Supporting Information

Palladium-catalyzed formation of phenolic compounds by a reaction of carbonyl compounds with carbon dioxide

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1 General Information

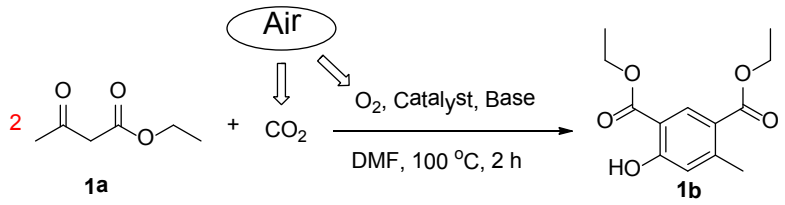
Methods. All manipulations were performed under an air atmosphere unless otherwise statement. Column chromatography was performed on silica gel (300−400 mesh). NMR spectra were obtained using a Bruker Avance 500 spectrometer (^{1}H at 500 MHz and ^{13}C at 125 MHz). Chemical shifts for ^{1}H NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$: δ 7.26 ppm). Chemical shifts for ^{13}C NMR spectra are reported in parts per million (ppm) from tetramethylsilane with the solvent as the internal standard ($CDCl_3$: δ 77.0 ppm). High resolution mass spectra (HRMS) were recorded on the Exactive Mass Spectrometer (Thermo Scientific, USA) equipped with ESI ionization source.

Materials. Unless stated otherwise, commercial reagents were used without further purification. All reagents were weighed and handled in air at room temperature.

2 General Experimental Procedure

The reaction mixture of carbonyl compounds **1** (0.6 mmol), $Pd(OAc)_2$ (6.7 mg, 5 mol %), K_2CO_3 (41.4 mg, 0.5 eq) and DMF (1 mL) in a 10 mL flask was stirred at 100 ^{o}C under an air atmosphere and monitored periodically by TLC. Upon completion, the reaction mixture was diluted with water (30 mL) and extracted with ethyl acetate (3 × 30 mL). The combined organic layers were washed with water and brine, dried over Na_2SO_4 and filtered. The solvent was removed under vacuum. The residue was purified by flash column chromatography to afford the product.

3 Optimization of Reaction Condtions[a]

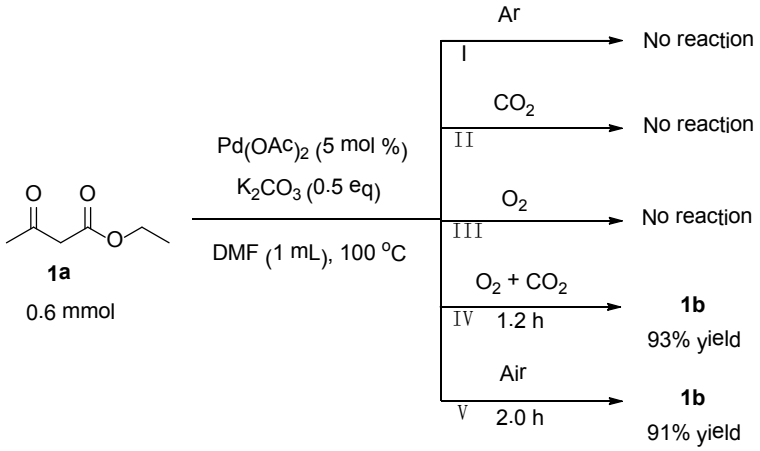


Entry	Catalyst	Base	Yield [%][b]
1	**$Pd(OAc)_2$**	**K_2CO_3 (0.5 eq)**	**91**
2	$Pd(OAc)_2$	K_2CO_3 (0.2 eq)	43
3	$Pd(OAc)_2$	K_2CO_3 (1.0 eq)	66
2	$InCl_3$	K_2CO_3	0
3	$In(OTf)_3$	K_2CO_3	0
4	$FeCl_3$	K_2CO_3	20
5	$Fe(OTf)_3$	K_2CO_3	28
6	$CuCl_2$	K_2CO_3	0
7	$Cu(OTf)_2$	K_2CO_3	0
8	CuCl	K_2CO_3	0
9	$BiCl_3$	K_2CO_3	31
10	$Pd(OAc)_2$	Cs_2CO_3	56
11	$Pd(OAc)_2$	$NaHCO_3$	47
12	$Pd(OAc)_2$	CH_3COONa	0
13	$Pd(OAc)_2$	$HOCH_2CH_2NH_2$	0
14	$Pd(OAc)_2$	KOH	0

[a] Reaction conditions: **1a** (0.6 mmol), air (1 atm), catalyst (5 mol %), base (0.5 equiv), DMF (1 mL), 100 °C, 2 h. [b] Isolated yield of pure product based on **1a**.

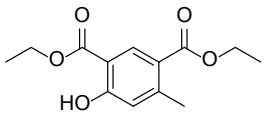
4 Contrast Experiment

In order to prove the CO_2 was come from the air, we did a series of control experiments. When the reaction was proceed under the Ar, CO_2, or O_2 atmosphere, there was no desired product observed. Interesting, the reaction were conducted well in the presence of the mixture of O_2 and CO_2, what is more, the yield of the product was slightly higher than in the air atmosphere. On the basis of the above experimental observations, we came to the conclusion that the CO_2 did participate in the reaction. Meanwhile, O_2 played an important role in this process.



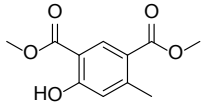
Scheme 1 I. In the presence of Argon. II. In the presence of CO_2. III. In the presence of O_2. IV. In the presence of O_2 (20%) and CO_2 (80%). V. In the presence of air.

5 Characterization of the Compounds



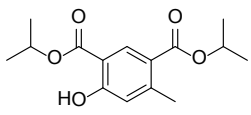
1b

Diethyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.09 (s, 1H), 8.47 (s, 1H), 6.83 (s, 1H), 4.43 (q, *J* = 7.1 Hz, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.60 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.70, 166.50, 163.80, 149.02, 133.73, 121.42, 120.26, 110.38, 61.66, 60.70, 22.46, 14.36, 14.20; **HRMS** (m/z) (ESI): calcd for $C_{13}H_{16}O_5$[M-H$^+$]: 251.09187; found: 251.09267.



2b

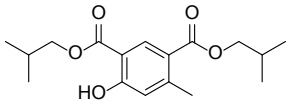
Dimethyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), white solid (mp 108-110 °C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.98 (s, 1H), 8.49 (s, 1H), 6.84 (s, 1H), 3.97 (s, 3H), 3.87 (s, 3H), 2.61 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.99, 166.67, 163.76, 149.46, 133.86, 120.91, 120.31, 110.08, 52.40, 51.75, 22.46; **HRMS** (m/z) (ESI): calcd for $C_{11}H_{12}O_5$ [M-H$^+$]: 223.06057; found: 223.06104.



3b

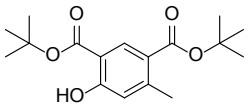
Diisopropyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.17 (s,

1H), 8.42 (s, 1H), 6.81 (s, 1H), 5.29 (sep, J = 6.3 Hz, 1H), 5.22 (sep, J = 6.3 Hz, 1H), 2.59 (s, 3H), 1.40 (d, J = 6.3 Hz, 6H), 1.37 (d, J = 6.2 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.28, 166.30, 163.71, 148.51, 133.66, 121.84, 120.14, 110.66, 69.62, 68.30, 22.59, 21.98, 21.80; **HRMS** (m/z) (ESI): calcd for $C_{15}H_{20}O_5$ [M-H$^+$]: 279.12317; found: 279.12399.



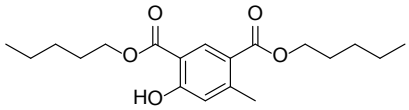
4b

Diisobutyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), pale yellow solid (mp 123-125 ^{o}C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.05 (s, 1H), 8.54 (s, 1H), 6.84 (s, 1H), 4.14 (d, J = 6.5 Hz, 2H), 4.07 (d, J = 6.4 Hz, 2H), 2.62 (s, 3H), 2.12-2.05 (m, 2H), 1.04 (d, J = 4.8 Hz, 6H), 1.03 (d, J = 4.8 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.61, 166.37, 163.77, 149.19, 133.81, 121.25, 120.25, 110.34, 71.40, 70.82, 27.88, 27.79, 22.51, 19.23, 19.03; **HRMS** (m/z) (ESI): calcd for $C_{17}H_{24}O_5$ [M-H$^+$]: 307.15447; found: 307.15546.



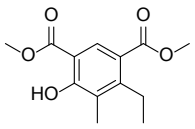
5b

Di-tert-butyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.22 (s, 1H), 8.35 (s, 1H), 6.77 (s, 1H), 2.56 (s, 3H), 1.61 (s, 9H), 1.59 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.35, 166.04, 163.65, 147.98, 133.96, 122.80, 120.06, 111.53, 83.17, 80.99, 28.32, 28.18, 22.54; **HRMS** (m/z) (ESI): calcd for $C_{17}H_{24}O_5$ [M-H$^+$]: 307.15447; found: 307.15531.



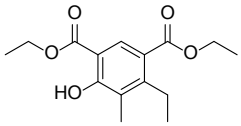
6b

Dipentyl 4-hydroxy-6-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.08 (s, 1H), 8.48 (s, 1H), 6.83 (s, 1H), 4.35 (t, J = 6.7 Hz, 2H), 4.28 (t, J = 6.7 Hz, 2H), 2.61 (s, 3H), 1.83-1.74 (m, 4H), 1.44-1.40 (m, 8H), 0.94 (t, J = 7.1, 3H), 0.93 (t, J = 7.1, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 169.71, 166.51, 163.75, 149.06, 133.78, 121.33, 120.23, 110.35, 65.73, 64.88, 28.39, 28.28, 28.19, 28.05, 22.51, 22.32, 22.28, 13.97, 13.93; **HRMS** (m/z) (ESI): calcd for $C_{19}H_{28}O_5$ [M-H$^+$]: 335.18577; found: 335.18668.



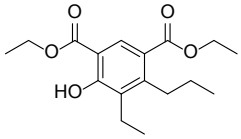
7b

Dimethyl 4-ethyl-6-hydroxy-5-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), white solid (mp 58-60 °C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.39 (s, 1H), 8.30 (s, 1H), 3.96 (s, 3H), 3.87 (s, 3H), 3.02 (q, *J* = 7.5 Hz, 2H), 2.26 (s, 3H), 1.19 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.52, 167.49, 162.21, 152.25, 130.73, 125.75, 120.99, 109.05, 52.37, 51.86, 24.05, 14.09, 10.80; **HRMS** (m/z) (ESI): calcd for $C_{13}H_{16}O_5$ [M-H$^+$]: 251.09187; found: 251.09244.



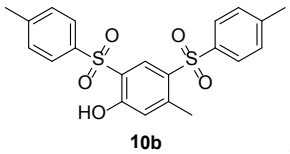
8b

Diethyl 4-ethyl-6-hydroxy-5-methylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), white solid (mp 84-86 °C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.49 (s, 1H), 8.25 (s, 1H), 4.42 (q, *J* = 7.2 Hz, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.99 (q, *J* = 7.5 Hz, 2H), 2.26 (s, 3H), 1.42 (t, *J* = 7.0 Hz, 3H), 1.39 (t, *J* = 7.0 Hz, 3H), 1.19 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.22, 167.52, 162.18, 151.62, 130.42, 125.62, 121.70, 109.35, 61.61, 60.80, 24.10, 14.31, 14.20, 14.17, 10.83; **HRMS** (m/z) (ESI): calcd for $C_{15}H_{20}O_5$ [M-H$^+$]: 279.12317; found: 279.12354.



9b

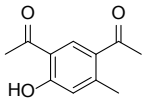
Diethyl 5-ethyl-4-hydroxy-6-propylisophthalate. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.45 (s, 1H), 8.25 (s, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 2.95-2.91 (m, 2H), 2.74 (q, *J* = 7.5 Hz, 2H), 1.60-1.52 (m, 2H), 1.42 (t, *J* = 6.5 Hz, 3H), 1.39 (t, *J* = 6.5 Hz, 3H), 1.15 (t, *J* =. 7.5 Hz, 3H), 1.03 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.21, 167.60, 162.08, 149.63, 130.62, 126.38, 121.98, 109.48, 61.55, 60.77, 32.21, 24.69, 19.00, 14.56, 14.31, 14.20, 13.89; **HRMS** (m/z) (ESI): calcd for $C_{17}H_{24}O_5$ [M-H$^+$]: 307.15447; found: 307.15536



10b

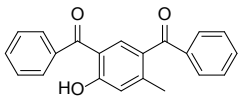
5-Methyl-2,4-ditosylphenol. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow solid (mp 98-100 °C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.71 (s, 1H),

8.49 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.81 (s, 1H), 2.44 (s, 3H), 2.41 (s, 3H), 2.35 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.06, 146.44, 145.55, 144.40, 137.86, 137.65, 132.17, 131.69, 130.36, 129.81, 127.74, 127.05, 122.64, 122.14, 21.65, 21.56, 20.42; **HRMS** (m/z) (ESI): calcd for $C_{21}H_{20}O_5S_2$ [M-H$^+$]: 415.06732; found: 415.06833.



