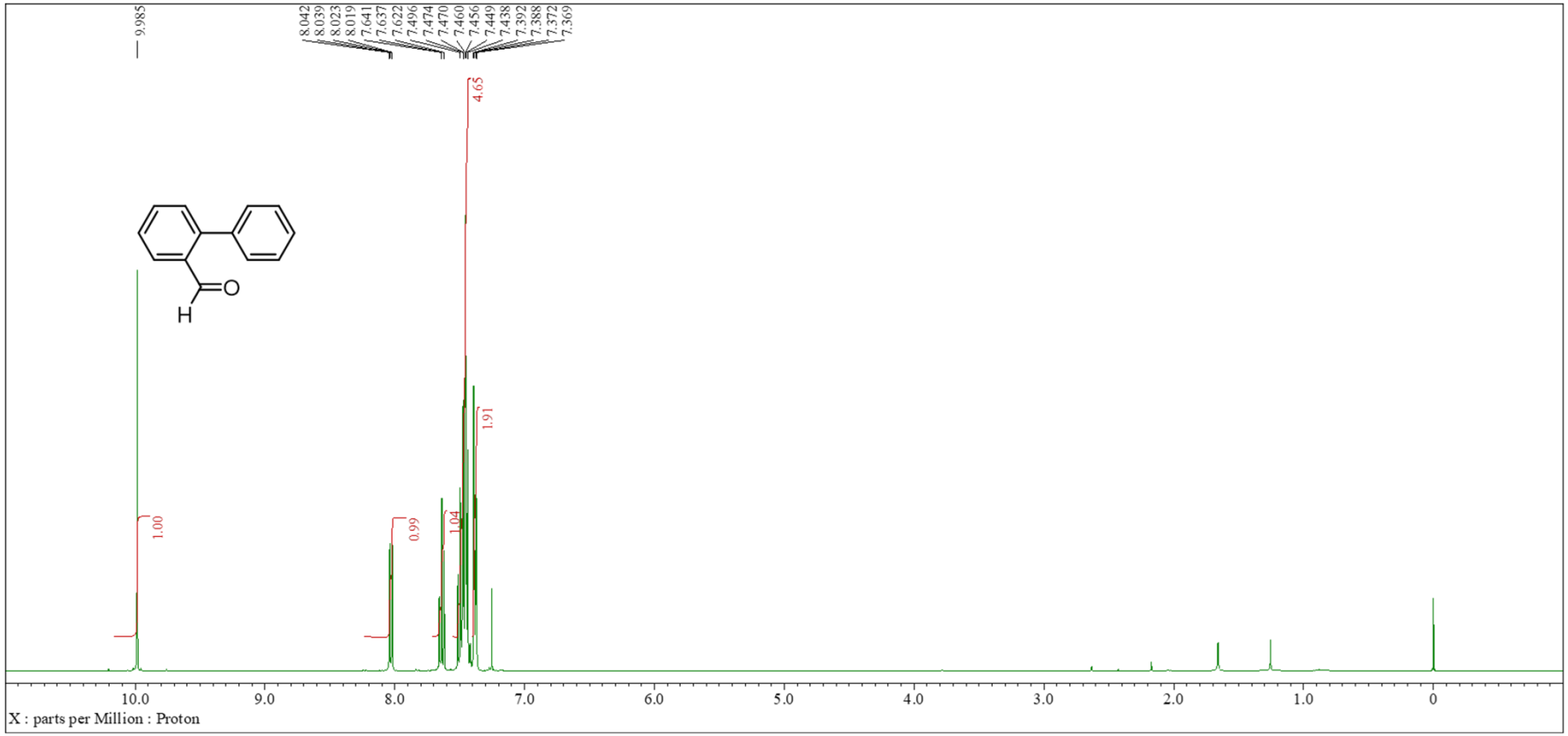
X : parts per Million : Carbon13

^{13}C NMR of **2c**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0.99
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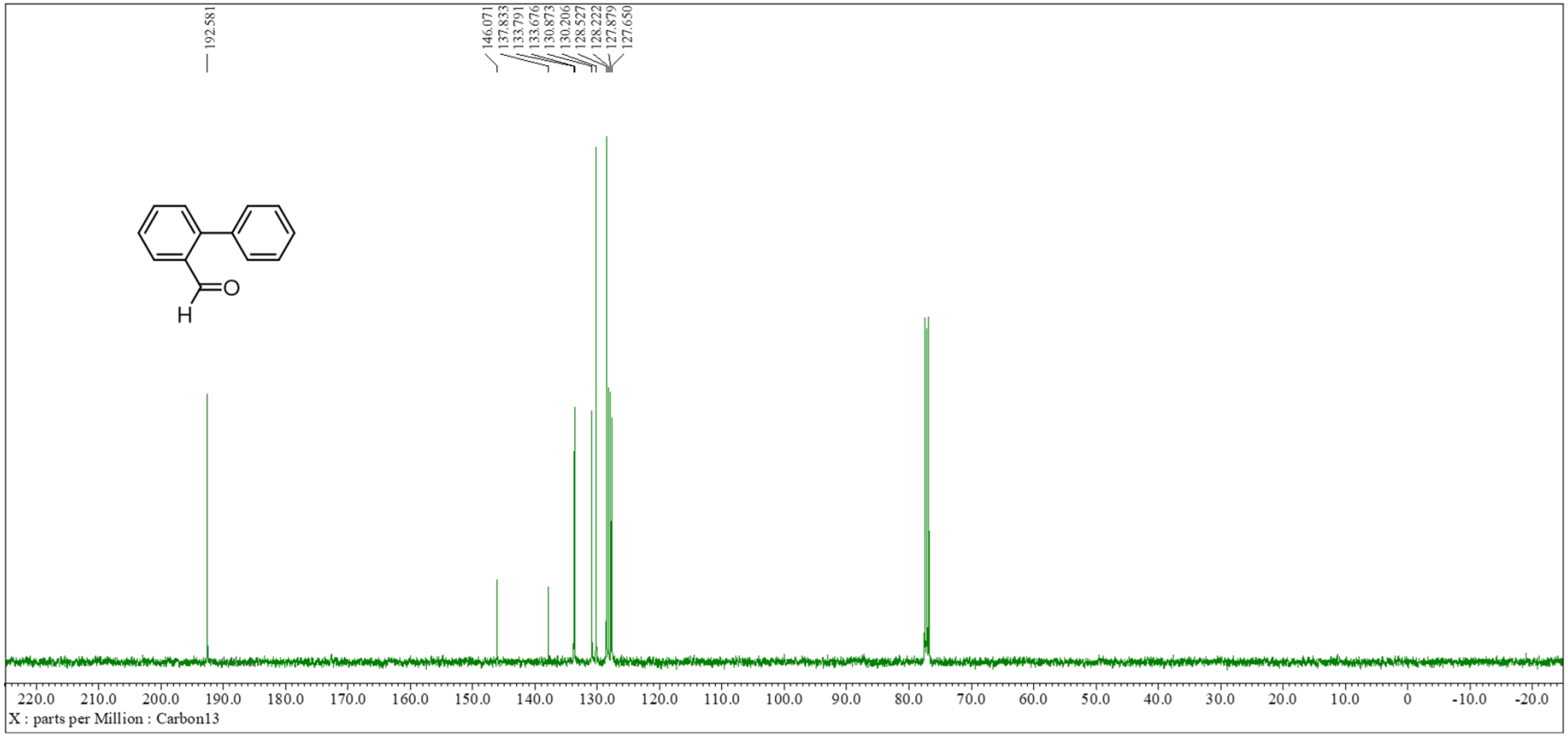
^{1}H NMR of **2d**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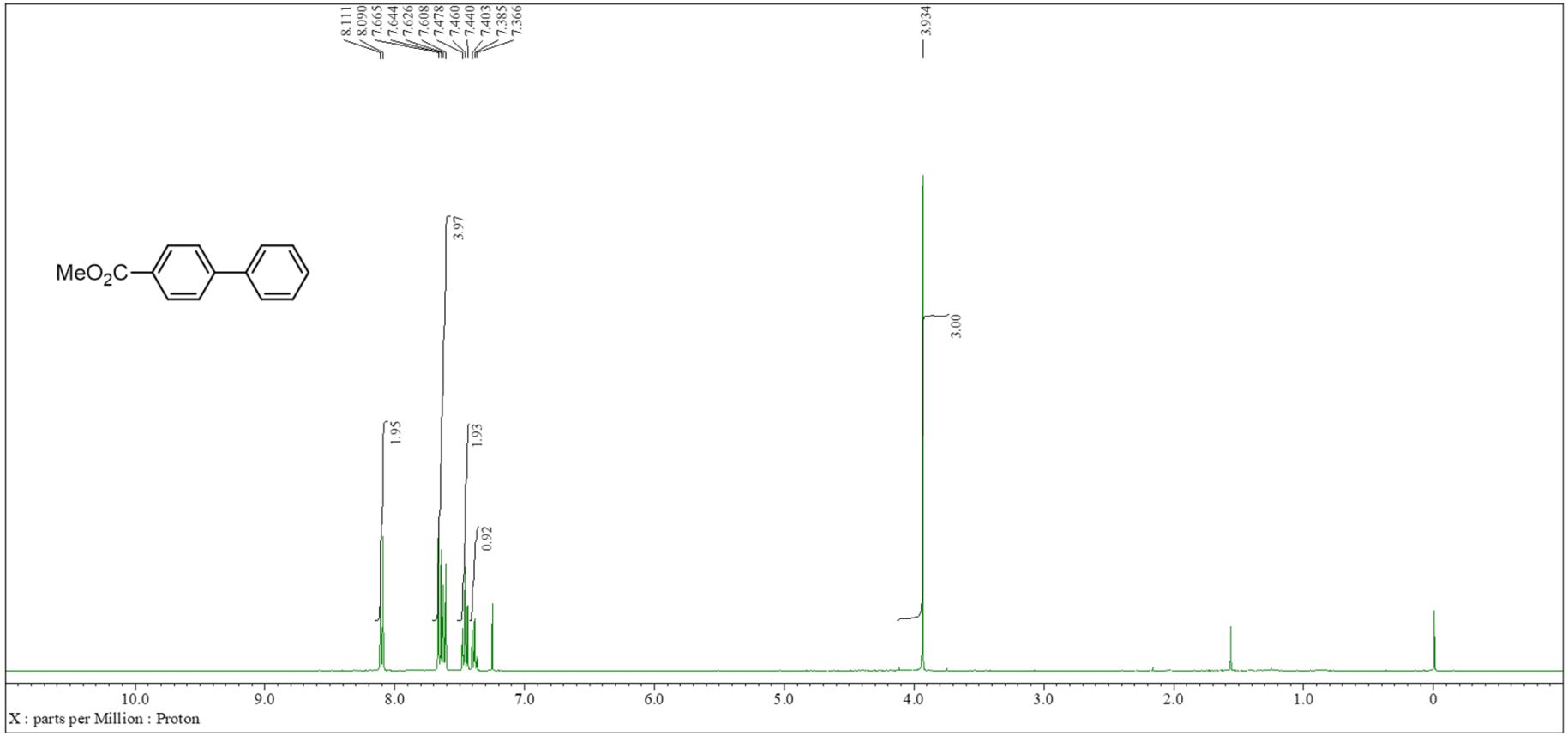
