Electronic Supplementary Material (ESI) for Chemical Communications

Cu^{II}-Catalyzed Decarboxylative Acylation of Acyl C–H of Formamides with α-Oxocarboxylic Acids Leading to α-Ketoamides

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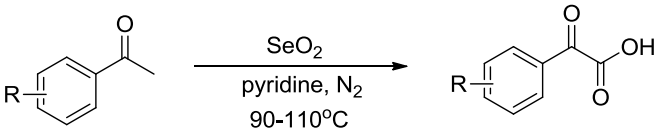
Table of Contents for Supporting Information

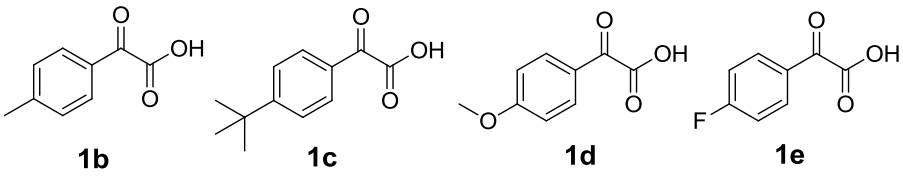
1. General considerations

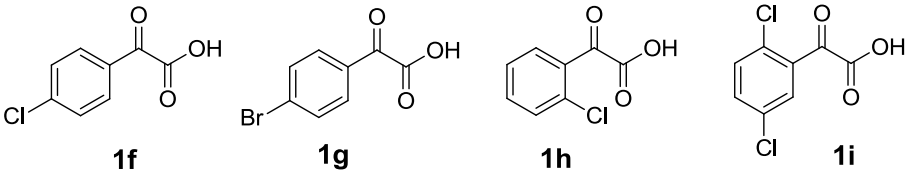
All the reactions of α-oxocarboxylic acids and formamides were carried out under an air atmosphere. ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker Avance NMR spectrometer (400 MHz or 100 MHz, respectively) with $CDCl_3$ as solvent and recorded in ppm relative to internal tetramethylsilane standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in Hertz (Hz). High resolution mass spectroscopy data of the product were collected on a Waters Micromass GCT instrument. Solvents and general chemicals were purchased from commercial suppliers and used without further purification.

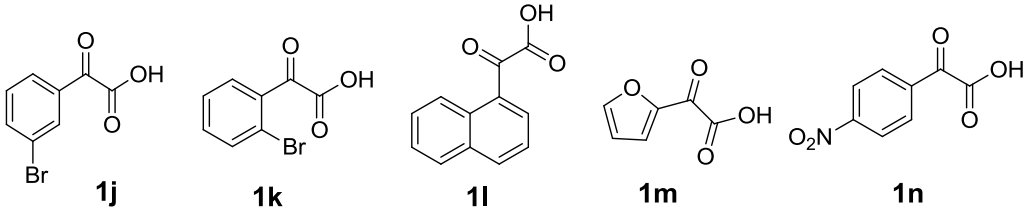
2. Starting materials

For this study, all formamides (**2a**–**2h**) and α-oxocarboxylic acid (**1a**) were purchased from commercial sources. Other α-oxocarboxylic acids (**1b–1n**) can be prepared from oxidation of corresponding methyl ketones with SeO_2 according to the reported procedure.[1]

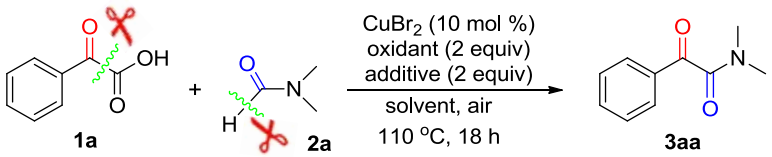








3. Optimization of oxidant, additive, solvent and temperature (TS1) [a]



Entry	Oxidant	Additive	Solvent	Yield (%)[b]
1	H_2O_2	PivOH	toluene	<10 [c]
2	TBHP	PivOH	toluene	<5 [d]
3	TBPB	PivOH	toluene	23
4	BQ	PivOH	toluene	<10
5	$K_2S_2O_8$	PivOH	toluene	trace
6	–	PivOH	toluene	20
7	O_2	PivOH	toluene	34
8	DTBP	TFA	toluene	14
9	DTBP	HOAc	toluene	<5
10	DTBP	$PhCO_2H$	toluene	<10
11	DTBP	CF_3SO_3H	toluene	NR
12	DTBP	pyridine	toluene	24
13	DTBP	NEt_3	toluene	trace
14	DTBP	K_2CO_3	toluene	NR
15	DTBP	K_3PO_4	toluene	NR
16	DTBP	–	toluene	43
17	DTBP	PivOH	toluene	81
18	DTBP	PivOH	–	61
19	DTBP	PivOH	*t*-AmOH	37
20	DTBP	PivOH	dioxane	41
21	DTBP	PivOH	CH_2ClCH_2Cl	35
22	DTBP	PivOH	$CH_3OCH_2CH_2OCH_3$	35
23	DTBP	PivOH	CH_2Cl_2	42
24	DTBP	PivOH	DMA	39
25	DTBP	PivOH	benzene	30
26	DTBP	PivOH	CH_3CN	27
27	DTBP	PivOH	CH_3COOEt	25
28	DTBP	PivOH	THF	24
29	DTBP	PivOH	EtOH	10
30	DTBP	PivOH	NMP	trace
31	DTBP	PivOH	CH_3NO_2	trace
32	DTBP	PivOH	DMSO	NR
33	DTBP	PivOH	HOAc	NR
34	DTBP	PivOH	H_2O	NR
35	DTBP	PivOH	toluene	72 [e]
36	DTBP	PivOH	toluene	77 [f]

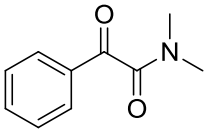
[a] Reaction conditions: **1a** (0.50 mmol), **2a** (5.0 equiv), $CuBr_2$ (10 mol %), oxidant (2.0 equiv), additive (2.0 equiv), solvent (1.5 mL), air atmosphere, 110 °C, 18 h. [b] Isolated yields. [c] H_2O_2 (30% in water). [d] TBHP (*tert*-butyl hydroperoxide, 70% in water). [e] 100 °C. [f] 120 °C.

4. General procedure

Under air atmosphere, a sealable reaction tube with a Teflon-coated screw cap equipped with a magnetic stir bar was charged with 2-oxo-2-phenylacetic acid (**1a**, 0.50 mmol), *N*,*N*-dimethylformamide (**2a**, DMF, 2.5 mmol), $CuBr_2$ (0.05 mmol), di-*tert*-butyl peroxide (DTBP, 1.0 mmol), pivalic acid (PivOH, 1.0 mmol), and toluene (1.5 mL). The rubber septum was then replaced by a Teflon-coated screw cap, and the reaction vessel placed in an oil bath at 110 ^{o}C for 18 h. After the reaction was completed, it was cooled to room temperature and quenched with water and extracted with ethyl acetate and then dried with Na_2SO_4. The resulting solution was directly filtered through a pad of silica gel using a sintered glass funnel, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluant: petroleum ether/ethyl acetate) to give the desired product *N*,*N*-dimethyl-2-oxo-2-phenylacetamide (**3aa**).

5. Characterization data for all products

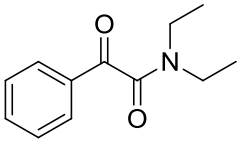
N,*N*-Dimethyl-2-oxo-2-phenylacetamide



3aa:[2] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.96–7.94 (m, 2H), 7.66–7.62 (m, 1H), 7.53–7.49 (m, 2H), 3.12 (s, 3H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.74, 167.04, 134.65, 133.13, 129.63, 128.98, 37.01, 33.99.

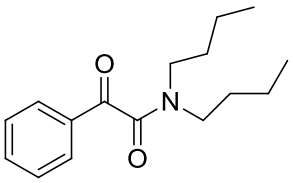
N,*N*-Diethyl-2-oxo-2-phenylacetanmide



3ab:[3] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95–7.93 (m, 2H), 7.65–7.61 (m, 1H), 7.52–7.49 (m, 2H), 3.56 (q, *J* = 7.2 Hz, 2H), 3.24 (q, *J* = 7.2 Hz, 2H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.55, 166.74, 134.50, 133.32, 129.59, 128.92, 42.10, 38.81, 14.07, 12.80.

N,*N*-Dibutyl-2-oxo-2-phenylacetamide

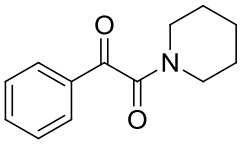


3ac:[4] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94–7.92 (m, 2H), 7.64–7.60 (m, 1H), 7.51–7.48 (m, 2H), 3.49 (t, *J* = 8.0 Hz, 2H), 3.14 (t, *J* = 8.0 Hz, 2H), 1.71–1.63 (m, 2H), 1.57–1.49 (m, 2H), 1.46–1.37 (m, 2H), 1.25–1.14 (m, 2H), 0.99 (t, *J* = 8.0 Hz, 3H), 0.81 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.55, 167.07, 134.44, 133.38, 129.57, 128.89,

47.42, 44.03, 30.61, 29.43, 20.21, 19.73, 13.80, 13.49.

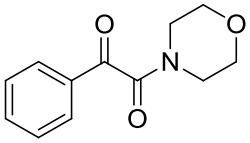
1-Phenyl-2-(piperidin-1-yl)ethane-1,2-dione



3ad:[3,4] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.96–7.94 (m, 2H), 7.65–7.62 (m, 1H), 7.53–7.49 (m, 2H), 3.71 (s, 2H), 3.29 (t, *J* = 5.6 Hz, 2H), 1.70 (s, 4H), 1.55 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.91, 165.45, 134.59, 133.31, 129.54, 128.97, 47.02, 42.15, 26.19, 25.43, 24.37.

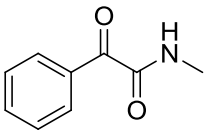
1-Morpholino-2-phenylethane-1,2-dione



3ae:[3,4] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.96–7.94 (m, 2H), 7.66–7.63 (m, 1H), 7.53–7.49 (m, 2H), 3.78 (s, 4H), 3.65–3.63 (m, 2H), 3.38–3.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.13, 165.45, 134.89, 133.09, 129.64, 129.07, 66.71, 66.63, 46.25, 41.62.

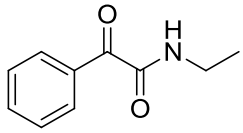
N-Methyl-2-oxo-2-phenylacetamide



3af: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.36–8.35 (m, 2H), 7.65–7.61 (m, 1H), 7.51–7.47 (m, 2H), 7.11 (s, 1H), 2.98 (d, *J* = 4.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 187.65, 162.42, 134.34, 133.36, 131.20, 128.46, 25.98. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1665, 1595. HRMS (EI) ($[M]^+$) Calcd. for $C_9H_9NO_2$: 163.0633, Found: 163.0636.

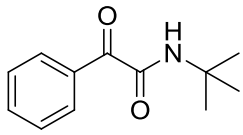
N-Ethyl-2-oxo-2-phenylacetamide



3ag: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35–8.33 (m, 2H), 7.64–7.61 (m, 1H), 7.50–7.46 (m, 2H), 7.11 (s, 1H), 3.48–3.41 (m, 2H), 1.26 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 187.92, 161.69, 134.30, 133.41, 131.18, 128.44, 34.36, 14.45. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1663, 1595. HRMS (EI) ($[M]^+$) Calcd. for $C_{10}H_{11}NO_2$: 177.0790, Found: 177.0786.

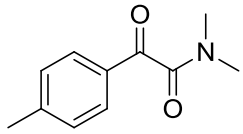
N-*tert*-Butyl-2-oxo-2-phenylacetamide



3ah: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.32–8.30 (m, 2H), 7.63–7.59 (m, 1H), 7.49–7.45 (m, 2H), 6.93 (s, 1H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 188.57, 161.14, 134.10, 133.43, 131.19, 128.35, 51.65, 28.38. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1667, 1597. HRMS (EI) ($[M]^+$) Calcd. for $C_{12}H_{15}NO_2$: 205.1103, Found: 205.1099.

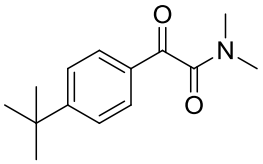
N,*N*-Dimethyl-2-oxo-2-*p*-tolylacetaminde



3ba:[5] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85–7.83 (m, 2H), 7.31–7.29 (m, 2H), 3.11 (s, 3H), 2.95 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.50, 167.28, 145.94, 130.69, 129.76, 129.71, 37.03, 33.96, 21.85.

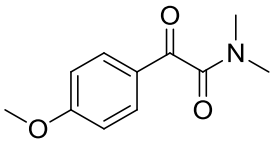
2-(4-*tert*-Butylphenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ca: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.88 (d, *J* = 8.4 Hz, 2H), 7.53–7.51 (m, 2H), 3.12 (s, 3H), 2.96 (s, 3H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 191.49, 167.29, 158.79, 130.57, 129.63, 126.00, 37.06, 35.34, 33.97, 30.97. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1678, 1650. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{14}H_{20}NO_2$:234.1494 Found: 234.1491.

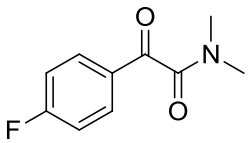
2-(4-Methoxyphenyl)-*N*,*N*-dimethy-2-oxoacetamide



3da:[6] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.90 (d, *J* = 8.8 Hz, 2H), 6.98–6.95 (m, 2H), 3.86 (s, 3H), 3.09 (s, 3H), 2.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.46, 167.38, 164.84, 132.08, 127.01, 114.31, 55.60, 37.05, 33.94.

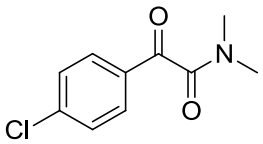
2-(4-Fluorophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ea:[7] White solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.00–7.97 (m, 2H), 7.20–7.16 (m, 2H), 3.11 (s, 3H), 2.97(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 189.97, 166.66 (d, *J* = 256.0 Hz), 166.60, 132.47 (d, *J* = 10.0 Hz), 129.67 (d, *J* = 3.0 Hz), 116.29 (d, *J* = 22.0 Hz), 37.02, 34.05.

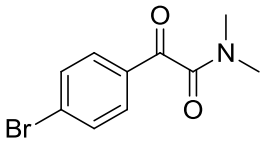
2-(4-Chlorophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3fa:[7] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91–7.89 (m, 2H), 7.50–7.48 (m, 2H), 3.12 (s, 3H), 2.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.26, 166.47, 141.31, 131.53, 131.01, 129.37, 37.02, 34.08.

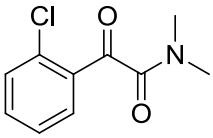
2-(4-Bromophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ga: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82–7.80 (m, 2H), 7.66–7.64 (m, 2H), 3.11 (s, 3H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.48, 166.43, 132.37, 131.92, 131.04, 130.16, 37.02, 34.09. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1679, 1646. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{10}H_{11}BrNO_2$: 255.9973, Found: 255.9970.

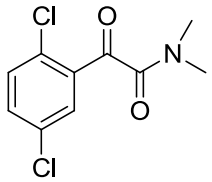
2-(2-Chlorophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ha: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.89–7.87 (m, 1H), 7.52–7.48 (m, 1H), 7.44–7.37 (m, 2H), 3.07 (s, 3H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.14, 166.93, 134.27, 133.72, 133.45, 132.22, 130.76, 127.27, 37.04, 34.50. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1679, 1650. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{10}H_{11}ClNO_2$: 212.0478, Found: 212.0475.

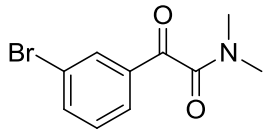
2-(2,5-Dichlorophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ia: Yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.84–7.83 (m, 1H)，7.47–7.44 (m, 1H), 7.38–7.36 (m, 1H), 3.08 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 188.67, 166.18, 134.91, 133.99, 133.67, 131.85, 131.74, 131.69, 37.04, 34.60. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1675, 1648. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{10}H_{10}Cl_2NO_2$: 246.0089, Found: 246.0087.

