Supporting Information

The first palladium-catalyzed 1,4-addition of terminal alkenes to acrylate esters

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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 APCI or ECI ionization source.

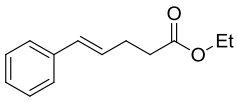
Materials. Unless stated otherwise, commercial reagents were used without further purification. All reagents were weighed and handled in air at room temperature.

2 General Experimental Procedure

The reaction mixture of alkenes **1** (0.5 mmol), acrylate esters **2** (0.75 mmol), $PdCl_2$ (6 mol%), and PhCl (2 mL) in a 15 mL sealed tube was stirred at 110 ^{o}C for 72 h, 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 (*E*)-alkenyl esters.

3 Characterization of the Compounds

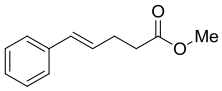
(*E*)-Ethyl 5-phenylpent-4-enoate (3aa)



Yellowish oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.35-7.33 (m, 2H), 7.31-7.28 (m, 2H), 7.22-7.19 (m, 1H), 6.44 (d, *J* = 15.8 Hz, 1H), 6.22 (dt, *J* = 15.8, 6.6 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 2.57-2.53 (m, 2H), 2.51-2.46 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 137.3, 130.9, 128.5, 127.1, 126.0, 60.4, 34.0, 28.3, 14.2; **ESI HRMS** exact mass calcd for $(C_{13}H_{16}O_2Na)^+$ requires m/z 227.10480, found m/z 227.10374.

The NMR data was in good agreement with that reported in the literature.[1]

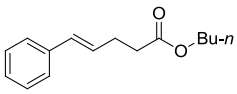
(*E*)-Methyl 5-phenylpent-4-enoate (3ab)



Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.4 Hz, 2H), 7.31-7.28 (m, 2H), 7.22 (d, *J* = 7.2 Hz, 1H), 6.44 (d, *J* = 15.9 Hz, 1H), 6.21 (dt, *J* = 15.8, 6.5 Hz, 1H), 3.70 (s, 3H), 2.57-2.53 (m, 2H), 2.51-2.48 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.4, 137.3, 131.0, 128.5, 128.4, 127.1, 126.0, 51.6, 33.8, 28.2; **ESI HRMS** exact mass calcd for $(C_{12}H_{15}O_2)^+$ requires m/z 191.10720, found m/z 191.10664.

The NMR data was in good agreement with that reported in the literature.[2]

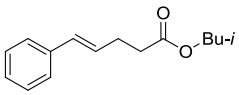
(*E*)-Butyl 5-phenylpent-4-enoate (3ac)



Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.3 Hz, 2H), 7.31-7.28 (m, 2H), 7.22-7.20 (m, 1H), 6.44 (d, *J* = 15.9 Hz, 1H), 6.22 (dt, *J* = 15.8, 6.6 Hz, 1H), 4.11 (t, *J* = 6.7 Hz, 2H), 2.57-2.53 (m, 2H), 2.52-2.47 (m, 2H), 1.65-1.59 (m, 2H), 1.43-1.35 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 137.3, 130.9, 128.4, 127.1, 126.0, 64.3, 34.0, 30.6, 28.3, 19.1, 13.6; **APCI**

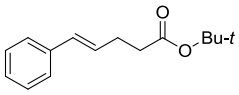
HRMS exact mass calcd for $(C_{15}H_{21}O_2)^+$ requires m/z 233.15415, found m/z 233.15385.

(*E*)-Isobutyl 5-phenylpent-4-enoate (3ad)



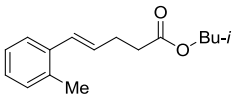
Yellowish oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.34 (m, 2H), 7.32-7.29 (m, 2H), 7.23-7.20 (m, 1H), 6.45 (d, *J* = 15.9 Hz, 1H), 6.23 (dt, *J* = 15.8, 6.5 Hz, 1H), 3.90 (d, *J* = 6.7 Hz, 2H), 2.59-2.54 (m, 2H), 2.53-2.49 (m, 2H), 1.97-1.92 (m, 1H), 0.95 (s, 3H), 0.94 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 137.3, 130.9, 128.4, 127.1, 127.0, 126.0, 70.5, 34.0, 28.3, 27.7, 19.0; **APCI HRMS** exact mass calcd for $(C_{15}H_{21}O_2)^+$ requires m/z 233.15415, found m/z 233.15387.

(*E*)-Tert-butyl 5-phenylpent-4-enoate (3ae)



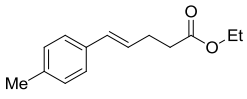
Yellow oil; **^{1}H NMR** (500 MHz,$CDCl_3$) δ 7.33 (d, *J* = 7.0 Hz, 2H), 7.31-7.28 (m, 3H), 6.42 (d, *J* = 15.9 Hz, 1H), 6.21 (dt, *J* = 15.8, 6.7 Hz, 1H), 2.52-2.48 (m, 2H), 2.41-2.38 (m, 2H), 1.45 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.4, 139.7, 130.7, 128.8, 128.5, 127.0, 126.0, 80.3, 35.2, 29.7, 28.1; **APCI HRMS** exact mass calcd for $(C_{15}H_{21}O_2)^+$ requires m/z 233.15415, found m/z 233.15297.

(*E*)-Isobutyl 5-(o-tolyl)pent-4-enoate (3bd)



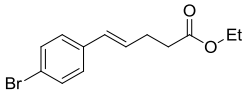
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 5.7 Hz, 1H), 7.18-7.13 (m, 3H), 6.65 (d, *J* = 15.7 Hz, 1H), 6.10 (dt, *J* = 15.5, 6.6 Hz, 1H), 3.90 (d, *J* = 6.7 Hz, 2H), 2.61-2.57 (m, 2H), 2.55-2.51 (m, 2H), 2.34 (s, 3H), 1.98-1.91 (m, 1H), 0.96 (s, 3H), 0.95 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 136.5, 135.0, 130.1, 129.8, 128.8, 127.0, 126.0, 125.5, 70.5, 34.2, 28.6, 27.7, 19.7, 19.1; **APCI HRMS** exact mass calcd for $(C_{16}H_{23}O_2)^+$ requires m/z 247.16980, found m/z 247.16870.

(*E*)-Mthyl 5-(p-tolyl)pent-4-enoate (3ca)



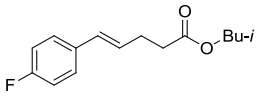
Yellowish oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 6.40 (d, *J* = 15.9 Hz, 1H), 6.15 (dt, *J* = 15.8, 6.6 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 2.56-2.49 (m, 2H), 2.49-2.45 (m, 2H), 2.33 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.1, 136.9, 134.6, 130.7, 129.2, 127.4, 125.9, 60.4, 34.1, 28.3, 21.1, 14.3; **APCI HRMS** exact mass calcd for $(C_{14}H_{19}O_2)^+$ requires m/z 219.13850, found m/z 219.13763.

(*E*)-Ethyl 5-(4-bromophenyl)pent-4-enoate (3da)



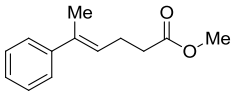
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 1.9 Hz, 1H), 7.40 (d, *J* = 1.8 Hz, 1H), 7.20 (d, *J* = 2.0 Hz, 1H), 7.18 (d, *J* = 1.7 Hz, 1H), 6.36 (d, *J* = 15.9 Hz, 1H), 6.20 (dt, *J* = 15.8, 6.4 Hz, 1H), 4.14 (q, *J* = 7.1 Hz, 2H), 2.54-2.50 (m, 2H), 2.49-2.45 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.9, 136.3, 131.6, 129.8, 129.4, 127.6, 120.8, 60.4, 33.9, 28.3, 14.3; **APCI HRMS** exact mass calcd for $(C_{13}H_{16}O_2Br)^+$ requires m/z 283.03337, found m/z 283.03040.

(*E*)-Isobutyl 5-(4-fluorophenyl)pent-4-enoate (3ed)



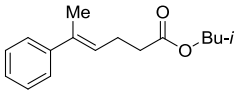
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30-7.26 (m, 2H), 6.99-6.94 (m, 2H), 6.39 (d, *J* = 15.9 Hz, 1H), 6.12 (dt, *J* = 15.8, 6.4 Hz, 1H), 3.87 (d, *J* = 6.6 Hz, 2H), 2.55-2.47 (m, 4H), 1.96-1.88 (m, 1H), 0.93 (s, 3H), 0.92 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.0, 163.0 and161.0, 133.5, 129.7, 128.2, 127.5, 127.4, 115.4 and 115.2, 70.6, 34.0, 28.2, 27.7, 19.0; **APCI HRMS** exact mass calcd for $(C_{15}H_{20}O_2F)^+$ requires m/z 251.14473, found m/z 251.14366.

(*E*)-Methyl 5-phenylhex-4-enoate (3fb)



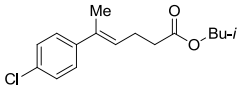
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.5 Hz, 2H), 7.34-7.31 (m, 2H), 7.25 (d, *J* = 7.4 Hz, 1H), 5.78-5.72 (m, 1H), 3.71 (s, 3H), 2.57-2.54 (m, 2H), 2.50-2.47 (m, 2H), 2.08 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.5, 143.5, 136.2, 128.1, 126.7, 125.9, 125.6, 51.5, 33.8, 24.2, 15.7; **ESI HRMS** exact mass calcd for $(C_{13}H_{17}O_2)^+$ requires m/z 205.12285, found m/z 205.12259.

(*E*)-Isobutyl 5-phenylhex-4-enoate (3fd)



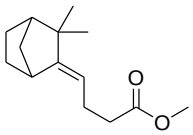
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.35 (m, 2H), 7.32-7.29 (m, 2H), 7.24-7.21 (m, 1H), 5.76-5.72 (m, 1H), 3.88 (d, *J* = 6.7 Hz, 2H), 2.57-2.52 (m, 2H), 2.49-2.45 (m, 2H), 2.06 (s, 3H), 1.95-1.91 (m, 1H), 0.94 (s, 3H), 0.93 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.3, 143.6, 139.0, 128.1, 126.7, 126.1, 125.6, 70.6, 34.2, 27.7, 24.3, 19.1, 15.8; **APCI HRMS** exact mass calcd for $(C_{16}H_{23}O_2)^+$ requires m/z 247.16980, found m/z 247.16943.

(*E*)-Isobutyl 5-(4-chlorophenyl)hex-4-enoate (3gd)



Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30-7.26 (m, 4H), 5.75-5.72 (m, 1H), 3.89 (d, *J* = 6.7 Hz, 2H), 2.55-2.52 (m, 2H), 2.50-2.47 (m, 2H), 2.36-2.30 (m, 1H), 2.04 (s, 3H), 0.95 (s, 3H), 0.94 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 173.1, 142.0, 135.1, 132.4, 128.2, 126.9, 126.6, 70.6, 34.0, 27.7, 24.3, 19.0, 15.8; **APCI HRMS** exact mass calcd for $(C_{16}H_{22}O_2Cl)^+$ requires m/z 281.13083, found m/z 281.13016.

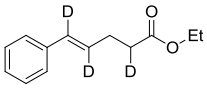
(*Z*)-Methyl 4-(3,3-dimethylbicyclo[2.2.1]heptan-2-ylidene)butanoate (3ib)



Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.77-5.71 (m, 1H), 3.73 (s,

3H), 3.29-3.28 (m, 1H), 2.34-2.29 (m, 1H), 2.04-1.96 (m, 2H), 1.78-1.73 (m, 1H), 1.73-1.67 (m, 2H), 1.67-1.63 (m, 1H), 1.47-1.40 (m, 1H), 1.33-1.29 (m, 1H), 1.25-1.23 (m, 1H), 1.21-1.16 (m, 1H), 1.07 (s, 3H), 1.04 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 171.5, 168.2, 117.0, 51.3, 47.7, 43.2, 42.6, 37.4, 28.4, 28.3, 28.1, 25.3, 23.6; **APCI HRMS** exact mass calcd for $(C_{14}H_{23}O_2)^+$ requires m/z 223.16980, found m/z 233.16942.

D-(*E*)-Ethyl 5-phenylpent-4-enoate (3aa-*d*)



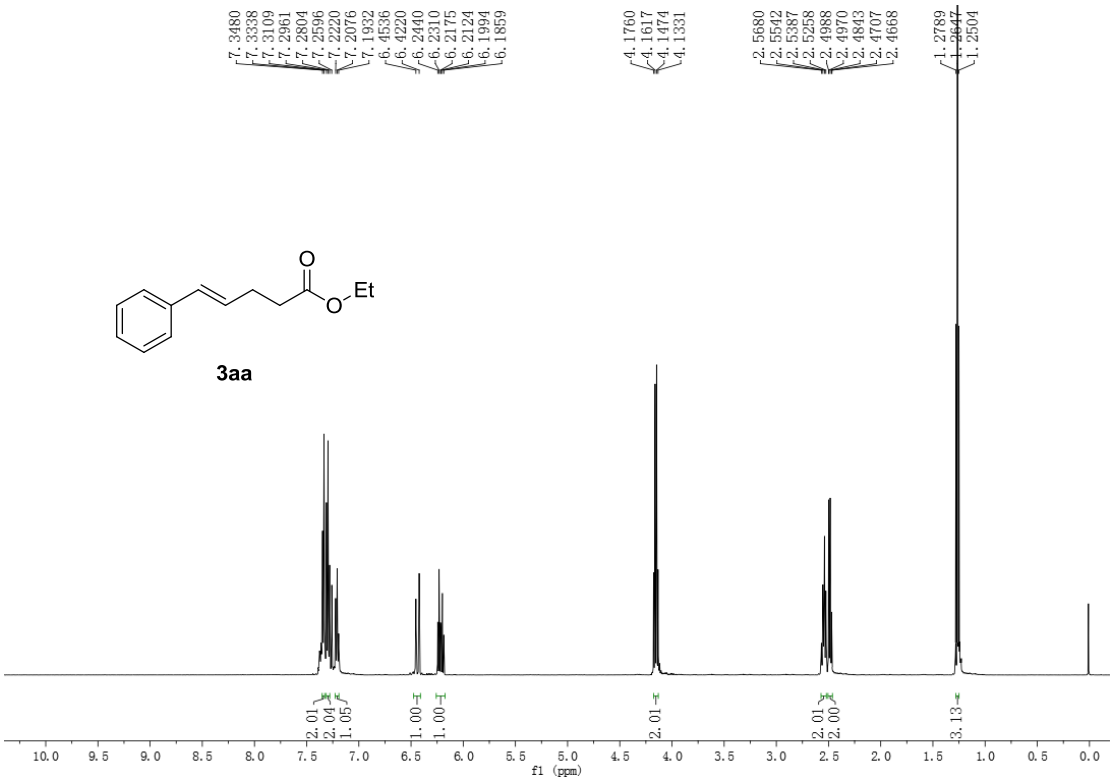
Yellow oil; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, J = 7.3 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.21 (t, J = 7.2 Hz, 1H), 4.15 (q, J = 7.1 Hz, 2H), 2.53 (d, J = 6.4 Hz, 1H), 2.48 (dd, J = 11.3, 4.5 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H).

