Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Alcohol Assisted C-C Bond Breaking: Copper-Catalyzed Deacetylative α-Arylation of β-keto Esters and Amides

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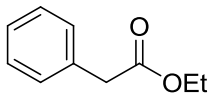
General Information

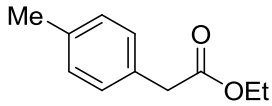
Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (boiling point is between 30-60 ^{o}C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum to the indicated solvent, and they are listed as volume/volume ratios. NMR spectra were recorded on a Varian Mercury spectrometers at 300 MHz (^{1}H NMR), 75 MHz (^{13}C NMR). Tetramethylsilane was used as an internal standard. All ^{1}H NMR spectra were reported in delta (δ) units, parts per million (ppm) downfield from the internal standard. Coupling constants are reported in Hertz (Hz). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument, accurate masses are reported for the molecular ion ($[M]^{+}$). Selective ratios were recorded with a Varian GC 2000 gas chromatography instrument with a FID detector. And GC yield were determined by the same instrument while naphthalene was used as the internal standard. GC-Ms spectra were recorded on a Varian GC-Ms 3900-2100T.

General Procedures for the Deacetylative Arylation of β-Keto Esters and Amides:



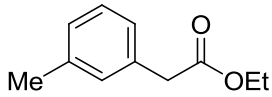
Ethyl 2-phenylacetate (3aa).[1] A mixture of iodobenzene **1a** (1.0 mmol), ethyl acetoacetate **2a** (3.0 mmol), CuI (10 mol %), K_3PO_4 (3.0 mmol), and alcohol additive (3.0 mmol) in DMSO (4 mL) was stirred in N_2 at 80 ^{o}C. After completion of the reaction, as indicated by GC or GC-MS, the mixture was quenched with diluted hydrochloride (2 mL, 2M), the solution was extracted with ethyl acetate (3 × 5 mL).

The organic layers were combined, and dried over sodium sulfate. The pure product was obtained by flash column chromatography on silica gel (petroleum ether/ethyl acetate, 50:1) to afford **3aa** in 82% yield. The spectroscopic data of all the products are presented below. All the known compounds gave satisfactory spectroscopic values and are analogue to spectroscopic data reported in the literature. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.27-7.22 (m, 5H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.53 (s, 2H), 1.17 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.9, 134.4, 129.5, 128.8, 127.3, 61.1, 41.7, 14.4.



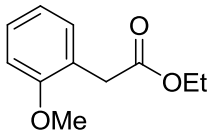
Ethyl 2-*p*-tolylacetate (3ba).[2]

Isolated yield: 81%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.11-7.03 (m, 4H), 4.05 (q, *J* = 7.1 Hz, 2H), 3.49 (s, 2H), 2.25 (s, 3H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.1, 136.8, 131.3, 129.5, 129.3, 61.0, 41.2, 21.3, 14.4.



Ethyl 2-*m*-tolylacetate (3ca).[3]

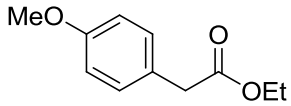
Isolated yield: 88%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.14 (t, *J* = 7.5 Hz, 1H), 7.02-6.99 (m, 3H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.50 (s, 2H), 2.26 (s, 3H), 1.18 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.0, 138.4, 134.3, 130.2, 128.7, 128.0, 126.5, 61.1, 41.6, 21.6, 14.4.



Ethyl 2-(2-methoxyphenyl)acetate (3da).[1]

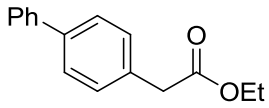
Isolated yield: 68%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.19-7.08 (m, 2H), 6.85-6.77 (m, 2H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.72 (s, 3H), 3.53 (s, 2H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C

NMR (75 MHz, $CDCl_3$): δ 172.1, 157.7, 131.0, 128.7, 123.3, 120.6, 110.6, 60.8, 55.6, 36.2, 14.4.



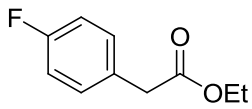
Ethyl 2-(4-methoxyphenyl)acetate (3ea).[2]

Isolated yield: 76%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.12 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 2H), 4.05 (q, *J* = 7.0 Hz, 2H), 3.70 (s, 3H), 3.46 (s, 2H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.2, 158.8, 130.5, 126.4, 114.1, 61.0, 55.4, 40.7, 14.4.



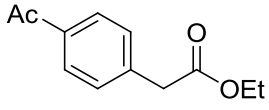
Ethyl 2-(biphenyl-4-yl)acetate (3fa).[4]

Isolated yield: 89%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48-7.43 (m, 4H), 7.34-7.24 (m, 5H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.54 (s, 2H), 1.15 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.8, 141.0, 140.2, 133.4, 129.9, 129.0, 127.5, 127.3, 61.1, 41.2, 14.4.



Ethyl 2-(4-fluorophenyl)acetate (3ga).[2]

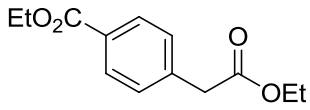
Isolated yield: 81%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.19-7.14 (m, 2H), 6.95-6.90 (m, 2H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.50 (s, 2H), 1.17 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.7, 163.8, 160.6, 131.1, 131.0, 115.7, 115.5, 61.2, 40.7, 14.4.



Ethyl 2-(4-acetylphenyl)acetate (3ha).[2]

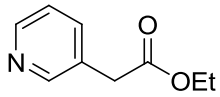
Isolated yield: 88%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.39 (d,

J = 7.8 Hz, 2H), 4.16 (q, *J* = 7.0 Hz, 2H), 3.68 (s, 2H), 2.60 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 198.0, 171.0, 139.7, 136.2, 131.7, 129.9, 129.8, 129.0, 128.8, 128.3, 61.4, 41.5, 26.9, 14.4.



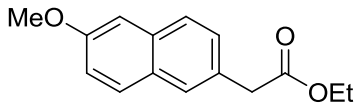
Ethyl 4-(2-ethoxy-2-oxoethyl)benzoate (3ia).[2]

Isolated yield: 87%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.09 (q, *J* = 7.1 Hz, 2H), 3.60 (s, 2H), 1.32 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.2, 166.7, 139.4, 131.5, 130.3, 130.1, 129.6, 61.4, 61.2, 41.6, 14.6, 14.4.



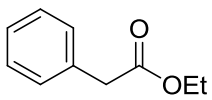
Ethyl 2-(pyridin-3-yl)acetate (3ja).[1]

Isolated yield: 73%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.53 (s, 2H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.29-7.24 (m, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.63 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 170.8, 150.4, 148.5, 136.9, 130.0, 123.5, 61.3, 38.5, 14.2.



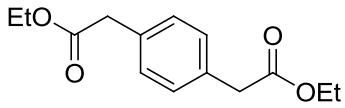
Ethyl 2-(6-methoxynaphthalen-2-yl)acetate (3ka).[5]

Isolated yield: 75%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.70-7.64 (m, 3H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.14-7.10 (m, 2H), 4.15 (q, *J* = 6.9 Hz, 2H), 3.88 (s, 3H), 3.72 (s, 2H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.0, 157.8, 133.8, 129.5, 129.4, 129.1, 128.1, 128.0, 127.3, 119.2, 105.8, 61.1, 55.5, 41.6, 14.4.



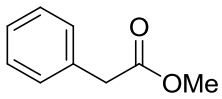
Ethyl 2-phenylacetate (3la).[1]

Isolated yield: 38%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.27-7.16 (m, 5H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.53 (s, 2H), 1.17 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.9, 134.4, 129.5, 128.8, 127.3, 61.1, 41.7, 14.4.



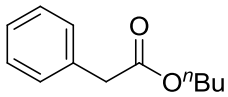
Diethyl 2,2'-(1,4-phenylene)diacetate (3ma).[2]

Isolated yield: 80%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.24 (s, 4H), 4.14 (q, *J* = 7.0 Hz, 4H), 3.59 (s, 4H), 1.25 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.8, 133.1, 130.4, 129.6, 128.6, 61.0, 41.2, 14.3.



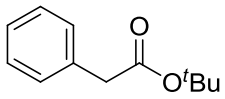
Methyl 2-phenylacetate (3ab).[6]

Isolated yield: 75%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.24-7.18 (m, 5H), 3.60 (s, 3H), 3.55 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.3, 134.2, 129.5, 128.8, 127.3, 52.3, 41.4.



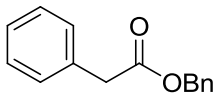
Butyl 2-phenylacetate (3ac).[7]

Isolated yield: 87%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35-7.23 (m, 5H), 4.09 (t, *J* = 6.8 Hz, 2H), 3.61 (s, 2H), 1.64-1.55 (m, 2H), 1.40-1.30 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.0, 134.4, 129.5, 128.8, 127.2, 65.0, 41.7, 30.8, 19.3, 13.9.



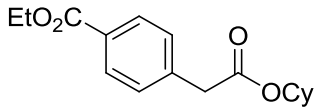
***tert*-Butyl 2-phenylacetate (3ad).[8]**

Isolated yield: 70%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.37-7.04 (m, 5H), 3.45 (s, 2H), 1.36 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.2, 134.9, 130.2, 129.4, 128.7, 127.1, 121.9, 81.0, 42.9, 28.3.



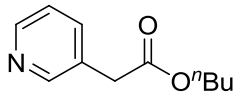
Benzyl 2-phenylacetate (3ae).[9]

Isolated yield: 67%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.33-7.24 (m, 10H), 5.13 (s, 2H), 3.67 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.6, 136.0, 134.1, 129.5, 128.8, 128.7, 128.4, 128.3, 127.3, 66.8, 41.5.



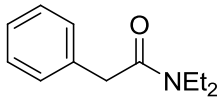
Ethyl 4-(2-(cyclohexyloxy)-2-oxoethyl)benzoate (3if).

Isolated yield: 72%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 4.70-4.68 (m, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 3.56 (s, 2H), 1.73-1.70 (m, 2H), 1.60-1.57 (m, 2H), 1.33-1.17 (m, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 170.6, 166.7, 139.7, 130.2, 130.0, 129.5, 73.6, 61.2, 42.1, 31.7, 25.6, 23.9, 14.6. HRMS (APCI) calcd for $C_{17}H_{22}O_4$ $[M]^+$: 290.1518; found 290.1519.



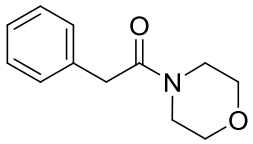
Butyl 2-(pyridin-3-yl)acetate (3jc).

Isolated yield: 59%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.53 (s, 2H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.29-7.25 (m, 1H), 4.11 (t, *J* = 6.8 Hz, 2H), 3.63 (s, 2H), 1.66-1.56 (m, 2H), 1.39-1.29 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.0, 150.6, 148.7, 137.1, 130.1, 123.6, 65.3, 38.8, 30.8, 19.3, 13.9. HRMS (APCI) calcd for $C_{11}H_{15}NO_2$ $[M]^+$:193.1103; found 193.1100.



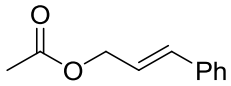
***N*,*N*-diethyl-2-phenylacetamide (3ag).[10]**

Isolated yield: 45%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.24-7.15 (m, 5H), 3.61 (s, 2H), 3.30 (q, *J* = 6.9 Hz, 2H), 3.20 (q, *J* = 7.0 Hz, 2H), 1.06-0.97 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 170.4, 135.5, 129.3, 128.7, 126.7, 42.5, 40.9, 40.3, 14.2, 13.0.



1-Morpholino-2-phenylethanone (3ah).[10]

Isolated yield: 44%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.27-7.14 (m, 5H), 3.65 (s, 2H), 3.59-3.56 (m, 4H), 3.38-3.36 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.9, 135.0, 129.1, 128.8, 127.2, 67.0, 66.7, 46.8, 42.4, 41.1.



(Z)-3-phenylallyl acetate.[11]

Isolated yield: 75%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40-7.25 (m, 5H), 6.65 (d, *J* = 15.9 Hz, 1H), 6.33-6.23 (m, 1H), 4.72 (d, *J* = 6.3 Hz, 2H), 2.10 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.1, 136.3, 134.4, 128.8, 128.3, 126.8, 123.3, 65.3, 21.2.