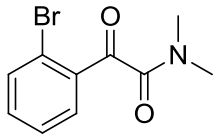
2-(3-Bromophenyl)-*N*,*N*-dimethyl-2-oxoaceamide



3ja: Yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.09 (s, 1H), 7.88 (d, *J* = 8.0 Hz,1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.41–7.37 (m, 1H), 3.13 (s, 3H), 2.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.05, 166.20, 137.48, 134.92, 132.38, 130.54, 128.27, 123.25, 37.03, 34.12. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1683, 1650. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{10}H_{11}BrNO_2$: 255.9973, Found: 255.9971.

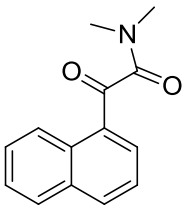
2-(2-Bromophenyl)-*N*,*N*-dimethyl-2-oxoacetamide



3ka: Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83–7.81 (m, 1H), 7.64–7.62 (m, 1H), 7.45–7.37 (m, 2H), 3.09 (s, 3H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.79, 166.27, 135.37, 134.06, 134.03, 132.57, 127.69, 121.48, 37.18, 34.61. IR (KBr, cm^{-1}): ($\nu_{C=O}$) 1675, 1646. HRMS (ESI) $[M+H]^+$ Calcd. for $C_{10}H_{11}BrNO_2$: 255.9973, Found: 255.9975.

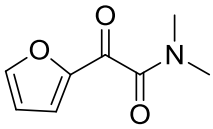
N,*N*-Dimethyl-2-(naphthalen-1-yl)-2-oxoacetamide



3la:[7] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.27–9.25 (m, 1H), 8.12–8.10 (m, 1H), 8.01–7.99 (m, 1H), 7.93–7.91 (m, 1H), 7.72–7.68 (m, 1H), 7.61–7.52 (m, 2H), 3.16 (s, 3H), 3.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.20, 167.68, 135.84, 134.29, 134.08, 130.98, 129.29, 128.72, 128.51, 126.97, 125.80, 124.54, 37.17, 34.15.

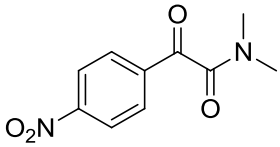
2-(Furan-2-yl)-*N*,*N*-dimethyl-2-oxoacetamide



3ma:[7] Yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.69 (s, 1H), 7.34 (br, s, 1H), 6.59–6.58 (m, 1H), 3.05 (s, 3H), 3.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 178.50, 165.41, 150.17, 148.69, 122.28, 112.82, 37.14, 34.45.

N,*N*-Dimethyl-2-(4-nitrophenyl)-2-oxoacetamide



3na:[7] Yellow solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.34–8.32 (m, 2H), 8.14–8.13 (m, 2H), 3.14 (s, 3H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 189.24, 165.60, 151.08, 137.57, 130.76, 124.05, 37.05, 34.28.

6. References

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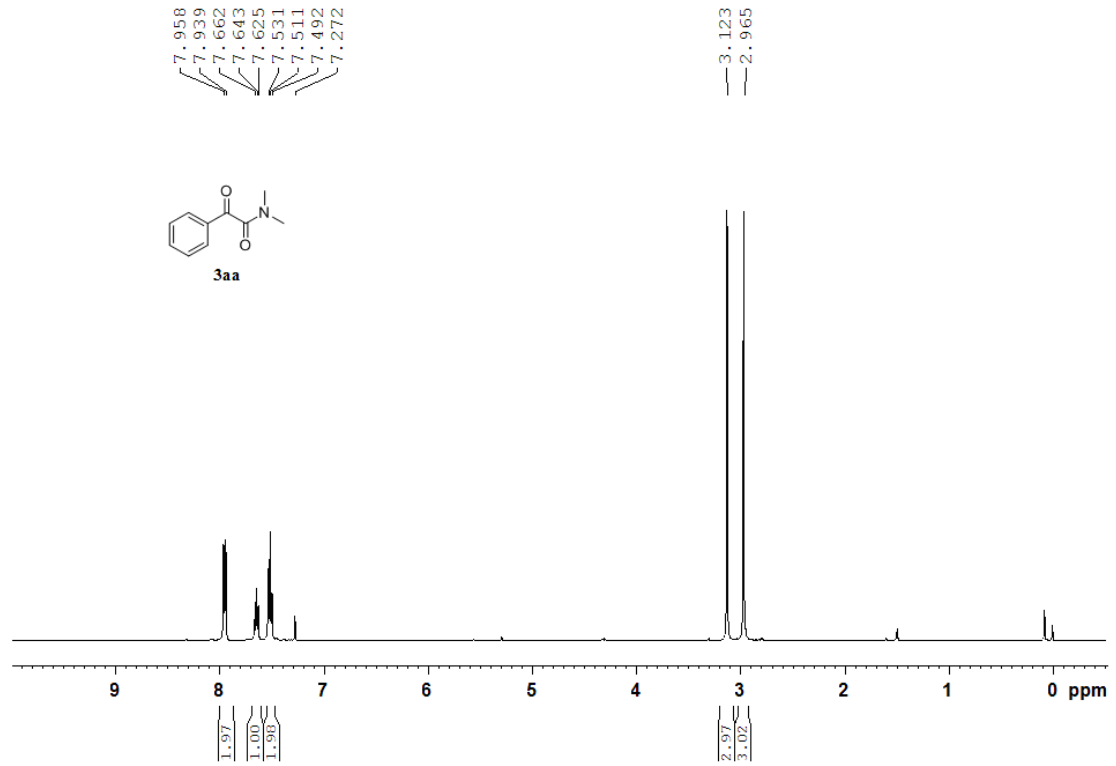
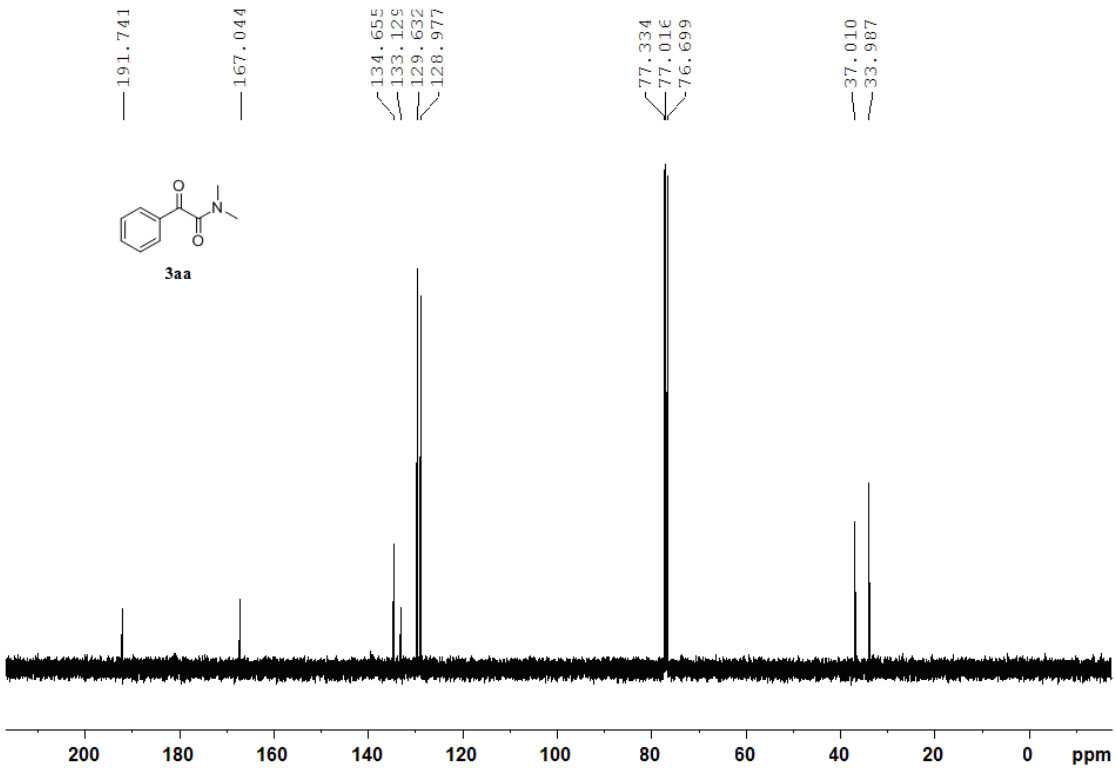
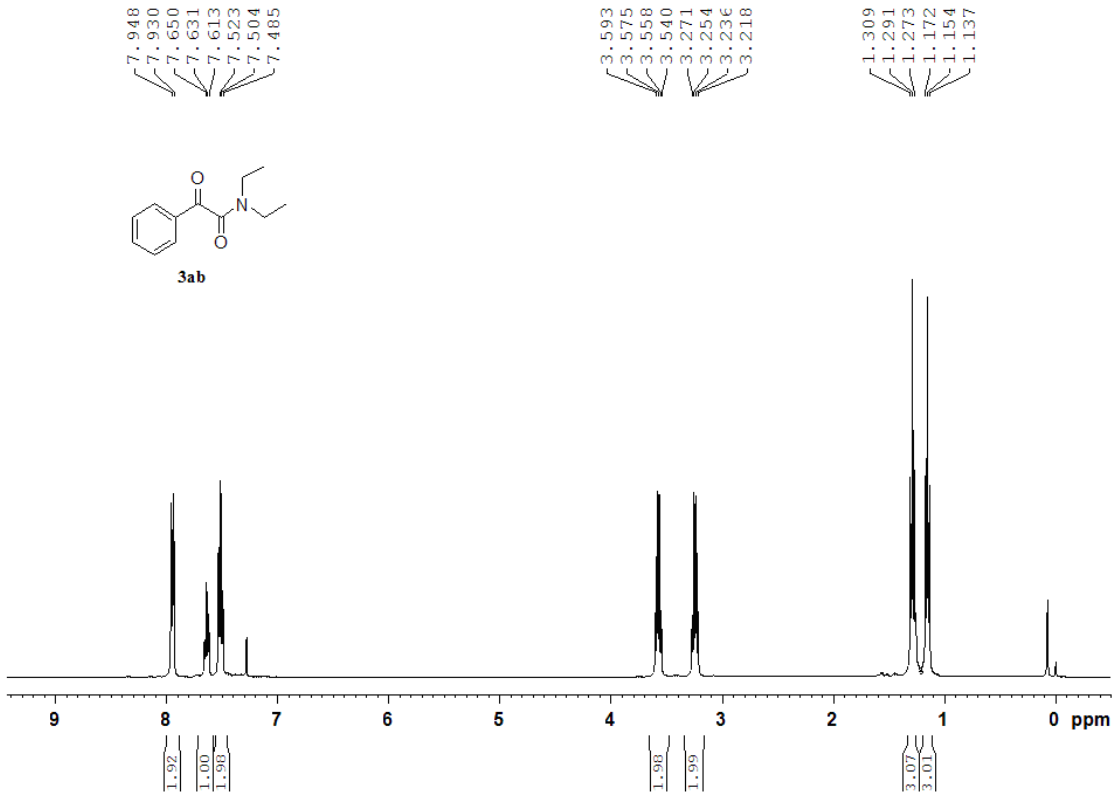
7. ^{1}H and ^{13}C NMR spectra of the products



