Supporting Information

Molecular Pd(II) Complex Incorporated into MOF as a Highly Active Single-Site Heterogeneous Catalyst for C–Cl Bond Activation

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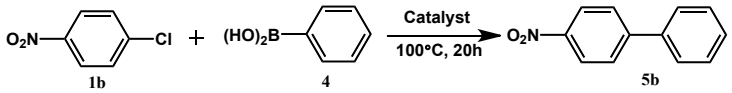
1. Catalyst characterization and catalytic reaction

Table S1. Suzuki–Miyaura coupling of 4-nitro-1-chlorobenzene with Pd(II) doped UiO-67[a]



1b 4 5b

Entry	Cat (mol %)	Base (equiv)	Solvent	Yield (%)[b]
1	Pd doped UiO-67	K_2CO_3(3)	DMF	4
2	Pd doped UiO-67	K_2CO_3(3)	Dioxane	15
3	Pd doped UiO-67	K_2CO_3(3)	Methanol (MeOH)	0
4	Pd doped UiO-67	K_2CO_3(3)	Ethanol (EtOH)	36
5	Pd doped UiO-67	K_2CO_3(3)	DMF/MeOH = 20:1	70
6	Pd doped UiO-67	K_2CO_3(3)	DMF/EtOH = 20:1	87
7	Pd doped UiO-67	K_3PO_4(3)	DMF/EtOH = 20:1	38
8	Pd doped UiO-67	Cs_2CO_3(3)	DMF/EtOH = 20:1	30
9	**Pd doped UiO-67**	**KOH**	**DMF/EtOH = 20:1**	**99**
10	UiO-67	KOH	DMF/EtOH = 20:1	--
11	Me_2L	KOH	DMF/EtOH = 20:1	50
12	$PdCl_2(CH_3CN)_2$	KOH	DMF/EtOH = 20:1	--
13	$PdCl_2(PPh_3)_2$	KOH	DMF/EtOH = 20:1	<3%

[a] Reaction conditions: 4-nitro-1-chlorobenzene (0.5 mmol), phenylboronic acid (0.75 mmol), base (1.5 mmol), solvent (5 mL), and Pd(II) doped UiO-67 (0.46 mol% Pd), 100 °C, 20 h, under N_2. [b] Yields were determined by GC-MS analysis.

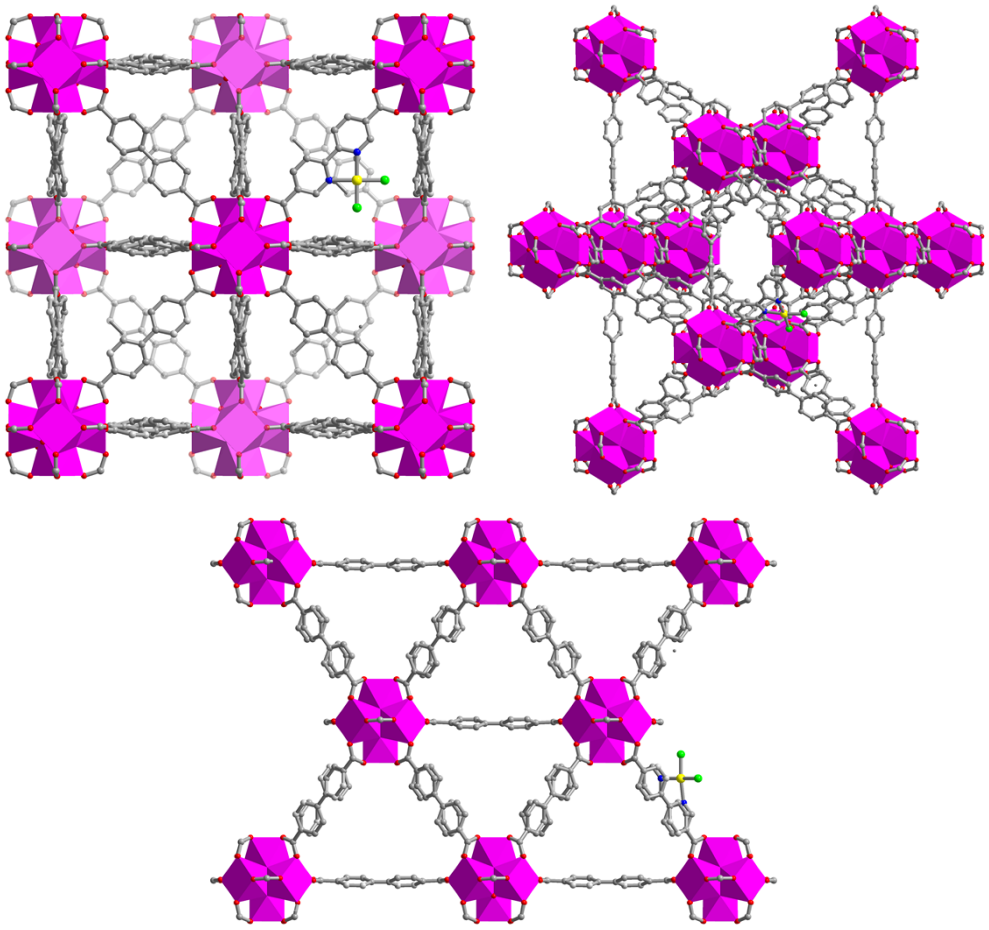


Figure S1. Structure of Pd(II) doped UiO-67 viewed from different directions. The molar ratio of (mol L_1/(mol L_1 + mol L_2)) of the displayed structural model is ca. 4.17 mol % (comparable to 4.0 mol % in the actual MOF as measured by AAS).

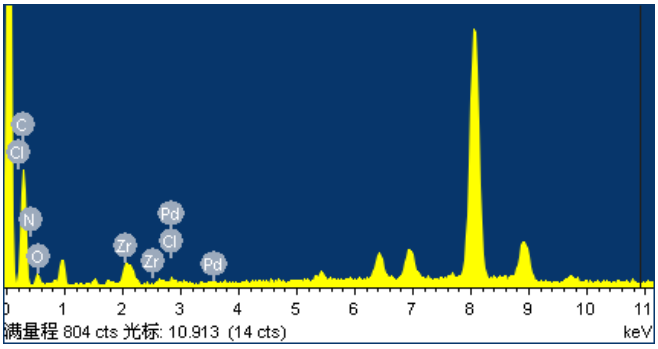


Figure S2. The EDX pattern of Pd(II) doped UiO-67, the unlabeled peaks belong to the copper support.

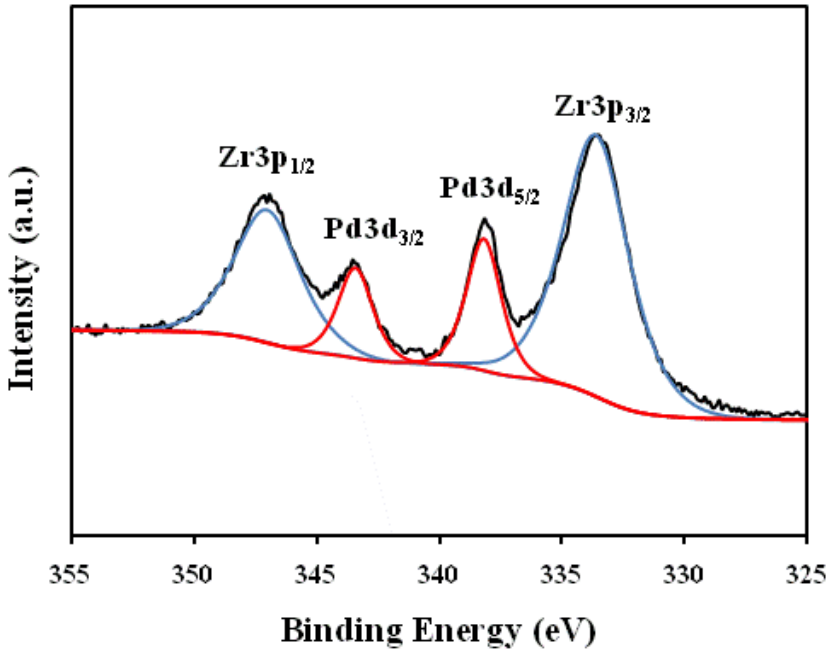


Figure S3. XPS spectra (Pd 3d level) for the recovered catalyst.

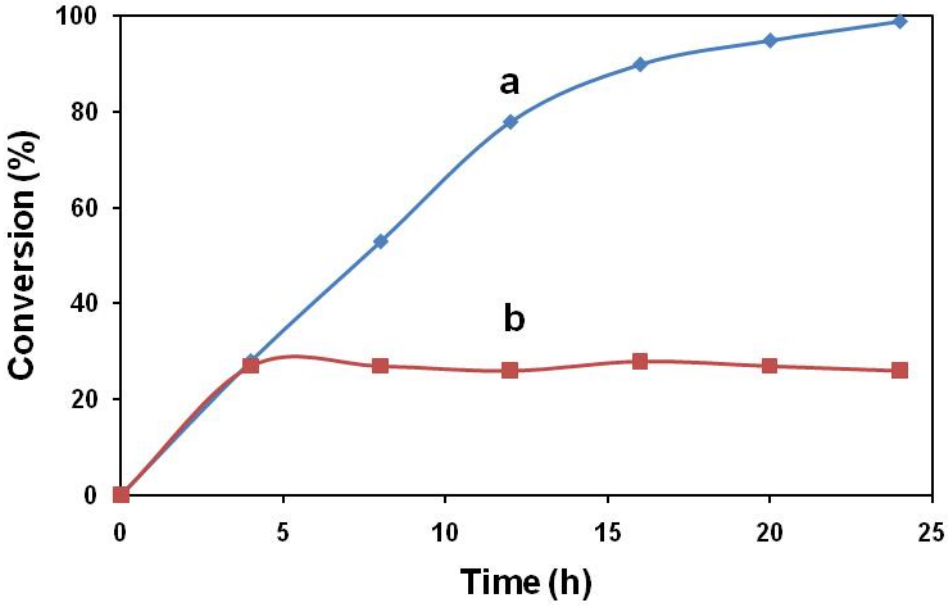
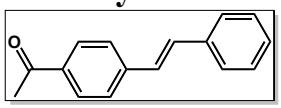


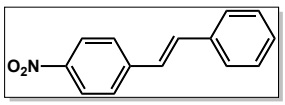
Figure S4. Activity profile for the cross-coupling of 4-chloroacetophenone with phenylethylene. Reaction conditions: 4-chloroacetophenone (0.5 mmol), phenylethylene (0.75 mmol), K_2CO_3 (3 equiv), tetrabutylammonium bromide (0.3 mmol), Pd(II) doped UiO-67 (0.46 mol% Pd), DMF (5 mL), 100 ºC. (a) With catalyst, and (b) with filtrate.

2. Analytical data for compounds



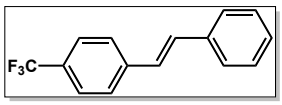
(E)-4-Acetylstilbene (3a)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.86 (d, J=8.4 Hz, 2H), 7.49 (d, J=8.4 Hz, 2H), 7.45 (d, J=7.6 Hz, 2H), 7.29 (t, J=7.4 Hz, 2H), 7.21 (t, J=7.2 Hz, 1H), 7.14 (d, J=16.4 Hz, 1H), 7.04 (d, J=16.0 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.4, 142.0, 136.7, 135.9, 131.4, 128.8, 128.7, 128.3, 127.4, 126.8, 126.5, 26.5.



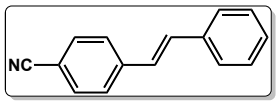
(E)-4-Nitrostilbene (3b)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.15 (d, J=8.8 Hz, 2H), 7.56 (d, J=8.8 Hz, 2H), 7.48 (d, J=7.2 Hz, 2H), 7.33 (t, J=7.4 Hz, 2H), 7.26 (t, J=7.4 Hz, 1H),7.20 (d, J=16.0 Hz, 1H), 7.07 (d, J=16.4 Hz, 1H). 13C NMR (100 MHz, $CDCl_3$) δ = 146.8, 143.9, 136.2, 133.3, 128.9, 128.8, 127.0, 126.9, 126.3, 124.1.



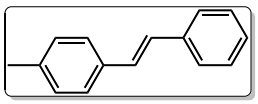
(E)-1-Styryl-4-(trifluoromethyl)benzene (3c)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.51 (s, 4H), 7.44 (d, J=7.2 Hz, 2H), 7.29 (t, J=7.4 Hz, 2H), 7.21 (t, J=7.2 Hz, 1H), 7.10 (d, J=16.4 Hz, 1H), 7.02 (d, J=16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 140.8, 136.6, 131.2, 129.4, 129.1, 128.8, 128.3, 127.1, 126.8, 126.6, 125.6, 122.9.



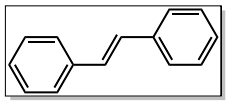
(E)-4-Styrylbenzonitrile (3d)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.51 (d, J=8.0 Hz, 2H), 7.46-7.41 (m, 4H), 7.28 (t, J=7.4 Hz, 2H), 7.21 (t, J=7.2 Hz, 1H), 7.09 (d, J=16.4 Hz, 1H), 6.97 (d, J=16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 141.7, 136.2, 132.4, 132.3, 128.8, 128.6, 126.8, 126.8, 126.6, 118.9, 110.5.



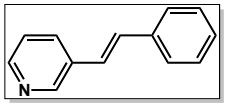
(E)-4-Methylstilbene (3e)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.41 (d, *J*=7.2 Hz, 2H), 7.32 (d, *J*=8.0 Hz, 2H), 7.26 (t, *J*=7.6 Hz, 2H), 7.15 (t, *J*=6.2 Hz, 1H), 7.08 (d, *J*=8.0 Hz, 2H), 6.99 (dd, *J*=19.2 Hz , 16.4 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, CDCl3) δ = 137.5, 137.5, 134.6, 129.4, 128.6, 127.7, 127.4, 126.4, 126.4, 21.2.