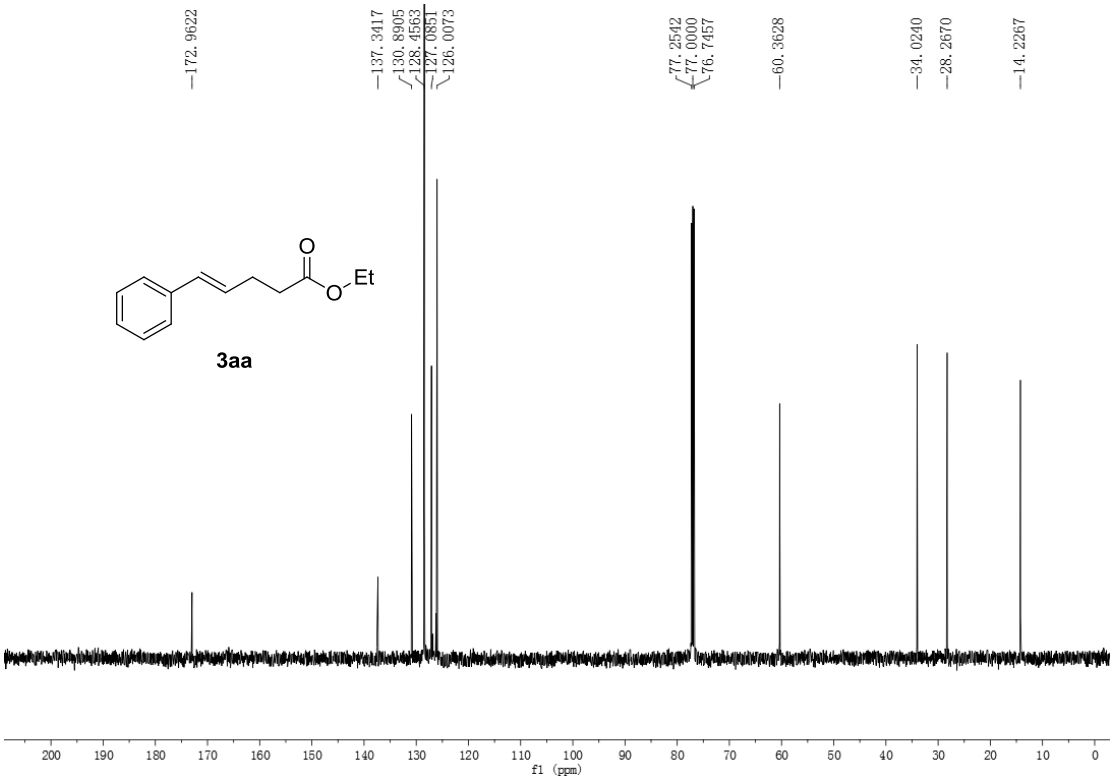
4 References

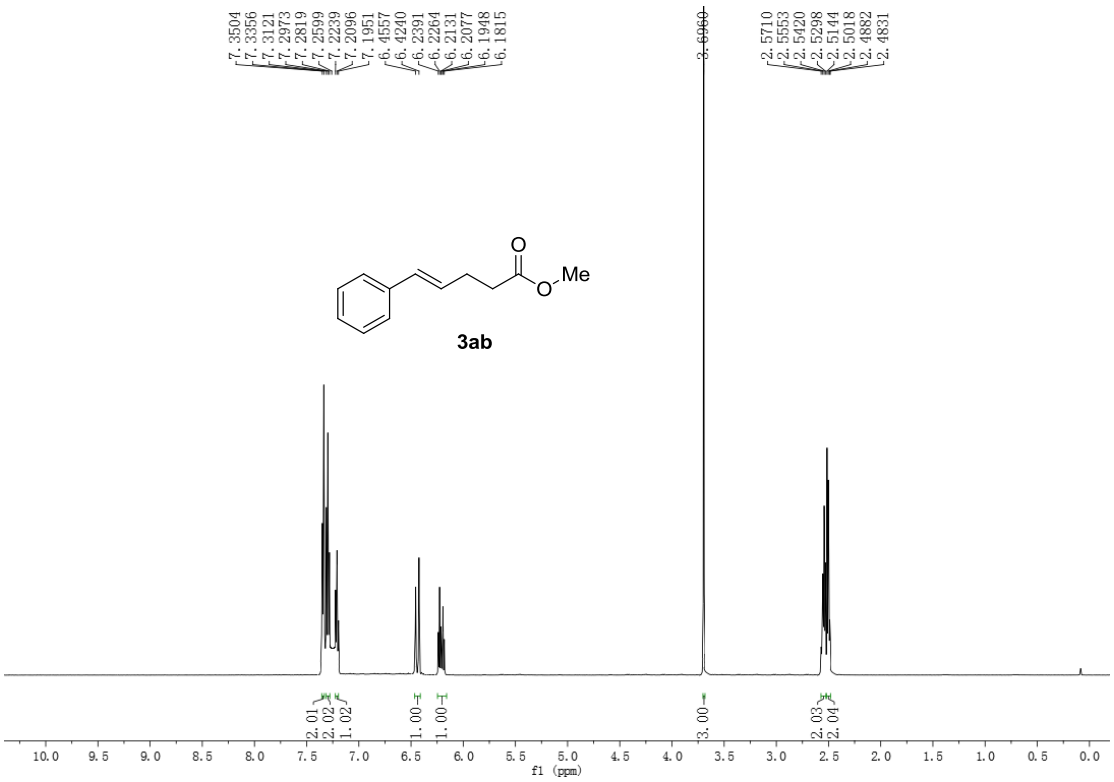
1 V. B. Phapale; M. Guisán-Ceinos; E. Buñuel; D. J. Cárdenas *Chem. Eur. J.* 2009, **15**, 12681-12688

2 C. M. Thompson; J. A. Frick *J. Org. Chem.* 1989, **54**, 890-896.

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



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6.1815
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2.5420
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2.5144
2.5018
2.4882
2.4831
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O
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1.00
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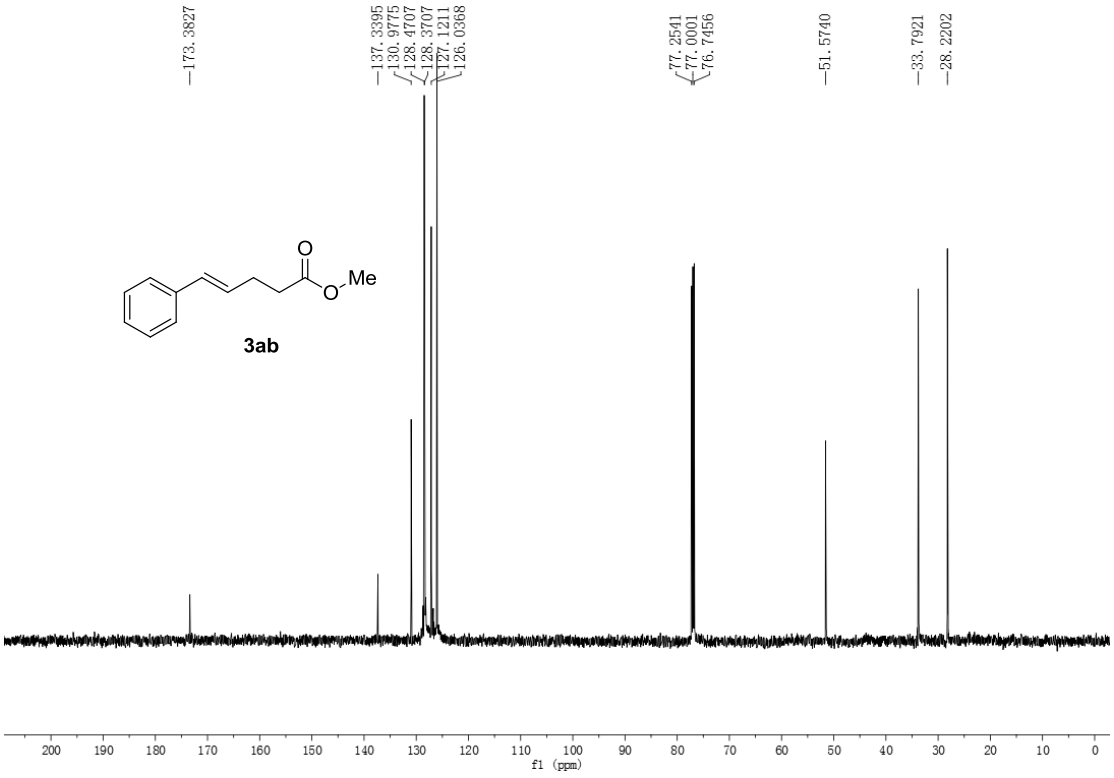
3.00
2.03
2.04
f1 (ppm)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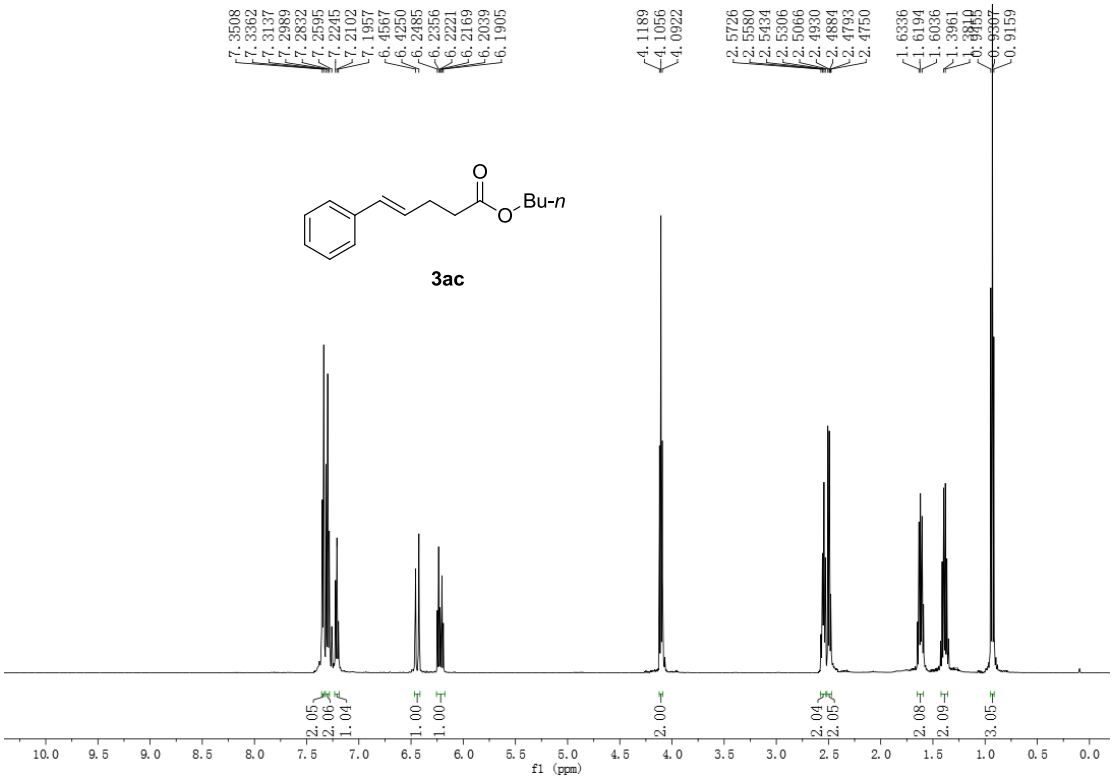
Me
3ab
f1 (ppm)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6.2169
6.2039
6.1905
4.1189
4.1056
4.0922
2.5726
2.5580
2.5434
2.5306
2.5066
2.4930
2.4884
2.4793
2.4750
1.6336
1.6194
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1.3961
0.9307
0.9159
O
O
Bu-n
3ac
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2.06
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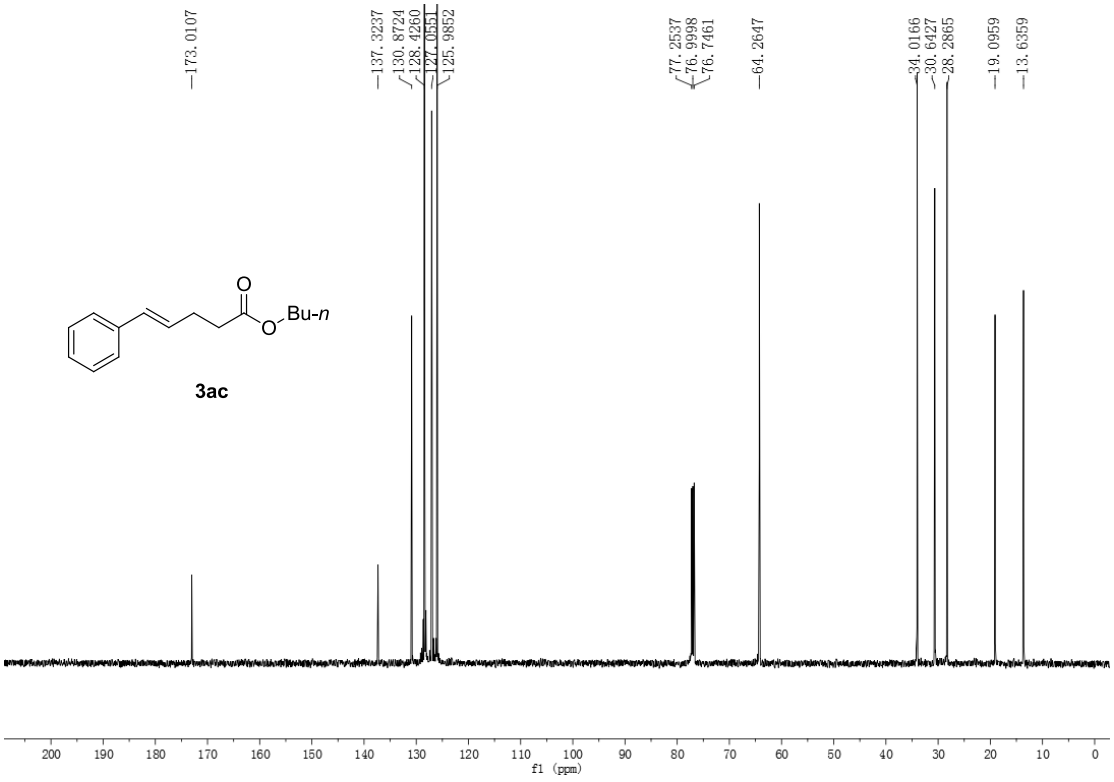
1.00
1.00
2.00
2.04
2.05
2.08
2.09
3.05
f1 (ppm)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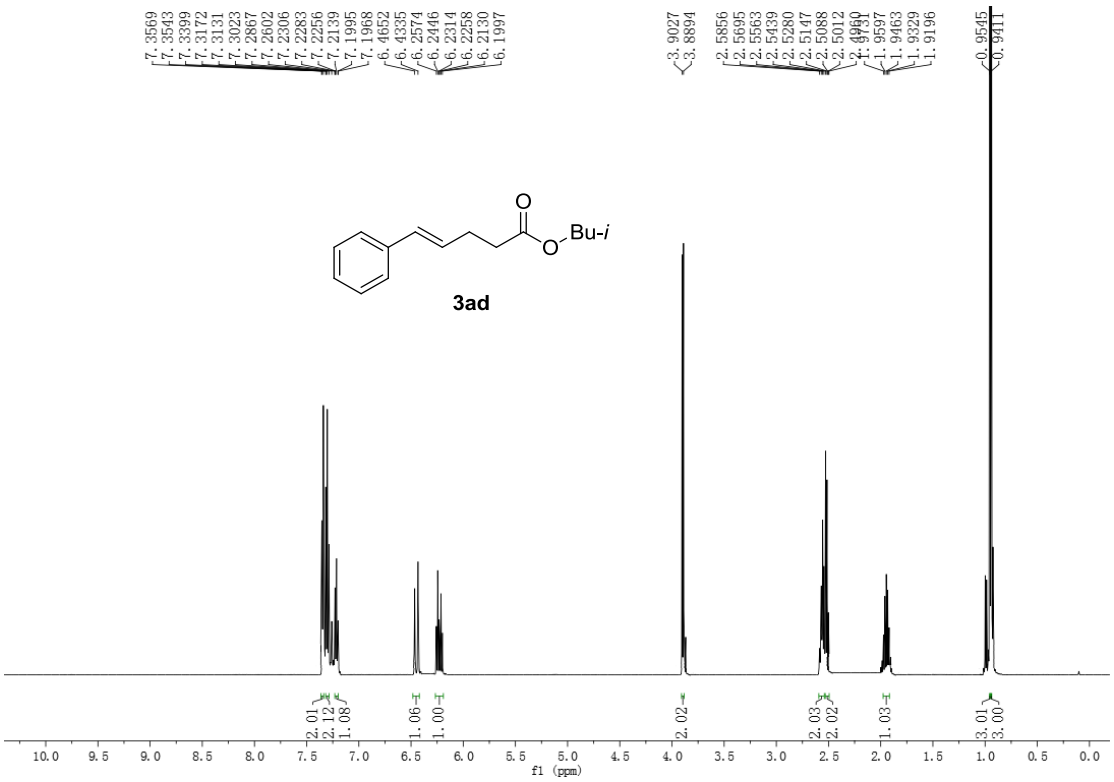
O
Bu-n
3ac
f1 (ppm)


