Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A general metal free approach to α-ketoamides via oxidative amidation-diketonization of terminal alkynes

*Ramesh Deshidi, Manjeet Kumar, Shekhar Devari and Bhahwal Ali Shah**

Academy of Scientific and Innovative Research (AcSIR); Natural Product Microbes, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu -Tawi, 180001.

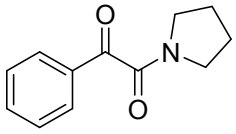
E-mail: bashah@iiim.res.in

General procedure for synthesis of α-ketoamides

TMSOTf (444 µl, 2mmol) was added to a solution of terminal alkyne (102 µL, 1mmol) in DMSO (1 ml) followed by the addition of iodine in catalytic amount and amine (1.5 mmol). The reaction mixture was then heated at 80 ^{o}C for 6 h and the product formation was monitored by TLC. After completion, reaction mixture was extracted with ethyl acetate (3 x 50ml). The combined organic layers were washed with brine solution, concentrated on rotary evaporator and purified by column chromatography using ethyl acetate and hexane to afford corresponding pure products.

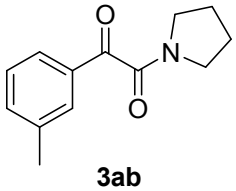
Note: Sometimes the TMSOTf evaporates during addition; in those cases further addition of TMSOTf may be required.

Spectroscopic Data:



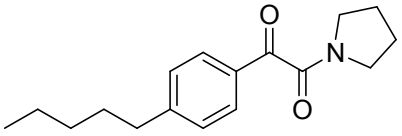
3aa

1-phenyl-2-(pyrrolidin-1-yl)ethane-1,2-dione (3aa): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.92 (m, 2H), 7.70 – 7.58 (m, 1H), 7.58 – 7.44 (m, 2H), 3.75 – 3.60 (m, 2H), 3.50 – 3.35 (m, 2H), 1.32 – 1.16 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 164.9, 134.5, 133.0, 129.8, 128.9, 46.6, 45.2, 25.9, 24.0.



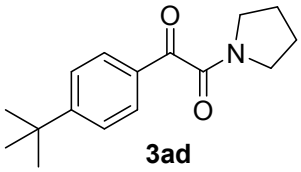
3ab

1-(pyrrolidin-1-yl)-2-(m-tolyl)ethane-1,2-dione (3ab): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 6.7 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 3.66 (t, *J* = 6.6 Hz, 2H), 3.42 (t, *J* = 6.4 Hz, 2H), 2.42 (s, 3H), 2.00 – 1.91 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 165.1, 138.9, 135.4, 133.0, 130.2, 128.8, 127.2, 46.7, 45.2, 25.9, 24.0.



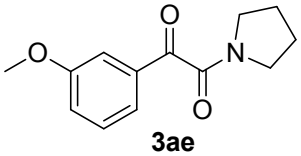
3ac

1-(4-pentylphenyl)-2-(pyrrolidin-1-yl)ethane-1,2-dione (3ac): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 3.66 (t, *J* = 6.6 Hz, 2H), 3.43 (t, *J* = 6.4 Hz, 2H), 2.67 (t, 2H), 1.95 (m, 2H), 1.63 (m, 4H), 1.37 – 1.27 (m, 6H), 0.89 (t, *J* = 4.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 165.2, 150.7, 130.7, 130.1, 129.0, 46.6, 45.2, 36.2, 31.4, 30.7, 25.9, 24.0, 22.5, 13.9.



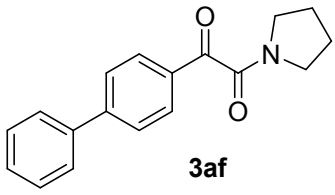
3ad

1-(4-(tert-butyl)phenyl)-2-(pyrrolidin-1-yl)ethane-1,2-dione (3ad); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 3.65 (t, *J* = 6.7 Hz, 2H), 3.42 (t, *J* = 6.4 Hz, 2H), 1.95 (m, 4H), 1.34 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.4, 165.2, 158.7, 130.3, 129.9, 125.9, 46.7, 45.2, 35.3, 31.0, 25.9, 24.0.



3ae

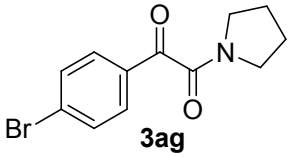
1-(3-methoxyphenyl)-2-(pyrrolidin-1-yl)ethane-1,2-dione (3ae); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.47 (m, 2H), 7.39 (dd, *J* = 18.4, 10.7 Hz, 1H), 7.17 (dt, *J* = 15.6, 7.9 Hz, 1H), 3.86 (d, *J* = 4.9 Hz, 3H), 3.65 (t, *J* = 6.7 Hz, 2H), 3.48 – 3.36 (m, 2H), 2.08 – 1.88 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 164.9, 160.0, 134.2, 130.0, 123.1, 121.5, 112.9, 55.5, 46.6, 45.2, 25.9, 24.0.



3af

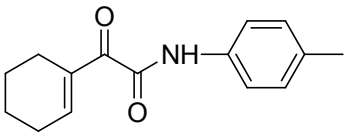
1-([1,1'-biphenyl]-4-yl)-2-(pyrrolidin-1-yl)ethane-1,2-dione (3af); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.56 (m, 2H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.3,

1H), 3.60 (t, *J* = 6.8 Hz, 2H), 3.39 (t, *J* = 6.6 Hz, 2H), 1.89 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191, 164.9, 147.3, 139.6, 131.7, 130.5, 129.02, 128.5, 127.6, 127.3, 46.7, 45.3, 25.9, 24.0.



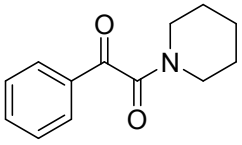
3ag

1-(4-bromophenyl)-2-(pyrrolidin-1-yl)ethane-1,2-dione (3ag); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.79 (m, 2H), 7.72 – 7.57 (m, 2H), 3.64 (t, *J* = 7.0 Hz, 2H), 3.44 (dd, *J* = 8.1, 5.3 Hz, 2H), 2.06 – 1.88 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 164.2, 132.3, 131.7, 131.3, 130.1, 46.8, 45.4, 25.9, 24.0.



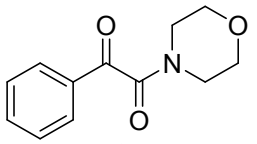
3ah

2-(cyclohex-1-en-1-yl)-2-oxo-N-(p-tolyl)acetamide: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (ddd, *J* = 5.6, 4.1, 1.6 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.19 – 7.13 (m, 2H), 2.42 – 2.26 (m, 7H), 1.76 – 1.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.7, 159.4, 151.0, 135.6, 134.7, 134.2, 129.6, 119.8, 26.9, 23.3, 21.7, 21.2.



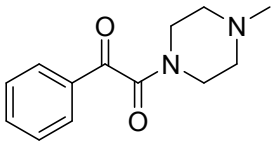
3ba

1-phenyl-2-(piperidin-1-yl)ethane-1,2-dione (3ba) : ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.90 (m, 2H), 7.71 – 7.59 (m, 1H), 7.56 – 7.46 (m, 2H), 3.70 (d, *J* = 5.5 Hz, 2H), 3.40 – 3.24 (m, 2H), 1.77 – 1.66 (m, 4H), 1.57 (dd, *J* = 17.4, 12.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 165.4, 134.5, 133.3, 129.5, 128.9, 47.0, 42.1, 26.2, 25.4, 24.4.



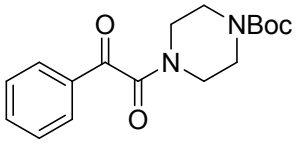
3ca

1-morpholino-2-phenylethane-1,2-dione (3ca): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.90 (m, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 3.81 (d, *J* = 6.4 Hz, 4H), 3.70 – 3.60 (m, 2H), 3.47 – 3.31 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 165.4, 134.9, 133.0, 129.6, 129.1, 66.6, 66.6, 46.2, 41.5.



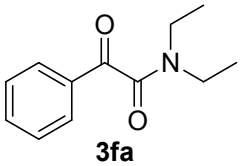
3da

1-(4-methylpiperazin-1-yl)-2-phenylethane-1,2-dione (3da): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.90 (m, 2H), 7.77 – 7.58 (m, 1H), 7.52 (dd, *J* = 10.7, 4.7 Hz, 2H), 3.91 – 3.76 (m, 2H), 3.46 – 3.32 (m, 2H), 2.64 – 2.47 (m, 2H), 2.40 (dd, *J* = 17.6, 12.5 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.56, 165.34, 134.81, 133.08, 129.55, 129.04, 54.81, 54.36, 45.83, 45.68, 41.04.



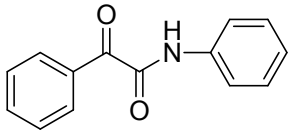
3ea

***tert*-butyl 4-(2-oxo-2-phenylacetyl)piperazine-1-carboxylate (3ea):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.92 (m, 2H), 7.68 – 7.61 (m, 1H), 7.55 – 7.49 (m, 2H), 3.83 – 3.70 (m, 2H), 3.66 – 3.53 (m, 2H), 3.50 – 3.40 (m, 2H), 3.37 – 3.29 (m, 2H), 1.52 – 1.44 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 165.6, 154.4, 130.0, 129.6, 129.1, 128.5, 128.3, 80.6, 45.7, 41.2, 28.3.



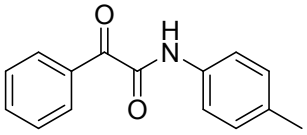
3fa

N,N-diethyl-2-oxo-2-phenylacetamide (3fa): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.81 (m, 2H), 7.70 – 7.54 (m, 1H), 7.56 – 7.39 (m, 2H), 3.57 (q, *J* = 7.2 Hz, 2H), 3.25 (q, *J* = 7.1 Hz, 2H), 1.38 – 1.20 (m, 3H), 1.20 – 1.05 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 166.7, 134.5, 130.1, 129.6, 128.9, 128.4, 42.1, 38.8, 14.1, 12.8.



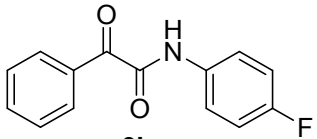
3ga

2-oxo-N,2-diphenylacetamide (3ga): ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (t, *J* = 11.5 Hz, 2H), 7.69 (t, *J* = 9.8 Hz, 2H), 7.62 (dt, *J* = 8.4, 5.7 Hz, 1H), 7.56 – 7.45 (m, 2H), 7.44 – 7.33 (m, 2H), 7.23 – 7.15 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.4, 158.9, 136.6, 134.6, 133.0, 131.5, 129.2, 128.6, 125.3, 119.9.



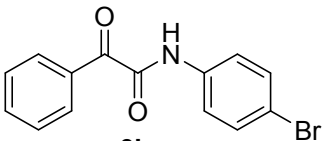
3ha

2-oxo-2-phenyl-N-(p-tolyl)acetamide (3ha): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.47 – 8.33 (m, 2H), 7.67 – 7.60 (m, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 2.34 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 187.5, 158.8, 135.0, 134.5, 134.1, 133.2, 131.5, 129.7, 128.5, 119.9, 20.9.



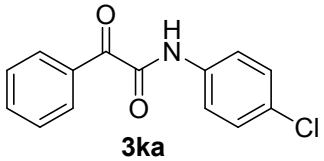
3ia

N-(4-fluorophenyl)-2-oxo-2-phenylacetamide (3ia): ^{1}H NMR (500 MHz, $CDCl_3$) 8.39 (d, *J* = 7.7 Hz, 2H), 7.73 – 7.61 (m, 3H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.08 (t, *J* = 8.6 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.3, 160.8, 158.9, 134.7, 133.0, 132.7, 131.5, 128.6, 121.7, 116.1, 115.9.



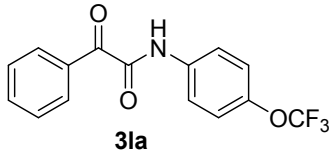
3ja

N-(4-bromophenyl)-2-oxo-2-phenylacetamide (3ja): ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.8 Hz, 2H), 7.66 (t, *J* = 6.4 Hz, 1H), 7.59 (t, *J* = 13.5 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.0, 158.8, 135.7, 134.8, 132.9, 132.2, 131.5, 128.6, 121.4, 118.0.