Reference

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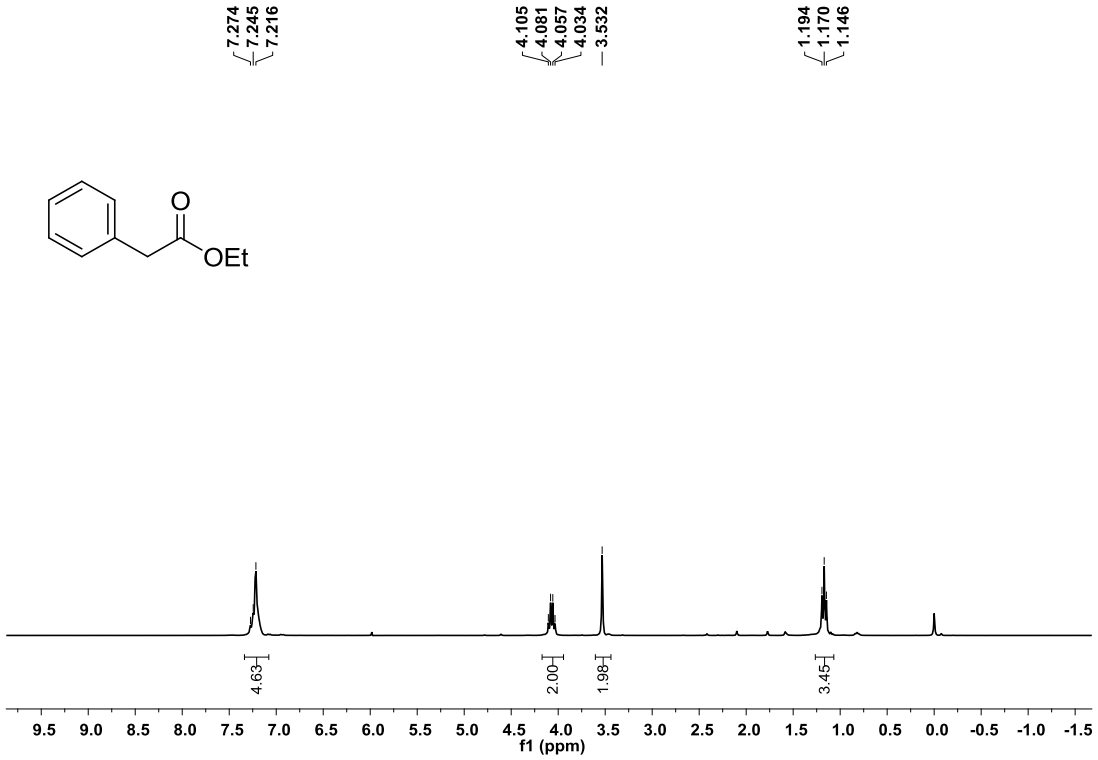
Spectrum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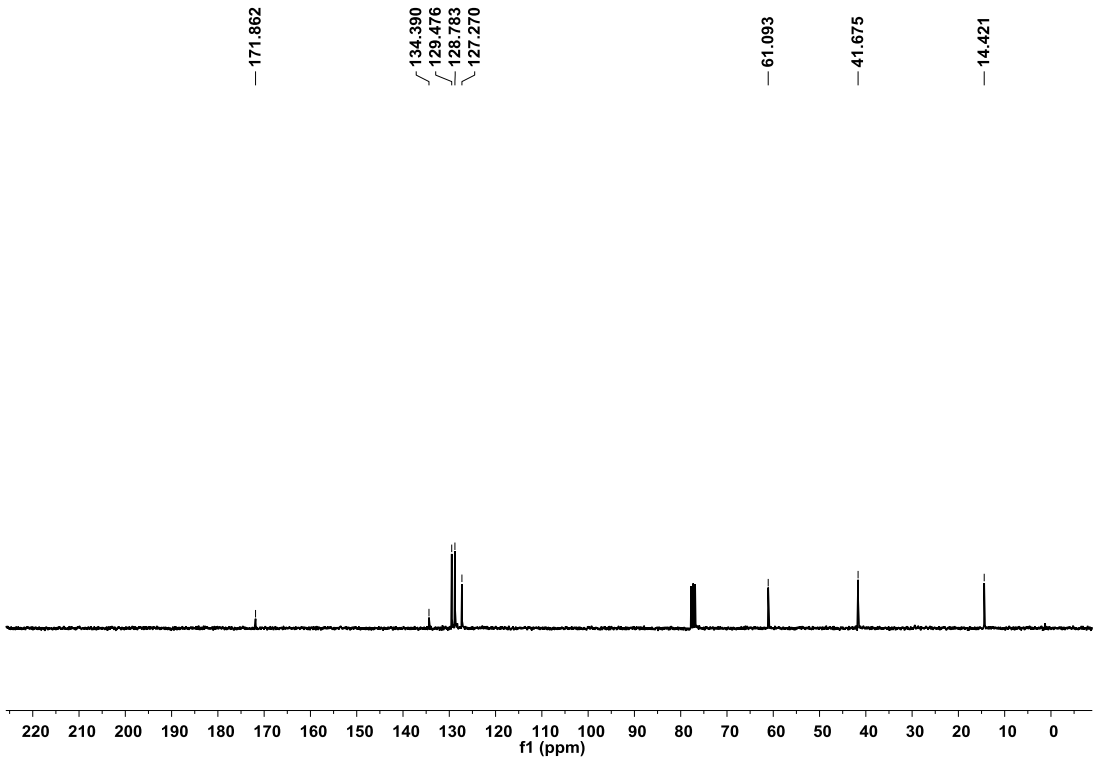
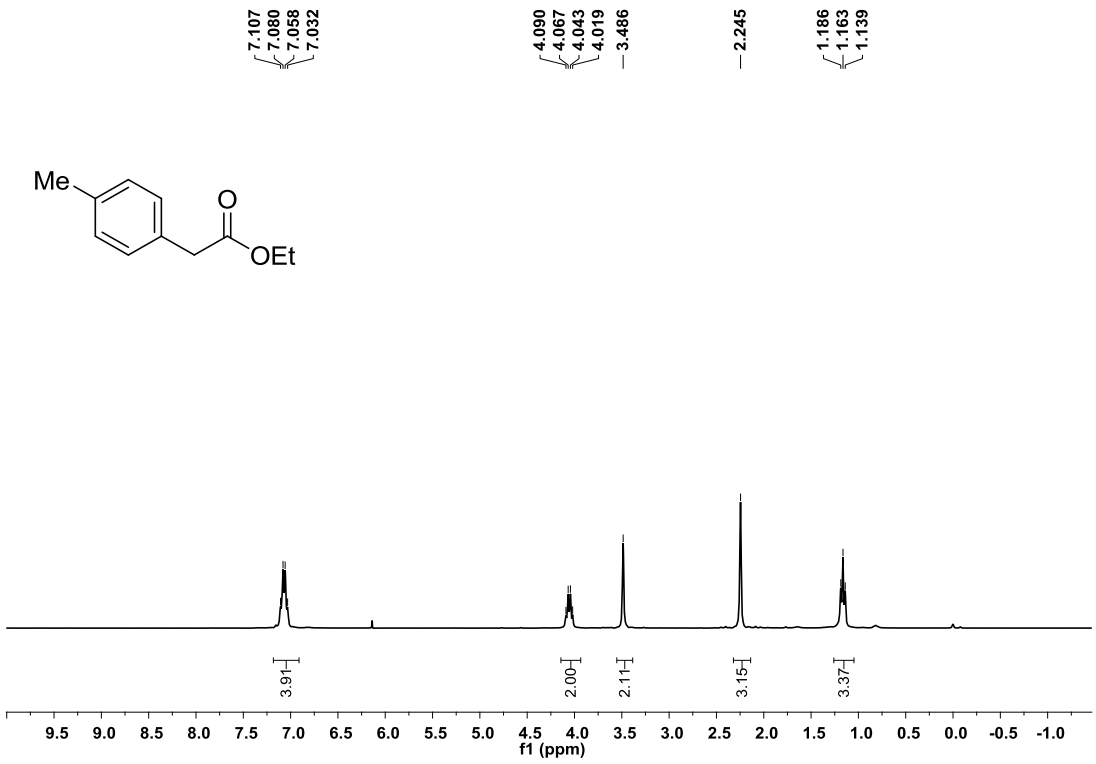
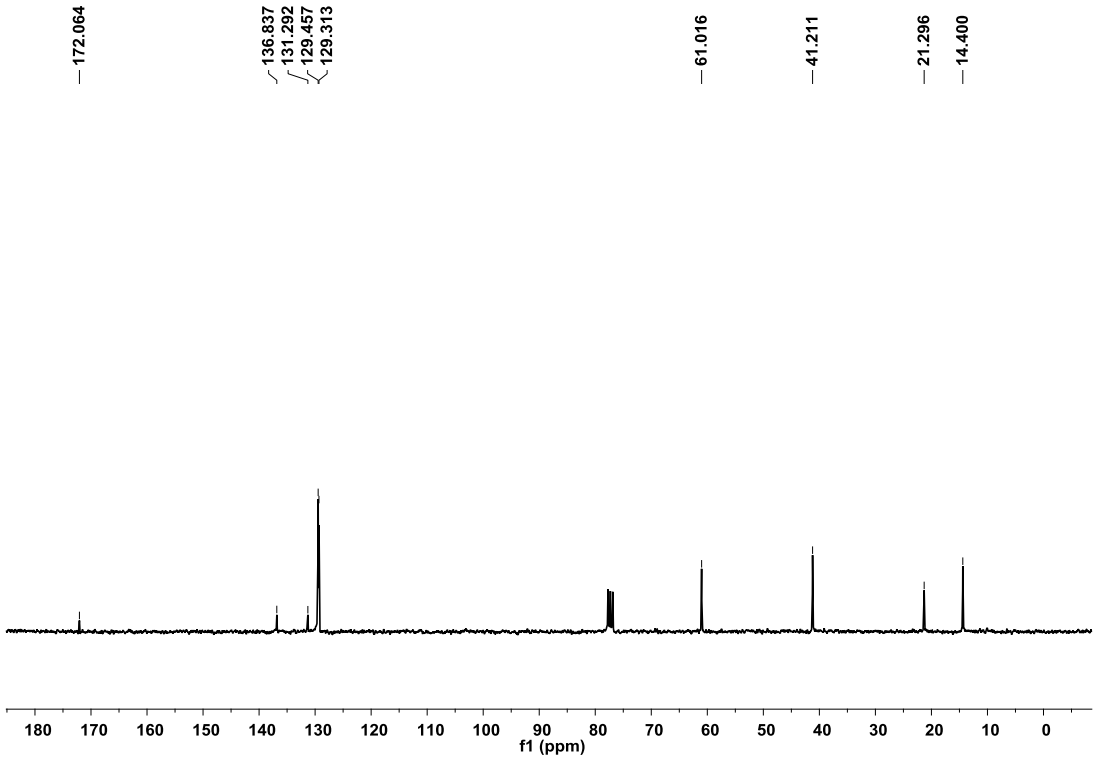
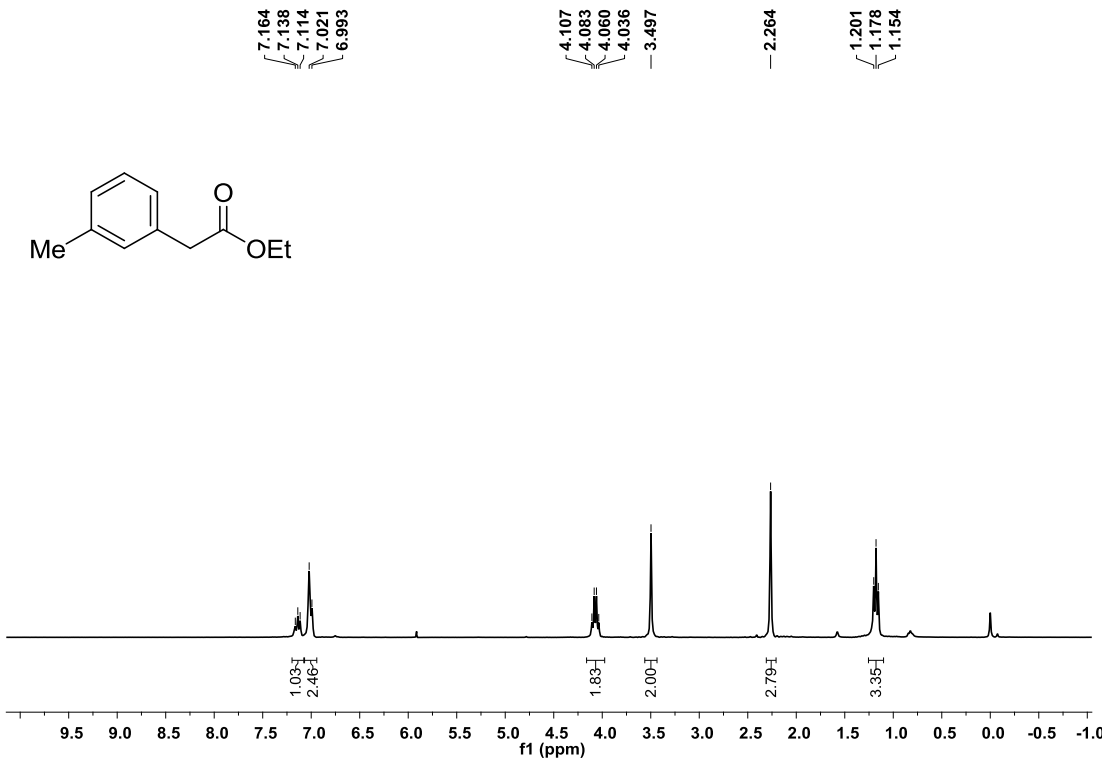
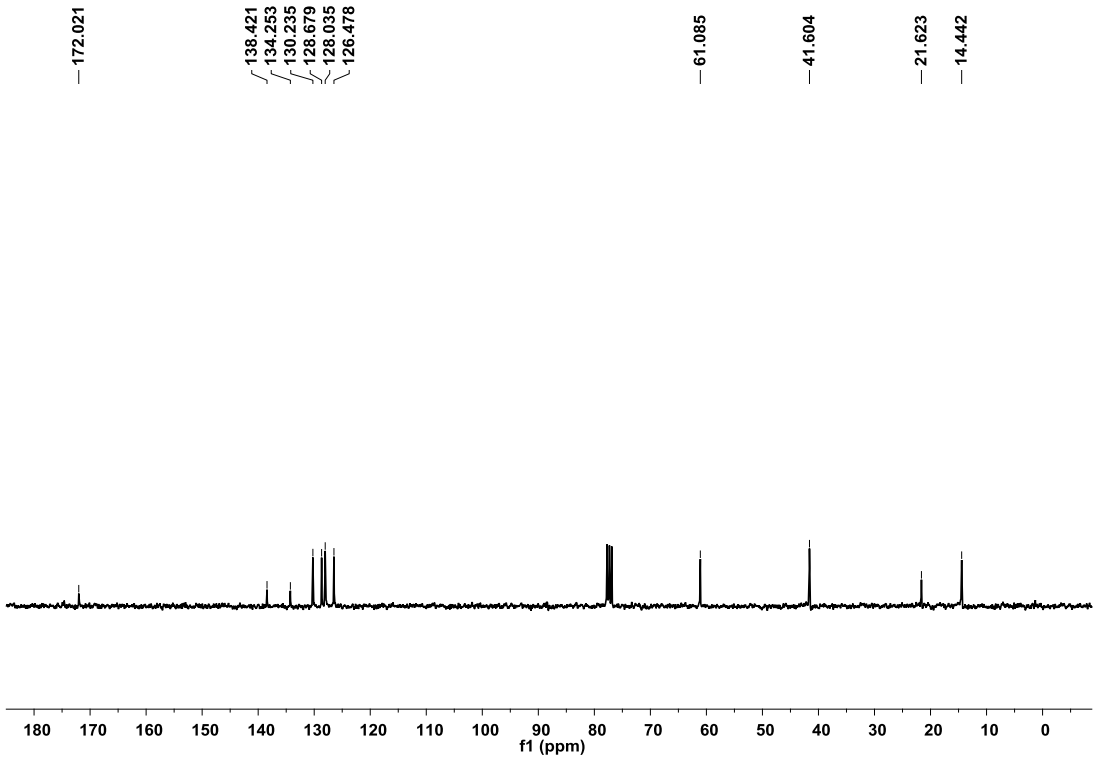
7.245
7.216
4.105
4.081
4.057
4.034
3.532
1.194
1.170
1.146
O
OEt
4.63
2.00
1.98
3.45
f1 (ppm)

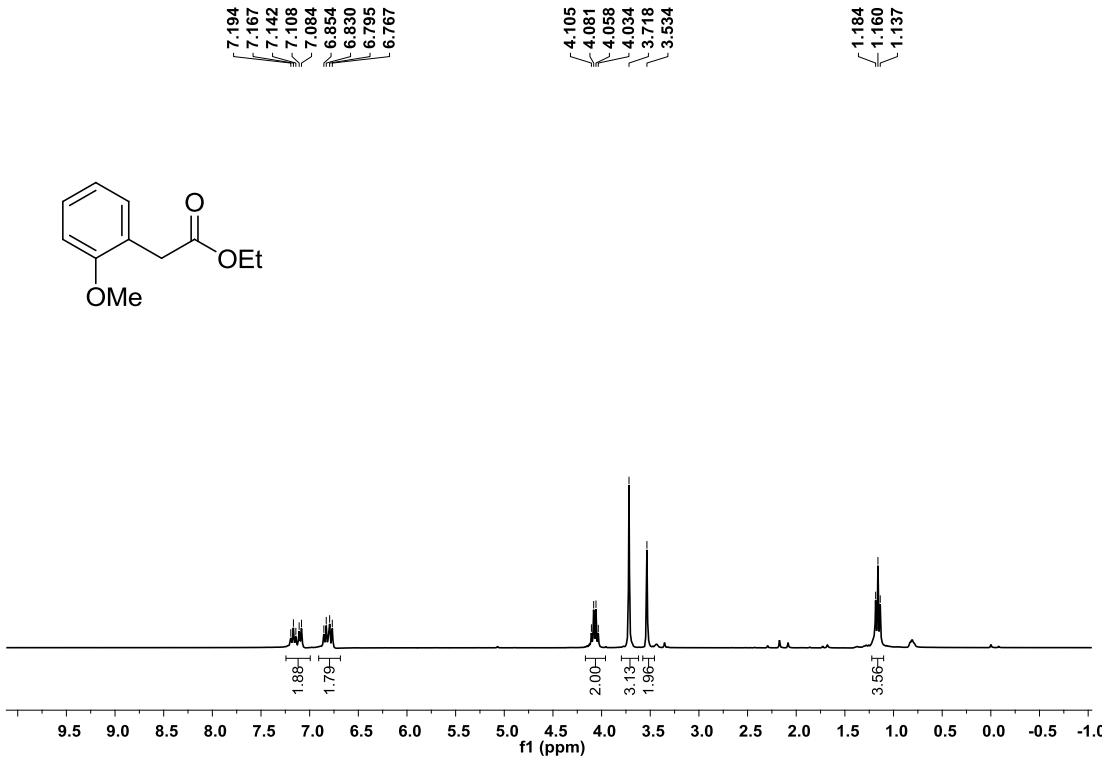

171.862
134.390
129.476
128.783
127.270
61.093
41.675
14.421
f1 (ppm)