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7.631
7.613
7.523
7.504
7.485
3.593
3.575
3.558
3.540
3.271
3.254
3.236
3.218
1.309
1.291
1.273
1.172
1.154
1.137
3ab
9
8
7
6
5
4
3
2
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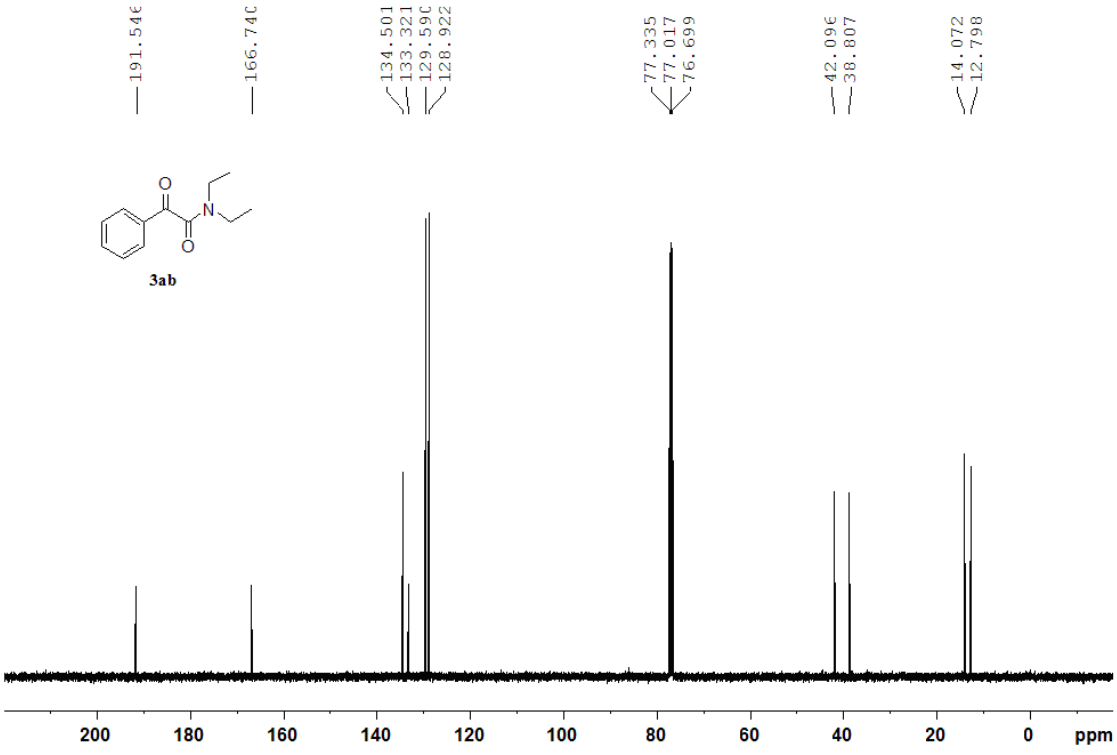
1.00
1.98
1.98
1.99
3.07
3.01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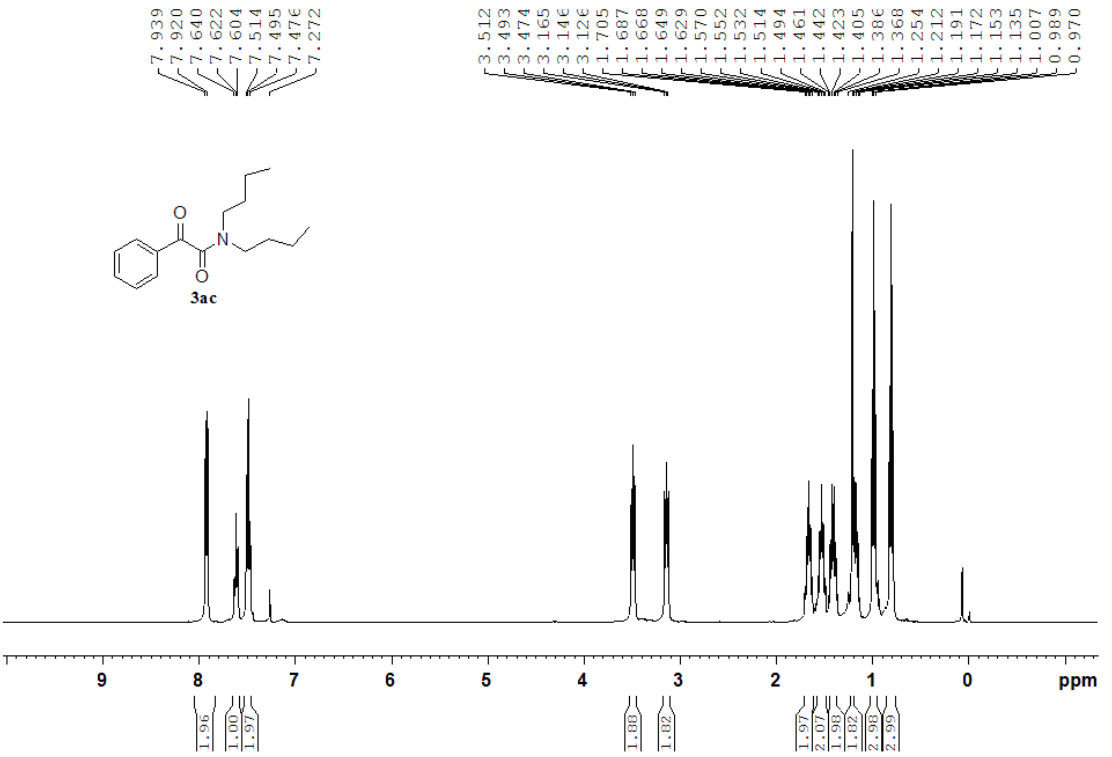
166.74
134.501
133.321
129.59
128.922
77.335
77.017
76.699
42.096
38.807
14.072
12.798
3ab
200
180
160
140
120
100
80
60
40
20
0
ppm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7.640
7.622
7.604
7.514
7.495
7.476
7.272
3.512
3.493
3.474
3.165
3.146
3.126
1.705
1.687
1.668
1.649
1.629
1.570
1.552
1.532
1.514
1.494
1.461
1.442
1.423
1.405
1.386
1.368
1.254
1.212
1.191
1.172
1.153
1.135
1.007
0.989
0.970
O
N
O
3ac
9
8
7
6
5
4
3
2
1
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ppm
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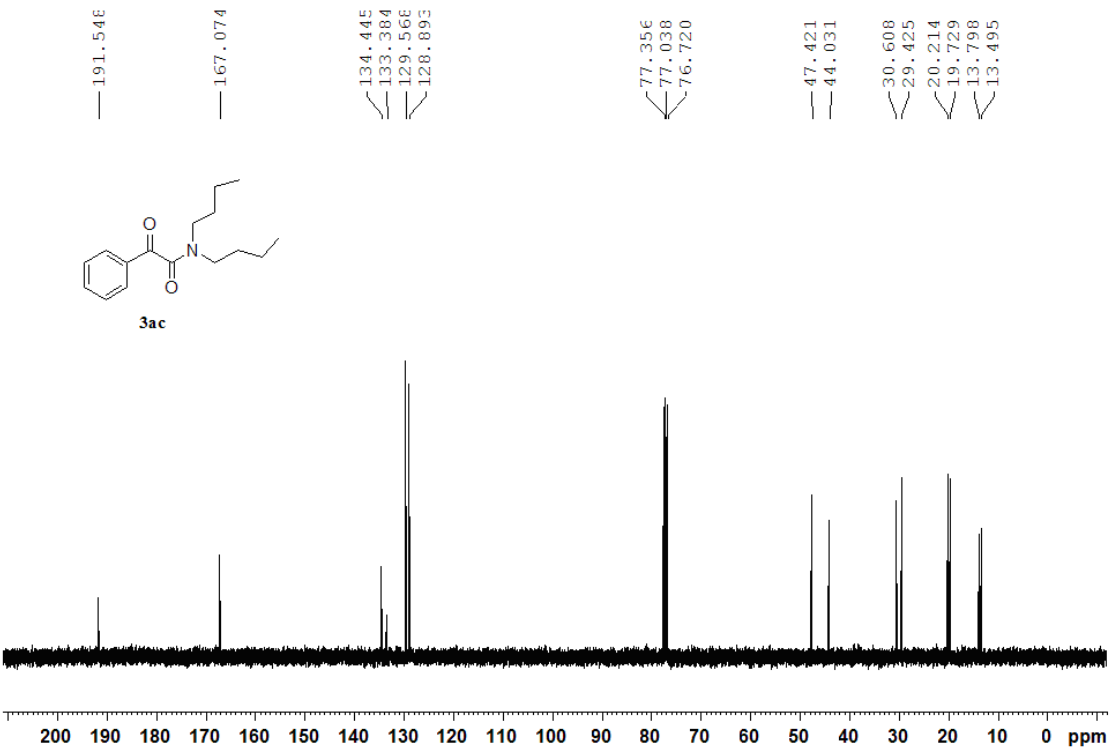
1.00
1.97
1.68
1.82
1.97
2.07
1.98
1.82
2.98
2.99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134.445
133.384
129.566
128.893
77.356
77.038
76.720
47.421
44.031
30.608
29.425
20.214
19.729
13.798
13.495
O
N
O
3ac
200
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170
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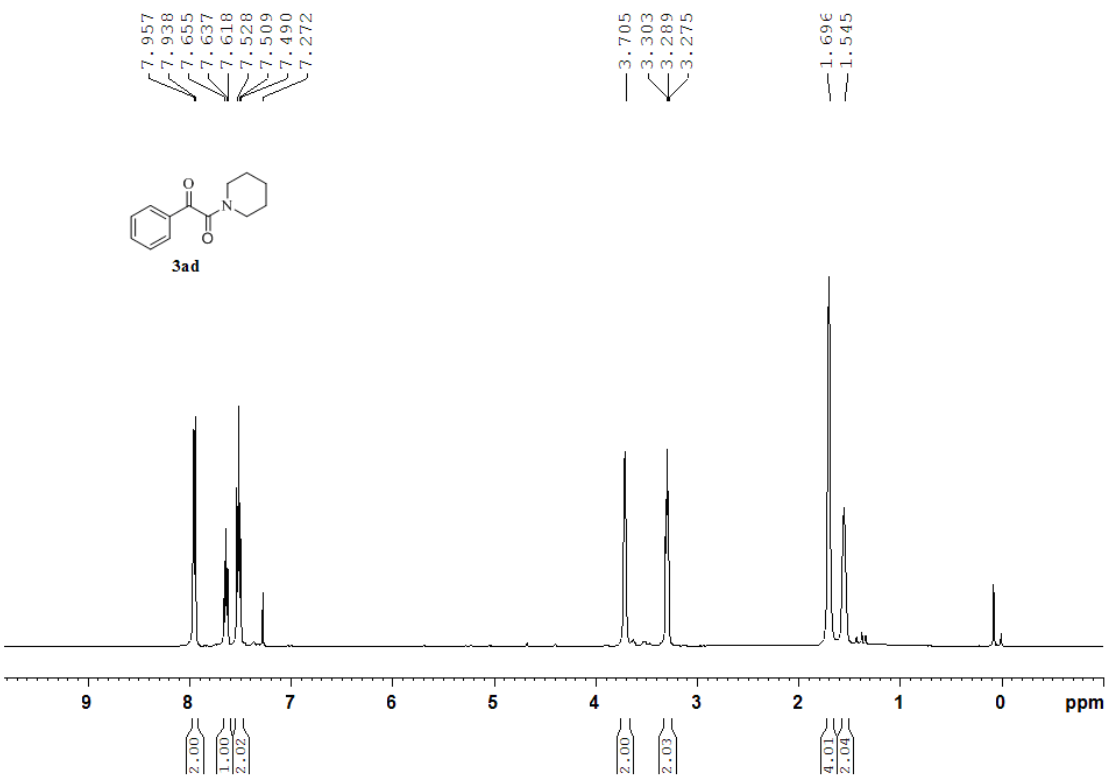
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.655
7.637
7.618
7.528
7.509
7.490
7.272
3.705
3.303
3.289
3.275
1.696
1.545
3ad
9
8
7
6
5
4
3
2
1
0
ppm
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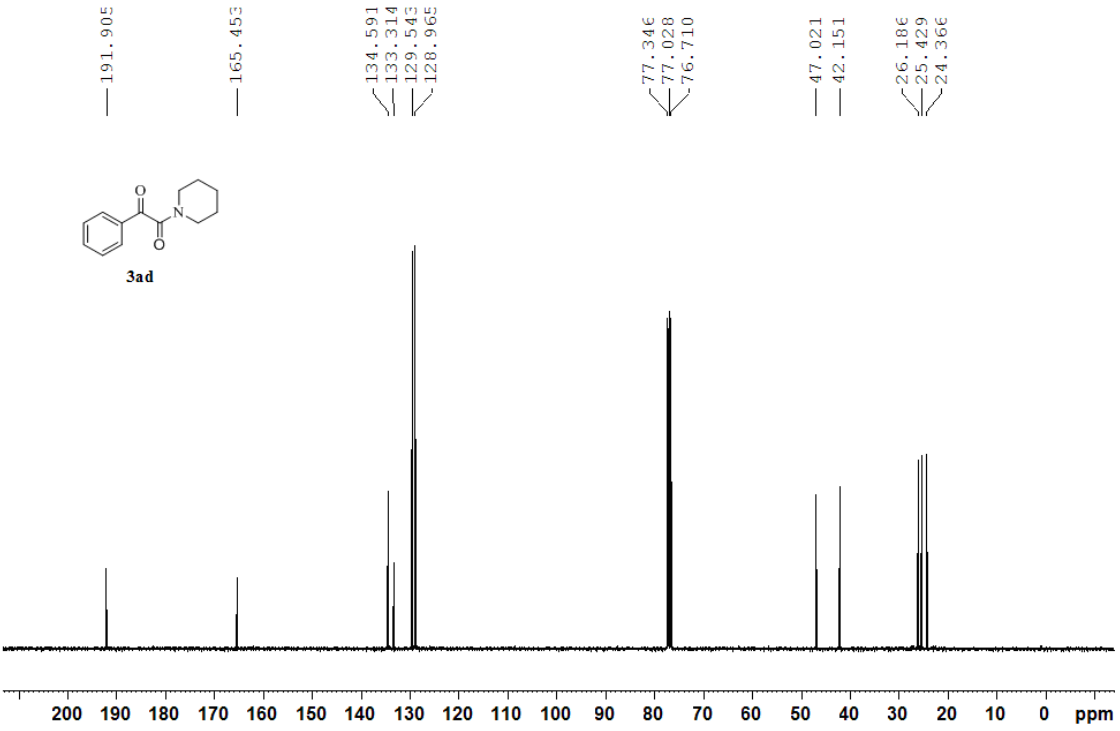
1.00
2.02
2.00
2.03
4.01