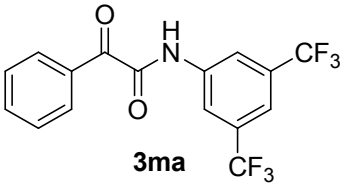
3ka

N-(4-chlorophenyl)-2-oxo-2-phenylacetamide (3ka): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.28 (m, 2H), 7.77 – 7.63 (m, 3H), 7.59 – 7.40 (m, 2H), 7.16 – 7.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.2, 161.1, 158.7, 134.7, 131.4, 128.5, 121.7, 121.6, 116.1, 115.8



3la

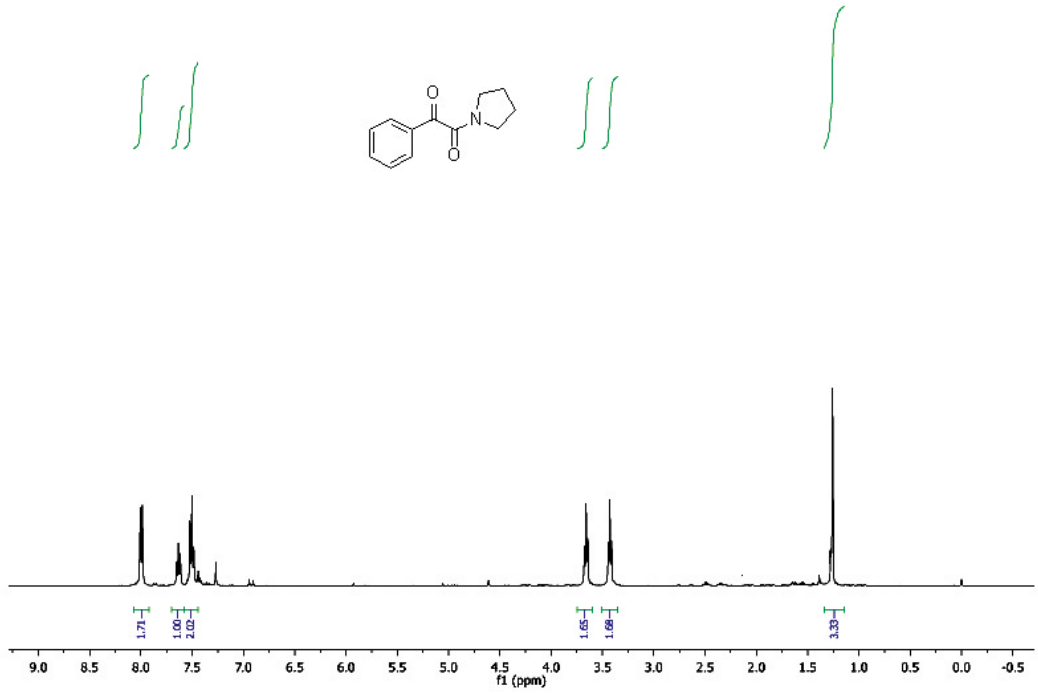
2-oxo-2-phenyl-N-(4-(trifluoromethoxy)phenyl)acetamide (3la): ^{1}H NMR (400 MHz, $CDCl_3$) 8.38 – 8.23 (m, 2H), 7.69 – 7.63 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.19 – 7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.1, 158.9, 145.9, 135.3, 134.8, 132.9, 131.5, 128.6, 121.9, 121.5, 121.2, 119.4.

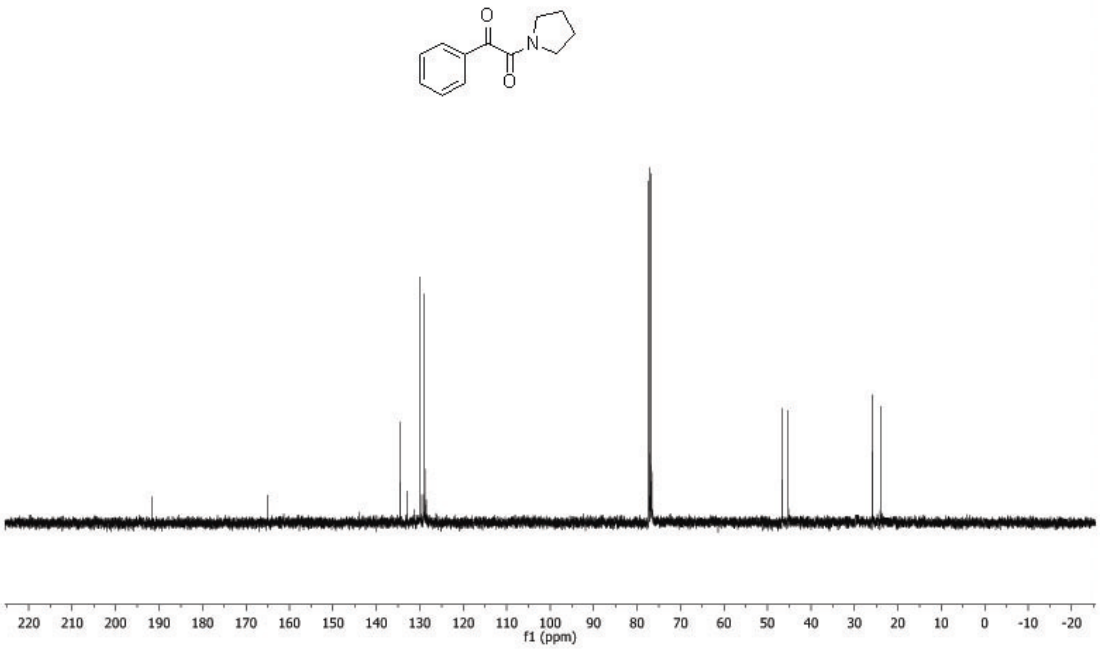


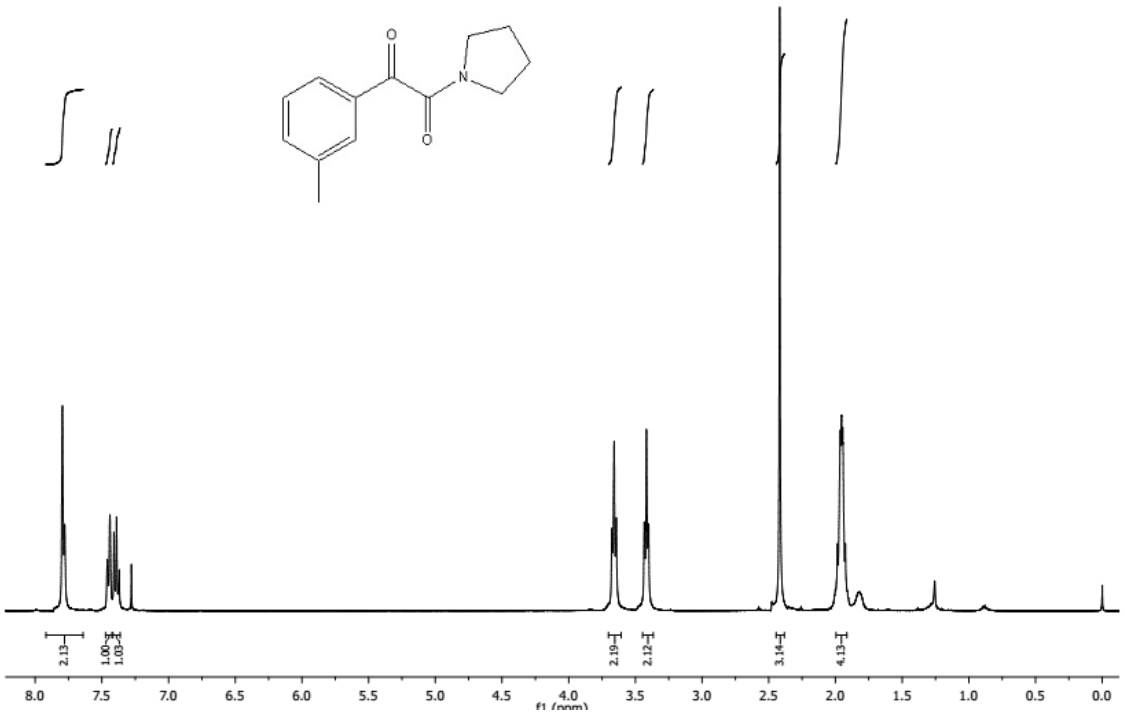
3ma

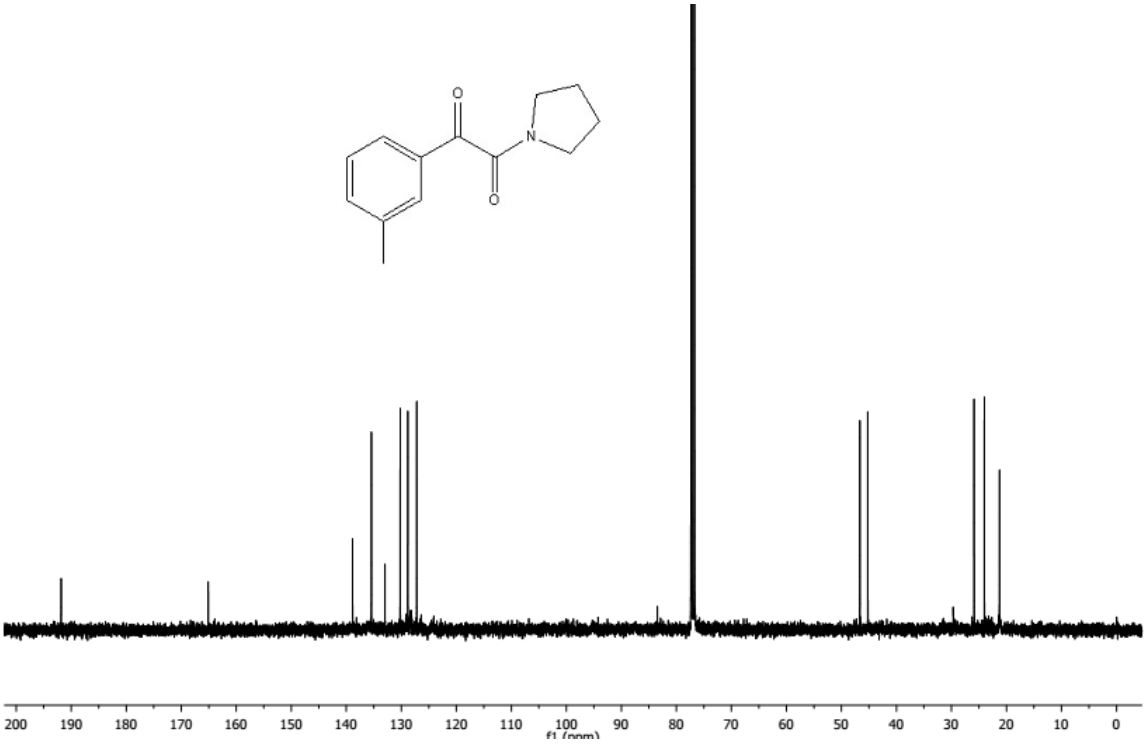
N-(3,5-bis(trifluoromethyl)phenyl)-2-oxo-2-phenylacetamide (3ma): ^{1}H NMR (400 MHz, $CDCl_3$) 8.42 (d, *J* = 7.7 Hz, 2H), 8.24 (s, 2H), 7.69 (d, *J* = 11.3 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.4, 159.1, 138.1, 135.2, 132.8, 132.5, 131.5, 128.8, 124.1, 121.8, 119.7, 118.5.

