Electronic Supplementary Material (ESI) for ChemComm.
This journal is © The Royal Society of Chemistry 2014

Supporting Information

The Bu_4NI-catalyzed alfa-acyloxylation of ketones with benzylic alcohols

Songjin Guo,[†] Jin-Tao Yu,[†] Qiang Dai,[†] Haitao Yang,[†] and Jiang Cheng*[,†,‡]

School of Petrochemical Engineering, Jiangsu Key Laboratory of Advanced Catalytic Materials & Technology, Jiangsu Province Key Laboratory of Fine Petrochemical Engineering, Changzhou University, Changzhou 213164, P. R. China, and State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, P. R. China

Email: jiangcheng@cczu.edu.cn

Table of Contents

1. General Considerations

All chemicals were used as received without further purification unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 300 or 400 MHz NMR spectrometer (75 or 100 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

2. Experimental Procedures.

Under air, a 20 mL of Schlenk tube equipped with a stir bar was charged with benzylic alcohol **1** (0.2 mmol), Ketone (0.4 mmol), Bu_4NI (14.8 mg, 20 mol %), TBHP (70% aqueous, 162 μL, 1.2 mmol), PhCN (2 mL). The tube was sealed with a Teflon lined cap. The reaction mixture was stirred at 90°C for 24h in oil bath. After the completion of the reaction (monitored by TLC), the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-EtOAc as the eluent to give the desired product.

3. The Reaction of Benzylic Alcohol in TBAI/TBHP

Under air, a 20 mL of Schlenk tube equipped with a stir bar was charged with benzylic alcohol **1** (0.2 mmol), Bu_4NI (14.8 mg, 20 mol %), TBHP (70% aqueous, 162 μL, 1.2 mmol), PhCN (2 mL). The tube was sealed with a Teflon lined cap. The reaction mixture was stirred at 40°C for 24 h in oil bath. After the completion of the reaction (monitored by TLC), the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-EtOAc as the eluent to give benzoic acid (57% yield) and *tert*-butyl perester (28% yield).

4. Characterization Data for the Products

Oxo-1-phenylpropan-2-yl benzoate (3aa):[1] 42.5 mg, 84% yield. White solid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.68 (d, *J* = 6.9 Hz, 3H), 6.21 (q, *J* = 6.9 Hz, 1H), 7.42-7.51 (m, 4H), 7.55-7.62 (m, 2H), 7.99-8.03 (m, 2H), 8.08-8.12 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 71.8, 128.4, 128.5, 128.8, 129.4, 129.8, 133.3, 133.6, 134.4, 165.9, 196.7.

1-Oxo-1-phenylpropan-2-yl 4-methoxybenzoate (3ba): 45.3 mg, 80% yield. White solid. m.p.: 107–109 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.65 (d, *J* = 6.9 Hz, 3H), 3.85 (s, 3H), 6.17 (q, *J* = 6.9 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 2H), 7.45-7.50 (m, 2H), 7.56-7.61 (m, 1H), 7.98-8.06 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.1, 55.4, 71.5, 113.6, 121.8, 128.5, 128.7, 131.9, 133.5, 134.5, 163.6, 165.6, 197.0. MS(EI) 284 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{17}H_{17}O_4$ $(M+H)^+$ 285.1121, found 285.1121.

1-Oxo-1-phenylpropan-2-yl 4-chlorobenzoate (3ca): 44.3 mg, 77% yield. White solid. m.p.: 102–104 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.67 (d, *J* = 6.9 Hz, 3H), 6.20 (q, *J* = 6.9 Hz, 1H), 7.40-7.45 (m, 2H), 7.47-7.52 (m, 2H), 7.58-7.64 (m, 1H), 7.98-8.05 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 72.1, 127.9, 128.5, 128.8, 128.8, 131.3, 133.7, 134.3, 139.8, 165.1, 196.5. MS(ESI) 288 (M^+); HRMS (EI) *m*/*z* calcd. for $C_{16}H_{14}ClO_3$ $(M+H)^+$ 289.0626, found 289.0619.

1-Oxo-1-phenylpropan-2-yl 4-bromobenzoate (3da): 47.3 mg, 71% yield. White solid. m.p.: 118–119 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.66 (d, *J* = 7.2 Hz, 3H), 6.19 (q, *J* = 7.2 Hz, 1H), 7.46-7.51 (m, 2H), 7.57-7.62 (m, 3H), 7.94-8.00 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 72.1, 128.3, 128.3, 128.4, 128.8, 131.3, 131.7, 133.6, 134.2, 165.2, 196.4. MS(EI) 332 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{16}H_{14}BrO_3$ $(M+Na)^+$ 354.9940, found 354.9933.

1-Oxo-1-phenylpropan-2-yl 4-fluorobenzoate (3ea): 44.0 mg, 81% yield. White solid. m.p.: 101–103 °C.^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.66 (d, *J* = 6.9 Hz , 3H), 6.20 (q, *J* = 7.2 Hz, 1H), 7.07-7.15 (m, 2H), 7.44-7.51 (m, 2H), 7.56-7.62 (m, 1H), 7.98-8.01 (m, 2H), 8.08-8.14 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 71.9, 115.5 (d, $J_{C\text{-}F}$ = 21.9 Hz), 125.7 (d, $J_{C\text{-}F}$ = 2.9 Hz), 128.4, 128.8, 132.4 (d, $J_{C\text{-}F}$ = 9.4 Hz), 133.6, 134.3, 164.9, 165.9 (d, $J_{C\text{-}F}$ = 252.8 Hz), 196.5. MS(EI) 272 (M^+); HRMS (ESI) *m*/*z*

calcd. for $C_{16}H_{14}FO_3$ $(M+H)^+$ 273.0921, found 273.0912.

1-Oxo-1-phenylpropan-2-yl 4-nitrobenzoate (3fa):[2] 38.8 mg, 65% yield. White solid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.71 (d, *J* = 6.9 Hz, 3H), 6.25 (q, *J* = 6.9 Hz, 1H), 7.49-7.54 (m, 2H), 7.60-7.65 (m, 1H), 7.98-8.00 (m, 2H), 8.25-8.32 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.3, 72.8, 123.5, 128.5, 128.9, 131.0, 133.9, 134.0, 134.9, 150.7, 164.1, 196.0.

1-Oxo-1-phenylpropan-2-yl 4-(benzoyloxy)benzoate (3ga): 46.0 mg, 61% yield. White solid. m.p.: 134–136 ^{o}C.^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.69 (d, *J* = 6.9 Hz, 3H), 6.22 (q, *J* = 6.9 Hz, 1H), 7.30-7.35 (m, 2H), 7.47-7.55 (m, 4H), 7.58-7.69 (m, 2H), 8.00-8.02 (m, 2H), 8.16-8.22 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 72.0, 121.8, 127.0, 128.5, 128.6, 128.8, 129.0, 130.2, 131.5, 133.6, 133.9, 134.3, 154.9, 164.5, 165.2, 196.6. MS(EI) 374 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{23}H_{19}O_5$ $(M+H)^+$ 375.1227, found 375.1230.

1-Oxo-1-phenylpropan-2-yl 2-methylbenzoate (3ha): 36.4 mg, 68% yield. White solid. m.p.: 51–52 ^{o}C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.66 (d, *J* = 7.2 Hz, 3H), 2.59 (s, 3H), 6.20 (q, *J* = 6.9 Hz, 1H), 7.23-7.28 (m, 2H), 7.38-7.62 (m, 4H), 8.00-8.02 (m 3H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.1, 21.6, 71.7, 125.7, 128.4, 128.8, 128.9, 130.8, 131.6, 132.2, 133.5, 134.4, 140.5, 166.9, 196.9. MS(EI) 268 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{17}H_{17}O_3$ $(M+H)^+$ 269.1172, found 269.1165.

Oxo-1-phenylpropan-2-yl 1-naphthoate (3ia): 53.7 mg, 88% yield. White solid. m.p.: 96–98 ^{o}C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.73 (d, *J* = 7.2 Hz, 3H), 6.33 (q, *J* = 7.2 Hz, 1H), 7.49-7.56 (m, 4H), 7.58-7.65 (m, 2H), 7.82-7.90 (m, 1H), 8.03-8.08 (m, 3H), 8.32 (d, *J* = 7.2 Hz, 1H), 8.92 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 71.9, 124.5, 125.7, 126.2, 126.3, 127.8, 128.5, 128.5, 128.8, 130.6, 131.3, 133.6, 133.6, 133.7, 134.4, 166.9, 196.9. MS(EI) 304 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{20}H_{17}O_3$ $(M+H)^+$ 305.1172, found 305.1174.

1-Oxo-1-phenylpropan-2-yl picolinate (3ja): 28.2 mg, 55% yield. White solid. m.p.: 90–92 ^{o}C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.71 (d, *J* = 7.2 Hz, 3H), 6.25 (q, *J* = 7.2 Hz, 1H), 7.44-7.49 (m, 3H), 7.54-7.60 (m, 1H), 7.82 (t, *J* = 7.7 Hz, 1H), 7.97-8.00 (m, 2H), 8.11-8.14 (m, 1H), 8.76-8.78 (m, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 72.8,

125.4, 127.1, 128.4, 128.7, 133.6, 134.2, 136.9, 147.4, 150.0, 164.5, 196.1. MS(EI) 255 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{15}H_{14}NO_3$ $(M+H)^+$ 256.0968, found 256.0966.

1-Oxo-1-phenylpropan-2-yl isobutyrate (3ka): 21.1 mg, 48% yield. Colorless oil. ^1H NMR ($CDCl_3$, 300 MHz) δ 1.18-1.21 (m, 6H), 1.53 (q, *J* = 6.9 Hz, 3H), 2.65 (hept, *J* = 6.9 Hz, 1H), 5.95 (q, *J*=6.9 Hz, 1H), 7.45-7.50 (m, 2H), 7.56-7.61 (m, 1H), 7.91-7.95 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 16.9, 18.8, 18.9, 33.7, 71.0, 128.4, 128.7, 133.5, 134.5, 176.6, 197.1. MS(EI) 220 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{13}H_{17}O_3$ $(M+H)^+$ 221.1172, found 221.1168.

1-Oxo-1-phenylpropan-2-yl cinnamate (3la): 28.6 mg, 51% yield. White solid. m.p.: 67–68 °C. ^1H NMR ($CDCl_3$, 300 MHz) δ 1.62 (d, *J* = 6.9 Hz, 3H), 6.12 (q, *J* = 7.2 Hz, 1H), 6.54 (d, *J* = 16.2 Hz, 1H), 7.38-7.41 (m, 3H), 7.47-7.63 (m, 5H), 7.72-7.78 (d, *J* = 16.2 Hz, 1H), 7.98-8.01 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.2, 71.4, 117.1, 128.2, 128.5, 128.8, 128.9, 130.5, 133.6, 134.2, 134.4, 145.9, 166.2, 196.9. MS(EI) 280 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{18}H_{16}NaO_3$ $(M+Na)^+$ 303.0992, found 303.0998.

1-(4-Bromophenyl)-1-oxopropan-2-yl benzoate (3ab):[3] 60.0 mg, 90% yield. White solid. ^1H NMR ($CDCl_3$, 300 MHz) δ 1.66 (d, *J* = 7.2 Hz, 3H), 6.12 (q, *J* = 6.9 Hz, 1H), 7.42-7.48 (m, 2H), 7.56-7.65 (m, 3H), 7.85-7.89 (m, 2H), 8.06-8.10 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.0, 71.7, 128.4, 128.8, 129.2, 129.8, 130.0, 132.1, 133.1, 133.4, 165.9, 195.8.

1-Oxo-1-phenylpentan-2-yl 4-methoxybenzoate (3ac): 45.0 mg, 72% yield. White solid. m.p.: 76–78 °C. ^1H NMR ($CDCl_3$, 300 MHz) δ 0.97-1.02 (m, 3H), 1.52-1.68 (m, 2H), 1.93-2.01 (m, 2H), 3.86 (s, 3H), 6.06-6.10 (m, 1H), 6.91-6.95 (m, 2H), 7.46-7.51 (m, 2H), 7.56-7.62 (m, 1H), 7.99-8.08 (m, 4H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 13.8, 19.0, 33.5, 55.4, 75.2, 113.6, 121.9, 128.4, 128.7, 131.9, 133.4, 134.9, 163.6, 165.9, 196.8. MS(EI) 312 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{19}H_{20}NaO_4$ $(M+Na)^+$ 335.1254, found 335.1258.

1-Oxo-1-(thiophen-2-yl)propan-2-yl 4-methoxybenzoate (3ad): 38.7 mg, 67% yield. White solid. m.p.: 110–111 °C. ^1H NMR ($CDCl_3$, 300 MHz) δ 1.69 (d, *J* = 7.2 Hz, 3H), 3.86 (s, 3H), 5.93 (q, *J* = 6.9 Hz, 1H), 6.93 (q, *J* = 8.7 Hz, 2H), 7.13-7.16 (m,

1H), 7.67-7.69 (m, 1H), 7.86-7.87 (m, 1H), 8.05 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 17.7, 55.4, 72.6, 113.7, 121.7, 128.2, 132.0, 132.7, 134.4, 140.5, 163.7, 165.6, 189.9. MS(EI) 290 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{15}H_{15}O_4S$ $(M+H)^+$ 291.0686, found 291.0683.

2-Oxocyclohexyl 4-methoxybenzoate (3ae): 17.0 mg, 34% yield. White solid. m.p.: 138–140 °C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.59-2.15 (m, 5H), 2.37-2.59 (m, 3H), 3.85 (s, 3H), 5.35-5.40 (m, 1H), 6.89-6.94 (m, 2H), 8.01-8.06 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 23.7, 27.2, 33.2, 40.7, 55.4, 76.7, 113.5, 121.9, 131.9, 163.5, 165.2, 204.7. MS(EI) 248 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{14}H_{16}NaO_4$ $(M+Na)^+$ 271.0941, found 271.0946.

(*E*)-4-Oxo-6-phenylhex-5-en-3-yl 4-methoxybenzoate (3af): 30.3 mg, 47% yield. White solid. m.p.: 93–94 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.10 (t, *J* = 7.6 Hz, 3H), 1.94-2.08 (m, 2H), 3.87 (s, 3H), 5.40-5.43 (m, 1H), 6.92-6.96 (m, 3H), 7.36-7.39 (m, 3H), 7.54-7.56 (m, 2H), 7.76 (d, *J* = 16 Hz, 1H), 8.08 (d *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 9.7, 24.4, 55.4, 79.1, 113.7, 121.0, 121.9, 128.5, 128.9, 130.8, 131.9, 134.3, 144.4, 163.7, 165.8, 196.2. MS(EI) 324 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{20}H_{21}O_4$ $(M+H)^+$ 325.1434, found 325.1429.

1-Oxo-1-(pyridin-4-yl)propan-2-yl 4-methoxybenzoate (3ag): 18.7 mg, 33% yield. Pale yellow solid. m.p.: 120–122 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.62 (d, *J* = 6.8Hz, 3H), 3.86 (s, 3H), 6.03 (q, *J* = 7.2 Hz, 1H), 6.92 (d, *J* = 8.8 Hz, 2H), 7.76 (d, *J* = 6.0 Hz, 2H), 8.00 (d, *J* = 8.8 Hz, 2H), 8.82 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 16.7, 55.5, 71.8, 113.8, 121.3, 121.3, 132.0, 140.8, 151.0, 163.8, 165.6, 197.0. MS(EI) 285 (M^+); HRMS (ESI) *m*/*z* calcd. for $C_{16}H_{15}NNaO_4$ $(M+Na)^+$ 308.0893, found 308.0890.