^{13}C NMR of **2d**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0.92
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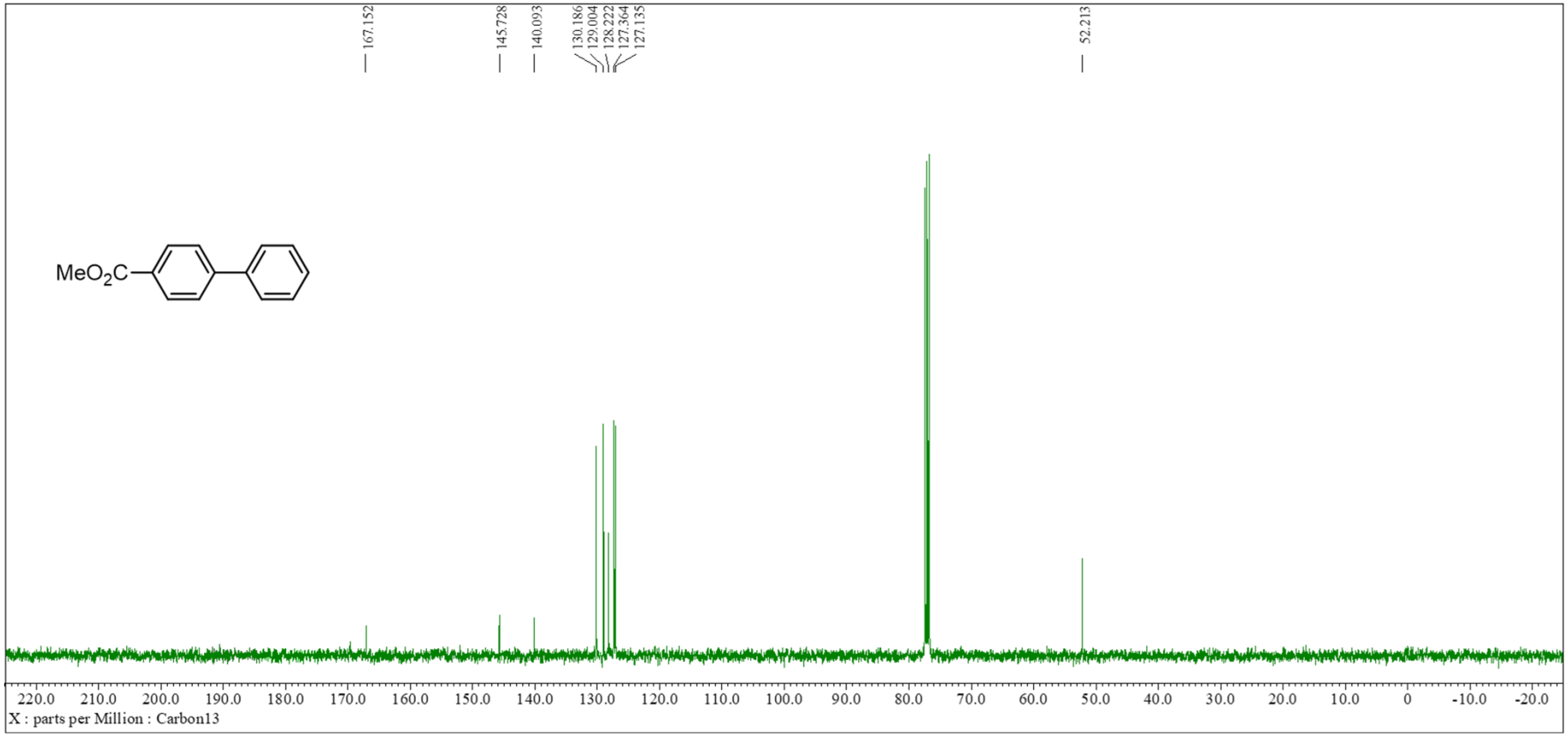
^{1}H NMR of **2e**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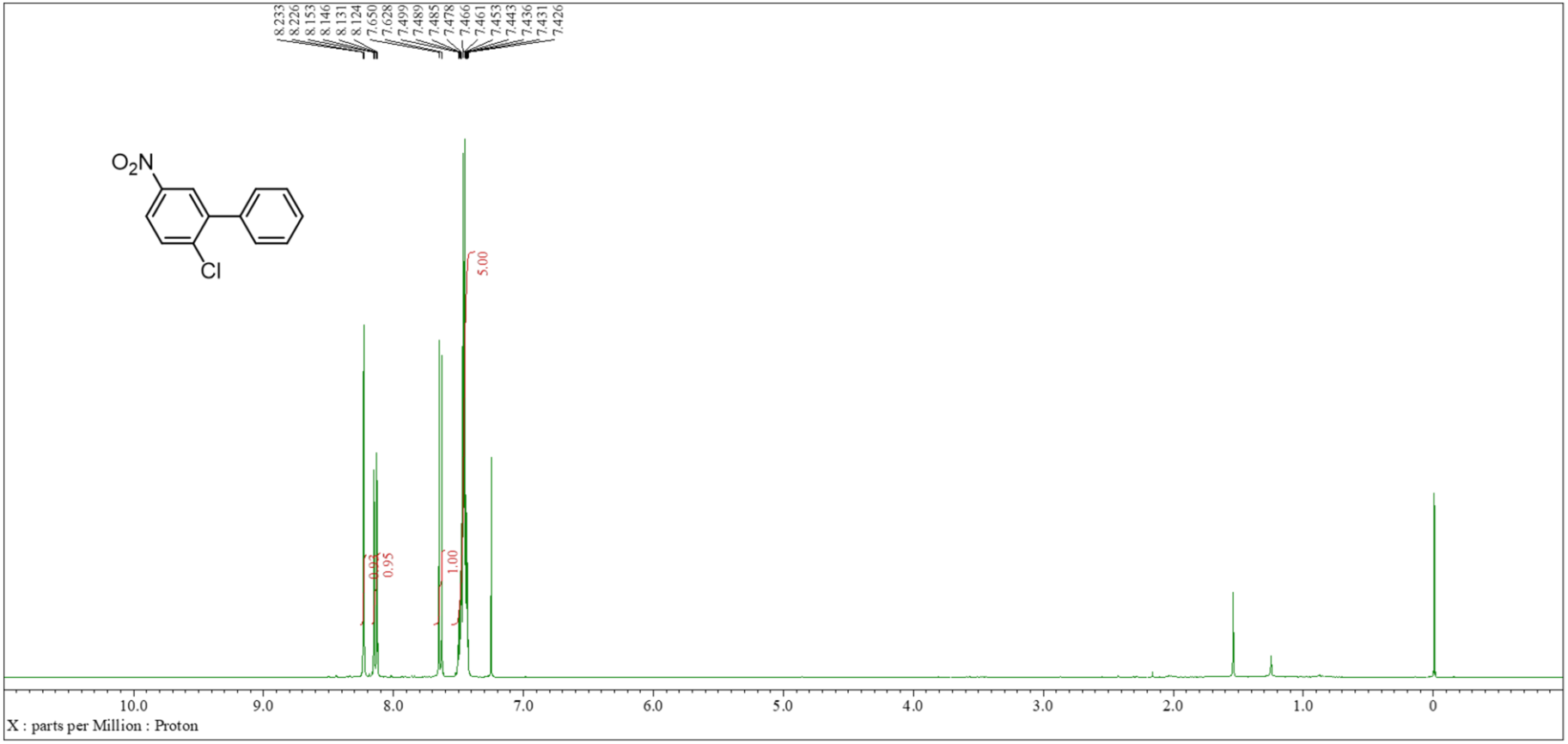
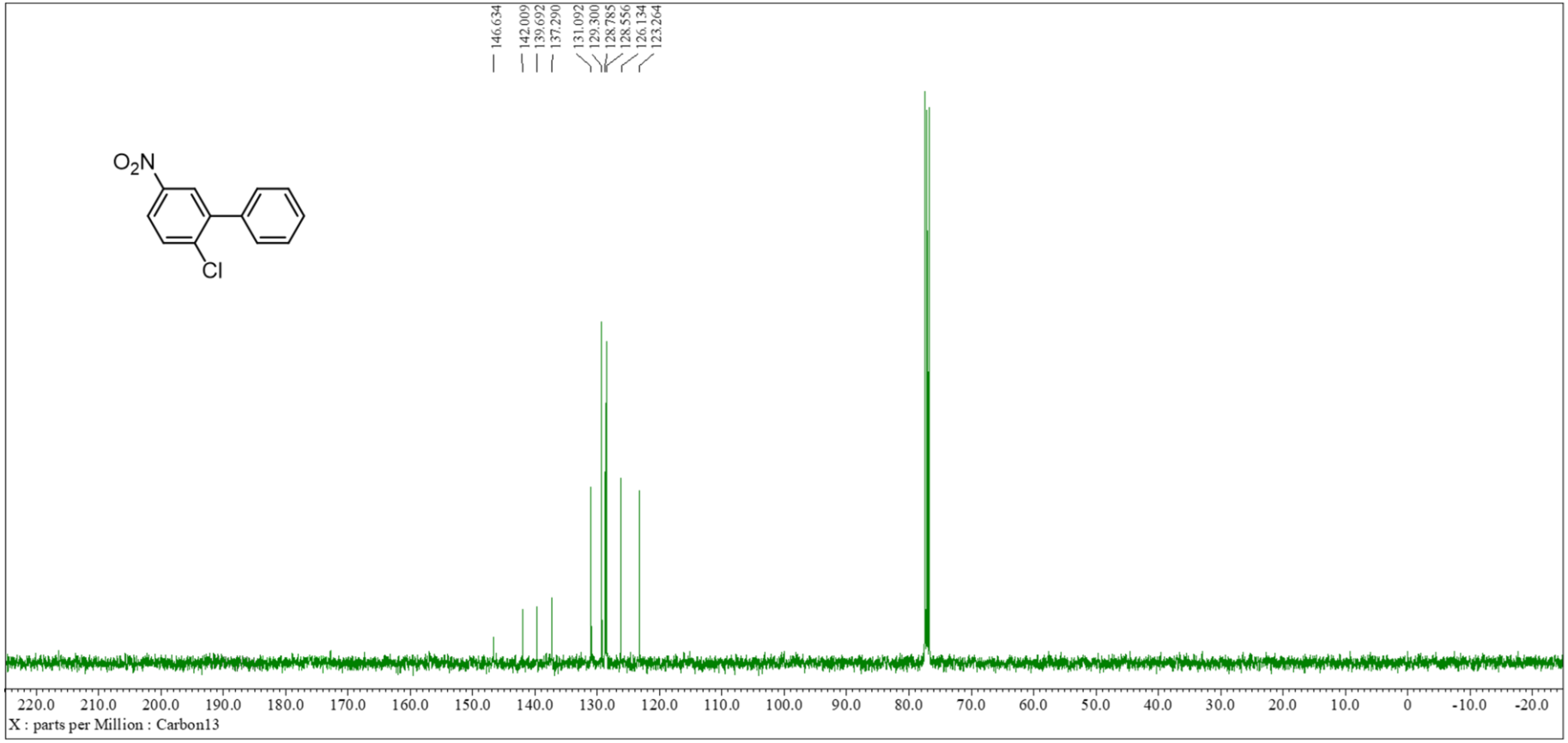
129.004
128.222
127.364
127.135
52.213
MeO2C
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