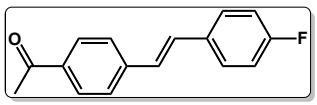
(E)-Stilbene (3f)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.57 (d, *J*=7.2 Hz, 4H), 7.42 (t, *J*=7.6 Hz, 4H), 7.32 (t, *J*=7.4 Hz, 2H), 7.17 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ =137.3, 128.7, 128.7, 127.6, 126.5.



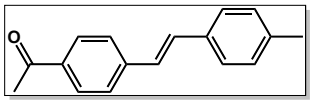
3-Styryl-pyridine (3g)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.63 (s, 1H), 8.39 (d, J=4.4 Hz, 1H), 7.72 (d, J=8.0 Hz, 1H), 7.43 (d, J=7.6 Hz, 2H), 7.28 (t, J=7.6 Hz, 2H), 7.22 – 7.16 (m, 2H), 7.06 (d, J=16.4 Hz, 1H), 6.96 (d, J=16.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 148.4, 136.6, 132.9, 132.6, 130.8, 128.7, 128.1, 126.6, 124.8, 123.5.



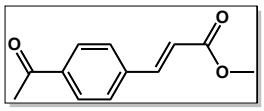
4-acetyl-4'-fluorostilbene (3h)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 (d, J=8.0, 2H), 7.49 (d, J=8.4, 2H), 7.43 (t, J=6.2, 2H), 7.10 (d, J=16.4, 1H), 6.98 (m, 3H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.4, 163.9, 161.46, 141.8, 136.0, 132.9, 132.9, 130.2, 128.9, 128.4, 128.3, 127.2, 127.2, 126.4, 115.9, 115.7, 26.5.



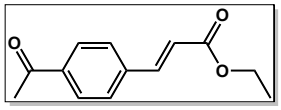
4-acetyl-4'-methylstilbene (3i)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.83 (d, J=8.4, 2H), 7.45 (d, J=8.0, 2H), 7.32 (d, J=8.0, 2H), 7.11 – 7.07 (m, 3H), 6.96 (d, J=16.4, 1H), 2.49 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.4, 142.2, 138.3, 135.7, 133.9, 131.3, 129.4, 128.8, 126.7, 126.4, 126.3, 26.5, 21.2.



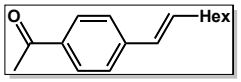
(E)-4-acetyl-methylcinnamate (3j)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (d, J=8.4 Hz, 2H), 7.58 (d, J=16.0 Hz, 1H), 7.48 (d, J=8.4 Hz, 2H), 6.40 (d, J=16.0 Hz, 1H), 3.71 (s, 3H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.0, 166.6, 143.0, 138.5, 137.8, 128.6, 127.9, 120.1, 51.6, 26.4.



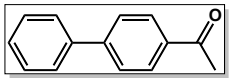
(E)-4-acetyl-ethylcinnamate (3k)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 (d, J=8.4 Hz, 2H), 7.59 (d, J=16.0 Hz, 1H), 7.50 (d, J=8.0 Hz, 2H), 6.42 (d, J=16.0 Hz, 1H), 4.18 (dd, J=14.4 Hz, 7.2 Hz, 2H), 2.51 (s, 3H), 1.25 (t, J=7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.1, 166.3, 142.8, 138.6, 137.8, 128.7, 128.0, 120.7, 60.6, 26.5, 14.1.



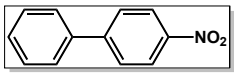
(E)-1-(4-Acetylphenyl)-1-octene (3l)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 (d, J=8.4 Hz, 2H), 7.31 (d, J=8.0 Hz, 2H), 6.34 – 6.25 (m, 2H), 2.48 (s, 3H), 2.14–1.95 (m, 2H), 1.39 – 1.21 (m, 8H), 0.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.4, 142.6, 135.3, 134.5, 128.9, 128.7, 125.8, 33.1, 31.6, 29.0, 28.8, 26.4, 22.5, 14.0.



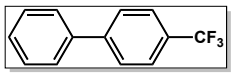
4-Acetyl-biphenyl (5a)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.03 (d, J=8.4 Hz, 2H), 7.69 (d, J=8.4 Hz, 2H), 7.63 (d, J=7.2 Hz, 2H), 7.49 –7.38 (m, 3H), 2.64 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 197.8, 145.7, 139.8, 135.9, 128.9, 128.9, 128.2, 127.3, 127.2 , 26.6.



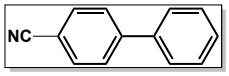
4-Nitrobiphenyl (5b)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.28 (d, J=8.8 Hz, 2H), 7.73 (d, J=8.8 Hz, 2H), 7.62 (d, J=8.0 Hz, 2H), 7.51– 7.42 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 147.6, 147.1, 138.7, 129.1, 128.9, 127.7, 127.3, 124.1.



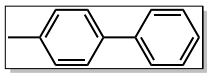
4-(Trifluoromethyl)biphenyl (5c)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60 –7.53 (m, 4H), 7.46 (d, J=7.2 Hz, 2H), 7.38 –7.34 (m, 2H), 7.33 –7.28 (m, 1H). ^{13}C NMR (100 MHz, CDCl3) δ = 145.5, 139.0, 132.4, 129.0, 128.5, 127.6, 127.1, 118.8, 110.8.



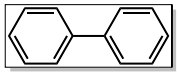
4-Carbbonitrilebiphenyl (5d)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.60 –7.54 (m, 4H), 7.47 (d, J=7.2 Hz, 2H), 7.37 (t, J=7.2 Hz, 2H), 7.31 (t, J=7.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 145.5, 139.0, 132.5, 129.0, 128.6, 127.6, 127.1, 118.8, 110.8.



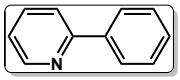
4-Methylbiphenyl (5e)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.57 (d, J=7.2 Hz, 1H), 7.49 (d, J=8.0 Hz, 2H), 7.42 (t, J=7.6 Hz, 2H), 7.31 (t, J=7.4 Hz, 1H), 7.24 (d, J=8.0 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 141.2, 138.3, 137.0, 129.5, 128.7, 127.0, 127.0, 21.1.



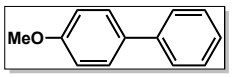
Biphenyl (5f)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.50 (d, J=7.2 Hz, 4H), 7.35 (t, J=7.4 Hz, 4H), 7.25 (t, J=7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 141.2, 128.7, 127.2, 127.2.



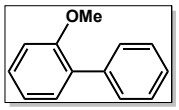
2-phenylpyridine (5g)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.72 (d, J=4.8 Hz, 1H), 8.04 (d, J=7.2 Hz, 2H), 7.71 – 7.66 (m, 2H), 7.49 (t, J=7.4 Hz, 2H), 7.43 (t, J=7.2 Hz, 1H), 7.20 –7.17 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.1, 149.4, 139.2, 136.4, 128.7, 128.5, 126.7, 121.8, 120.2.



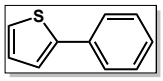
4-methoxybiphenyl (5h)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.53 (t, J=8.4 Hz, 4H), 7.41 (t, J=7.6 Hz, 2H), 7.29 (t, J=7.4 Hz, 1H), 6.97 (d, J=8.8 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.1, 140.8, 133.8, 128.7, 128.1, 126.7, 126.6, 114.2, 55.3.



2-methoxybiphenyl (5i)

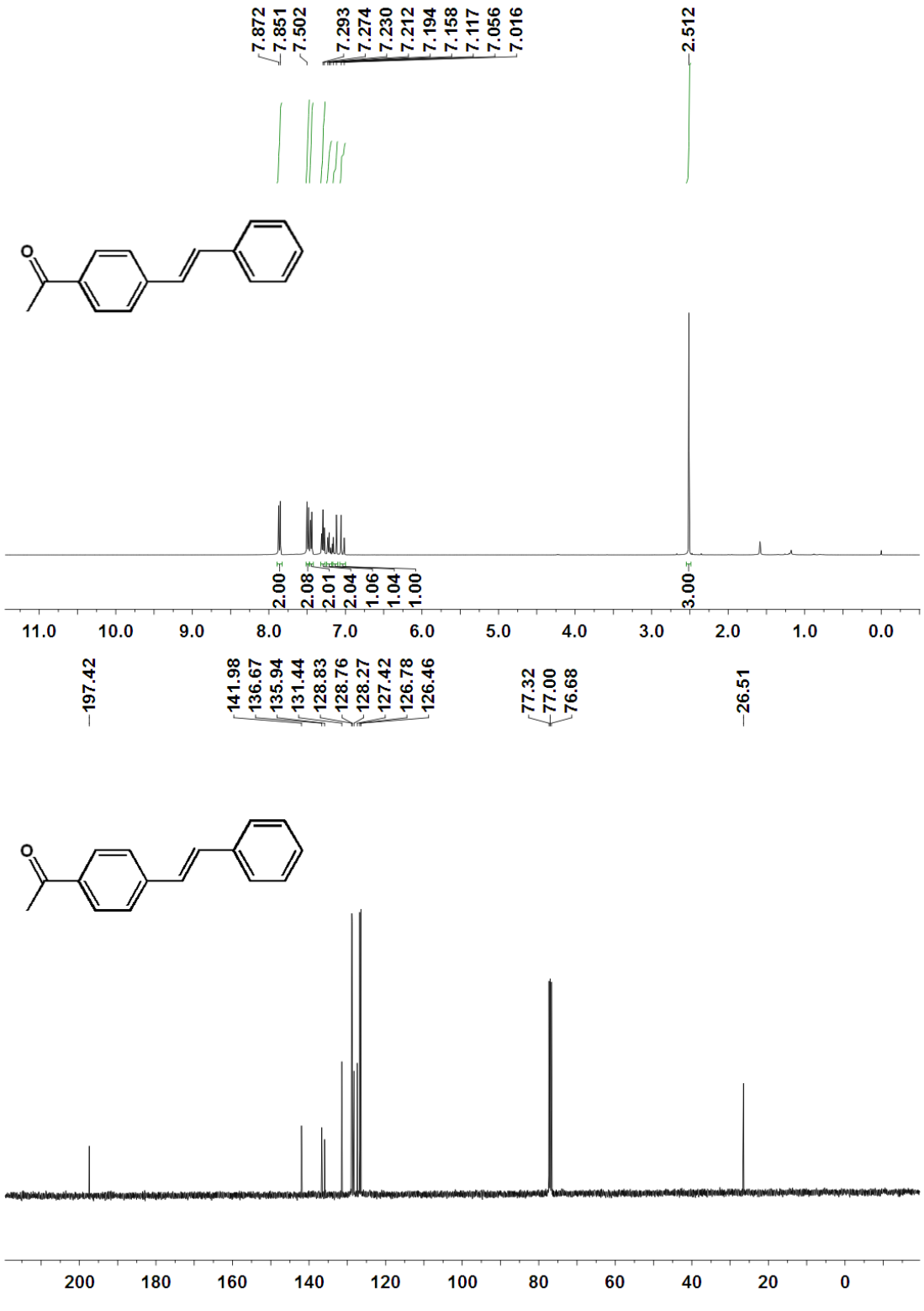
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.51 (d, J=7.6 Hz, 2H), 7.38 (t, J=7.6 Hz, 2H), 7.29 (t, J=8.0 Hz, 1H), 7.02 – 6.93 (m, 1H), 3.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 156.4, 138.5, 130.8, 130.7, 129.5, 128.6, 127.9, 126.9, 120.8, 111.2, 55.5.

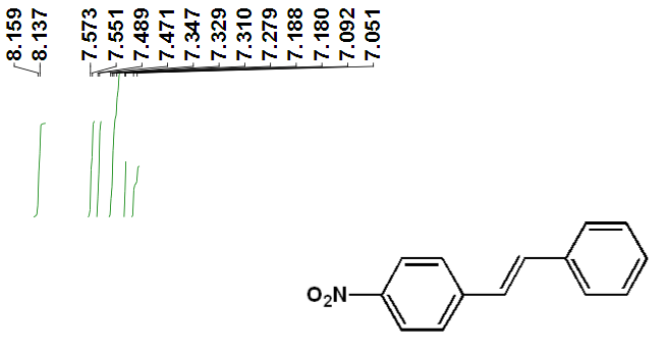


2-phenylthiophene (5j)

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.51 (d, J=7.6, 2H), 7.26 (t, J=6.8, 2H), 7.20 –7.14 (m, 3H), 6.97–6.95 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.5, 134.5, 129.0, 128.1, 127.5, 126.0, 124.9, 123.2.