11b

1,1'-(4-hydroxy-6-methyl-1,3-phenylene)Diethanone[1]. Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow solid (mp 106-108 ^{o}C): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 12.53 (s, 1H), 8.16 (s, 1H), 6.81 (s, 1H), 2.66 (s, 3H), 2.58 (s, 3H), 2.57 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 203.49, 198.28, 164.54, 149.30, 133.51, 128.85, 121.54, 115.63, 28.93, 26.27, 22.68; **HRMS** (m/z) (ESI): calcd for $C_{11}H_{12}O_3$ [M-H$^+$]: 191.07074; found: 191.07127.



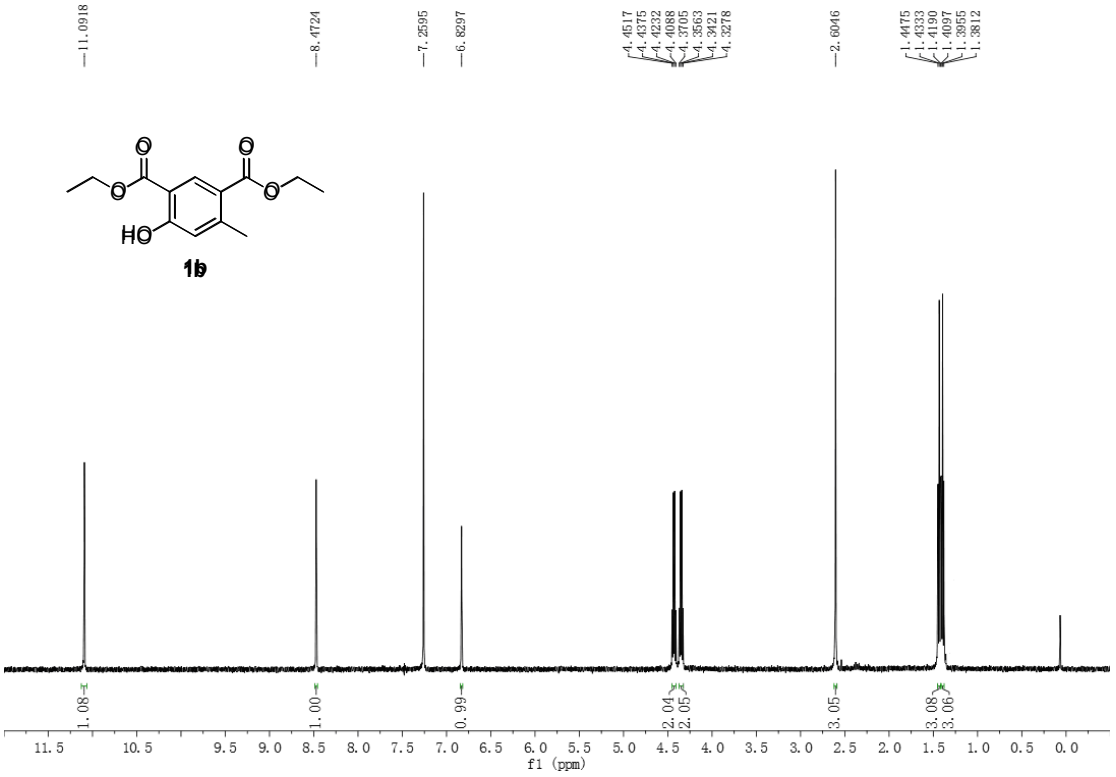
12b

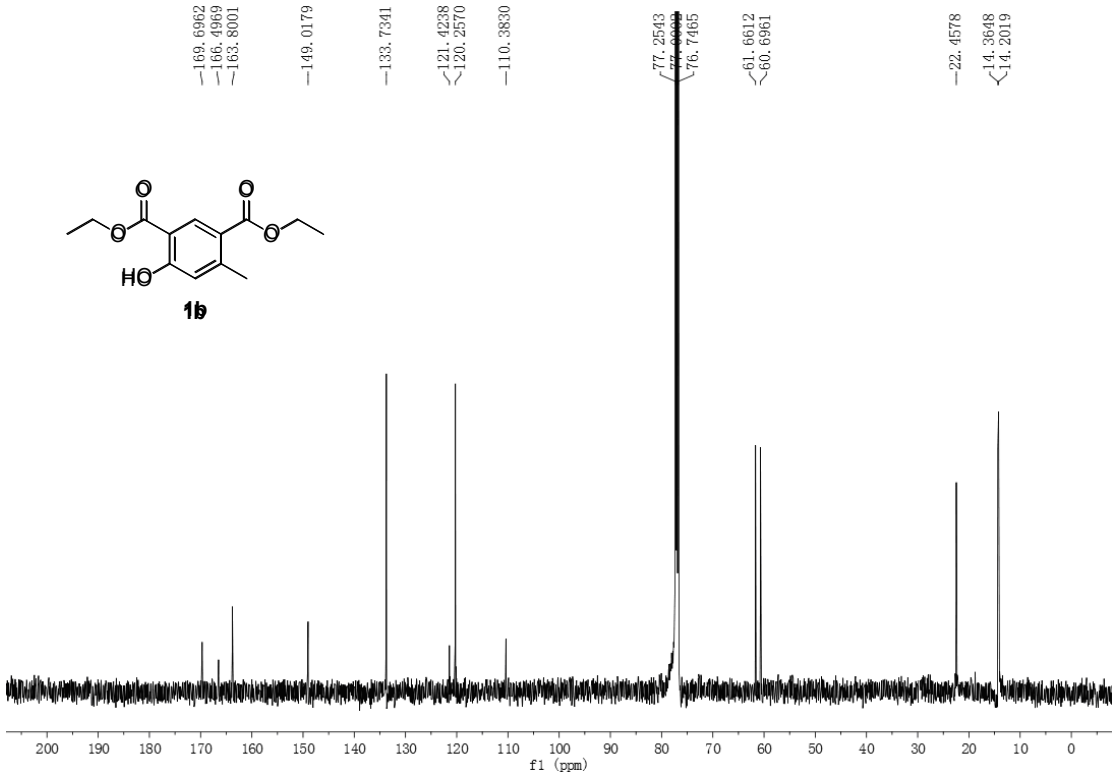
(4-hydroxy-6-methyl-1,3-phenylene)bis(phenylmethanone). Isolated by column chromatography (silica gel, PE /EA = 50/1), yellow oil: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 12.25 (s, 1H), 9.95 (s, 1H), 7.91-6.92 (m, 10H), 6.81 (s, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 200.95, 158.90, 145.86, 139.84, 139.66, 139.06, 132.87, 128.90, 128.79, 128.65, 128.19, 127.05, 122.02, 121.64, 113.26, 22.47; **HRMS** (m/z) (ESI): calcd for $C_{21}H_{16}O_3$ [M-H$^+$]: 315.10204; found: 315.10306.