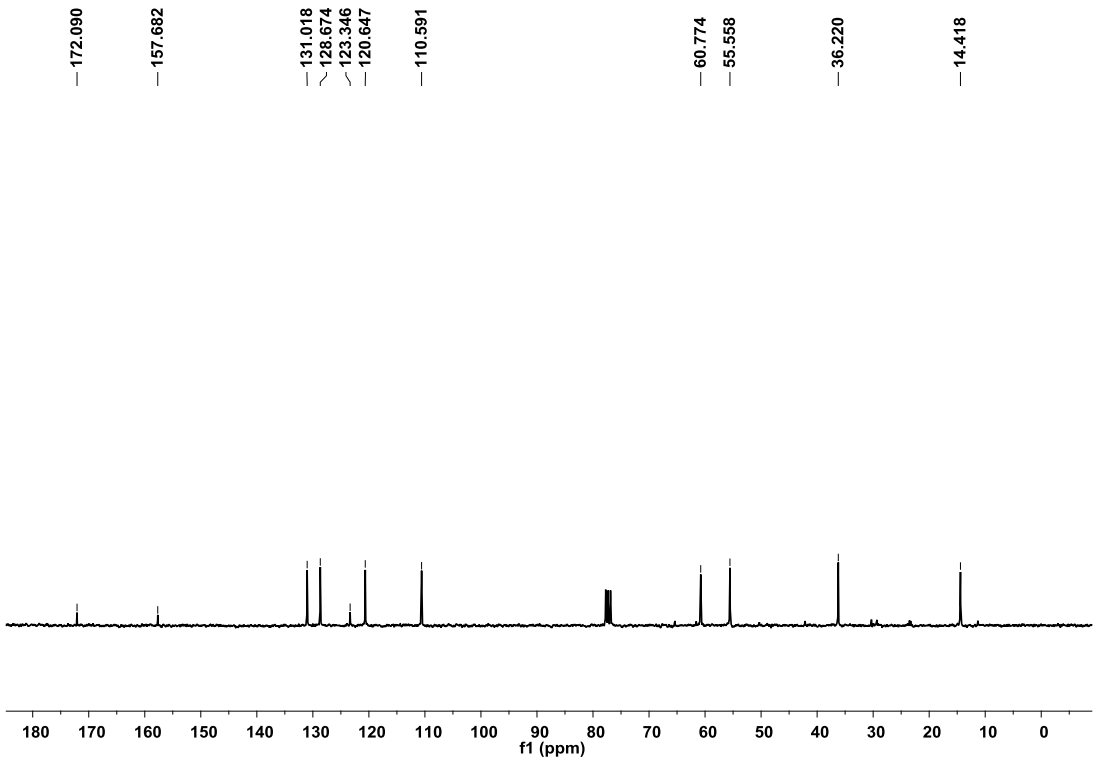

7.107
7.080
7.058
7.032
4.090
4.067
4.043
4.019
3.486
2.245
1.186
1.163
1.139
Me
O
OEt
3.91
2.00
2.11
3.15
3.37
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

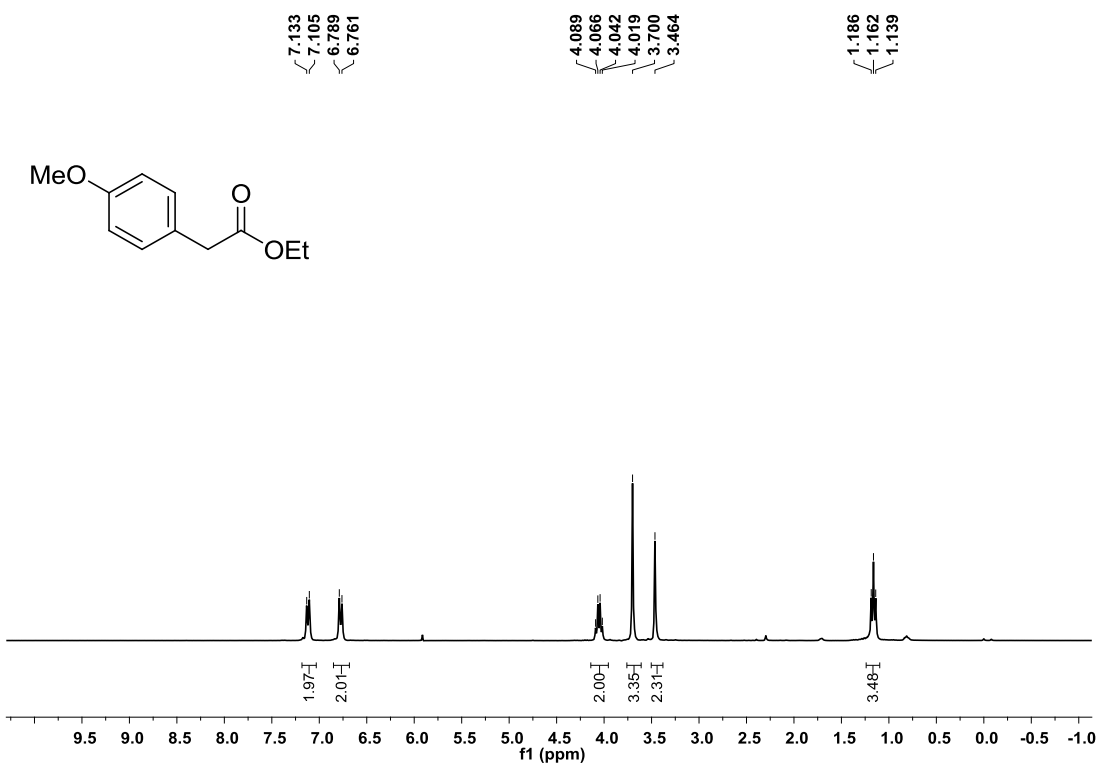

172.064
136.837
131.292
129.457
129.313
61.016
41.211
21.296
14.400
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

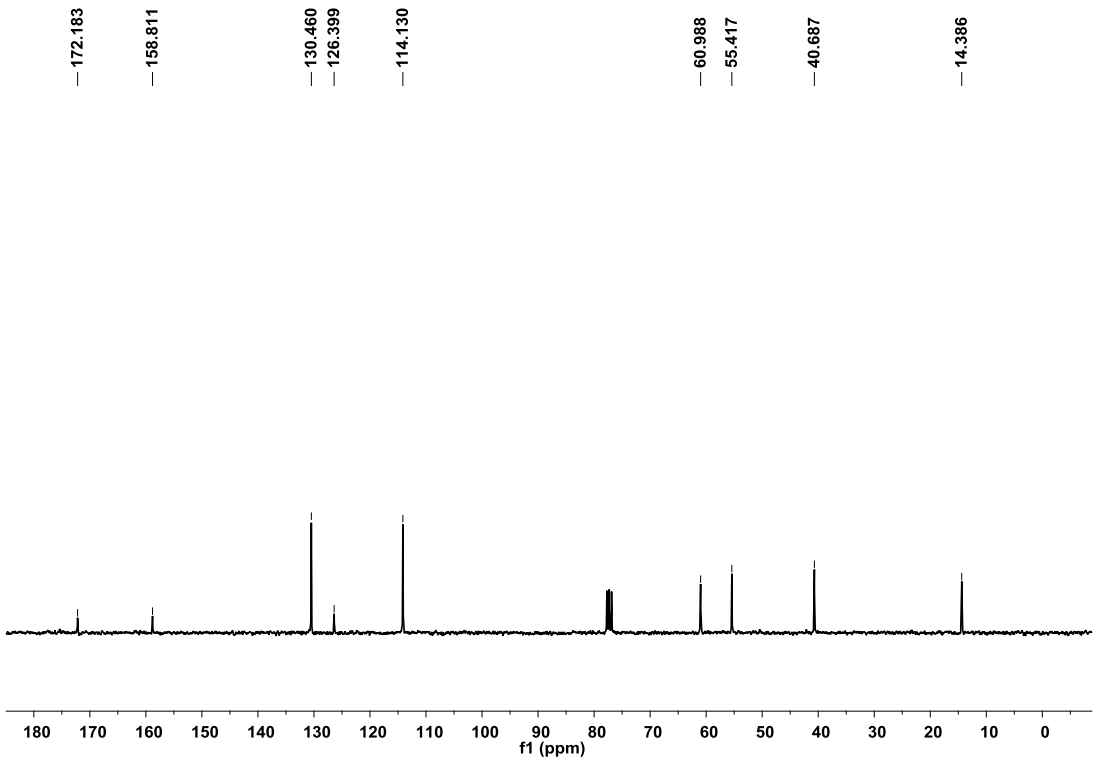

7.164
7.138
7.114
7.021
6.993
4.107
4.083
4.060
4.036
3.497
2.264
1.201
1.178
1.154
Me
O
OEt
1.03
2.46
1.83
2.00
2.79
3.35
f1 (ppm)

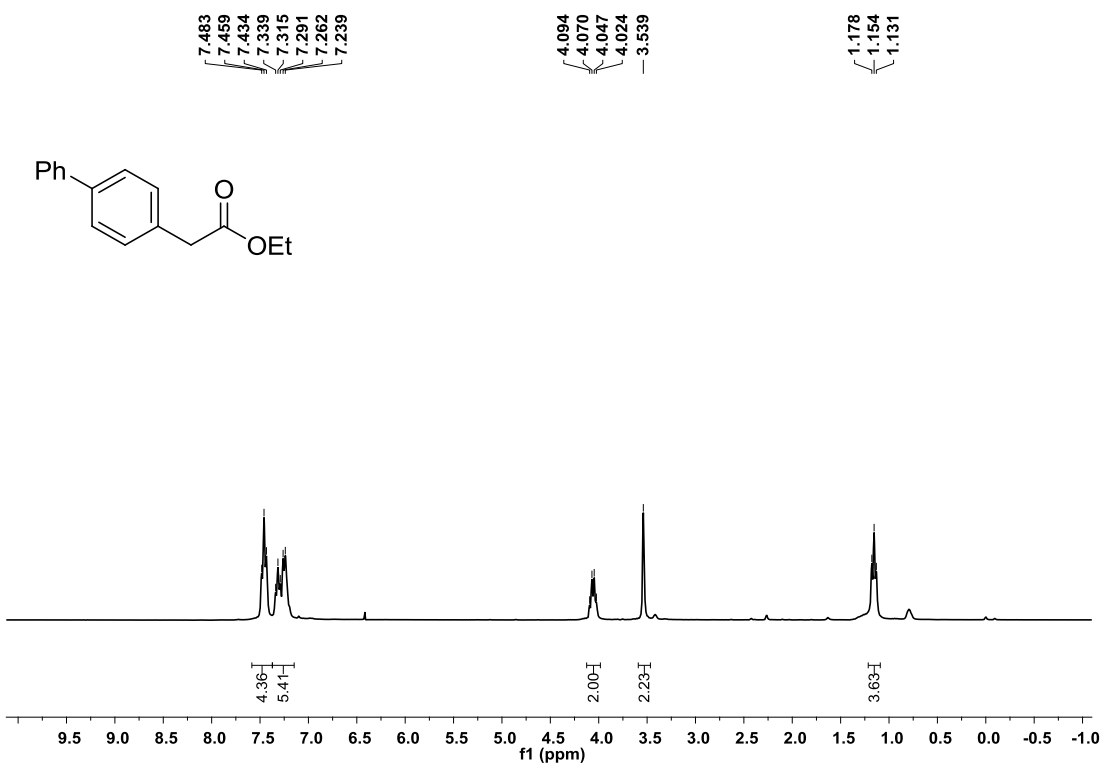

172.021
138.421
134.253
130.235
128.679
128.035
126.478
61.085
41.604
21.623
14.442
f1 (ppm)

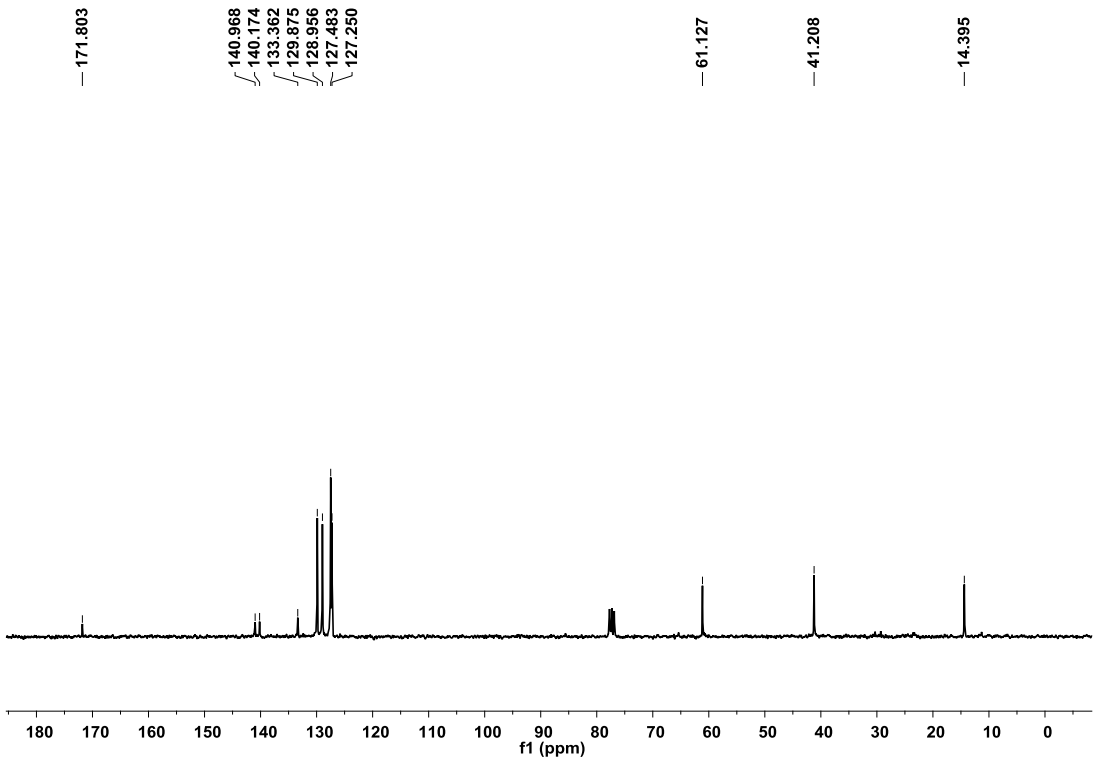

7.194
7.167
7.142
7.108
7.084
6.854
6.830
6.795
6.767
4.105
4.081
4.058
4.034
3.718
3.534
1.184
1.160
1.137
O
OEt
OMe
1.88
1.79
2.00
3.13
1.96
3.56
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

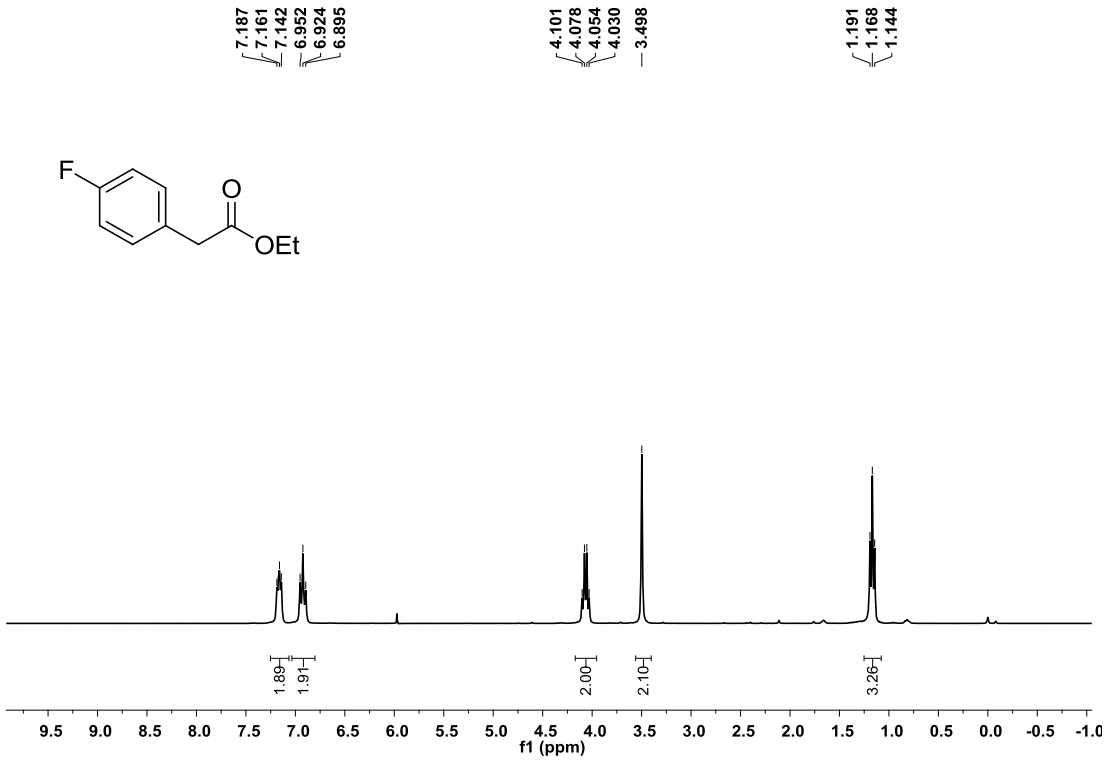

172.090
157.682
131.018
128.674
123.346
120.647
110.591
60.774
55.558
36.220
14.418
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