3. ^{1}H NMR and ^{13}C NMR spectra of products

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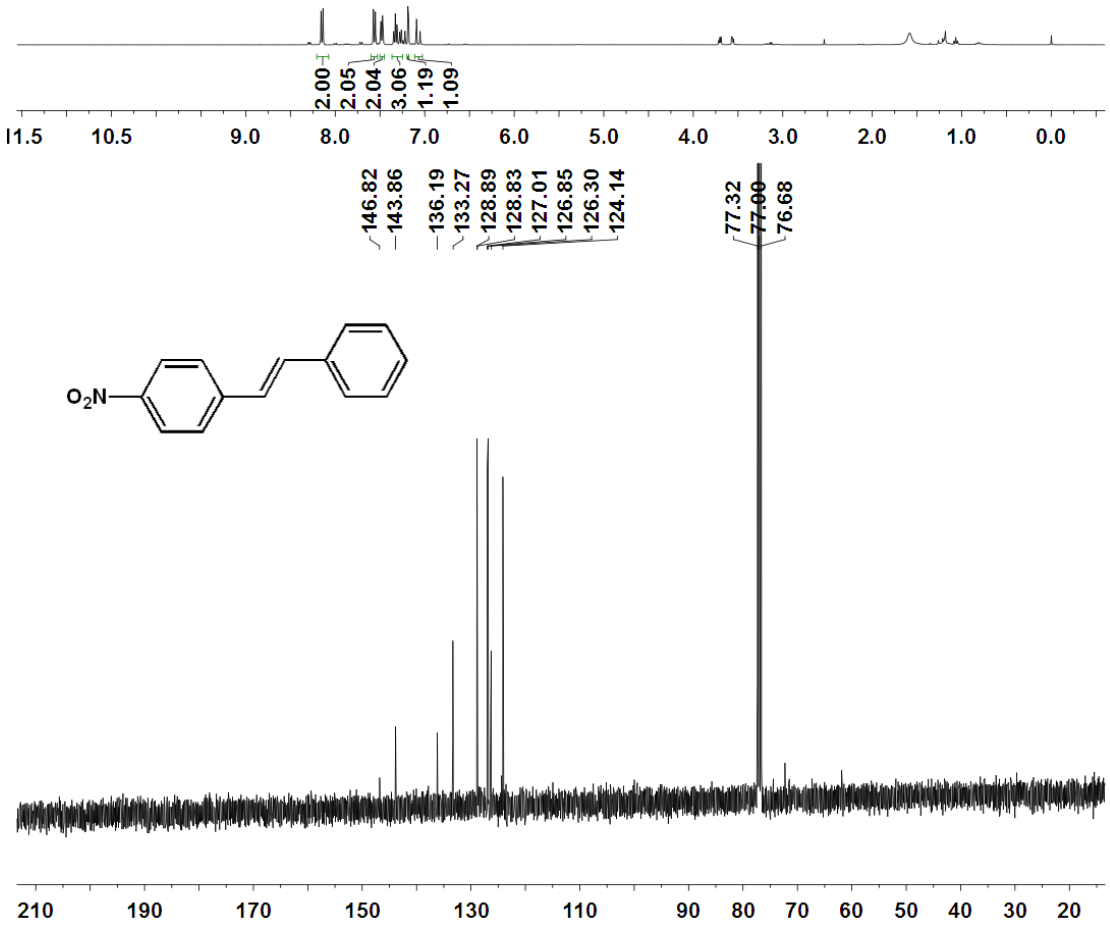
7.180
7.092
7.051
O2N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2.04
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1.09
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10.5
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7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
146.82
143.86
136.19
133.27
128.89
128.83
127.01
126.85
126.30
124.14
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77.00
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O2N
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150
130
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90
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60
50
40
30
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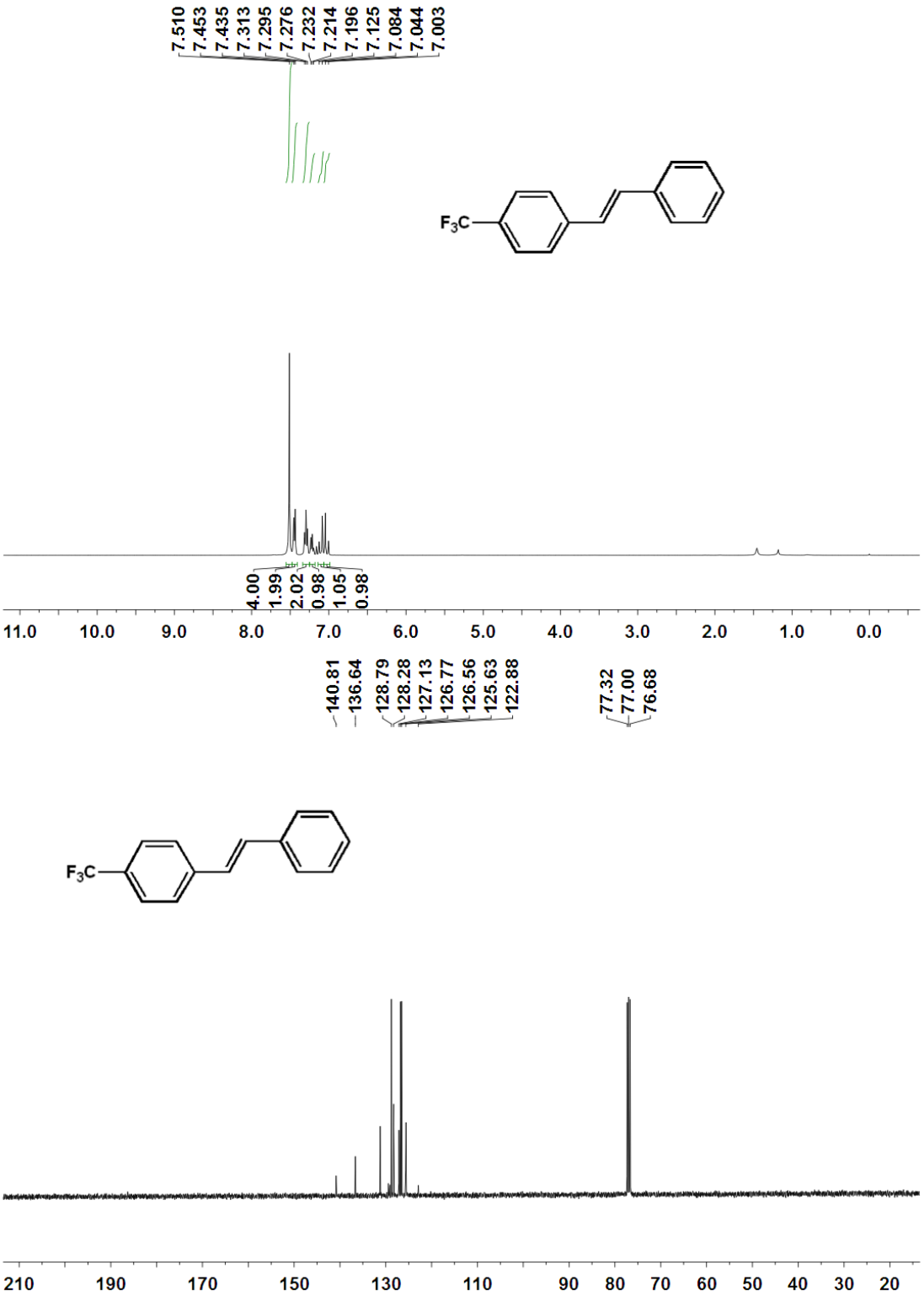
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7.214
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7.044
7.003
F3C
4.00
1.99
2.02
0.98
1.05
0.98
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
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0.0