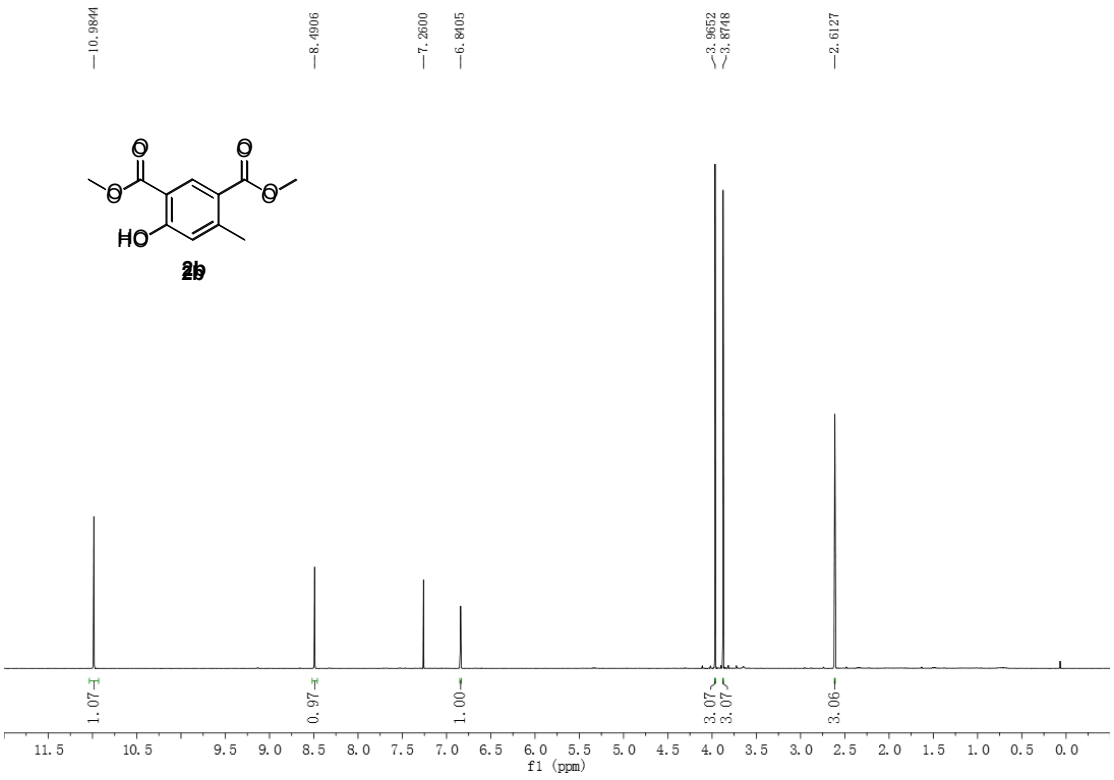
6 References

1. W. Su and C. Jin, *Synthetic commun.,* 2004, **34**, 4199.

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



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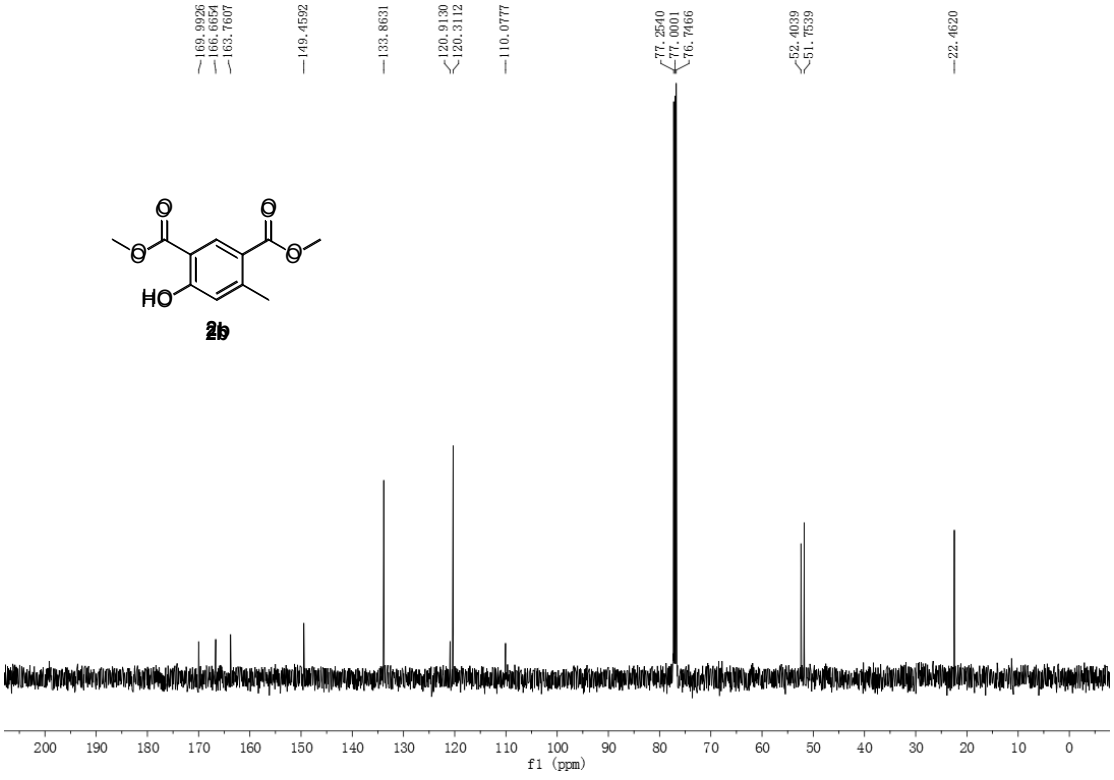
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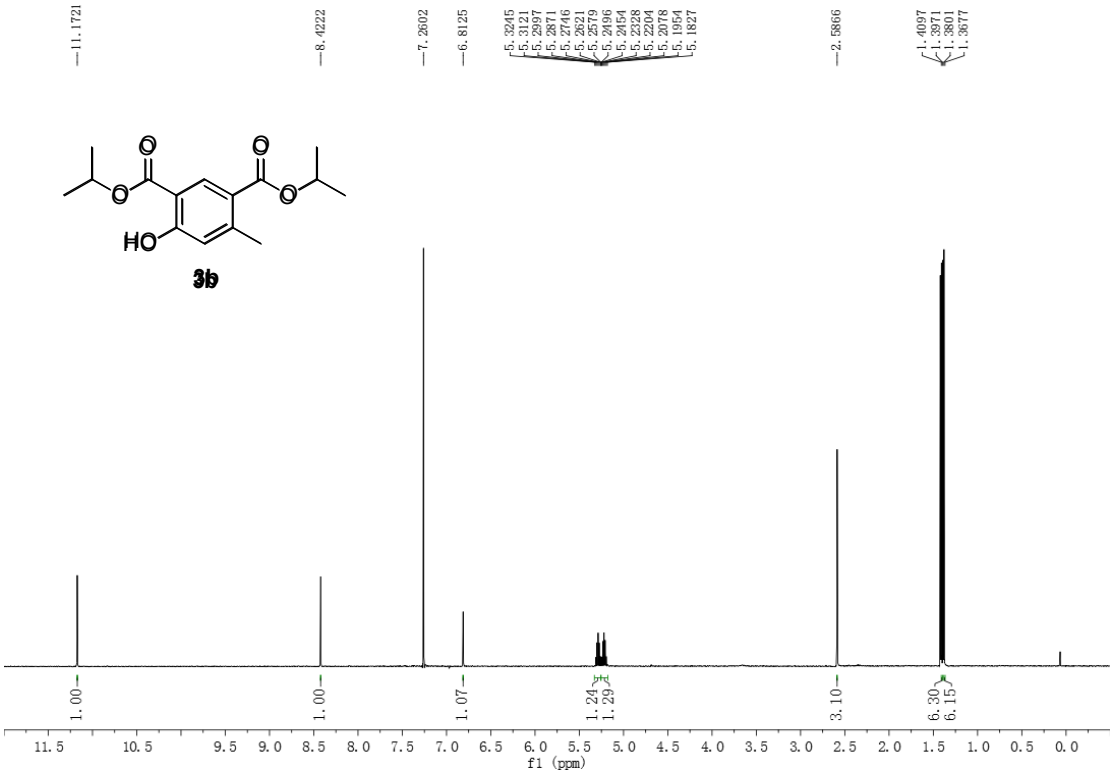
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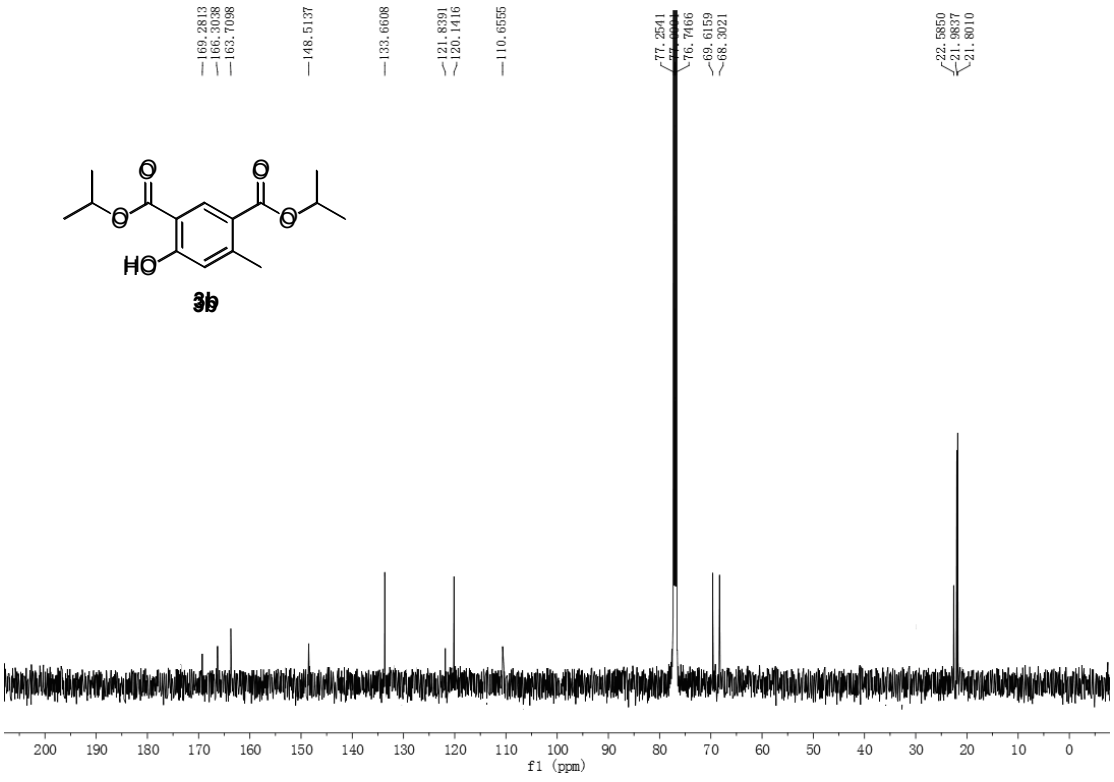
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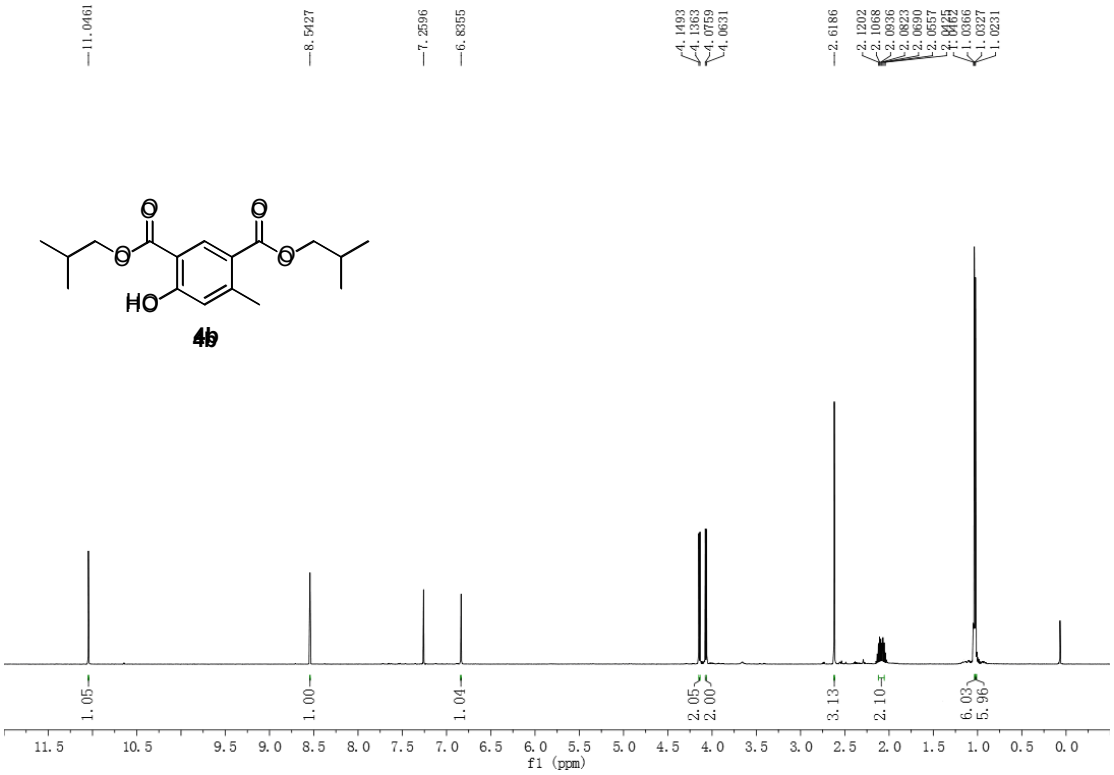
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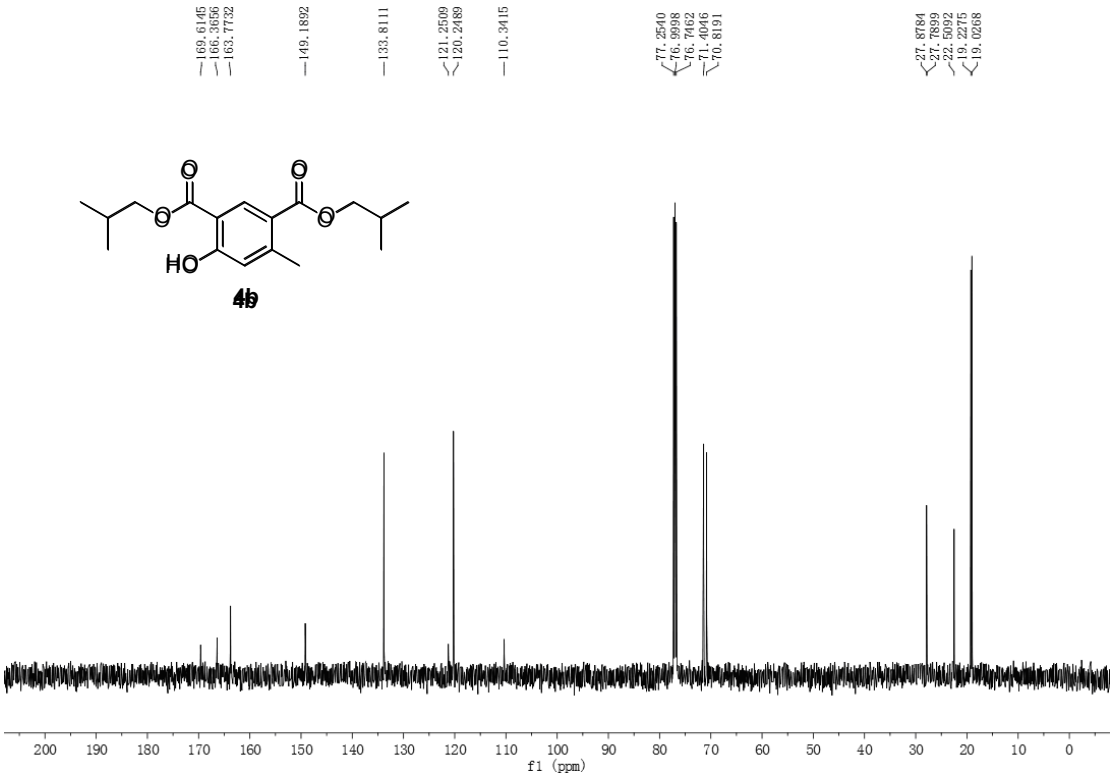
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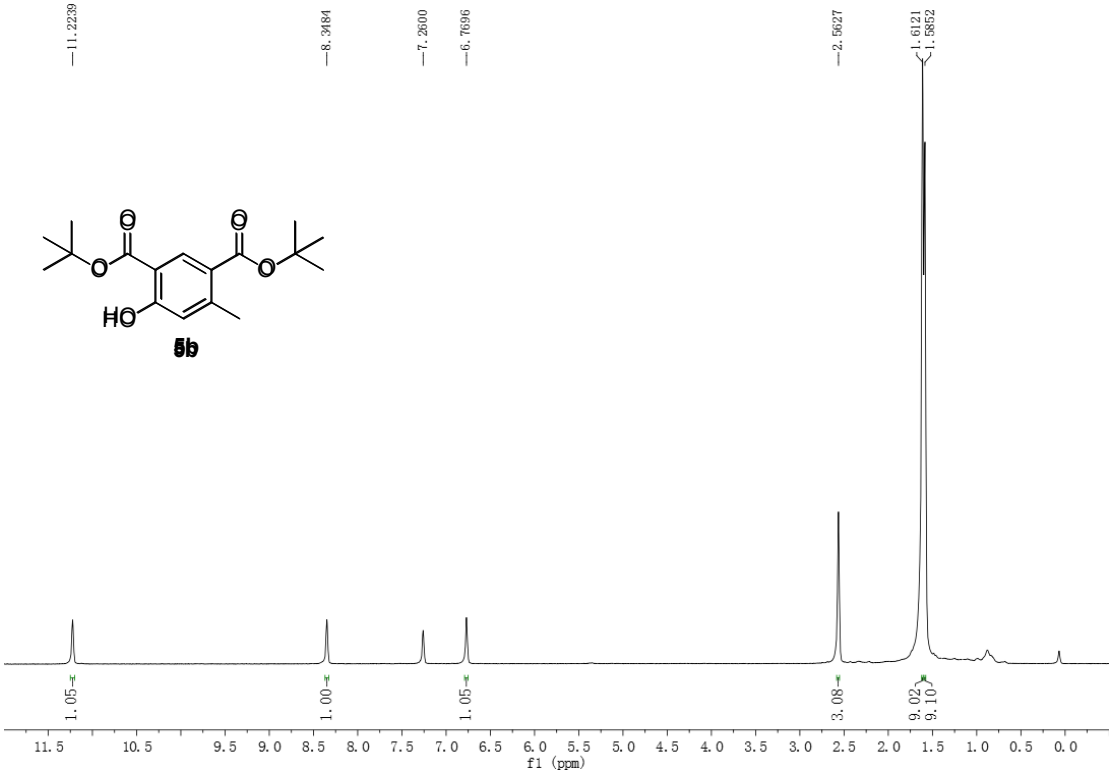
149.1892
133.8111
121.2509
120.2489
110.3415
77.2540
76.9998
76.7462
71.4046
70.8191
27.8784
27.7899
22.5092
19.2275
19.0268
HO
4b
f1 (ppm)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7.2600
6.7696
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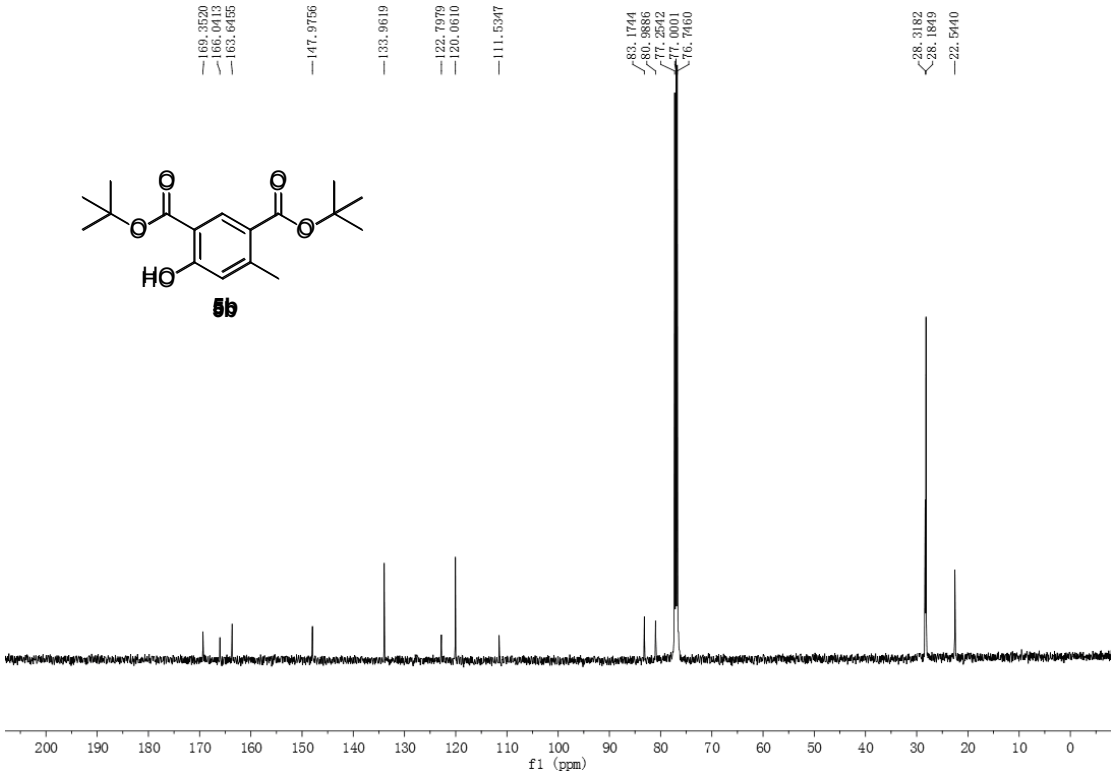
1.5852
1.05
1.00
1.05
3.08
9.02
9.10
f1 (ppm)