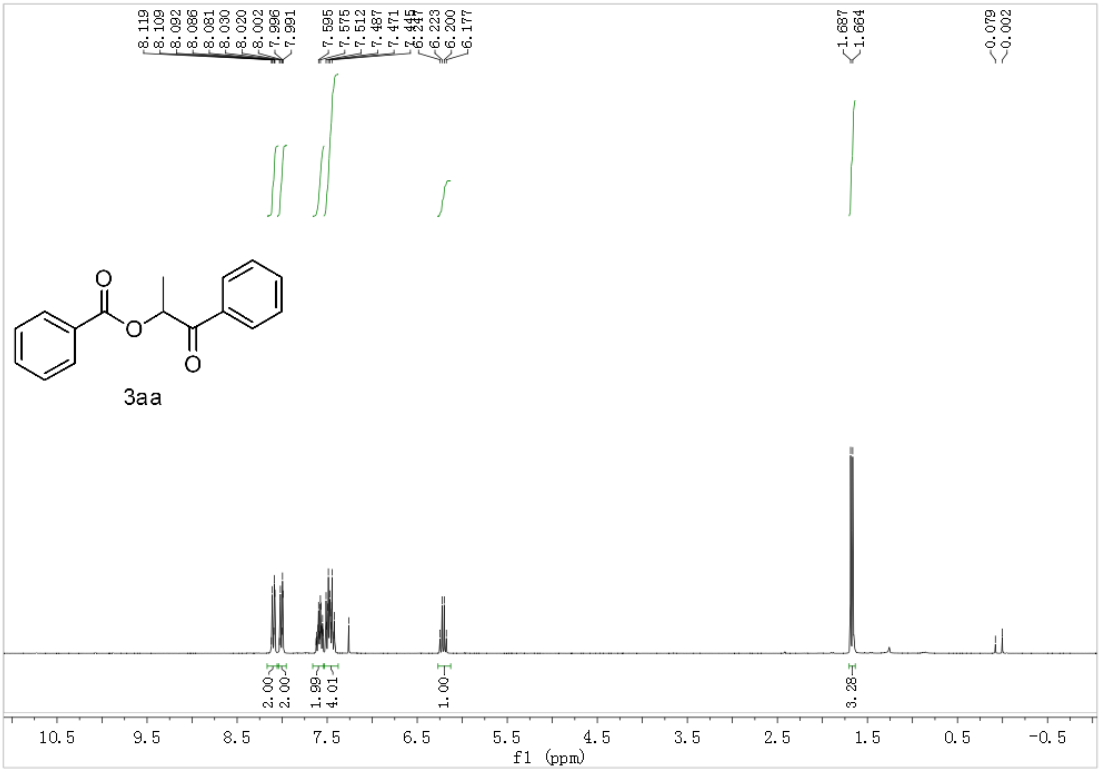
5. Reference

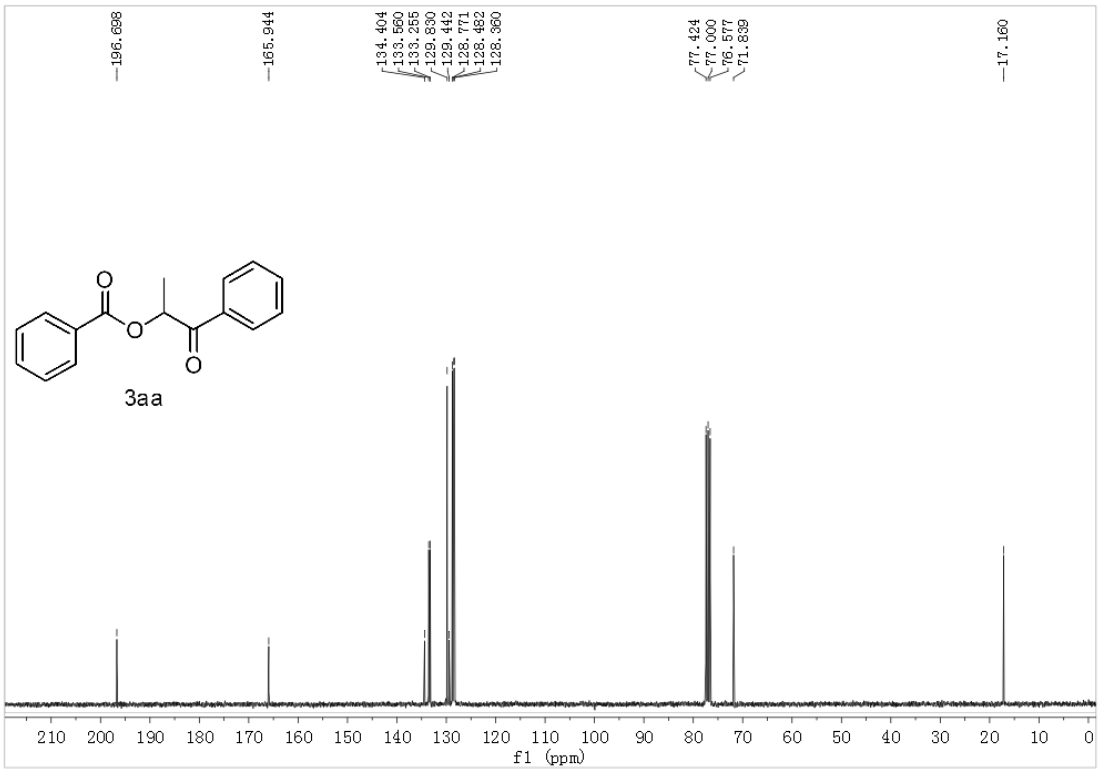
[1] M. Shindo, Y. Yoshimura, M. Hayashi, H. Soejima, T. Yoshikawa, K. Matsumoto, and K. Shishido, *Org. Lett.,* 2007, **9**, 1963.

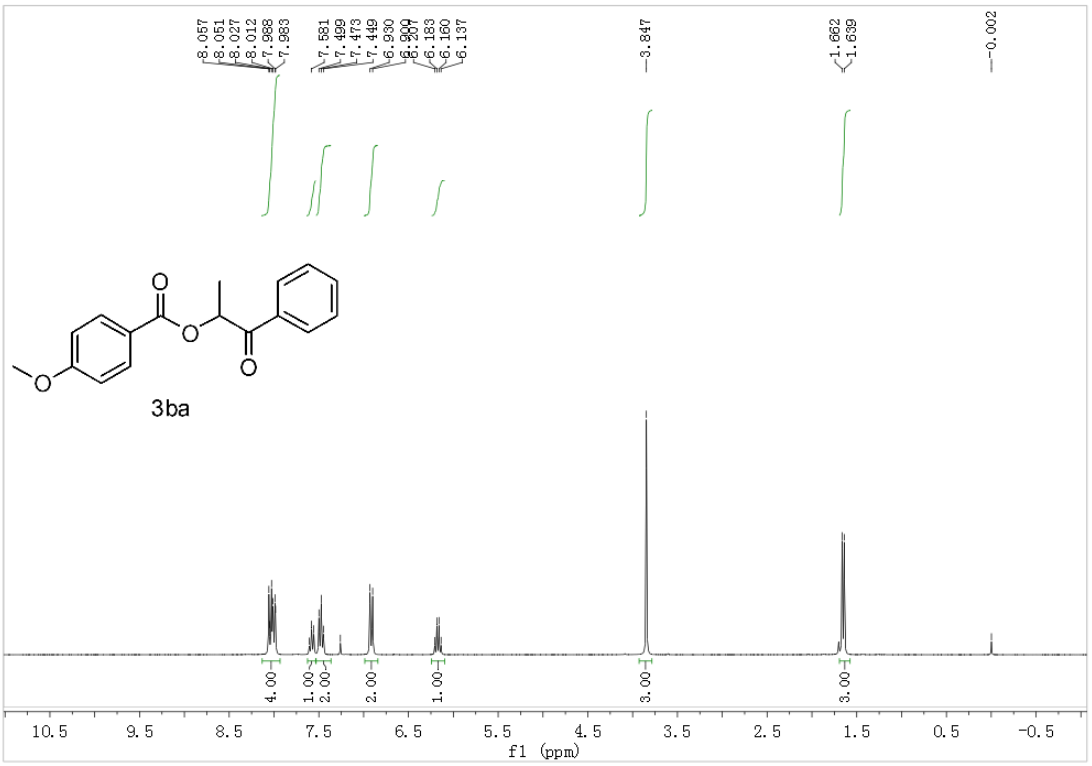
[2] M. Uyanik, D. Suzuki, T. Yasui, and K. Ishihara, *Angew. Chem., Int. Ed.*, 2011, **50**, 5331..

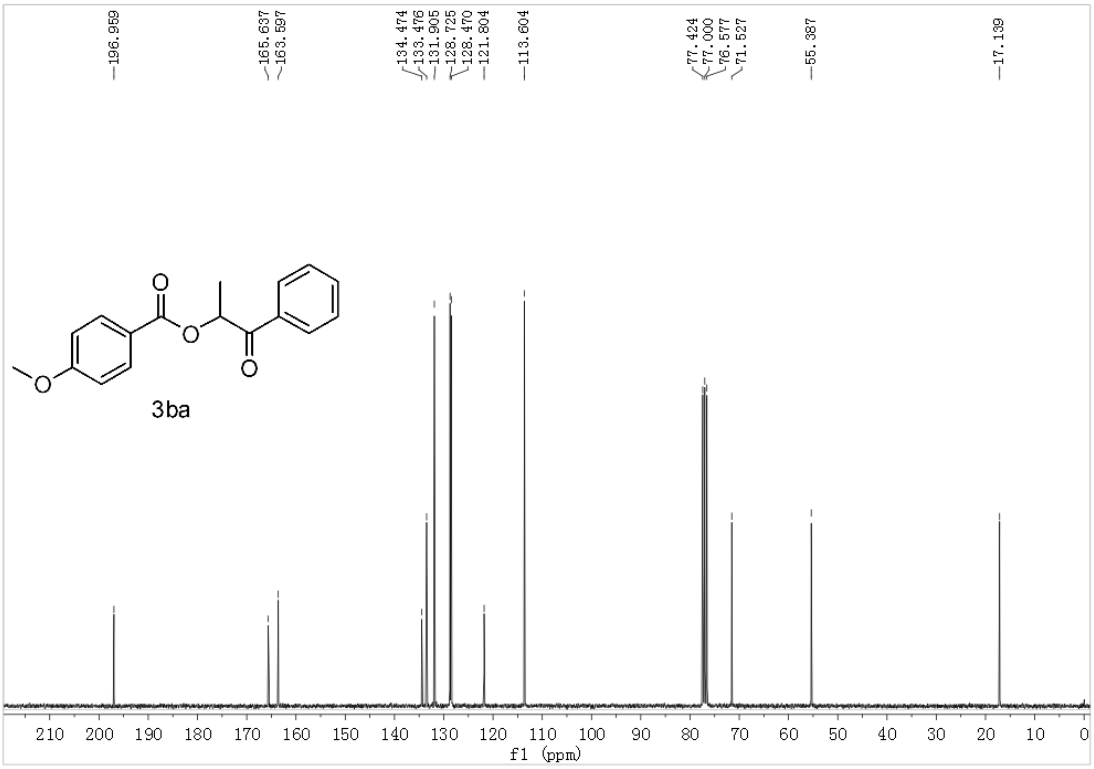
[3] C. S. Beshara, A. Hall, R. L. Jenkins, K. L. Jones, T. C. Jones, N. M. Killeen, P. H. Taylor, S. P. Thomas and N. C. O. Tomkinson, *Org. Lett.* 2005, **7**, 5729.

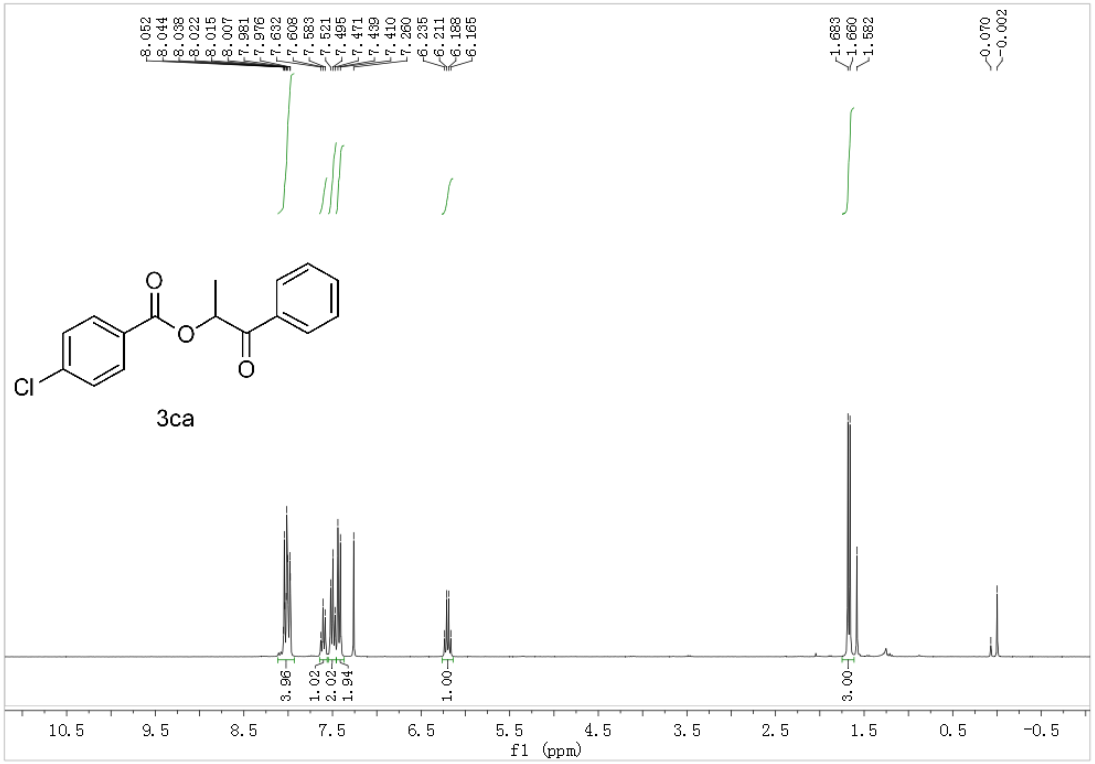
6. Copies of the ^{1}H NMR and ^{13}C NMR spectra