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127.13
126.77
126.56
125.63
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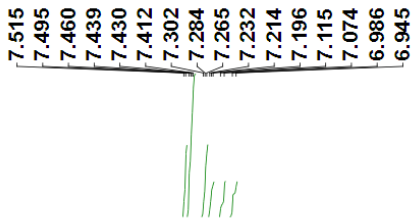
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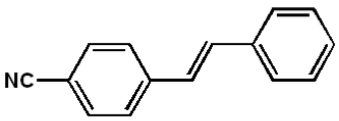
7.196
7.115
7.074
6.986
6.945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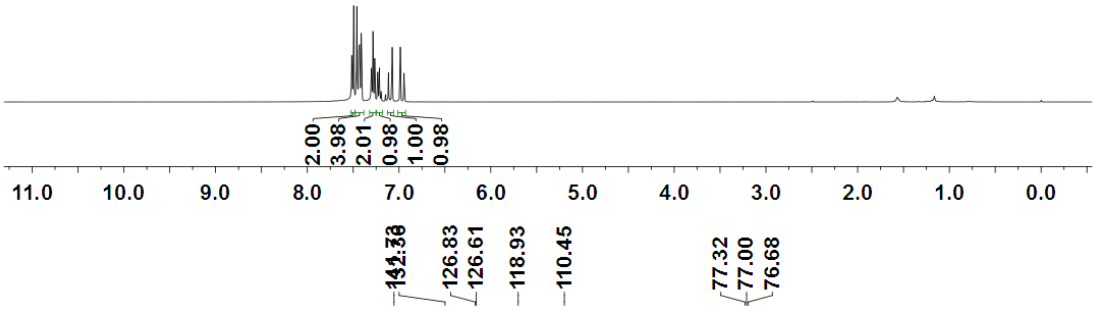
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118.93
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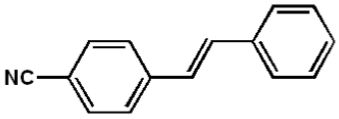
76.68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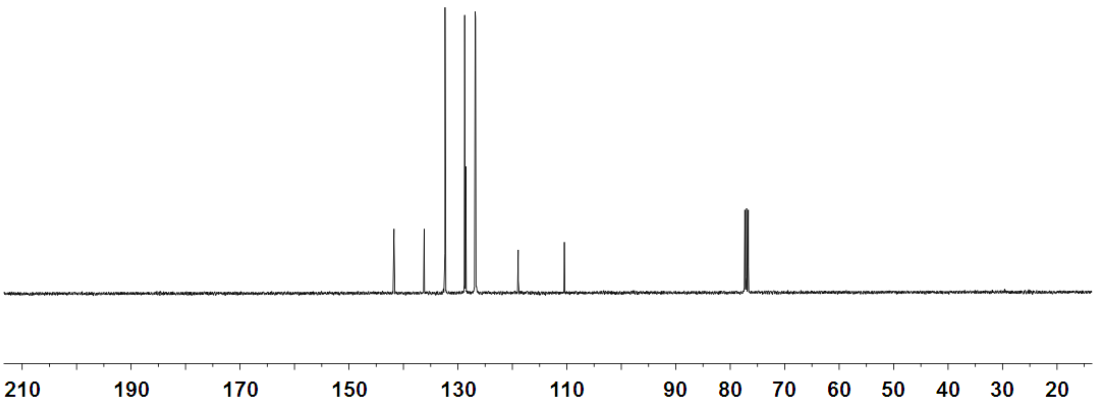
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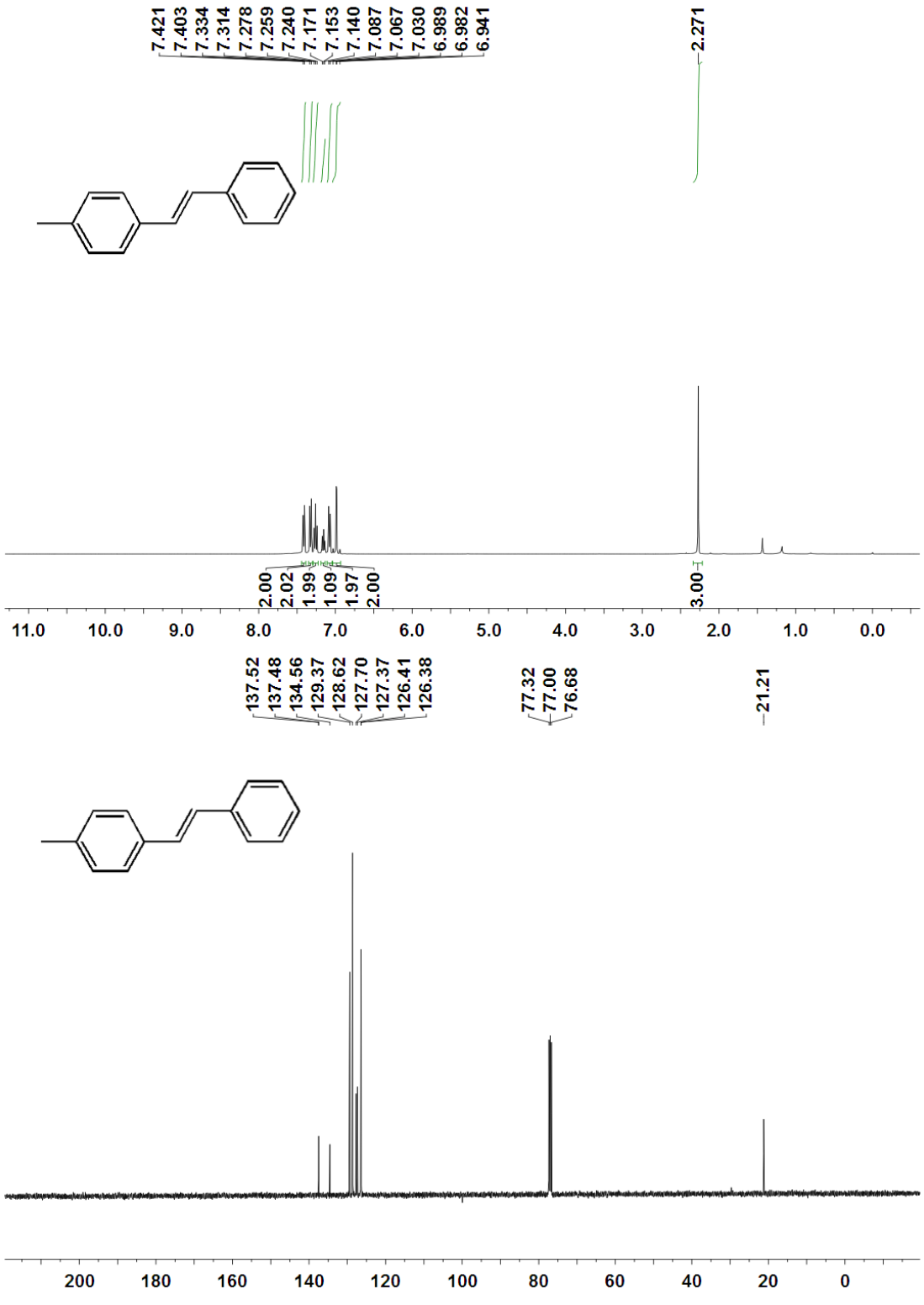
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6.982
6.941
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2.02
1.99
1.09
1.97
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3.00
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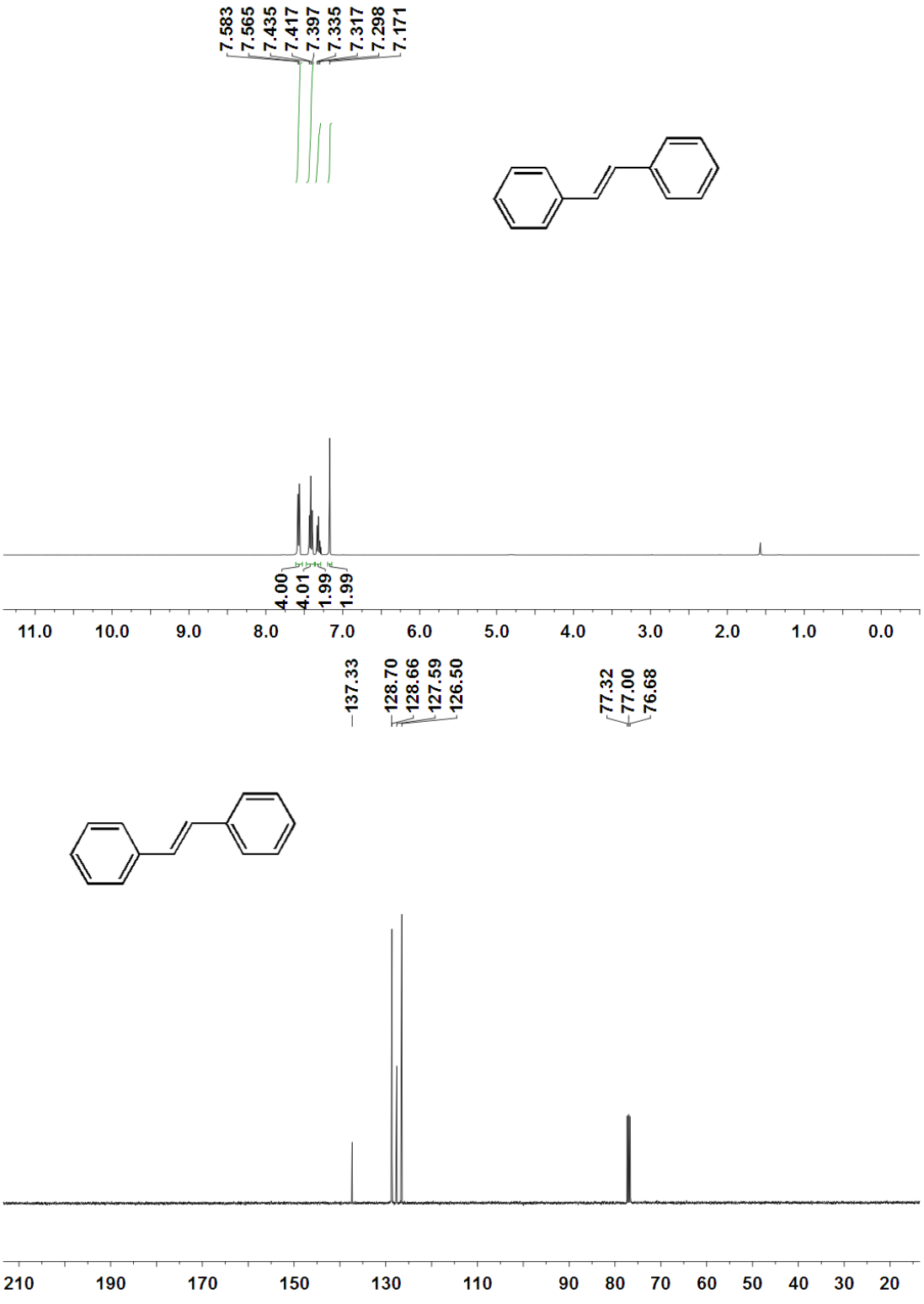
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0.0
137.33
128.70
128.66
127.59
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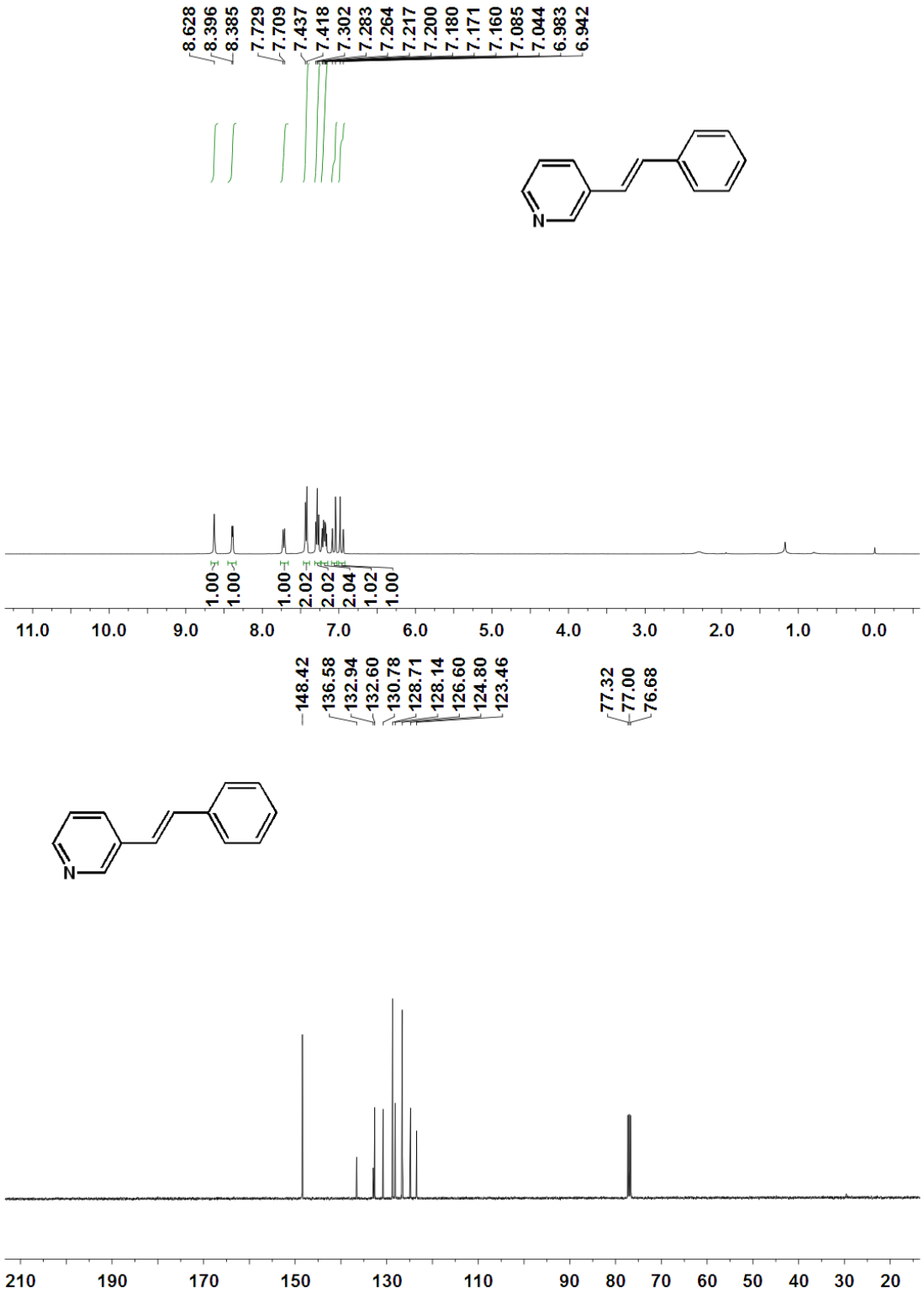