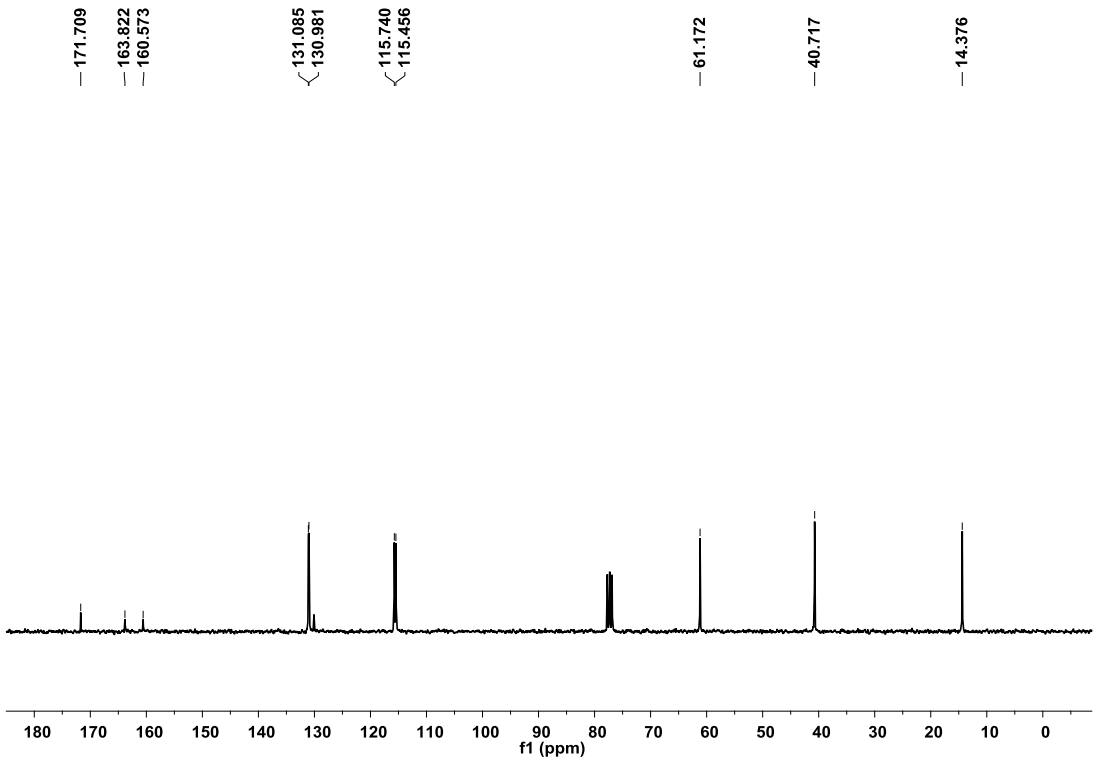

7.133
7.105
6.789
6.761
4.089
4.066
4.042
4.019
3.700
3.464
1.186
1.162
1.139
MeO
O
OEt
1.97
2.01
2.00
3.35
2.31
3.48
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

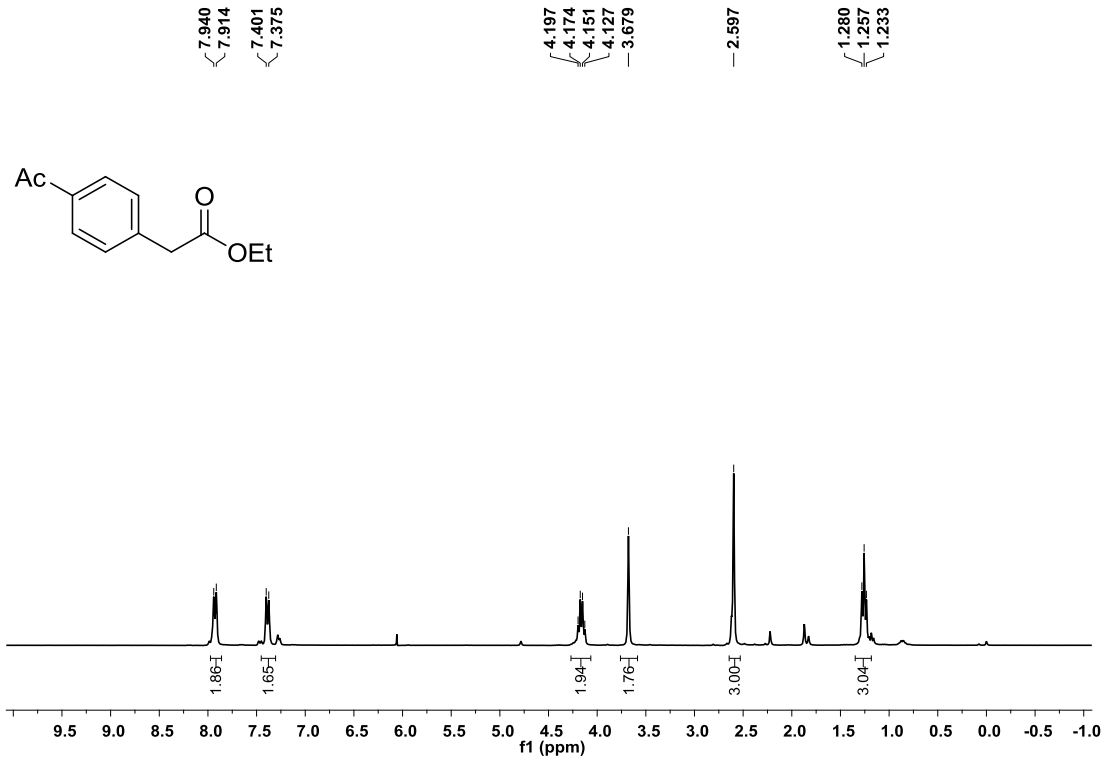

172.183
158.811
130.460
126.399
114.130
60.988
55.417
40.687
14.386
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

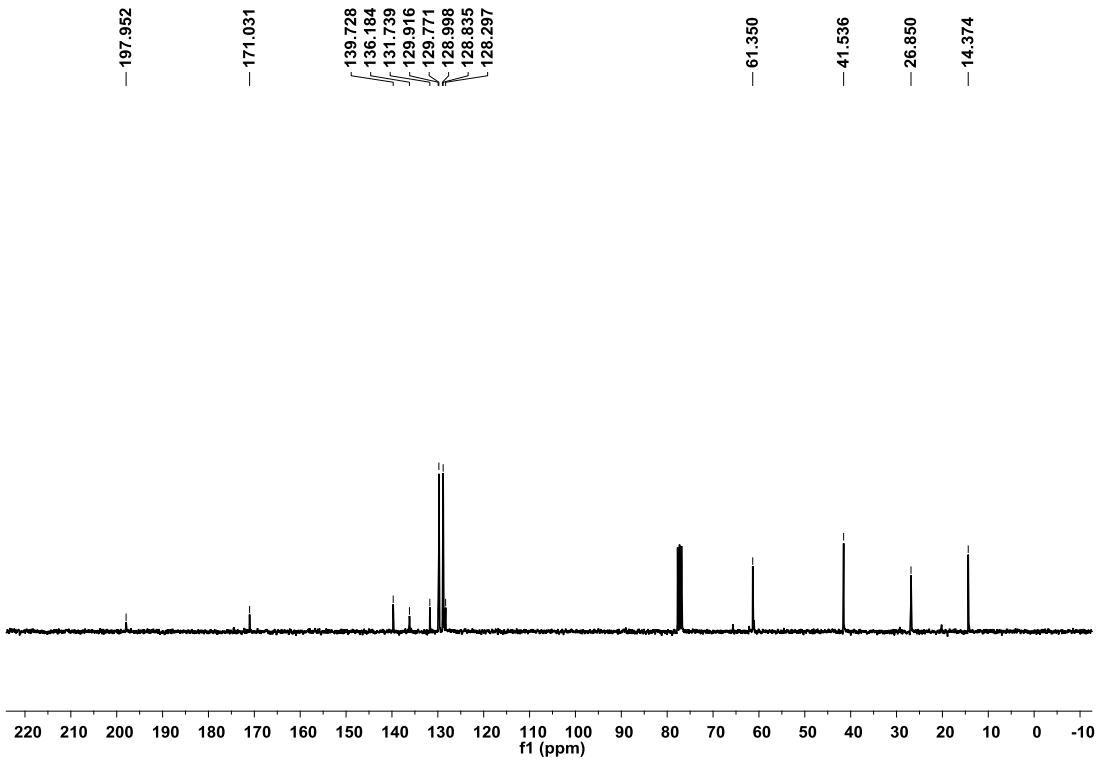

7.483
7.459
7.434
7.339
7.315
7.291
7.262
7.239
4.094
4.070
4.047
4.024
3.539
1.178
1.154
1.131
Ph
O
OEt
4.36
5.41
2.00
2.23
3.63
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


171.803
140.968
140.174
133.362
129.875
128.956
127.483
127.250
61.127
41.208
14.395
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

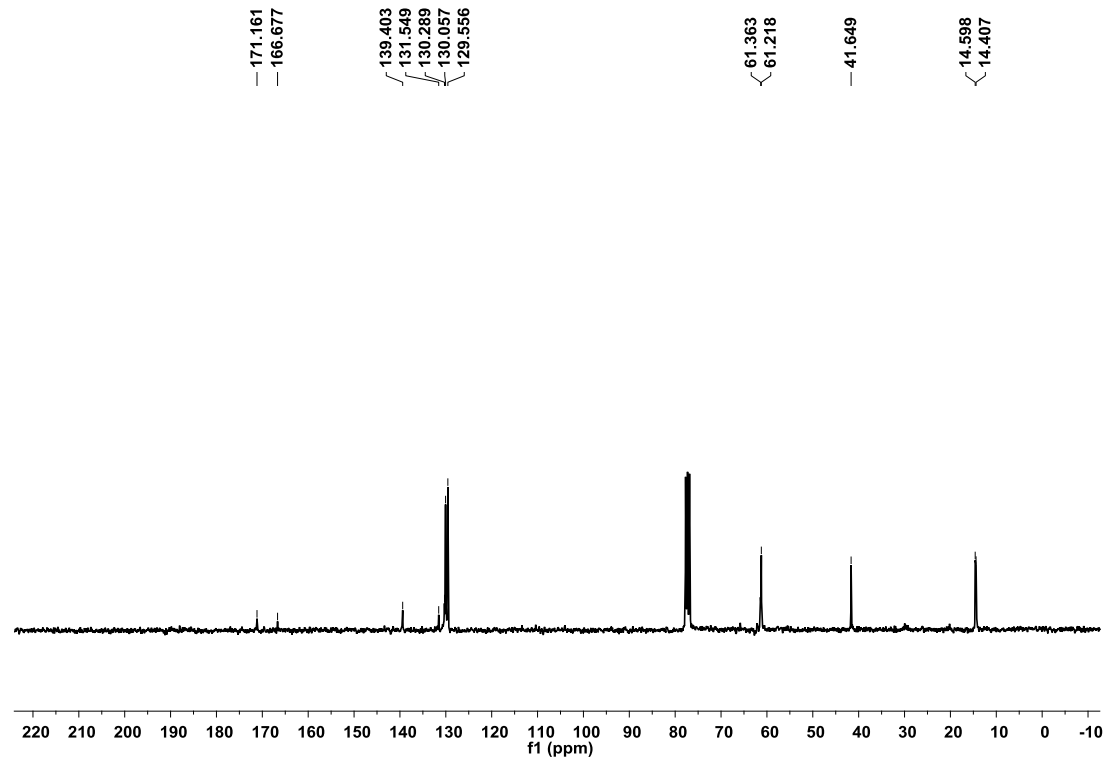





7.940
7.914
7.401
7.375
4.197
4.174
4.151
4.127
3.679
2.597
1.280
1.257
1.233
Ac
O
OEt
1.86
1.65
1.94
1.76
3.00
3.04
f1 (ppm)


197.952
171.031
139.728
136.184
131.739
129.916
129.771
128.998
128.835
128.297
61.350
41.536
26.850
14.374
f1 (ppm)


7.951
7.923
7.302
7.275
4.339
4.316
4.292
4.268
4.125
4.101
4.078
4.054
3.599
1.344
1.320
1.297
1.205
1.181
1.157
EtO2C
O
OEt
2.06
1.95
2.17
1.96
2.00
3.29
ppm (t1)


171.161
166.677
139.403
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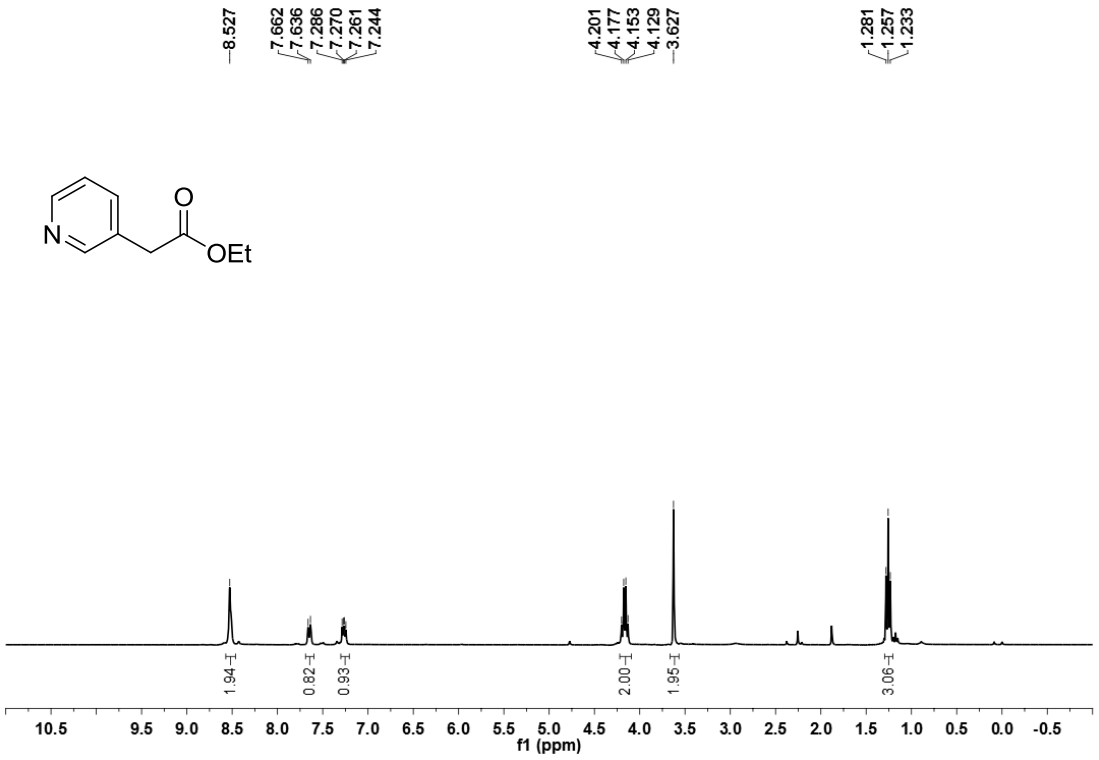
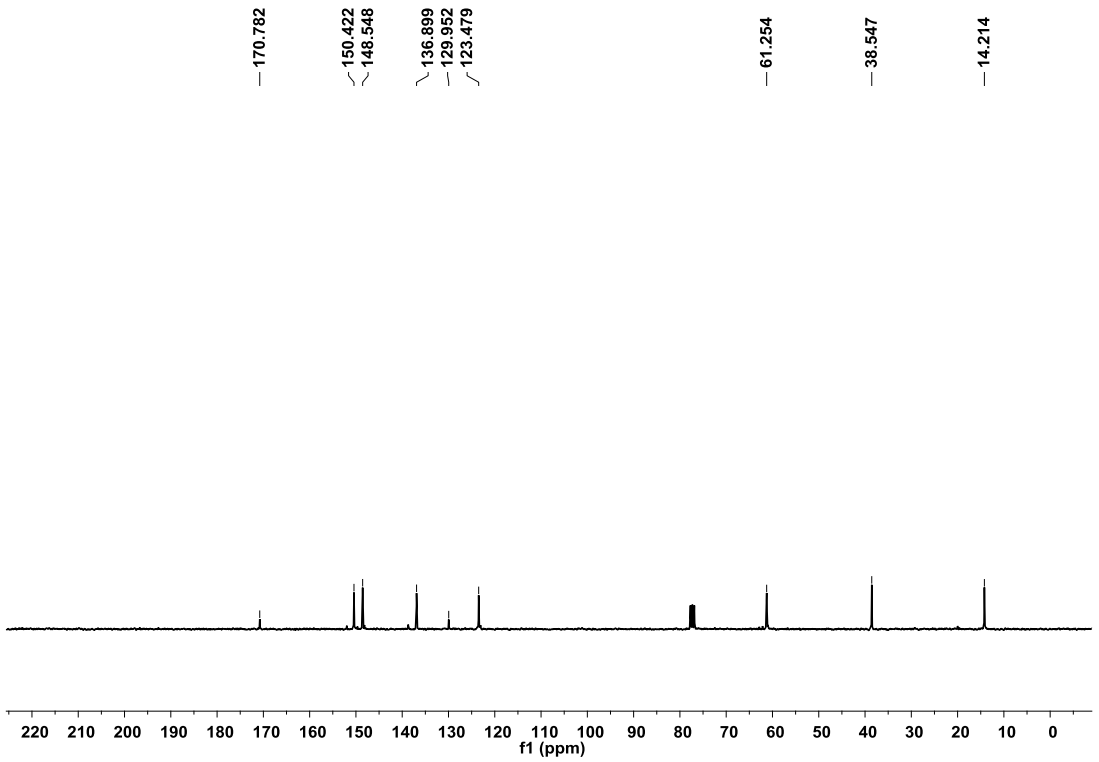
130.289
130.057
129.556
61.363
61.218
41.649
14.598
14.407
f1 (ppm)