5b


169.3520
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163.6455
147.9756
133.9619
122.7979
120.0610
111.5347
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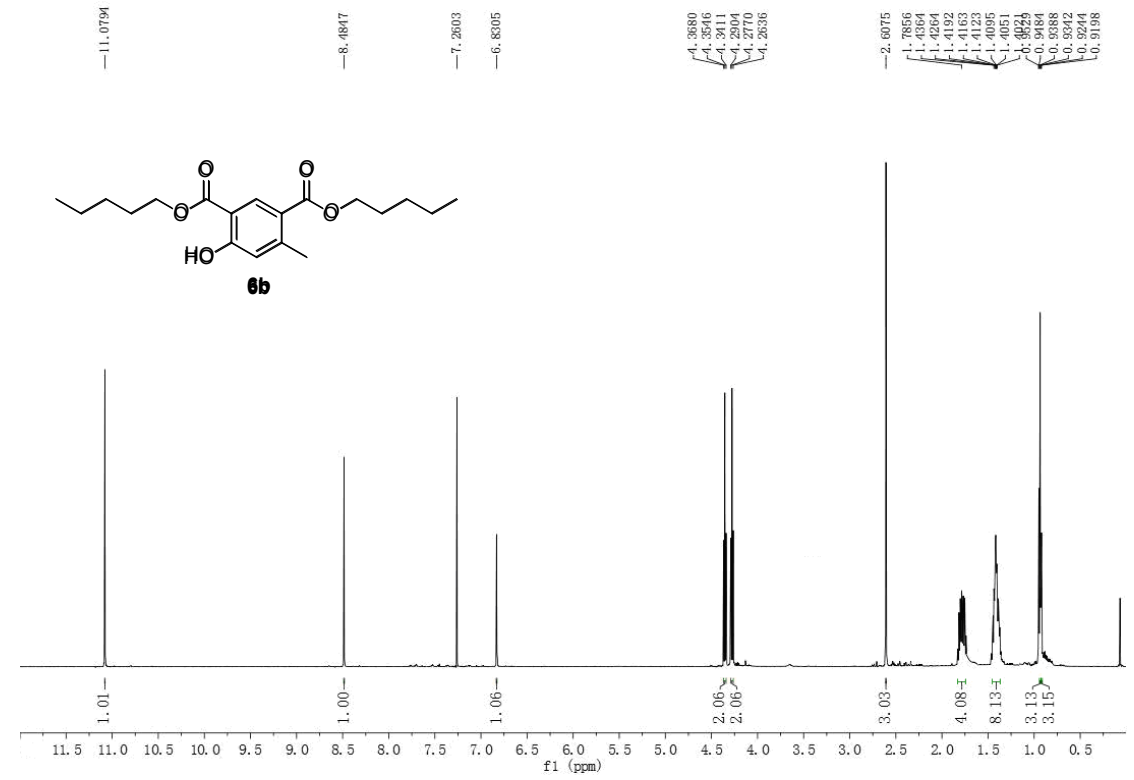
80.9886
77.2542
77.0001
76.7460
28.3182
28.1849
22.5440
f1 (ppm)

5b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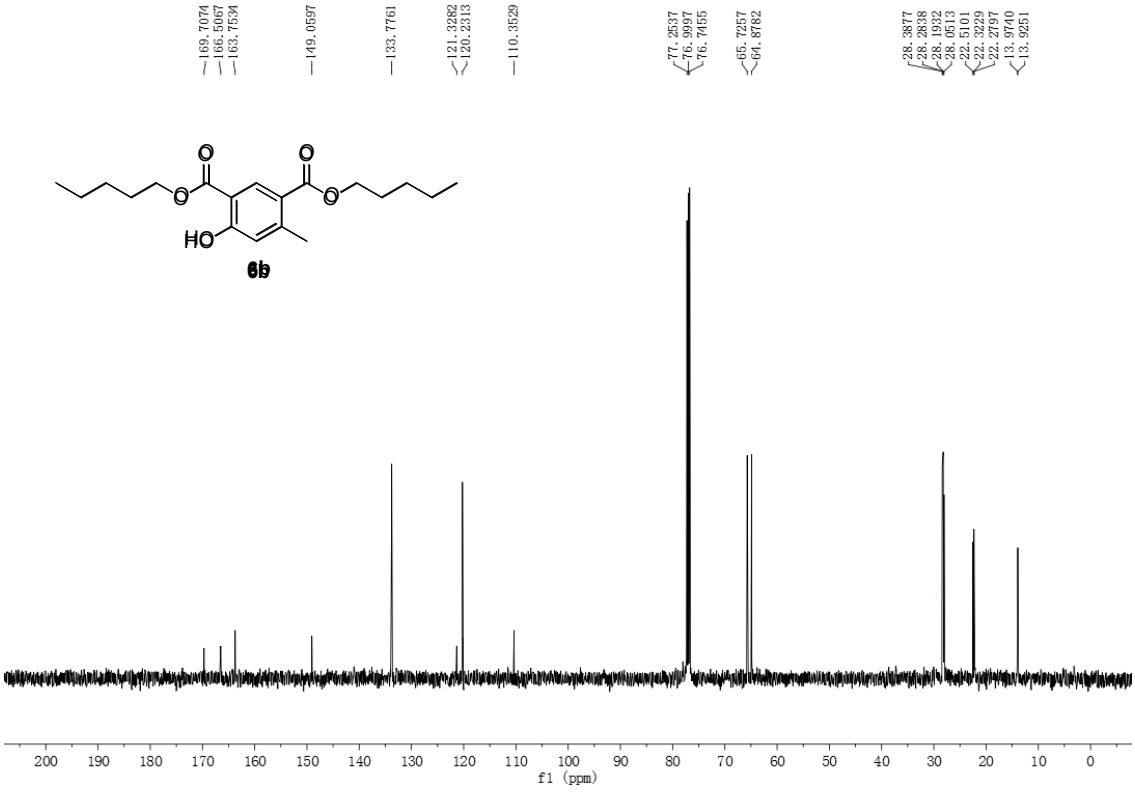
7.2603
6.8305
4.3680
4.3546
4.3411
4.2904
4.2770
4.2636
2.6075
1.7856
1.4364
1.4264
1.4192
1.4163
1.4123
1.4095
1.4051
0.9829
0.9484
0.9388
0.9342
0.9244
0.9198
HO
6b
1.01
1.00
1.06
2.06
2.06
3.03
4.08
8.13
3.13
3.15
f1 (ppm)


169.7074
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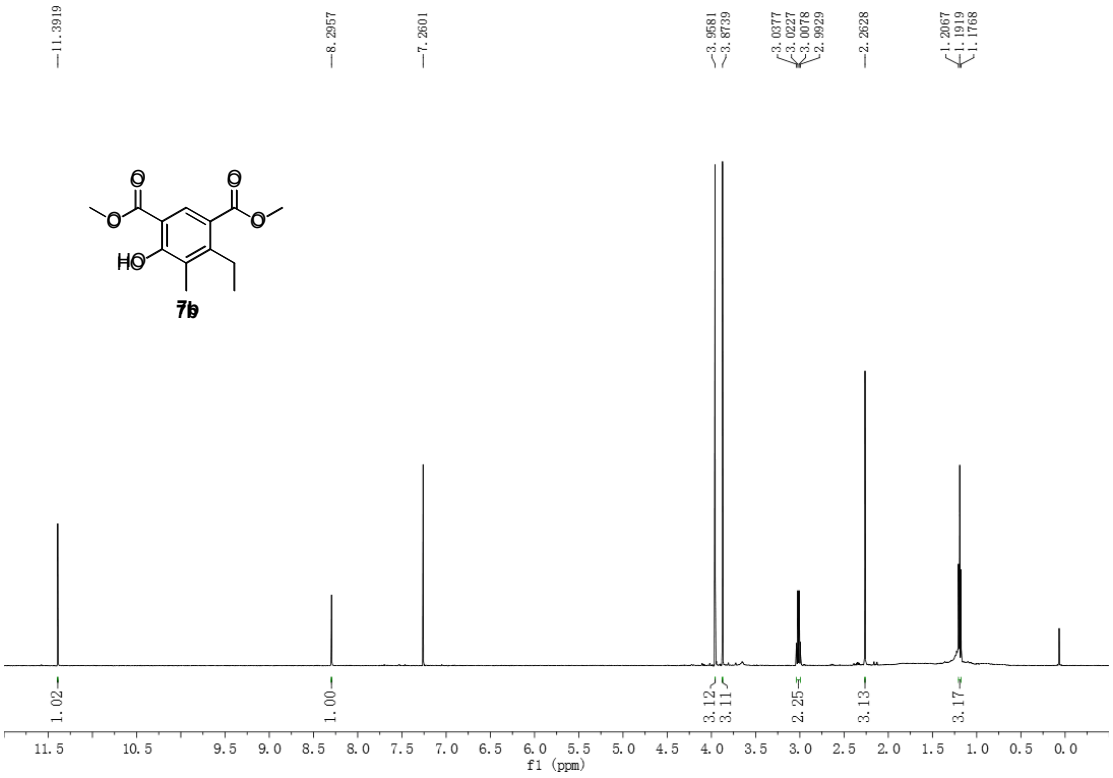
163.7534
149.0597
133.7761
121.3282
120.2313
110.3529
77.2537
76.9997
76.7455
65.7257
64.8782
28.3877
28.2838
28.1932
28.0513
22.5101
22.3229
22.2797
13.9740
13.9251
HO
6b
f1 (ppm)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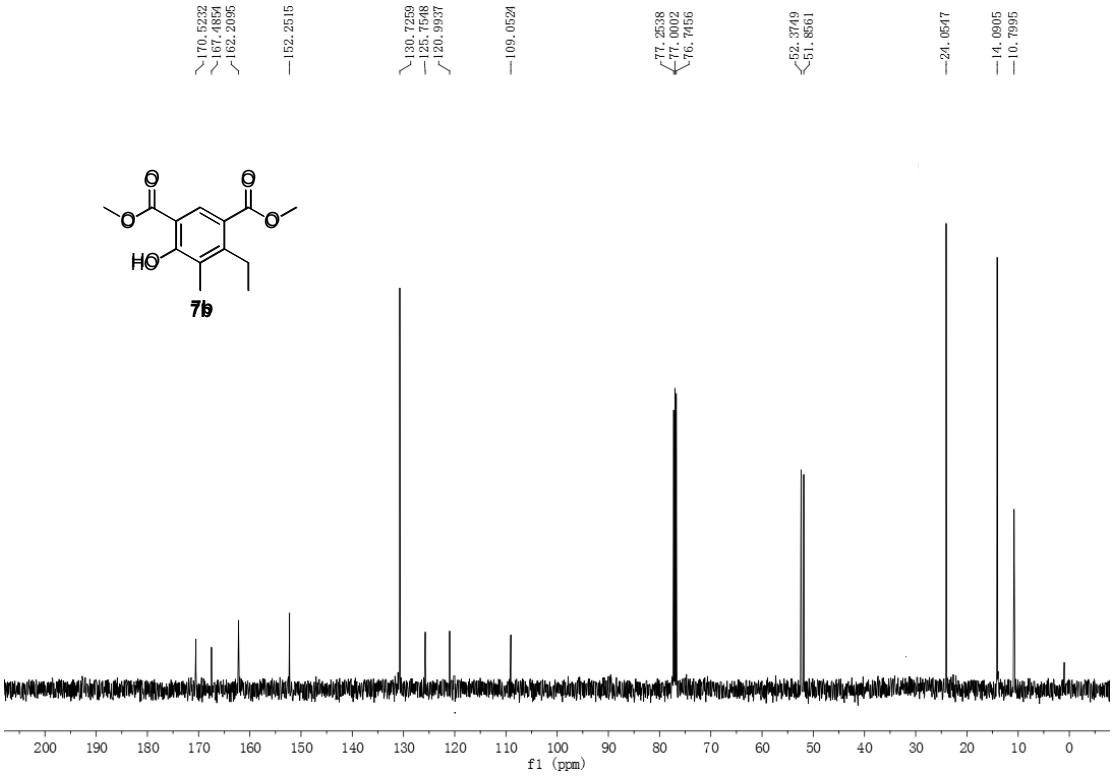
8.2957
7.2601
3.9681
3.8739
3.0377
3.0227
3.0078
2.9929
2.2628
1.2067
1.1919
1.1768
HO
7b
1.02
1.00
3.12
3.11
2.25
3.13
3.17
f1 (ppm)