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7.180
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7.160
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7.044
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6.942
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1.00
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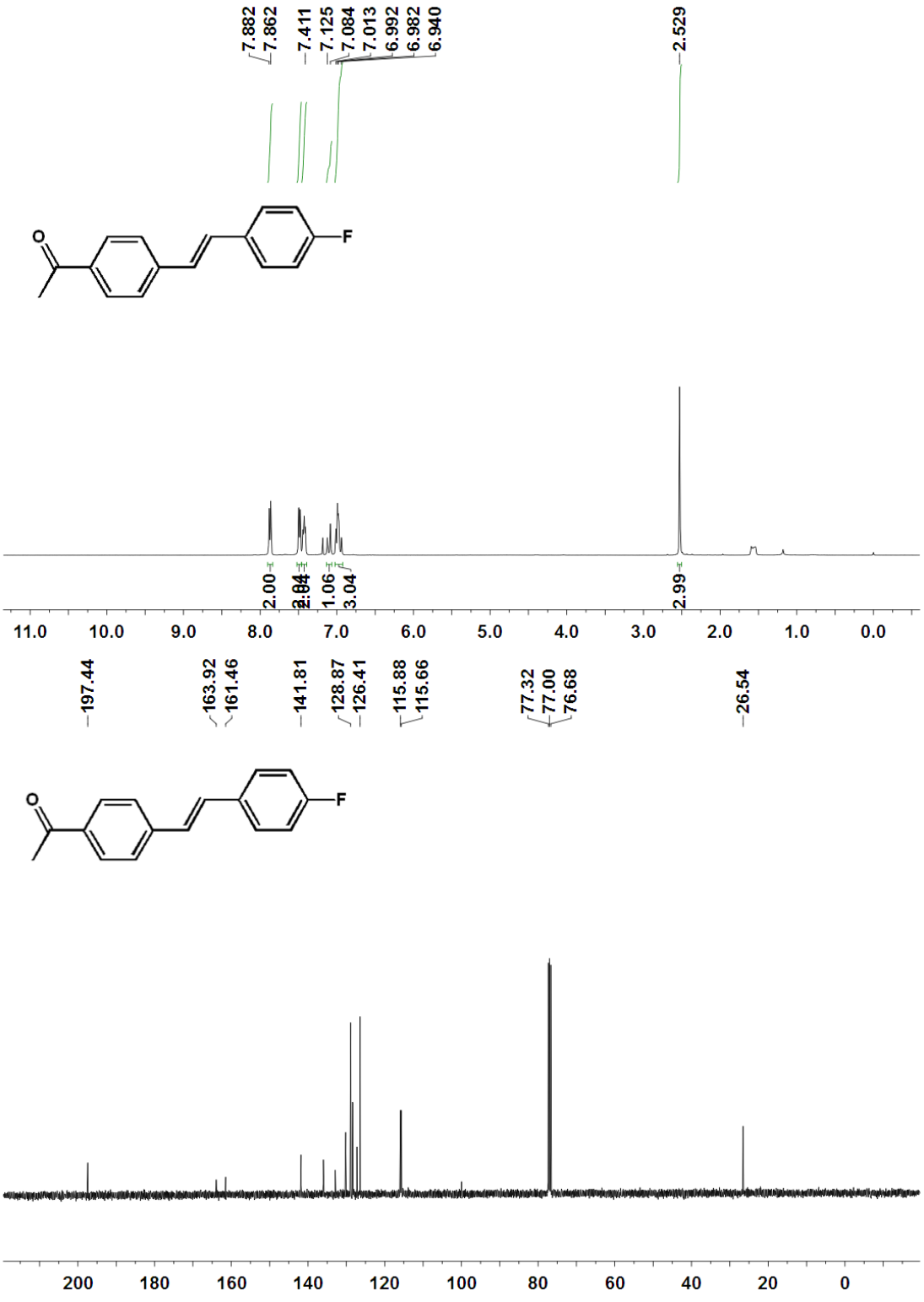
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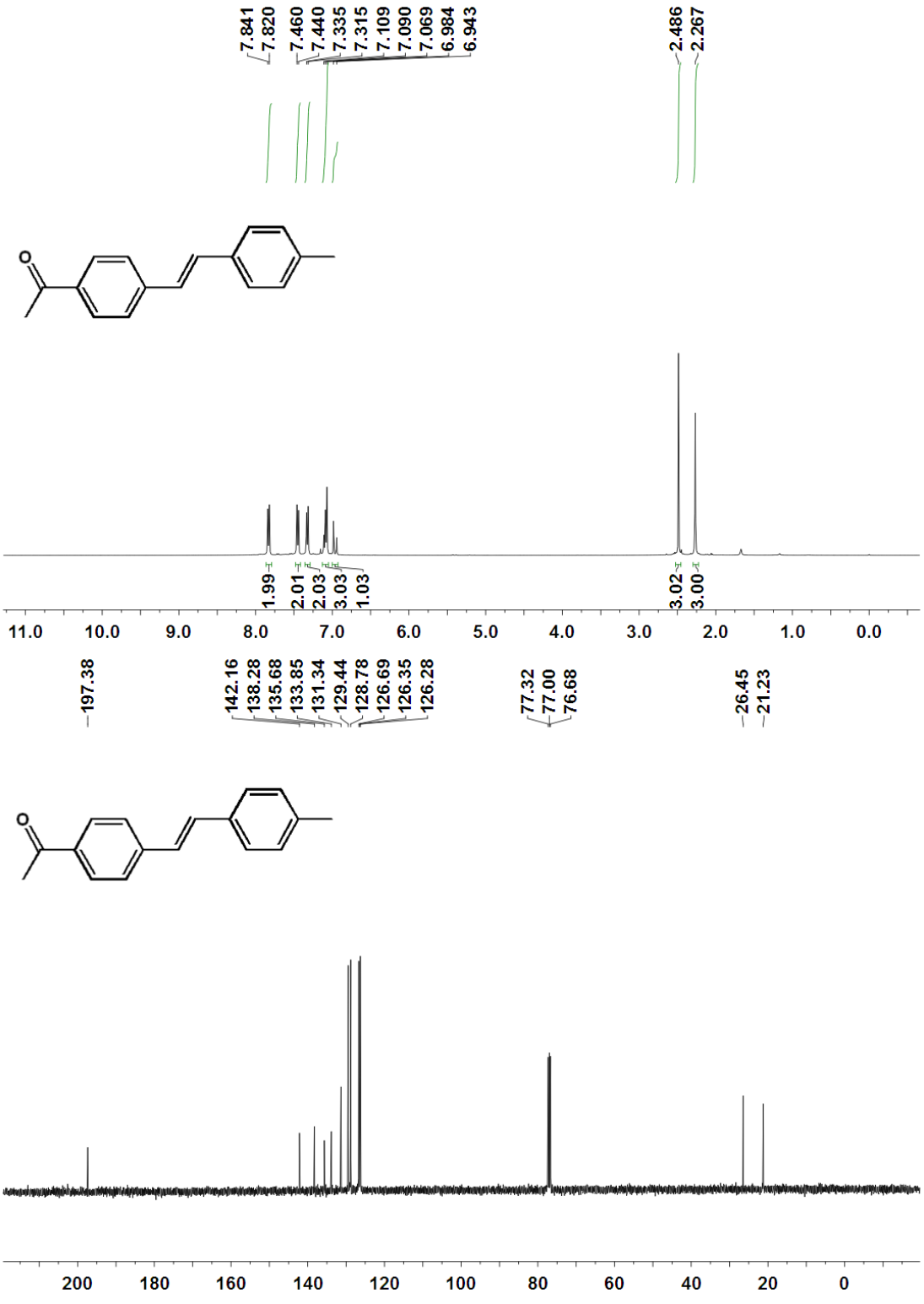
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7.0
6.0
5.0
4.0
3.0
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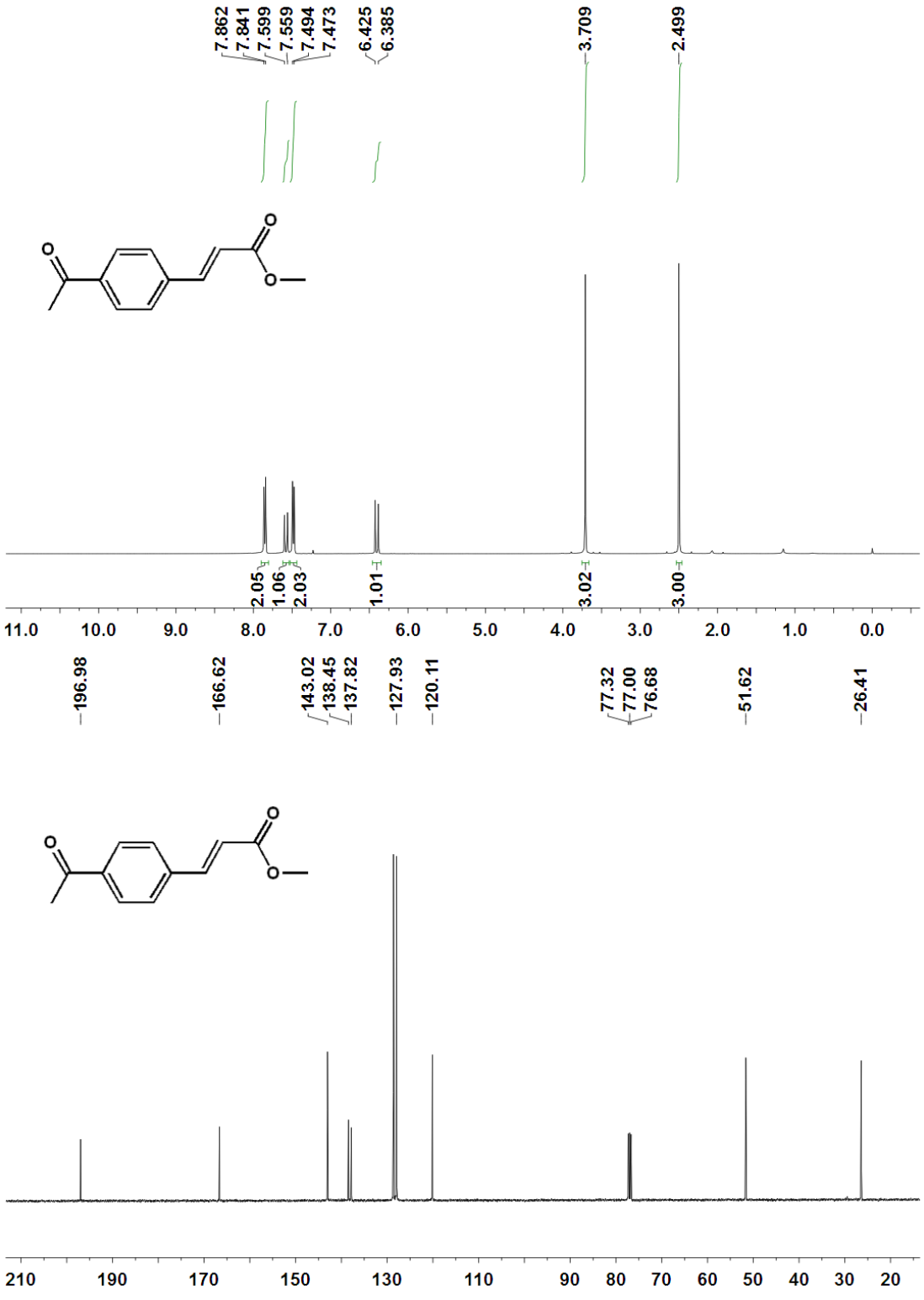
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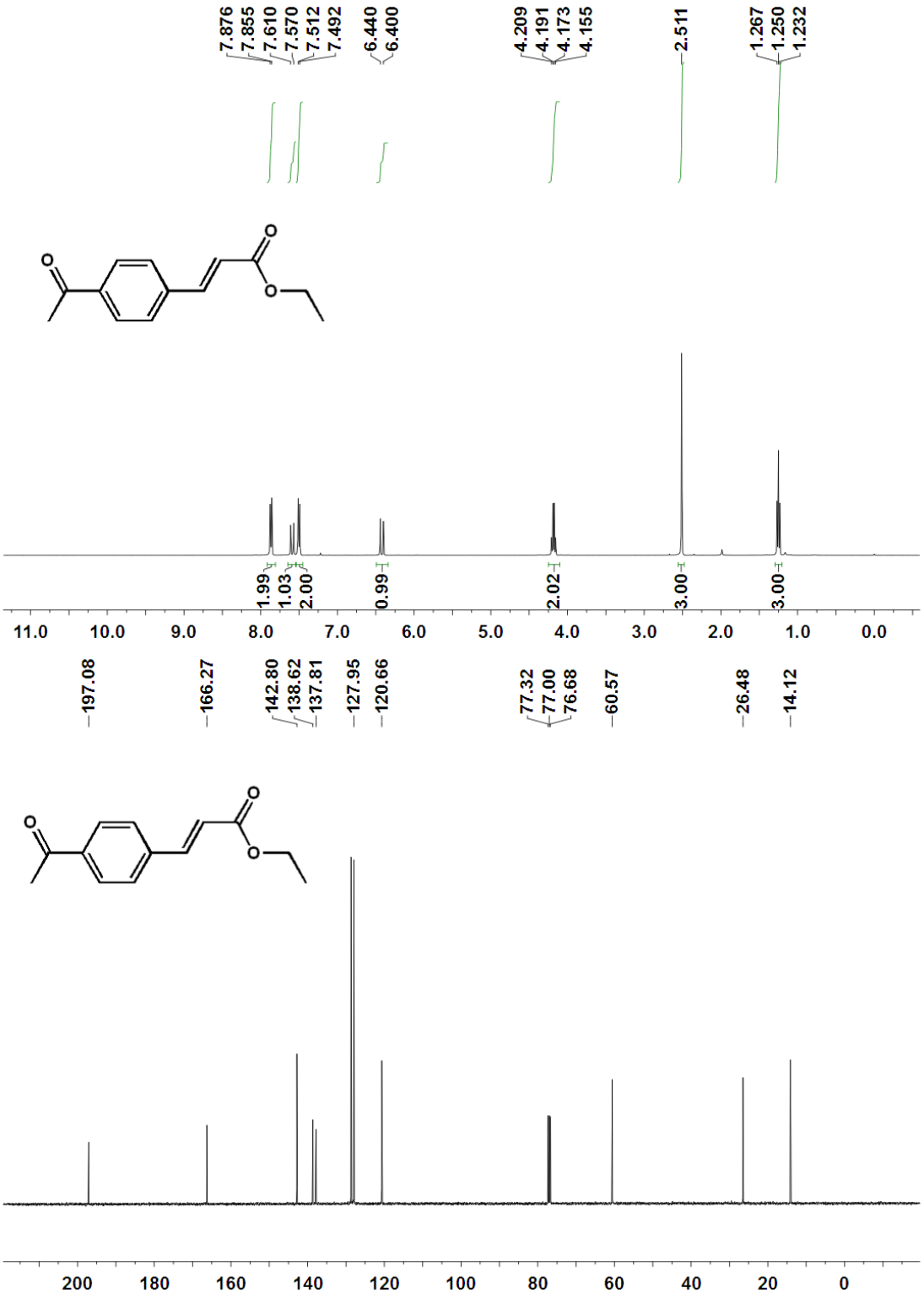
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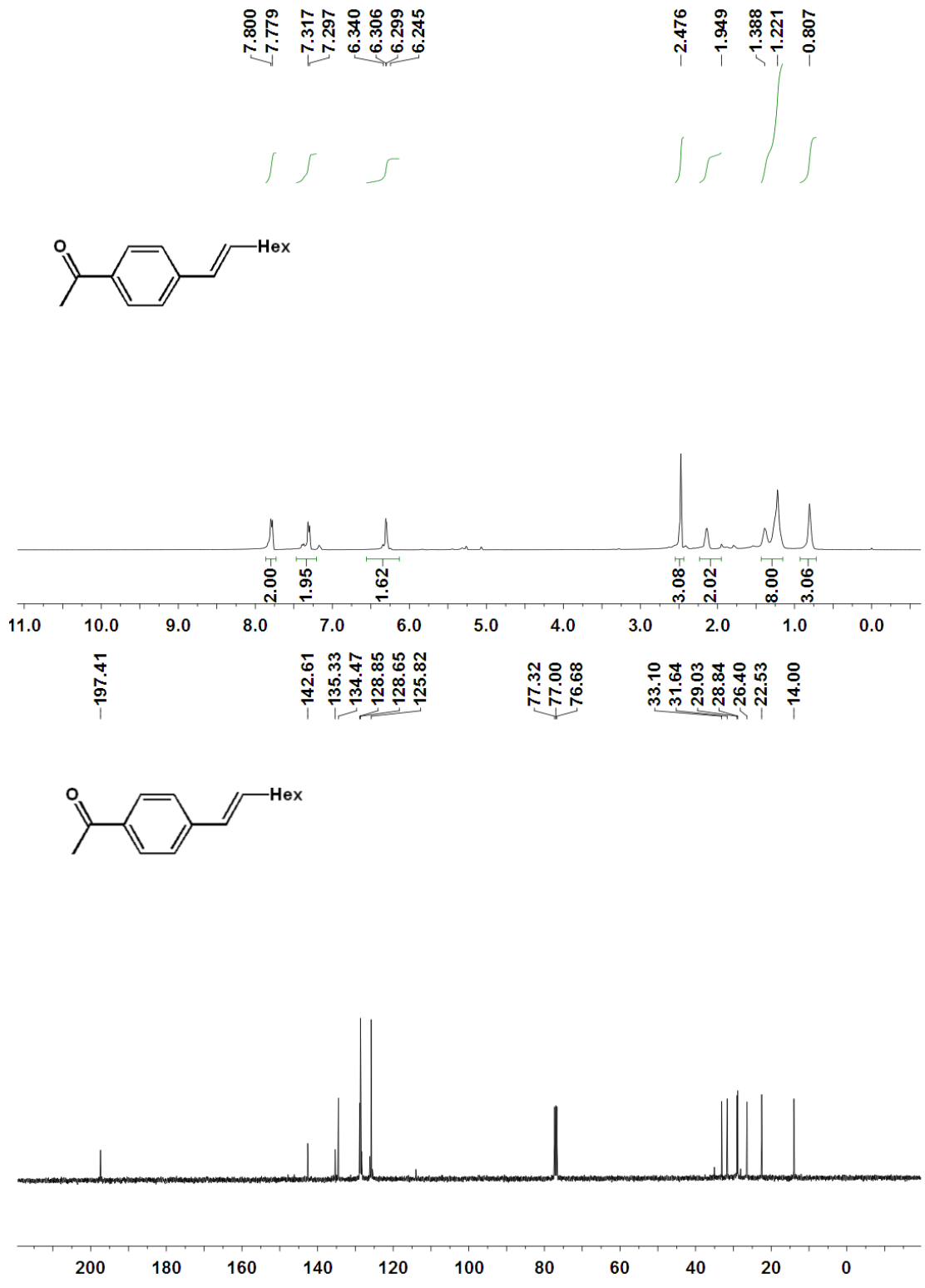
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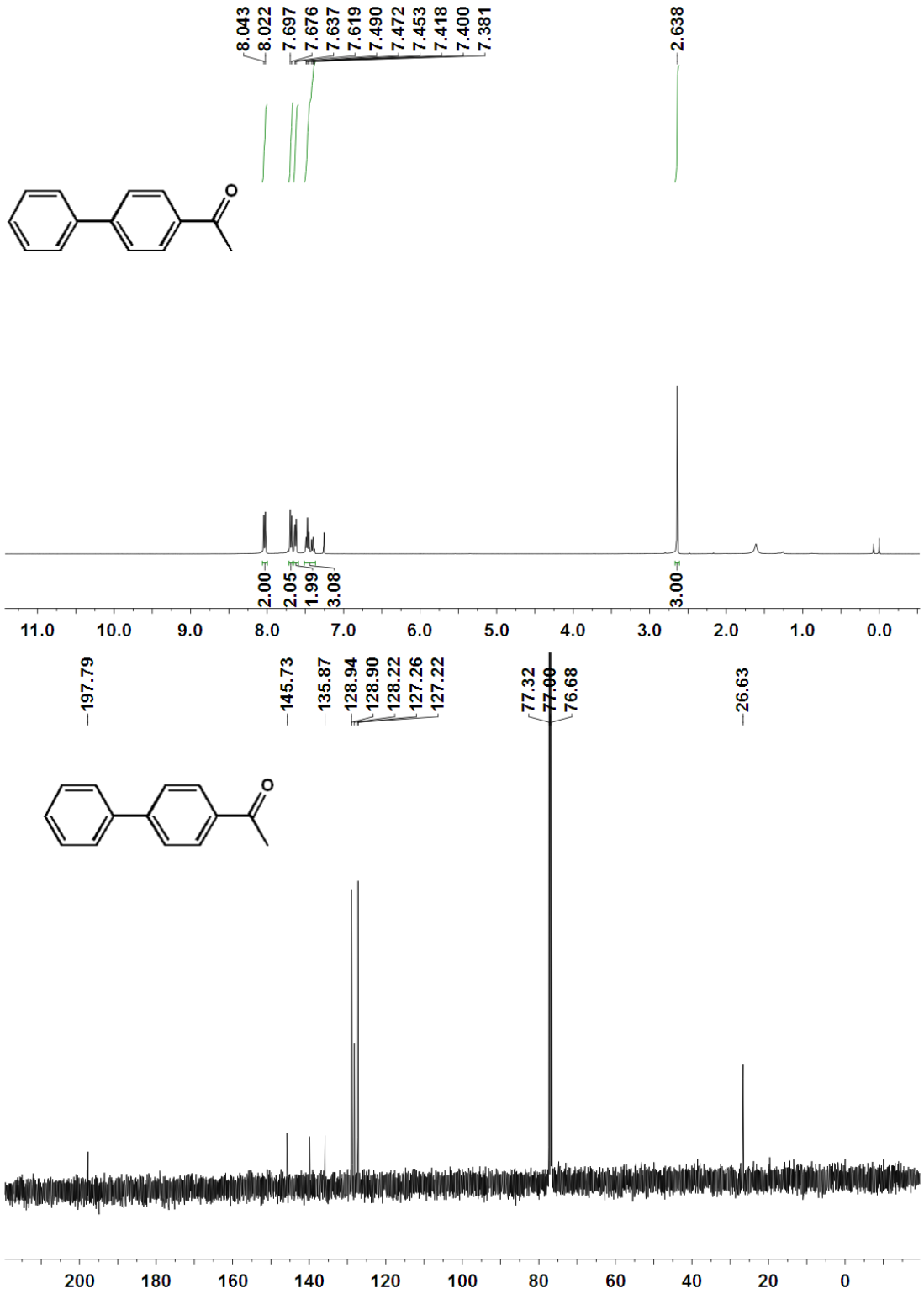
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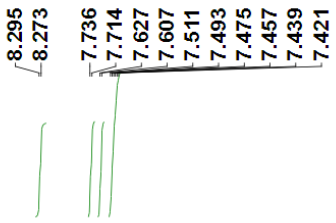
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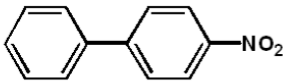
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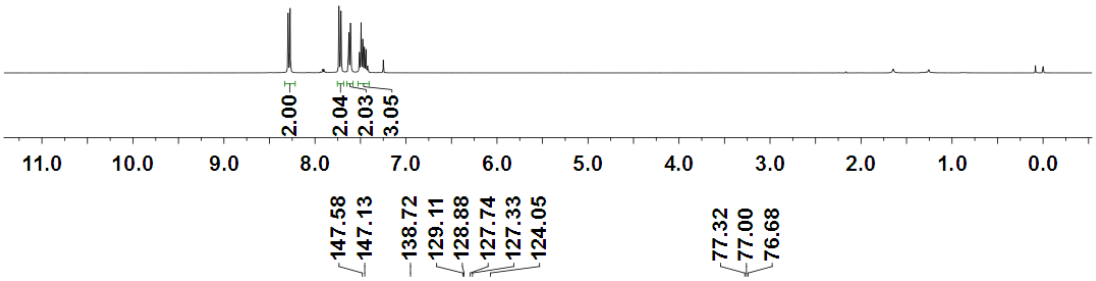