7.3569
7.3543
7.3399
7.3172
7.3131
7.3023
7.2867
7.2602
7.2306
7.2283
7.2256
7.2139
7.1995
7.1968
6.4652
6.4335
6.2574
6.2446
6.2314
6.2258
6.2130
6.1997
3.9027
3.8894
2.5856
2.5695
2.5563
2.5439
2.5280
2.5147
2.5088
2.5012
2.4960
2.4931
1.9597
1.9463
1.9329
1.9196
0.9545
0.9411
O
O
Bu-i
3ad
2.01
2.12
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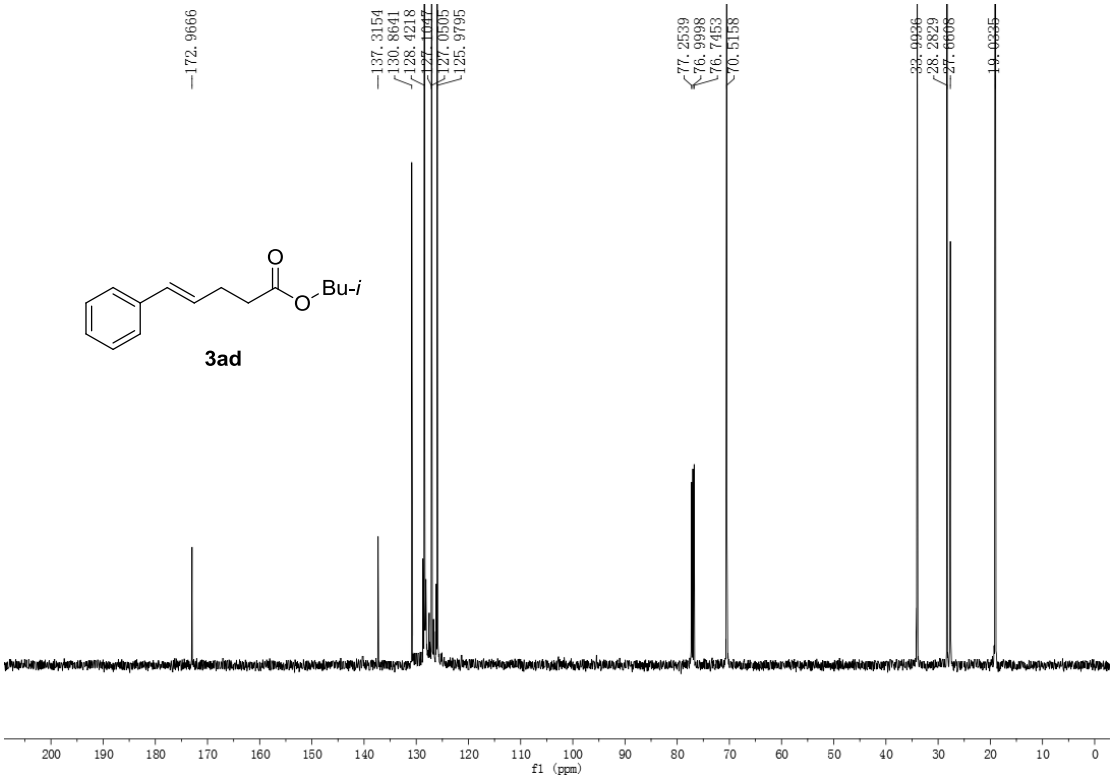
1.06
1.00
2.02
2.03
2.02
1.03
3.01
3.00
f1 (ppm)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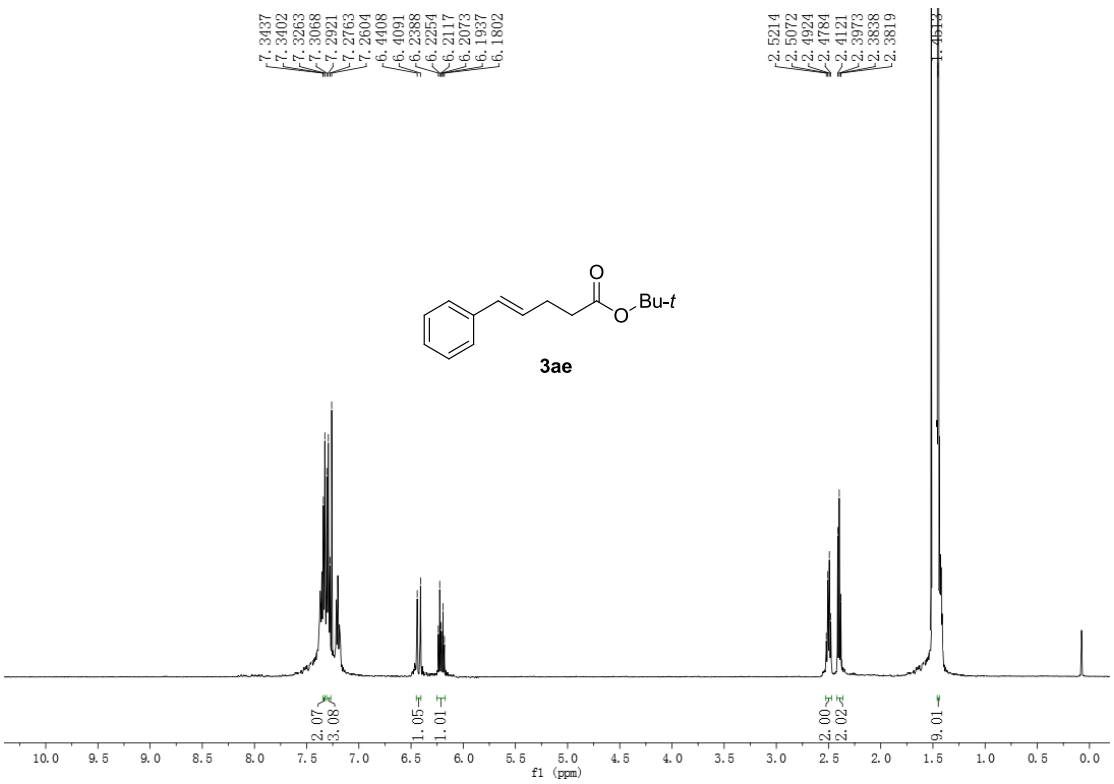
Bu-i
3ad
f1 (ppm)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6.4091
6.2388
6.2254
6.2117
6.2073
6.1937
6.1802
2.5214
2.5072
2.4924
2.4784
2.4121
2.3973
2.3838
2.3819
1.4615
O
O
Bu-t
3ae
2.07
3.08
1.05
1.01
2.00
2.02
9.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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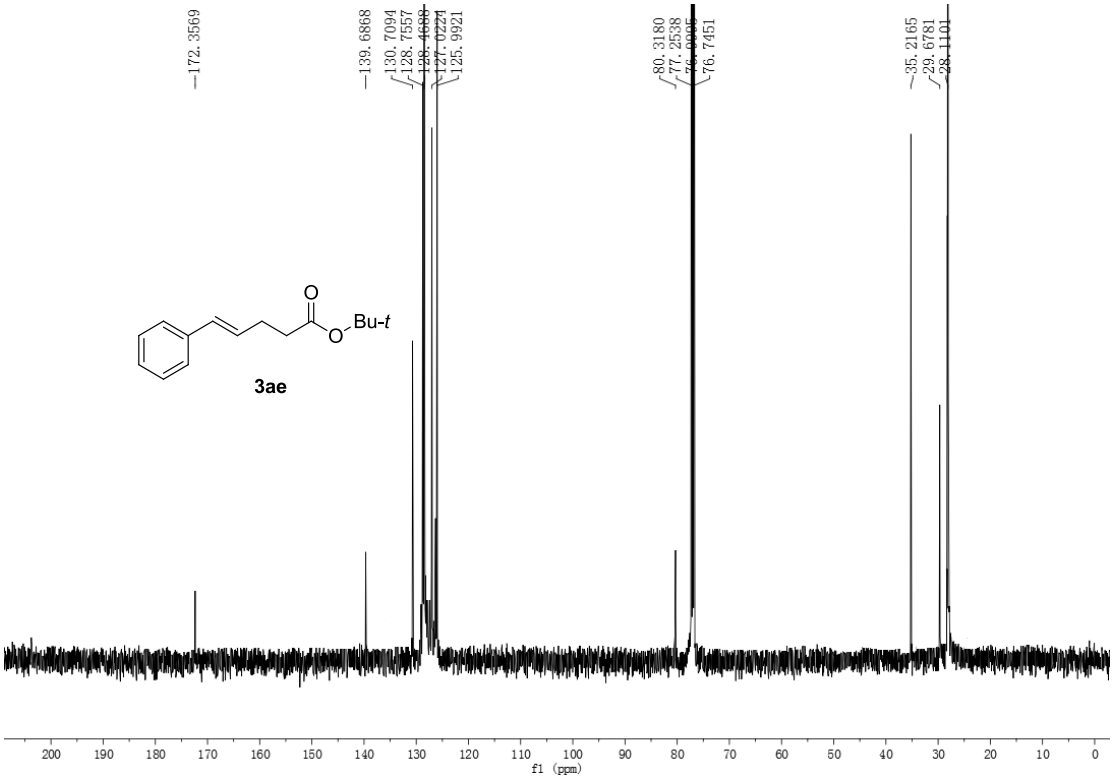
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127.0224
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76.7451
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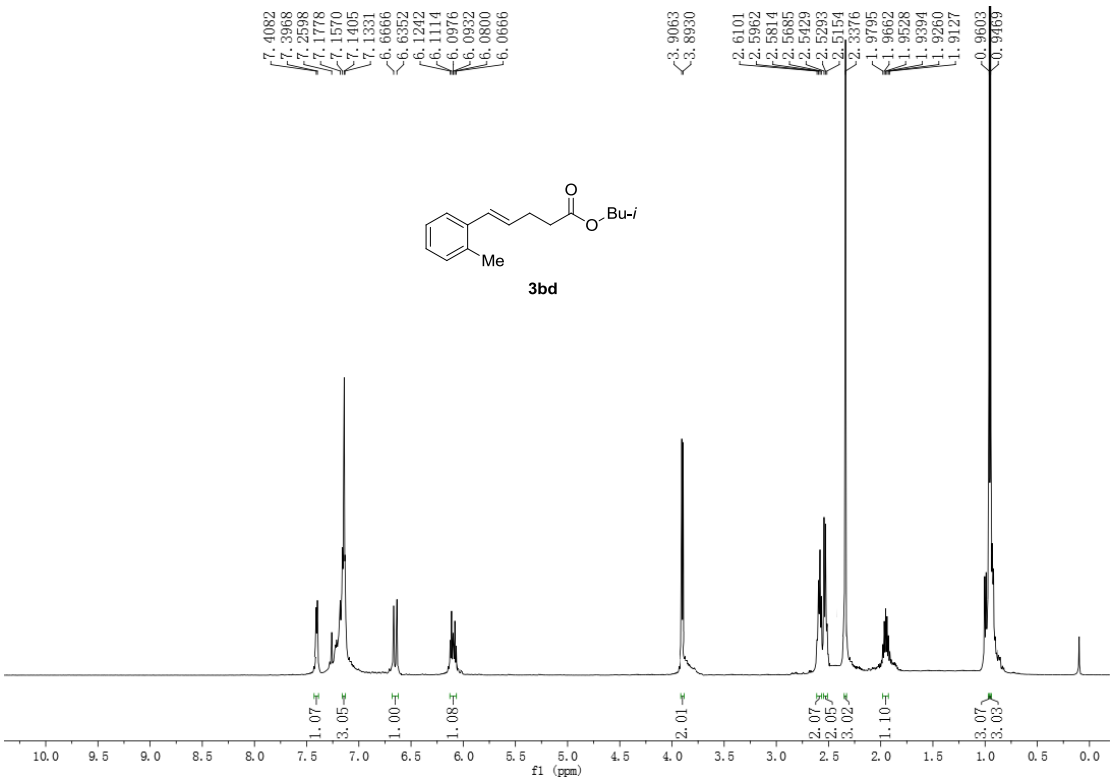
29.6781
28.1101
O
O
Bu-t
3ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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6.0932
6.0800
6.0666
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3.8930