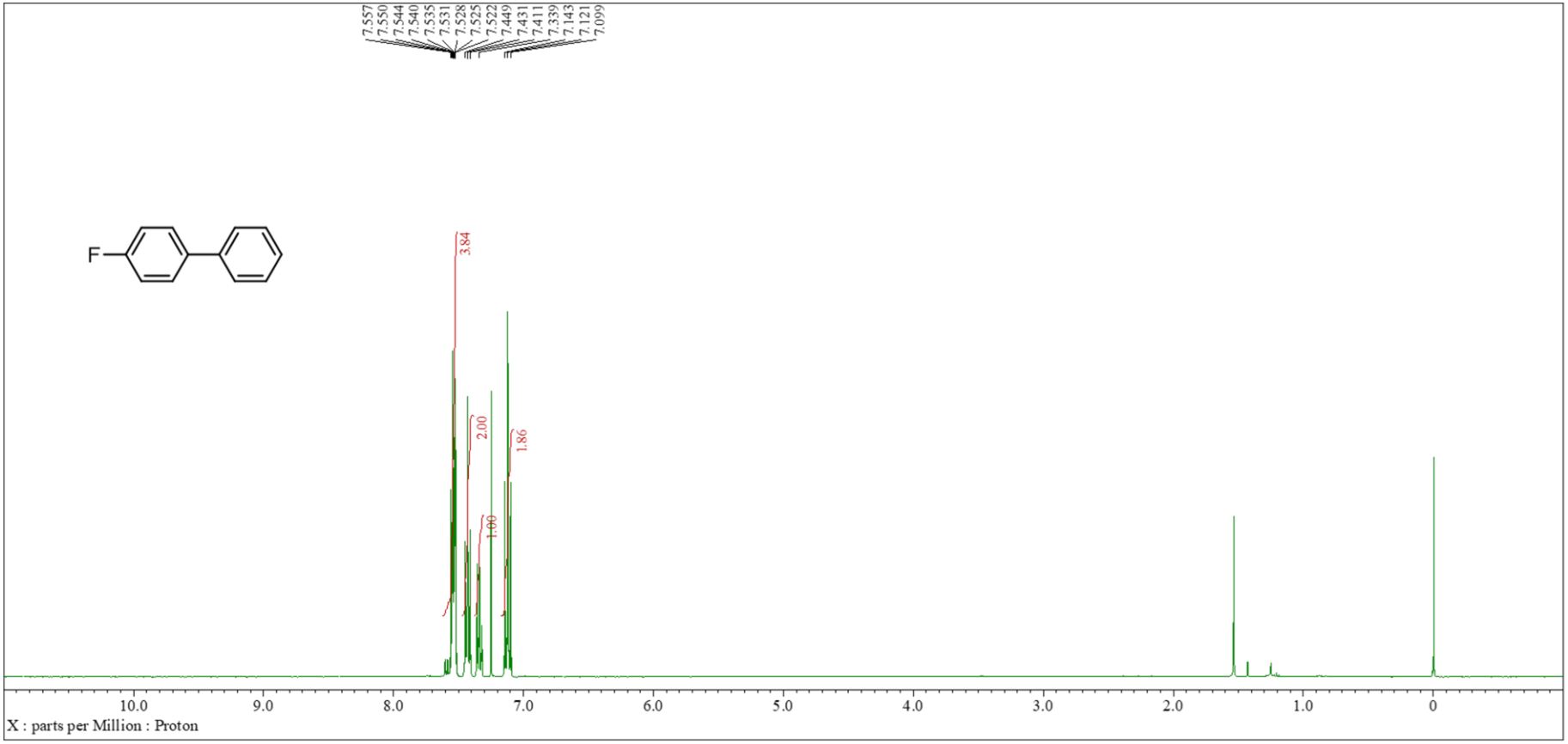
^{13}C NMR of **2e**


8.233
8.226
8.153
8.146
8.131
8.124
7.650
7.628
7.499
7.489
7.485
7.478
7.466
7.461
7.453
7.443
7.436
7.431
7.426
O2N
Cl
5.00
0.93
0.95
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

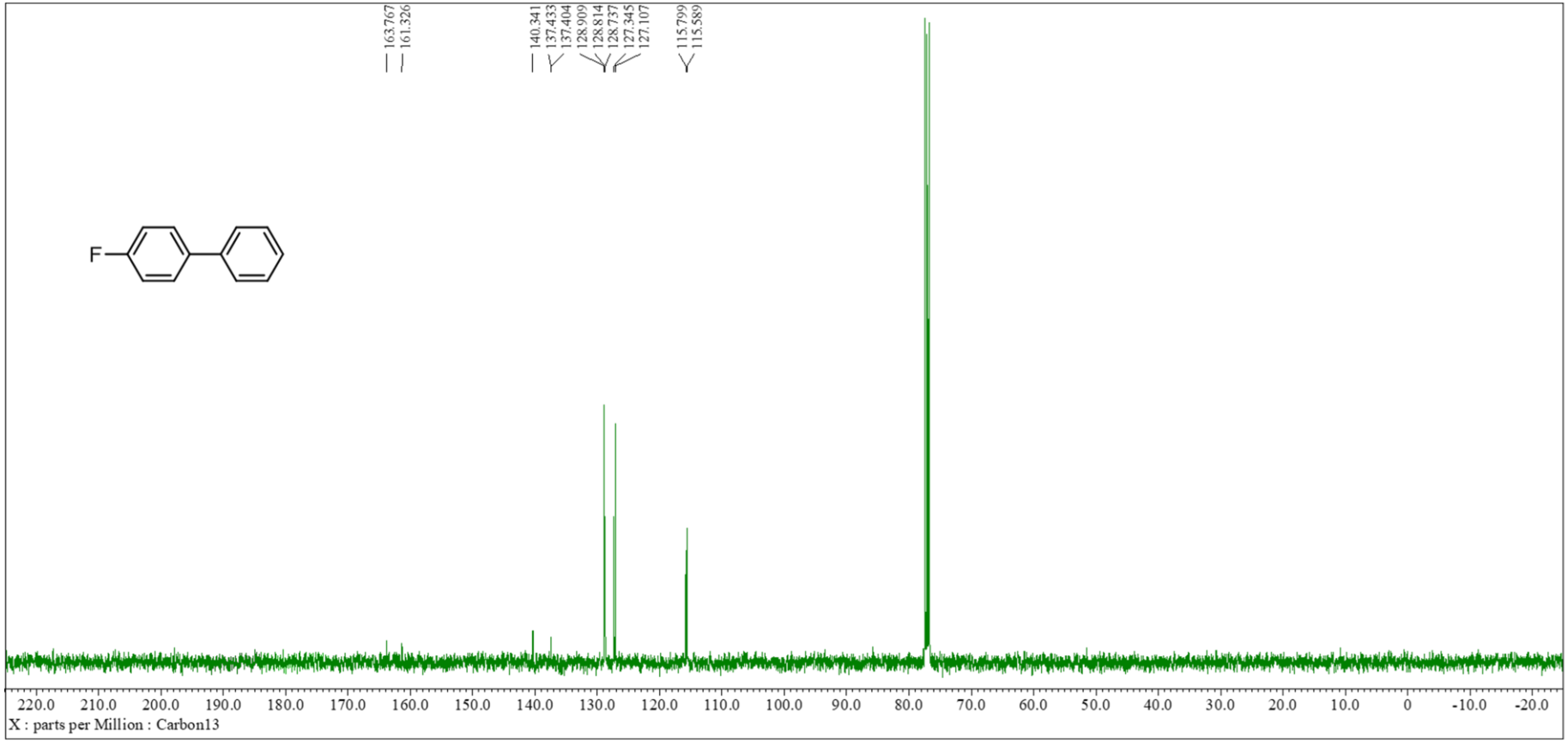
^{1}H NMR of **2f**


146.634
142.009
139.692
137.290
131.092
129.300
128.785
128.556
126.134
123.264
O2N
Cl
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