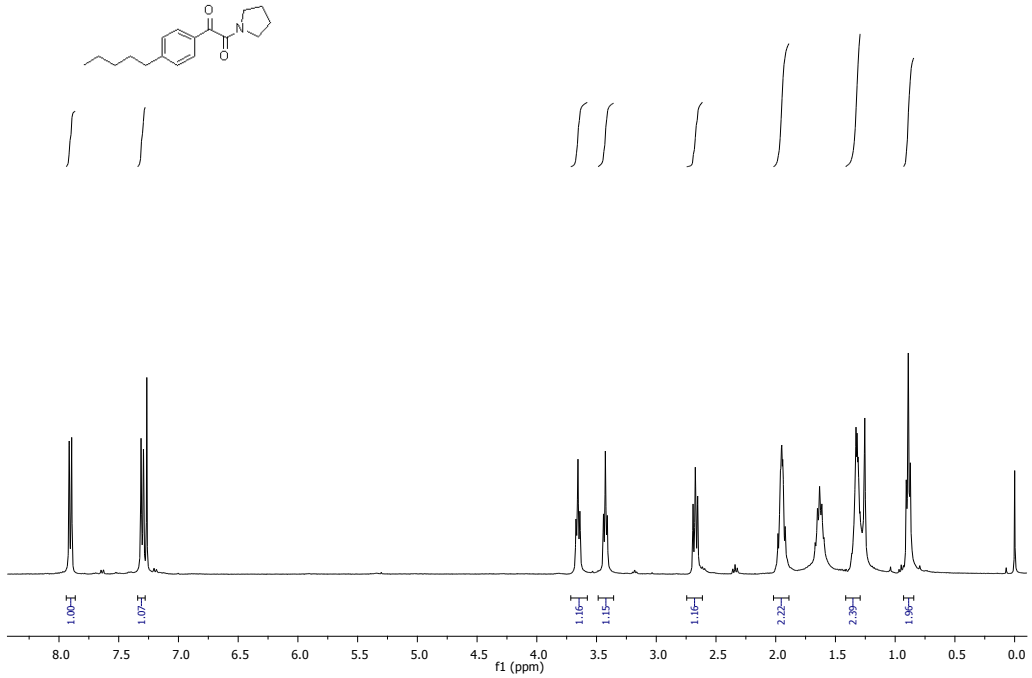
Spectral Graphs

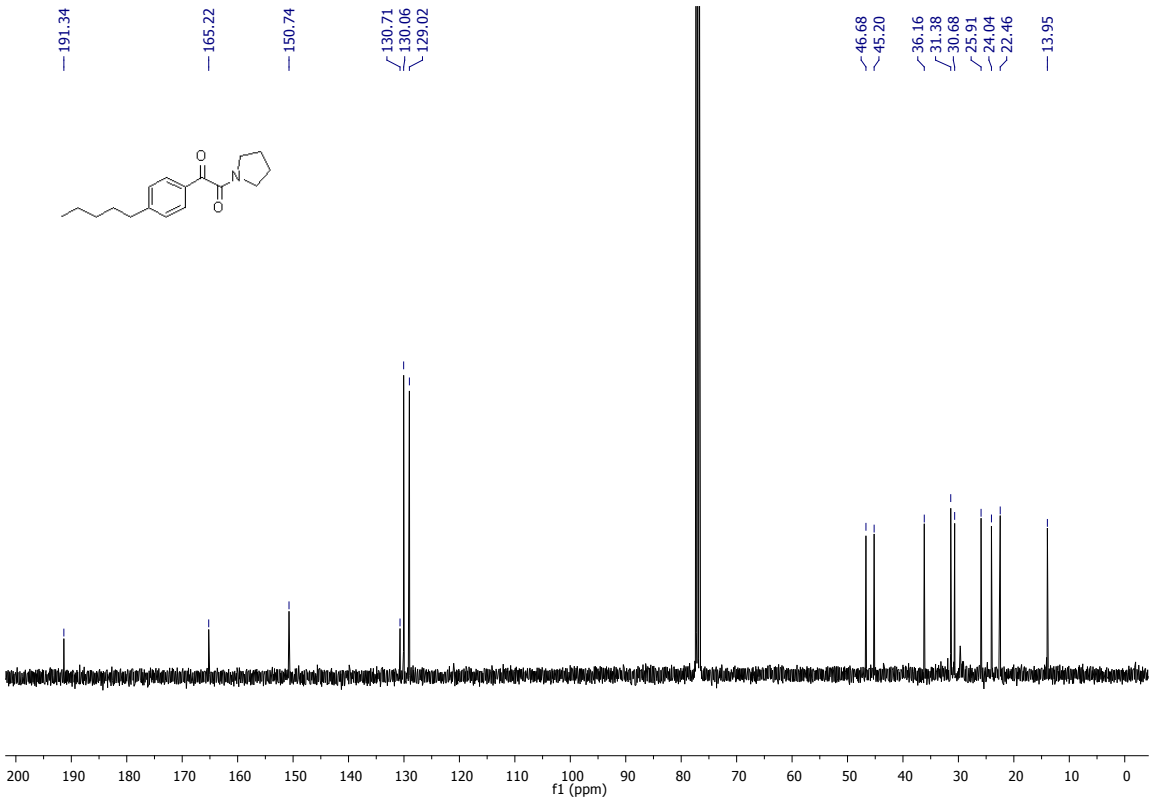


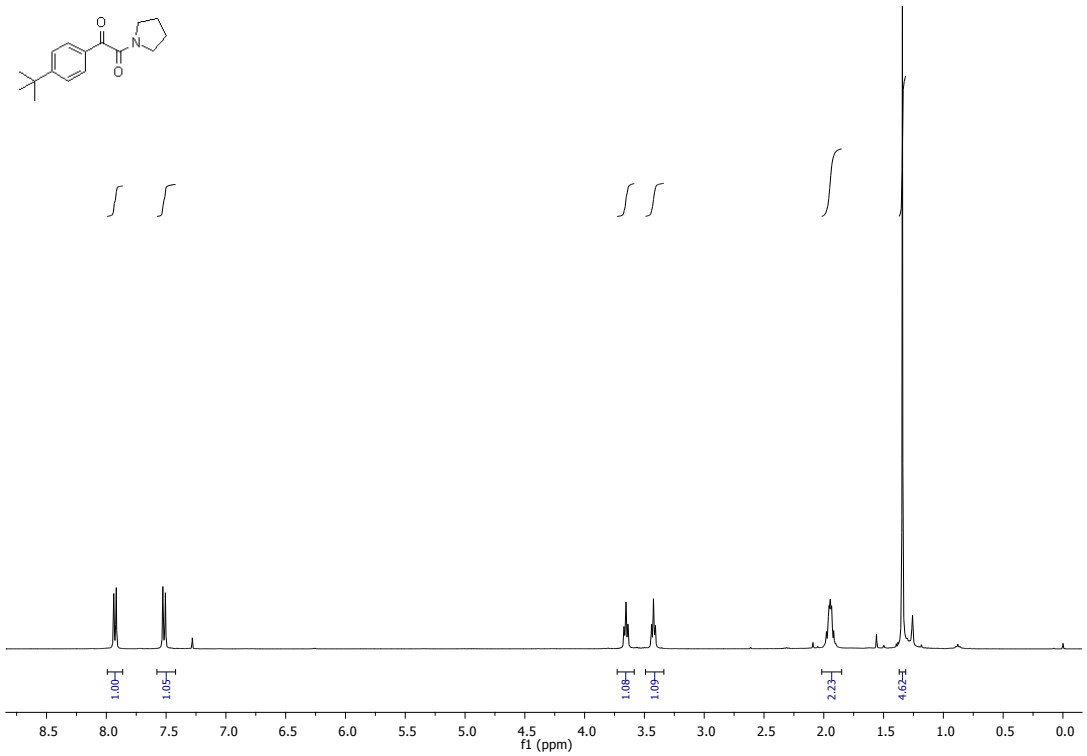


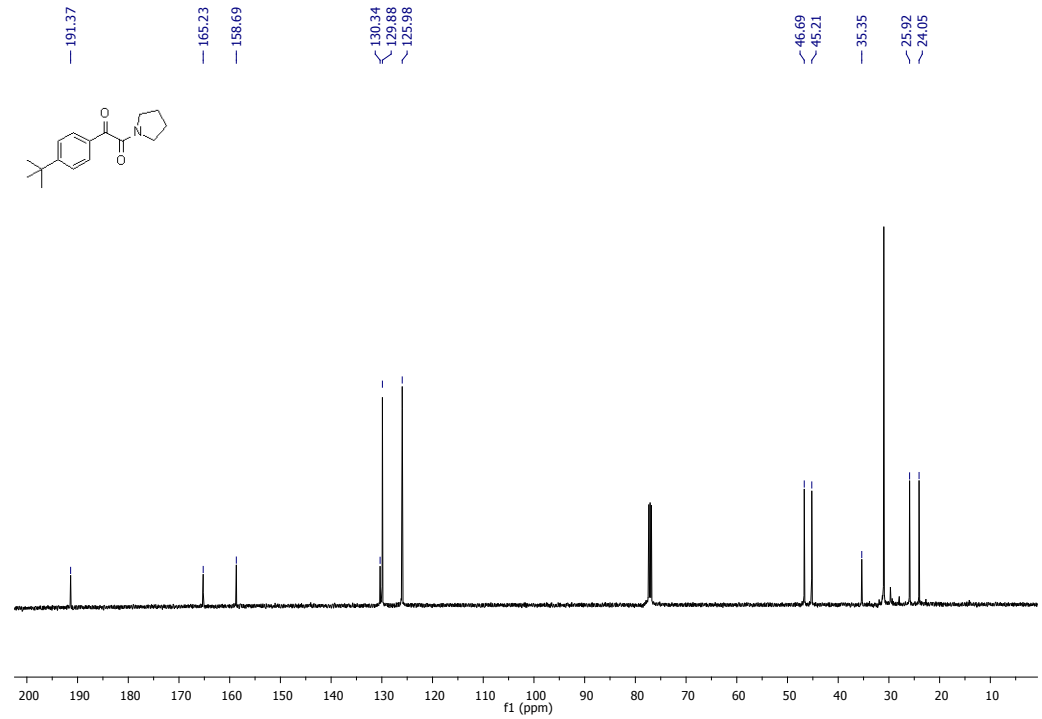

O
N
O
2.13
1.00
1.03
2.19
2.12
3.14
4.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

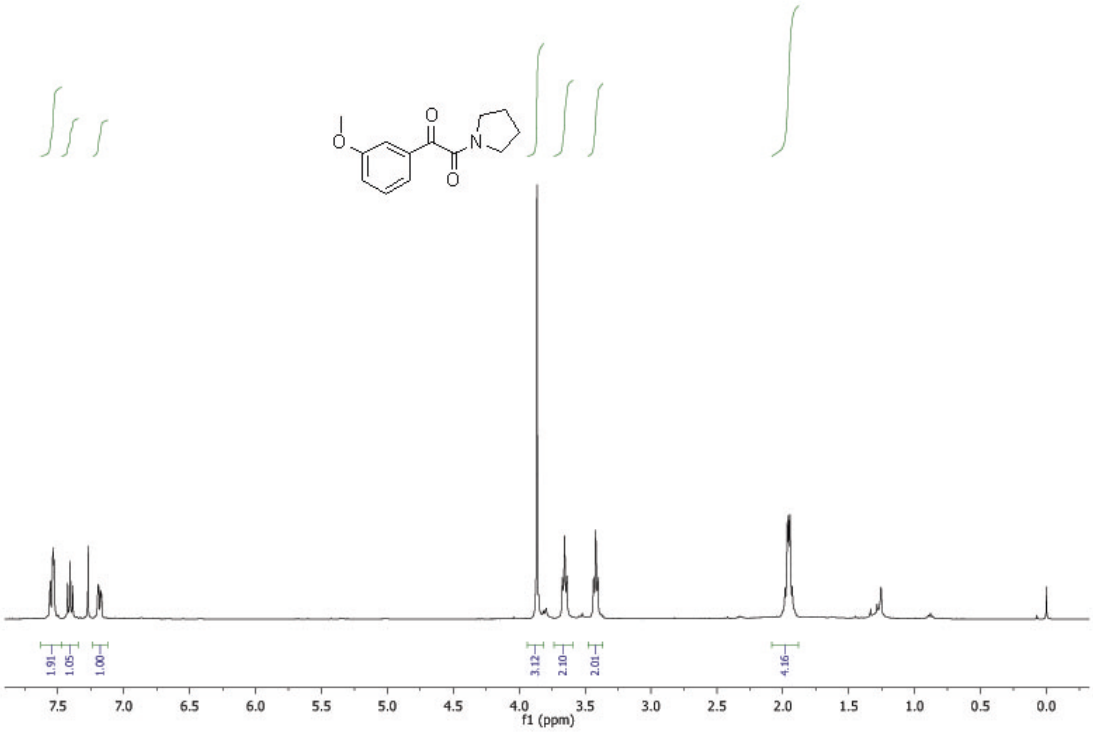

O
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

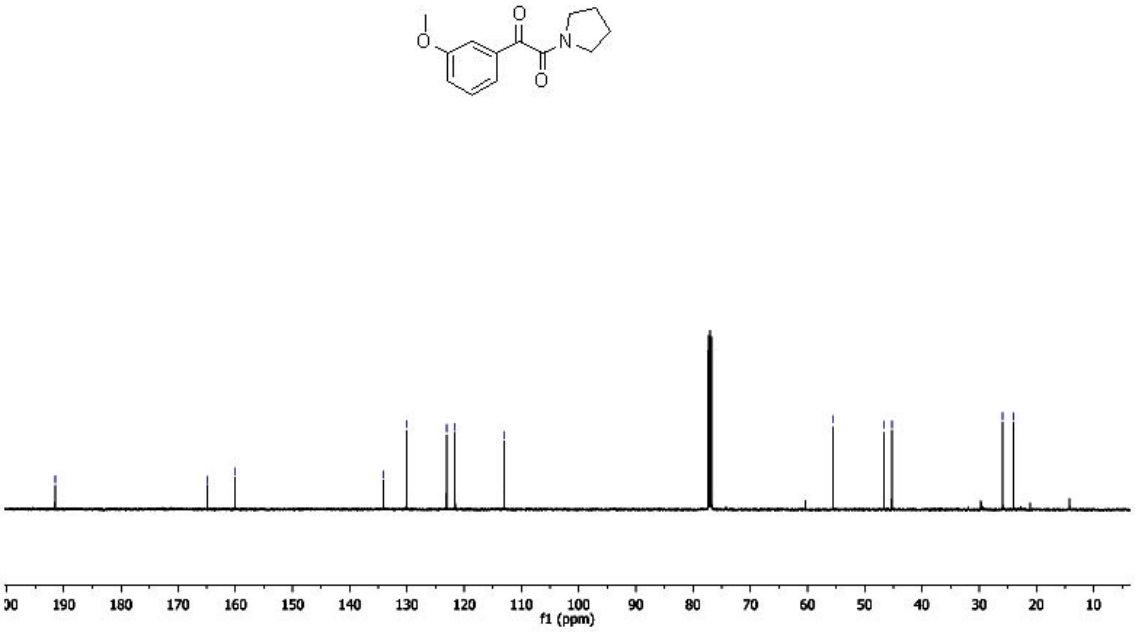

1.00
1.07
1.16
1.15
1.16
2.22
2.39
1.96
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

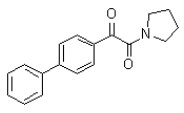

191.34
165.22
150.74
130.71
130.06
129.02
46.68
45.20
36.16
31.38
30.68
25.91
24.04
22.46
13.95
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

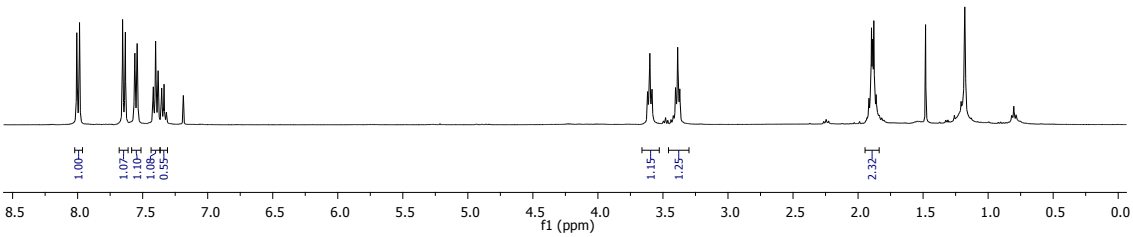

1.00
1.05
1.08
1.09
2.23
4.62
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