2.6101
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2.5814
2.5685
2.5429
2.5293
2.5154
2.3376
1.9795
1.9662
1.9528
1.9394
1.9260
1.9127
0.9603
0.9469
Bu-i
O
O
Me
3bd
1.07
3.05
1.00
1.08
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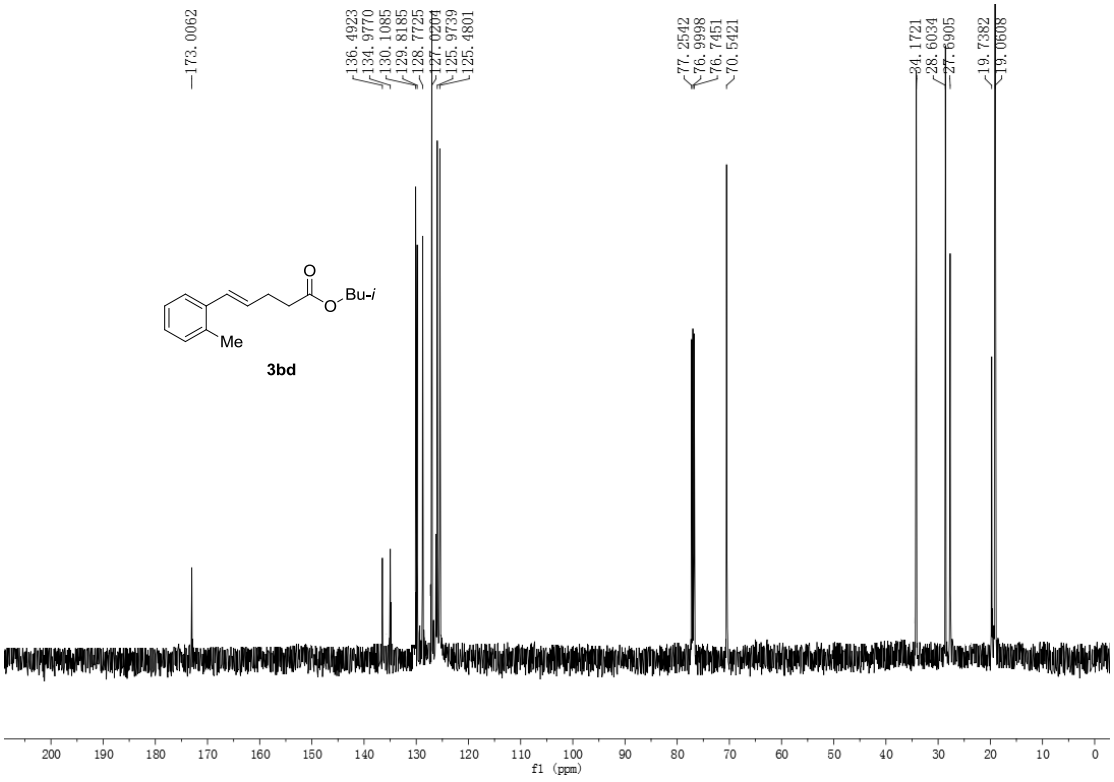
2.07
2.05
3.02
1.10
3.07
3.03
f1 (ppm)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76.7451
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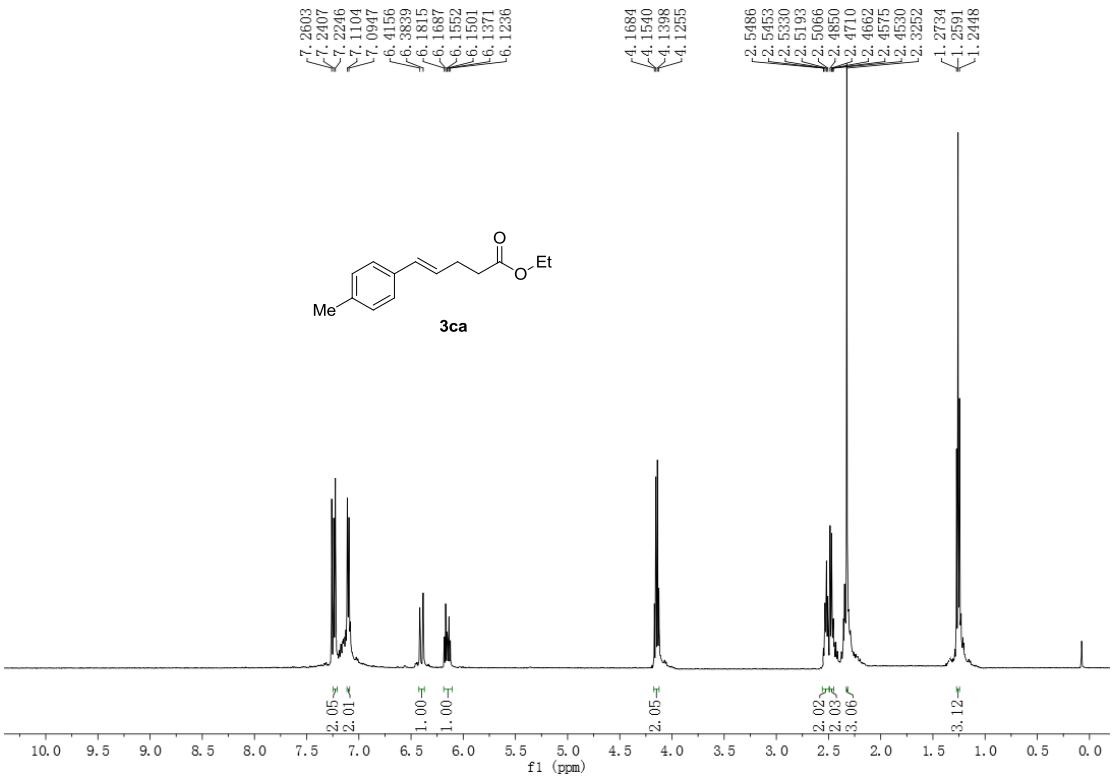
28.6034
27.6905
19.7382
19.0608
Bu-i
O
O
Me
3bd
f1 (ppm)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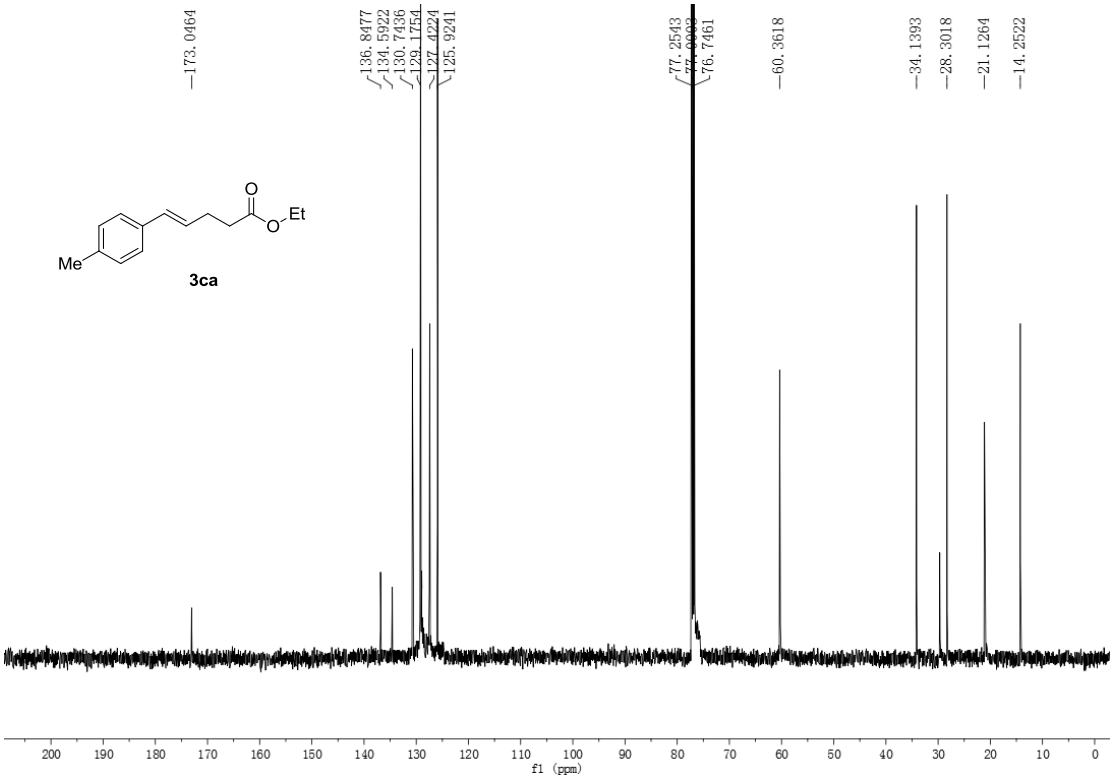
6.1501
6.1371
6.1236
4.1684
4.1540
4.1398
4.1255
2.5486
2.5453
2.5330
2.5193
2.5066
2.4850
2.4710
2.4662
2.4575
2.4530
2.3252
1.2734
1.2591
1.2448
O
O
Et
Me
3ca
2.05
2.01
1.00
1.00
2.05
2.02
2.03
3.06
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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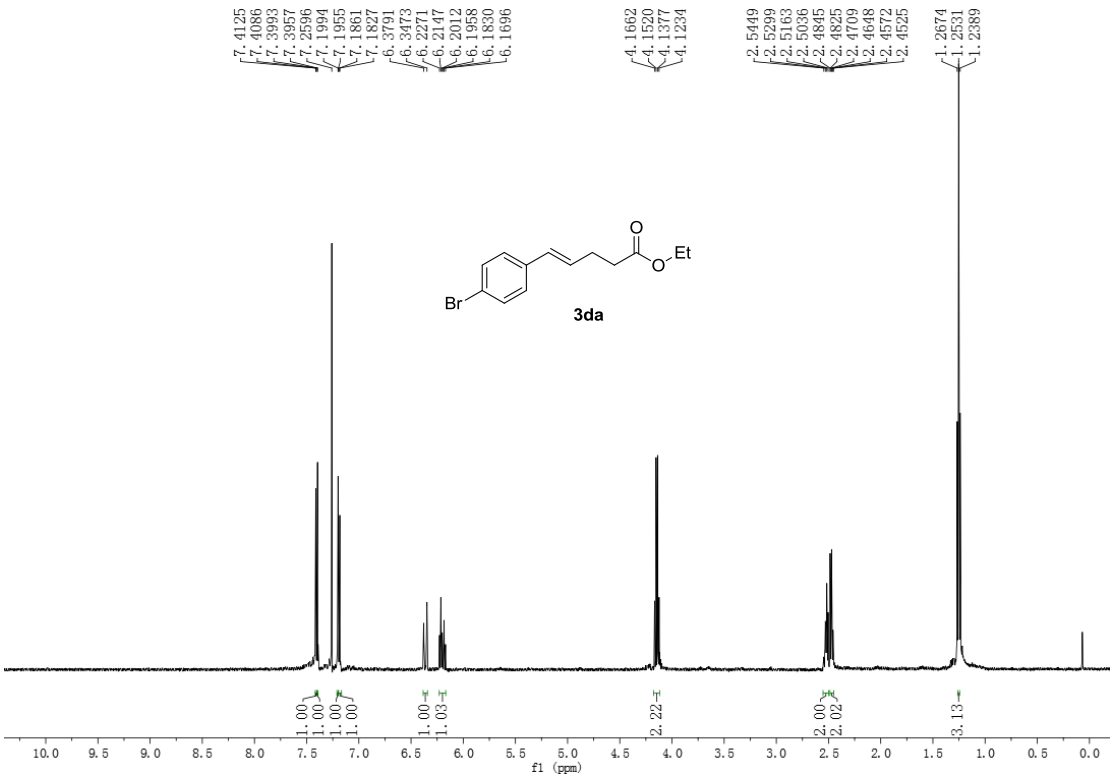
60.3618
34.1393
28.3018
21.1264
14.2522
O
O
Et
Me
3ca
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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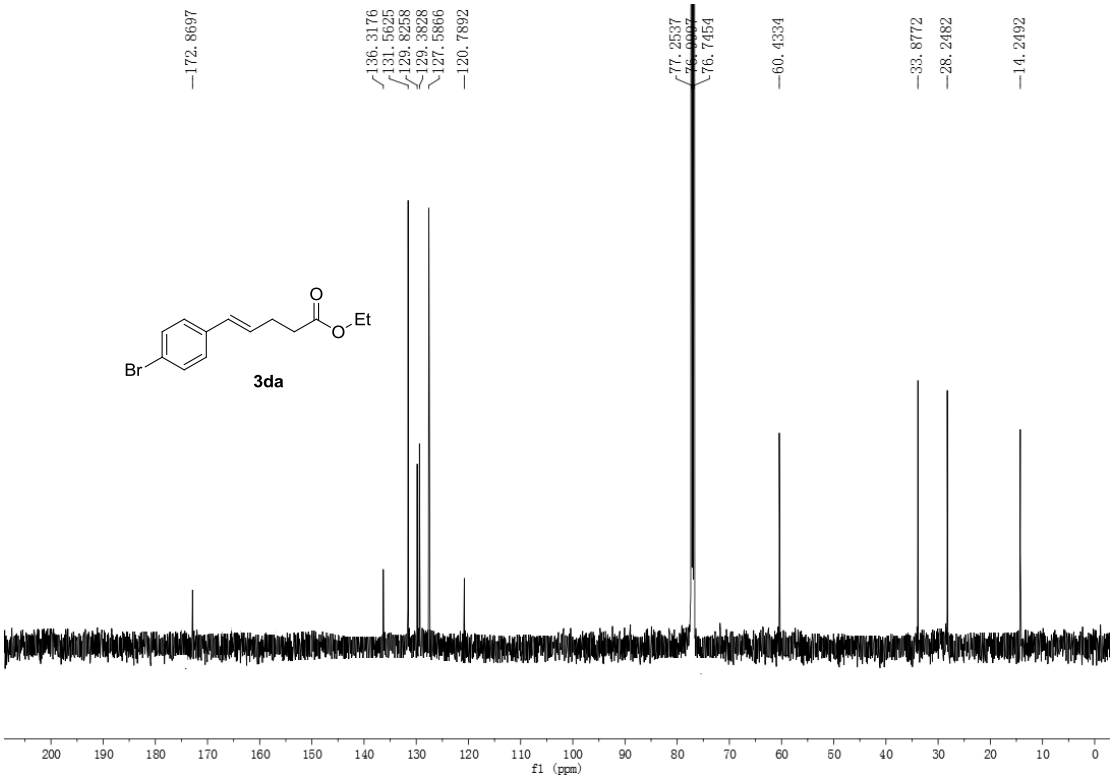
7.3957
7.2596
7.1994
7.1955
7.1861
7.1827
6.3791
6.3473
6.2271
6.2147
6.2012
6.1958
6.1830
6.1696
4.1662
4.1520
4.1377
4.1234
2.5449
2.5299
2.5163
2.5036
2.4845
2.4825