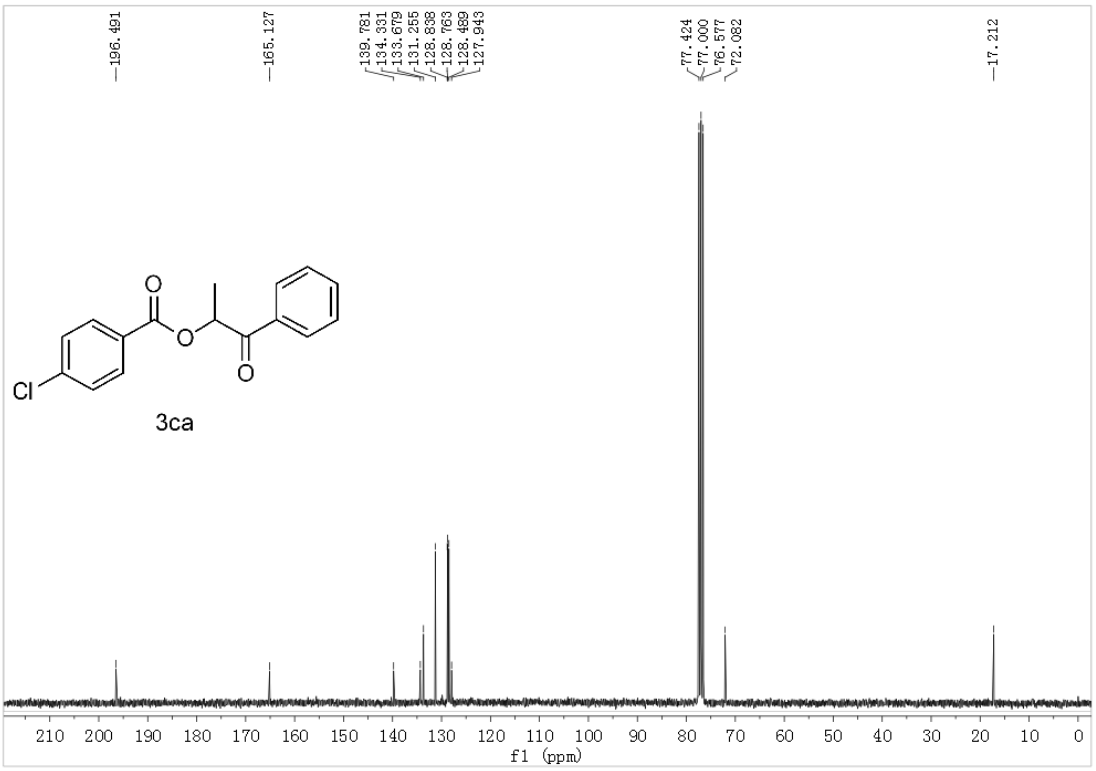


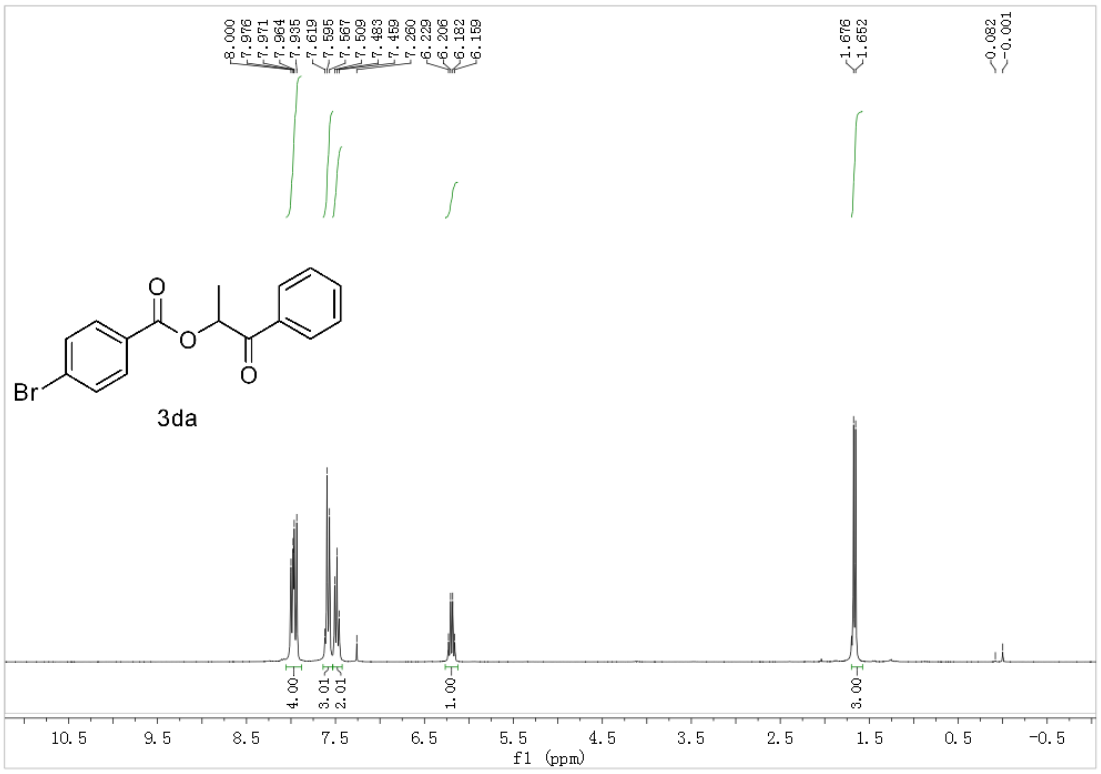


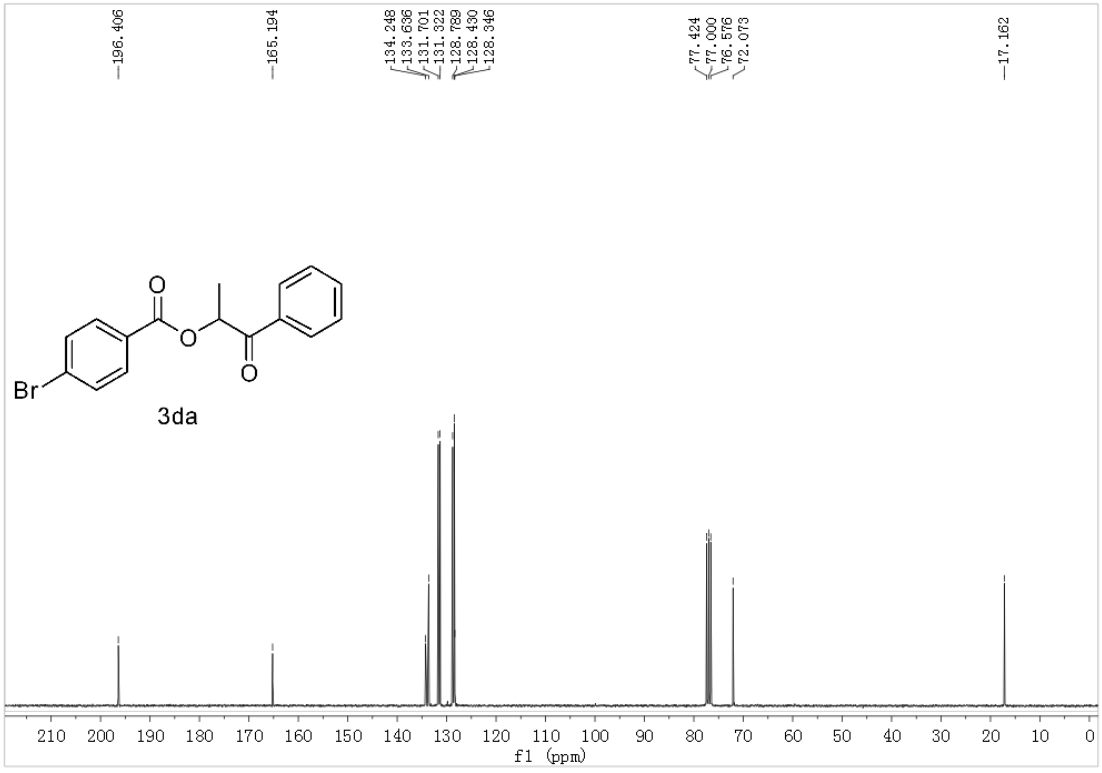

8.057
8.051
8.027
8.012
7.988
7.983
7.581
7.499
7.473
7.449
6.930
6.207
6.183
6.160
6.137
3.847
1.662
1.639
0.002
3ba
4.00
1.00
2.00
2.00
1.00
3.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

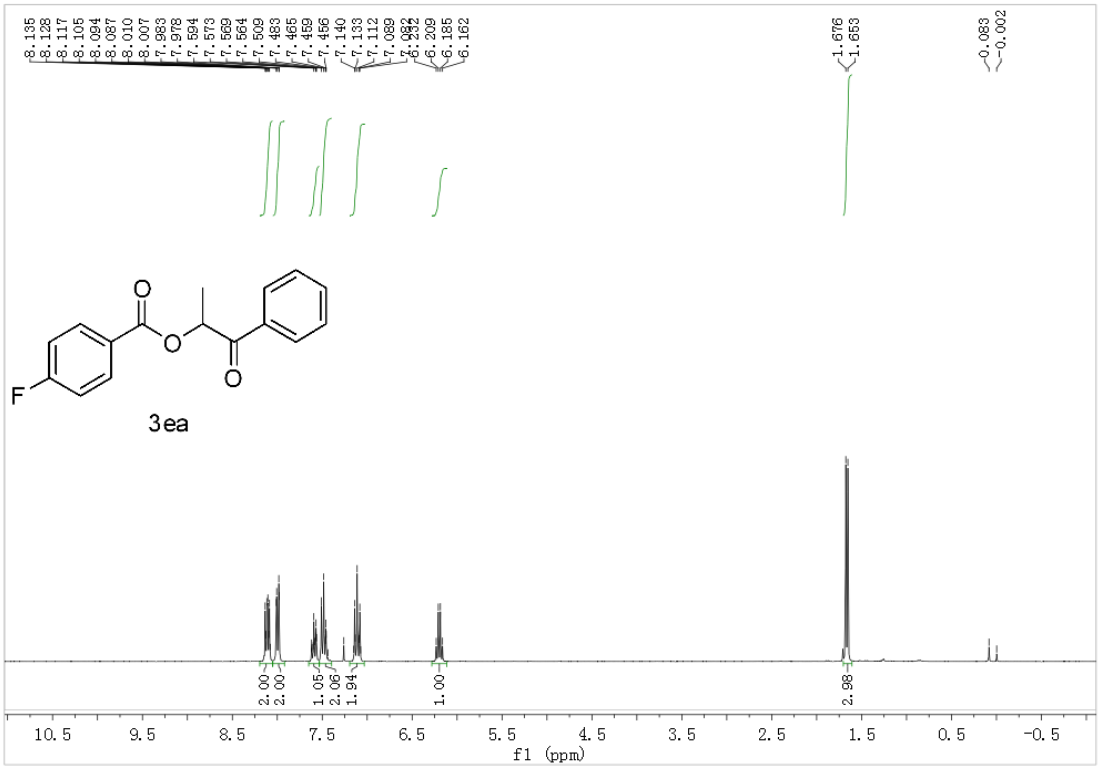

196.959
165.637
163.597
134.474
133.476
131.905
128.725
128.470
121.804
113.604
77.424
77.000
76.577
71.527
55.387
17.139
3ba
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

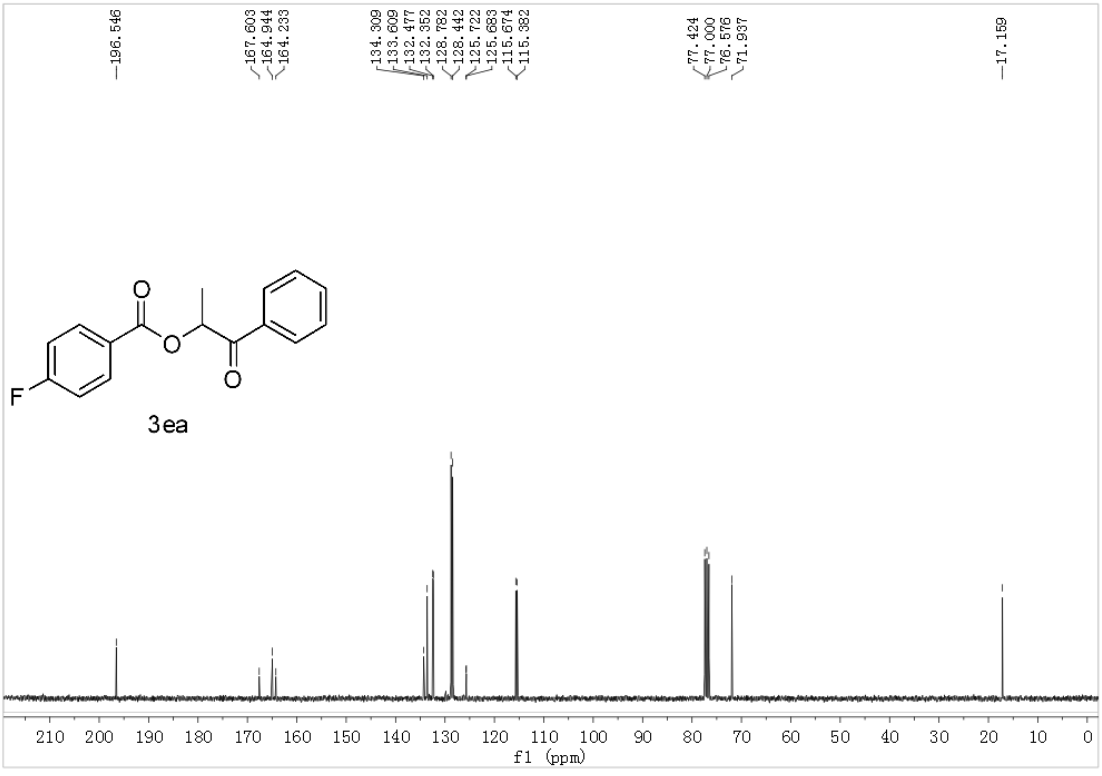

8.052
8.044
8.038
8.022
8.015
8.007
7.981
7.976
7.632
7.608
7.583
7.521
7.496
7.471
7.439
7.410
7.260
6.235
6.211
6.188
6.165
1.683
1.660
1.582
0.070
-0.002
O
O
O
Cl
3ca
3.96
1.02
2.02
1.94
1.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

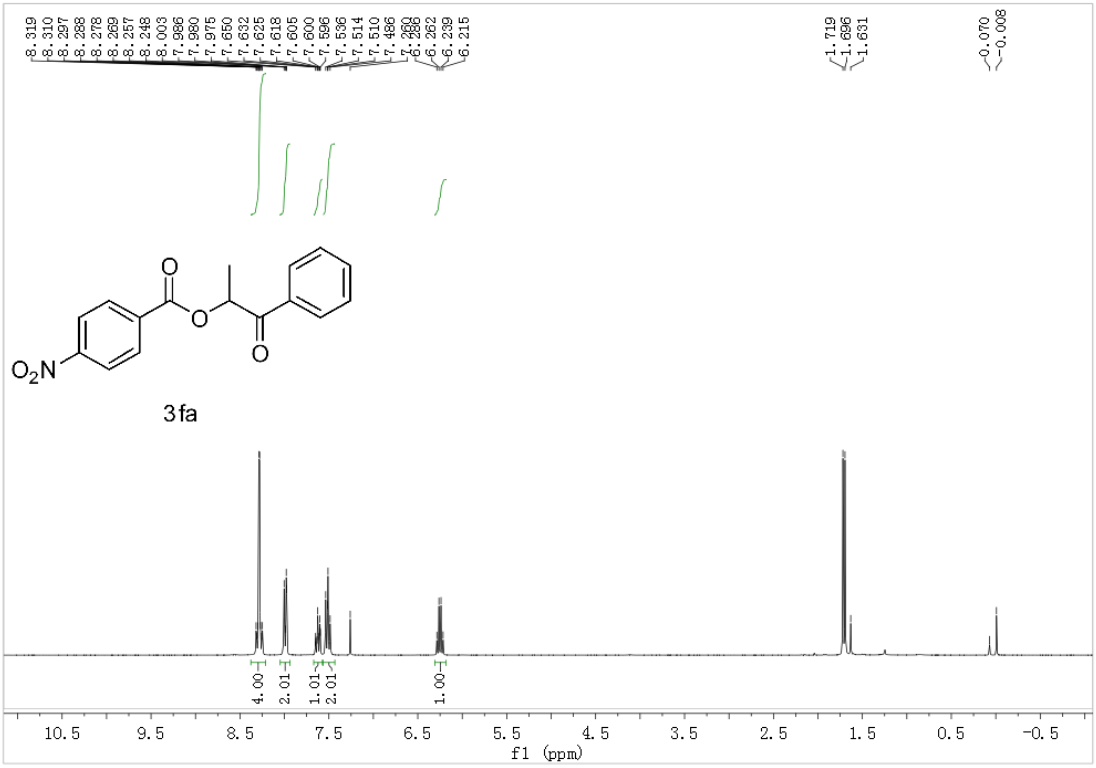

196.491
165.127
139.781
134.331
133.679
131.255
128.838
128.763
128.489
127.943
77.424
77.000
76.577
72.082
17.212
O
O
O
Cl
3ca
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