191.37
165.23
158.69
130.34
129.88
125.98
46.69
45.21
35.35
25.92
24.05
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

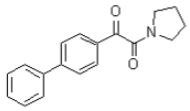

O
O
N
O
1.91
1.05
1.00
3.12
2.10
2.01
4.16
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

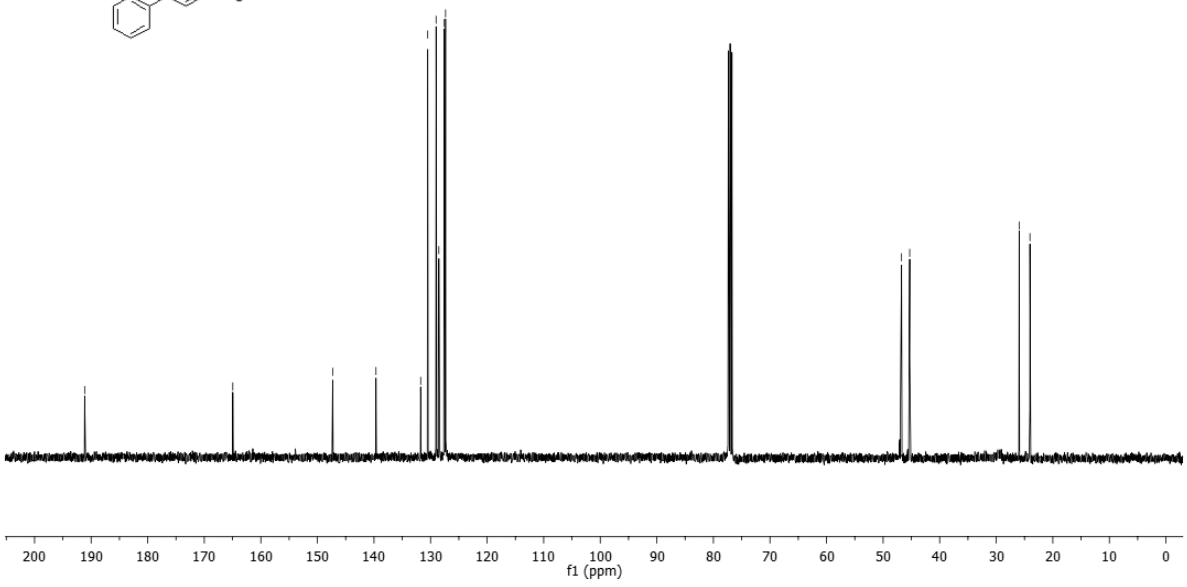

O
O
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

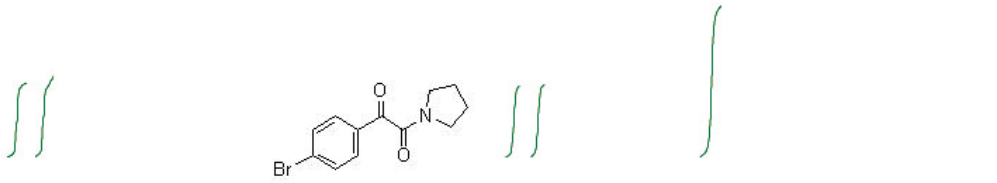

O
N
O

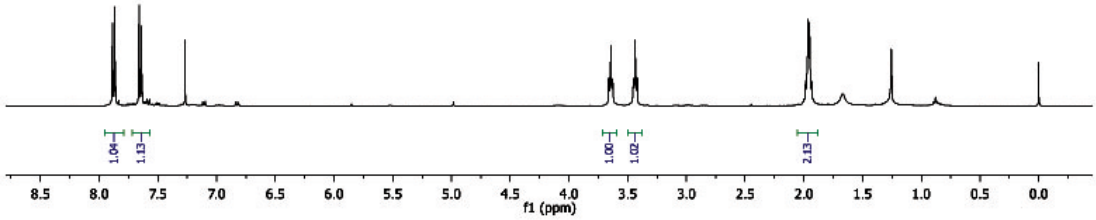

1.00
1.07
1.10
1.08
0.55
1.15
1.25
2.32
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

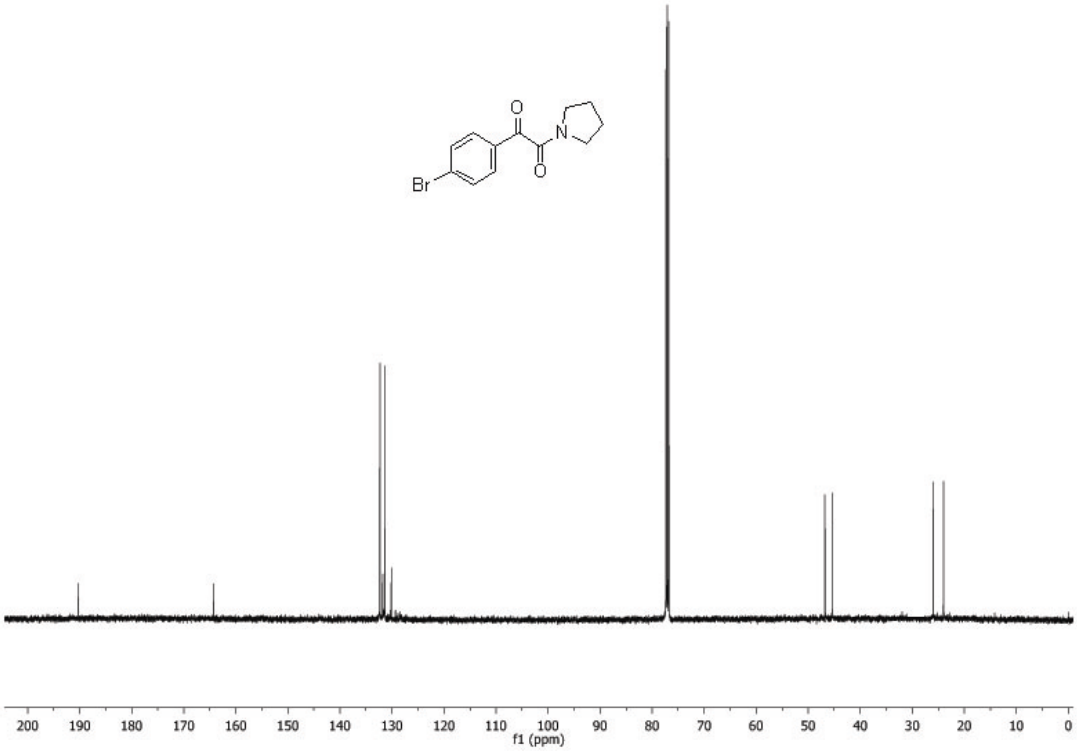

191.14
164.96
147.30
139.65
131.75
130.50
129.02
128.53
127.57
127.35
46.74
45.30
25.94
24.04