2.4709
2.4648
2.4572
2.4525
1.2674
1.2531
1.2389
O
O
Et
Br
3da
1.00
1.00
1.00
1.00
1.00
1.03
2.22
2.00
2.02
3.13
f1 (ppm)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120.7892
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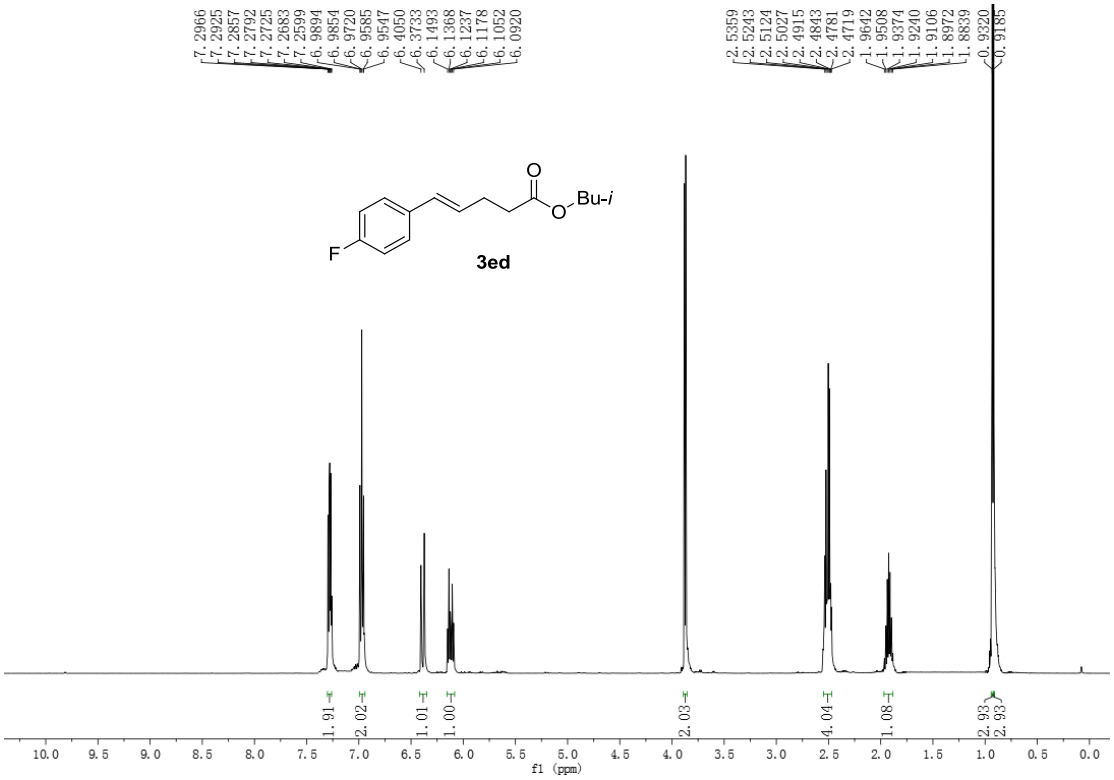
O
Et
Br
3da
f1 (ppm)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6.9547
6.4050
6.3733
6.1493
6.1368
6.1237
6.1178
6.1052
6.0920
2.5359
2.5243
2.5124
2.5027
2.4915
2.4843
2.4781
2.4719
1.9642
1.9508
1.9374
1.9240
1.9106
1.8972
1.8839
0.9320
0.9185
O
O
Bu-i
F
3ed
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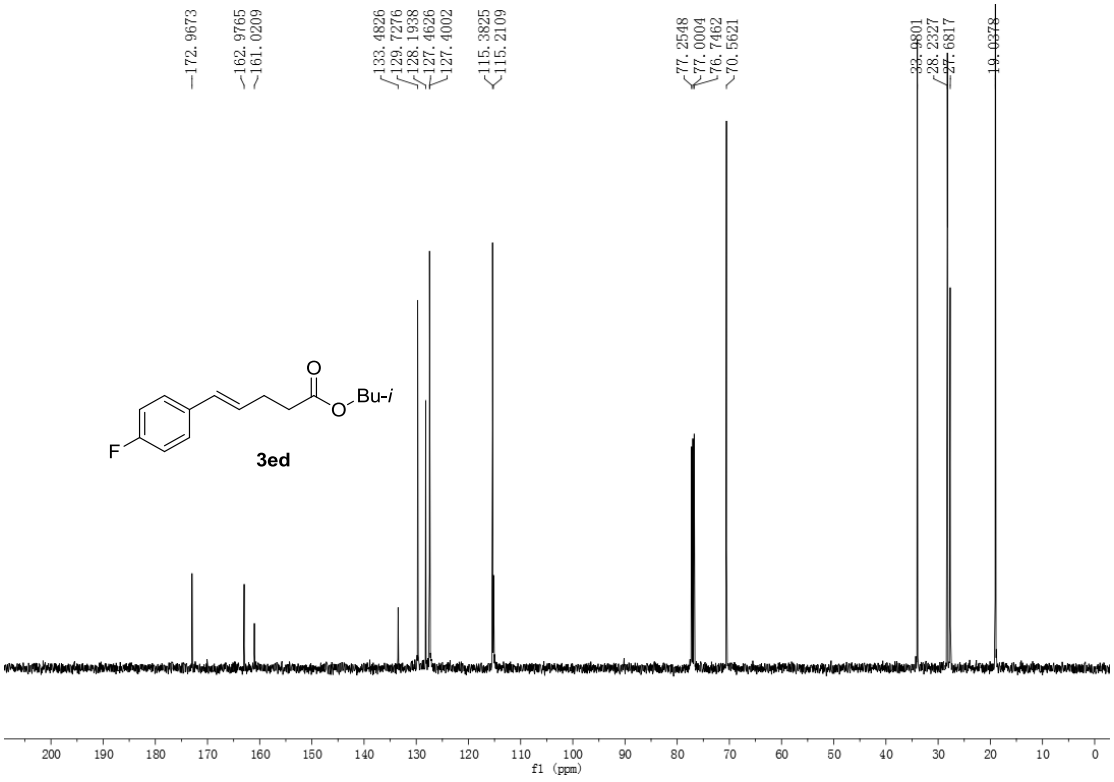
2.03
4.04
1.08
2.93
2.93
f1 (ppm)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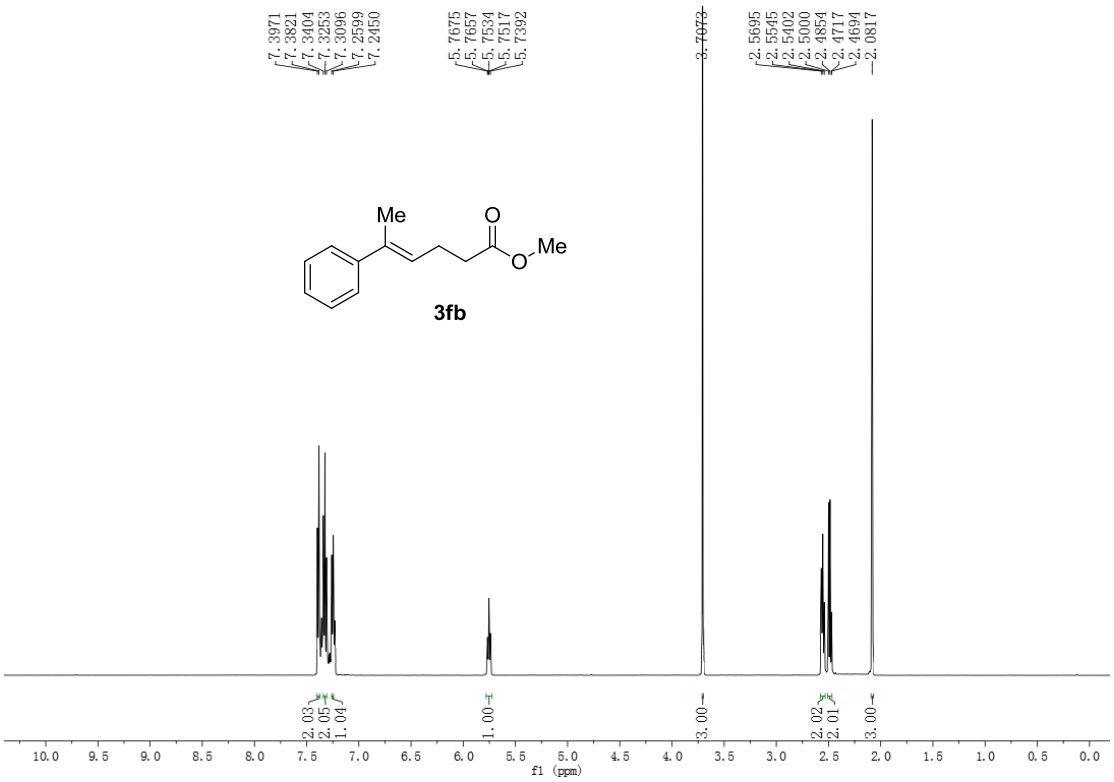
129.7276
128.1938
127.4626
127.4002
115.3825
115.2109
77.2548
77.0004
76.7462
70.5621
33.9801
28.2327
27.6817
19.0378
O
O
Bu-i
F
3ed
f1 (ppm)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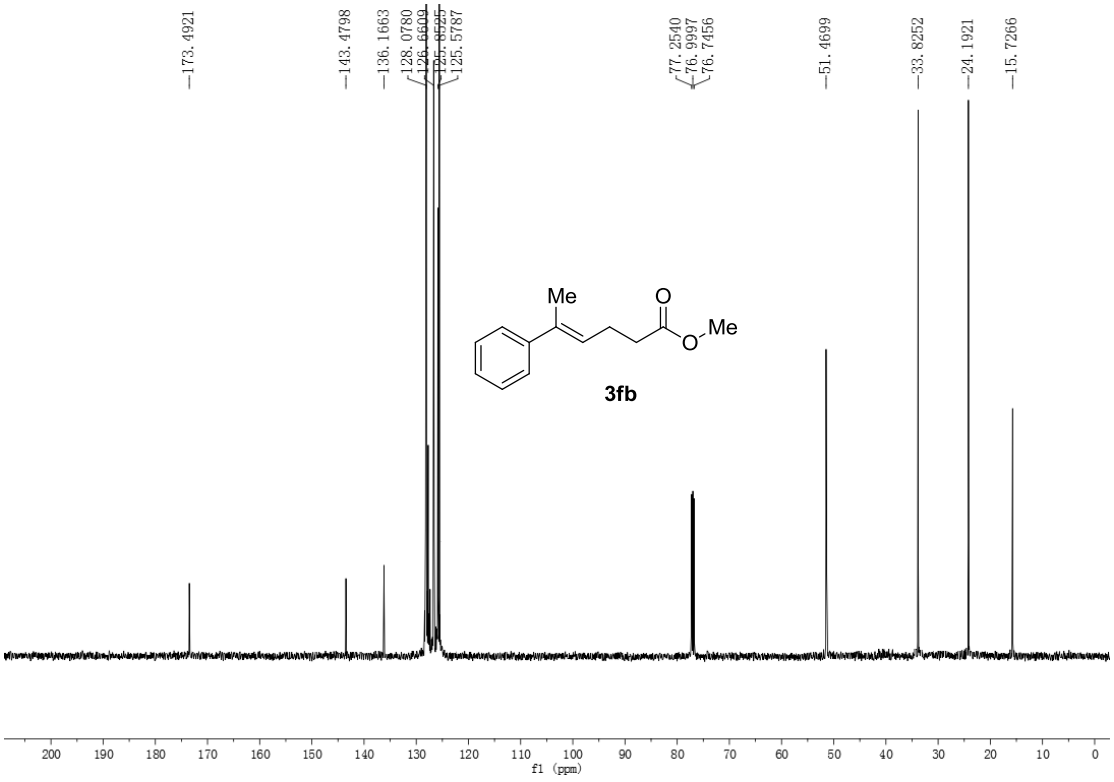
7.3096
7.2599
7.2450
5.7675
5.7657
5.7534
5.7517
5.7392
3.7073
2.5695
2.5545
2.5402
2.5000
2.4854
2.4717
2.4694
2.0817
Me
O
O
Me
3fb
2.03
2.05
1.04
1.00
3.00
2.02
2.01
3.00
f1 (ppm)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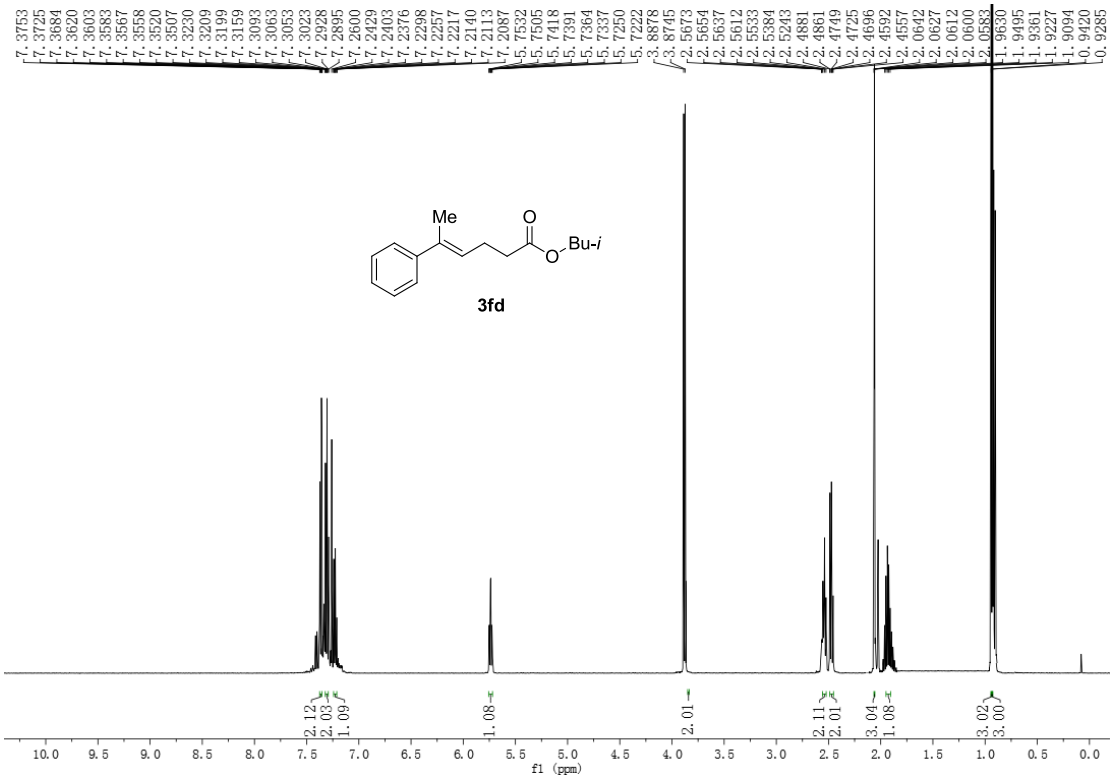
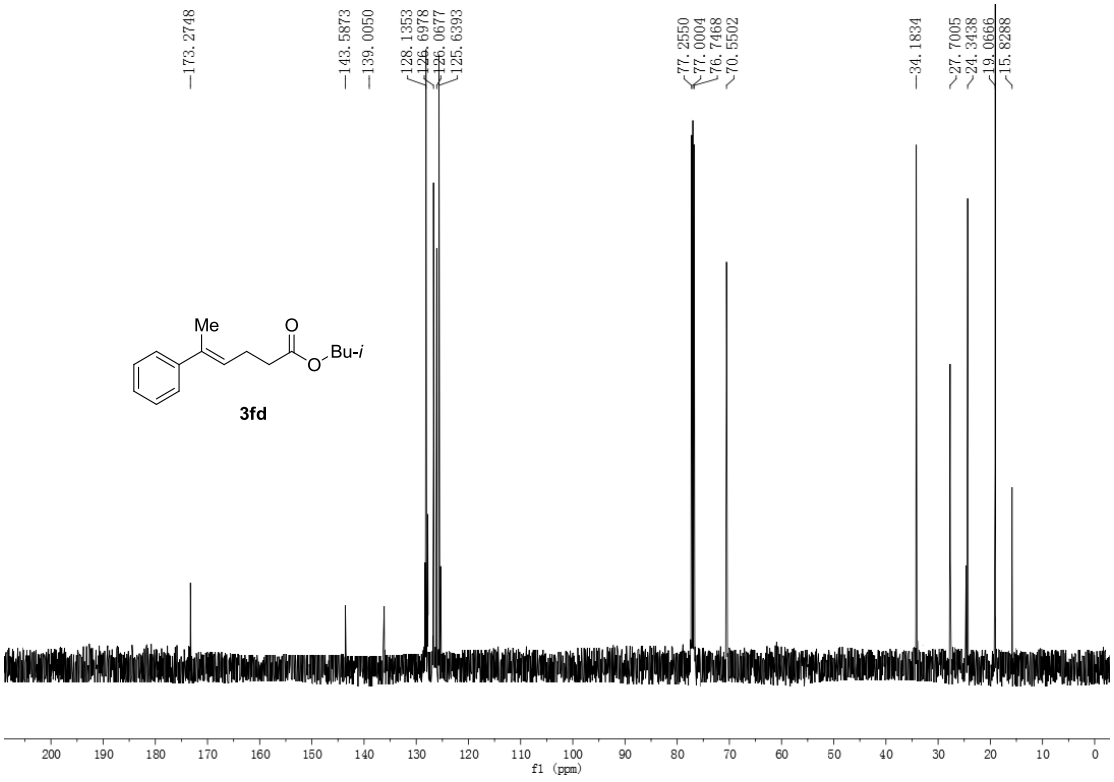
Me
O
O
Me
3fb
f1 (ppm)