8.527
7.662
7.636
7.286
7.270
7.261
7.244
4.201
4.177
4.153
4.129
3.627
1.281
1.257
1.233
N
O
OEt
1.94
0.82
0.93
2.00
1.95
3.06
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
-0.5
f1 (ppm)


170.782
150.422
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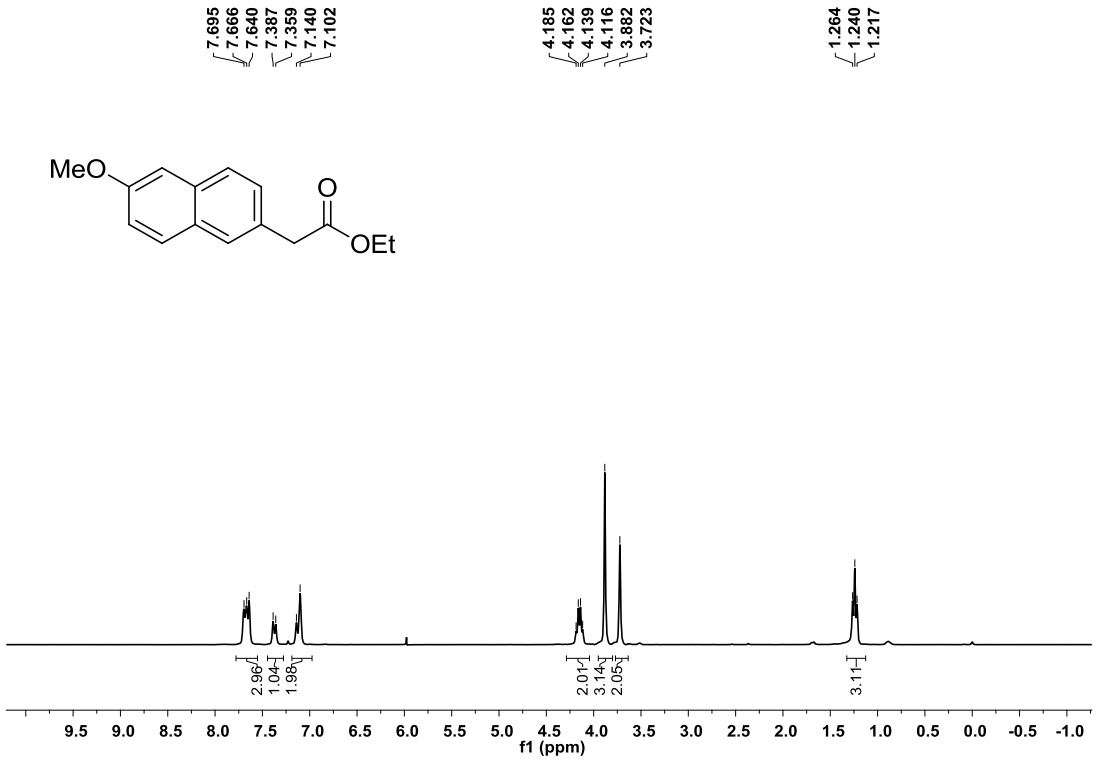
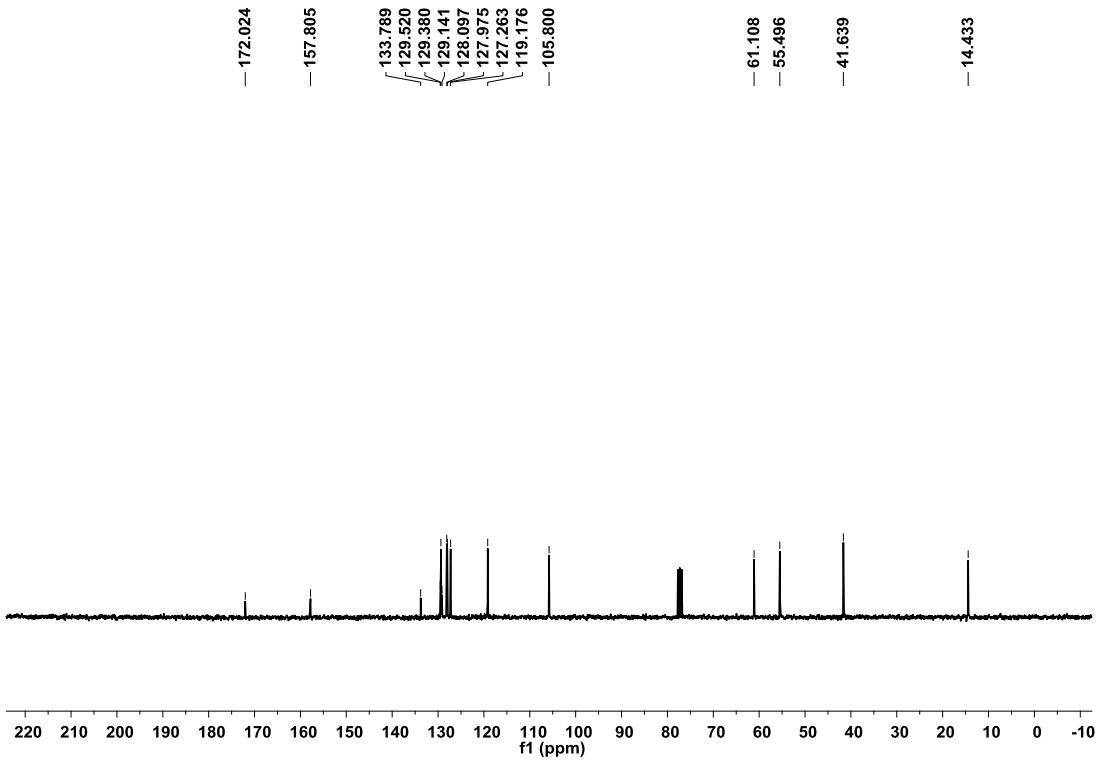
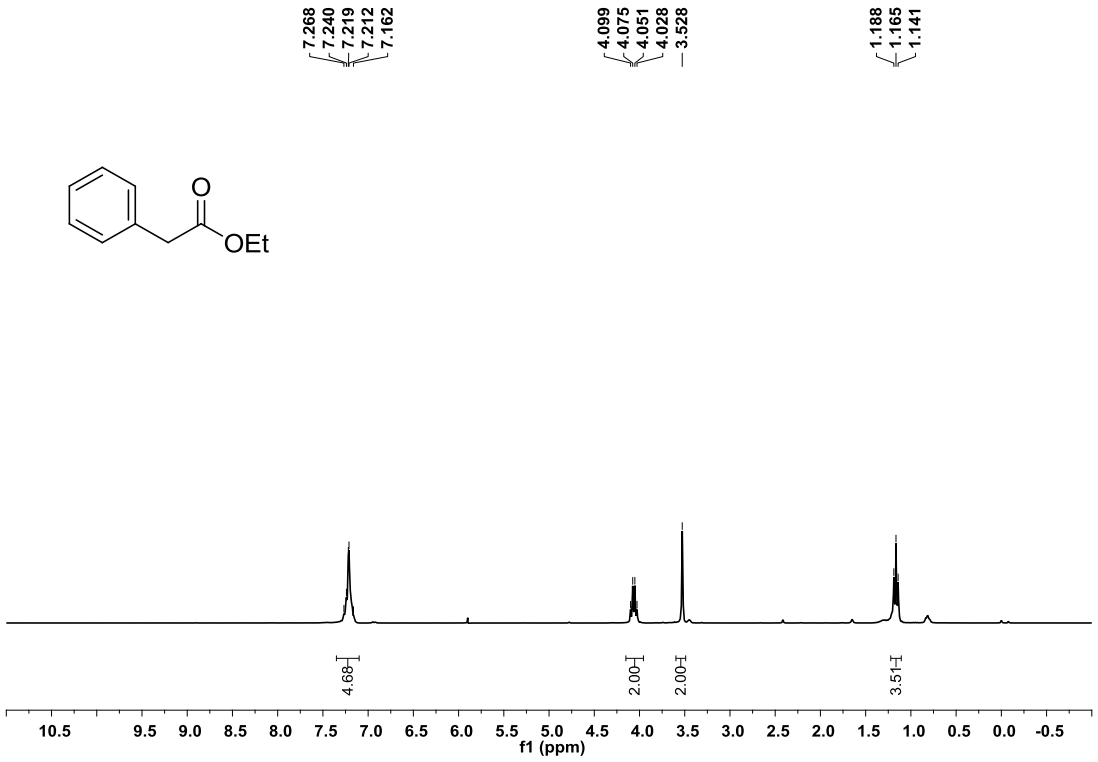
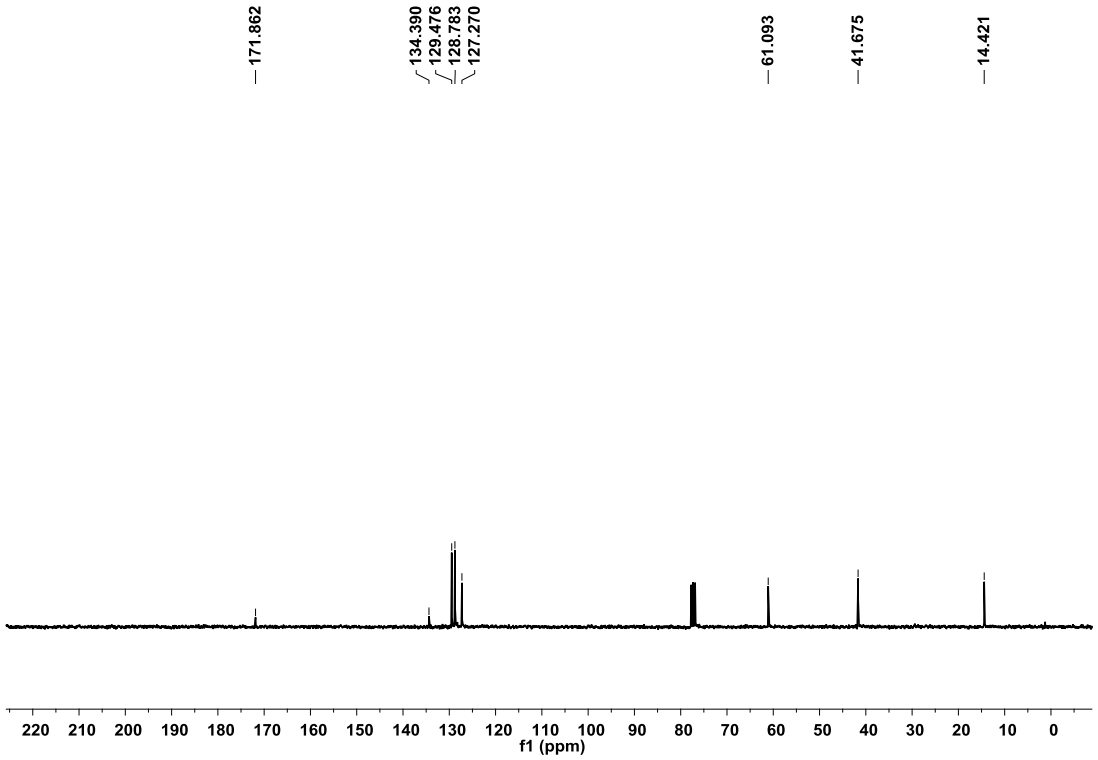
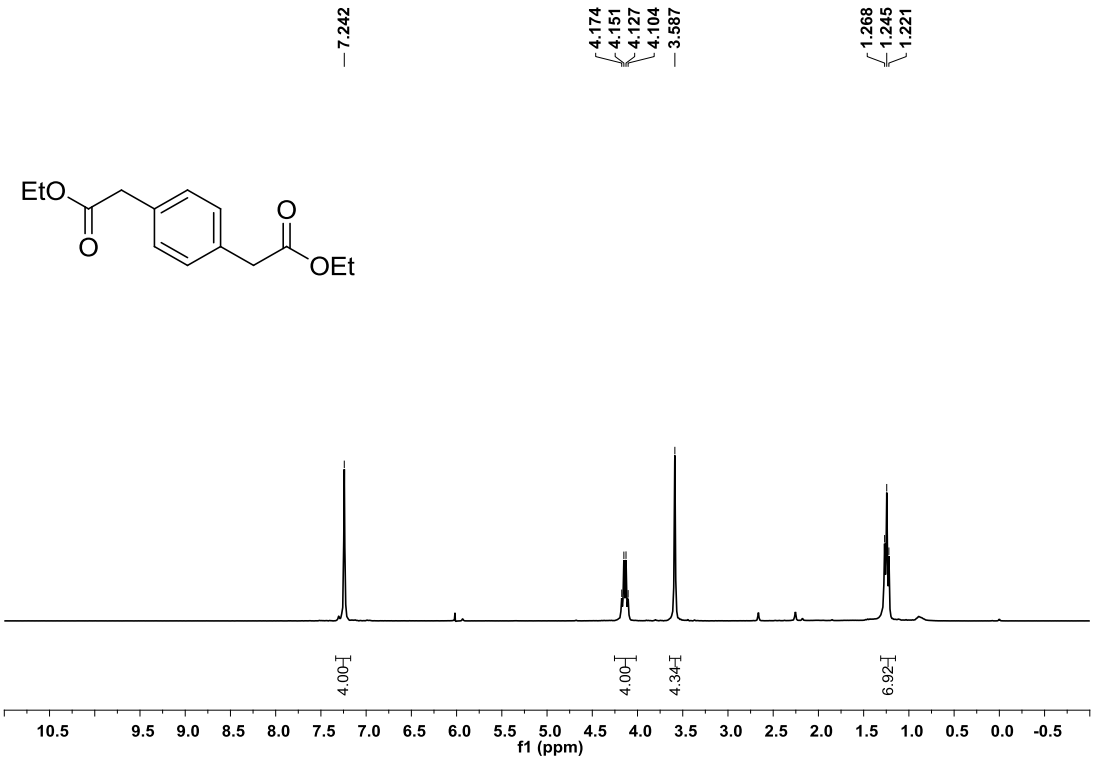
136.899
129.952
123.479
61.254
38.547
14.214
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