170.5232
167.4854
162.2095
152.2515
130.7259
125.7548
120.9937
109.0524
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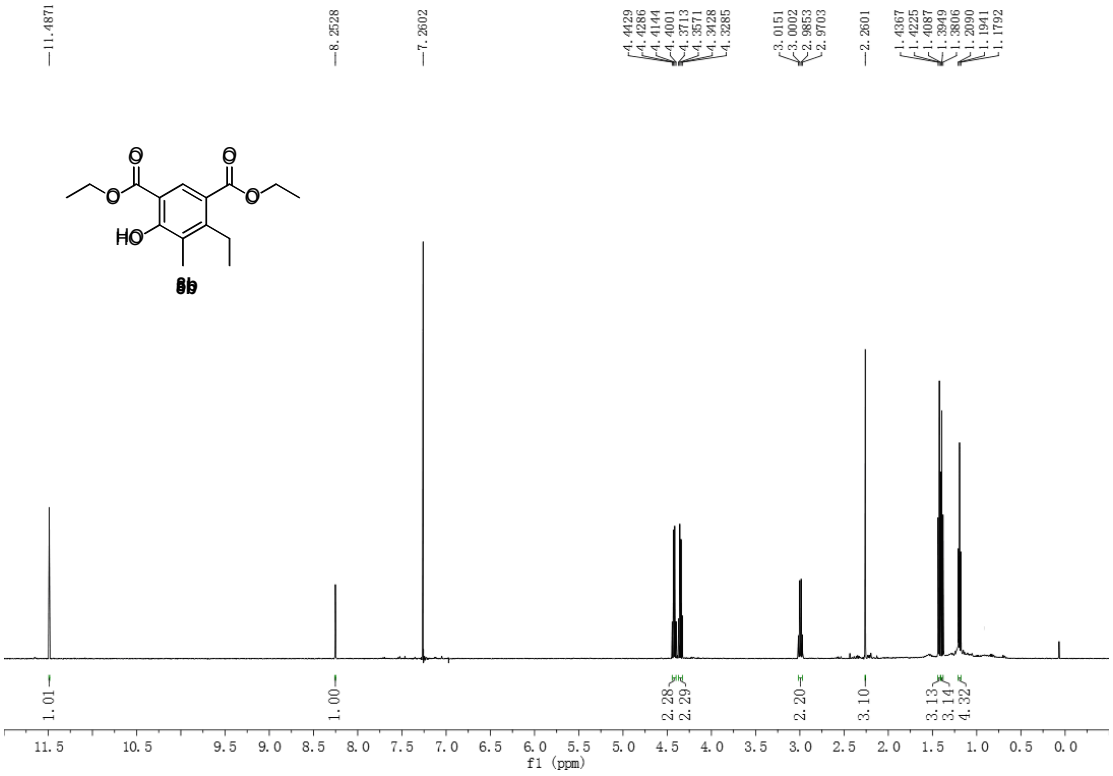
77.0002
76.7456
52.3749
51.8561
24.0547
14.0905
10.7995
HO
7b
f1 (ppm)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7.2602
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4.4001
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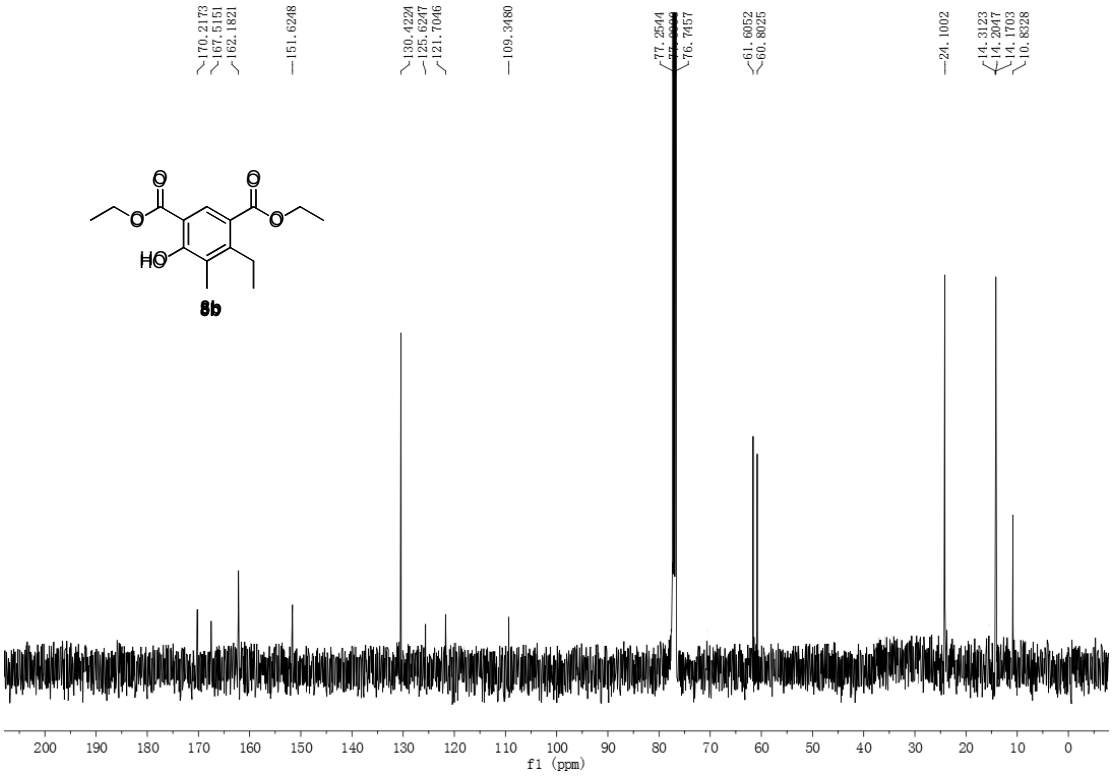
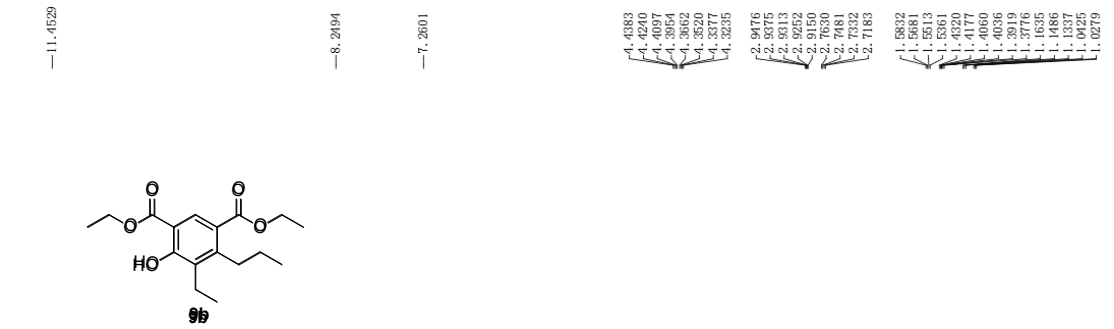
4.3571
4.3428
4.3285
3.0151
3.0002
2.9853
2.9703
2.2601
1.4367
1.4225
1.4087
1.3949
1.3806
1.2090
1.1941
1.1792
HO
8b
1.01
1.00
2.28
2.29
2.20
3.10
3.13
3.14
4.32
f1 (ppm)


170.2173
167.5151
162.1821
151.6248
130.4224
125.6247
121.7046
109.3480
77.2544
76.7457
61.6052
60.8025
24.1002
14.3123
14.2947
14.1703
10.8328
HO
8b
f1 (ppm)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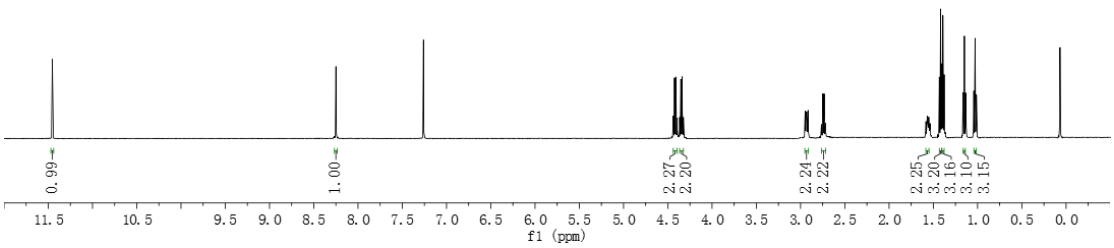
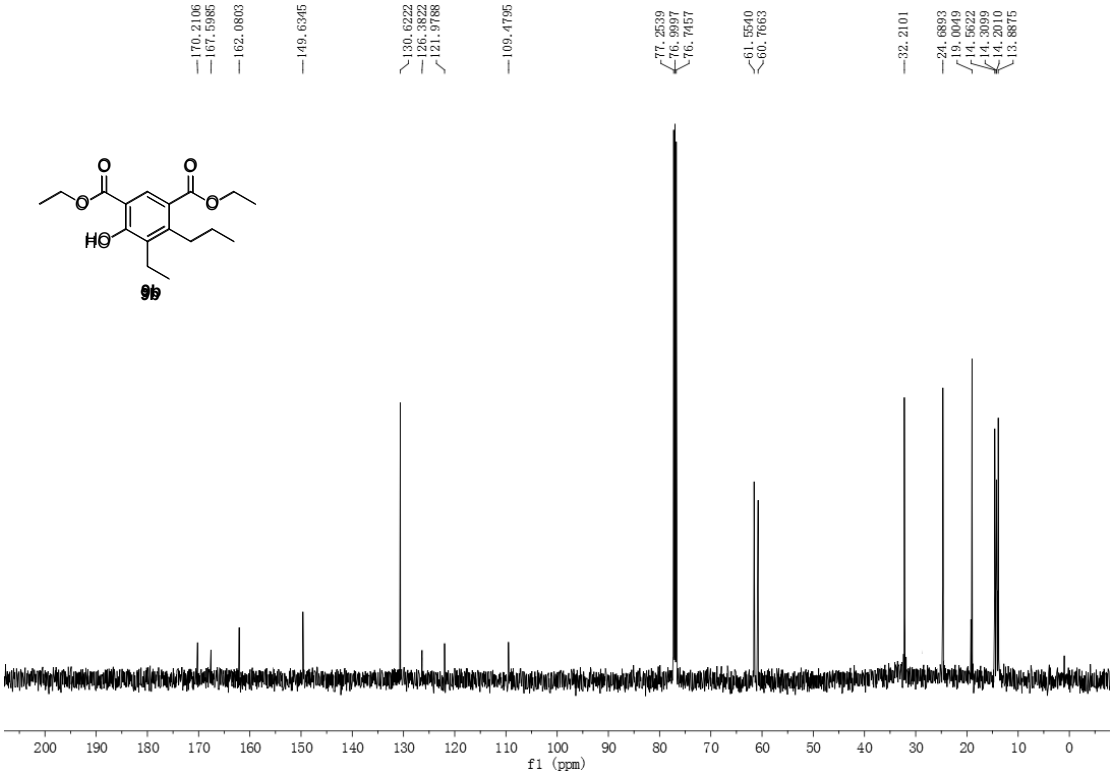
7.2601
4.4383
4.4240
4.4097
4.3954
4.3662
4.3520
4.3377
4.3235
2.9476
2.9375
2.9113
2.9252
2.9150
2.7630
2.7481
2.7332
2.7183
1.5832
1.5681
1.5513
1.5361
1.4320
1.4177
1.4060
1.4036
1.3919
1.3776
1.1635
1.1486
1.1337
1.0425
1.0279