Me
O
O
Bu-i
3fd
f1 (ppm)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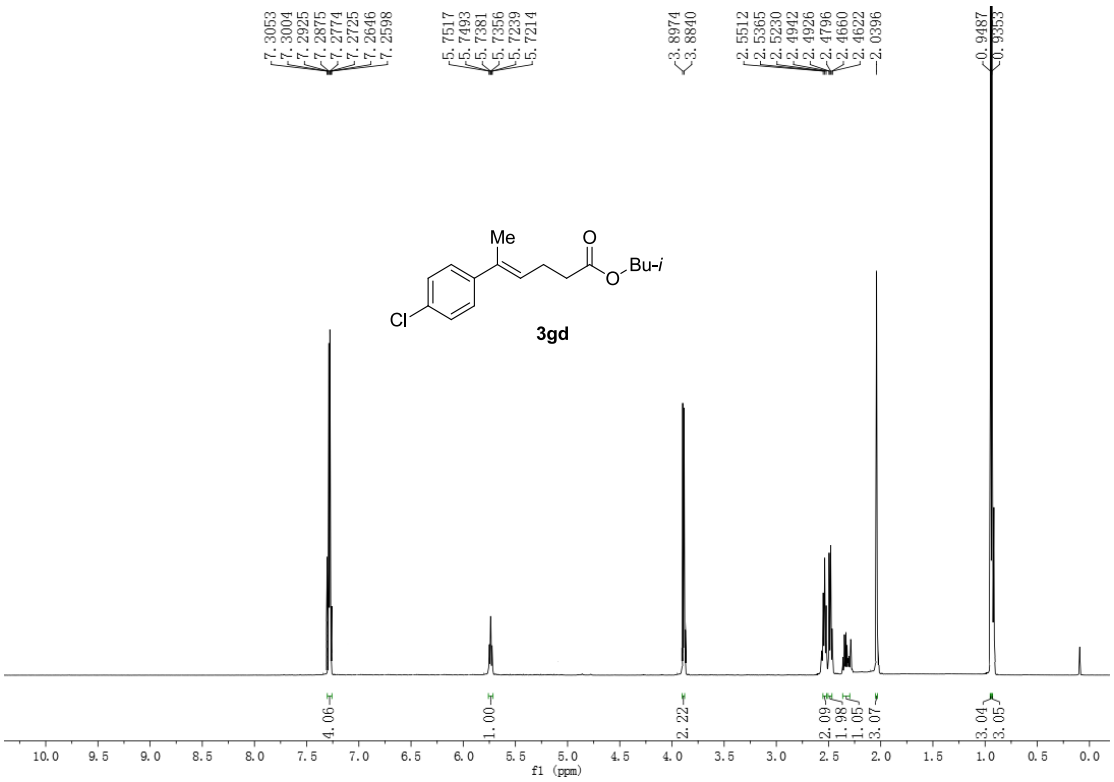
O
O
Bu-i
3fd
f1 (ppm)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5.7239
5.7214
3.8974
3.8840
2.5512
2.5365
2.5230
2.4942
2.4926
2.4796
2.4660
2.4622
2.0396
0.9487
0.9353
Me
O
Bu-i
O
Cl
3gd
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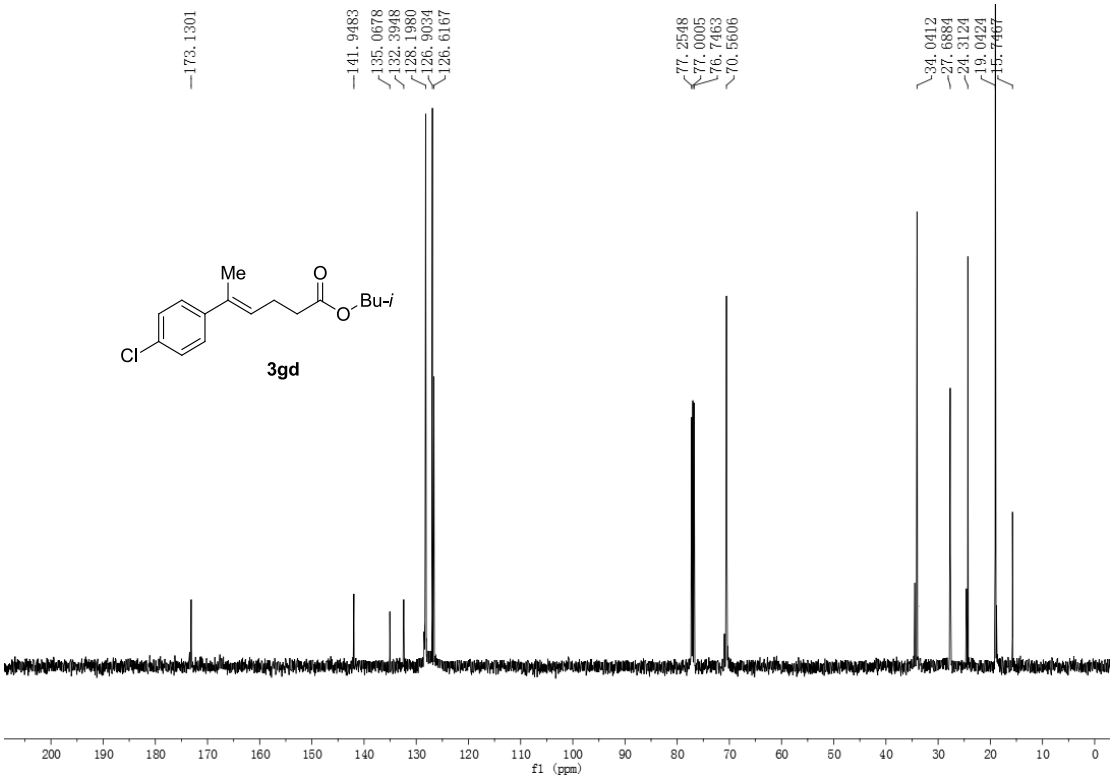
1.00
2.22
2.09
1.98
1.05
3.07
3.04
3.05
f1 (ppm)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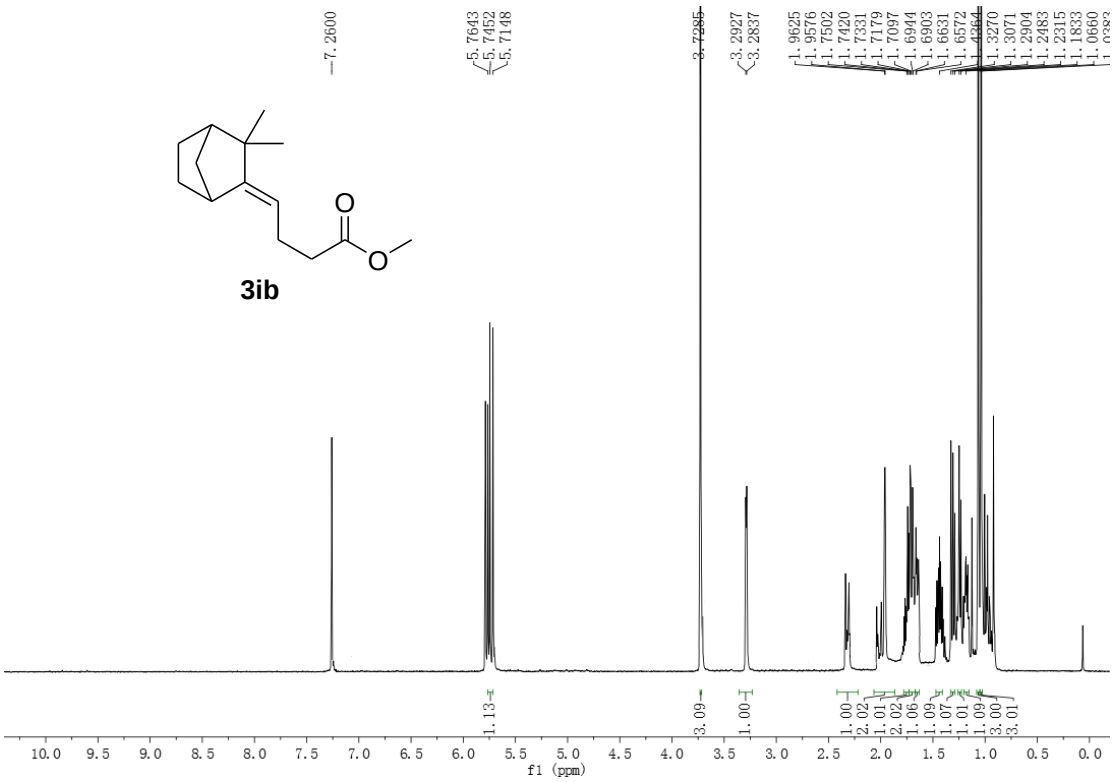
O
Bu-i
O
Cl
3gd
f1 (ppm)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3.2837
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1.9576
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1.7420
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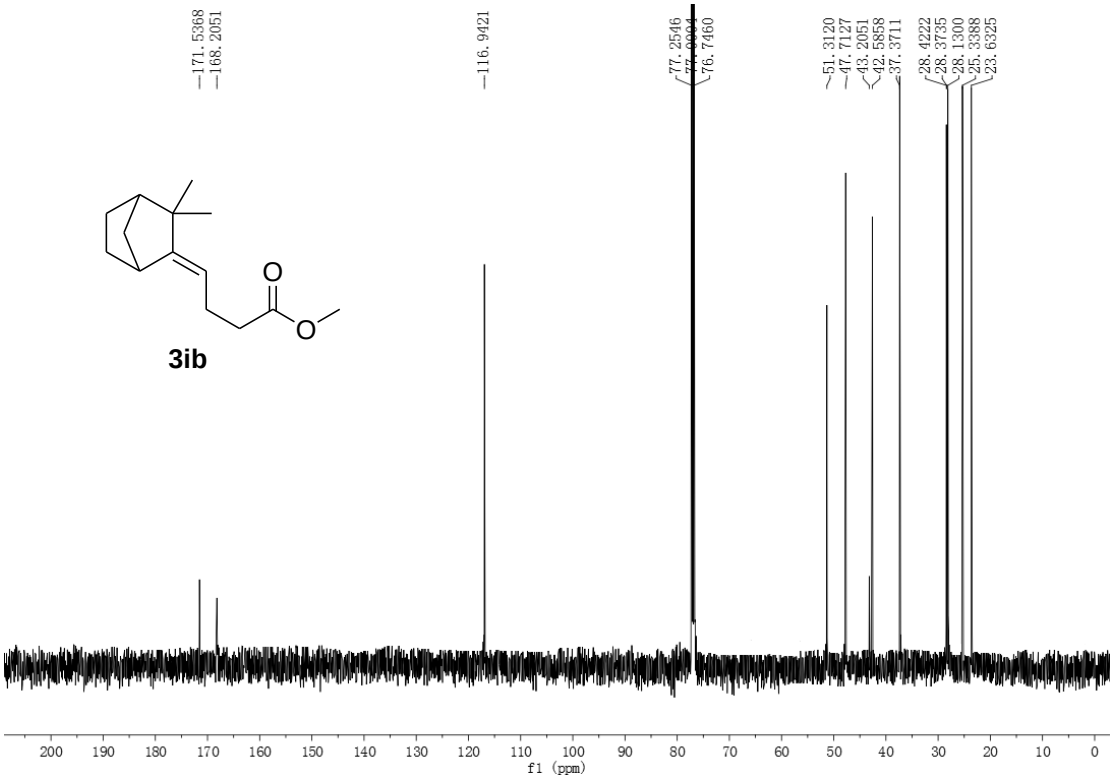
1.6903
1.6631
1.6572
1.4364
1.3270
1.3071
1.2904
1.2483
1.2315
1.1833
1.0660
O
O
3ib
1.13
3.09
1.00
1.00
2.02
1.01
2.02
1.06
1.09
1.07
1.01
1.09
3.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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42.5858
37.3711
28.4222
28.3735
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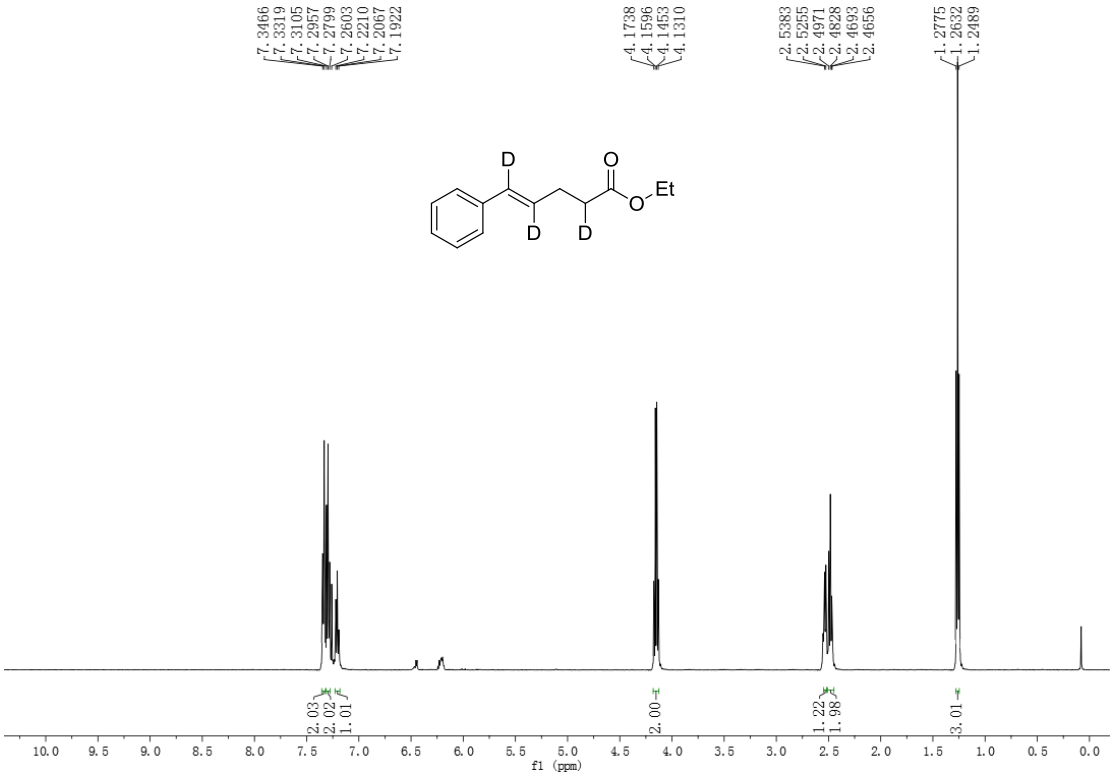
25.3388
23.6325
O
O
3ib
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2603
7.2210
7.2067
7.1922
4.1738
4.1596
4.1453
4.1310
2.5383
2.5255
2.4971
2.4828
2.4693
2.4656
1.2775
1.2632
1.2489
D
O
Et
O
D
D
2.03
2.02
1.01
2.00
1.22
1.98
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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2.0
1.5
1.0
0.5
0.0
f1 (ppm)