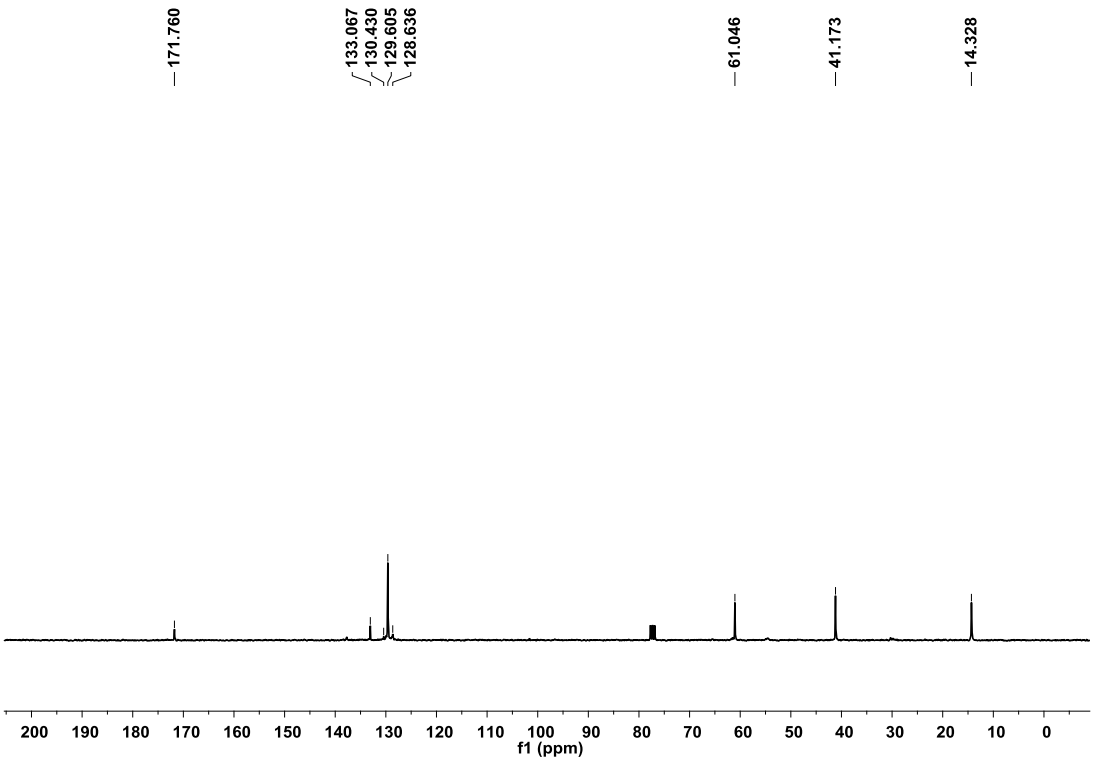


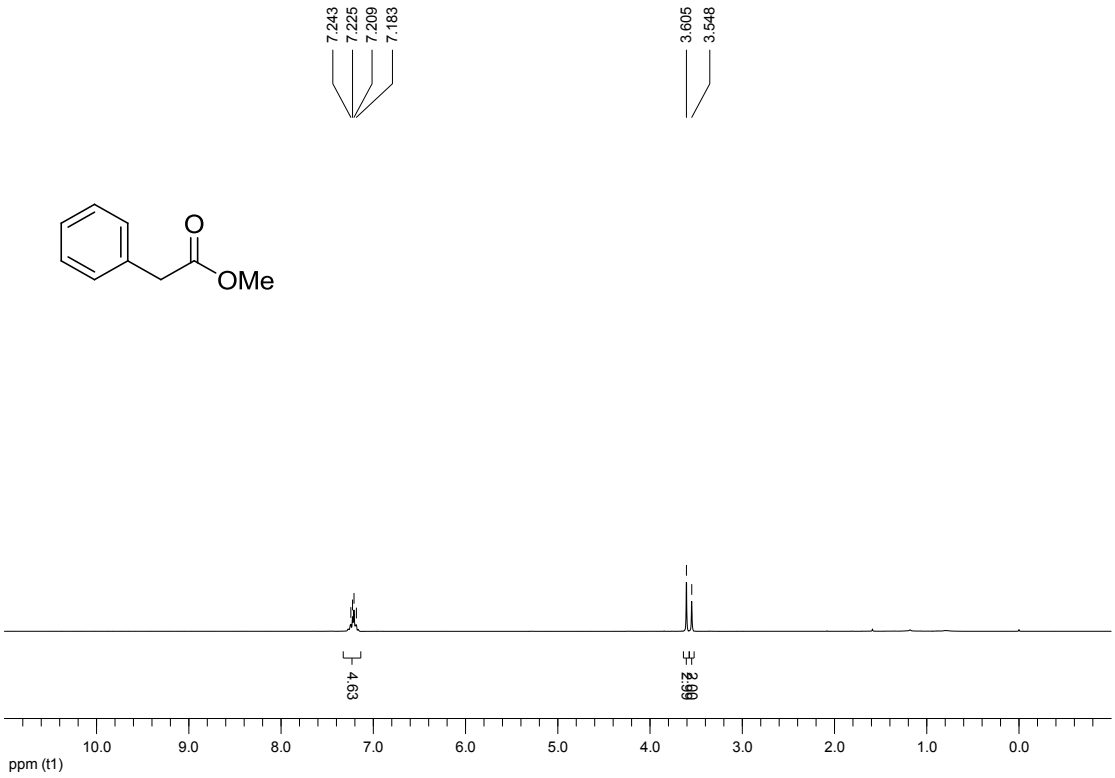


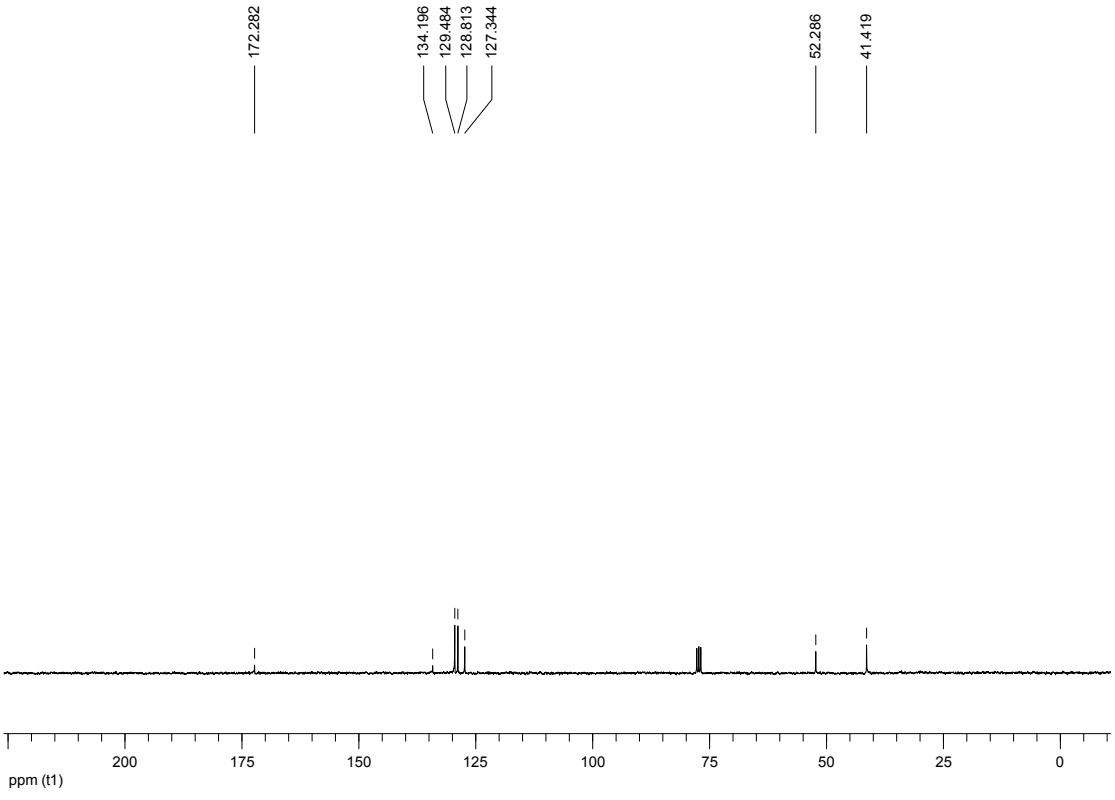

7.268
7.240
7.219
7.212
7.162
4.099
4.075
4.051
4.028
3.528
1.188
1.165
1.141
O
OEt
4.68
2.00
2.00
3.51
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

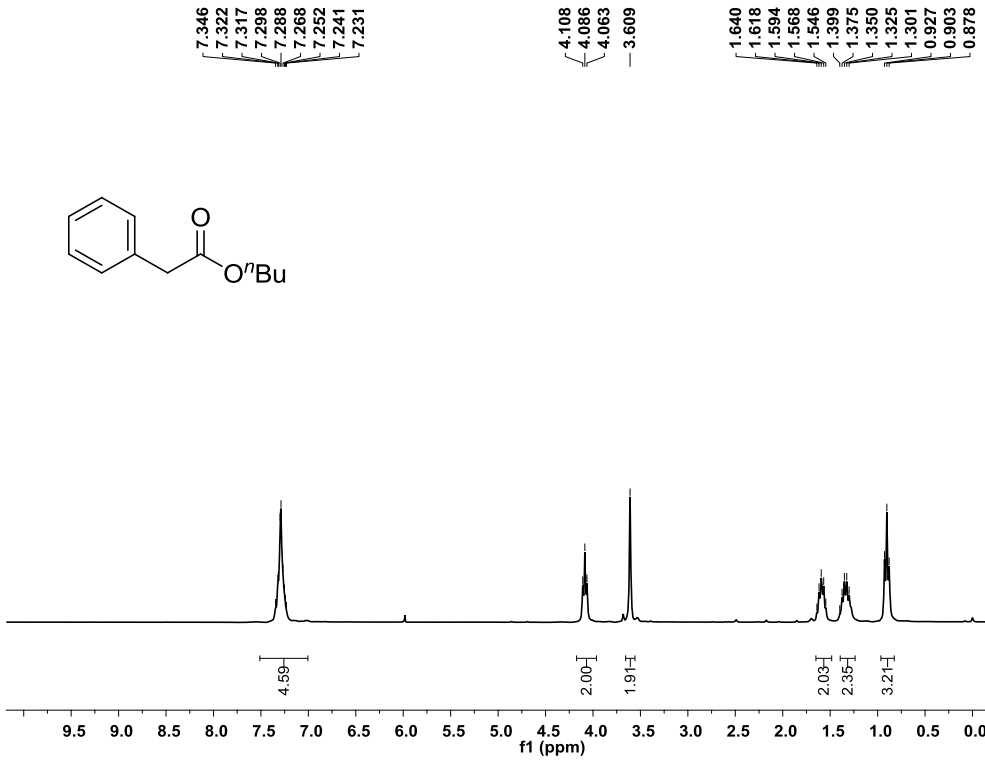

171.862
134.390
129.476
128.783
127.270
61.093
41.675
14.421
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)