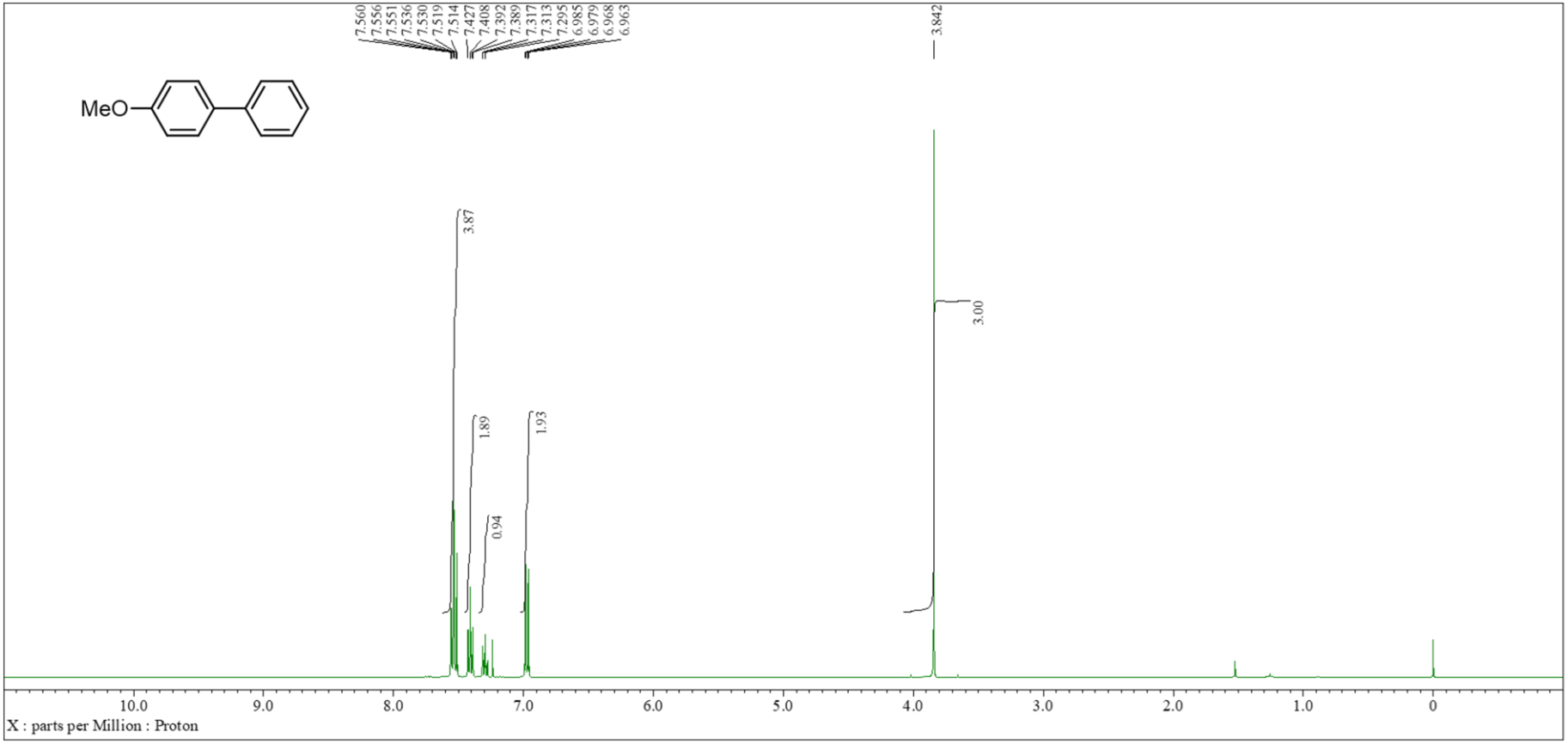
^{13}C NMR of **2f**


7.557
7.550
7.544
7.540
7.535
7.531
7.528
7.525
7.522
7.449
7.431
7.411
7.339
7.143
7.121
7.099
F
3.84
2.00
1.00
1.86
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

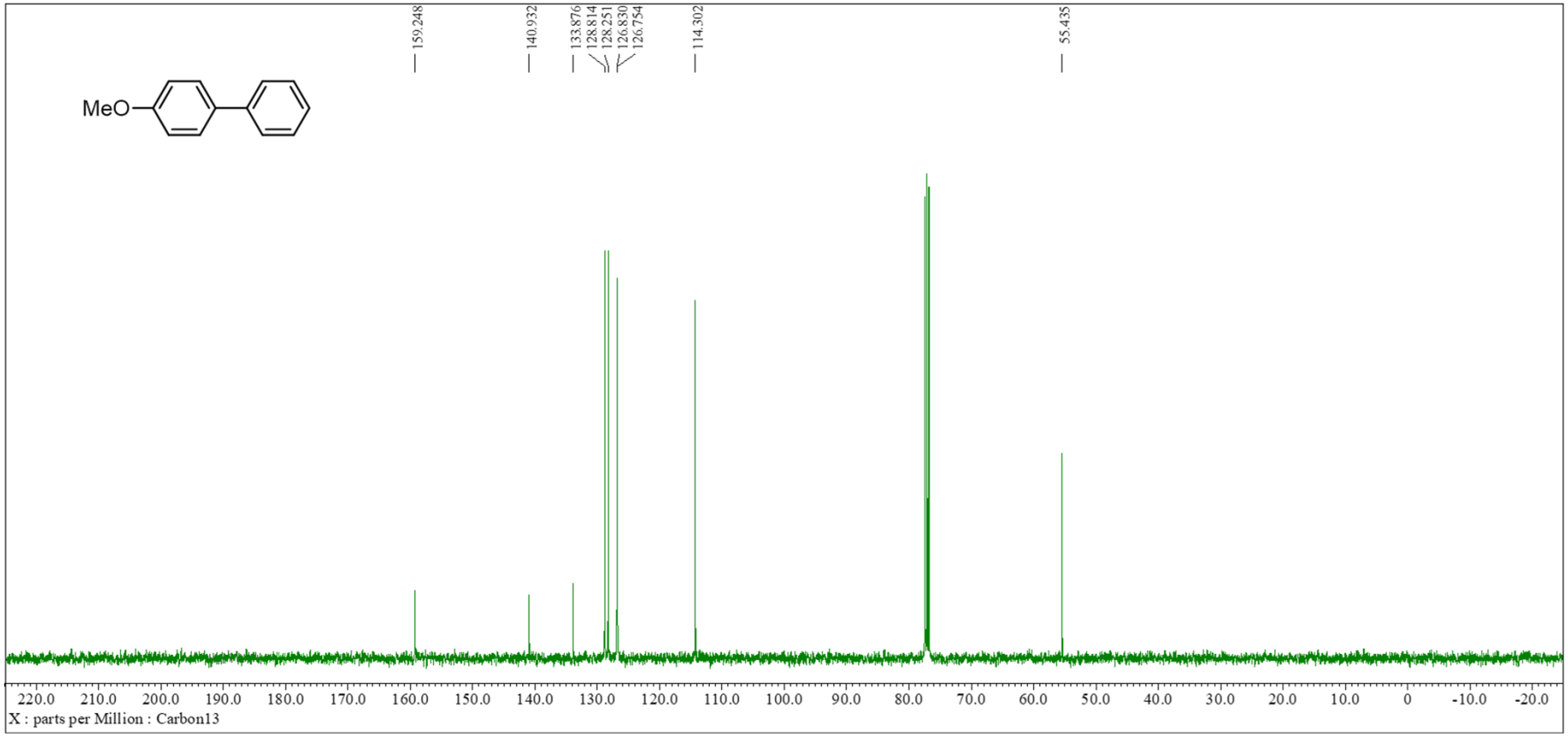
^{1}H NMR of **2g**


163.767
161.326
140.341
137.433
137.404
128.909
128.814
128.737
127.345
127.107
115.799
115.589
F
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