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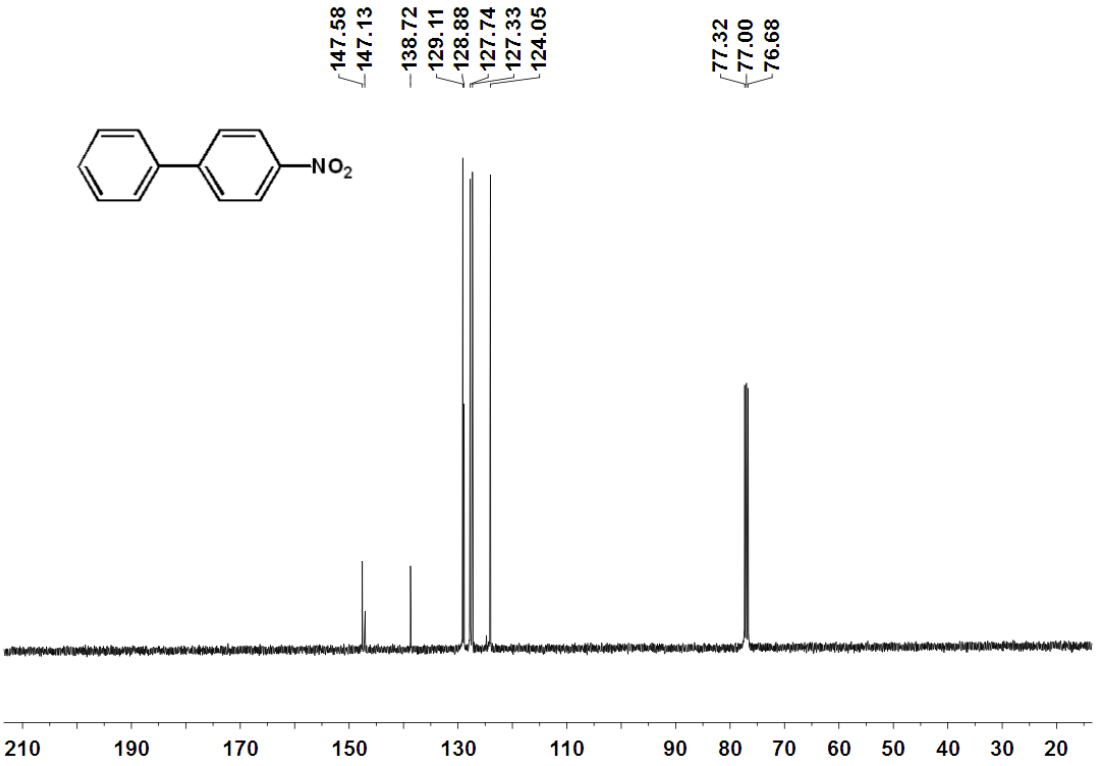
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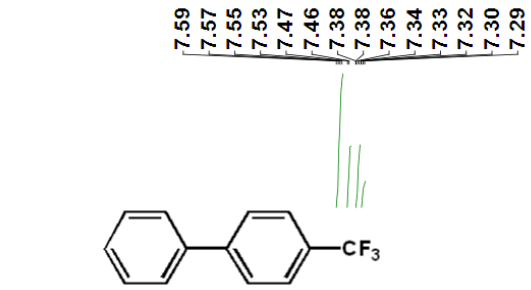
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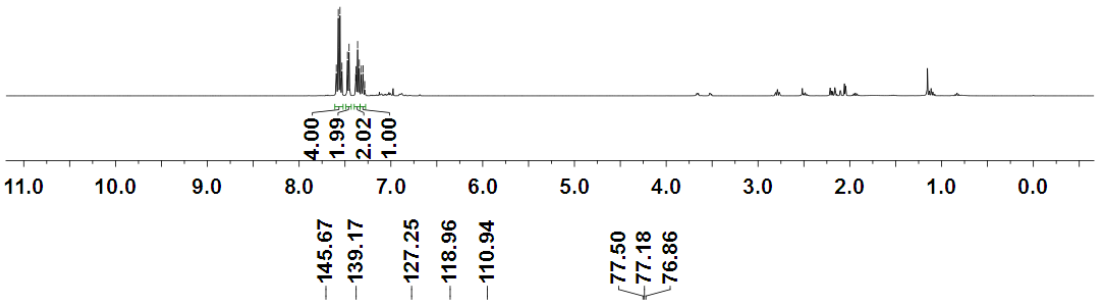
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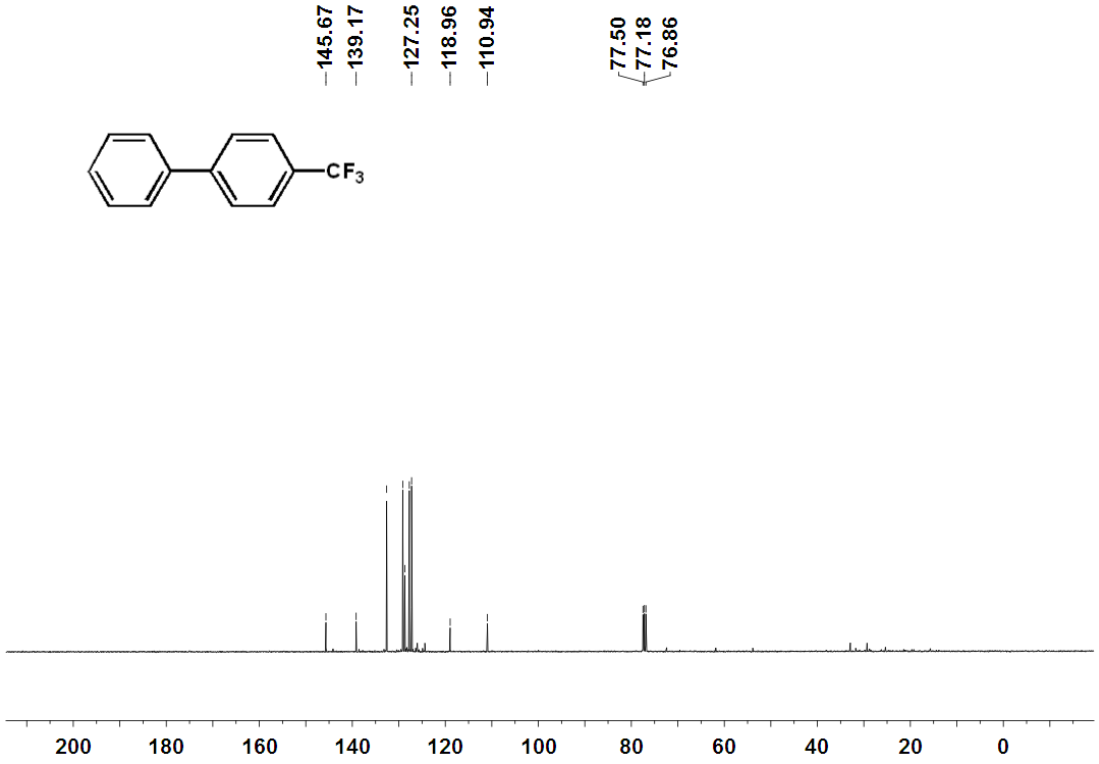
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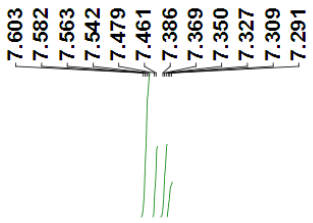
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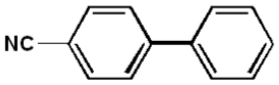
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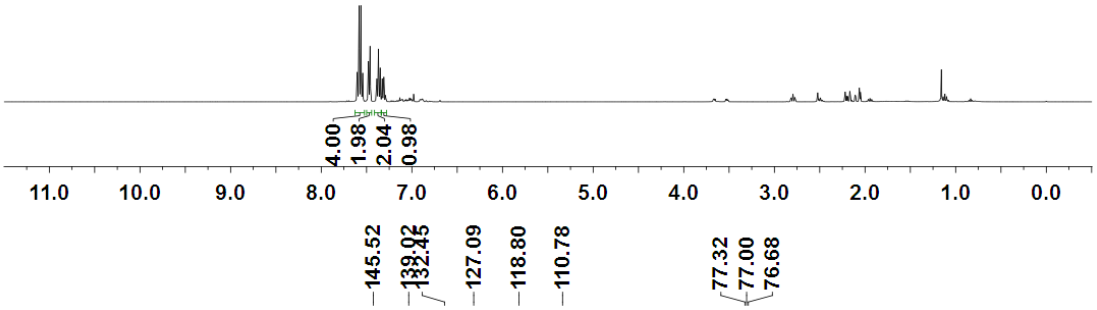
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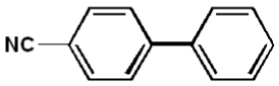
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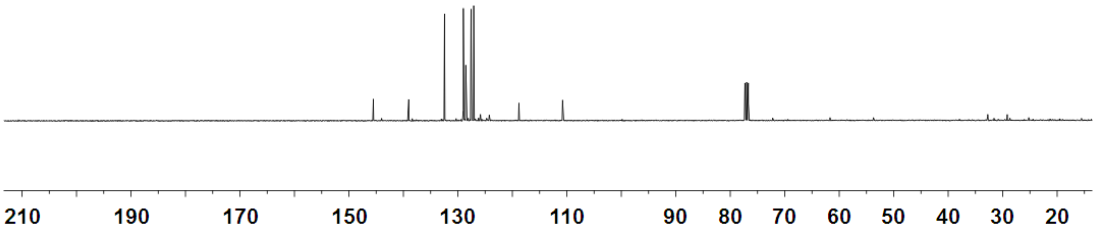
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30
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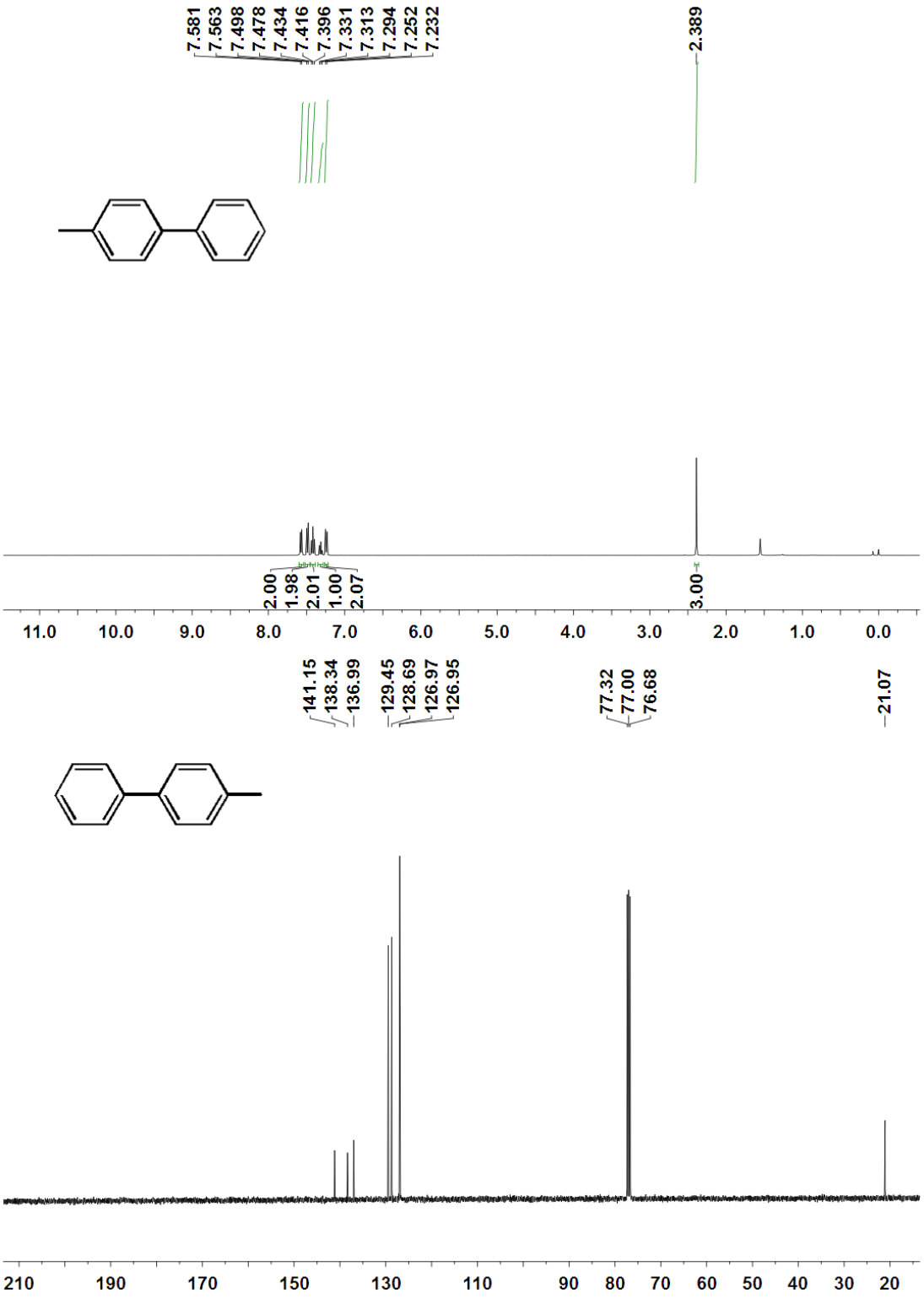
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7.331
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7.232
2.389
2.00
1.98
2.01
1.00
2.07
3.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
141.15
138.34
136.99