2.04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47.021
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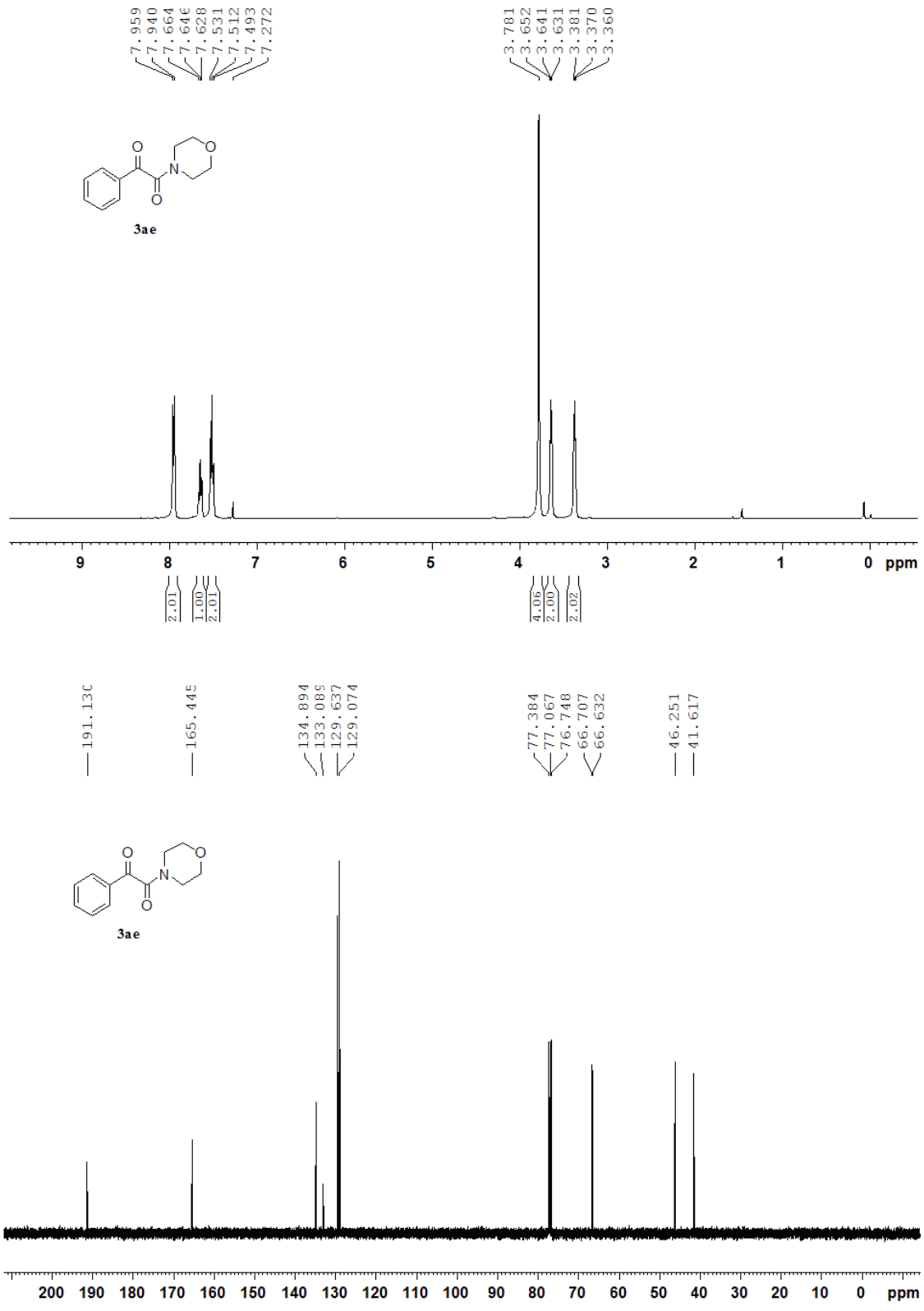
26.186
25.429
24.366
3ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.512
7.493
7.272
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3.641
3.631
3.381
3.370
3.360
3ae
9 8 7 6 5 4 3 2 1 0 ppm
2.01
1.00
2.01
4.06
2.00
2.02
191.130
165.445
134.894
133.089
129.637
129.074
77.384
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66.707
66.632
46.251
41.617
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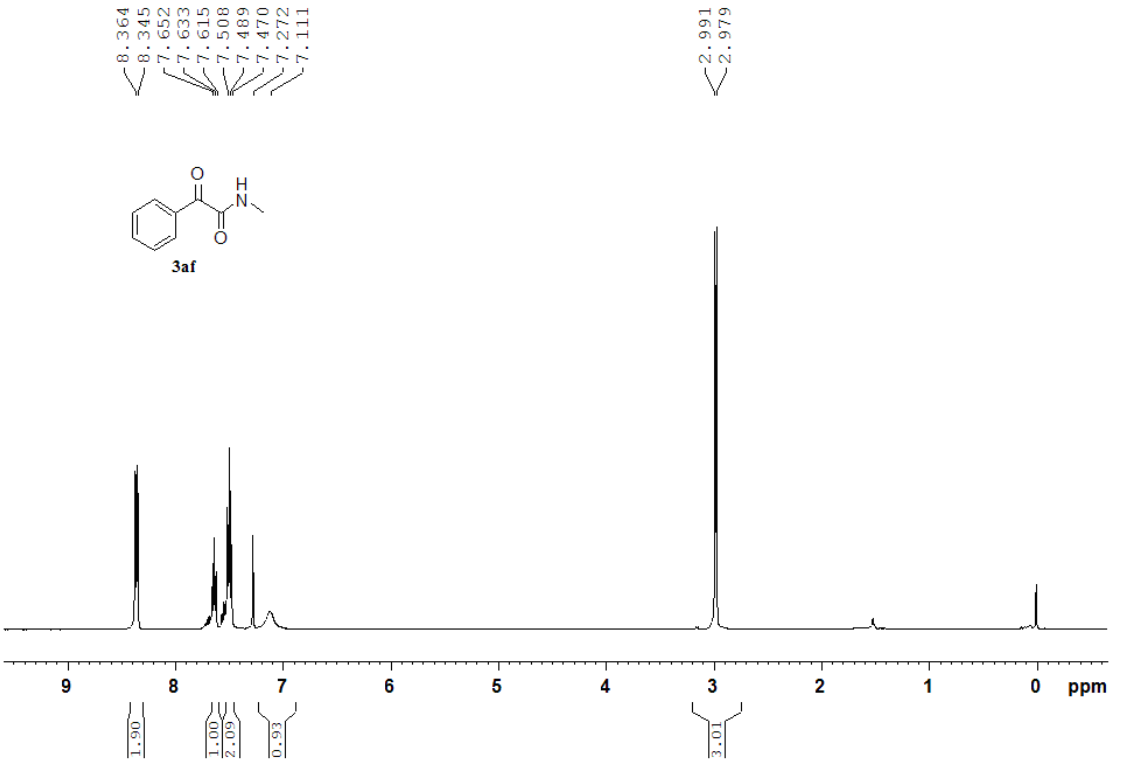
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7.470
7.272
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8
7
6
5
4
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2.09
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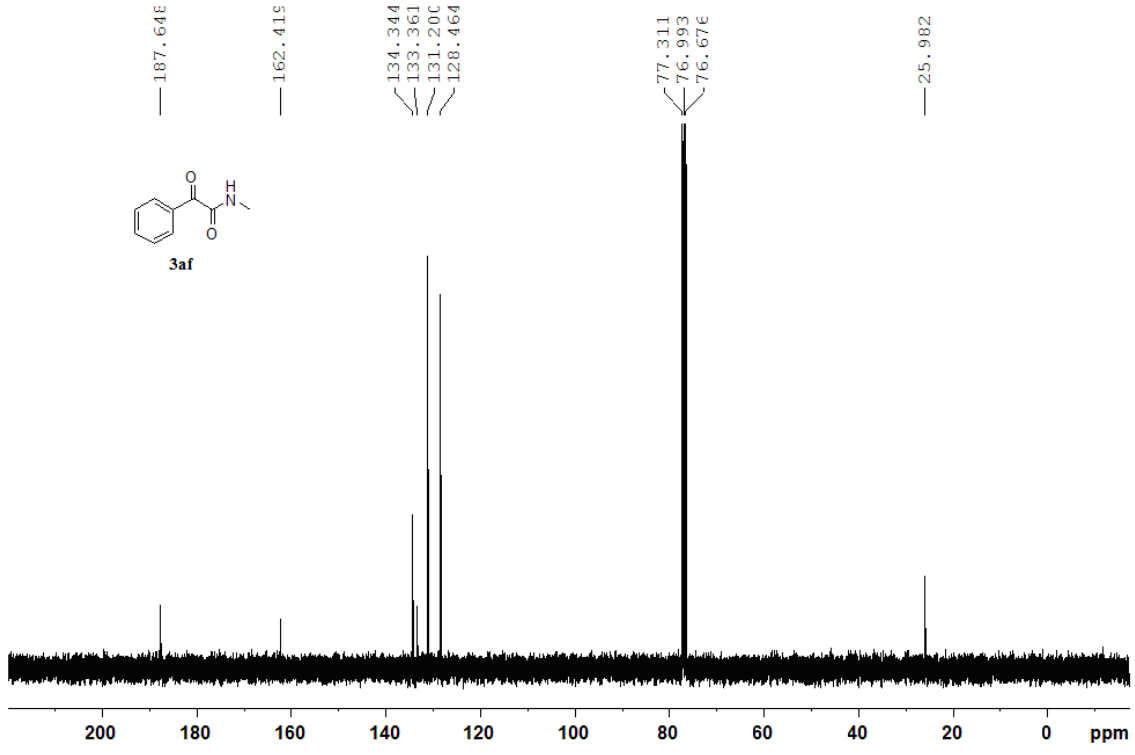
3.01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160
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120
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60
40
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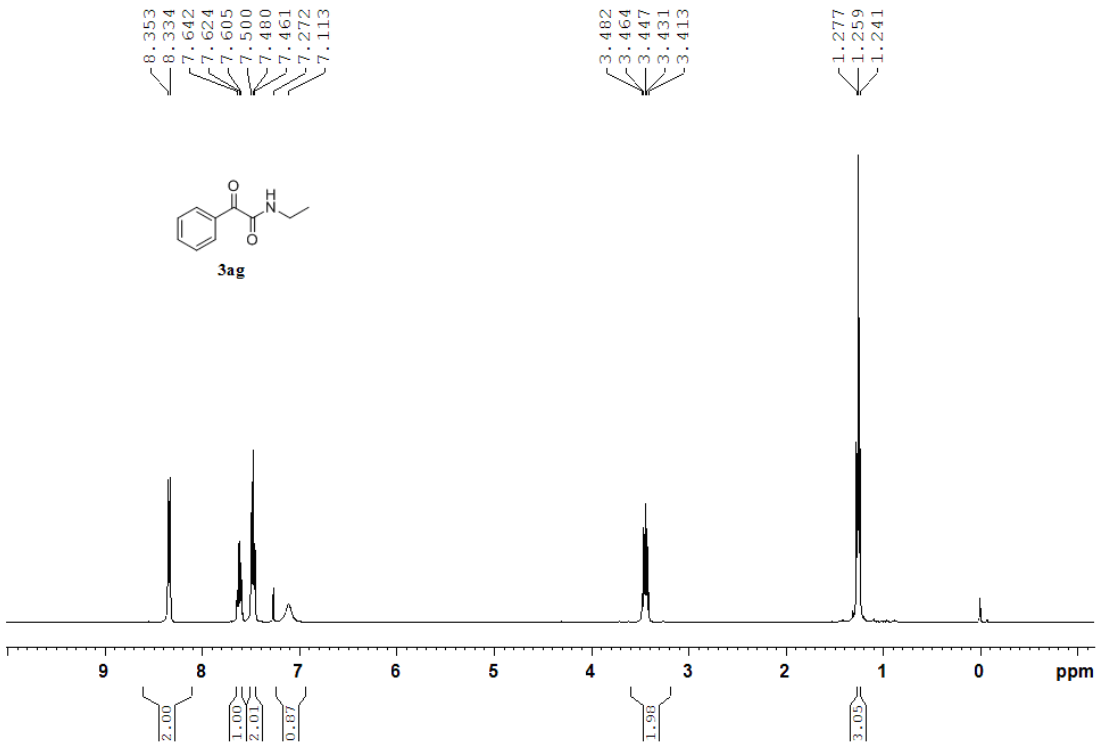
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7.113
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3.431
3.413
1.277
1.259
1.241
3ag
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1.00
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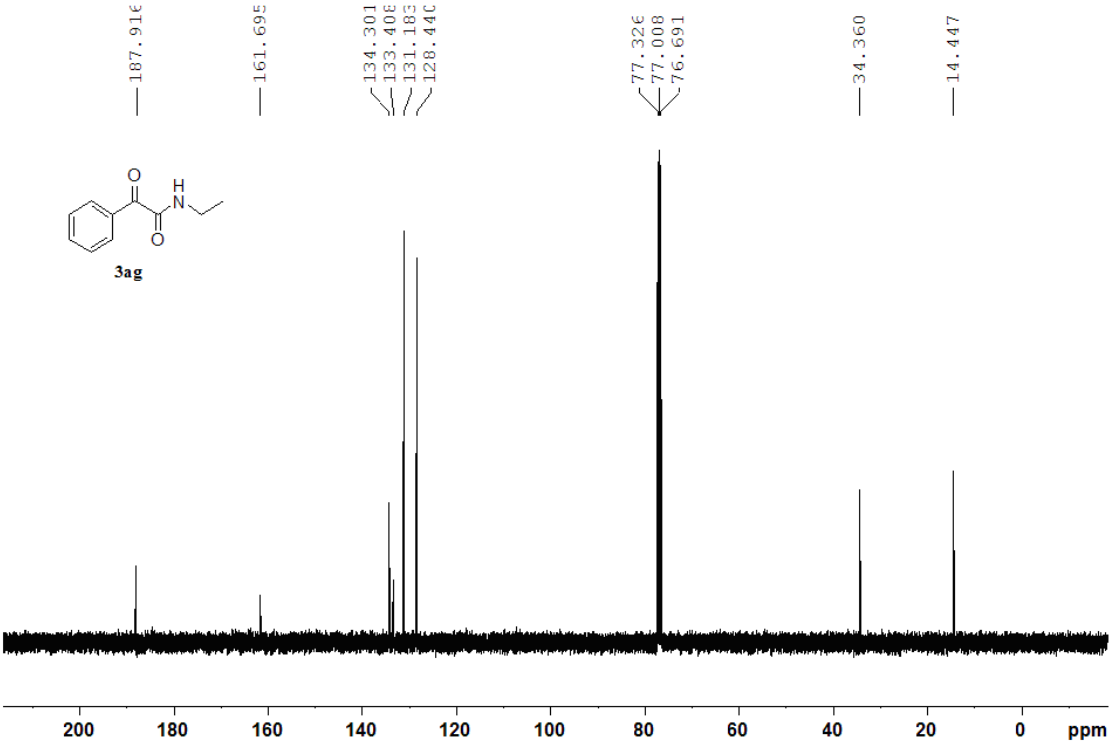
3.05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120
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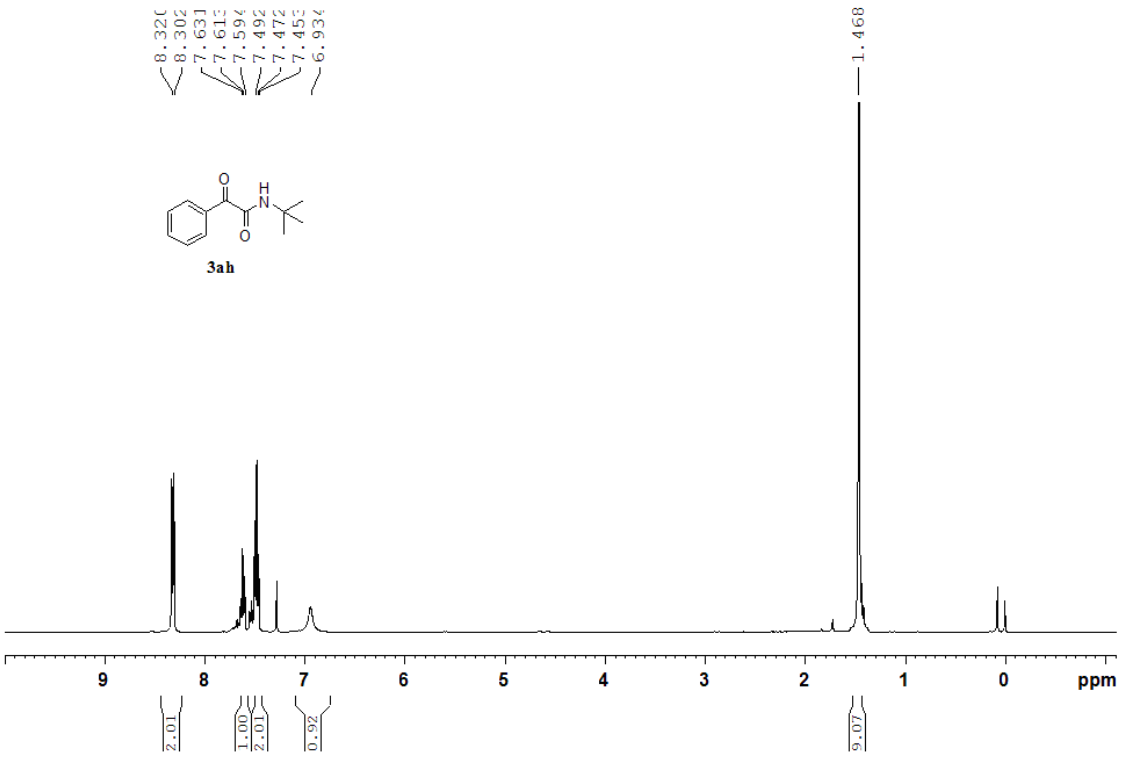
60
40
20
0
ppm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5