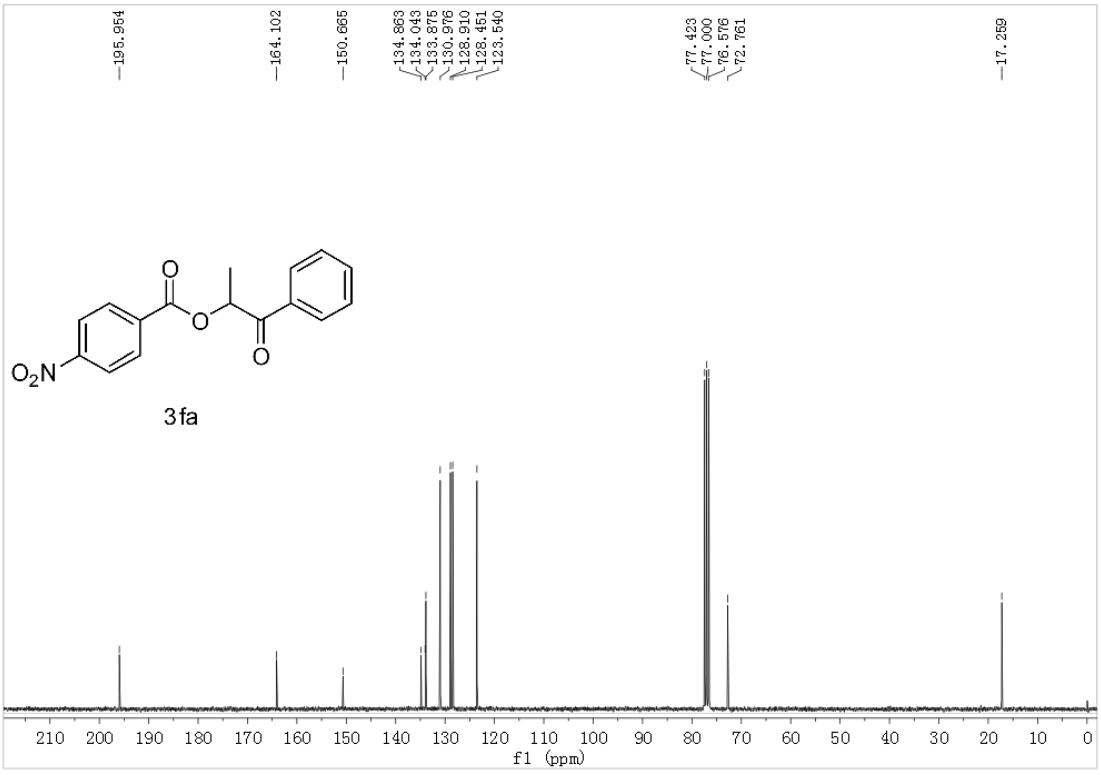

8.000
7.976
7.971
7.964
7.935
7.619
7.595
7.567
7.509
7.483
7.469
7.260
6.229
6.206
6.182
6.159
1.676
1.652
0.082
-0.001
Br
O
O
O
3da
4.00
3.01
2.01
1.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

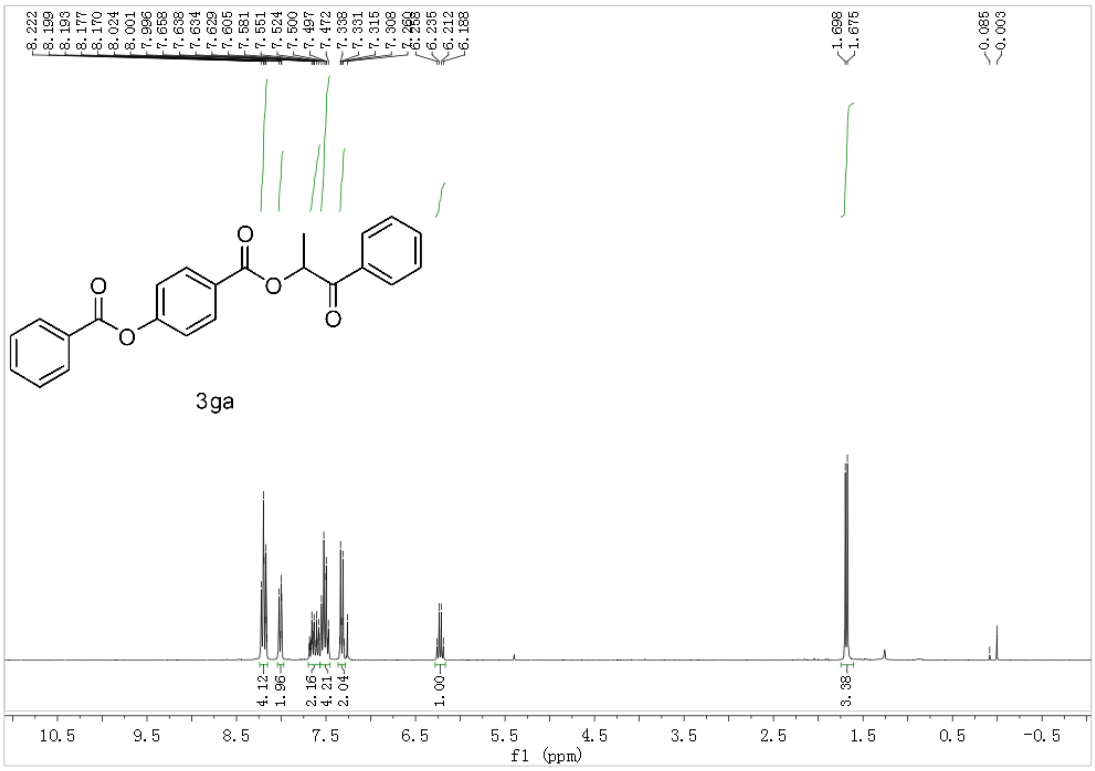

196.406
165.194
134.248
133.636
131.701
131.322
128.789
128.430
128.346
77.424
77.000
76.576
72.073
17.162
Br
O
O
O
3da
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

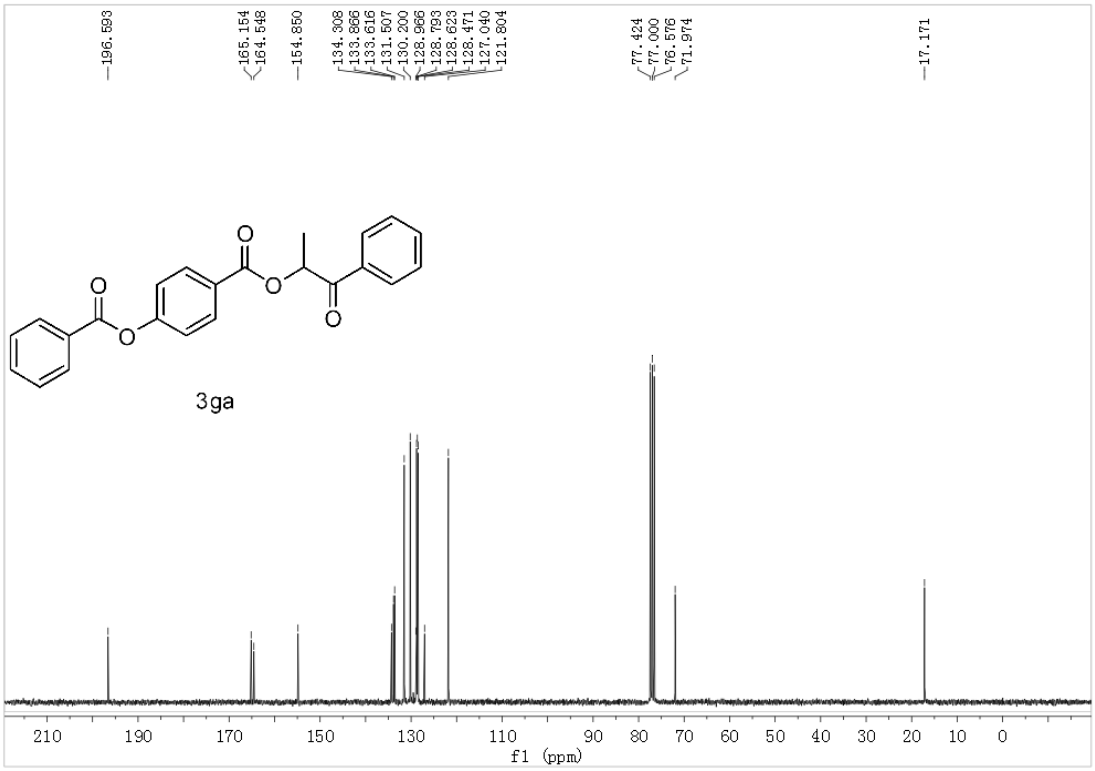

8.135
8.128
8.117
8.105
8.094
8.087
8.010
8.007
7.983
7.978
7.594
7.573
7.569
7.564
7.509
7.483
7.465
7.459
7.456
7.140
7.133
7.112
7.089
6.209
6.185
6.162
1.676
1.653
0.083
-0.002
O
O
O
F
3ea
2.00
2.00
1.05
2.06
1.94
1.00
2.98
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

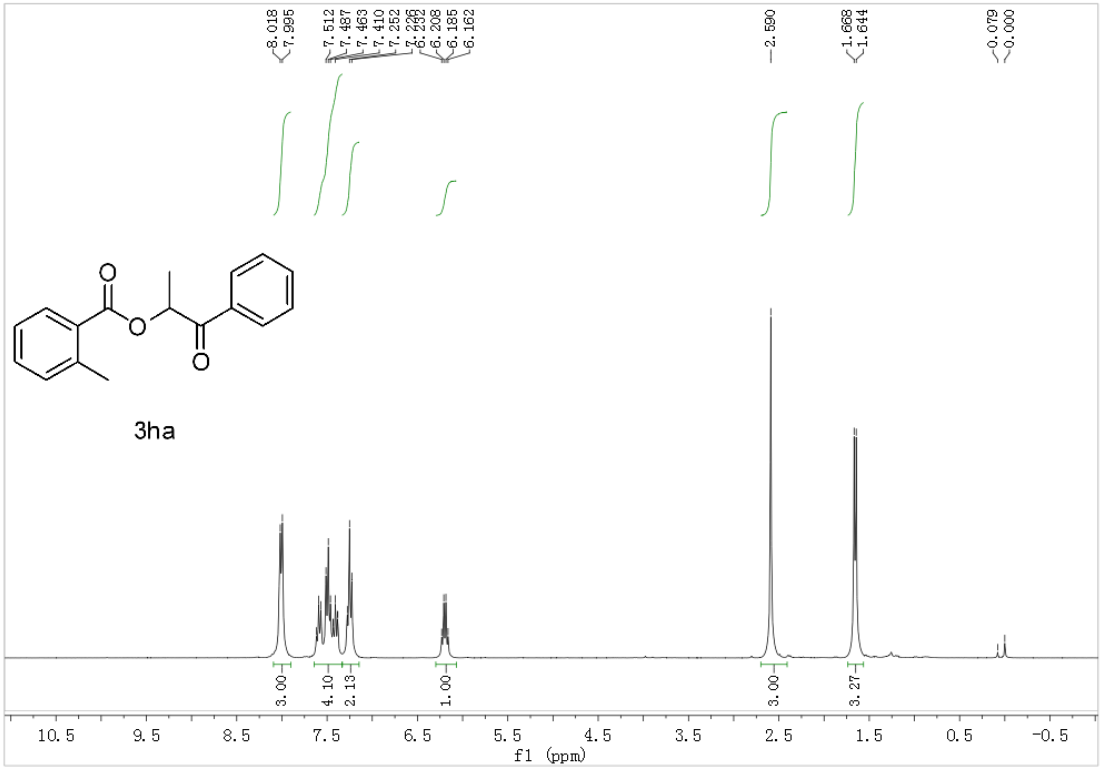

196.546
167.603
164.944
164.233
134.309
133.609
132.477
132.352
128.782
128.442
125.722
125.683
115.674
115.382
77.424
77.000
76.576
71.937
17.159
O
O
O
F
3ea
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

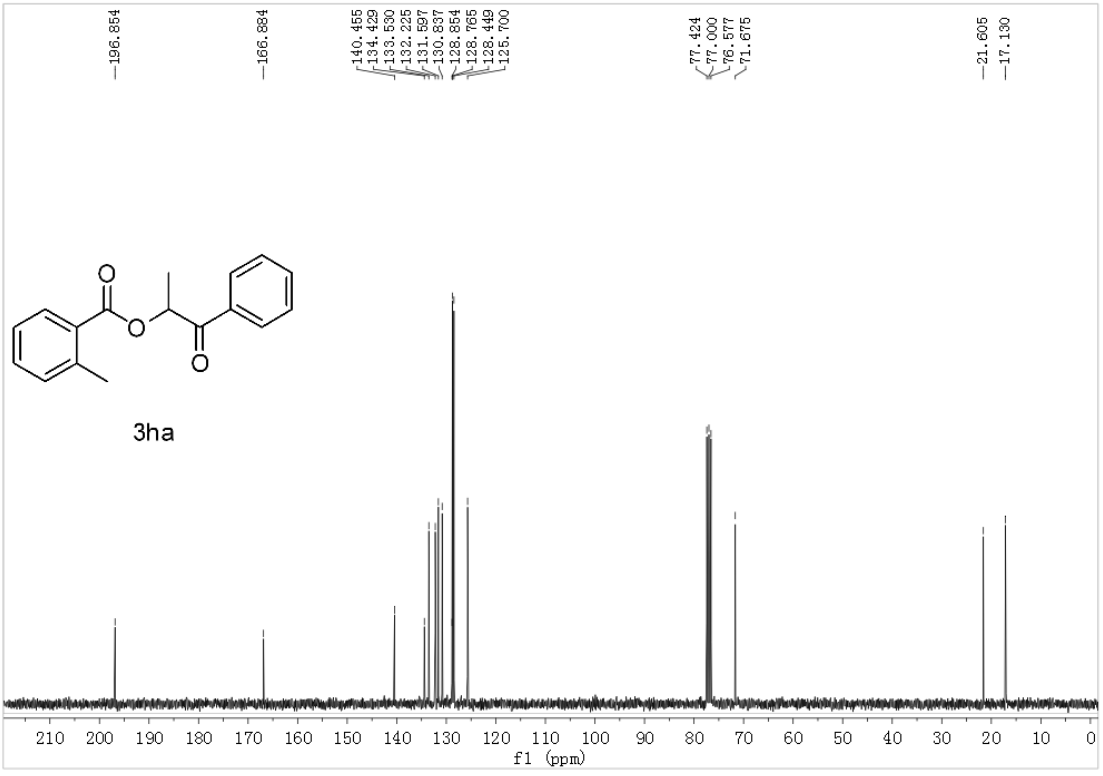

8.319
8.310
8.297
8.288
8.278
8.269
8.257
8.248
8.003
7.986
7.980
7.975
7.650
7.632
7.625
7.618
7.605
7.600
7.596
7.536
7.514
7.510
7.486
7.280
6.262
6.239
6.215
1.719
1.696
1.631
0.070
-0.008
O
O
O
O2N
3fa
4.00
2.01
1.01
2.01
1.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