O
O
O
O
HO

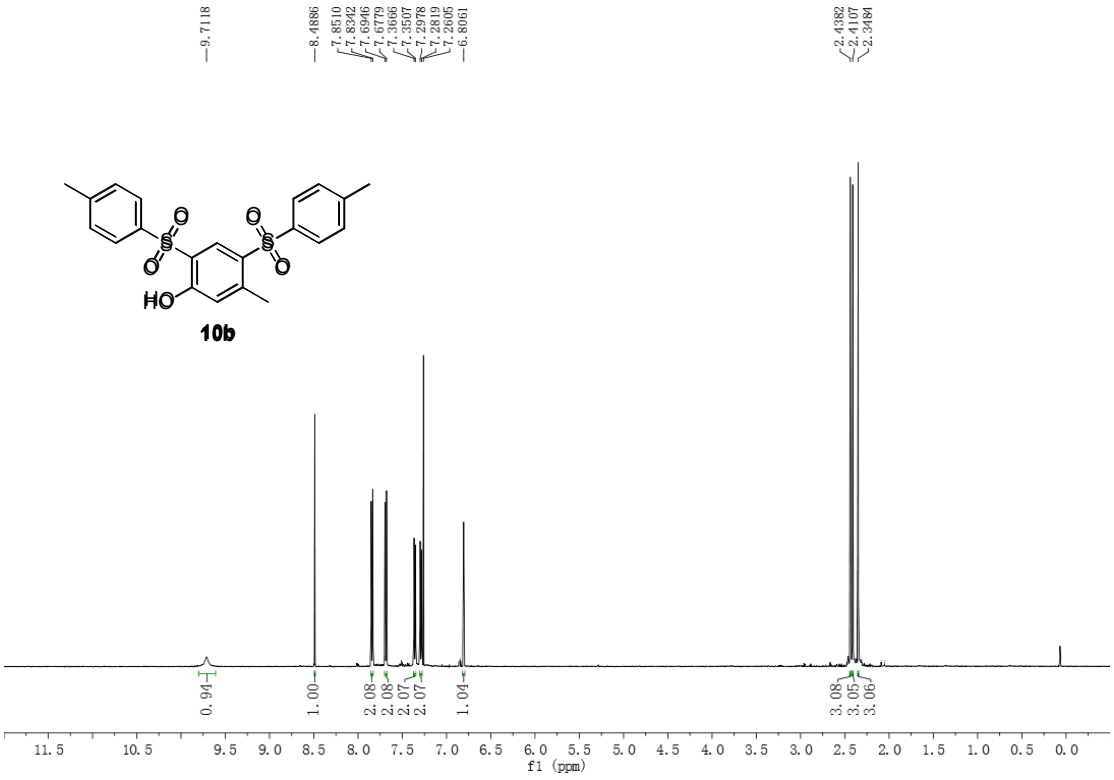
9b

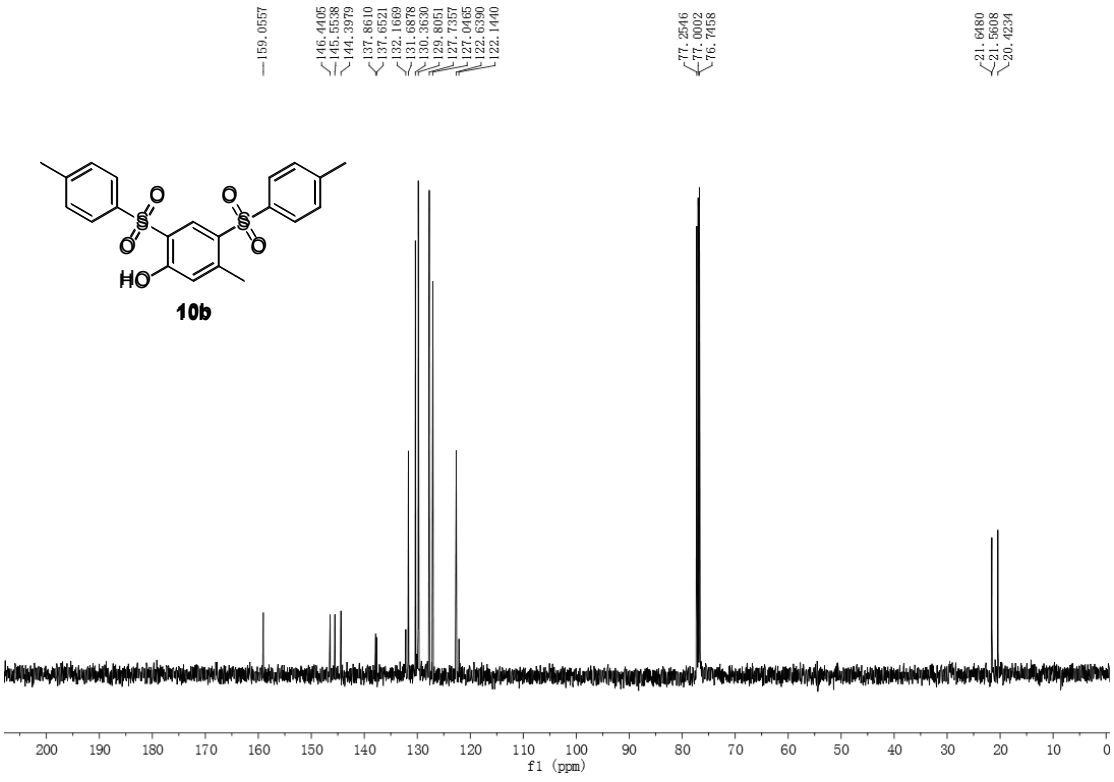

0.99
1.00
2.27
2.20
2.24
2.22
2.25
3.20
3.16
3.10
3.15
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

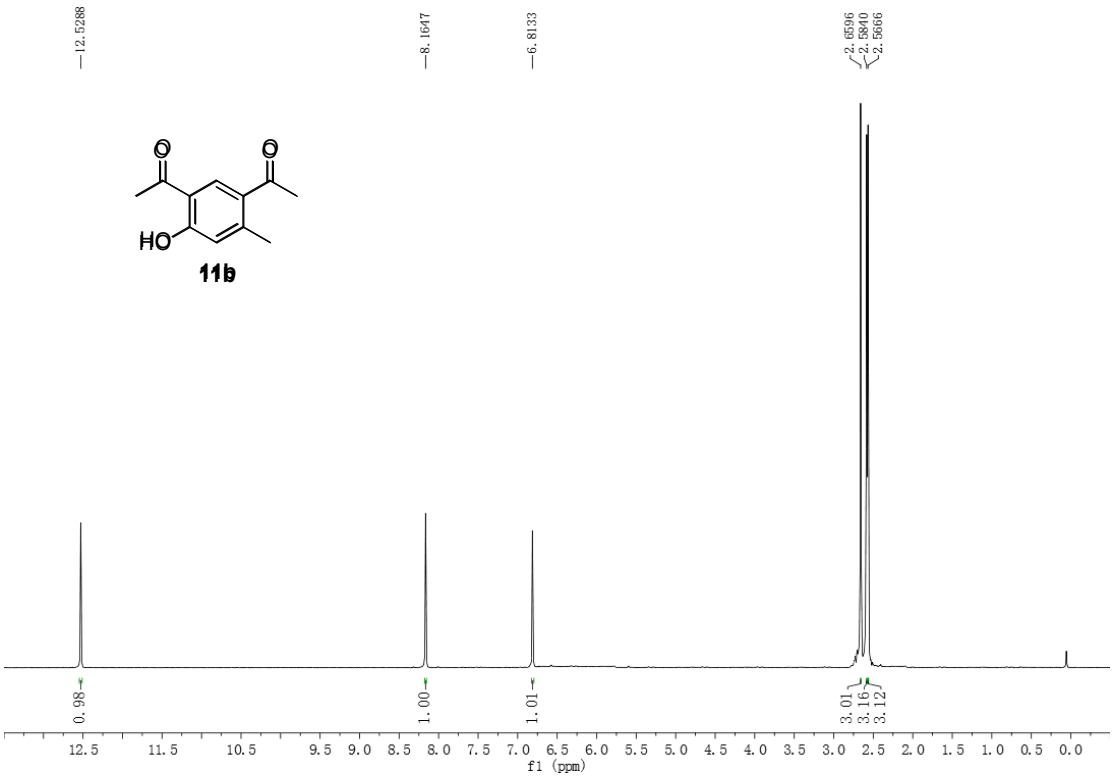

170.2106
167.5985
162.0803
149.6345
130.6222
126.3822
121.9788
109.4795
77.2539
76.9997
76.7457
61.5540
60.7663
32.2101
24.6893
19.0049
14.5622
14.3099
14.2010
13.8875
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