4
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2
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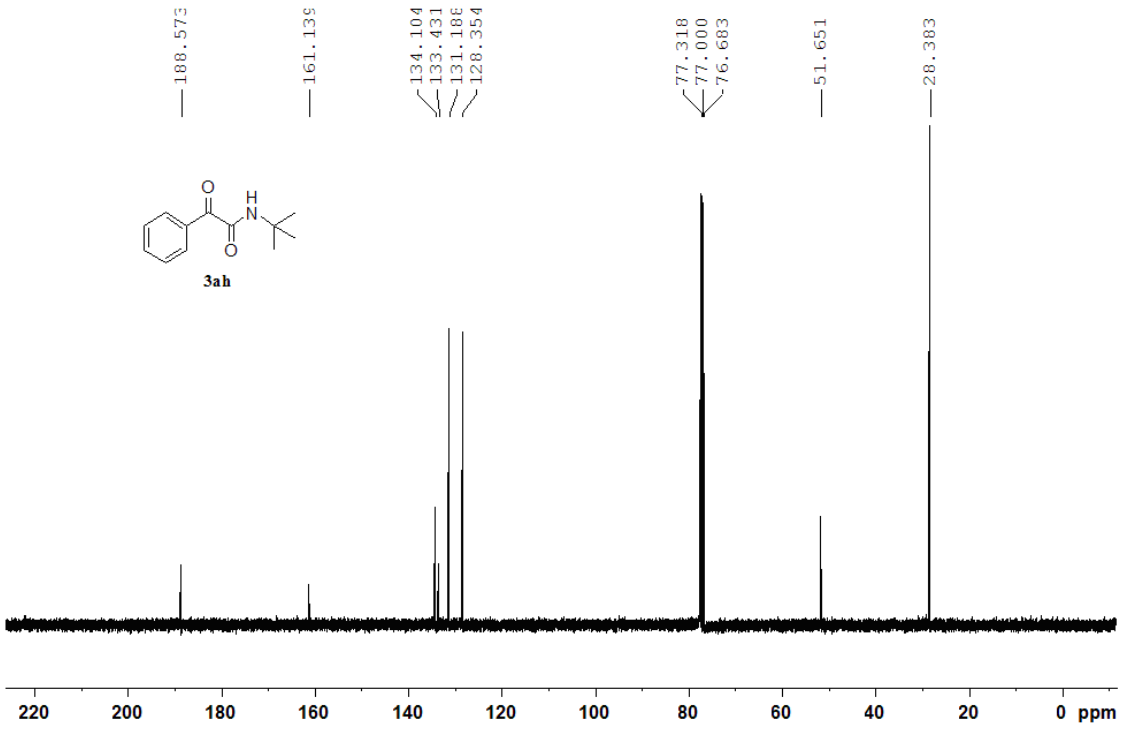
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20
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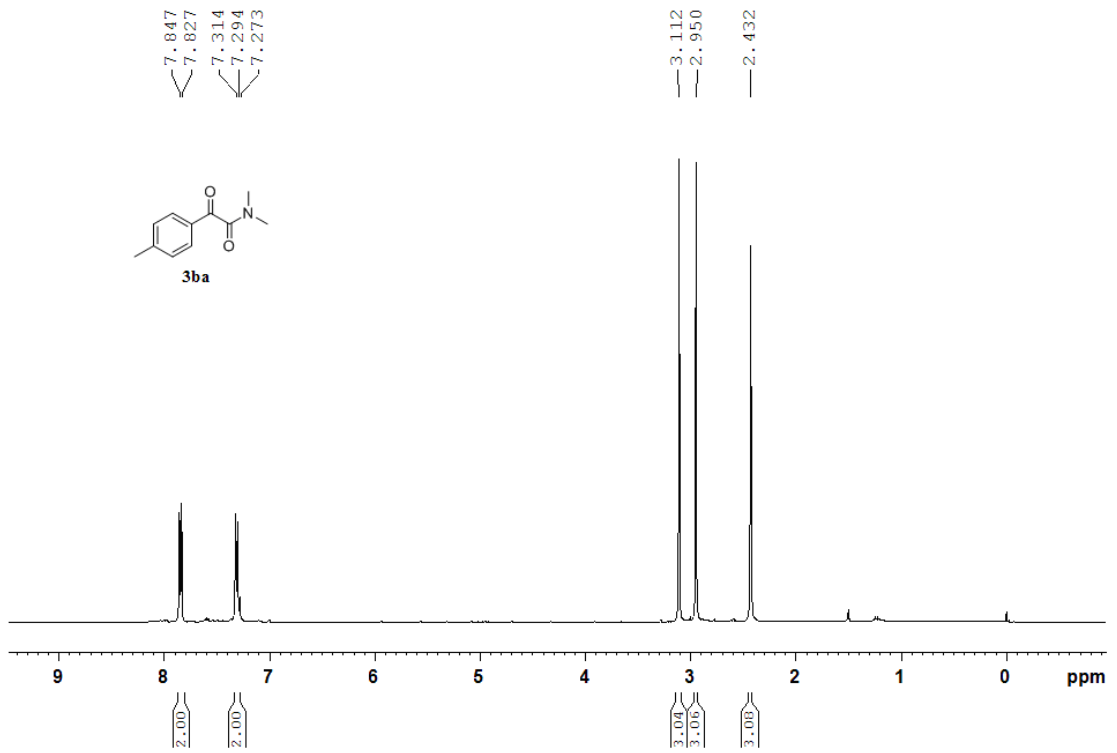
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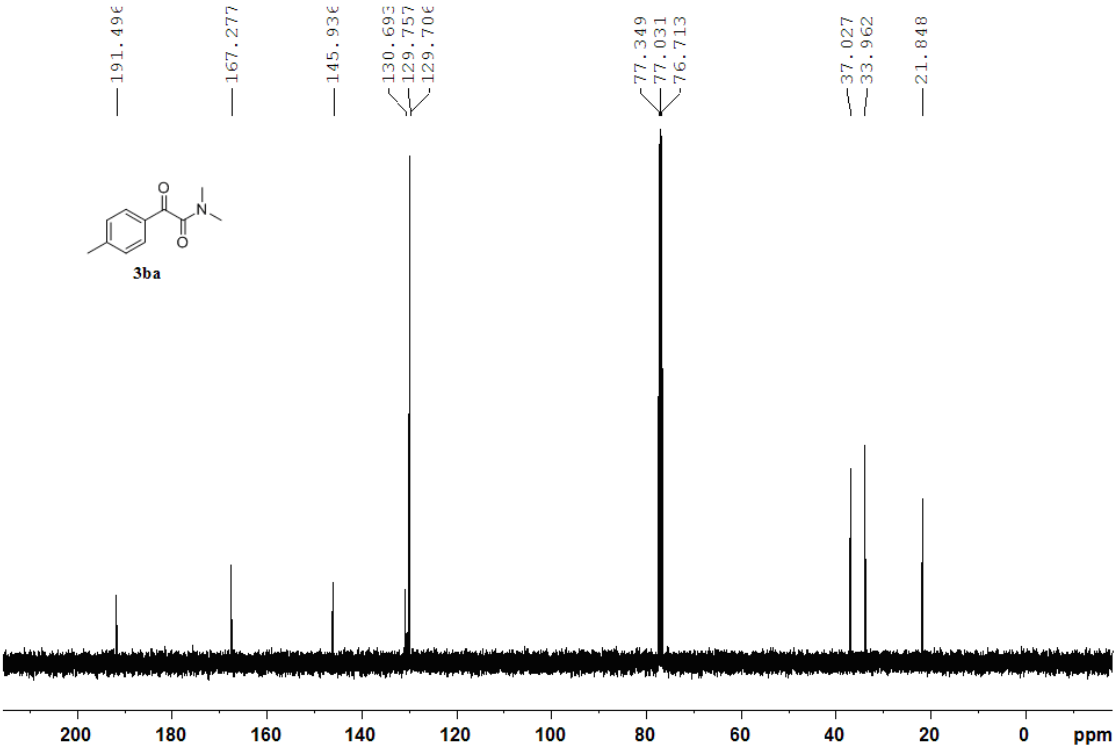
3.04
3.06
3.08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40
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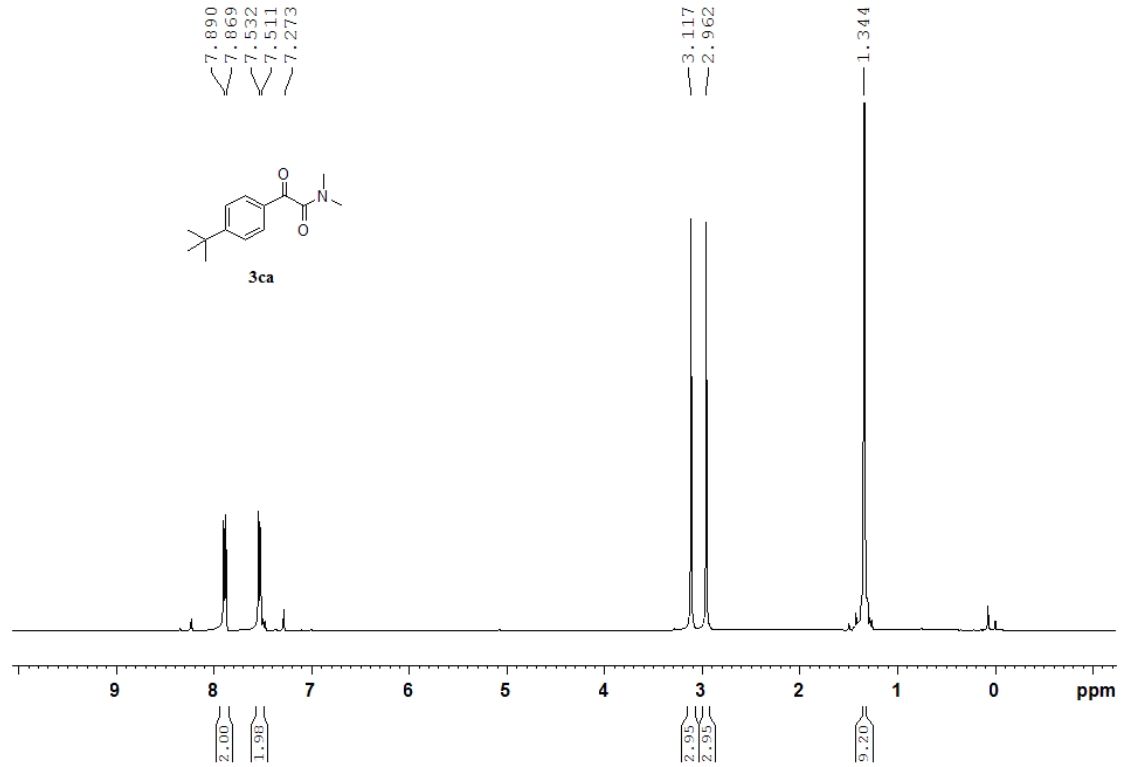
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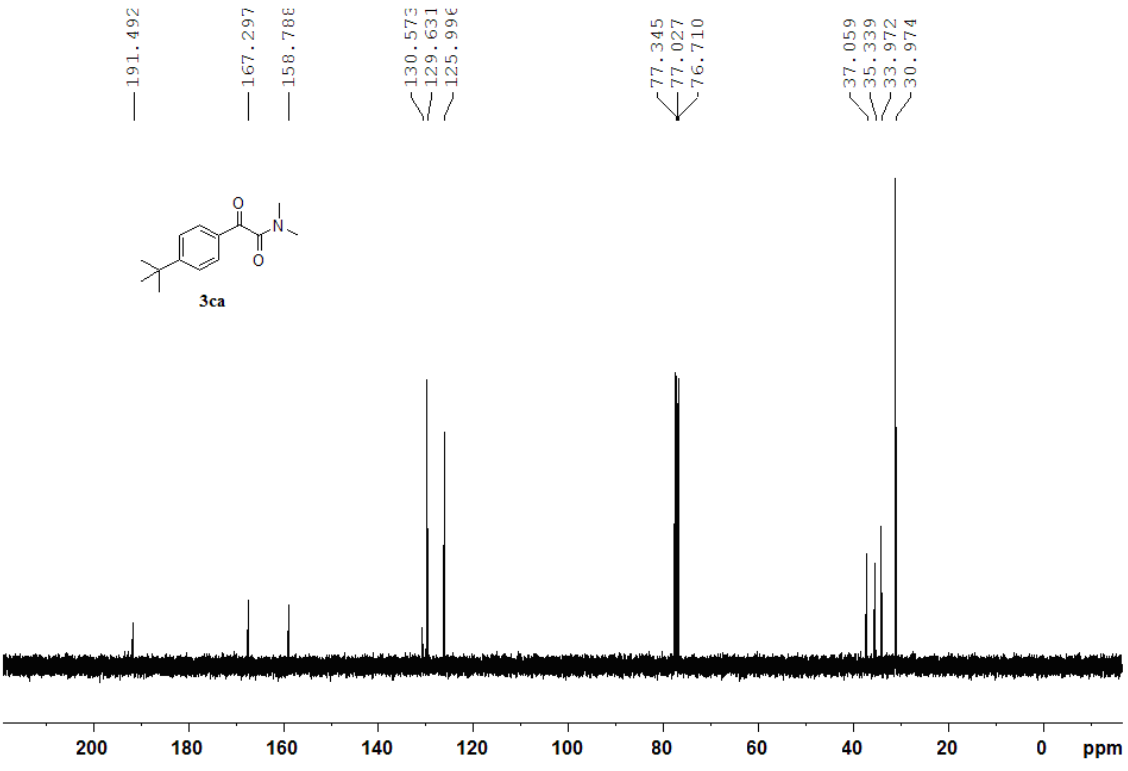
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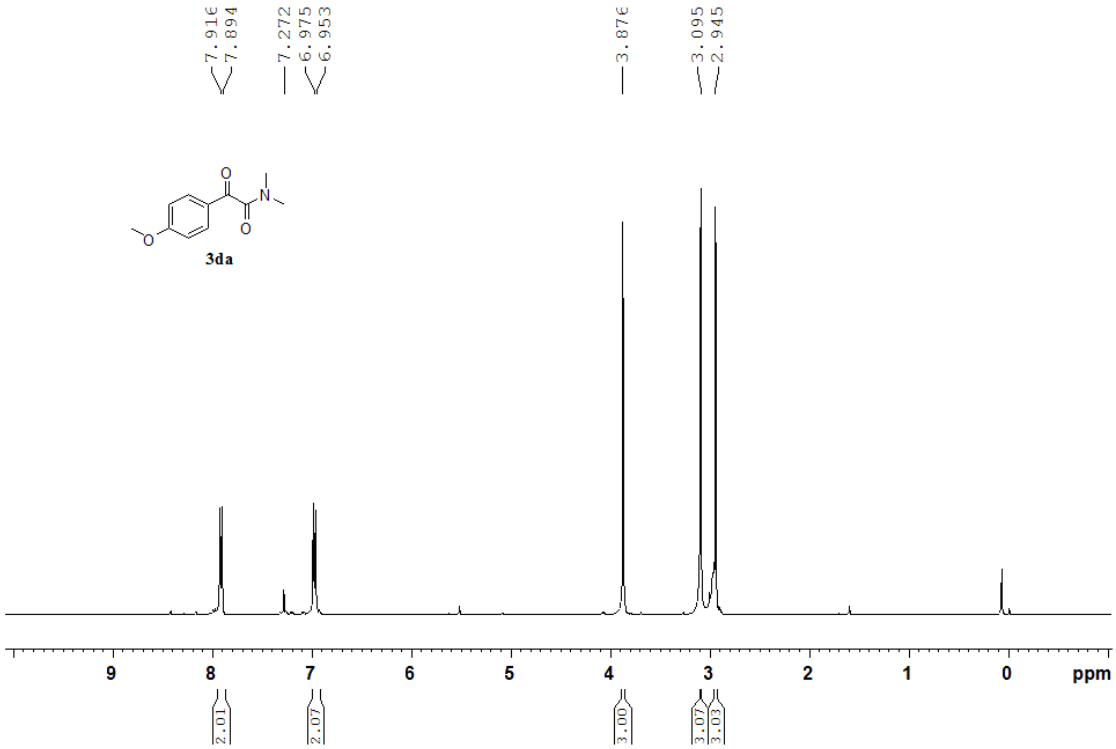
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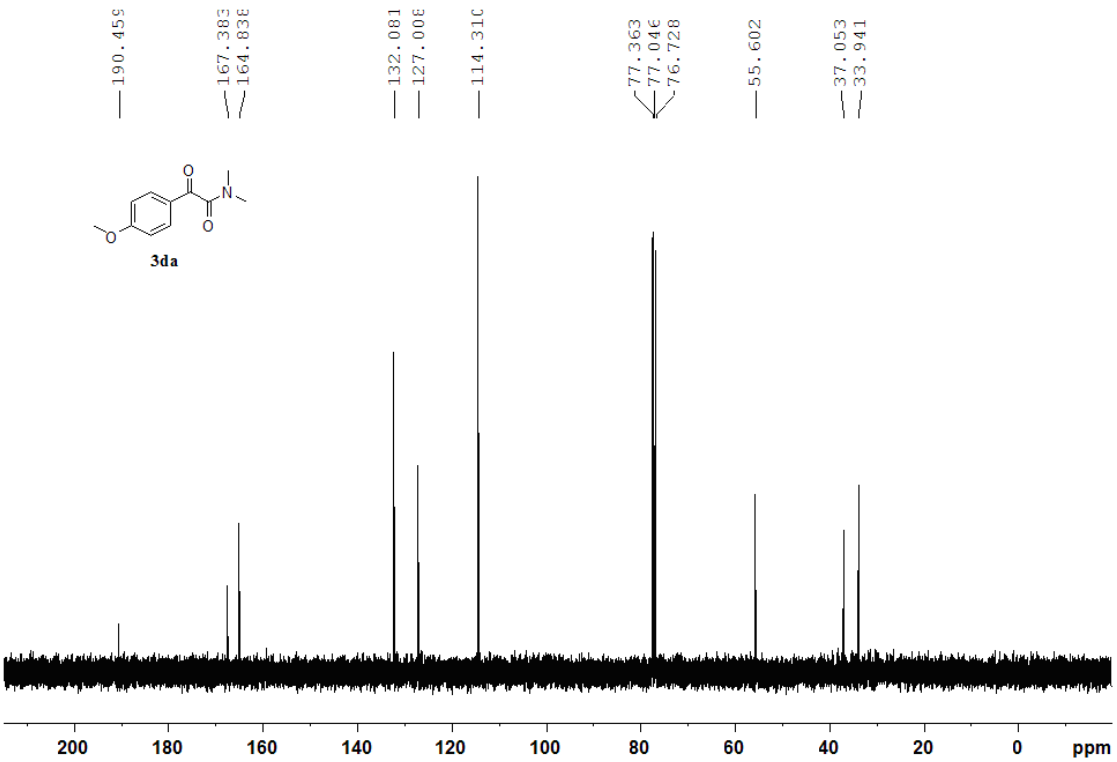
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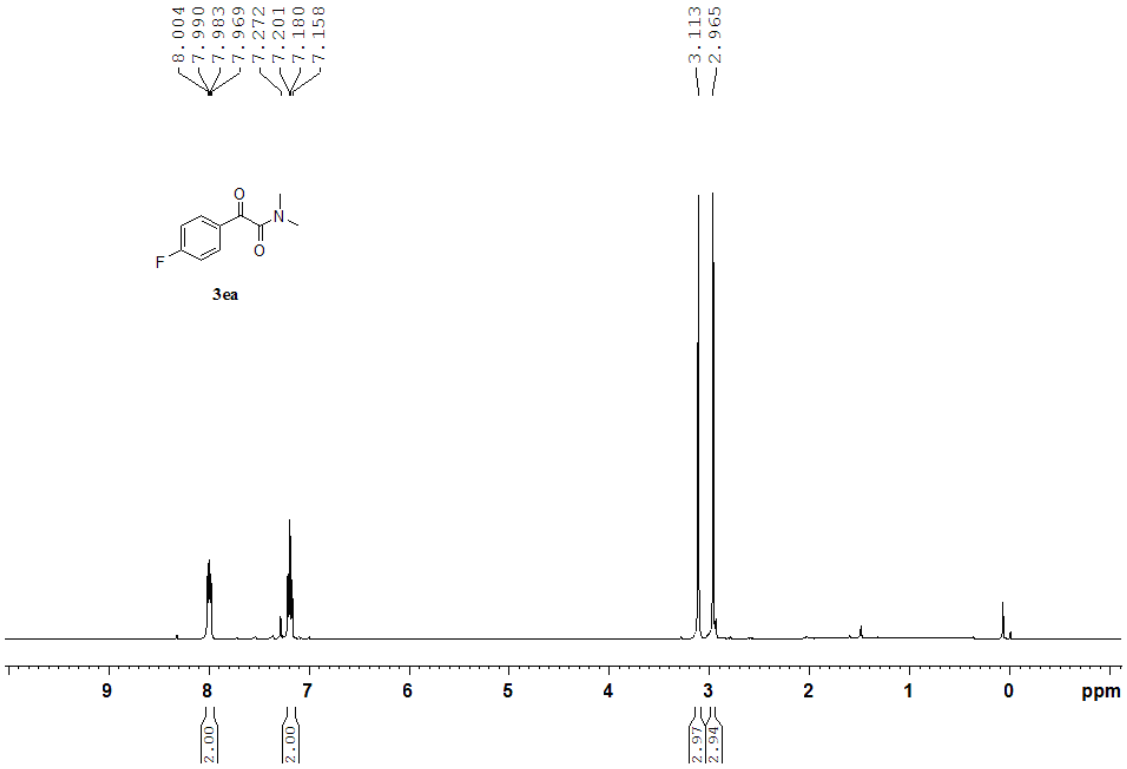
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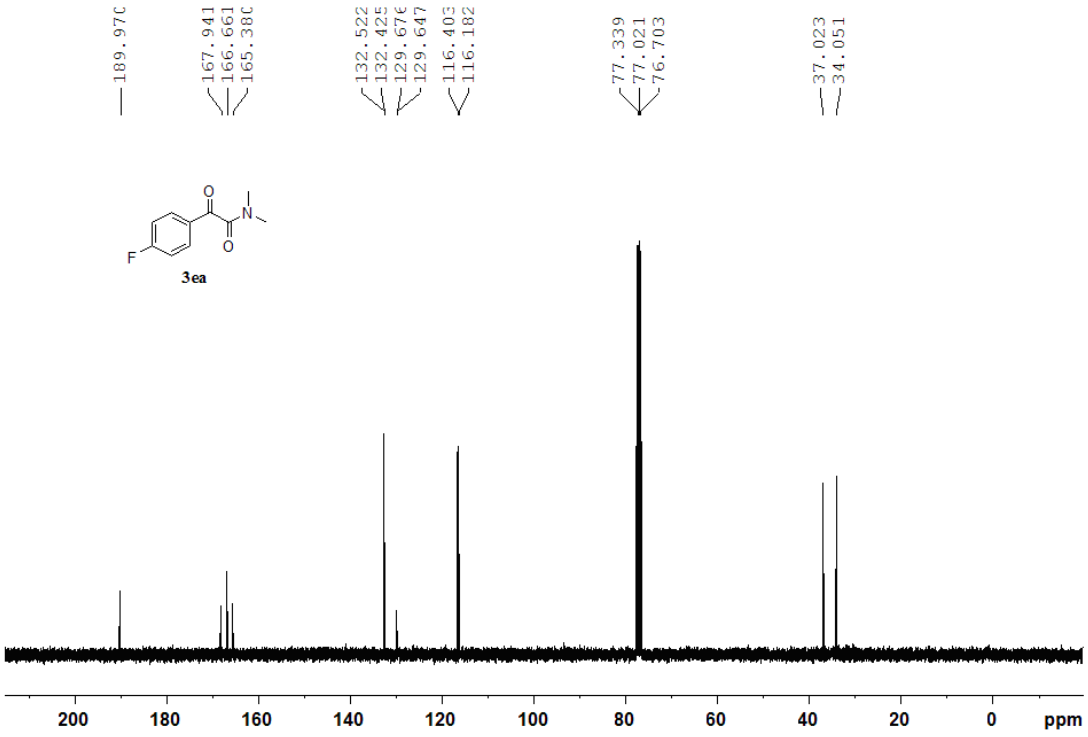
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76.703
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N
O
F
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120
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20
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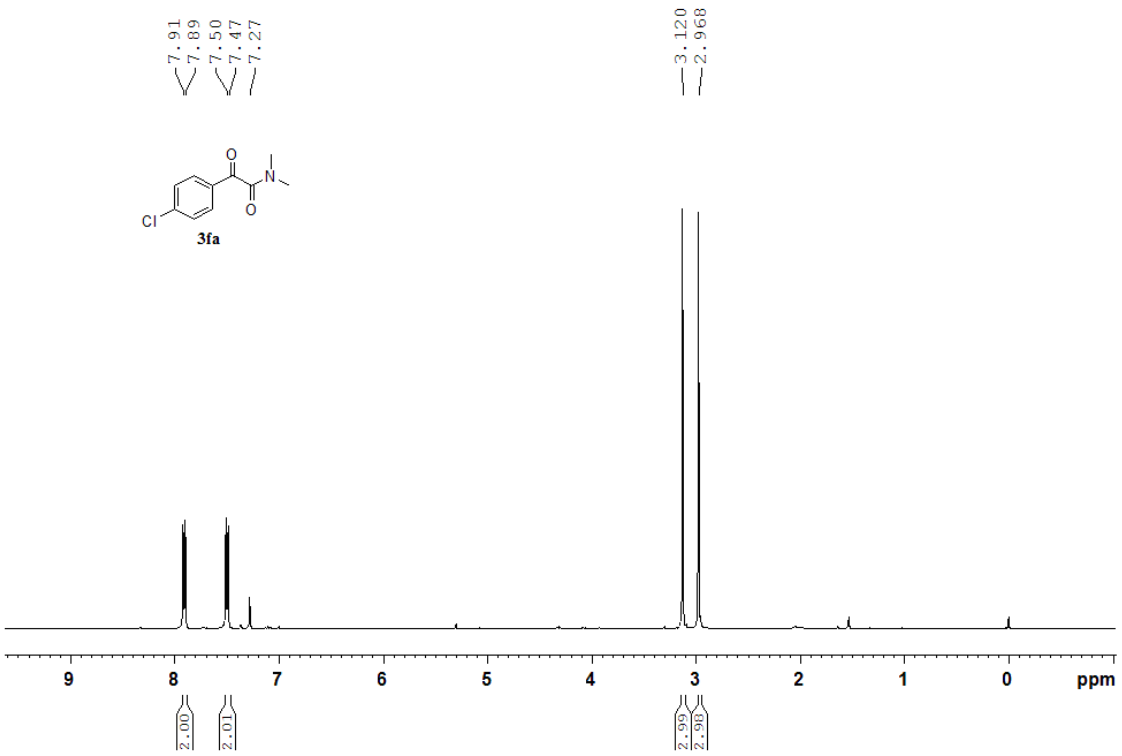
ppm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Cl
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7
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ppm
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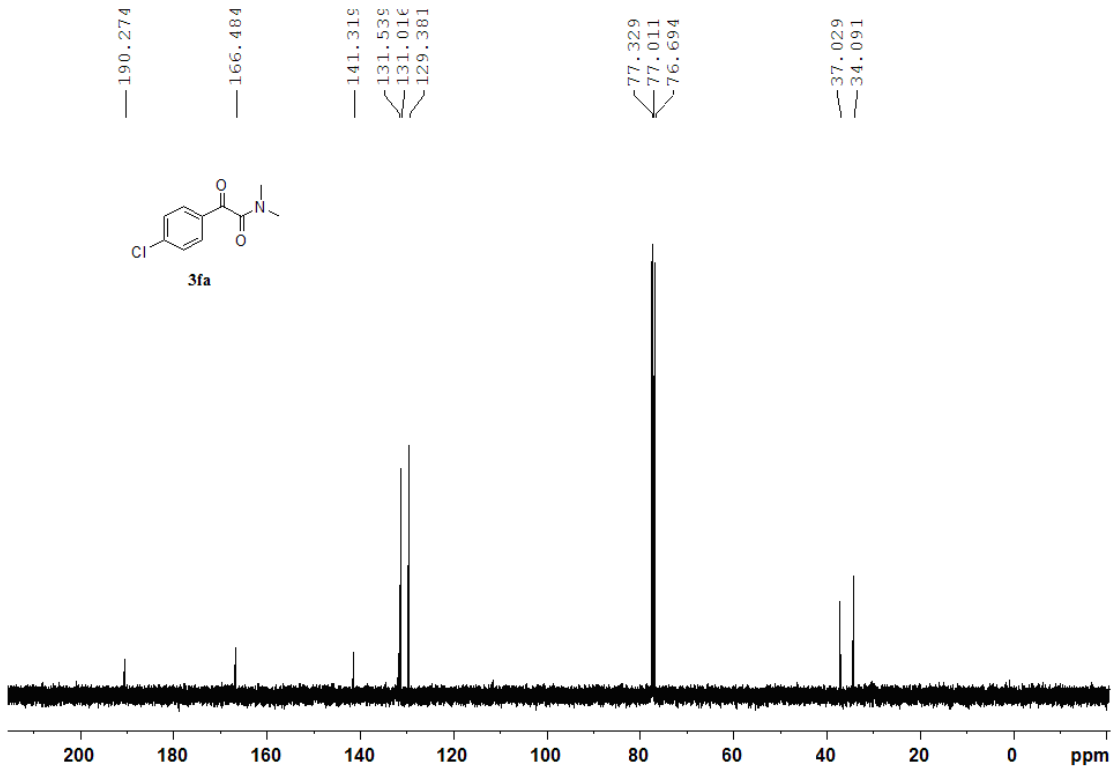
2.98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Cl