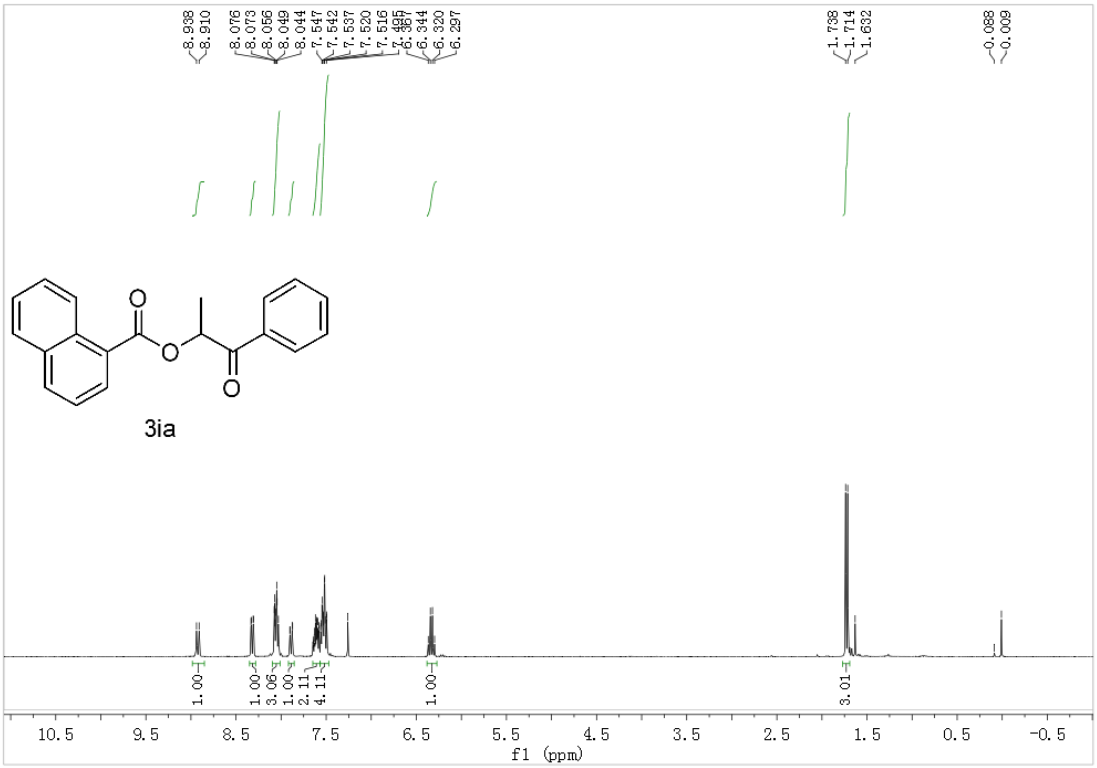

195.954
164.102
150.665
134.863
134.043
133.875
130.976
128.910
128.451
123.540
77.423
77.000
76.576
72.761
17.259
O
O
O
O2N
3fa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

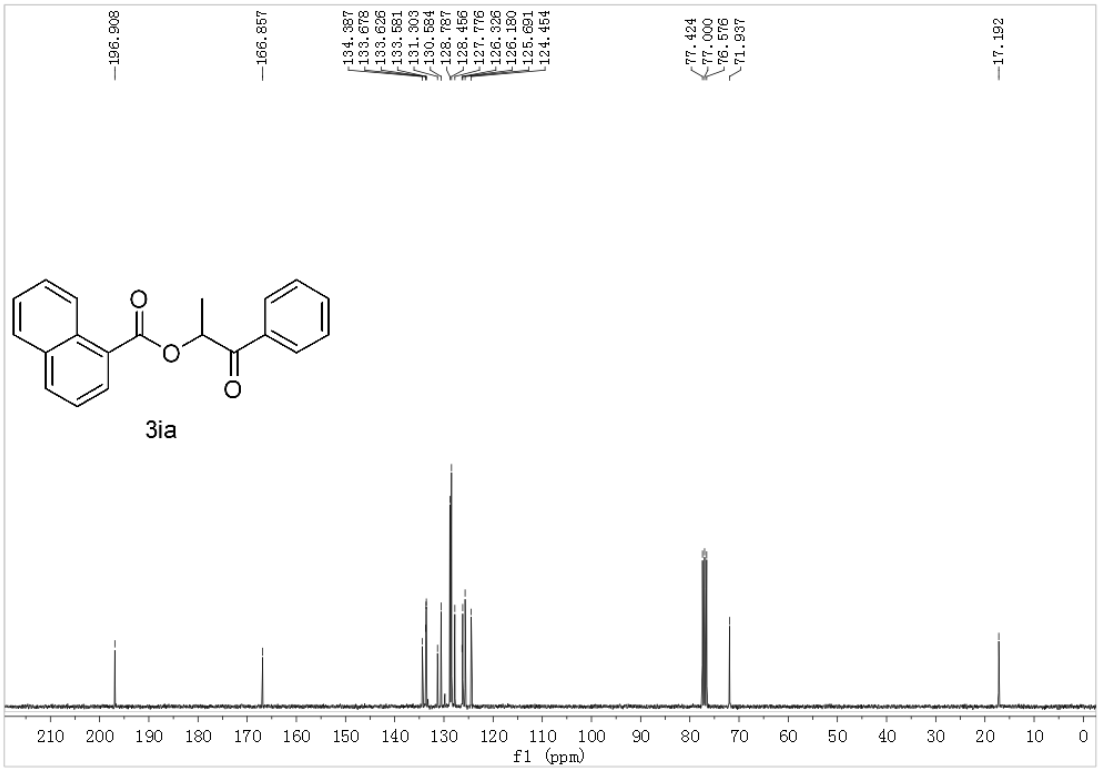

8.222
8.199
8.193
8.177
8.170
8.024
8.001
7.996
7.658
7.638
7.634
7.629
7.605
7.581
7.551
7.524
7.500
7.497
7.472
7.338
7.331
7.315
7.308
6.235
6.212
6.188
1.698
1.675
0.085
0.003
3ga
4.12
1.96
2.16
4.21
2.04
1.00
3.38
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

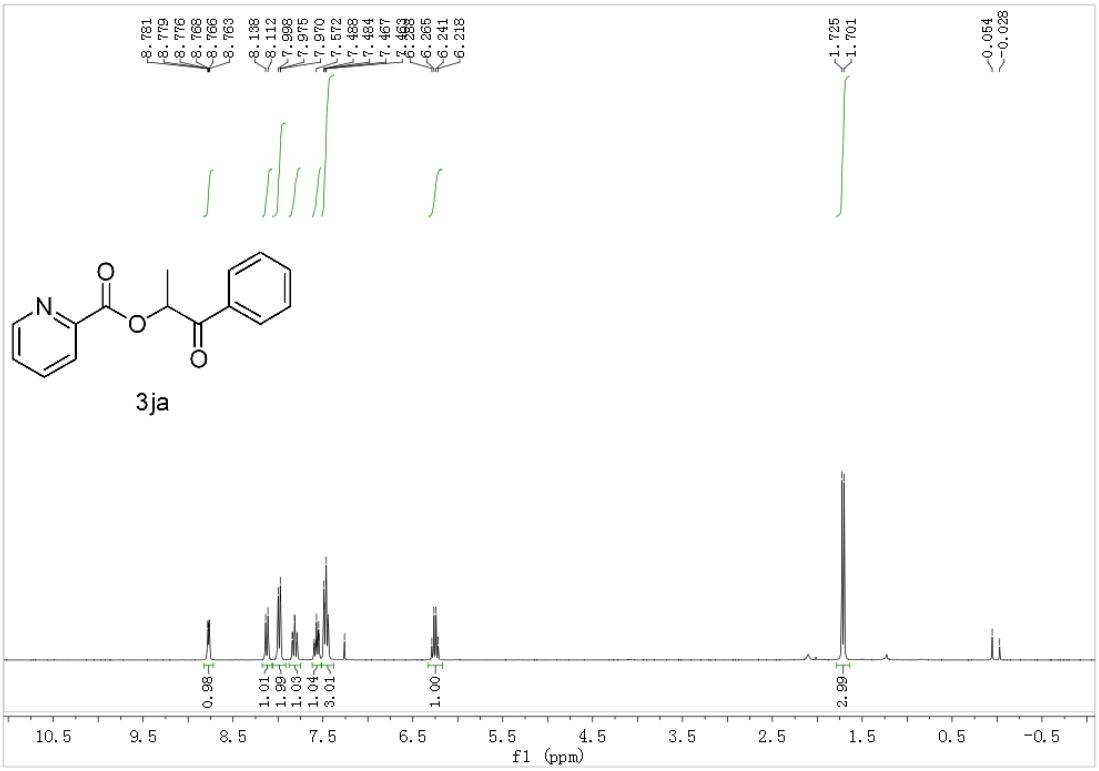

196.593
165.154
164.548
154.850
134.308
133.866
133.616
131.507
130.200
128.966
128.793
128.623
128.471
127.040
121.804
77.424
77.000
76.576
71.974
17.171
3ga
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

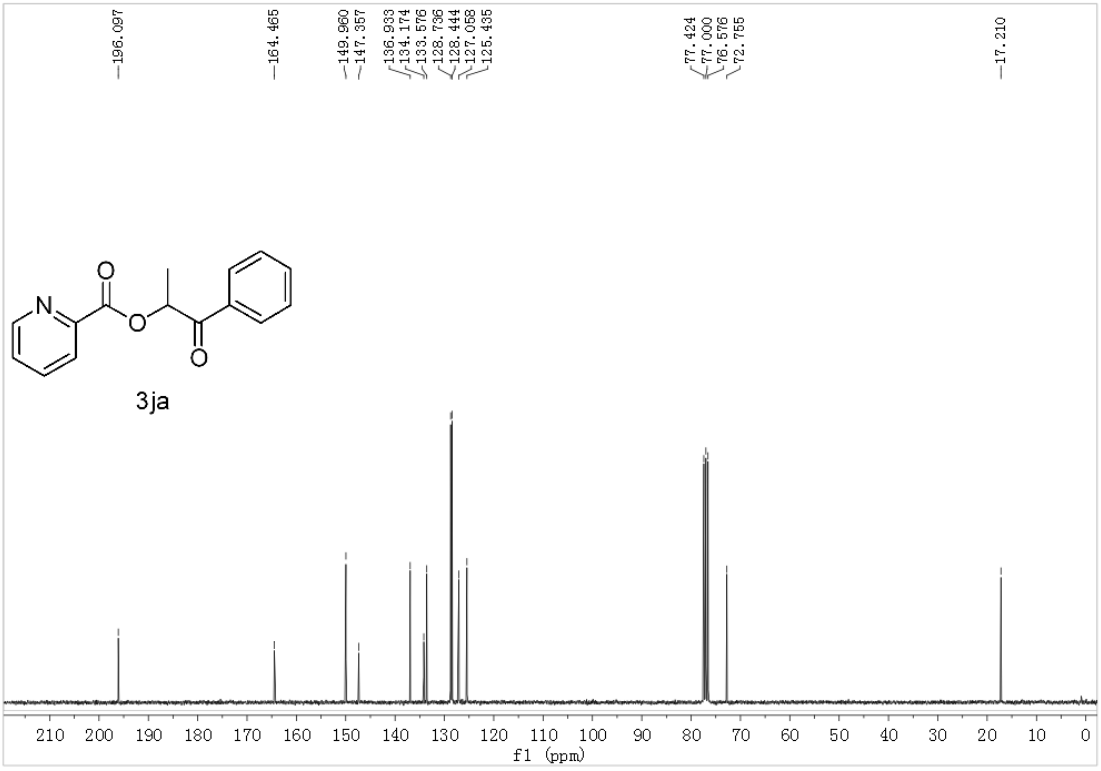

8.018
7.995
7.512
7.497
7.463
7.410
7.252
7.226
6.232
6.208
6.185
6.162
2.590
1.668
1.644
0.079
0.000
3ha
3.00
4.10
2.13
1.00
3.00
3.27
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

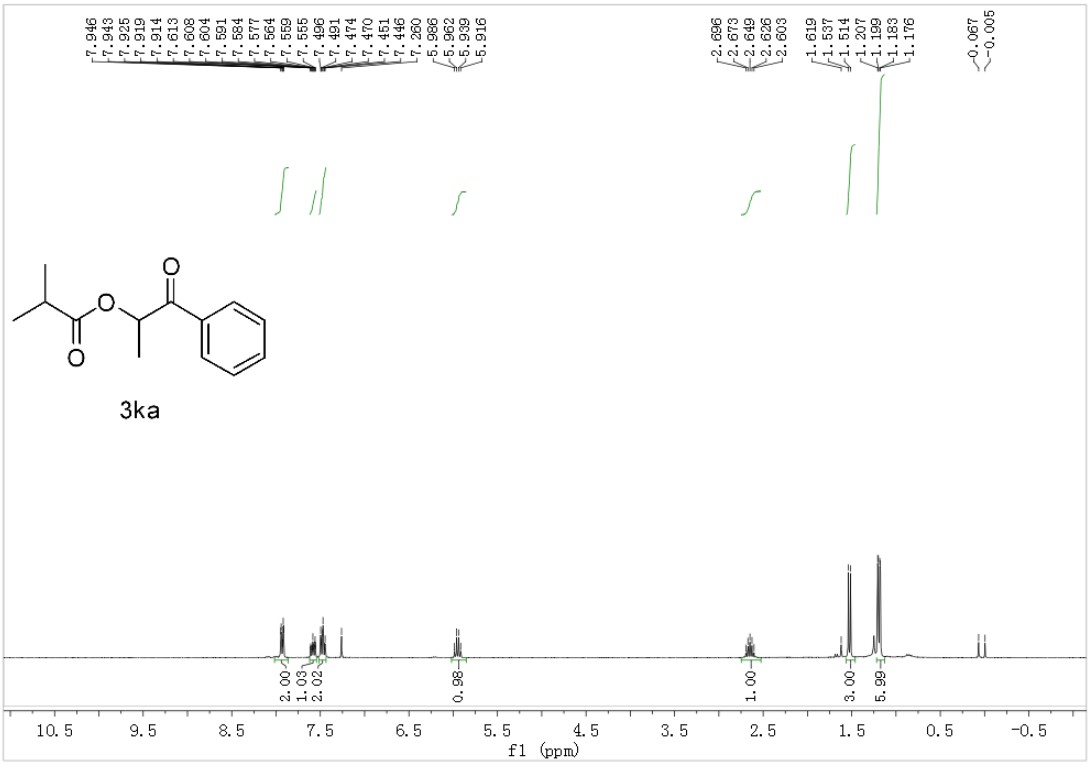

196.854
166.884
140.455
134.429
133.530
132.225
131.597
130.837
128.854
128.765
128.449
125.700
77.424
77.000
76.577
71.675
21.605
17.130
3ha
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