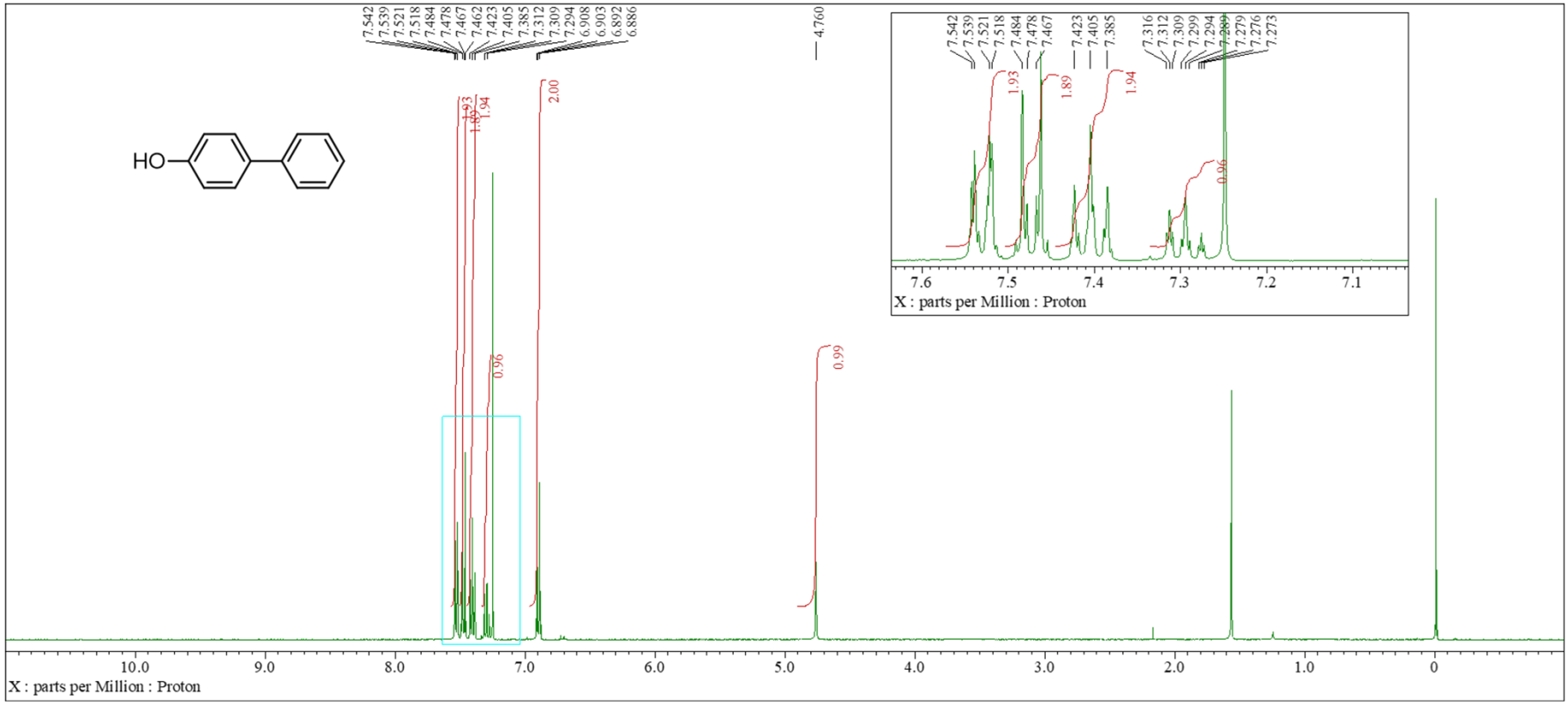
^{13}C NMR of **2g**


7.560
7.556
7.551
7.536
7.530
7.519
7.514
7.427
7.408
7.392
7.389
7.317
7.313
7.295
6.985
6.979
6.968
6.963
3.842
MeO
3.87
1.89
0.94
1.93
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

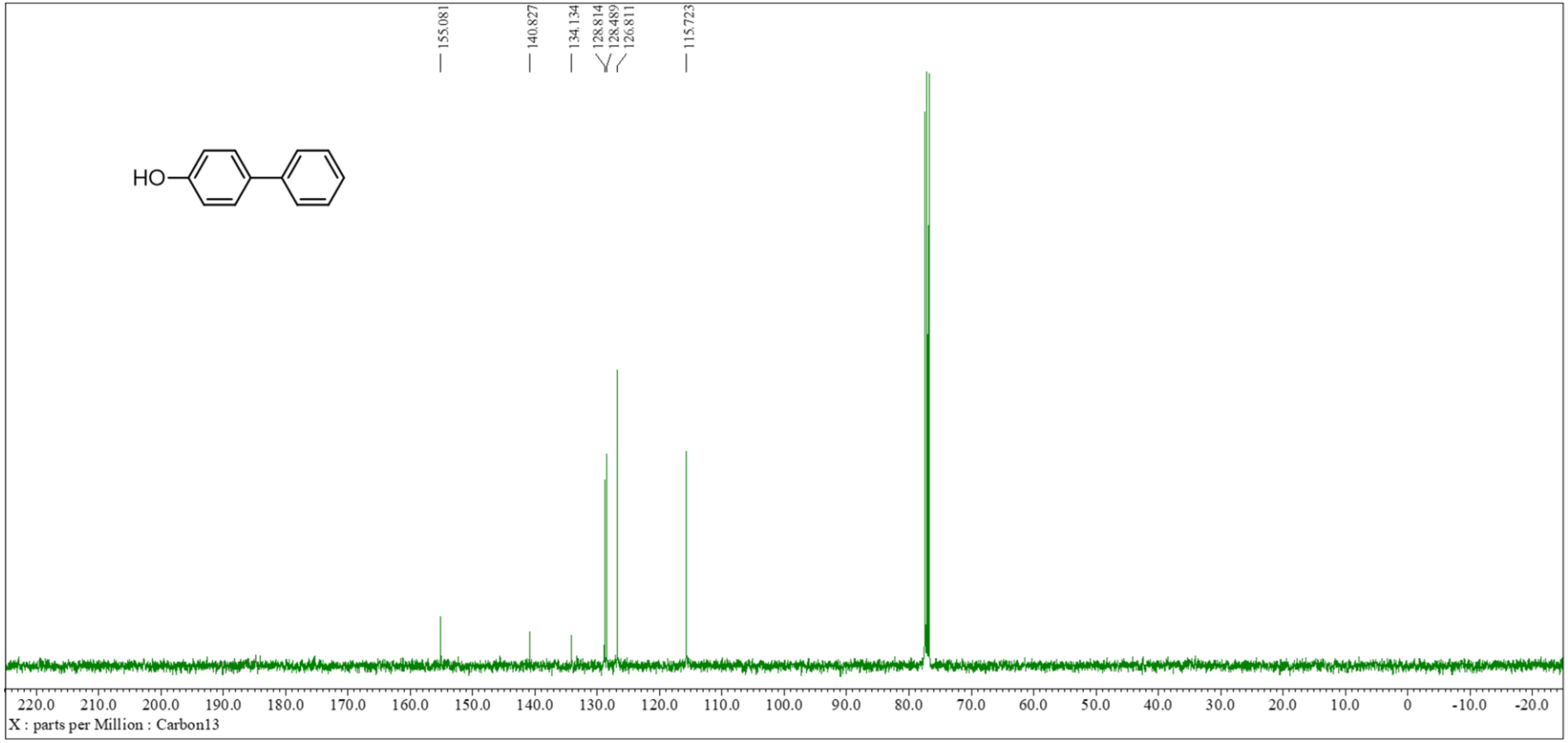
^{1}H NMR of **2h**


159.248
140.932
133.876
128.814
128.251
126.830
126.754
114.302
55.435
MeO
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

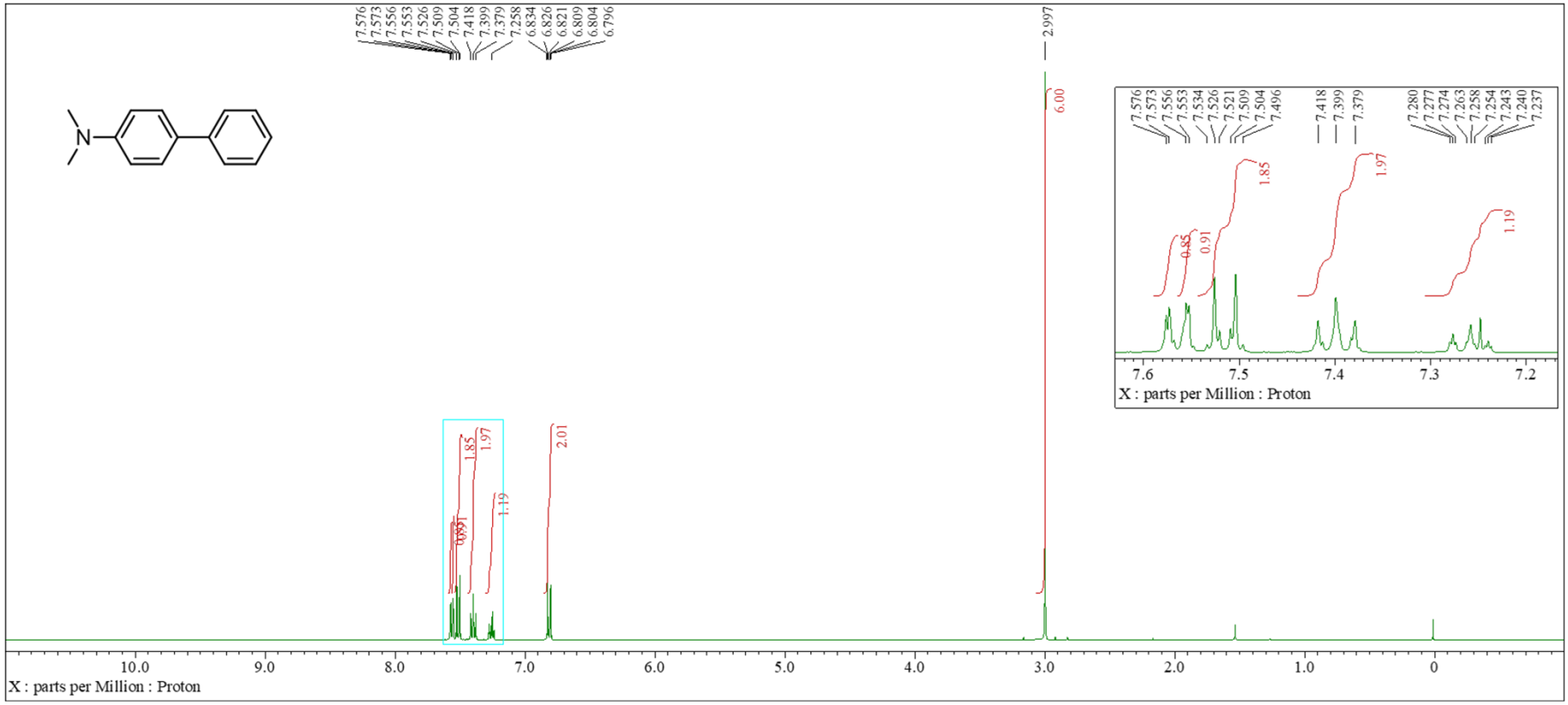
^{13}C NMR of **2h**


HO
7.542
7.539
7.521
7.518
7.484
7.478
7.467
7.462
7.423
7.405
7.385
7.312
7.309
7.294
6.908
6.903
6.892
6.886
4.760
1.93
1.94
2.00
0.96
0.99
7.316
7.299
7.289
7.279
7.276
7.273
1.89
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6
7.5
7.4
7.3
7.2
7.1