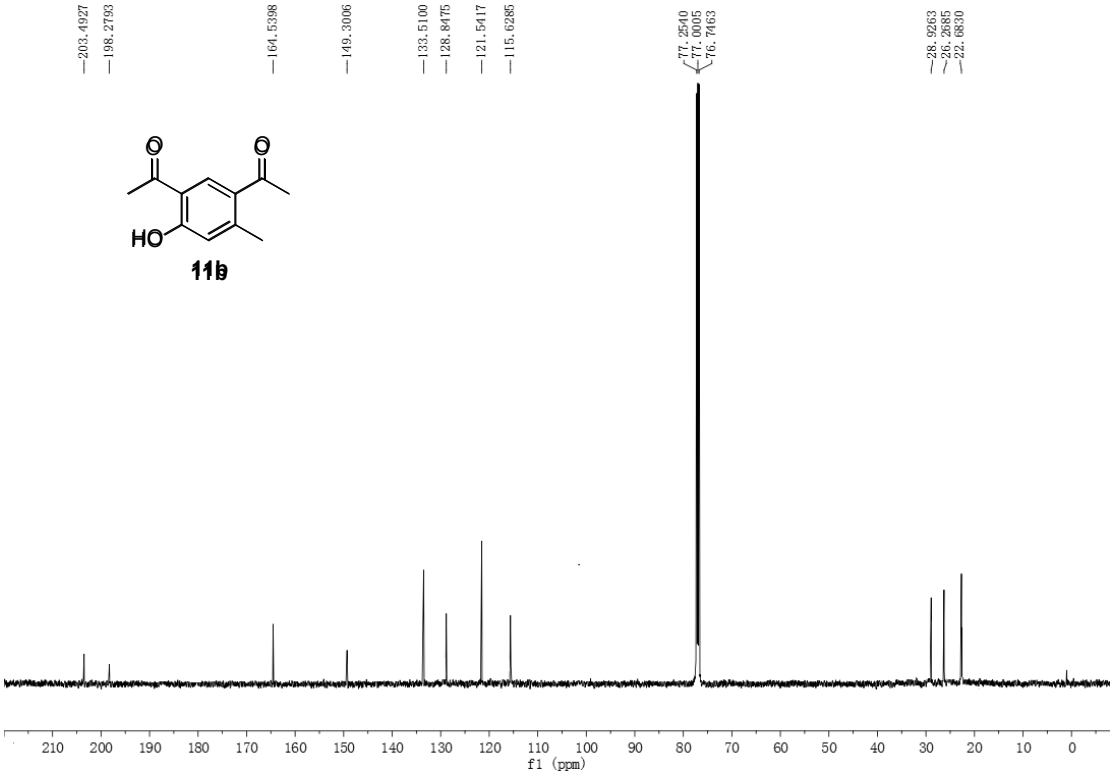
O
O
O
O
HO

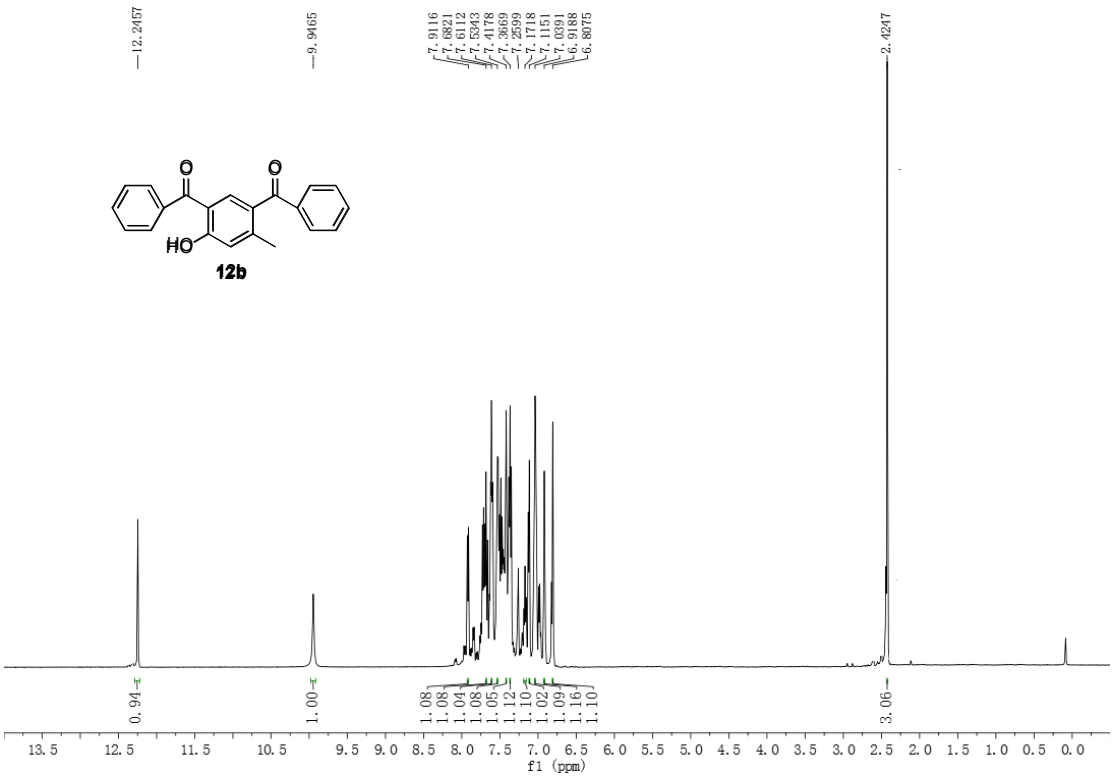
9b

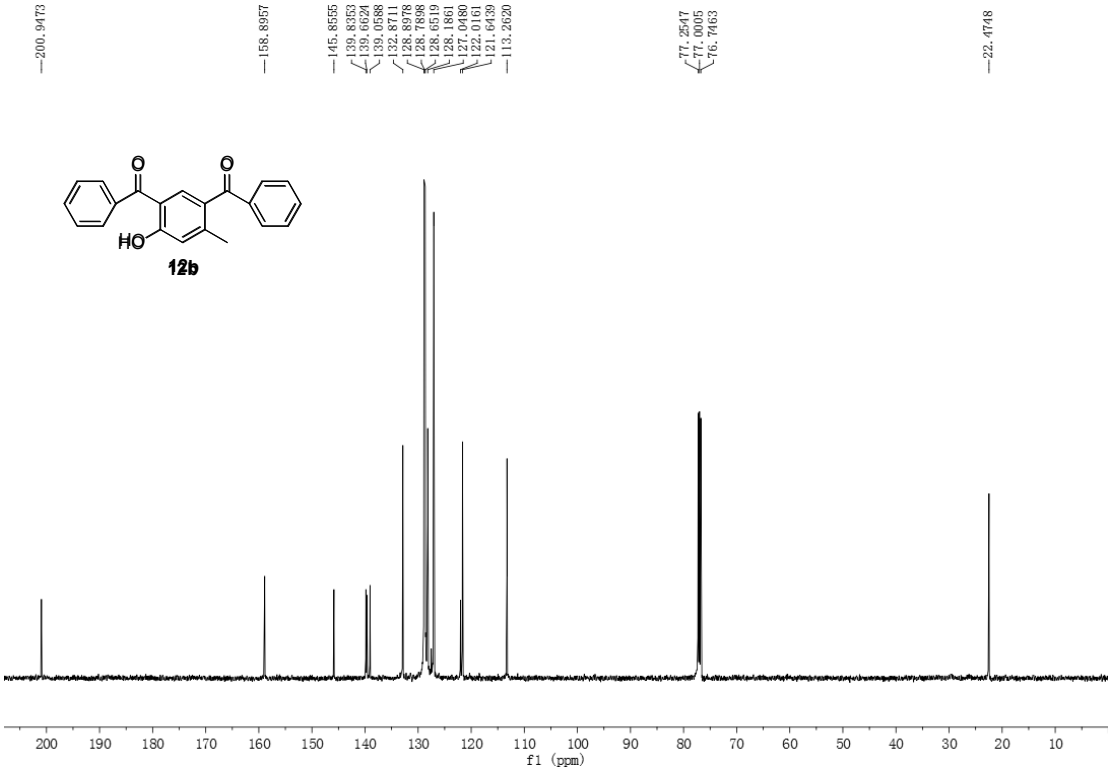

9.7118
8.4886
7.8510
7.8342
7.6946
7.6779
7.3666
7.3507
7.2978
7.2819
7.2605
6.8061
2.4382
2.4107
2.3494
HO
10b
0.94
1.00
2.08
2.08
2.07
2.07
1.04
3.08
3.05
3.06
f1 (ppm)


159.0557
146.4405
145.5538
144.3979
137.8610
137.6521
132.1669
131.6878
130.3630
129.8051
127.7357
127.0465
122.6390
122.1440
77.2546
77.0002
76.7458
21.6480
21.5608
20.4234
HO
10b
f1 (ppm)


12.5288
8.1647
6.8133
2.6596
2.5840
2.5666
HO
11b
0.98
1.00
1.01
3.01
3.16
3.12
f1 (ppm)


203.4927
198.2793
164.5398
149.3006
133.5100
128.8475
121.5417
115.6285
77.2540
77.0005
76.7463
28.9263
26.2685
22.6830
HO
11b
f1 (ppm)


12.2457
9.9465
7.9116
7.6821
7.6112
7.5343
7.4178
7.3669
7.2599
7.1718
7.1151
7.0391
6.9188
6.8075
2.4247
O
O
HO
12b
0.94
1.00
1.08
1.08
1.04
1.08
1.05
1.12
1.10
1.02
1.09
1.16
1.10
3.06
f1 (ppm)


200.9473
158.8957
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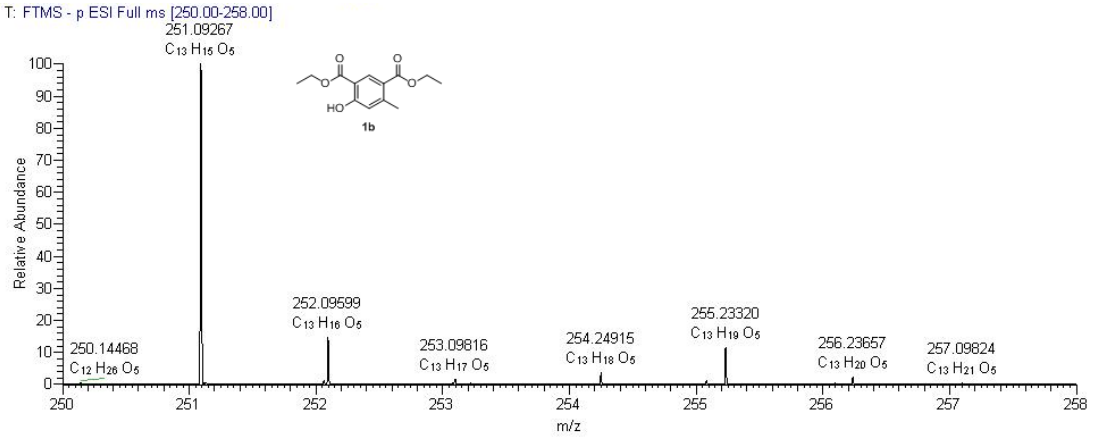
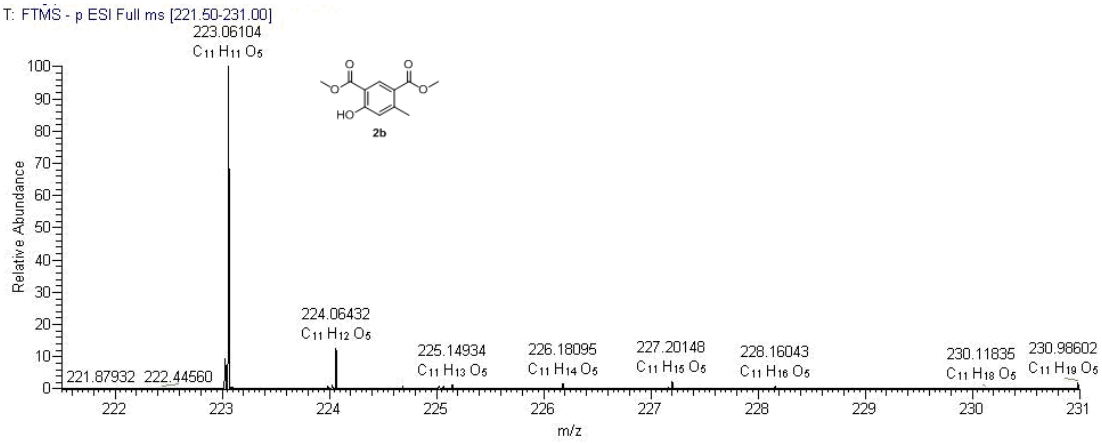
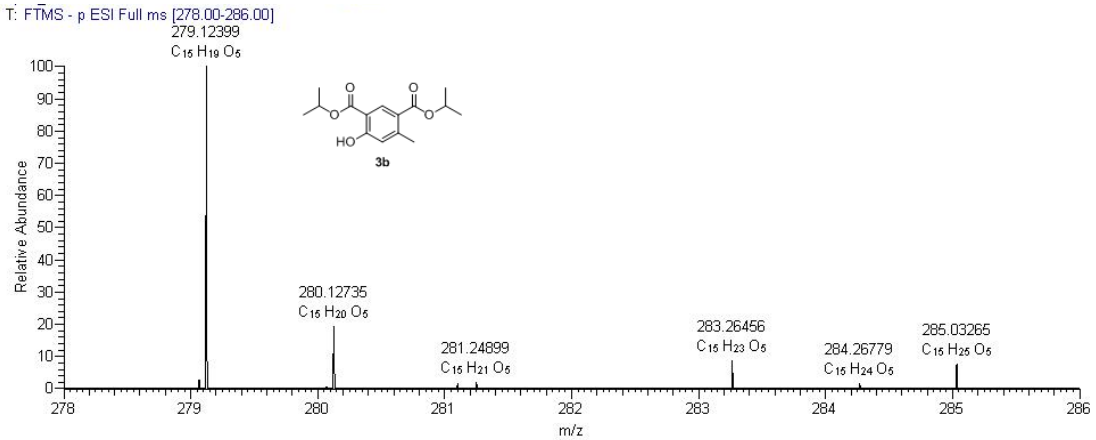
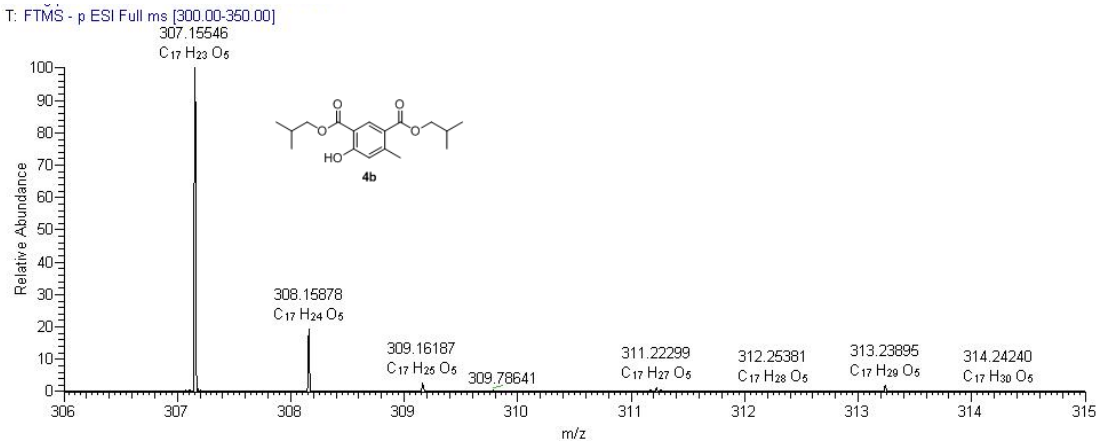
139.8353
139.6624
139.0588
132.8711
128.8978
128.7698
128.6519
128.1861
127.0480
122.0161
121.6439
113.2620
77.2547
77.0005
76.7463
22.4748
O
O
HO
12b
f1 (ppm)