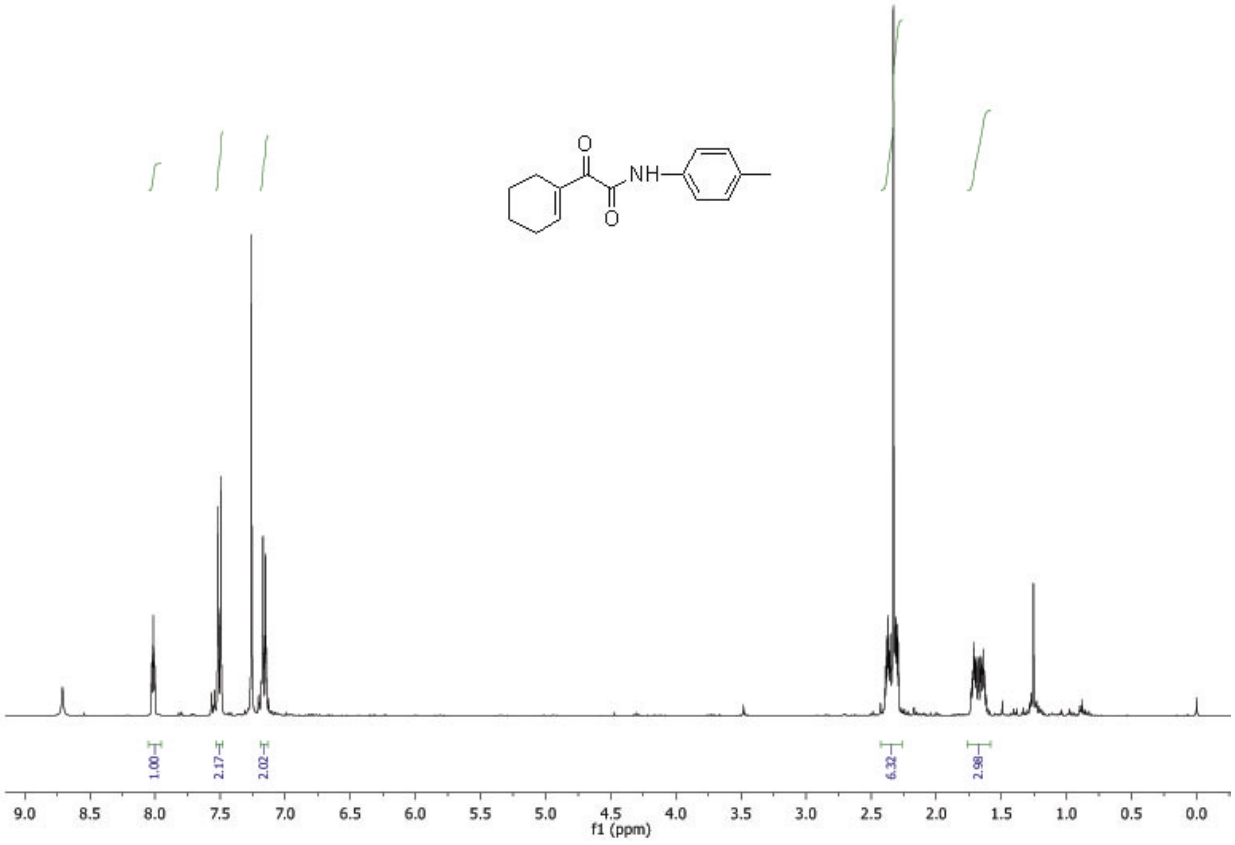

O
N
O

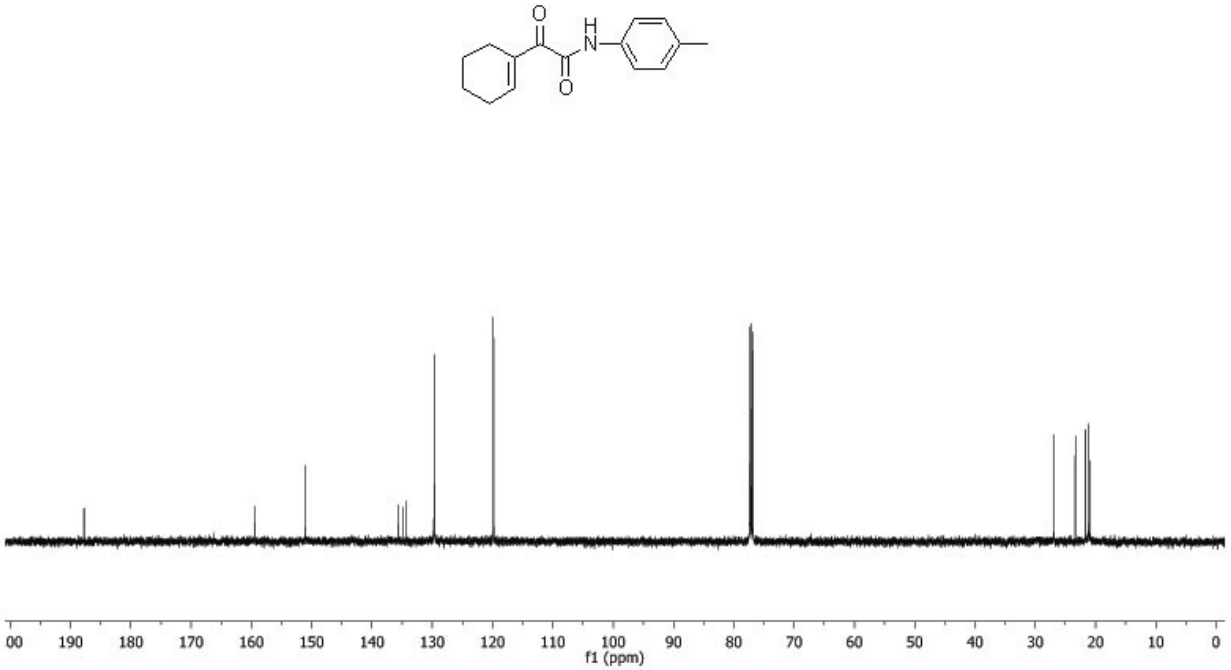

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

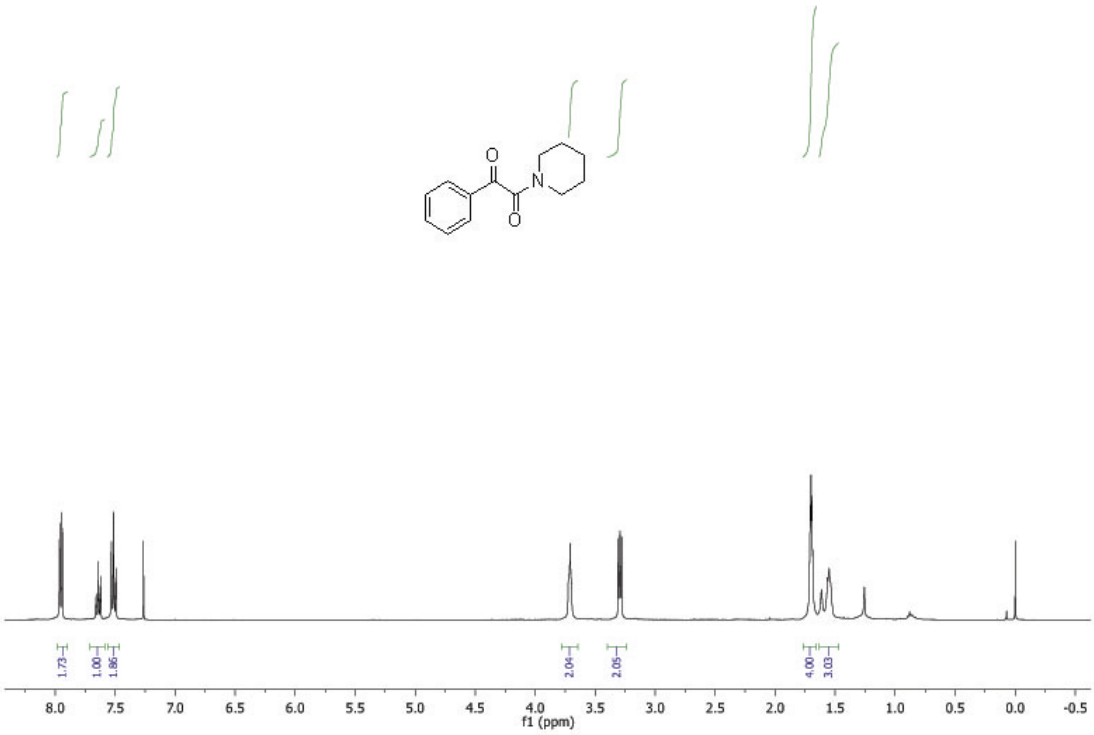

O
N
O
Br

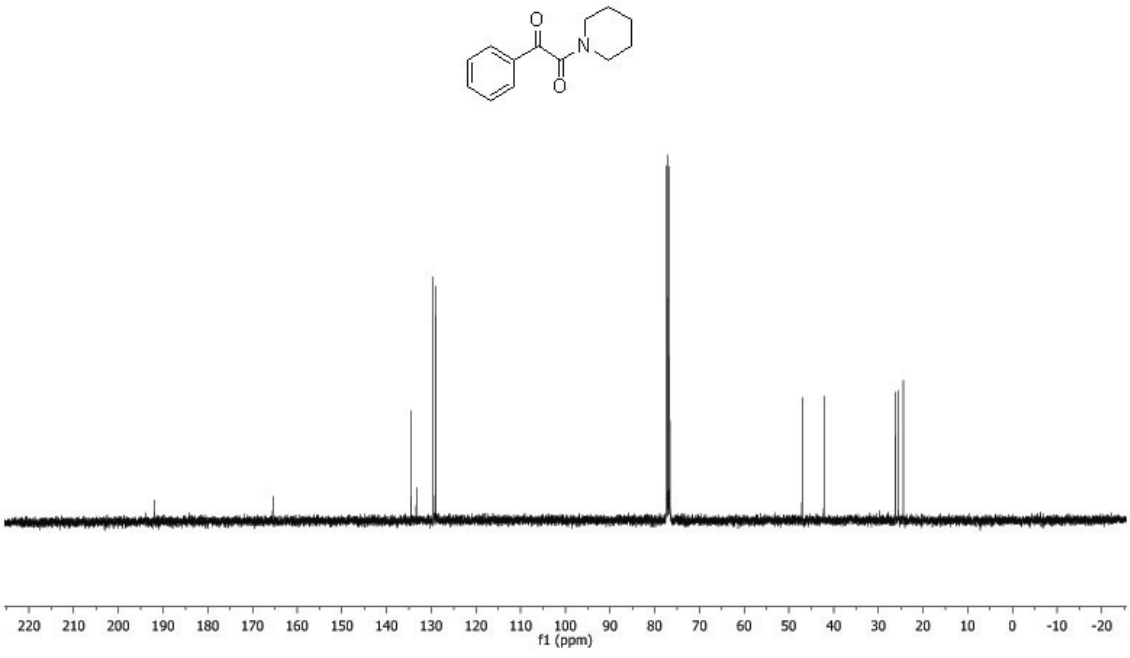

1.04
1.13
1.00
1.02
2.13
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

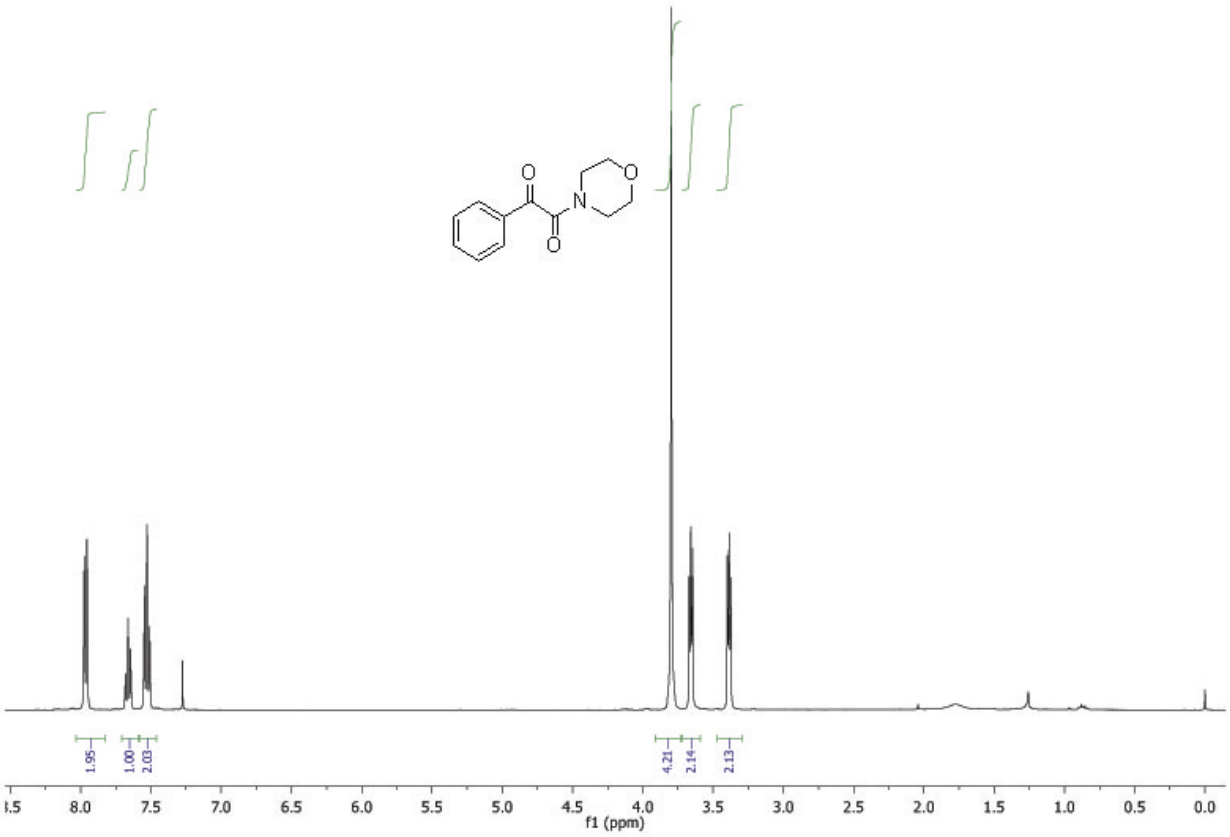

O
N
O
Br
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

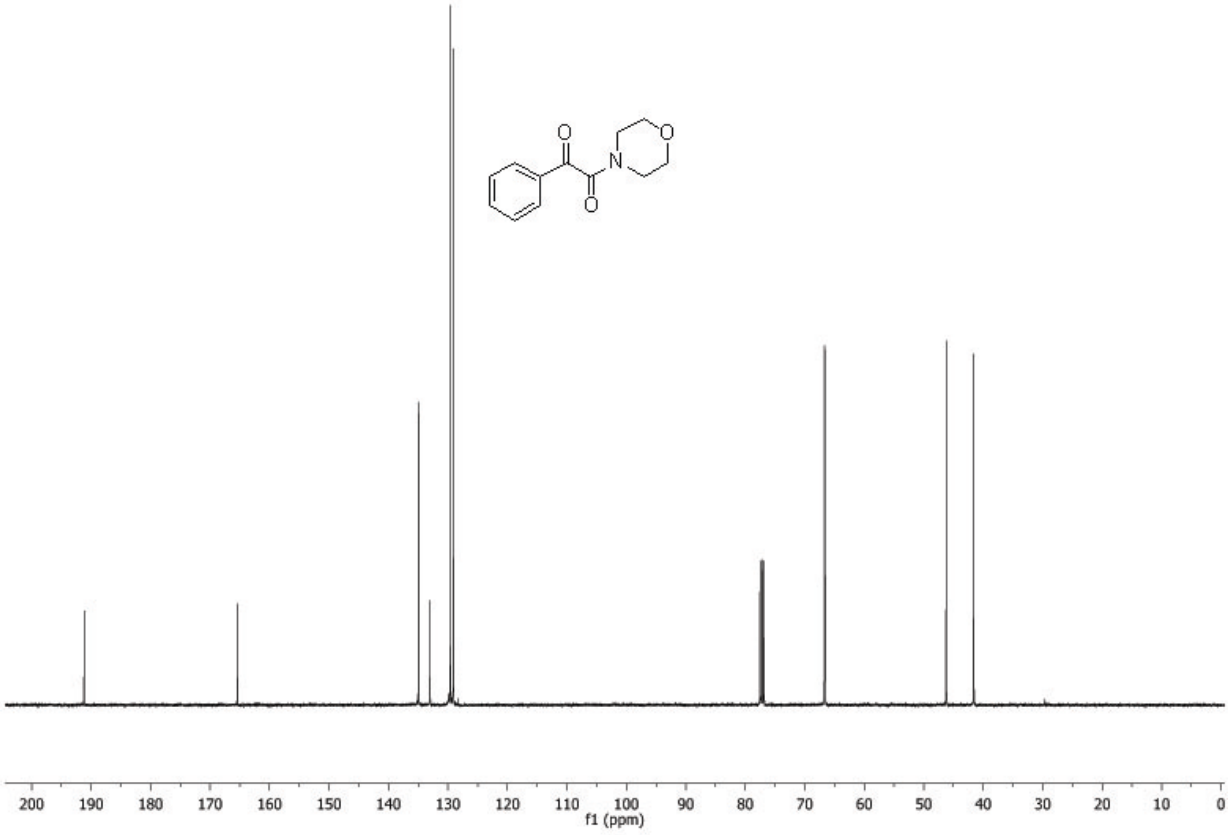

O
NH
O
1.00
2.17
2.02
6.32
2.98
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