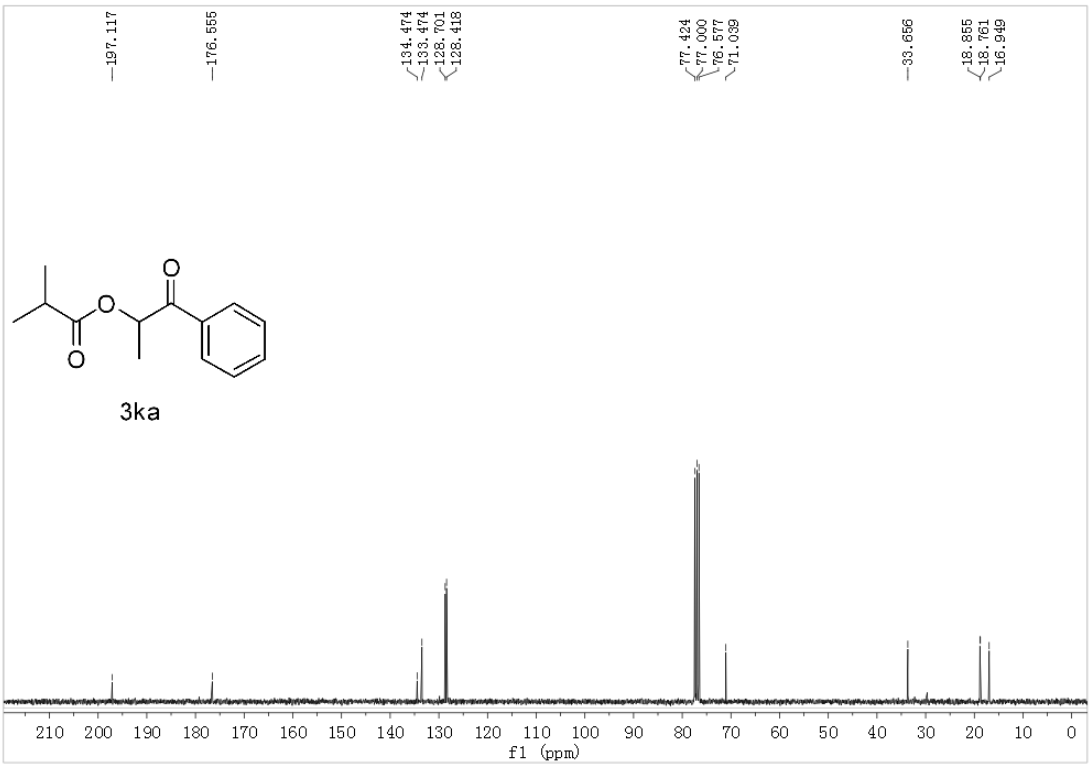

8.938
8.910
8.076
8.073
8.056
8.049
8.044
7.547
7.542
7.537
7.520
7.516
6.344
6.320
6.297
1.738
1.714
1.632
0.088
0.009
3ia
1.00
1.00
3.06
1.00
2.11
4.11
1.00
3.01
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

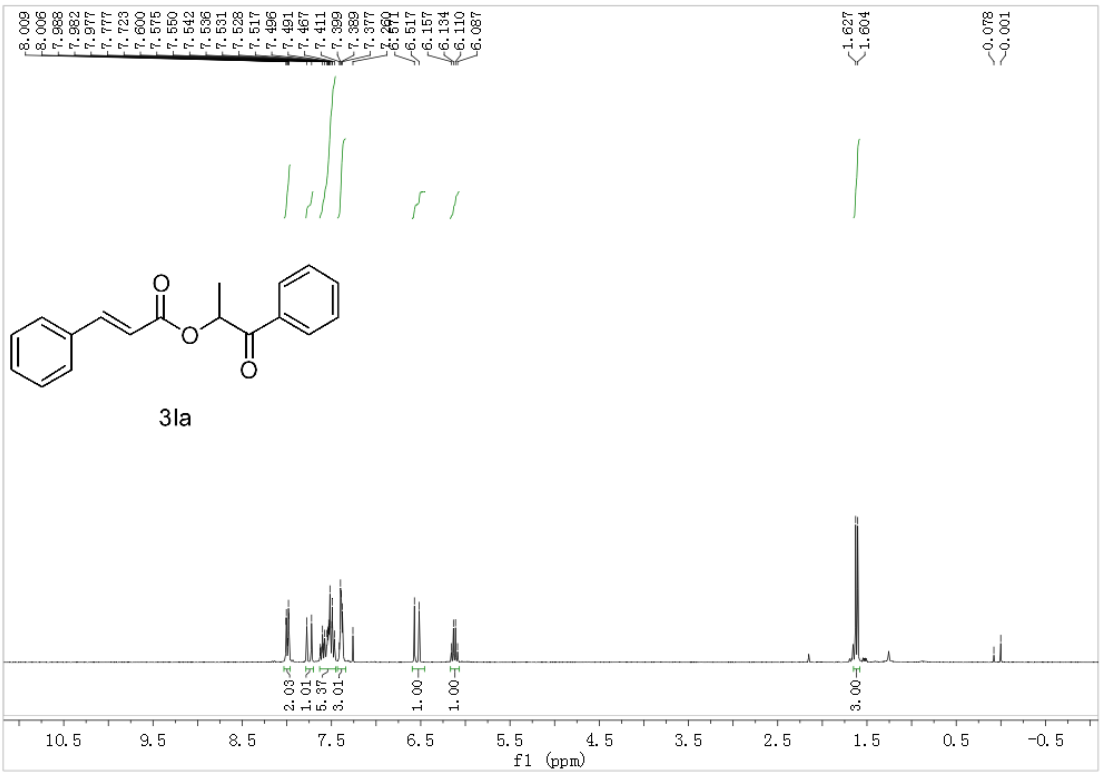

196.908
166.857
134.387
133.678
133.626
133.681
131.303
130.584
128.787
128.456
127.776
126.326
126.180
125.691
124.454
77.424
77.000
76.576
71.937
17.192
3ia
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

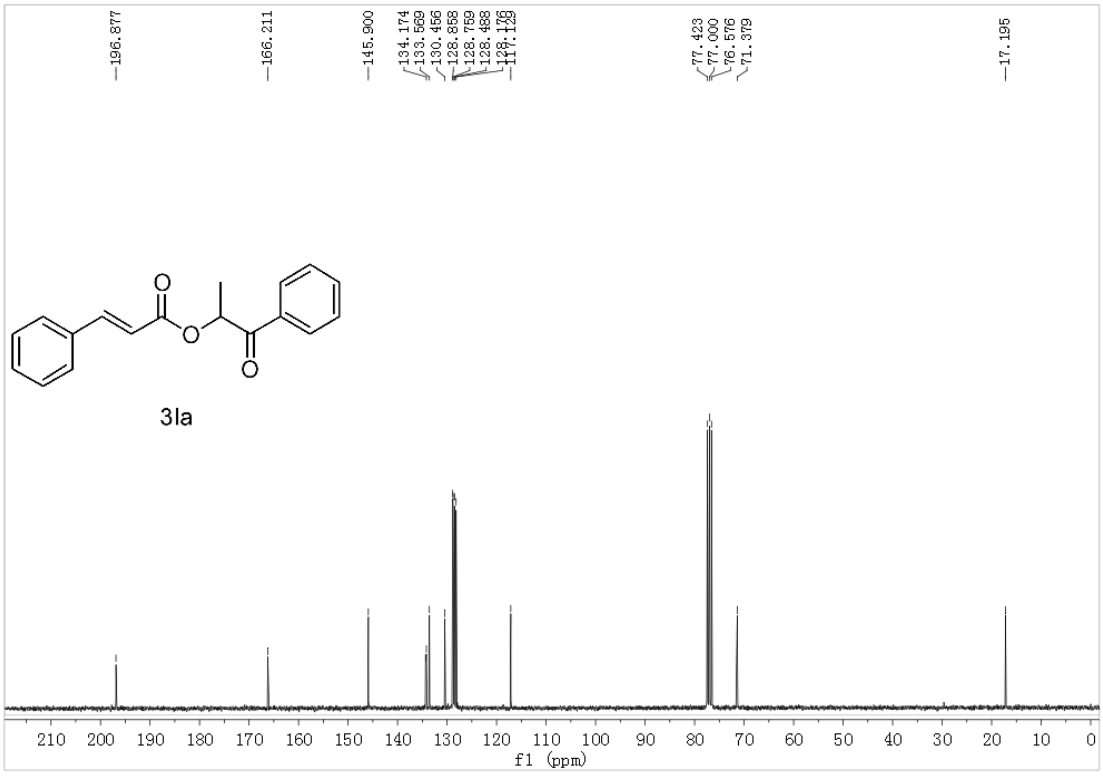

8.781
8.779
8.776
8.768
8.766
8.763
8.138
8.112
7.998
7.975
7.970
7.572
7.488
7.484
7.467
6.265
6.241
6.218
1.725
1.701
0.054
0.028
N
O
O
O
3ja
0.98
1.01
1.99
1.03
1.04
3.01
1.00
2.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

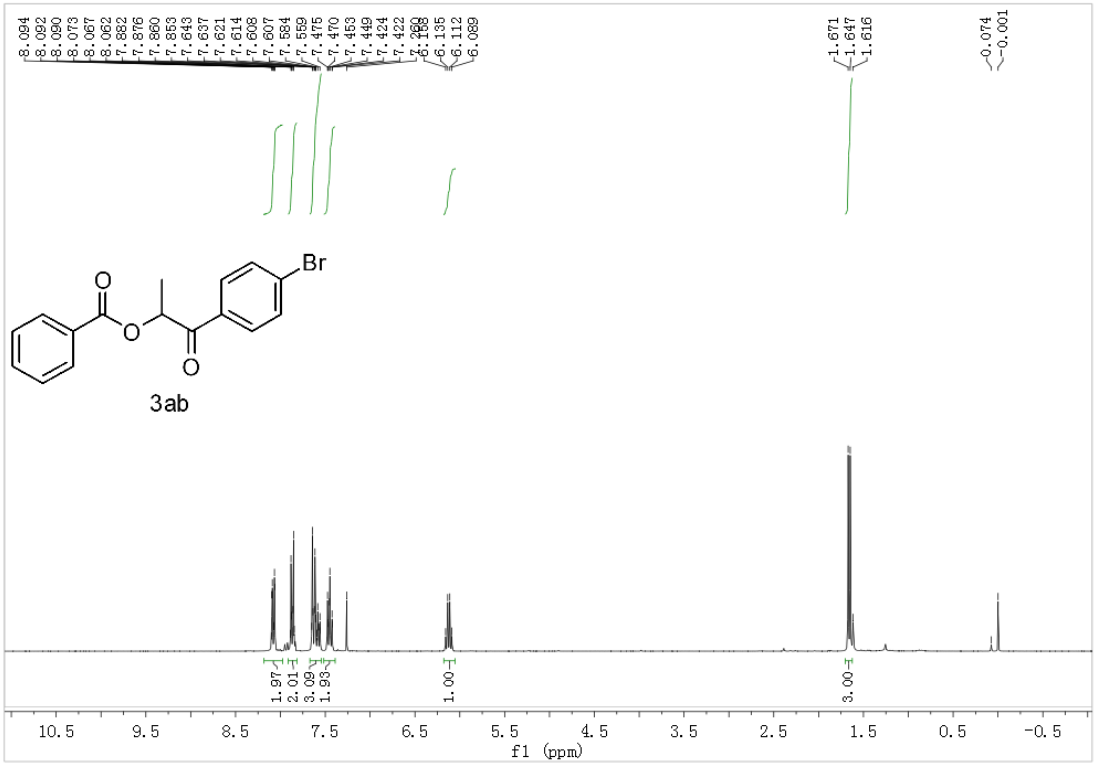

196.097
164.465
149.960
147.357
136.993
134.174
133.576
128.736
128.444
127.058
125.435
77.424
77.000
76.576
72.755
17.210
N
O
O
O
3ja
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

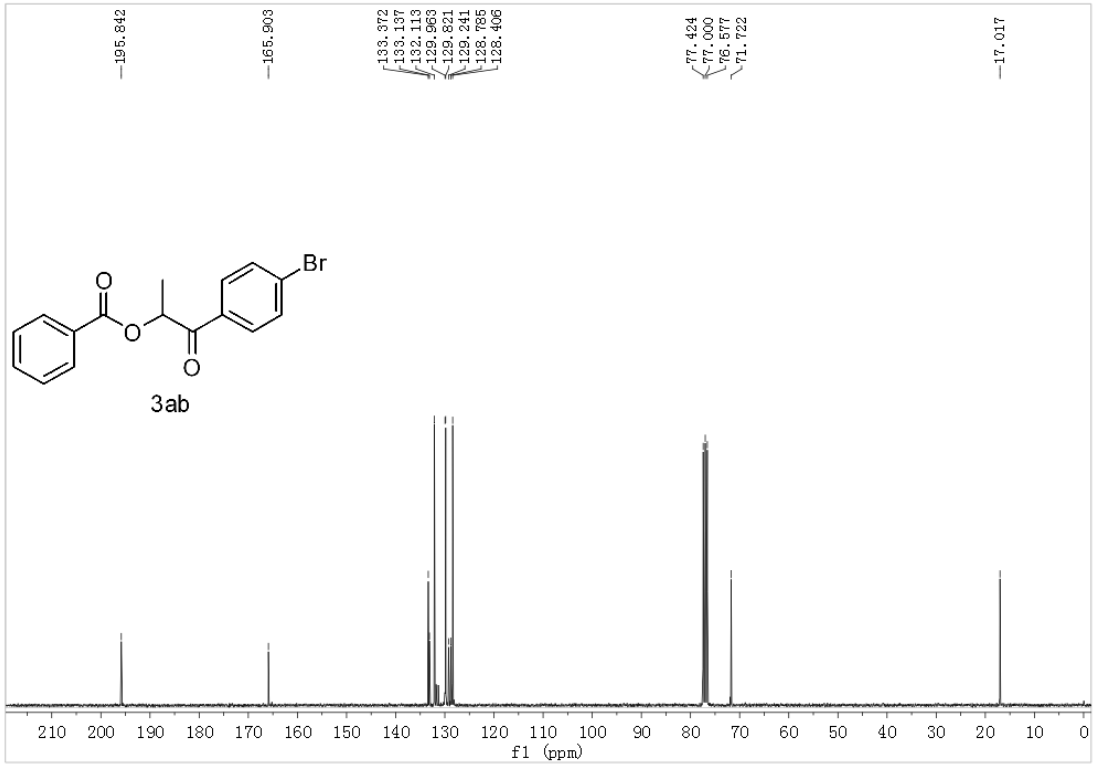

7.946
7.943
7.925
7.919
7.914
7.613
7.608
7.604
7.591
7.584
7.577
7.564
7.559
7.555
7.496
7.491
7.474
7.470
7.451
7.446
7.260
5.986
5.962
5.939
5.916
2.696
2.673
2.649
2.626
2.603
1.619
1.537
1.514
1.207
1.199
1.183
1.176
0.067
-0.005
3ka
2.00
1.03
2.02
0.98
1.00
3.00
5.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