^{1}H NMR of **2i**

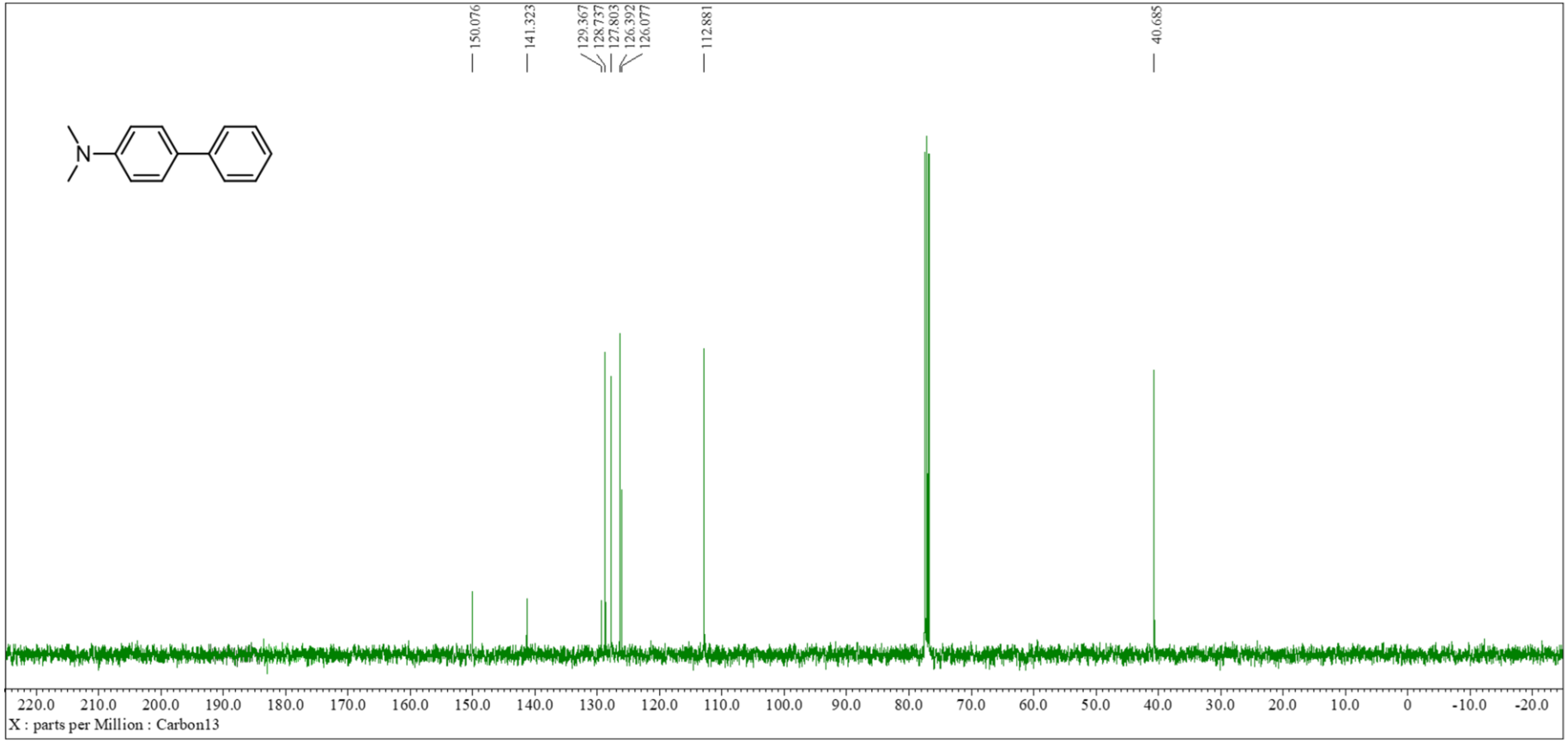

155.081
140.827
134.134
128.814
128.489
126.811
115.723
HO
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

^{13}C NMR of **2i**

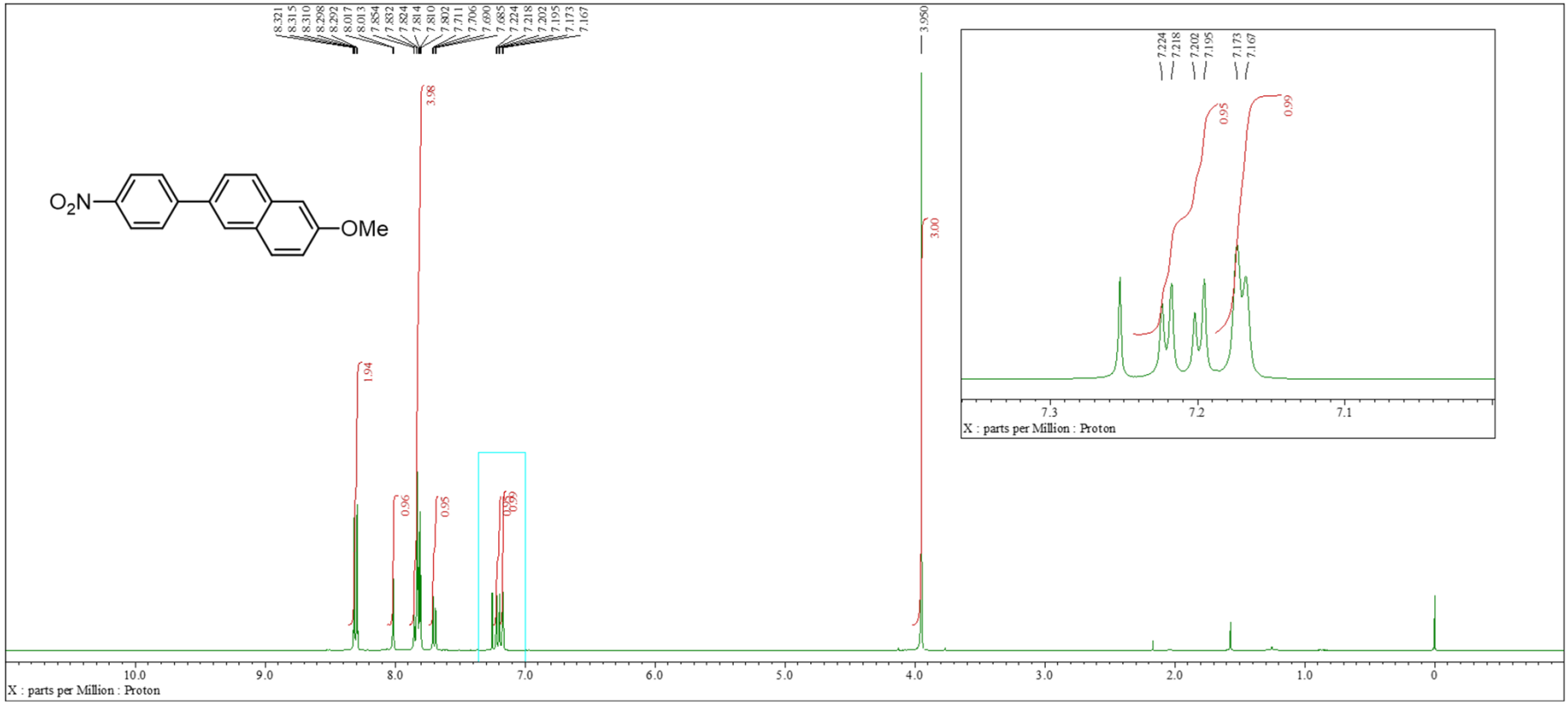


7.576
7.573
7.556
7.553
7.526
7.509
7.504
7.418
7.399
7.379
7.258
6.834
6.826
6.821
6.809
6.804
6.796
2.997
6.00
2.01
1.85
1.97
1.19
0.91
0.85
7.576
7.573
7.556
7.553
7.534
7.526
7.521
7.509
7.504
7.496
7.418
7.399
7.379
7.280
7.277
7.274
7.263
7.258
7.254
7.243
7.240
7.237
7.6
7.5
7.4
7.3
7.2
X : parts per Million : Proton
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