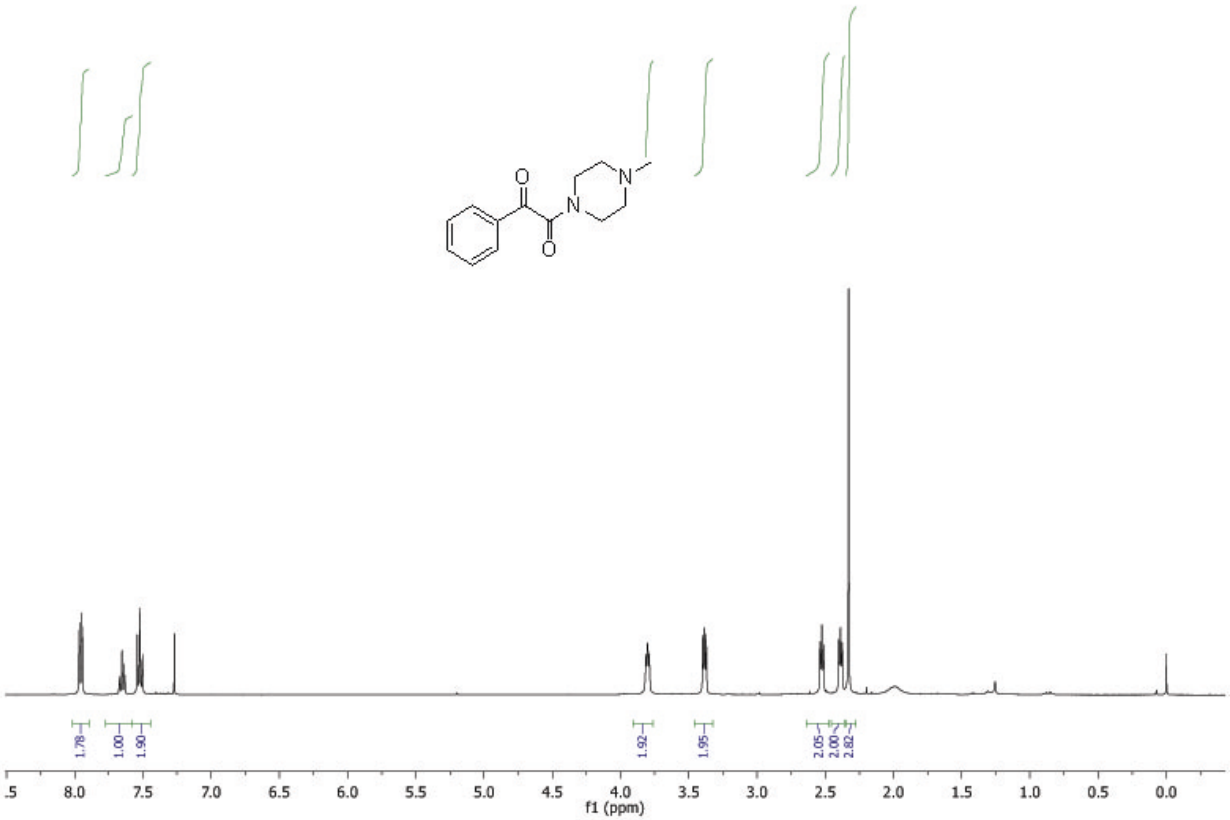

O
H
N
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

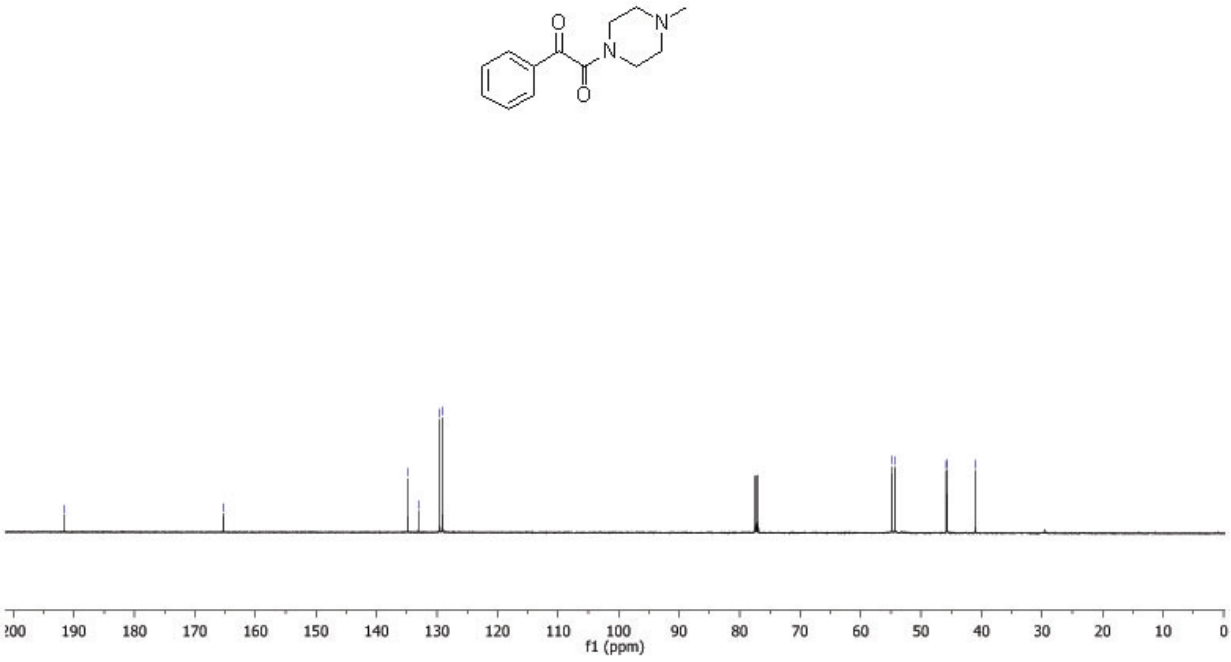

O
N
O
1.73
1.00
1.86
2.04
2.05
4.00
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

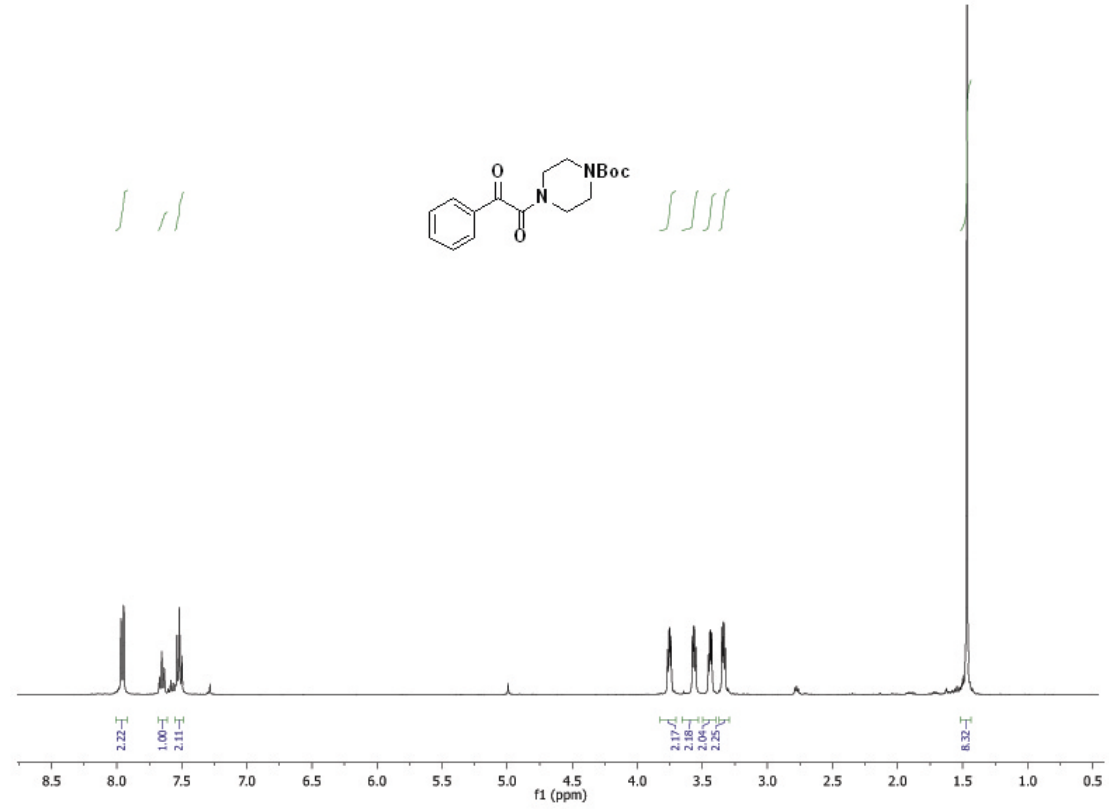

O
N
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

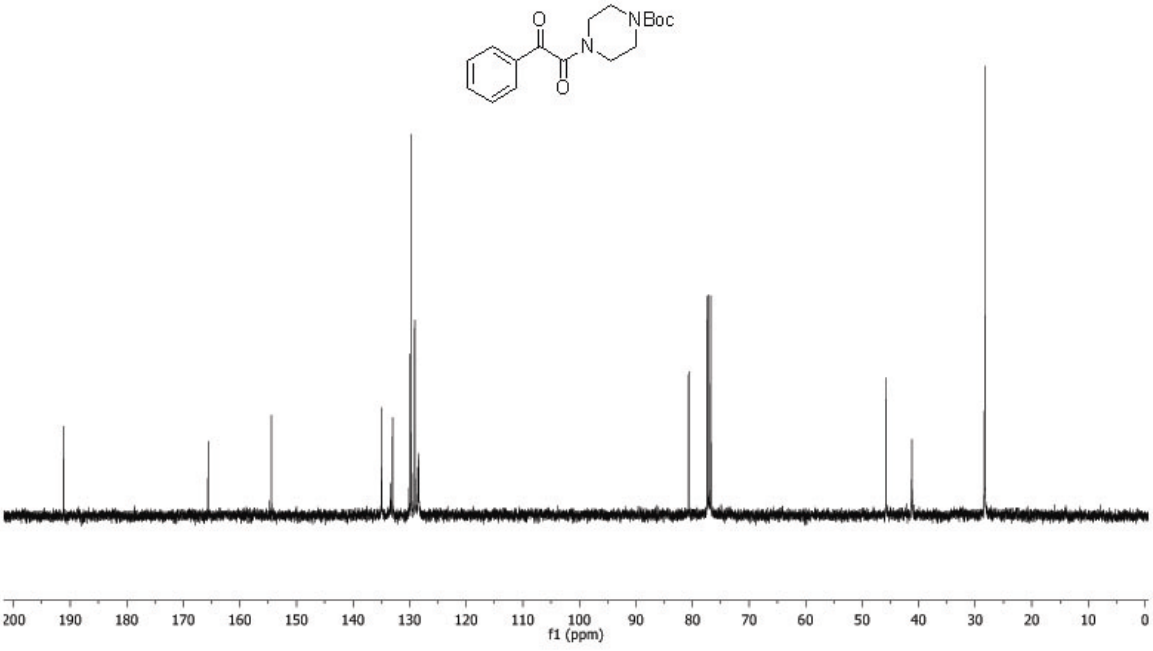

1.95
1.00
2.03
4.21
2.14
2.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

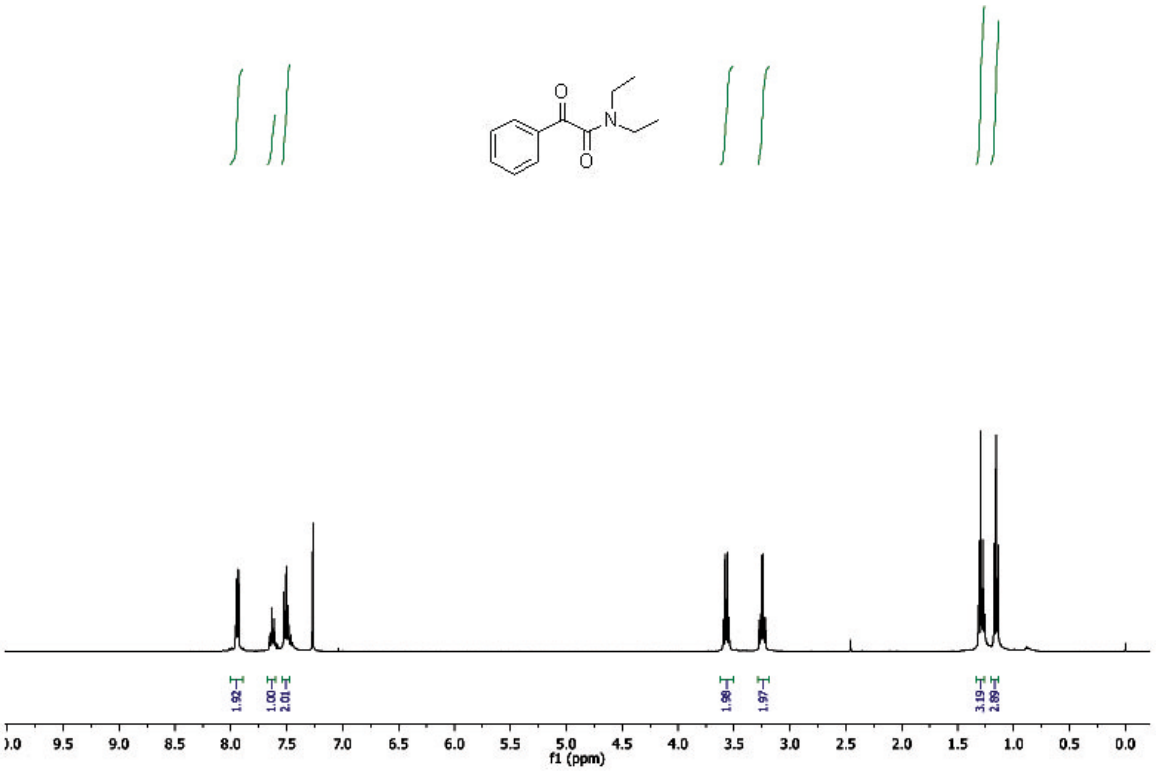

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

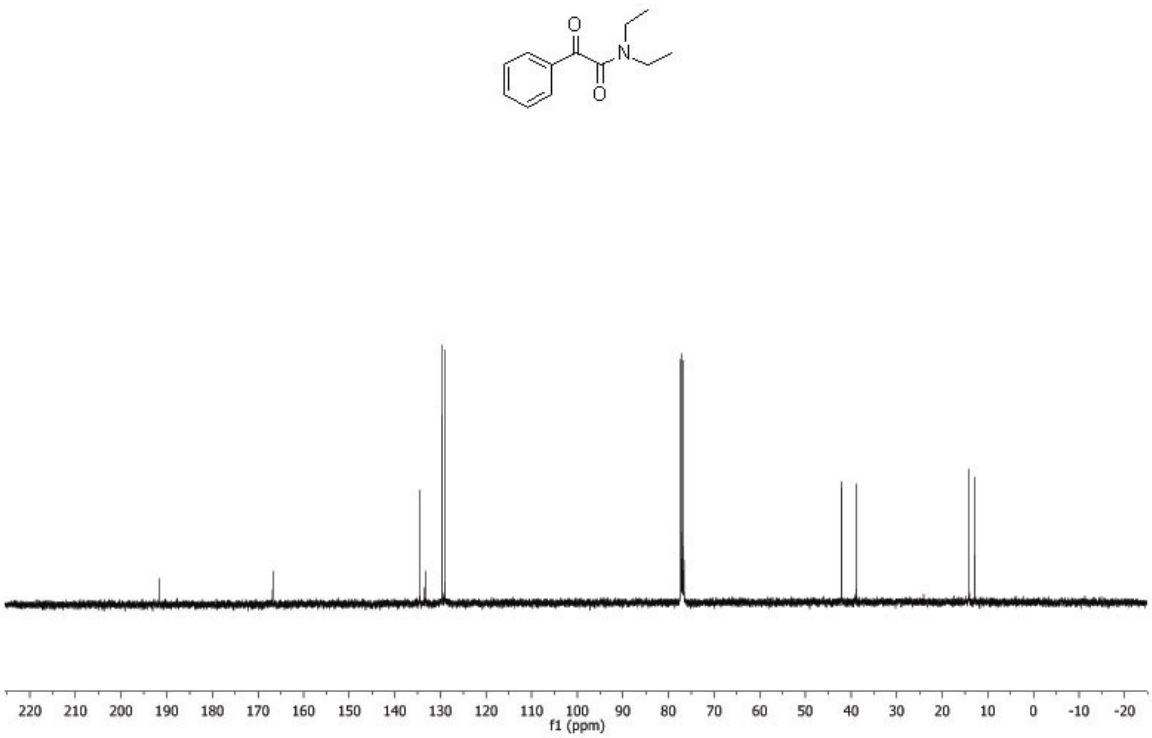

O
N
N
O
1.78
1.00
1.90
1.92
1.95
2.05
2.00
2.82
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