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60
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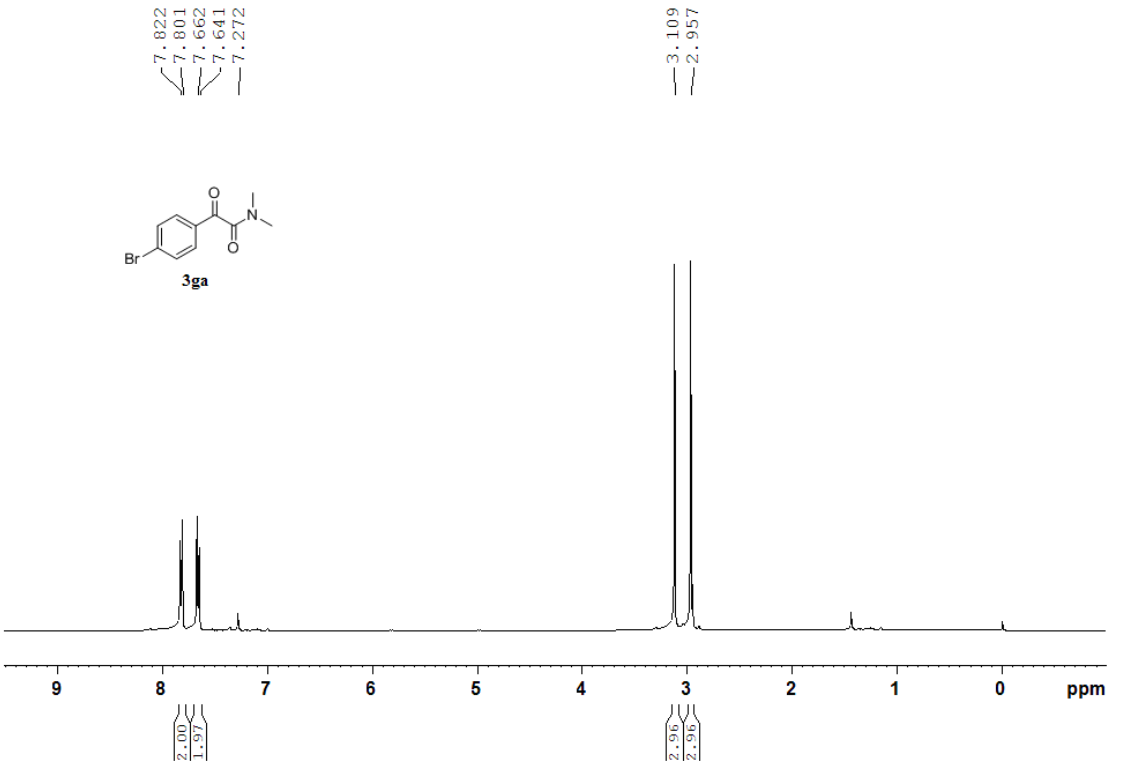
20
0
ppm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Br
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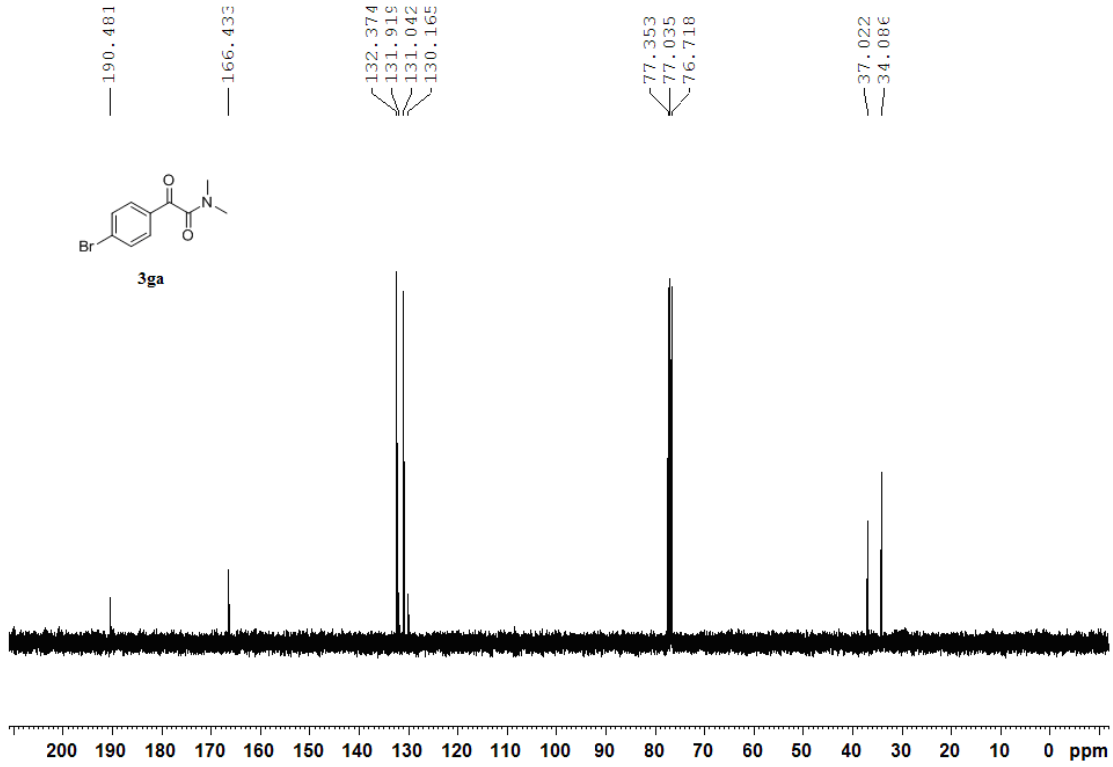
8
7
6
5
4
3
2
1
0
ppm
2.00
1.97
2.96
2.96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132.374
131.919
131.042
130.165
77.353
77.035
76.718
37.022
34.086
Br
O
N
O
3ga
200
190
180
170
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150
140
130
120
110
100
90
80
70
60
50
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30
20
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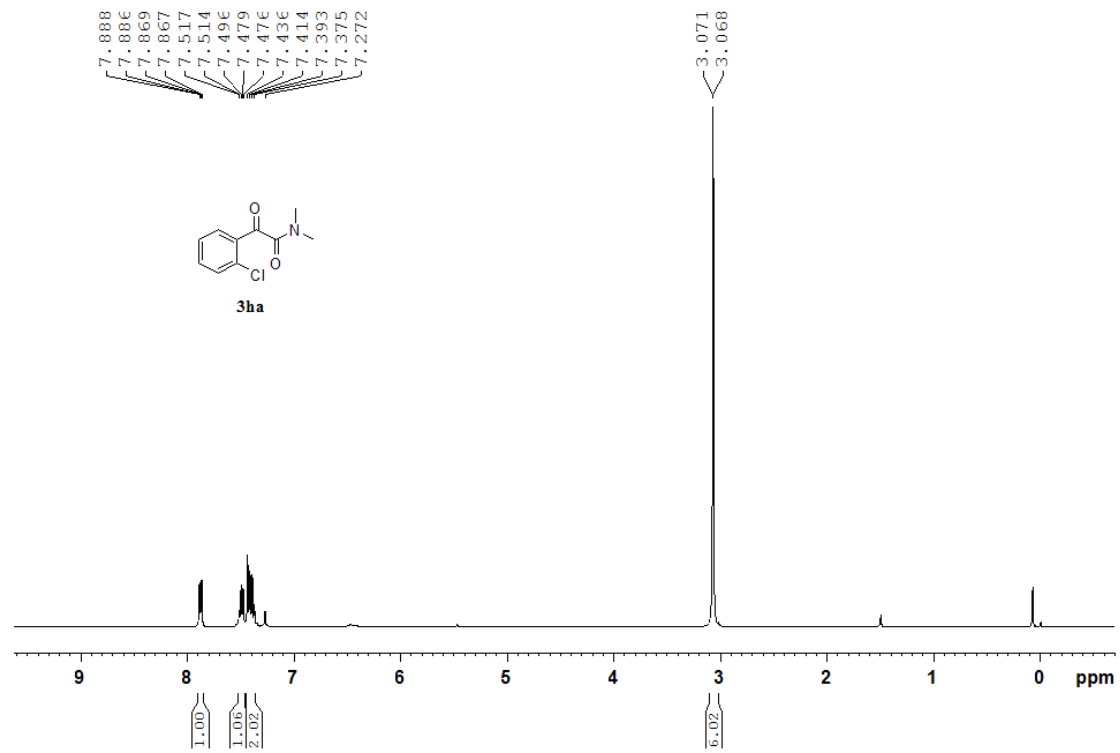
0
ppm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7.869
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7.514
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7.479
7.476
7.436
7.414
7.393
7.375
7.272
3.071
3.068
3ha
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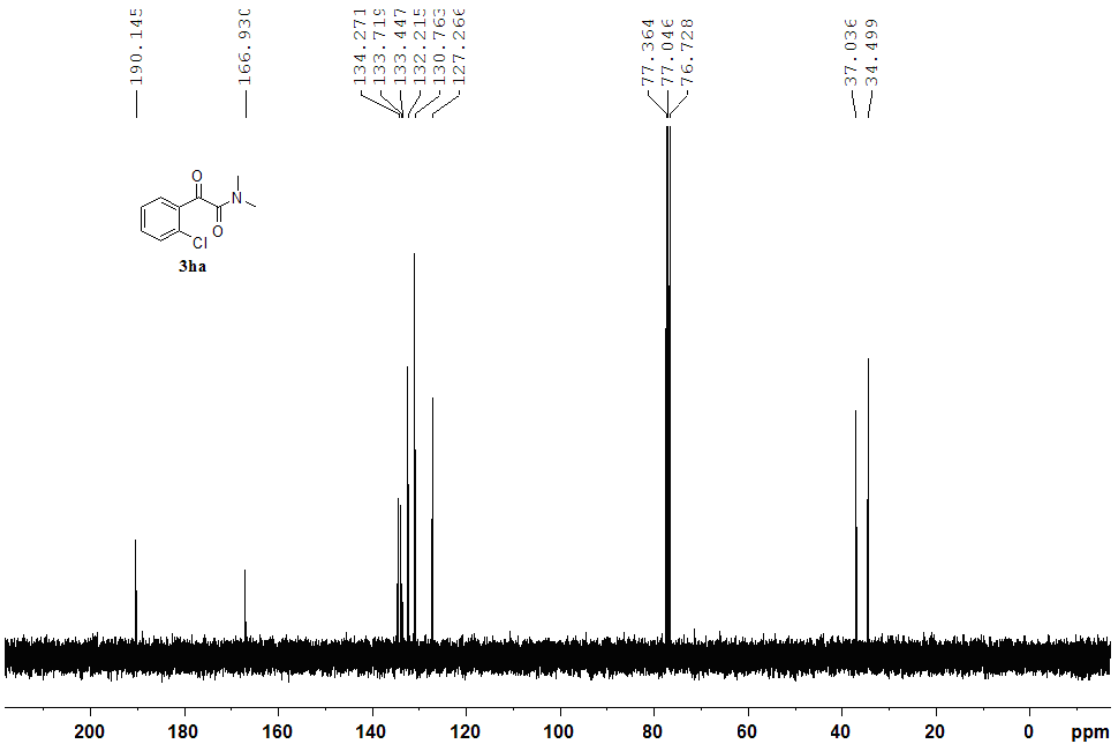
8
7
6
5
4
3
2
1
0
ppm
1.00
1.06
2.02
6.02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166.930
134.271
133.715
133.447
132.215
130.763
127.266
77.364
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37.036
34.499
3ha
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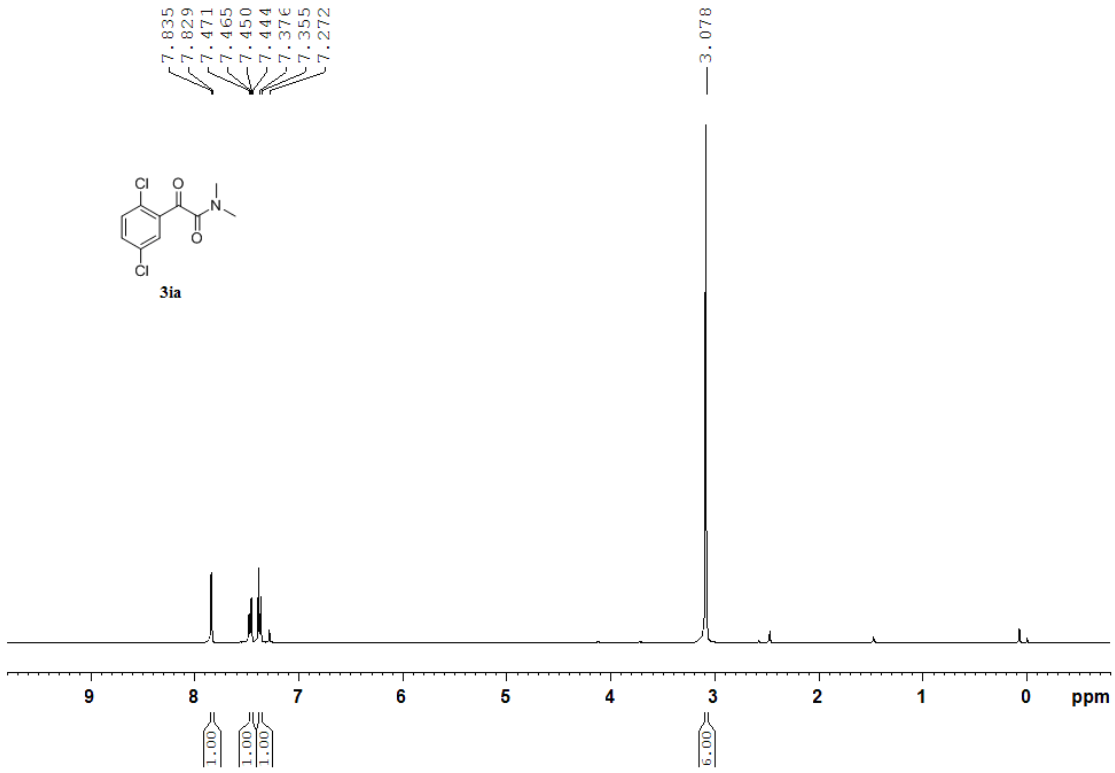
180
160
140
120
100
80
60
40
20
0
ppm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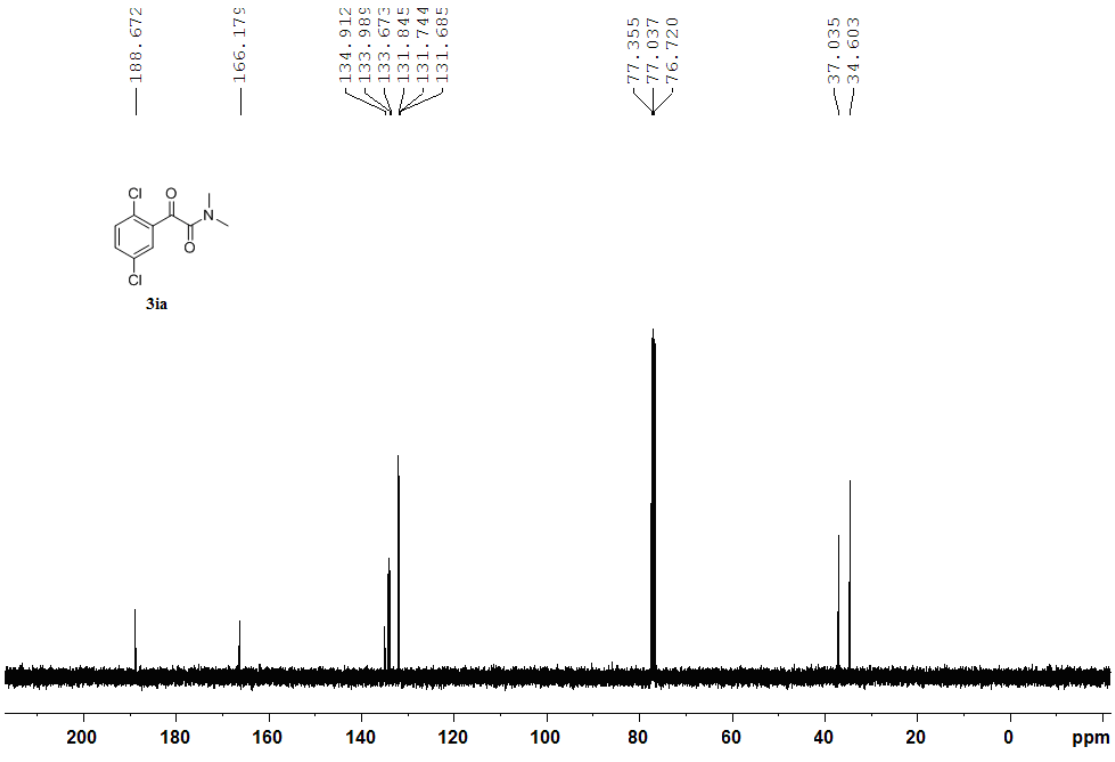
7.471
7.465
7.450
7.444
7.376
7.355
7.272
3.078
Cl
O
N
O
Cl
3ia
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
6.00