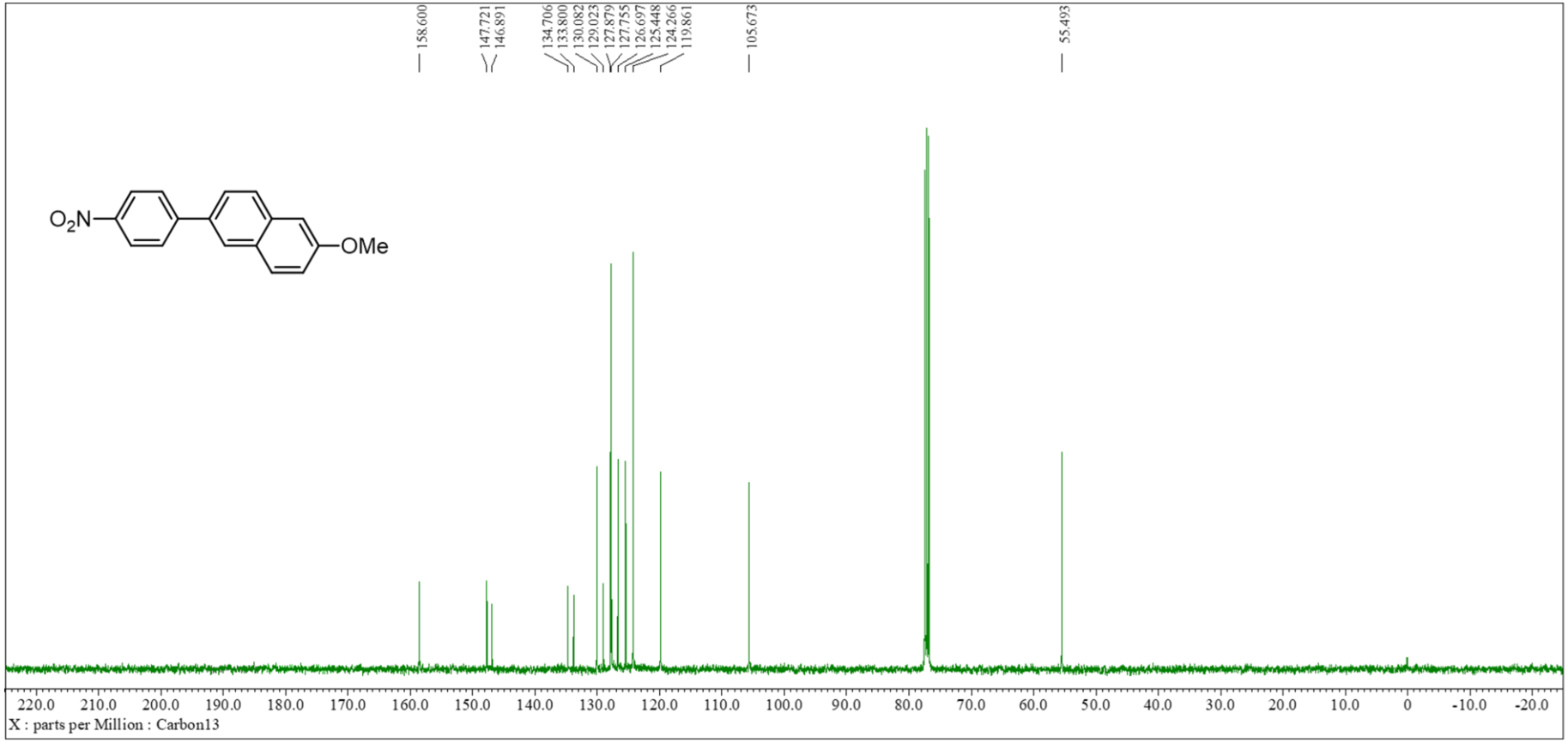
^{1}H NMR of **2j**


150.076
141.323
129.367
128.737
127.803
126.392
126.077
112.881
40.685
N
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

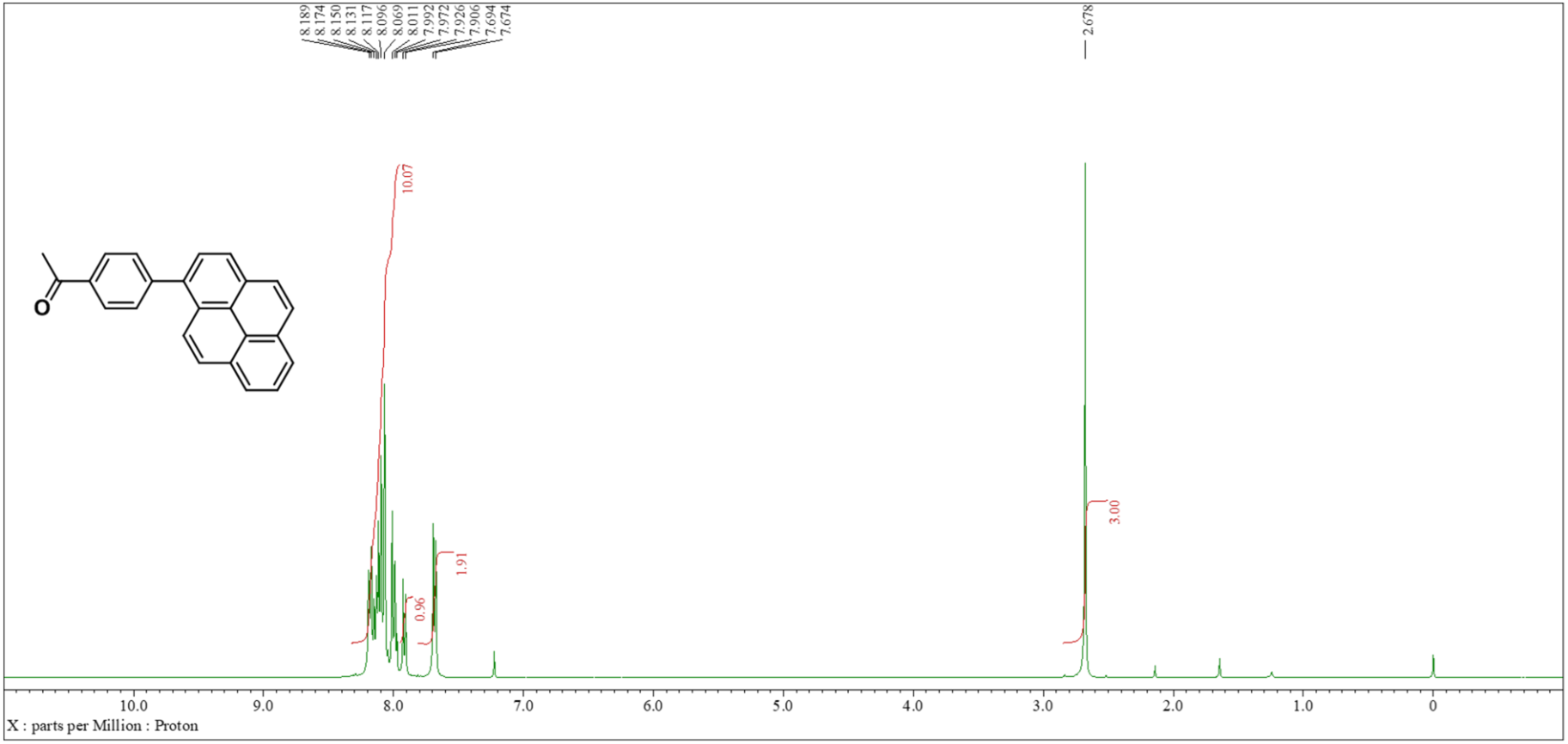
^{13}C NMR of **2j**


8.321
8.315
8.310
8.298
8.292
8.017
8.013
7.854
7.832
7.824
7.814
7.810
7.802
7.711
7.706
7.690
7.685
7.224
7.218
7.202
7.195
7.173
7.167
3.950
3.98
3.00
1.94
0.96
0.95
0.98
0.99
O2N
OMe
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton
7.224
7.218
7.202
7.195
7.173
7.167
0.95
0.99
7.3
7.2
7.1
X : parts per Million : Proton

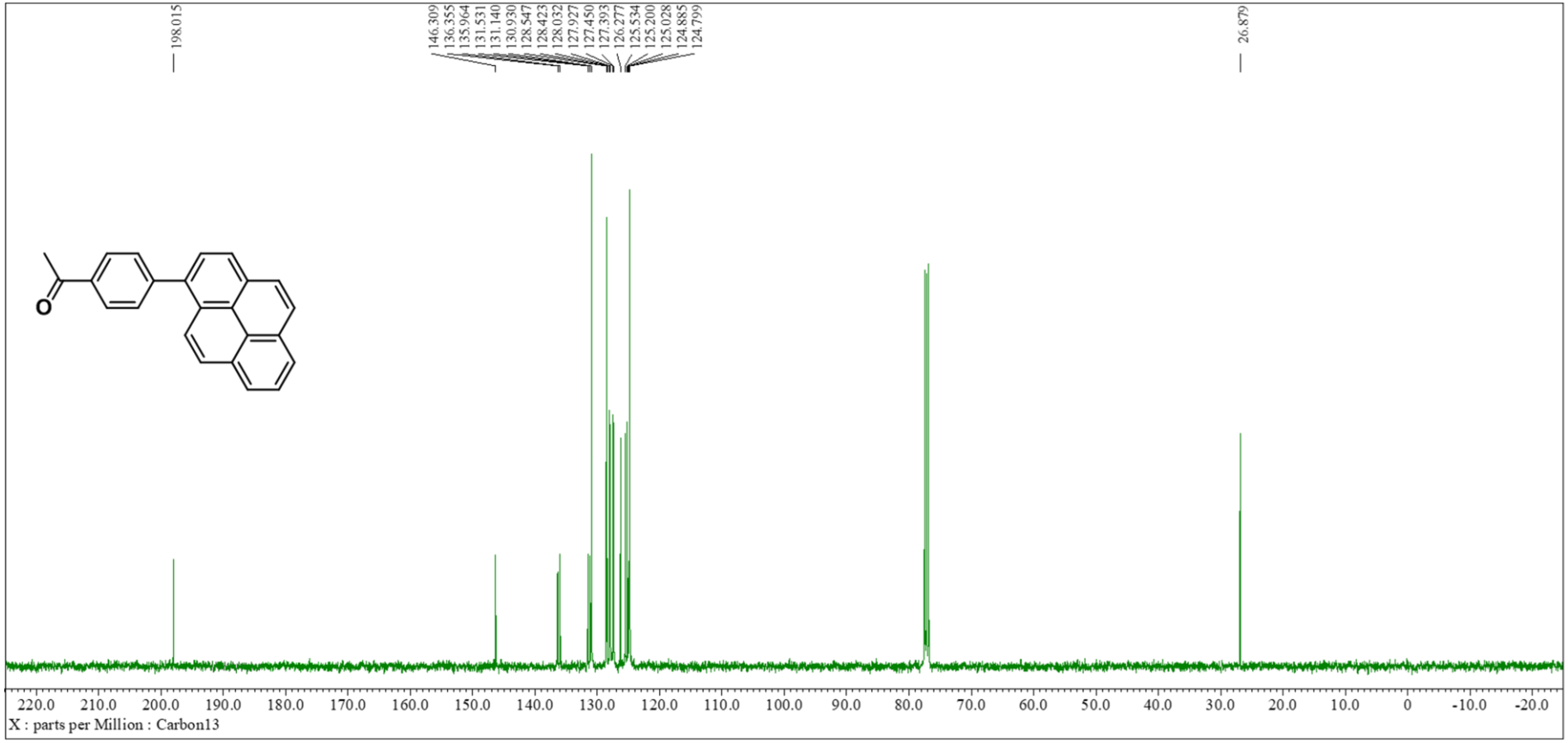
^{1}H NMR of **2k**


158.600
147.721
146.891
134.706
133.800
130.082
129.023
127.879
127.755
126.697
125.448
124.266
119.861
105.673
55.493
O2N
OMe
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