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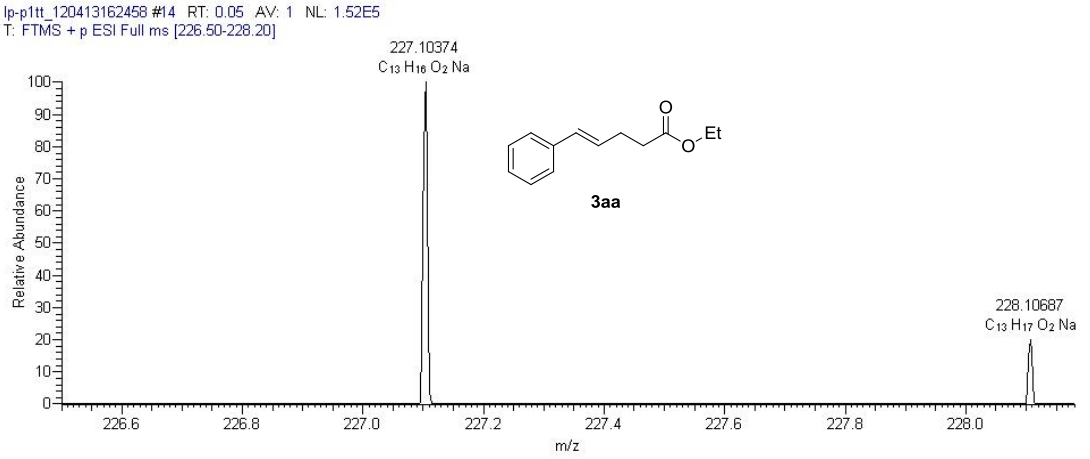
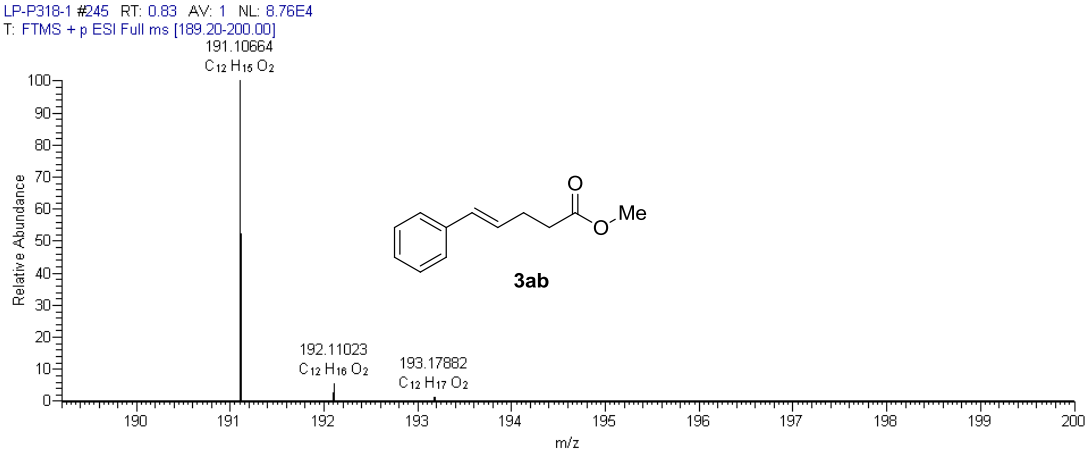
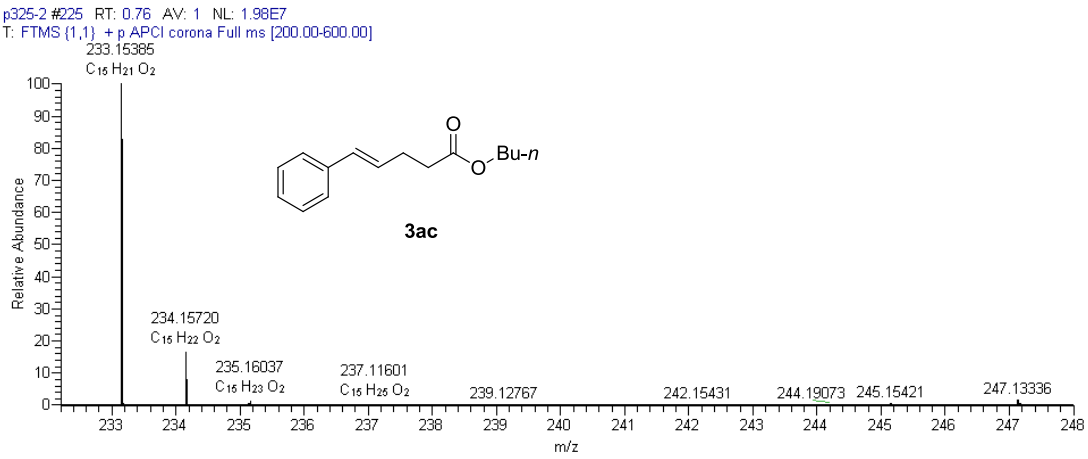
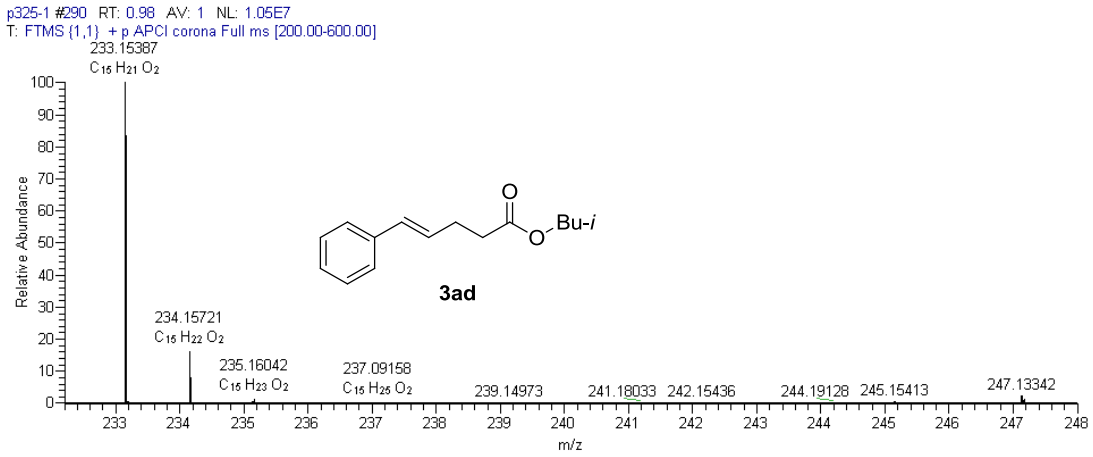
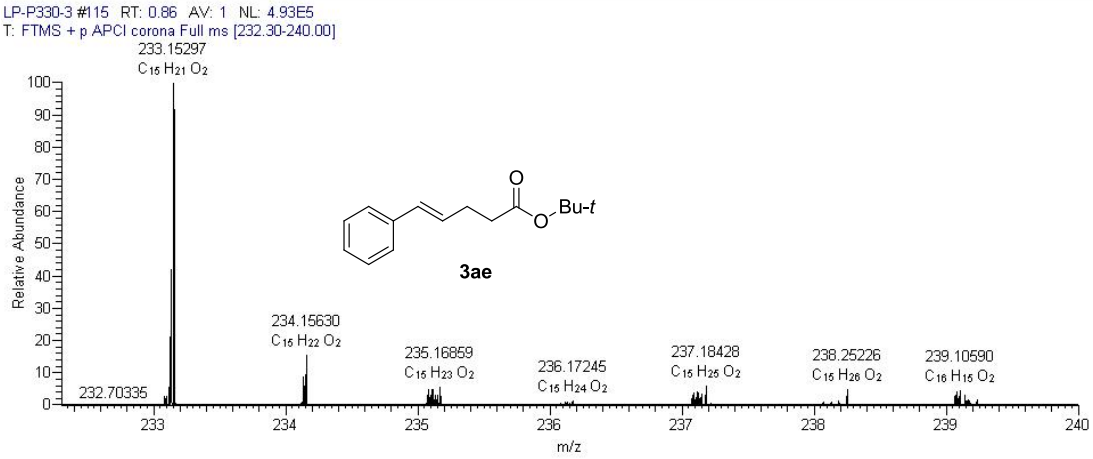
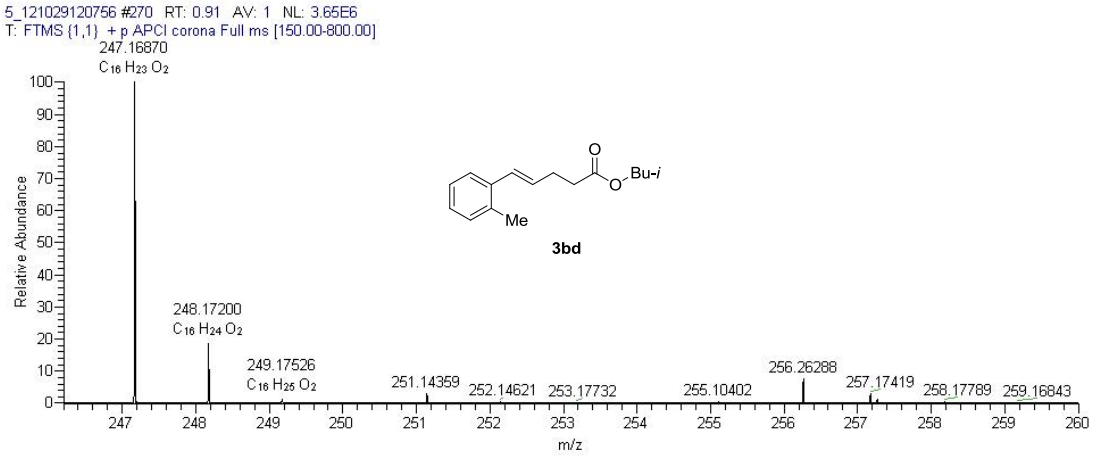