129.45
128.69
126.97
126.95
77.32
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76.68
21.07
210
190
170
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90
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30
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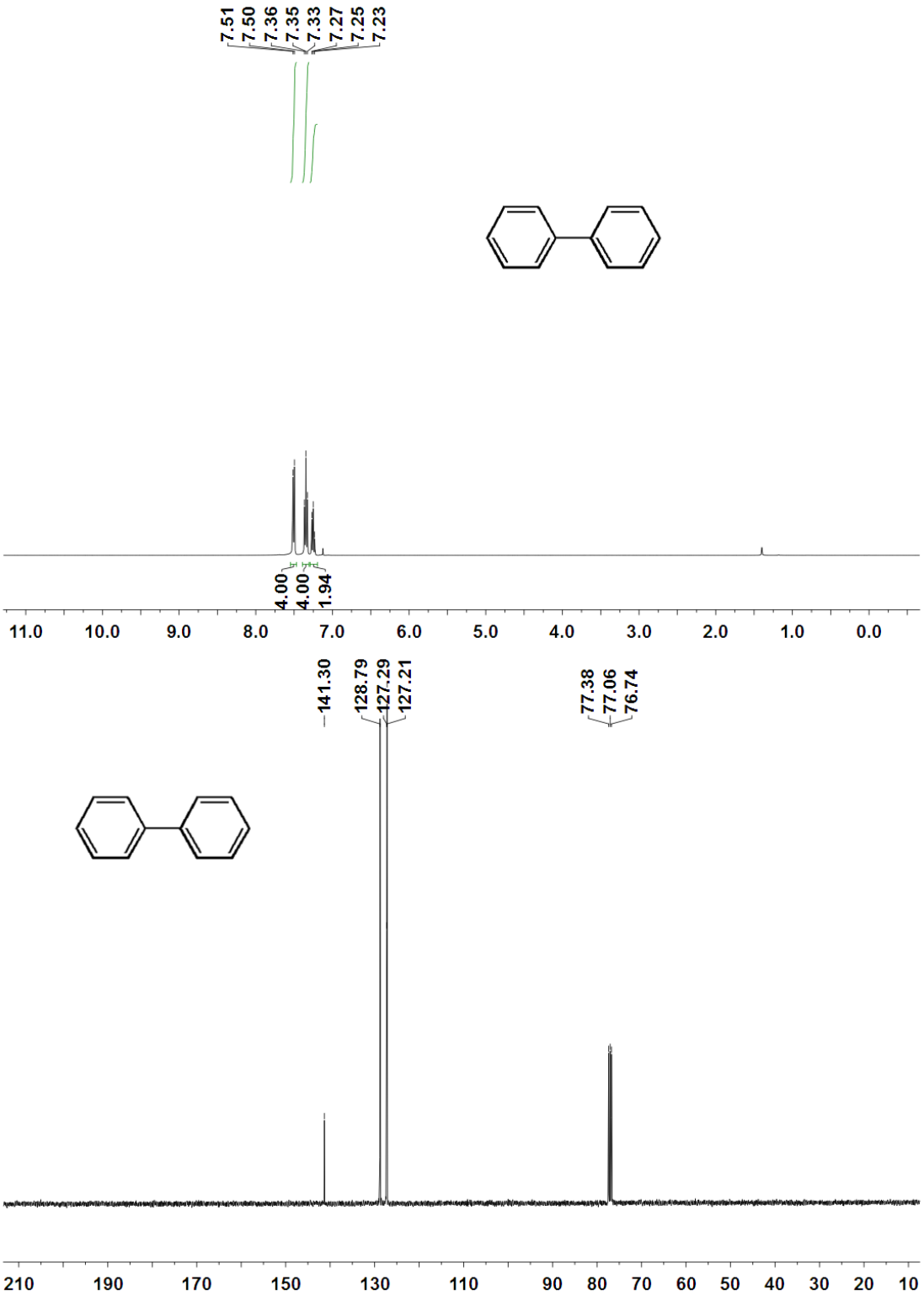
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7.50
7.36
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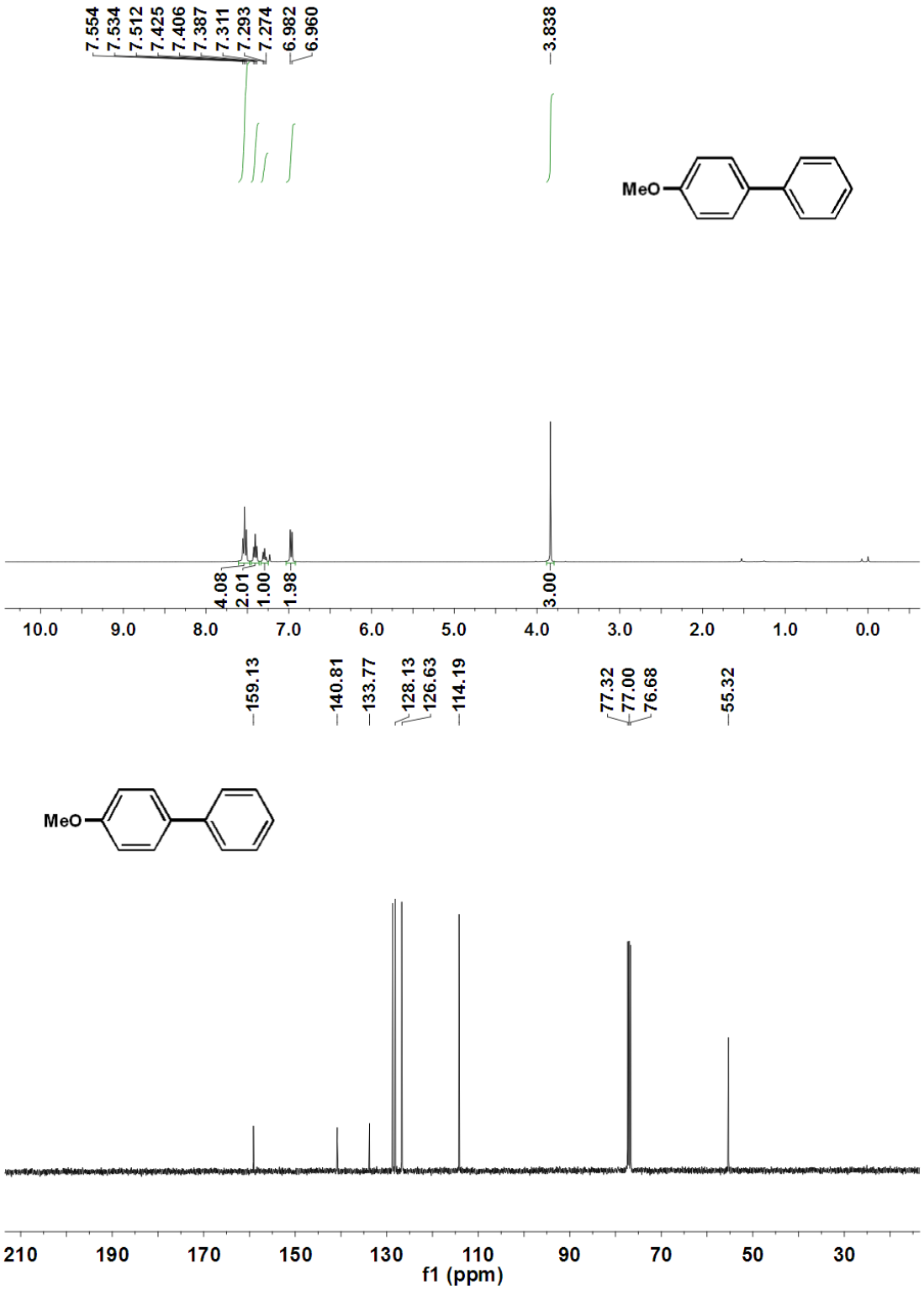
7.27
7.25
7.23
4.00
4.00
1.94
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
141.30
128.79
127.29
127.21
77.38
77.06
76.74
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10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7.512
7.425
7.406
7.387
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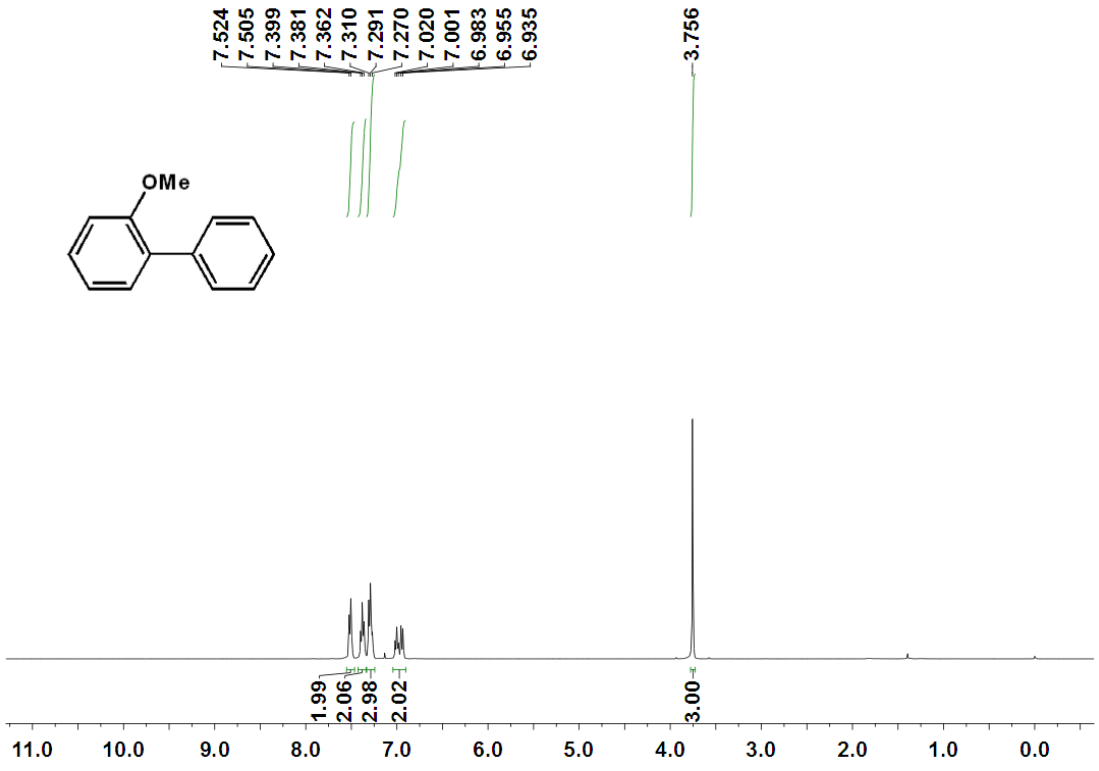
7.293
7.274
6.982
6.960
3.838
MeO
4.08
2.01
1.00
1.98
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
159.13
140.81
133.77
128.13
126.63
114.19
77.32
77.00
76.68
55.32
MeO
210
190
170
150
130
110
90
70
50
30
f1 (ppm)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7.505
7.399
7.381
7.362
7.310
7.291
7.270
7.020
7.001
6.983
6.955
6.935
3.756
OMe
1.99
2.06
2.98
2.02