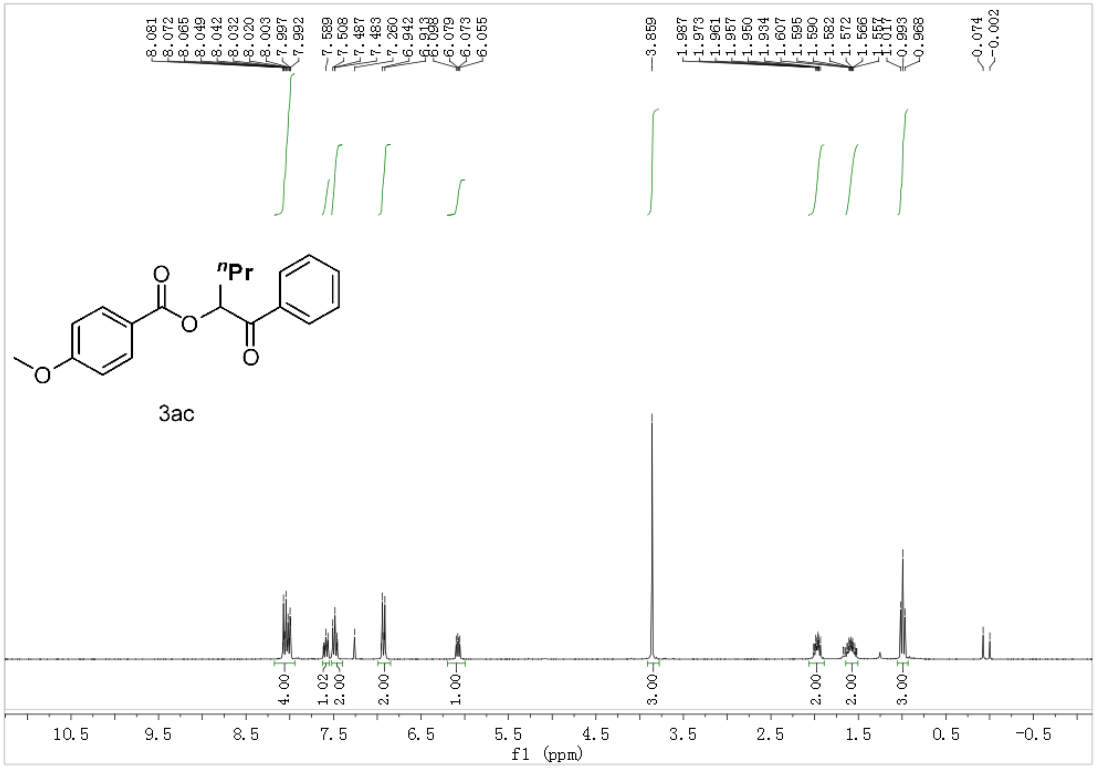

197.117
176.555
134.474
133.474
128.701
128.418
77.424
77.000
76.577
71.039
33.656
18.855
18.761
16.949
3ka
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

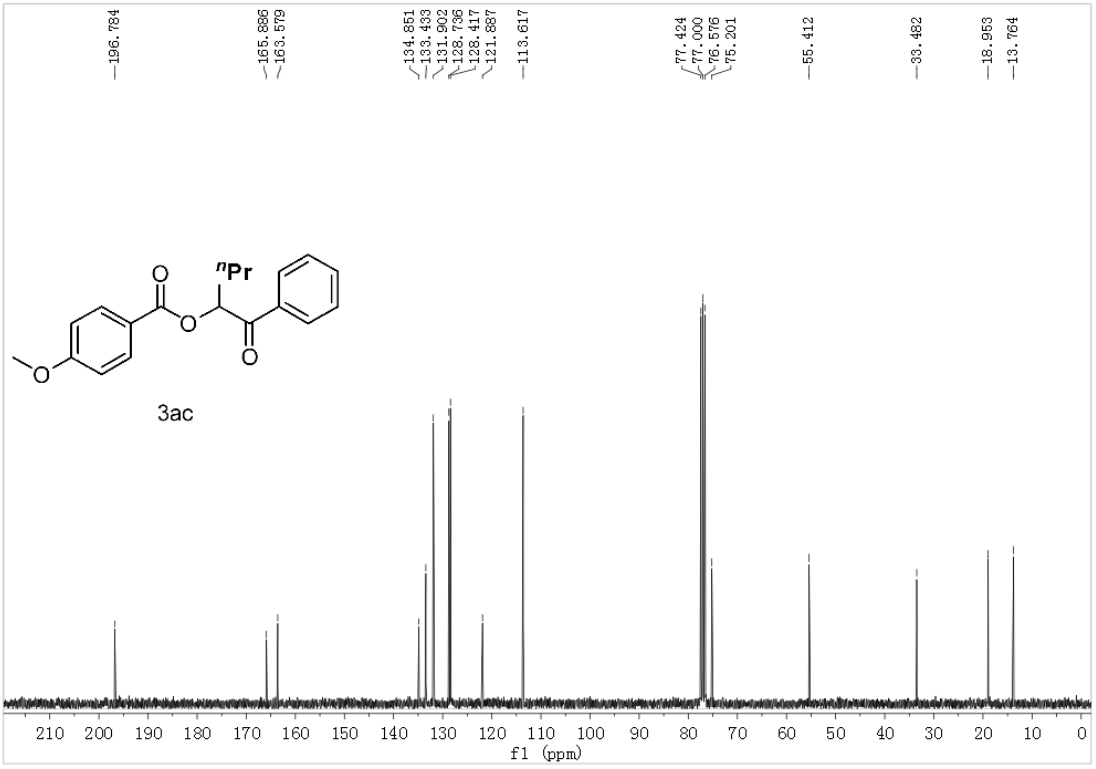

8.009
8.006
7.988
7.982
7.977
7.777
7.723
7.600
7.575
7.550
7.542
7.536
7.531
7.528
7.517
7.496
7.491
7.467
7.411
7.399
7.389
7.377
7.260
6.511
6.157
6.134
6.110
6.087
1.627
1.604
0.078
0.001
O
O
O
3la
2.03
1.01
5.37
3.01
1.00
1.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

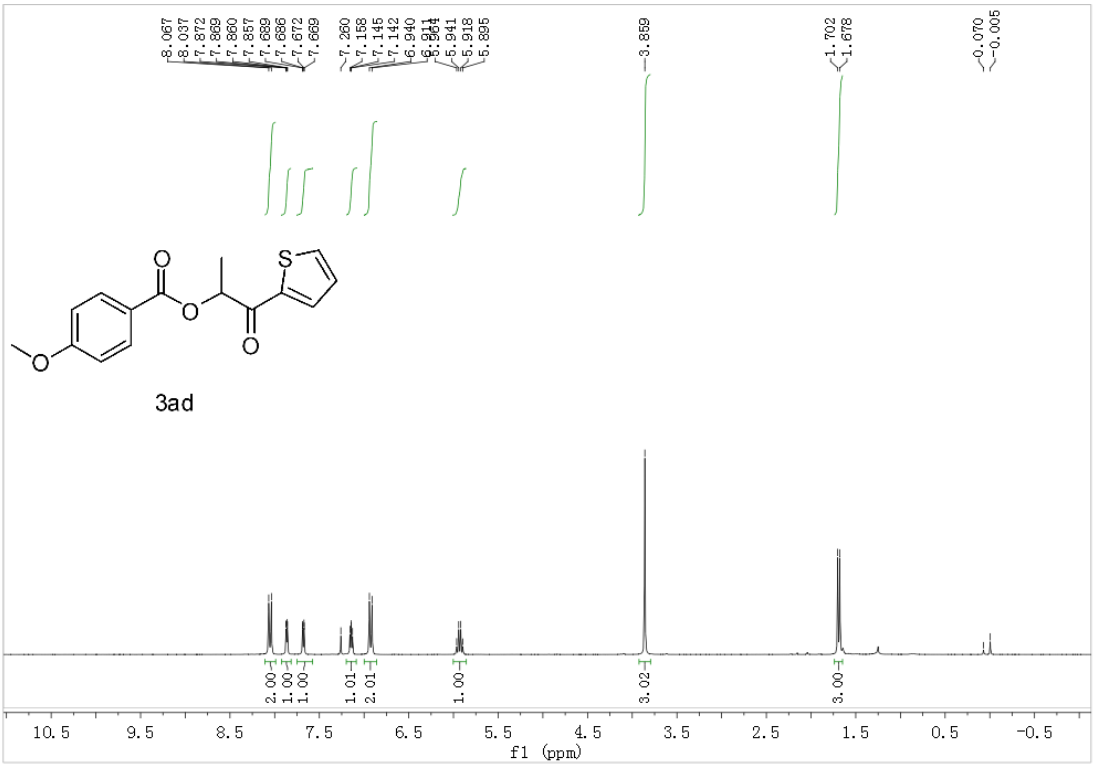

196.877
166.211
145.900
134.174
133.569
130.456
128.858
128.759
128.468
77.423
77.000
76.576
71.379
17.195
O
O
O
3la
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

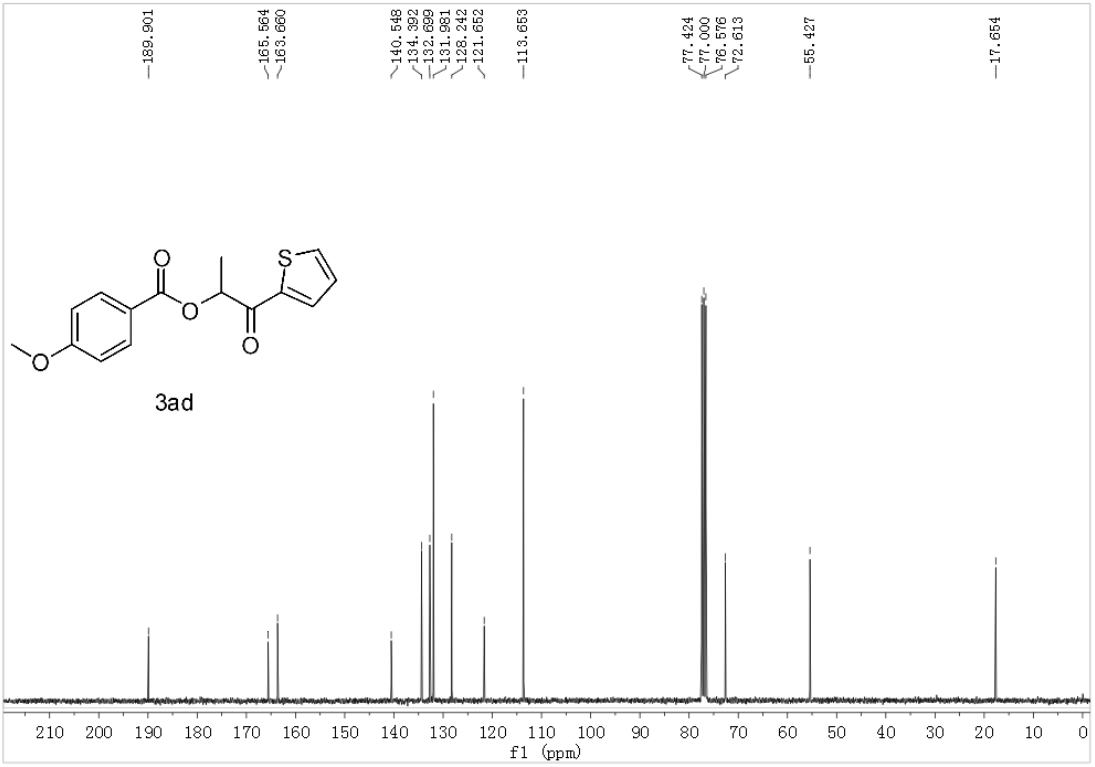

8.094
8.092
8.090
8.073
8.067
8.062
7.882
7.876
7.860
7.853
7.643
7.637
7.621
7.614
7.608
7.607
7.584
7.559
7.475
7.470
7.453
7.449
7.424
7.422
6.135
6.112
6.089
1.671
1.647
1.616
0.074
-0.001
Br
O
O
O
3ab
1.97
2.01
3.09
1.93
1.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

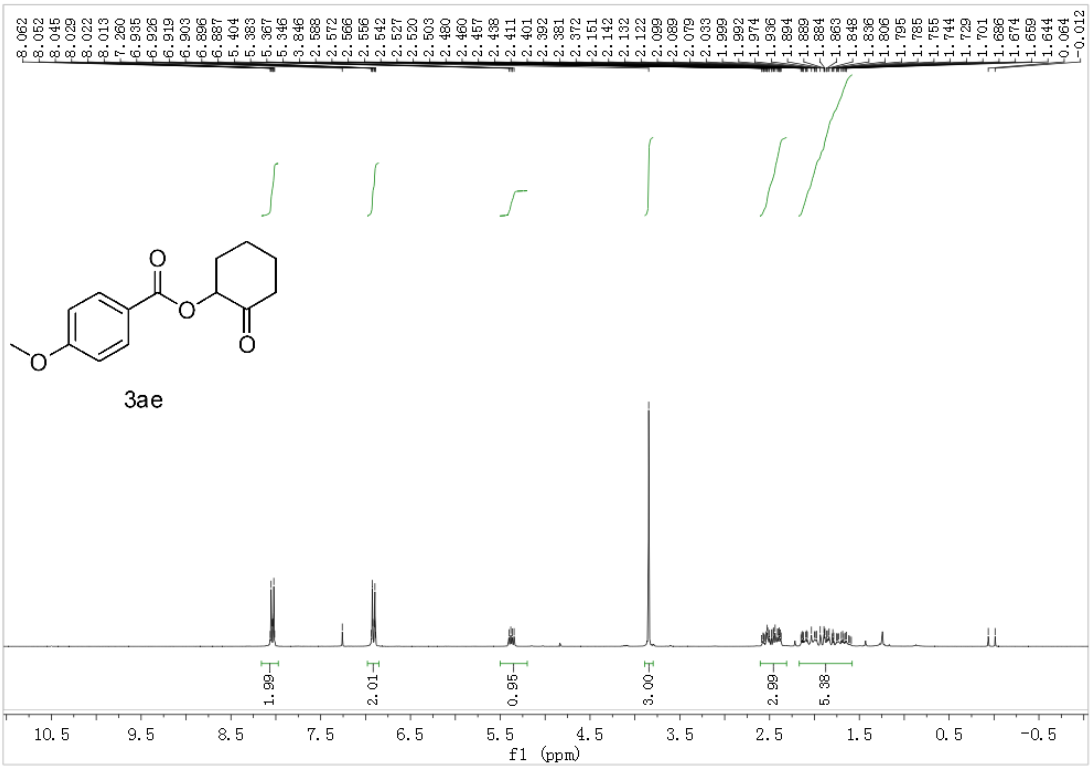

195.842
165.903
133.372
133.137
132.113
129.963
129.821
129.241
128.785
128.406
77.424
77.000
76.577
71.722
17.017
Br
O
O
O
3ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