188.672
166.179
134.912
133.989
133.673
131.845
131.744
131.685
77.355
77.037
76.720
37.035
34.603
Cl
O
N
O
Cl
3ia
200
180
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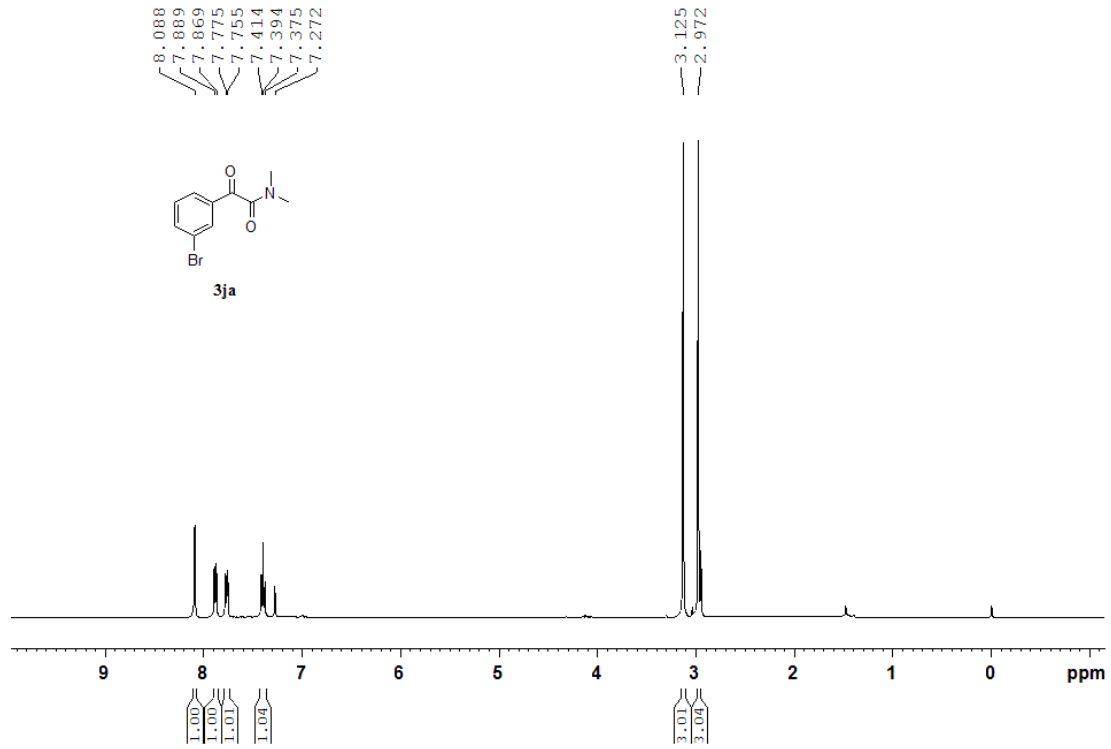
140
120
100
80
60
40
20
0
ppm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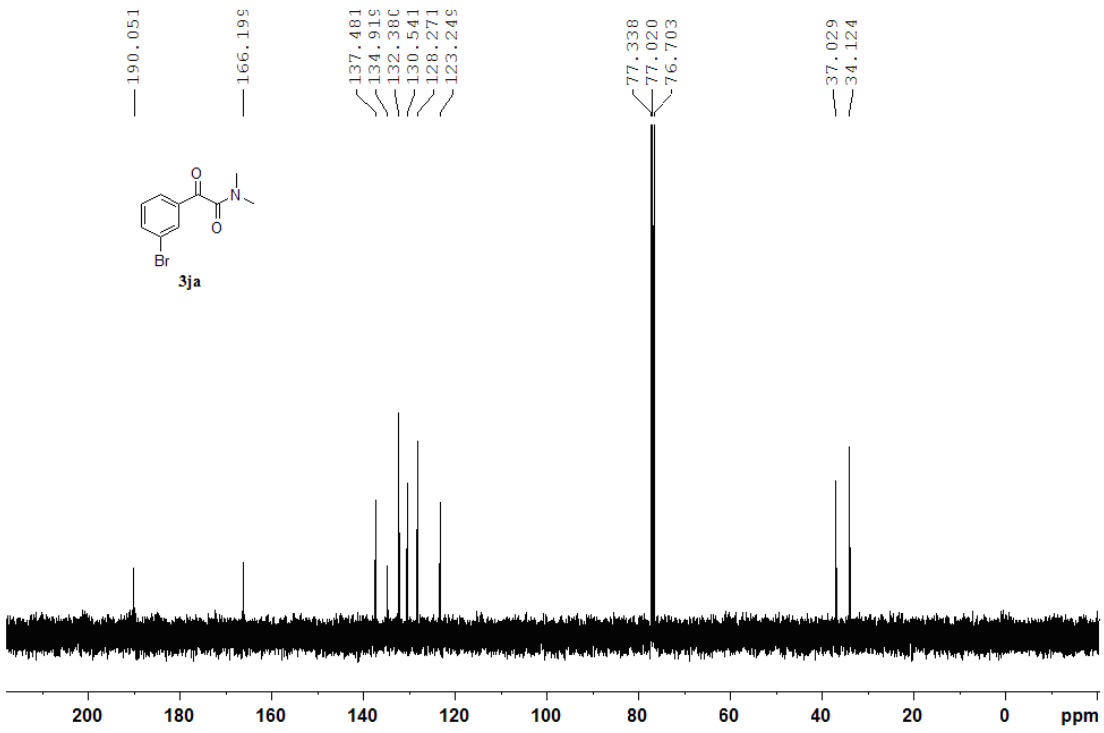
7.889
7.869
7.775
7.755
7.414
7.394
7.375
7.272
3.125
2.972
Br
3ja
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.01
1.04
3.01
3.04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137.481
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132.38
130.541
128.271
123.24
77.338
77.020
76.703
37.029
34.124
Br
3ja
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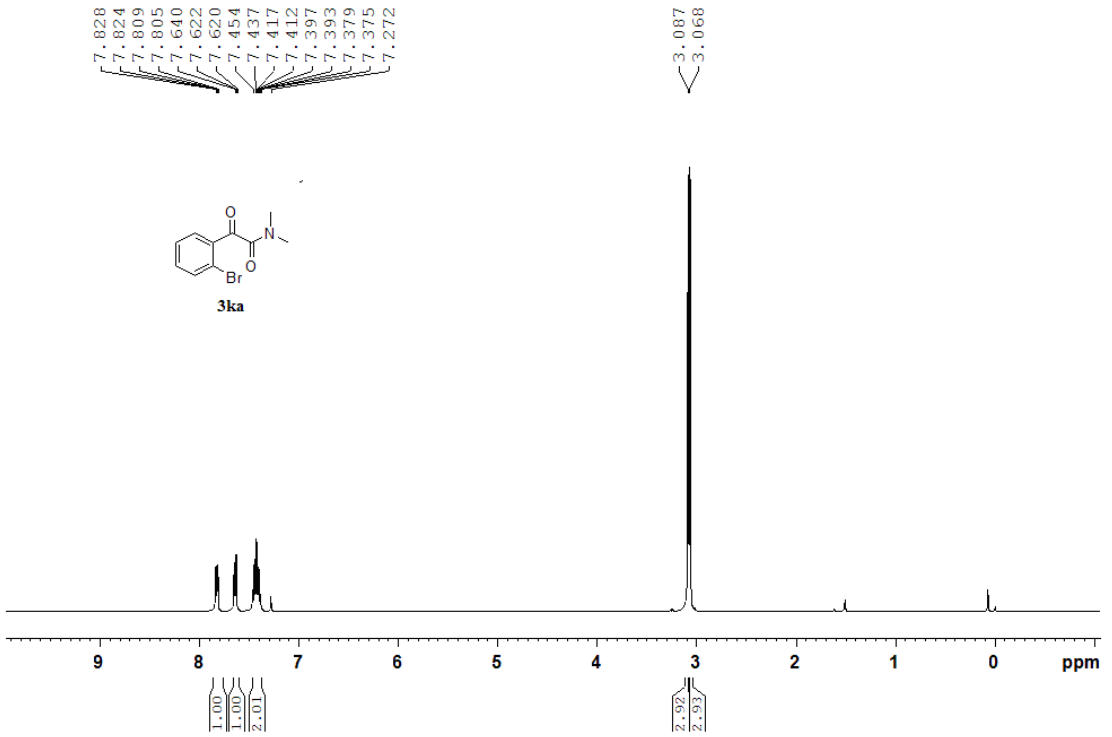
160
140
120
100
80
60
40
20
0
ppm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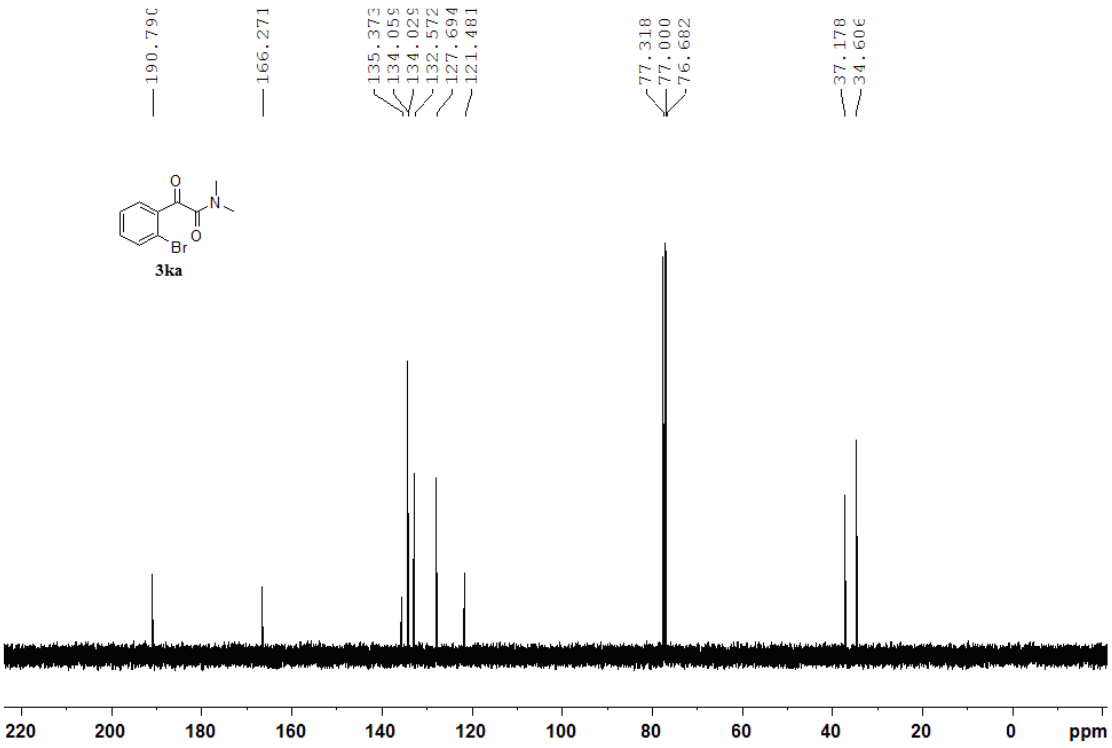
7.809
7.805
7.640
7.622
7.620
7.454
7.437
7.417
7.412
7.397
7.393
7.379
7.375
7.272
3.087
3.068
O
N
O
Br
3ka
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
2.01
2.92
2.93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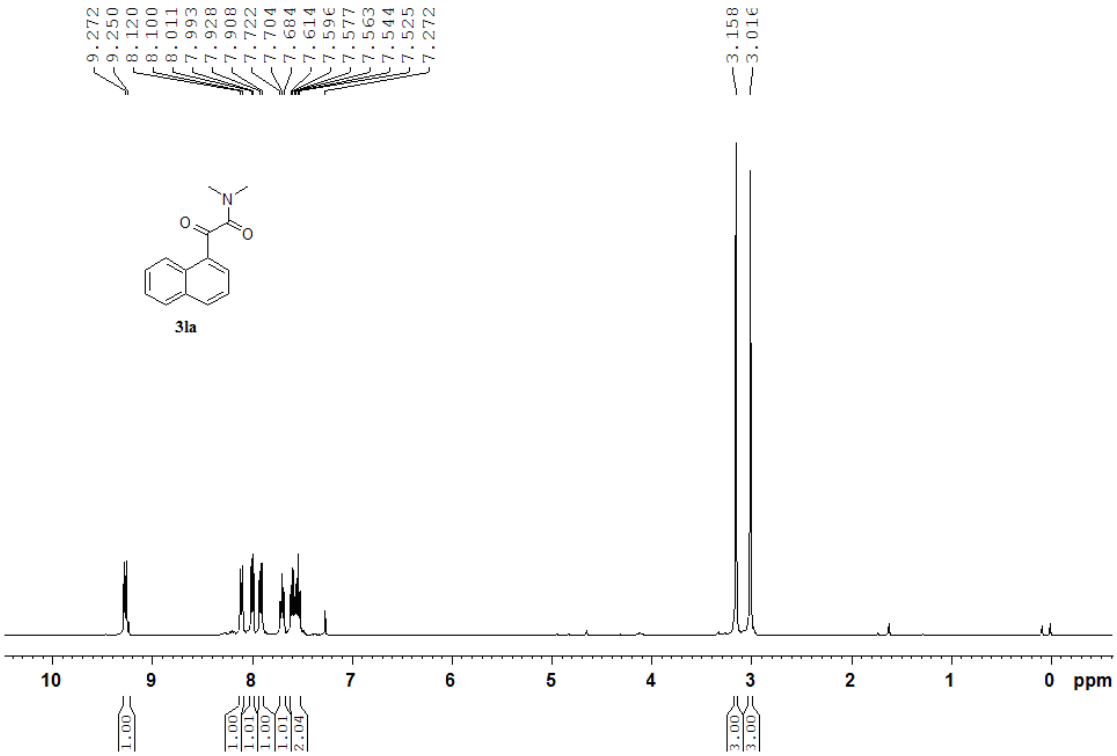
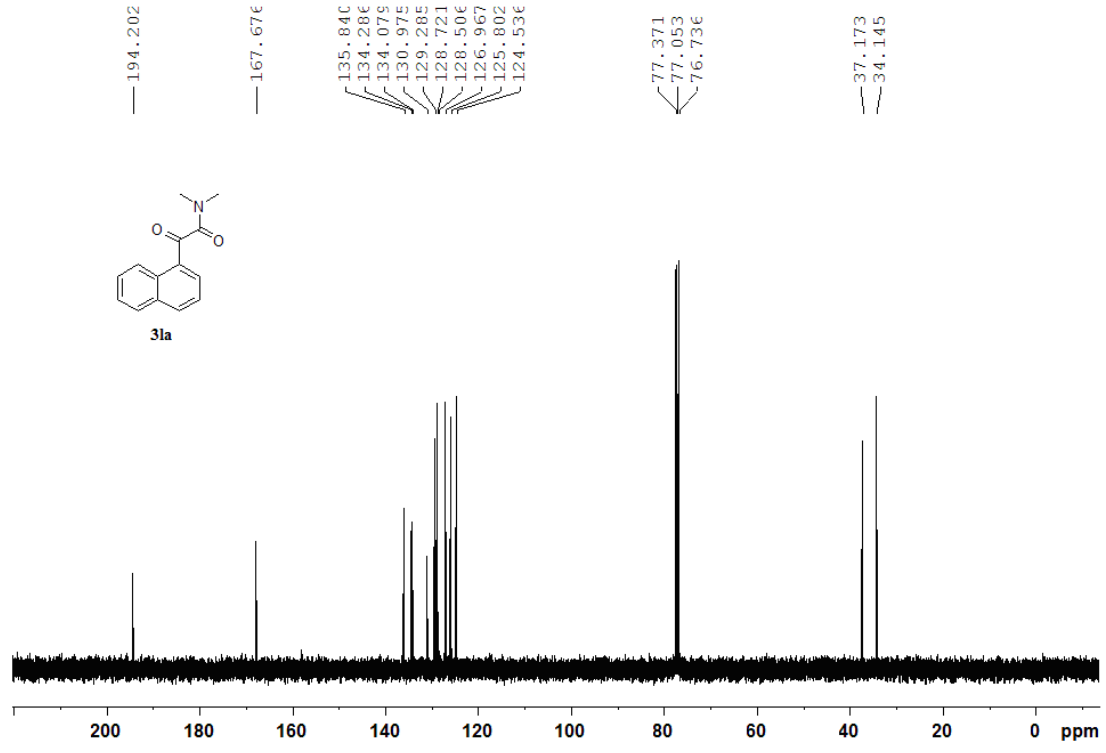
134.059
134.029
132.572
127.694
121.481
77.318
77.000
76.682
37.178
34.606
O
N
O
Br
3ka
220
200
180
160
140
120
100
80
60
40
20
0
ppm