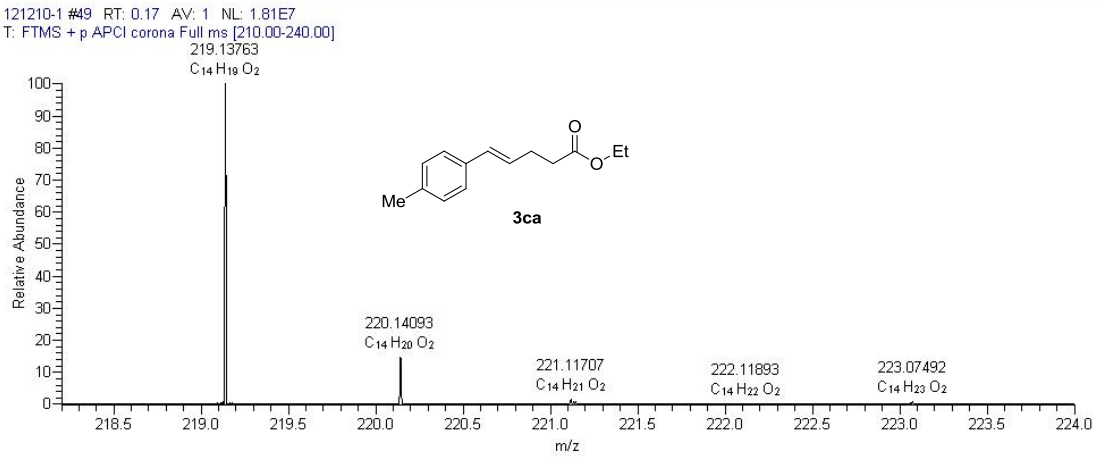


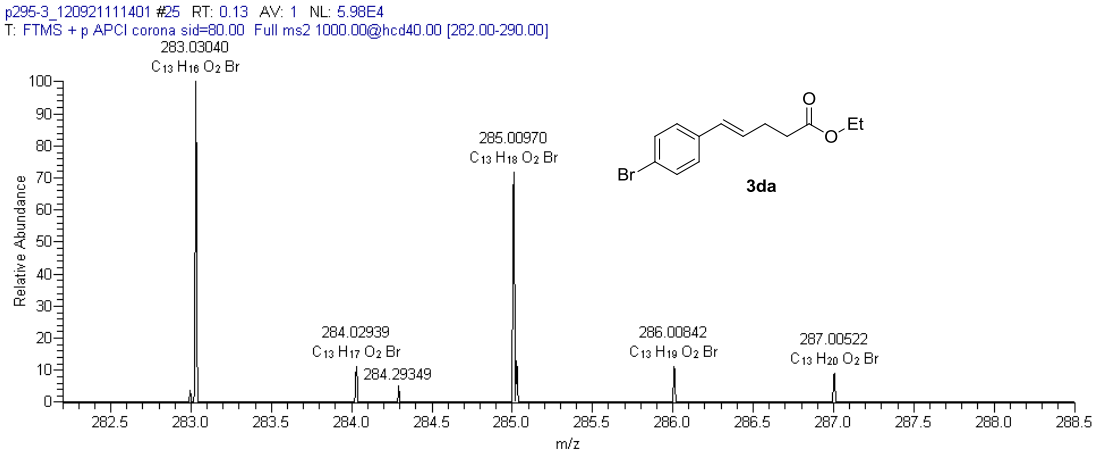


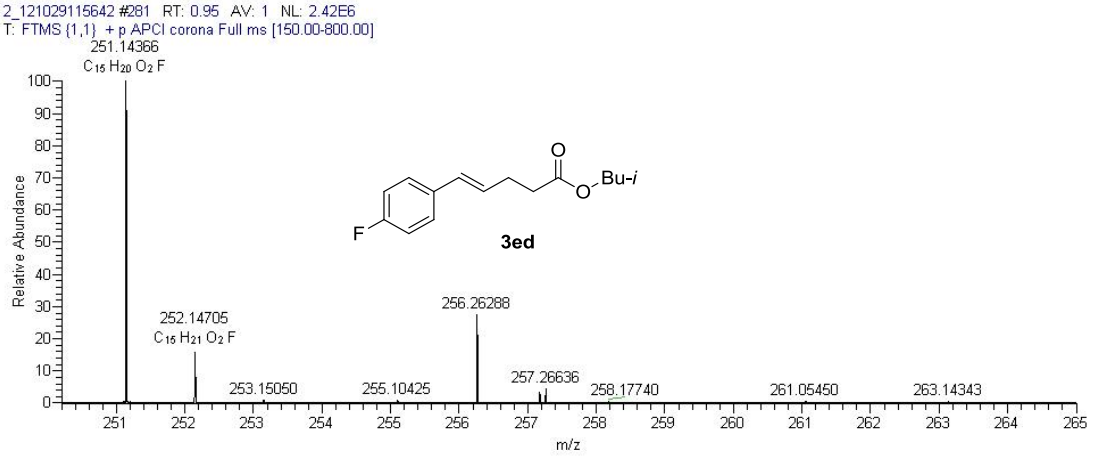

p325-1 #290 RT: 0.98 AV: 1 NL: 1.05E7
T: FTMS {1,1} + p APCI corona Full ms [200.00-600.00]
233.15387
C15 H21 O2
234.15721
C15 H22 O2
235.16042
C15 H23 O2
237.09158
C15 H25 O2
239.14973
241.18033
242.15436
244.19128
245.15413
247.13342
Relative Abundance
m/z
O
O
Bu-i
3ad

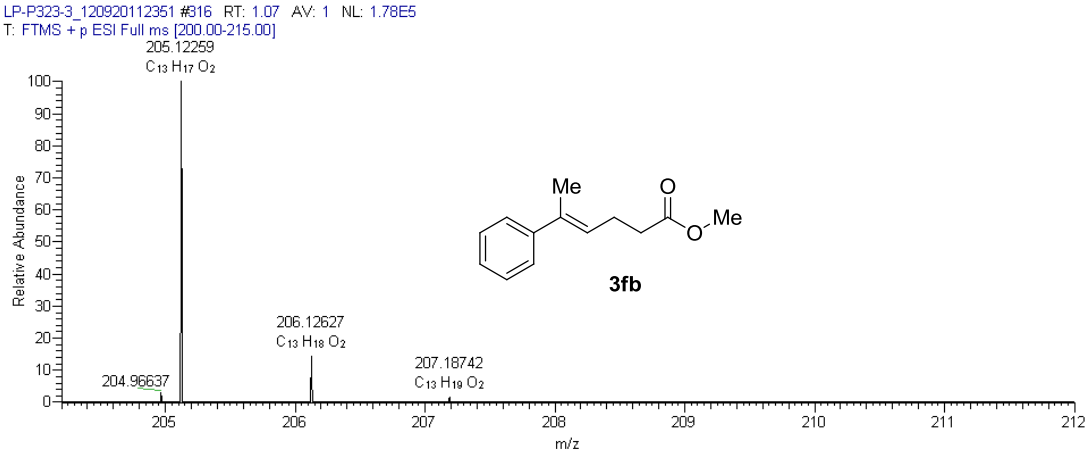

LP-P330-3 #115 RT: 0.86 AV: 1 NL: 4.93E5
T: FTMS + p APCI corona Full ms [232.30-240.00]
233.15297
C15 H21 O2
232.70335
234.15630
C15 H22 O2
235.16859
C15 H23 O2
236.17245
C15 H24 O2
237.18428
C15 H25 O2
238.25226
C15 H26 O2
239.10590
C16 H15 O2
Relative Abundance
m/z
O
O
Bu-t
3ae

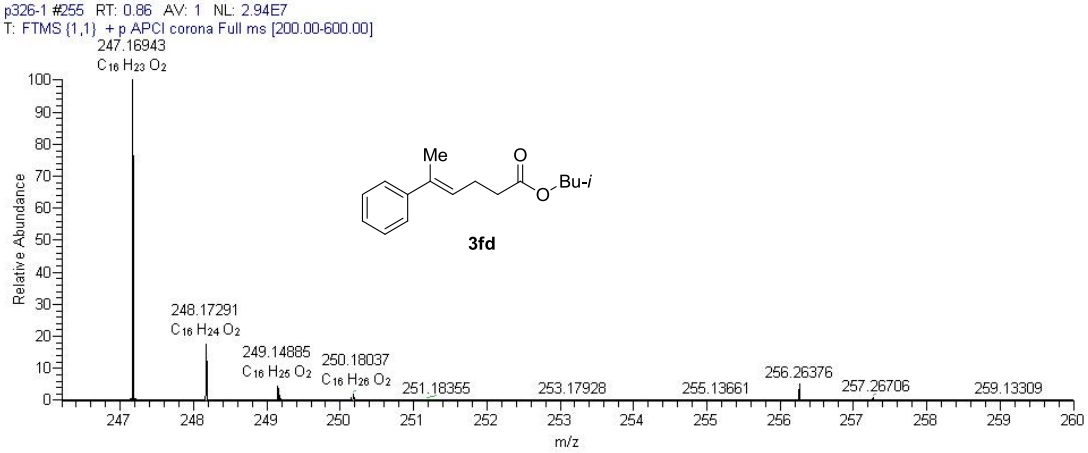

5_121029120756 #270 RT: 0.91 AV: 1 NL: 3.65E6
T: FTMS {1,1} + p APCI corona Full ms [150.00-800.00]
247.16870
C16 H23 O2
248.17200
C16 H24 O2
249.17526
C16 H25 O2
251.14359
252.14621
253.17732
255.10402
256.26288
257.17419
258.17789
259.16843
Relative Abundance
m/z
O
O
Bu-i
Me
3bd

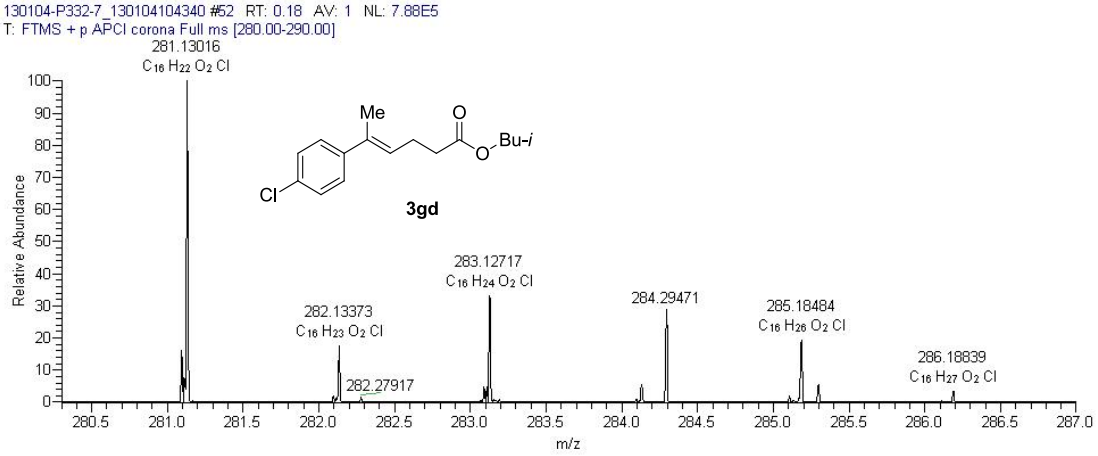

121210-1 #49 RT: 0.17 AV: 1 NL: 1.81E7
T: FTMS + p APCI corona Full ms [210.00-240.00]
219.13763
C14 H19 O2
220.14093
C14 H20 O2
221.11707
C14 H21 O2
222.11893
C14 H22 O2
223.07492
C14 H23 O2
Relative Abundance
m/z
Me
O
O
Et
3ca

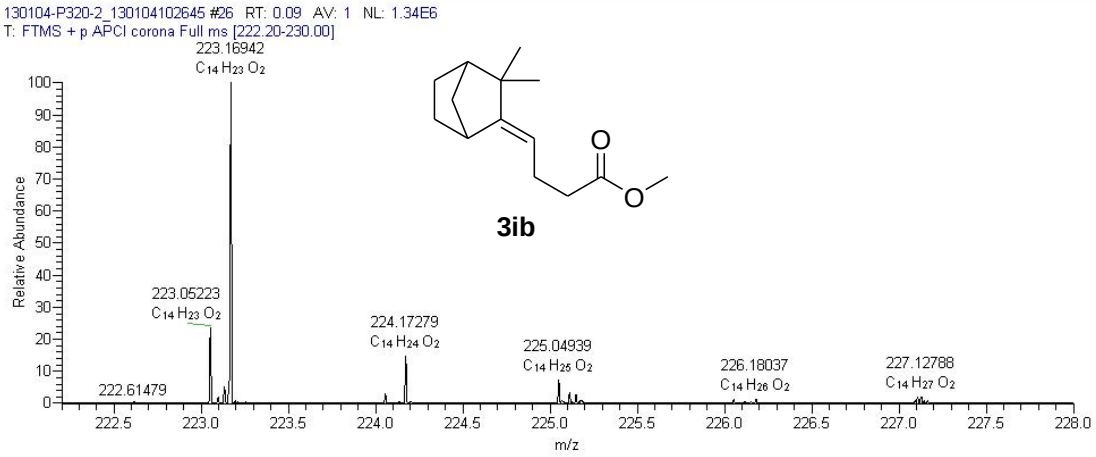

p295-3_120921111401 #25 RT: 0.13 AV: 1 NL: 5.98E4
T: FTMS + p APCI corona sid=80.00 Full ms2 1000.00@hcd40.00 [282.00-290.00]
283.03040
C13 H16 O2 Br
284.02939
C13 H17 O2 Br
284.29349
285.00970
C13 H18 O2 Br
286.00842
C13 H19 O2 Br
287.00522
C13 H20 O2 Br
Relative Abundance
m/z
Br
O
O
Et
3da


2_121029115642 #281 RT: 0.95 AV: 1 NL: 2.42E6
T: FTMS {1,1} + p APCI corona Full ms [150.00-800.00]
251.14366
C15 H20 O2 F
252.14705
C15 H21 O2 F
253.15050
255.10425
256.26288
257.26636
258.17740
261.05450
263.14343
Relative Abundance
m/z
F
O
O
Bu-i
3ed


LP-P323-3_120920112351 #316 RT: 1.07 AV: 1 NL: 1.78E5
T: FTMS + p ESI Full ms [200.00-215.00]
205.12259
C13 H17 O2
206.12627
C13 H18 O2
207.18742
C13 H19 O2
204.96637
Relative Abundance
m/z
Me
O
O
Me
3fb


p326-1 #255 RT: 0.86 AV: 1 NL: 2.94E7
T: FTMS {1,1} + p APCI corona Full ms [200.00-600.00]
247.16943
C16 H23 O2
248.17291
C16 H24 O2
249.14885
C16 H25 O2
250.18037
C16 H26 O2
251.18355
253.17928
255.13661
256.26376
257.26706
259.13309
Relative Abundance
m/z
Me
O
O
Bu-i
3fd


130104-P332-7_130104104340 #52 RT: 0.18 AV: 1 NL: 7.88E5
T: FTMS + p APCI corona Full ms [280.00-290.00]
281.13016
C16 H22 O2 Cl
282.13373
C16 H23 O2 Cl
282.27917
283.12717
C16 H24 O2 Cl
284.29471
285.18484
C16 H26 O2 Cl
286.18839
C16 H27 O2 Cl
Relative Abundance
m/z
Me
O
O
Bu-i
Cl
3gd


130104-P320-2_130104102645 #26 RT: 0.09 AV: 1 NL: 1.34E6
T: FTMS + p APCI corona Full ms [222.20-230.00]
223.16942
C14 H23 O2
223.05223
C14 H23 O2
224.17279
C14 H24 O2
225.04939
C14 H25 O2
226.18037
C14 H26 O2
227.12788
C14 H27 O2
222.61479
Relative Abundance
m/z
O
O
3ib