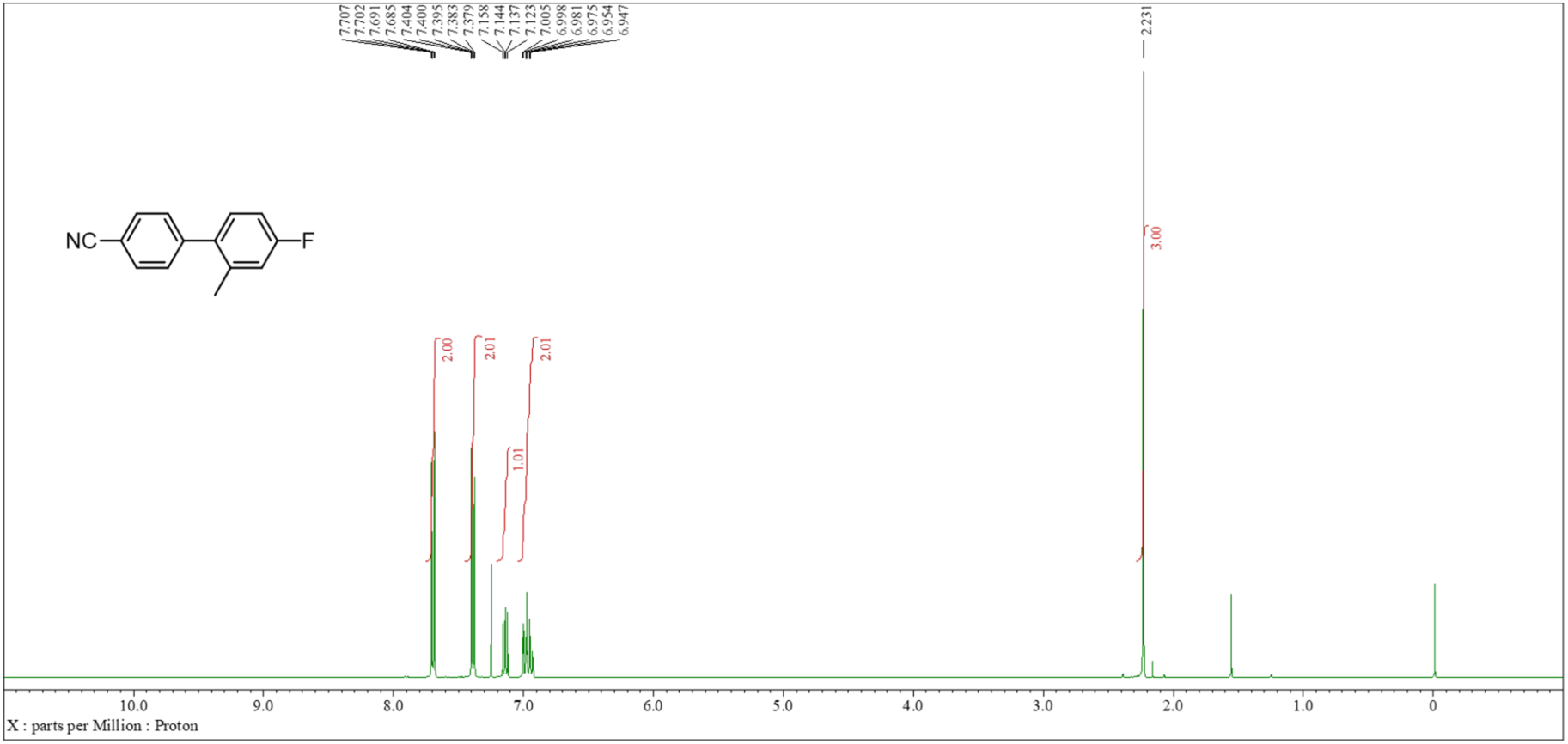
^{13}C NMR of **2k**


8.189
8.174
8.150
8.131
8.117
8.096
8.069
8.011
7.992
7.972
7.926
7.906
7.694
7.674
2.678
10.07
1.91
0.96
3.00
O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

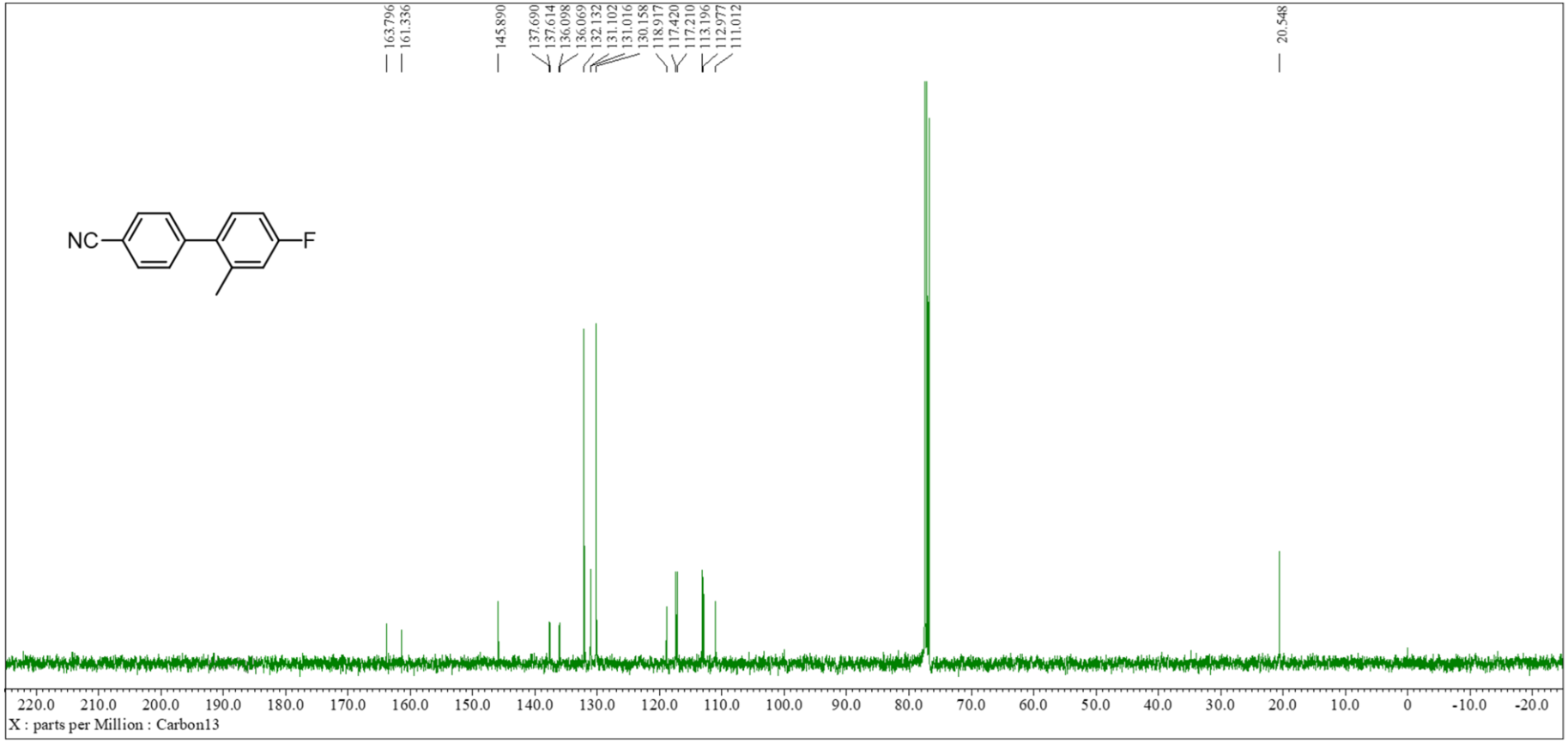
^{1}H NMR of **2l**


198.015
146.309
136.355
135.964
131.531
131.140
130.930
128.547
128.423
128.032
127.927
127.450
127.393
126.277
125.534
125.200
125.028
124.885
124.799
26.879
O
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

^{13}C NMR of **2l**


7.707
7.702
7.691
7.685
7.404
7.400
7.395
7.383
7.379
7.158
7.144
7.137
7.123
7.005
6.998
6.981
6.975
6.954
6.947
2.231
NC
F
2.00
2.01
1.01
2.01
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

^{1}H NMR of **2m**


163.796
161.336
145.890
137.690
137.614
136.098
136.069
132.132
131.102
131.016
130.158
118.917
117.420
117.210
113.196
112.977
111.012
20.548
NC
F
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
X : parts per Million : Carbon13

^{13}C NMR of **2m**