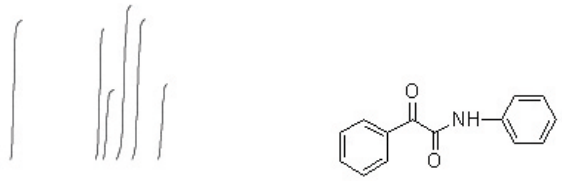

O
N
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

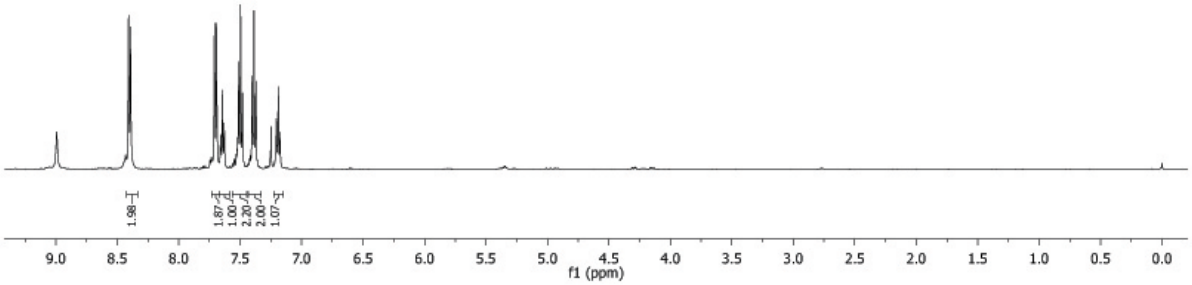

O
NBoc
N
O
2.22
1.00
2.11
2.17
2.18
2.04
2.25
8.32
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

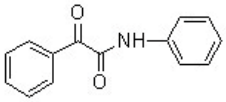

O
NBoc
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

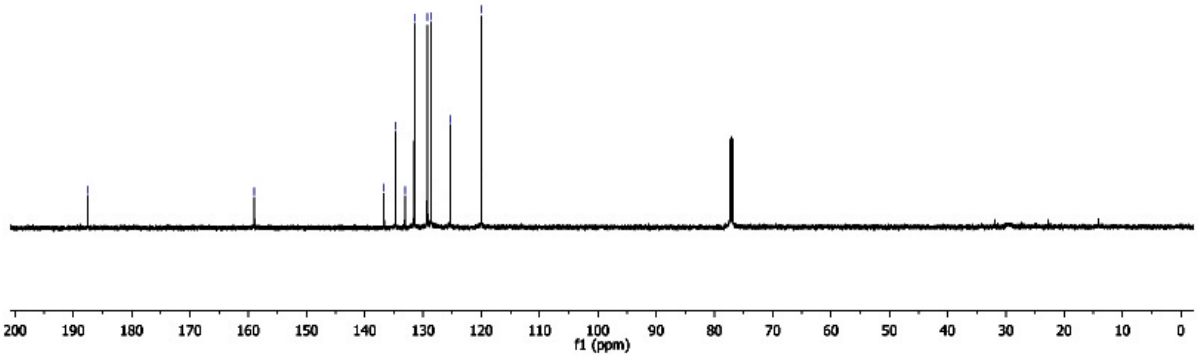

1.92
1.00
2.01
1.98
1.97
3.19
2.89
f1 (ppm)

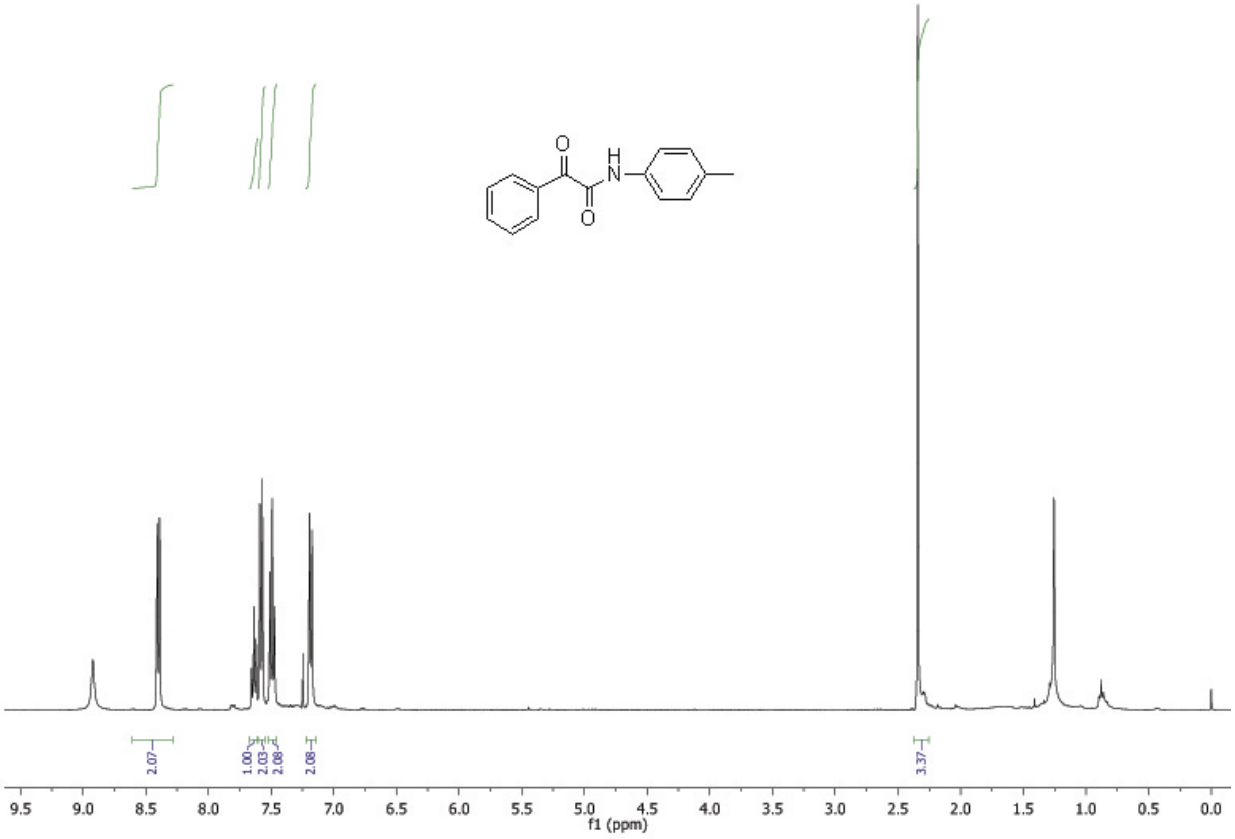

f1 (ppm)

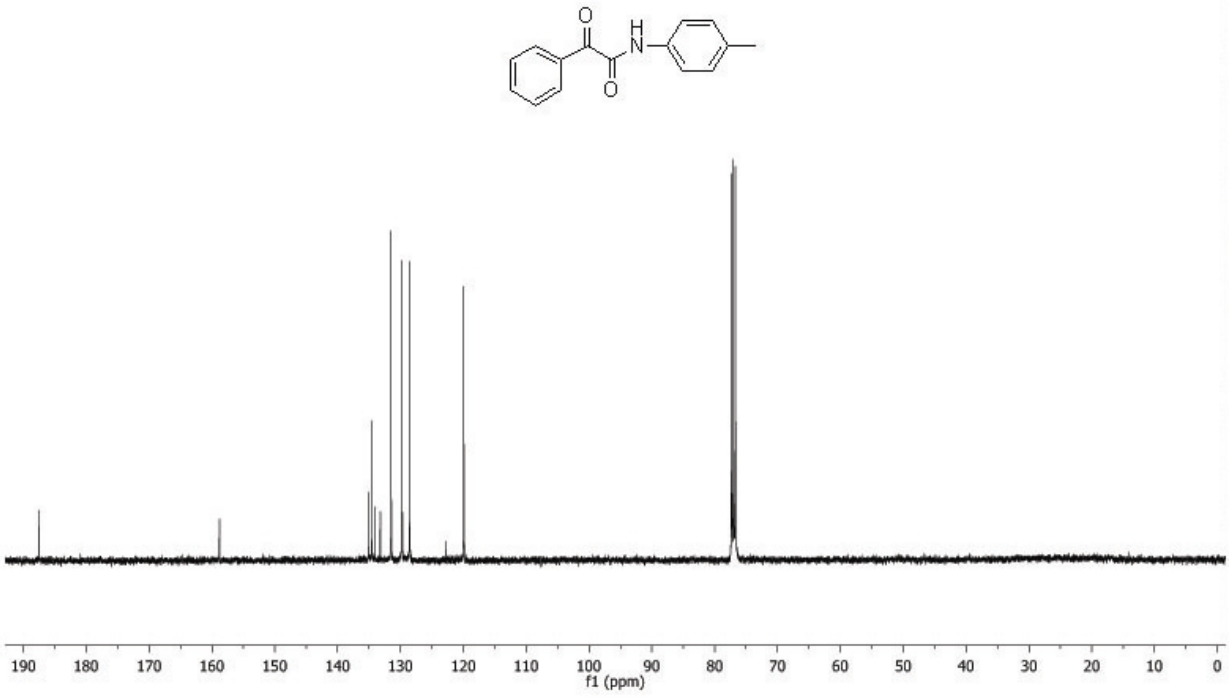

O
NH
O

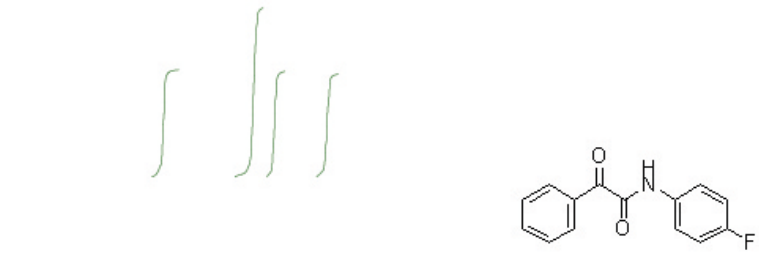

1.98
1.87
1.00
2.20
2.00
1.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

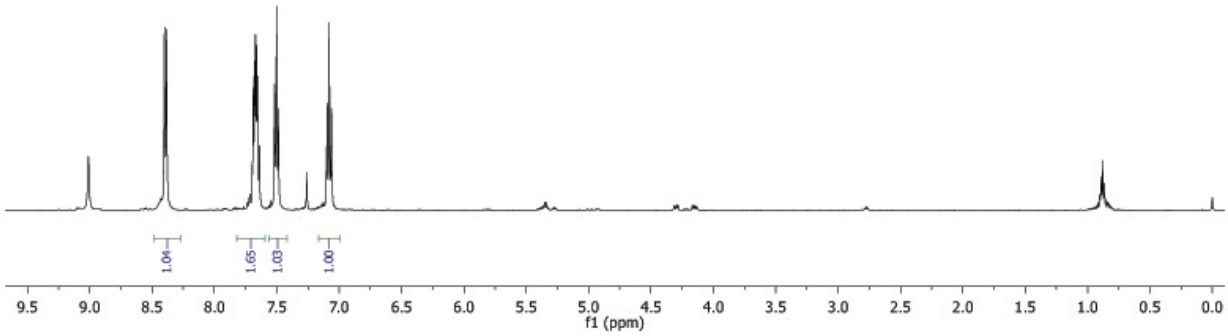

O
NH
O

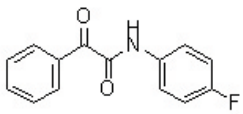

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

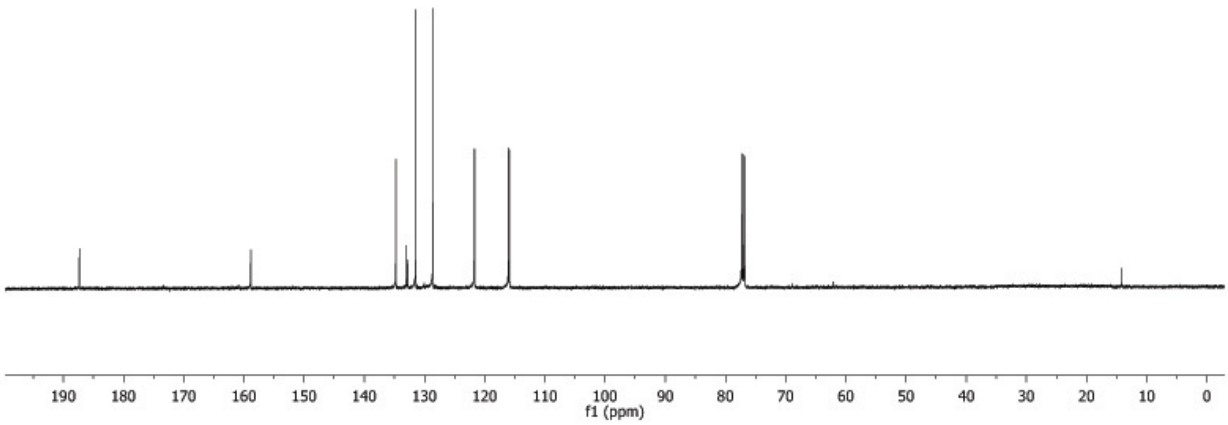

O
H
N
O
2.07
1.00
2.03
2.00
2.08
3.37
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