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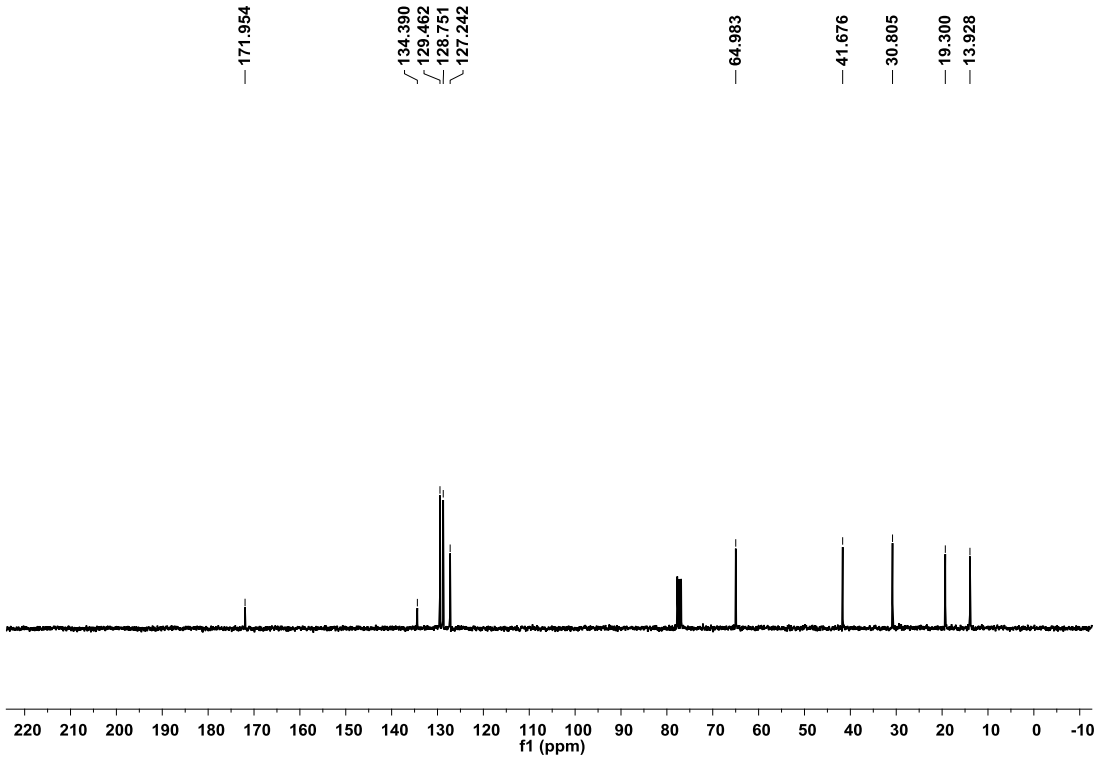
7.322
7.317
7.298
7.288
7.268
7.252
7.241
7.231
4.108
4.086
4.063
3.609
1.640
1.618
1.594
1.568
1.546
1.399
1.375
1.350
1.325
1.301
0.927
0.903
0.878
O
O^{n}Bu
4.59
2.00
1.91
2.03
2.35
3.21
f1 (ppm)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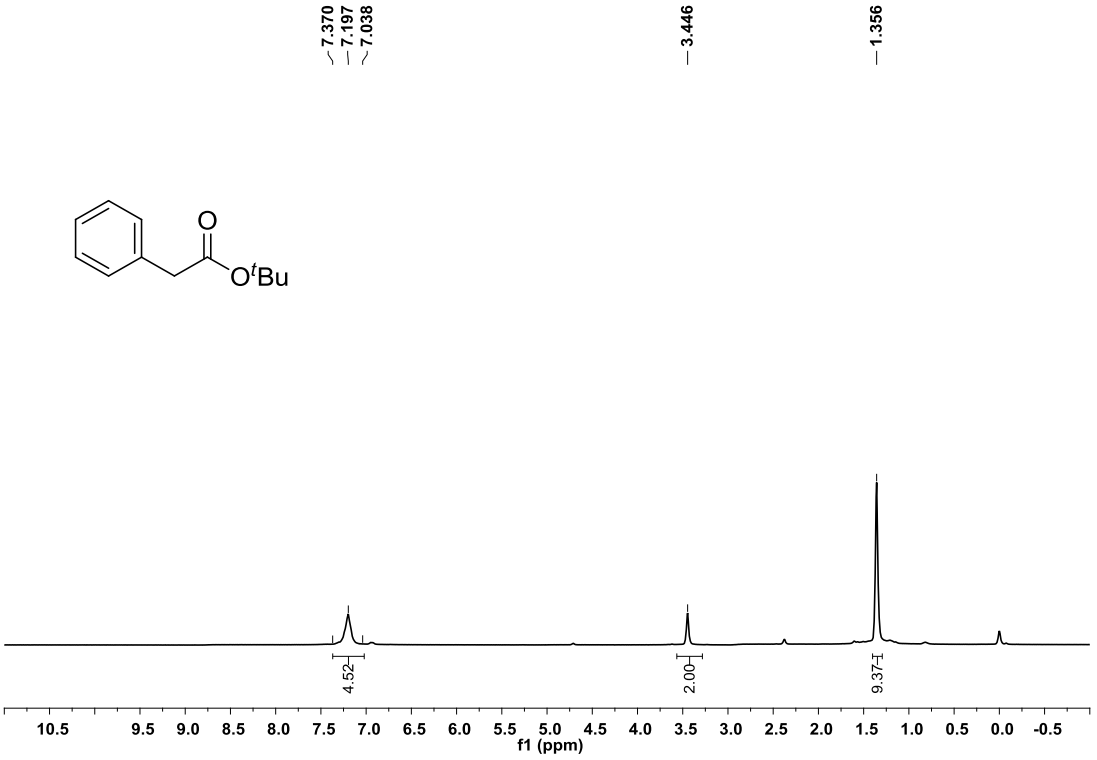
127.242
64.983
41.676
30.805
19.300
13.928
f1 (ppm)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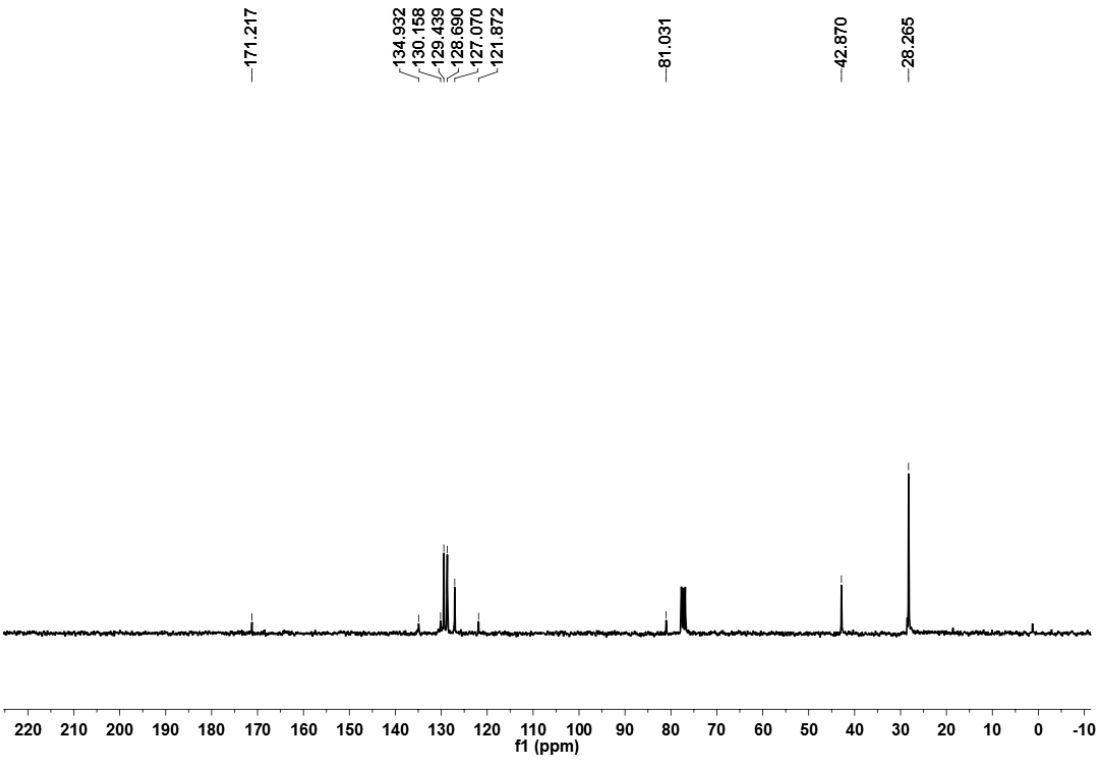
7.197
7.038
3.446
1.356
O
O^{t}Bu
4.52
2.00
9.37
f1 (ppm)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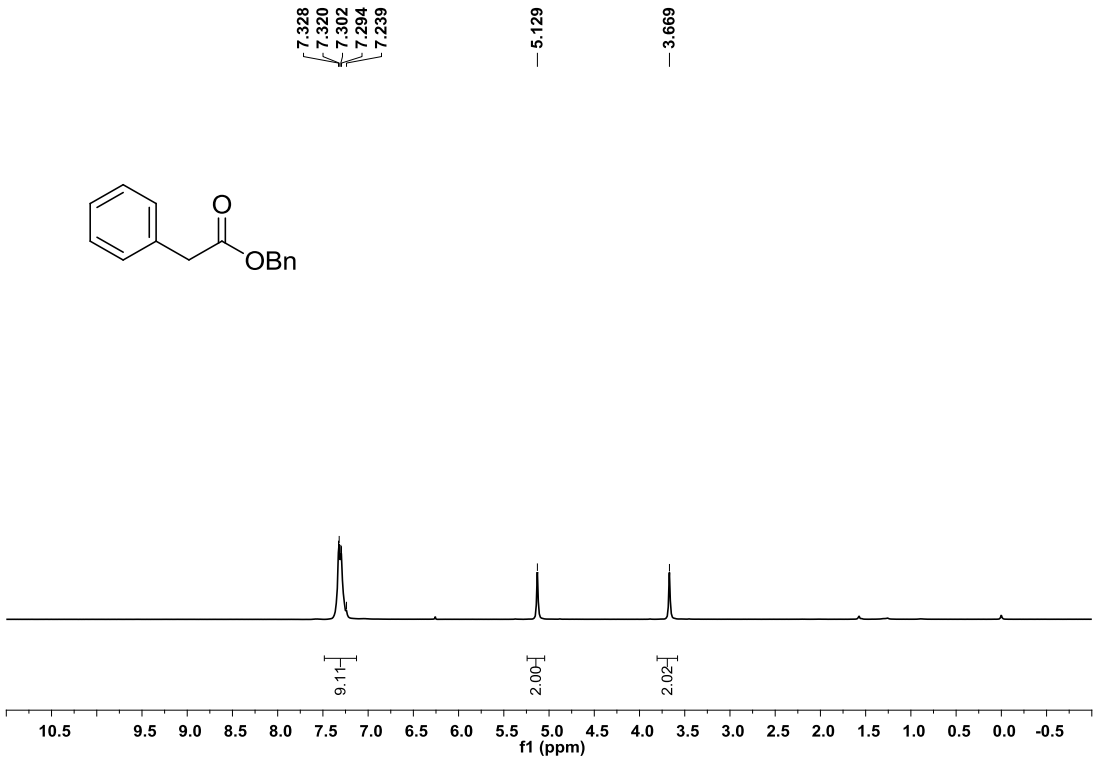
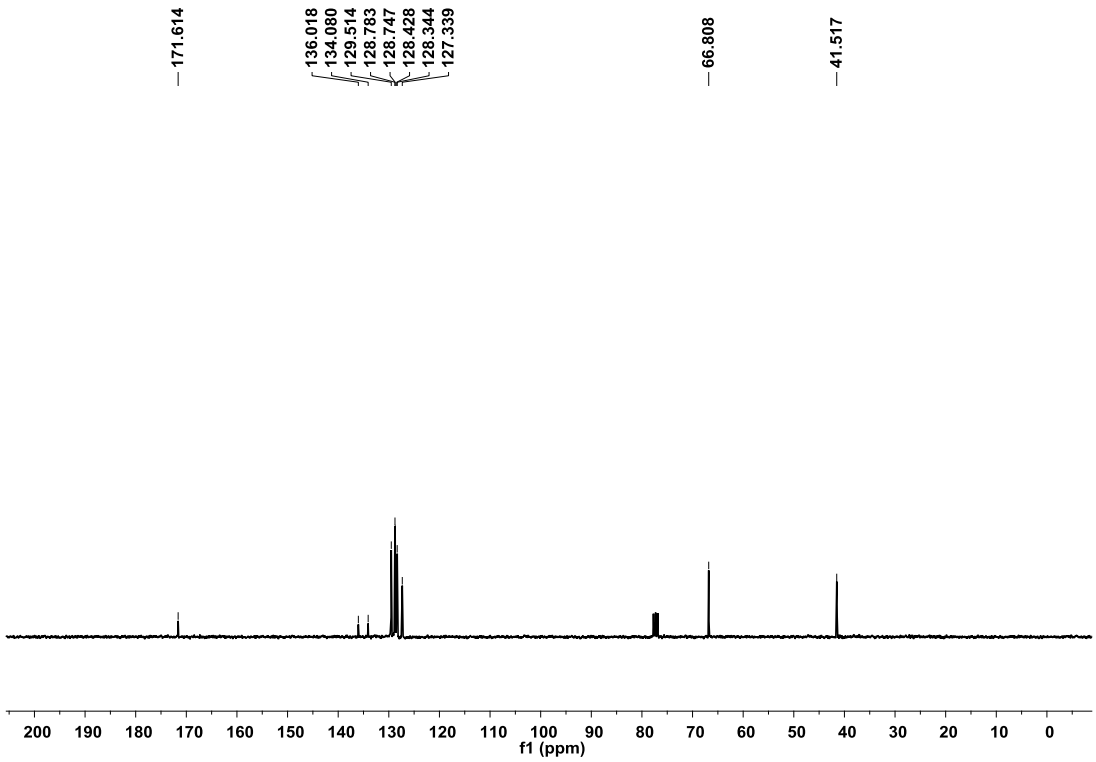
127.070
121.872
81.031
42.870
28.265
f1 (ppm)