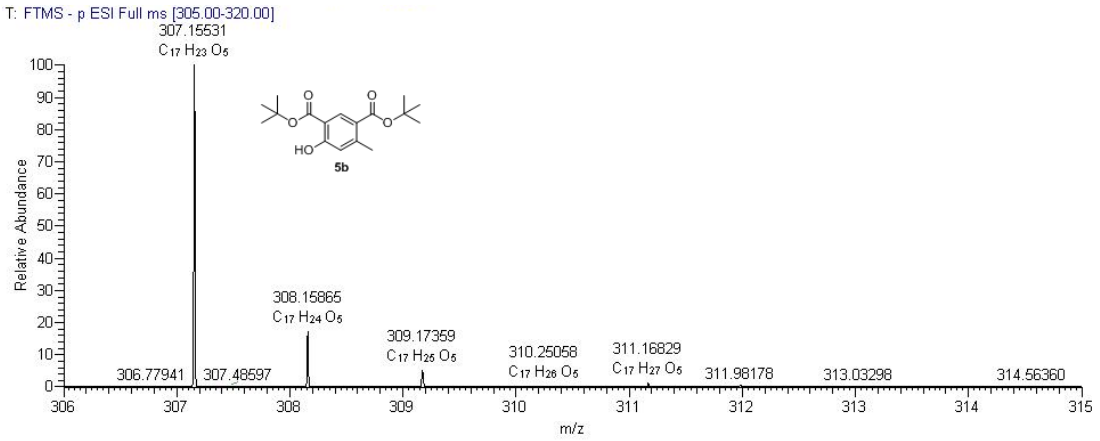
8 Copies of HRMS Spectra of Products

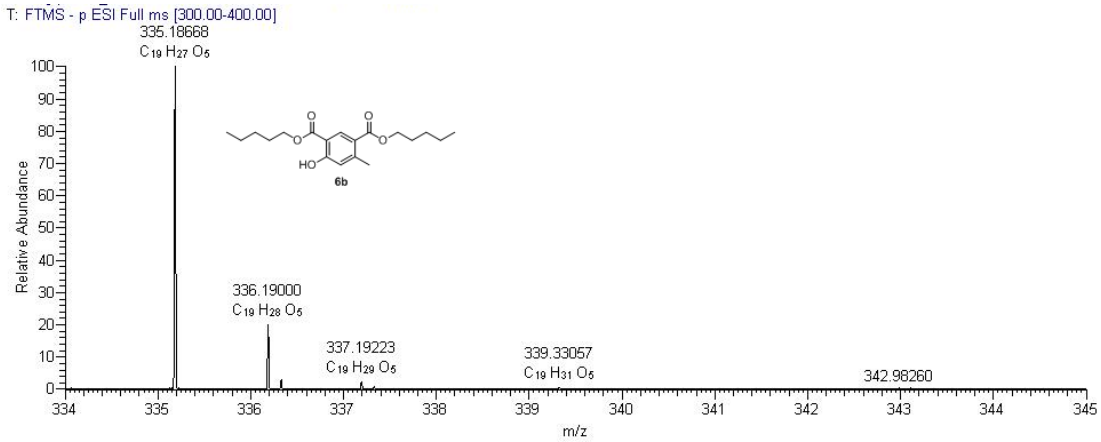


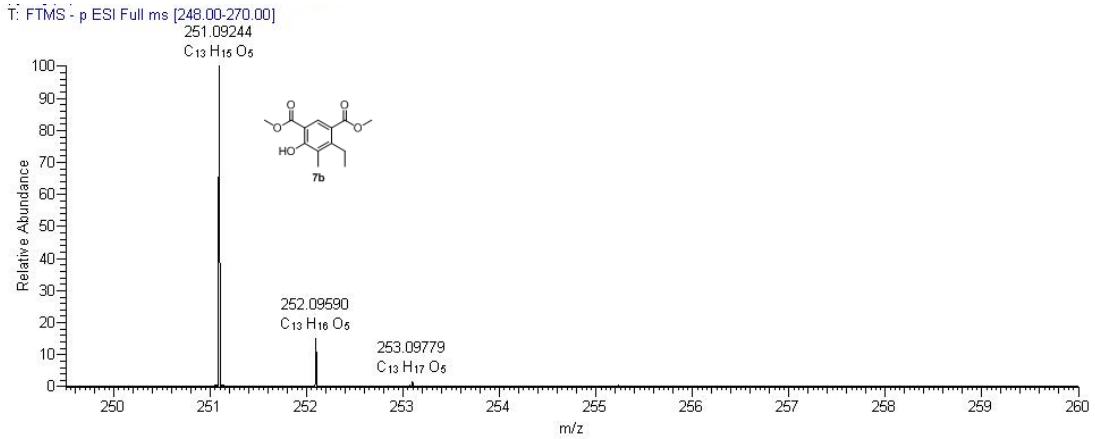


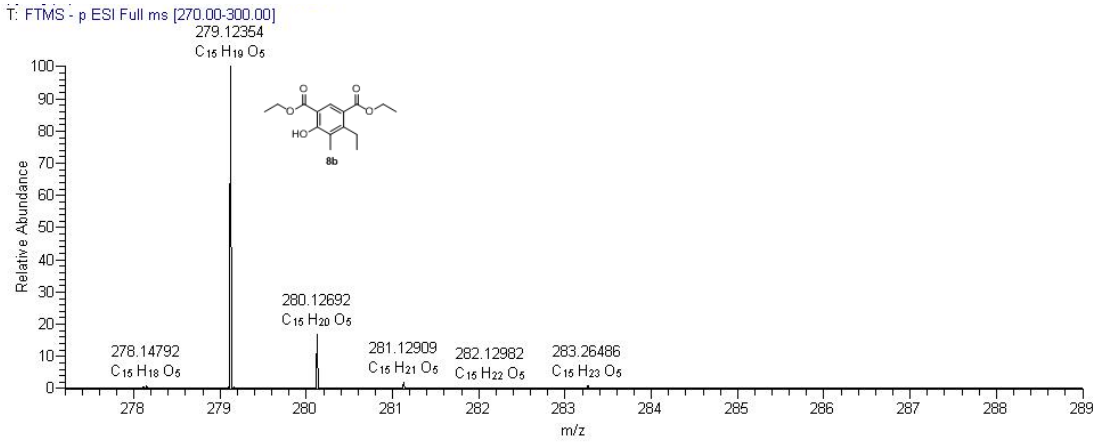


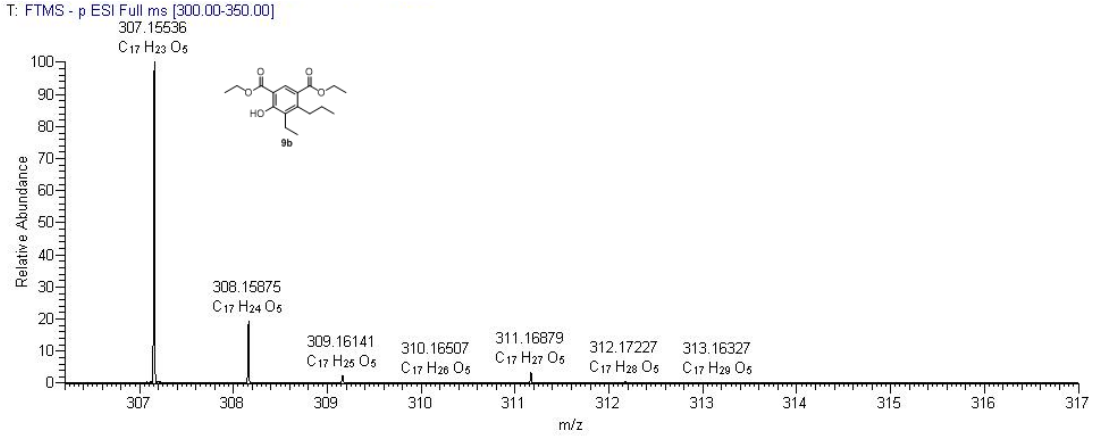

T: FTMS - p ESI Full ms [300.00-350.00]
307.15546
C17 H23 O5
4b
308.15878
C17 H24 O5
309.16187
C17 H25 O5
309.78641
311.22299
C17 H27 O5
312.25381
C17 H28 O5
313.23895
C17 H29 O5
314.24240
C17 H30 O5
Relative Abundance
m/z

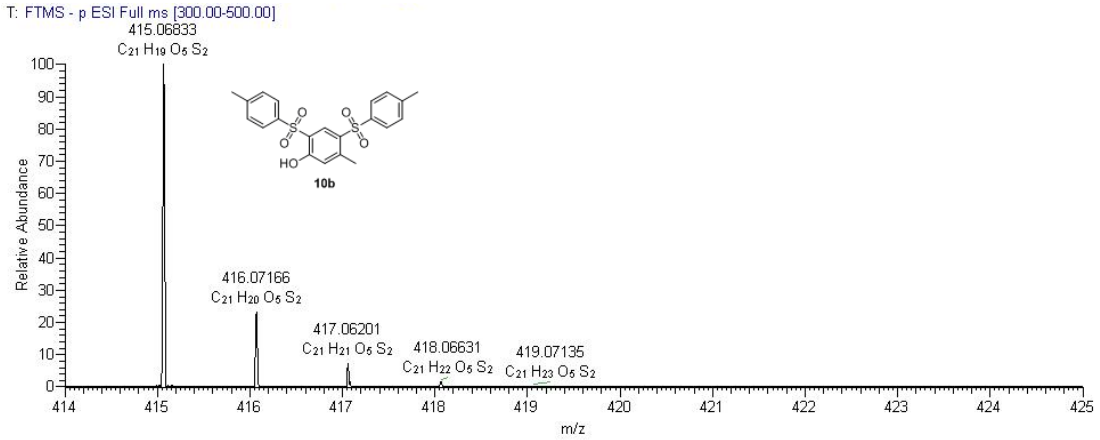

T: FTMS - p ESI Full ms [305.00-320.00]
307.15531
C17 H23 O5
5b
308.15865
C17 H24 O5
309.17359
C17 H25 O5
306.77941
307.48597
310.25058
C17 H26 O5
311.16829
C17 H27 O5
311.98178
313.03298
314.56360
Relative Abundance
m/z

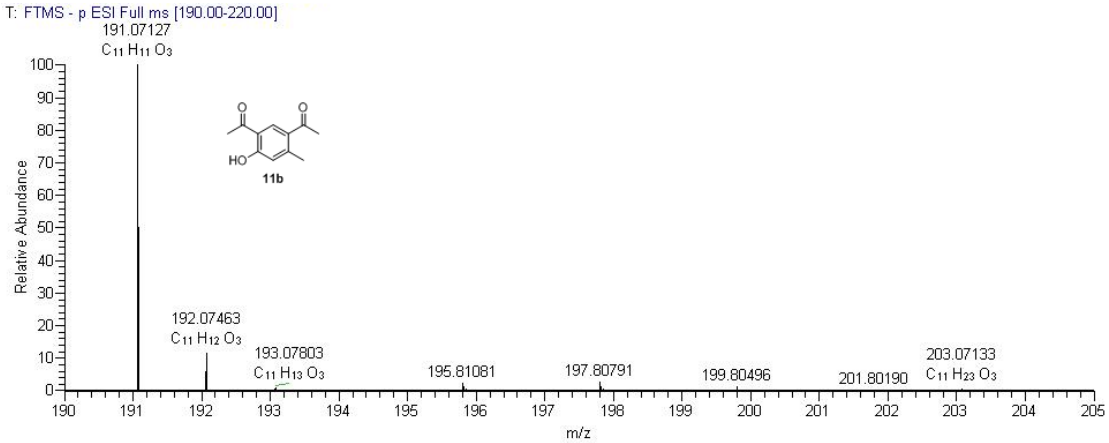

T: FTMS - p ESI Full ms [300.00-400.00]
335.18668
C19 H27 O5
6b
336.19000
C19 H28 O5
337.19223
C19 H29 O5
339.33057
C19 H31 O5
342.98260
Relative Abundance
m/z

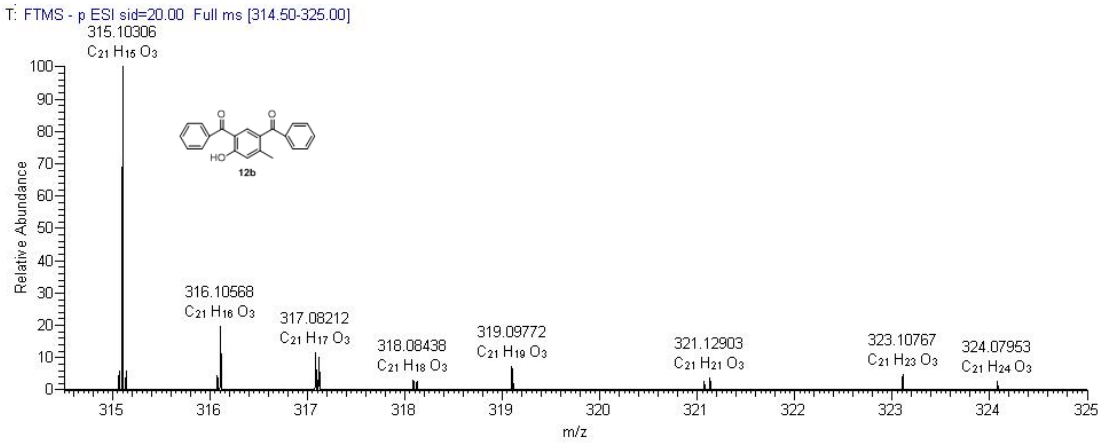

T: FTMS - p ESI Full ms [248.00-270.00]
251.09244
C13 H15 O5
7b
252.09590
C13 H16 O5
253.09779
C13 H17 O5
Relative Abundance
m/z


T: FTMS - p ESI Full ms [270.00-300.00]
279.12354
C15 H19 O5
280.12692
C15 H20 O5
278.14792
C15 H18 O5
281.12909
C15 H21 O5
282.12982
C15 H22 O5
283.26486
C15 H23 O5
8b
Relative Abundance
m/z


T: FTMS - p ESI Full ms [300.00-350.00]
307.15536
C17 H23 O5
308.15875
C17 H24 O5
309.16141
C17 H25 O5
310.16507
C17 H26 O5
311.16879
C17 H27 O5
312.17227
C17 H28 O5
313.16327
C17 H29 O5
9b
Relative Abundance
m/z


T: FTMS - p ESI Full ms [300.00-500.00]
415.06833
C21 H19 O5 S2
416.07166
C21 H20 O5 S2
417.06201
C21 H21 O5 S2
418.06631
C21 H22 O5 S2
419.07135
C21 H23 O5 S2
10b
Relative Abundance
m/z


T: FTMS - p ESI Full ms [190.00-220.00]
191.07127
C11 H11 O3
192.07463
C11 H12 O3
193.07803
C11 H13 O3
195.81081
197.80791
199.80496
201.80190
203.07133
C11 H23 O3
11b
Relative Abundance
m/z


T: FTMS - p ESI sid=20.00 Full ms [314.50-325.00]
315.10306
C21 H15 O3
316.10568
C21 H16 O3
317.08212
C21 H17 O3
318.08438
C21 H18 O3
319.09772
C21 H19 O3
321.12903
C21 H21 O3
323.10767
C21 H23 O3
324.07953
C21 H24 O3
12b
Relative Abundance
m/z