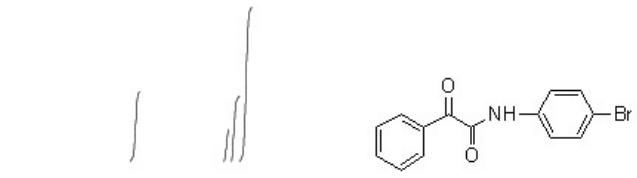

O
H
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

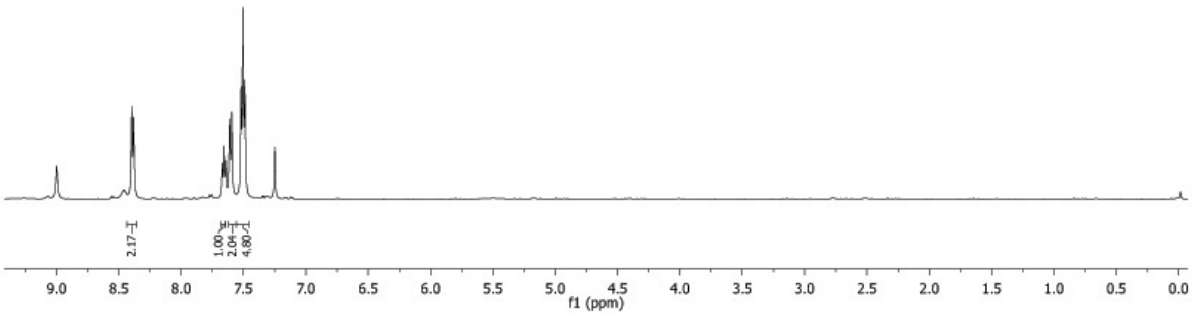

O
H
N
O
F

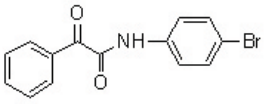

1.04
1.65
1.03
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

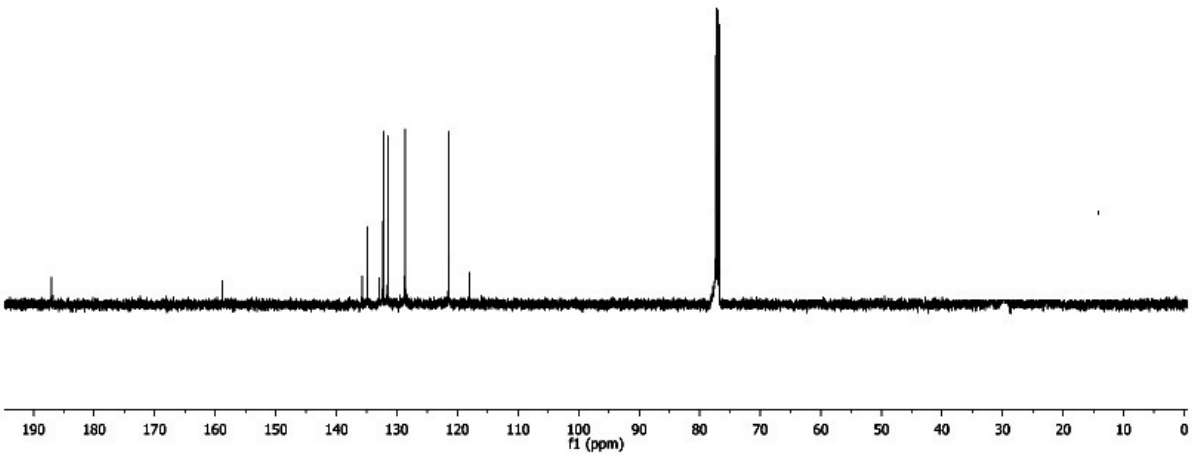

O
H
N
O
F

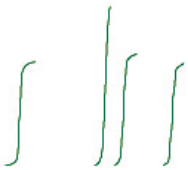

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

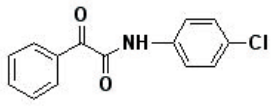

O
NH
Br
O

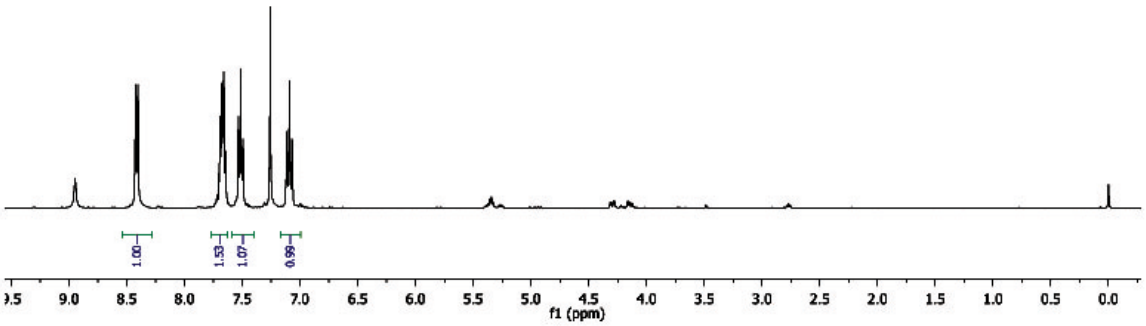

2.17
1.00
2.04
4.80
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

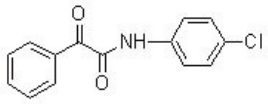

O
NH
Br
O


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

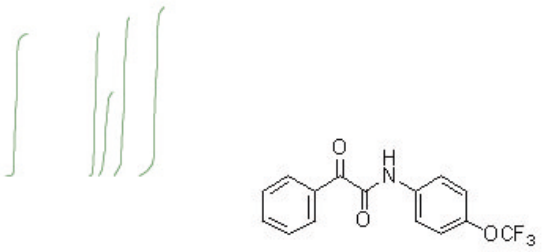


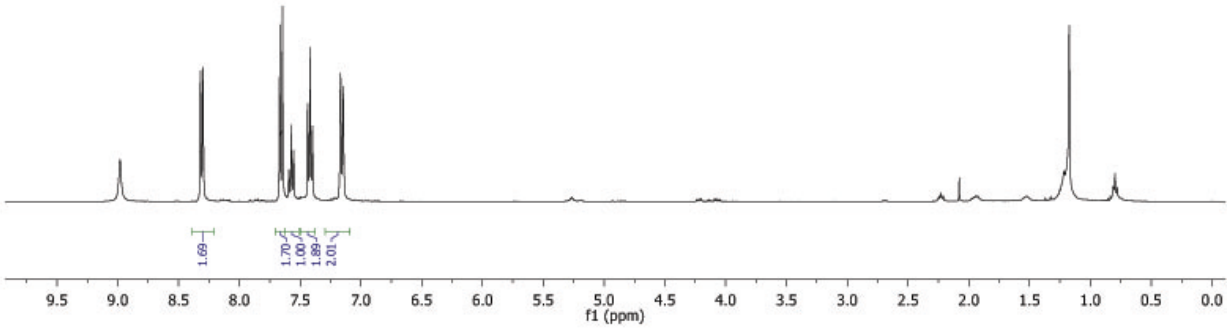

O
NH
Cl
O

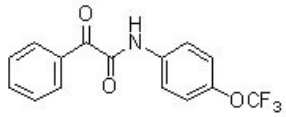

1.00
1.53
1.07
0.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

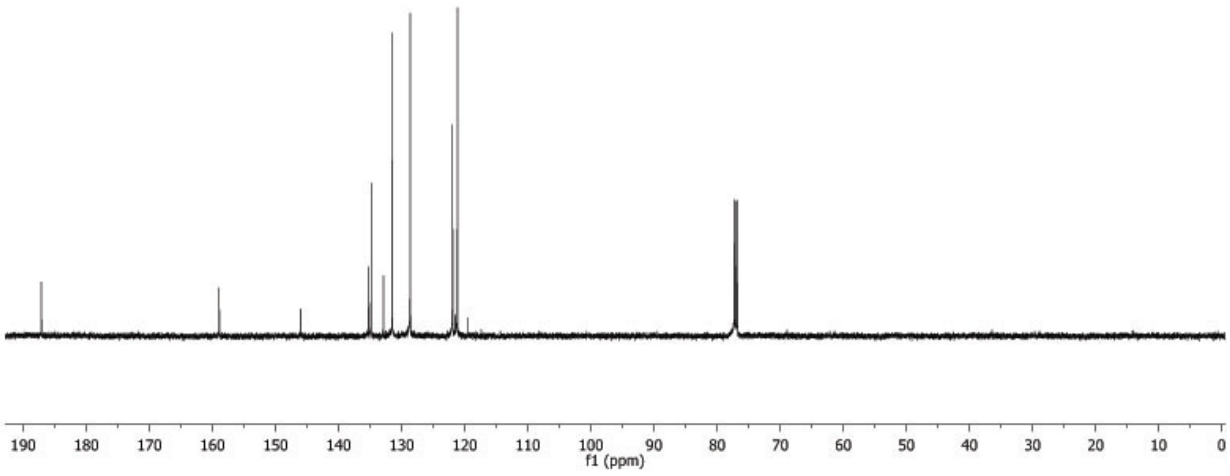

O
NH
Cl
O

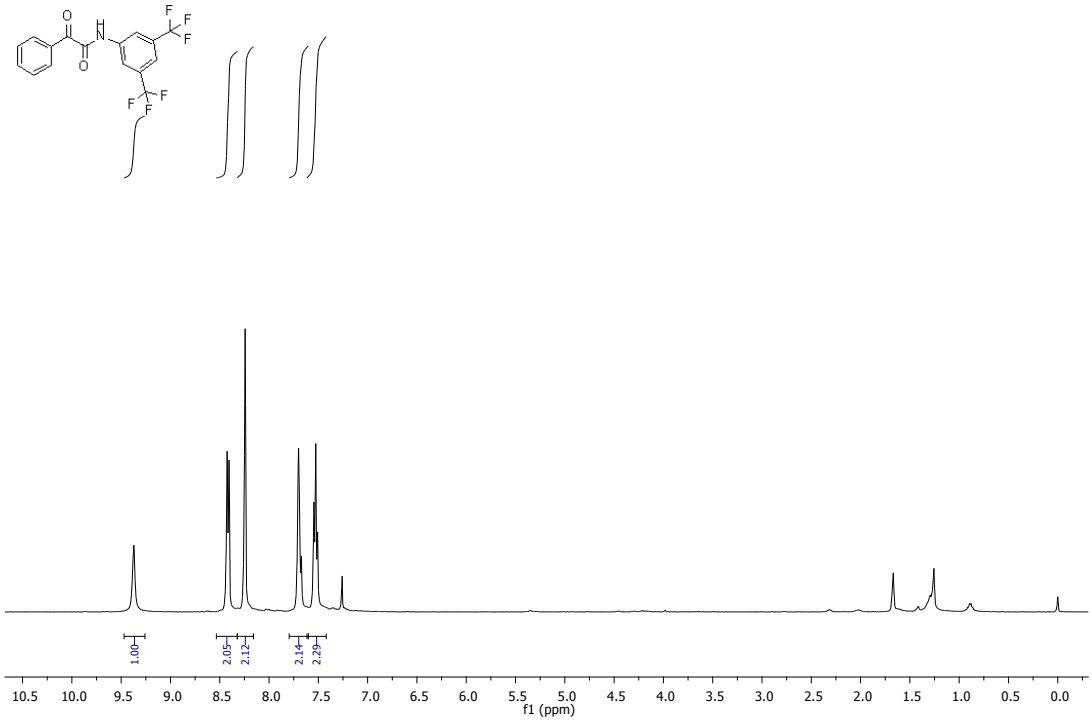
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


O
H
N
O
OCF3


1.69
1.70
1.00
1.89
2.01
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)


O
H
N
O
OCF3


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



186.36
159.09
138.15
135.23
132.80
132.51
131.55
128.77
124.06
121.89
119.72
118.56