7.926
7.899
7.284
7.258
4.703
4.690
4.678
4.320
4.297
4.273
4.249
3.563
1.734
1.702
1.596
1.574
1.328
1.303
1.280
1.230
1.197
1.170
EtO2C
O
OCy
1.67
1.74
0.95
1.94
2.00
2.35
2.37
8.99
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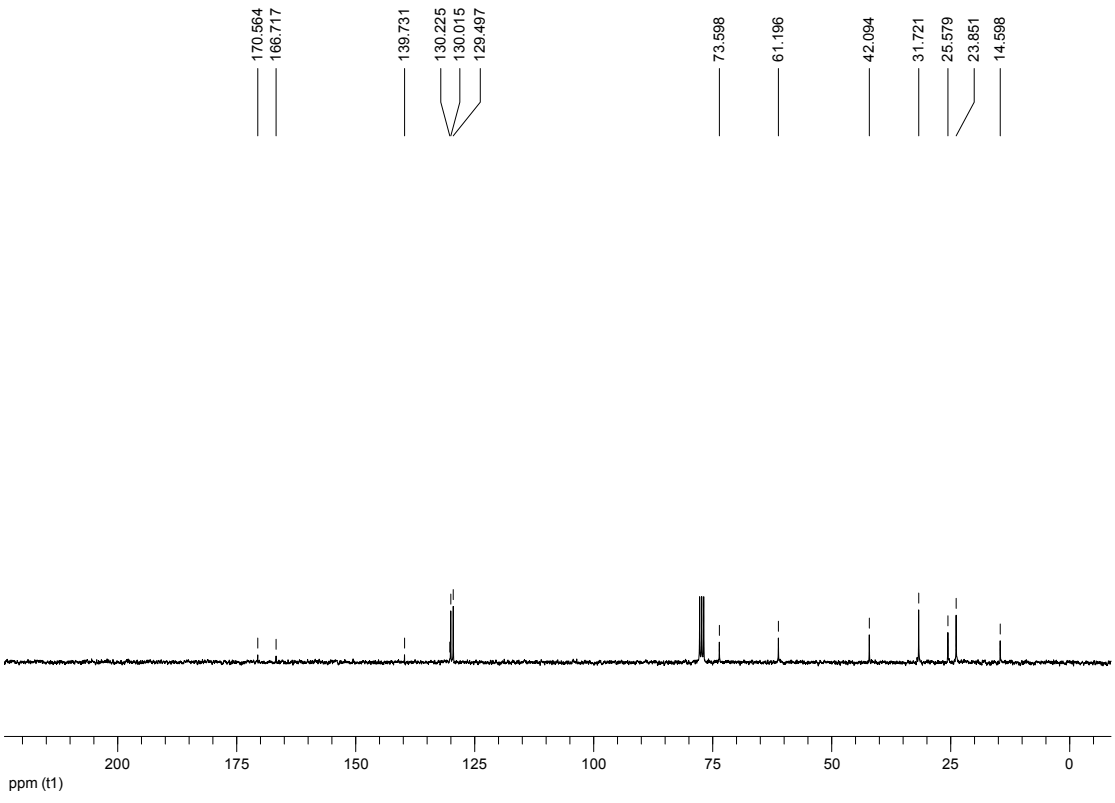
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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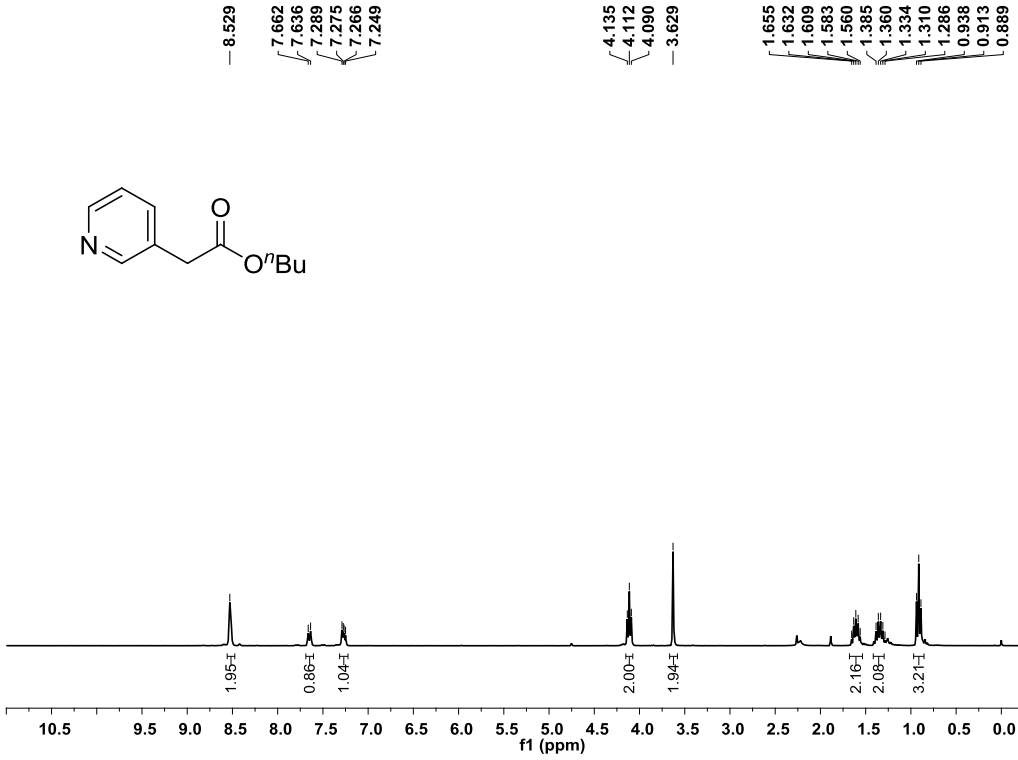
166.717
139.731
130.225
130.015
129.497
73.598
61.196
42.094
31.721
25.579
23.851
14.598
200
175
150
125
100
75
50
25
0
ppm (t1)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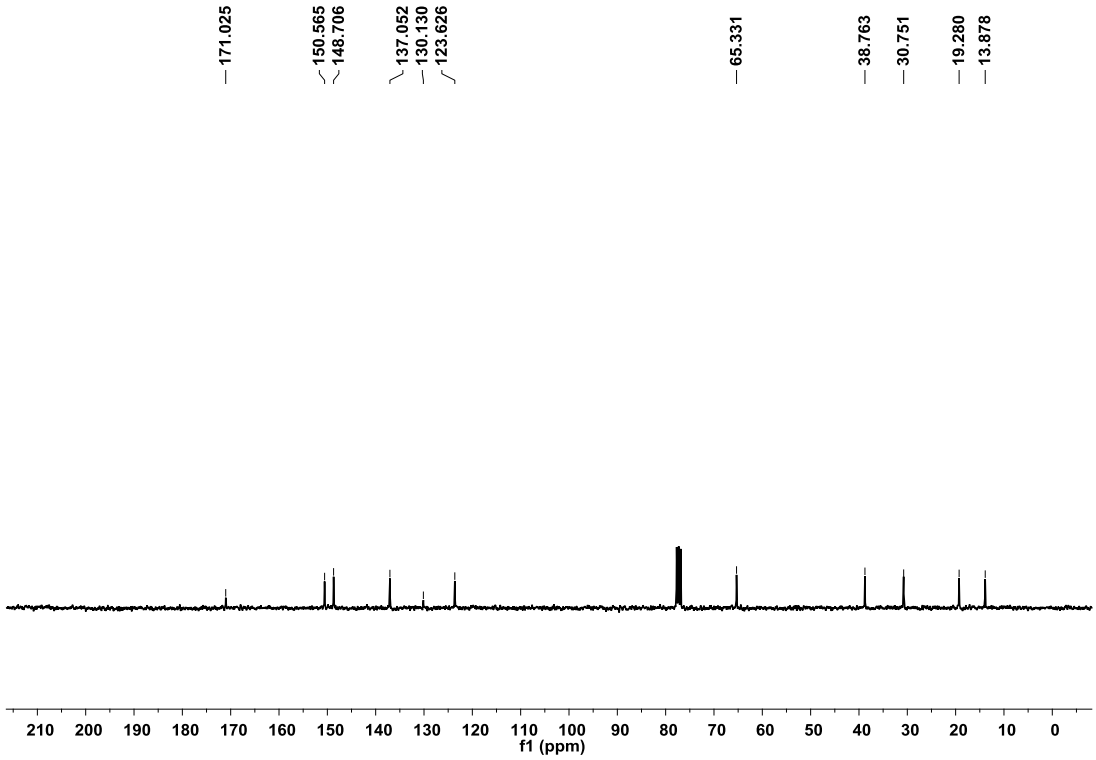
7.662
7.636
7.289
7.275
7.266
7.249
4.135
4.112
4.090
3.629
1.655
1.632
1.609
1.583
1.560
1.385
1.360
1.334
1.310
1.286
0.938
0.913
0.889
N
O
O^{n}Bu
1.95
0.86
1.04
2.00
1.94
2.16
2.08
3.21
f1 (ppm)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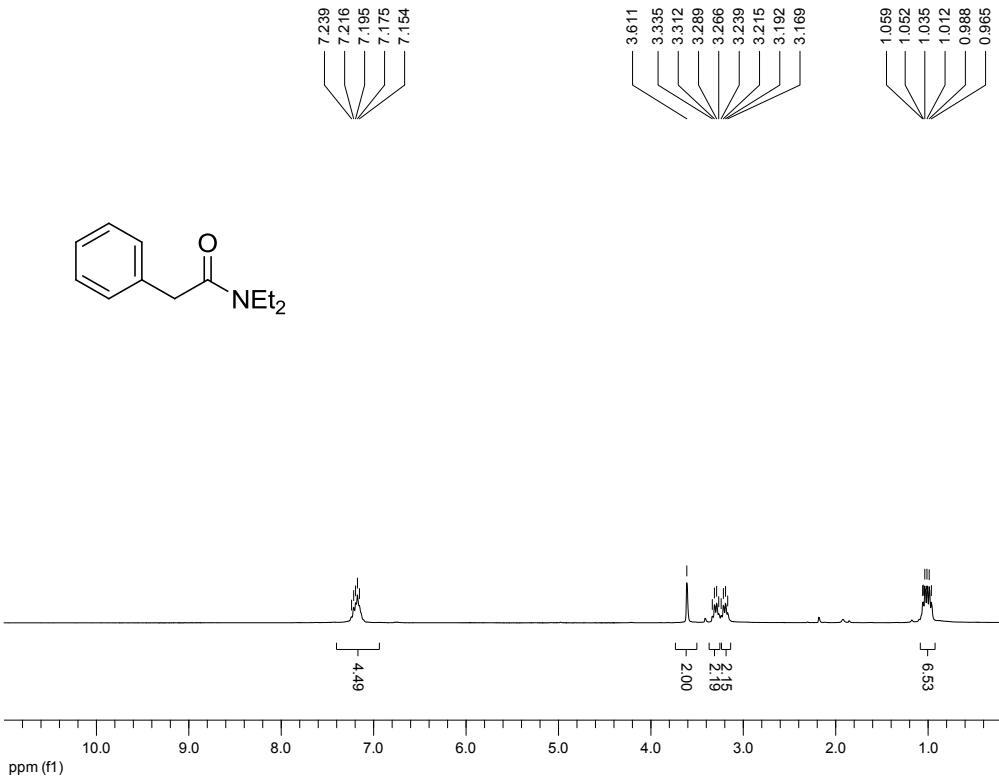
30.751
19.280
13.878
f1 (ppm)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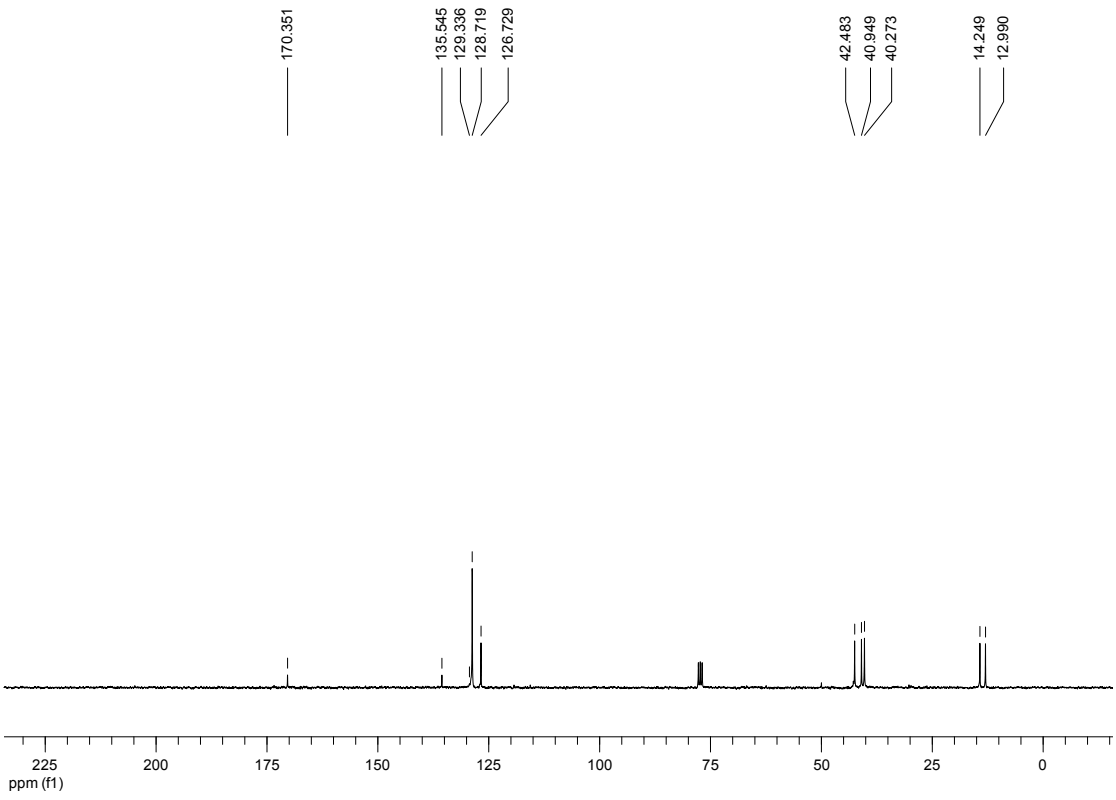
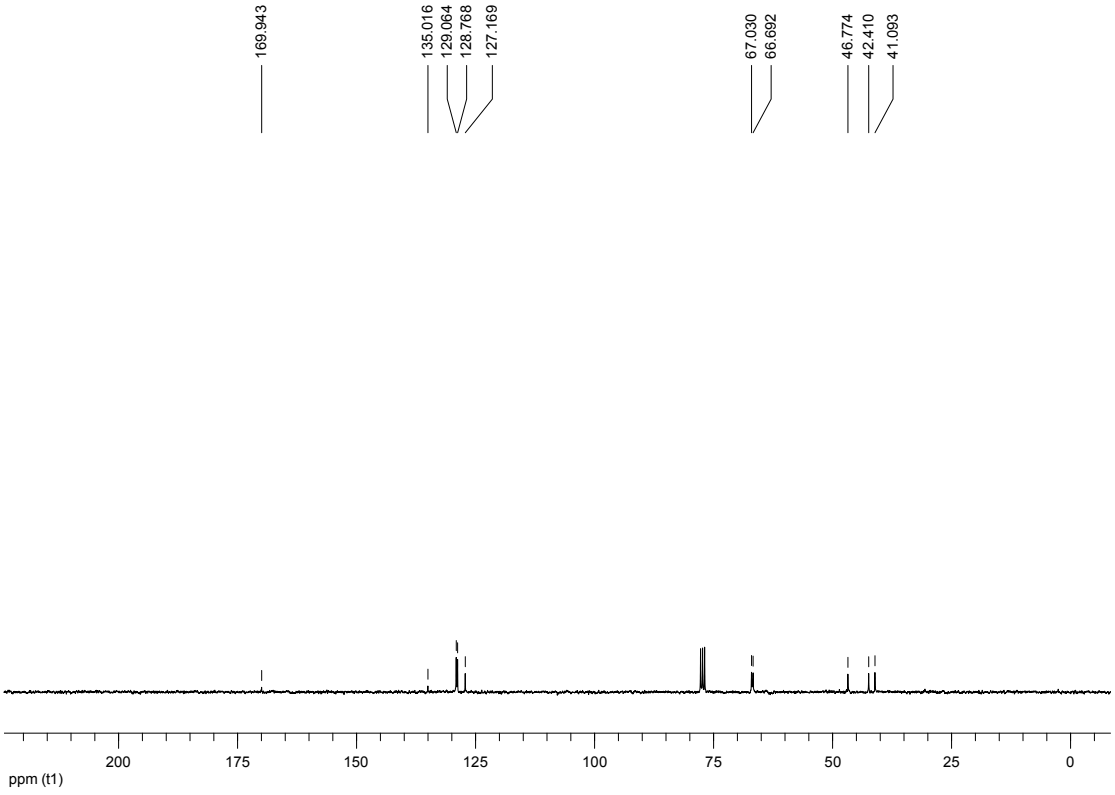
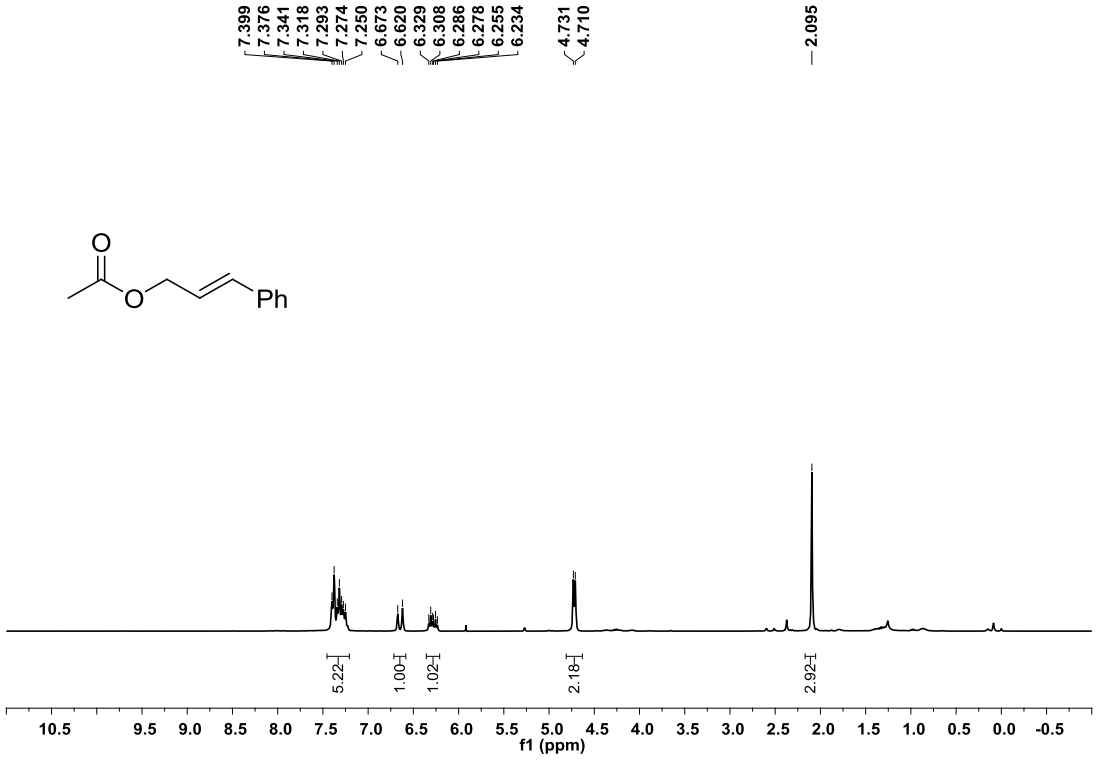
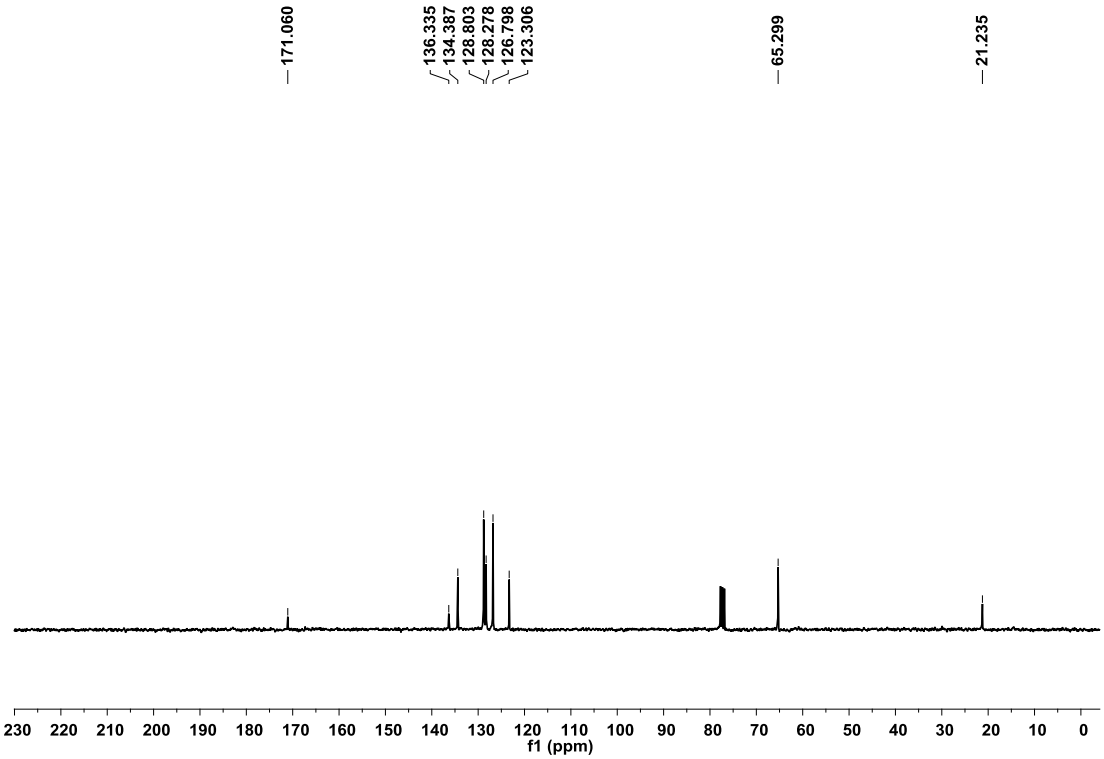
7.175
7.154
3.611
3.335
3.312
3.289
3.266
3.239
3.215
3.192
3.169
1.059
1.052
1.035
1.012
0.988
0.965
O
NEt2
4.49
2.00
2.15
2.19
9.53
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


170.351
135.545
129.336
128.719
126.729
42.483
40.949
40.273
14.249
12.990
225
200
175
150
125
100
75
50
25
0
ppm (f1)


7.271
7.247
7.223
7.189
7.168
7.144
3.654
3.590
3.563
3.384
3.363
O
N
O
3.97
2.86
3.92
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


169.943
135.016
129.064
128.768
127.169
67.030
66.692
46.774
42.410
41.093
200
175
150
125
100
75
50
25
0
ppm (t1)


7.399
7.376
7.341
7.318
7.293
7.274
7.250
6.673
6.620
6.329
6.308
6.286
6.278
6.255
6.234
4.731
4.710
2.095
O
O
Ph
5.22
1.00
1.02
2.18
2.92
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 -0.5
f1 (ppm)


171.060
136.335
134.387
128.803
128.278
126.798
123.306
65.299
21.235
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)