3.00
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2.0
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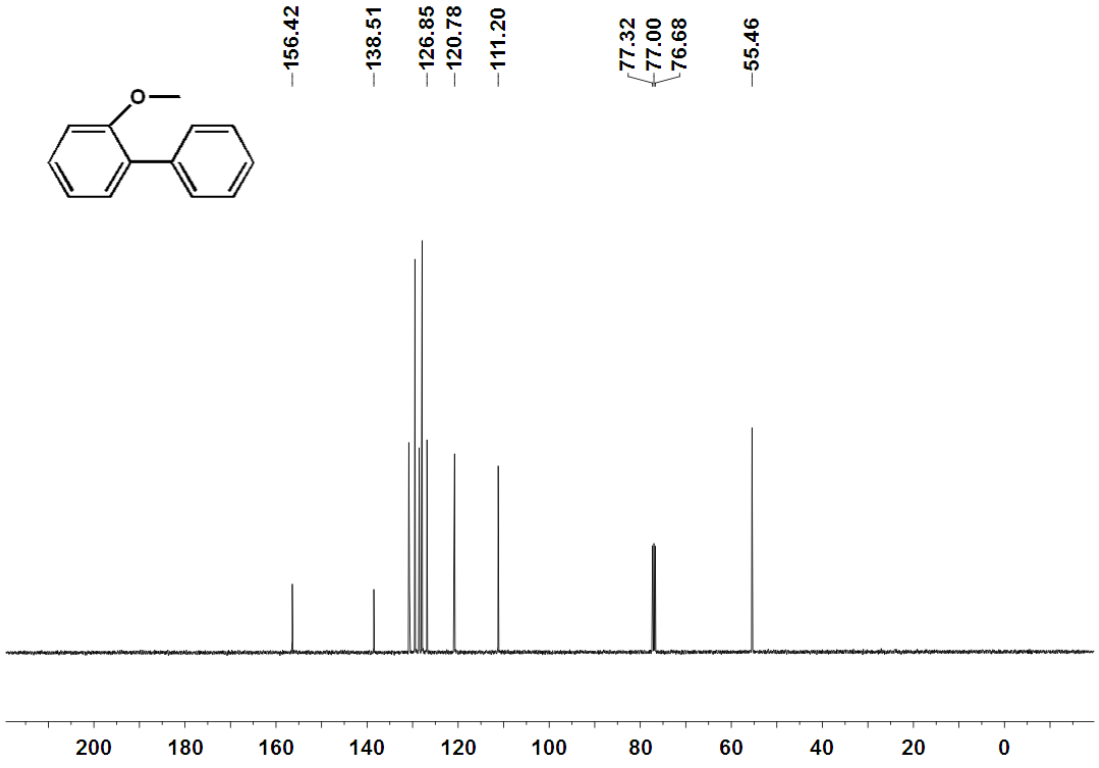
0.0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120.78
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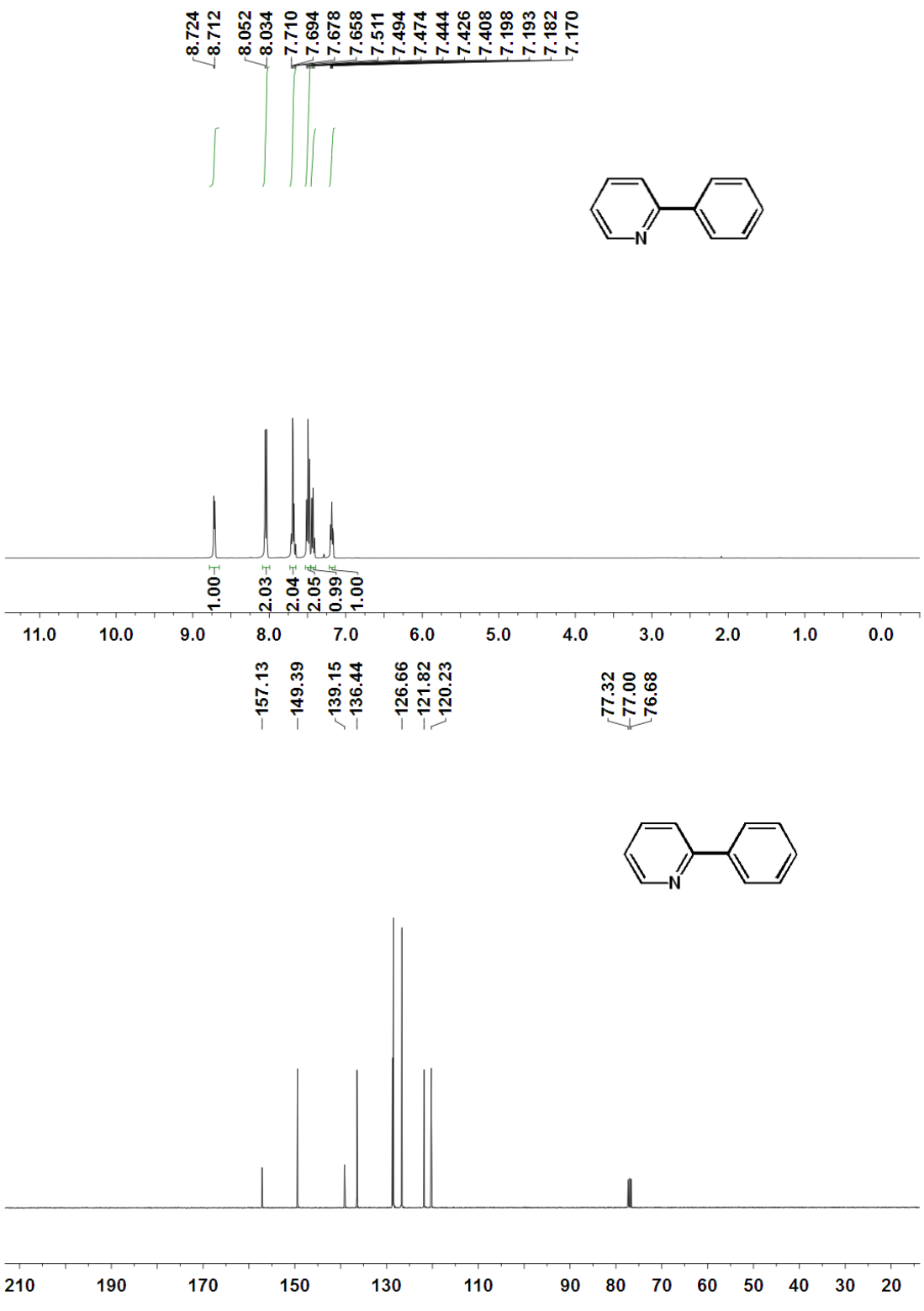
77.00
76.68
55.46
O
200
180
160
140
120
100
80
60
40
20
0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7.658
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7.474
7.444
7.426
7.408
7.198
7.193
7.182
7.170
N
1.00
2.03
2.04
2.05
0.99
1.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
157.13
149.39
139.15
136.44
126.66
121.82
120.23
77.32
77.00
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N
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190
170
150
130
110
90
80
70
60
50
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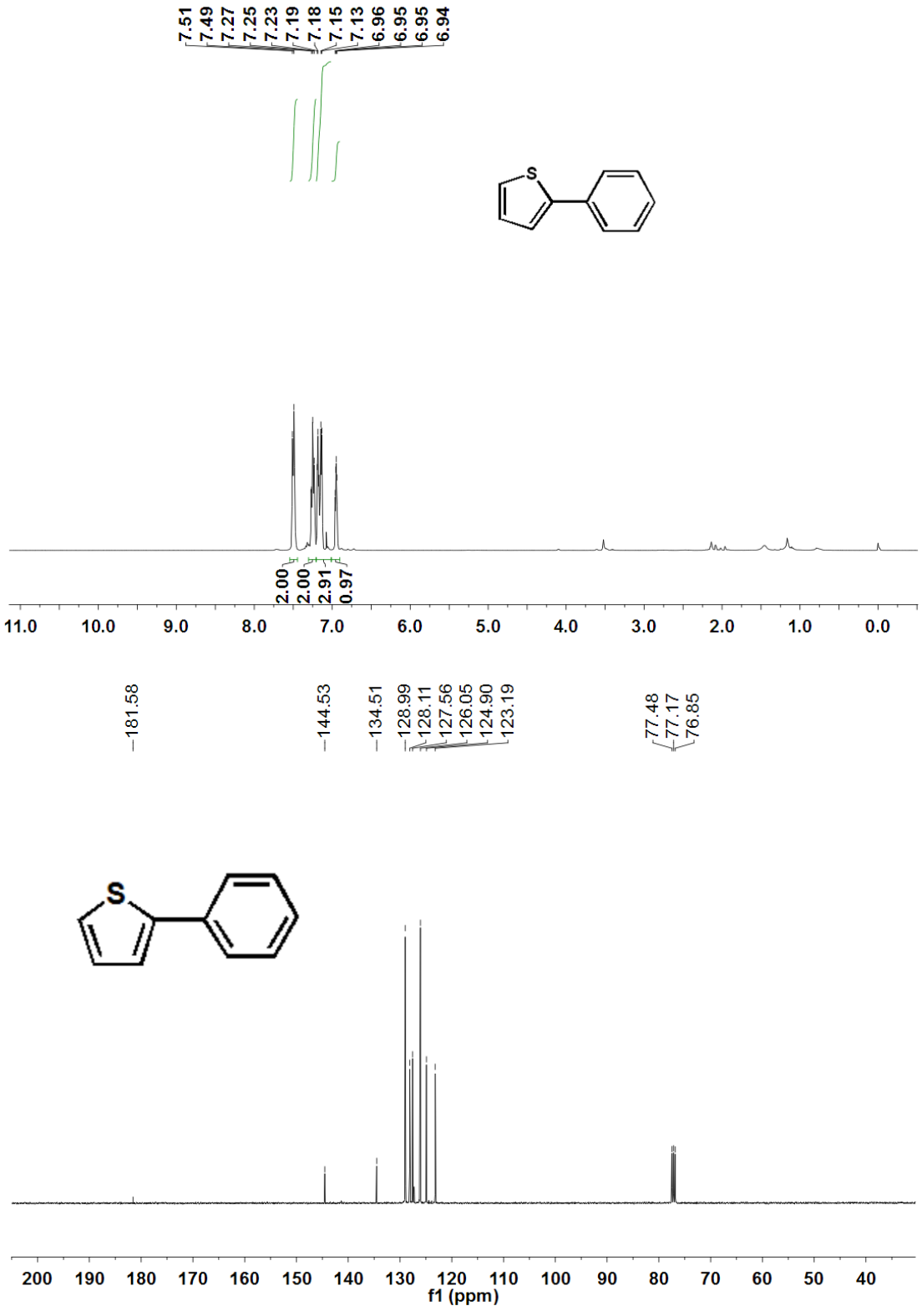
30
20


7.51
7.49
7.27
7.25
7.23
7.19
7.18
7.15
7.13
6.96
6.95
6.95
6.94
S
2.00
2.00
2.91
0.97
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
181.58
144.53
134.51
128.99
128.11
127.56
126.05
124.90
123.19
77.48
77.17
76.85
S
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
f1 (ppm)