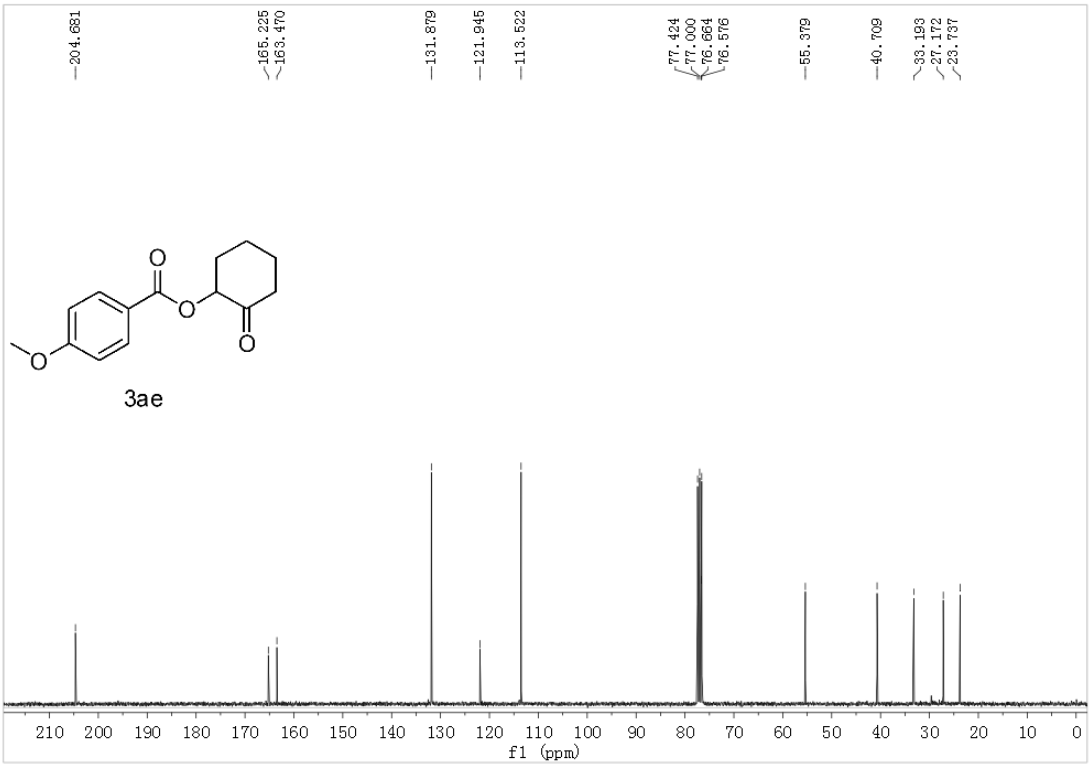

8.081
8.072
8.065
8.049
8.042
8.032
8.020
8.003
7.997
7.992
7.589
7.508
7.487
7.483
7.260
6.942
6.913
6.098
6.079
6.073
6.055
3.859
1.987
1.973
1.961
1.957
1.950
1.934
1.607
1.595
1.590
1.582
1.572
1.566
1.517
0.993
0.968
0.074
-0.002
nPr
O
O
O
O
3ac
4.00
1.02
2.00
2.00
1.00
3.00
2.00
2.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

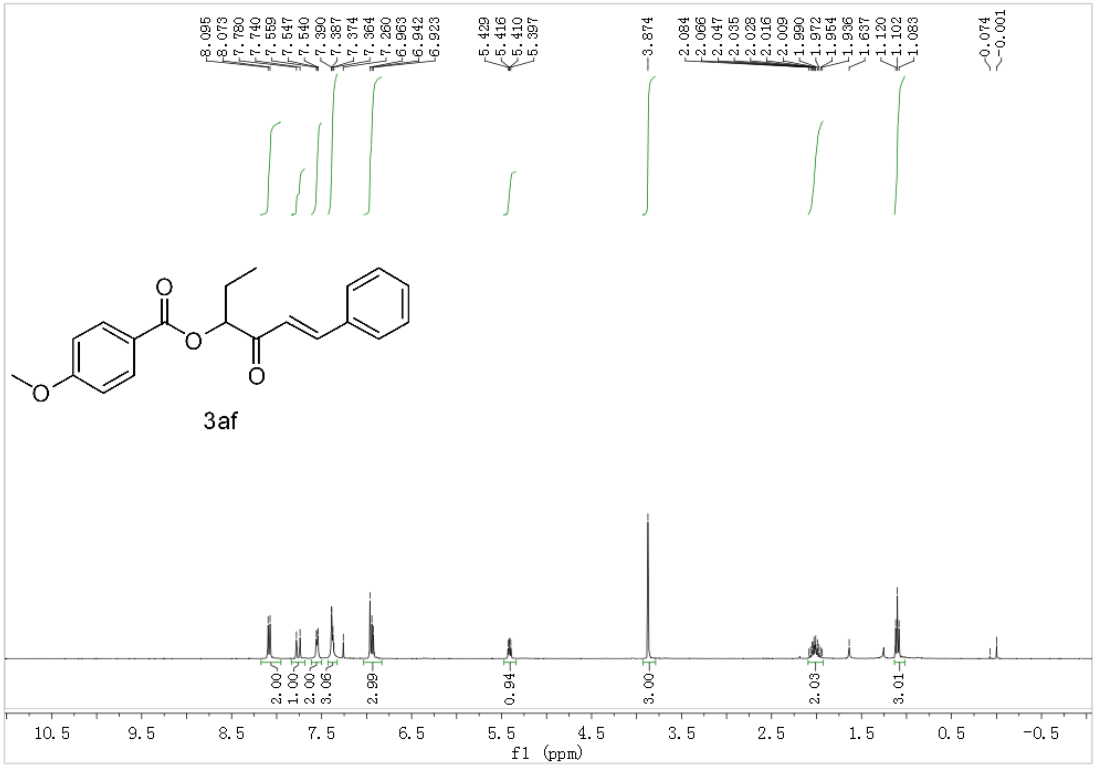

196.784
165.886
163.579
134.851
133.433
131.902
128.736
128.417
121.887
113.617
77.424
77.000
76.576
75.201
55.412
33.482
18.953
13.764
nPr
O
O
O
O
3ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

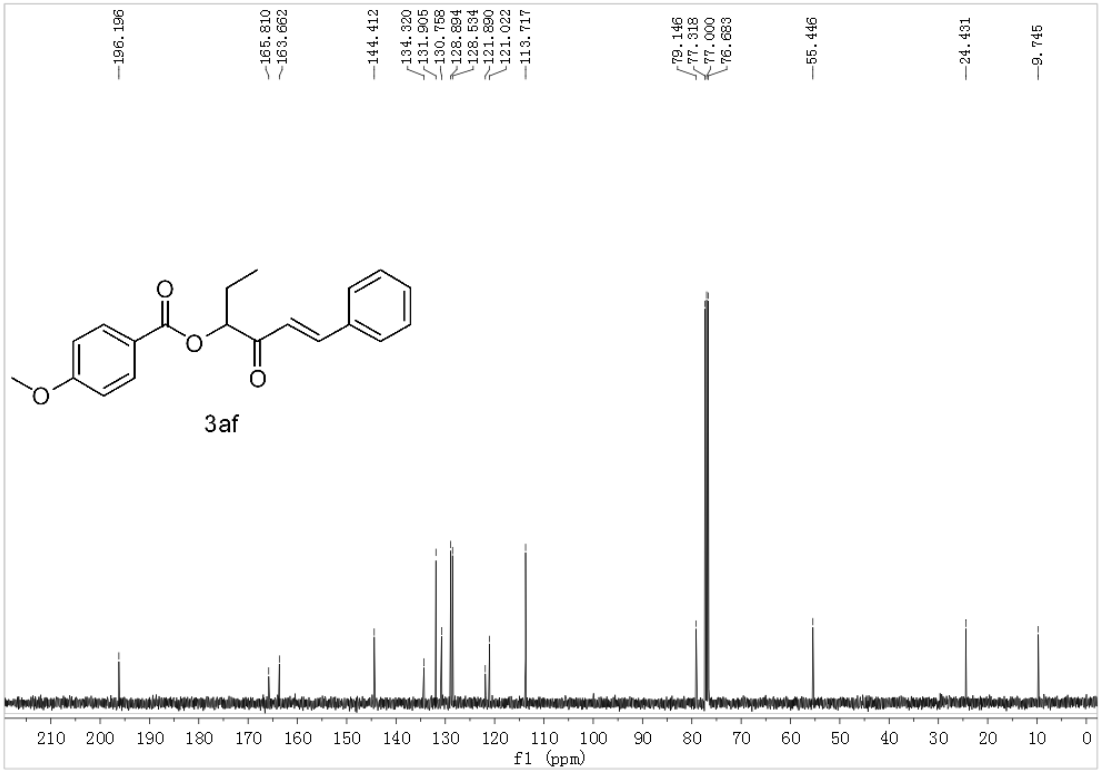

8.067
8.037
7.872
7.869
7.860
7.857
7.689
7.686
7.672
7.669
7.260
7.158
7.145
7.142
6.940
6.911
5.941
5.918
5.895
3.859
1.702
1.678
0.070
-0.005
O
O
O
S
O
3ad
2.00
1.00
1.00
1.01
2.01
1.00
3.02
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

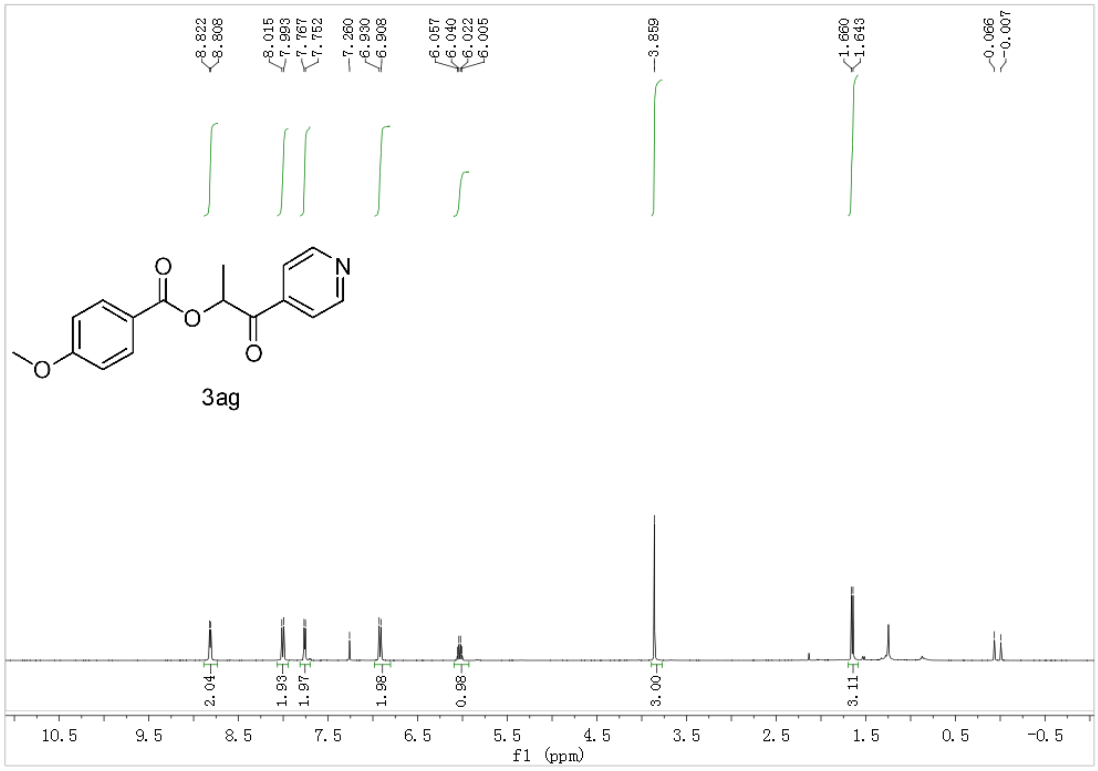

189.901
165.564
163.660
140.548
134.392
132.699
131.981
128.242
121.652
113.653
77.424
77.000
76.576
72.613
55.427
17.654
O
O
O
S
O
3ad
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

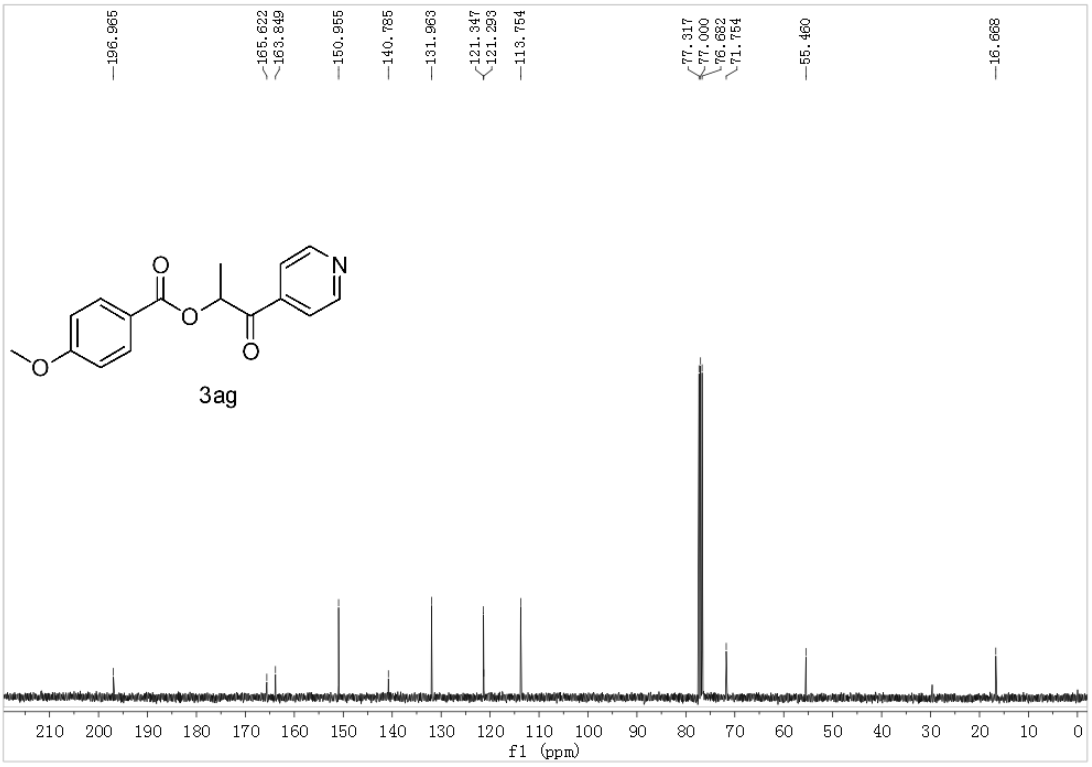

8.062
8.052
8.045
8.029
8.022
8.013
7.260
6.935
6.926
6.919
6.903
6.896
6.887
5.404
5.383
5.367
5.346
3.846
2.588
2.572
2.566
2.556
2.542
2.527
2.520
2.503
2.480
2.460
2.457
2.438
2.411
2.401
2.392
2.381
2.372
2.151
2.142
2.132
2.122
2.099
2.089
2.079
2.033
1.999
1.992
1.974
1.936
1.894
1.889
1.884
1.863
1.848
1.836
1.806
1.795
1.785
1.755
1.744
1.729
1.701
1.686
1.674
1.659
1.644
1.064
-0.012
O
O
O
O
3ae
1.99
2.01
0.95
3.00
2.99
5.38
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


204.681
165.225
163.470
131.879
121.945
113.522
77.424
77.000
76.664
76.576
55.379
40.709
33.193
27.172
23.737
O
O
O
O
3ae
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.095
8.073
7.780
7.740
7.559
7.547
7.540
7.390
7.387
7.374
7.364
7.260
6.963
6.942
6.923
5.429
5.416
5.410
5.397
3.874
2.084
2.066
2.047
2.035
2.028
2.016
2.009
1.990
1.972
1.954
1.936
1.637
1.120
1.102
1.083
0.074
-0.001
3af
2.00
1.00
2.00
3.06
2.99
0.94
3.00
2.03
3.01
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


196.196
165.810
163.662
144.412
134.320
131.905
130.758
128.894
128.534
121.890
121.022
113.717
79.146
77.318
77.000
76.683
55.446
24.431
9.745
3af
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.822
8.808
8.015
7.993
7.767
7.752
7.260
6.930
6.908
6.057
6.040
6.022
6.005
3.859
1.660
1.643
0.066
-0.007
3ag
2.04
1.93
1.97
1.98
0.98
3.00
3.11
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


196.965
165.622
163.849
150.955
140.786
131.963
121.347
121.293
113.754
77.317
77.000
76.682
71.754
55.460
16.668
3ag
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)