9.272
9.250
8.120
8.100
8.011
7.993
7.928
7.908
7.722
7.704
7.684
7.614
7.596
7.577
7.563
7.544
7.525
7.272
3.158
3.016
3la
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.01
2.04
3.00
3.00


194.202
167.676
135.840
134.286
134.079
130.975
129.285
128.721
128.506
126.967
125.802
124.536
77.371
77.053
76.736
37.173
34.145
3la
200
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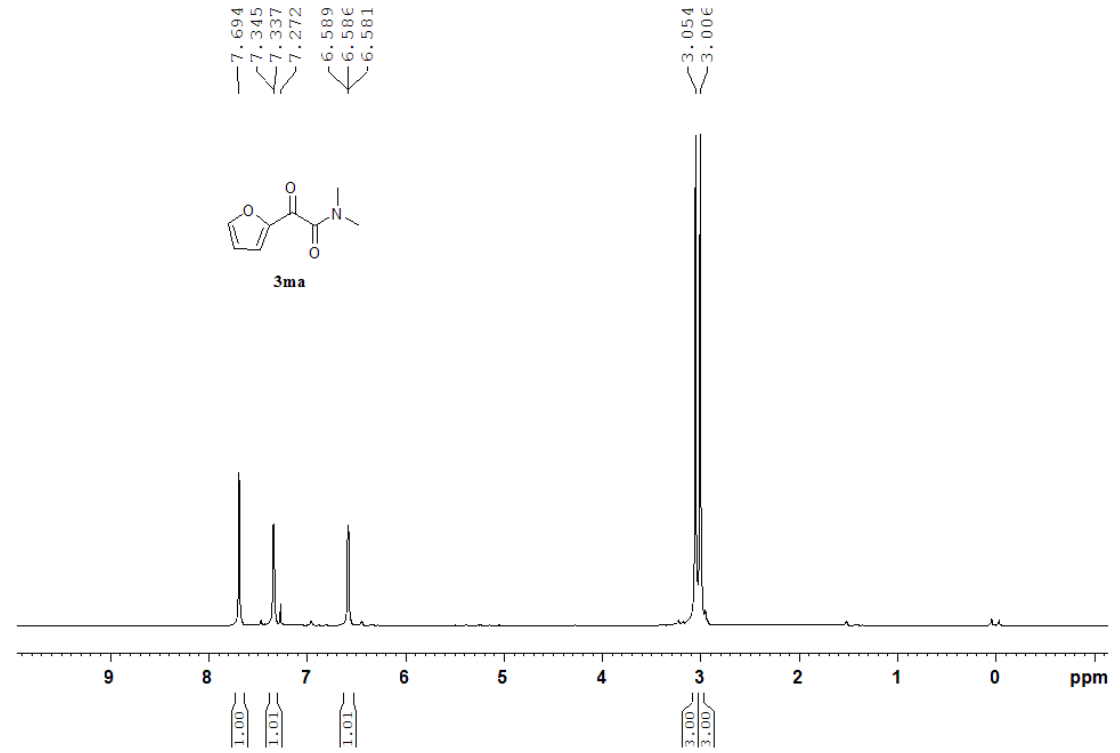
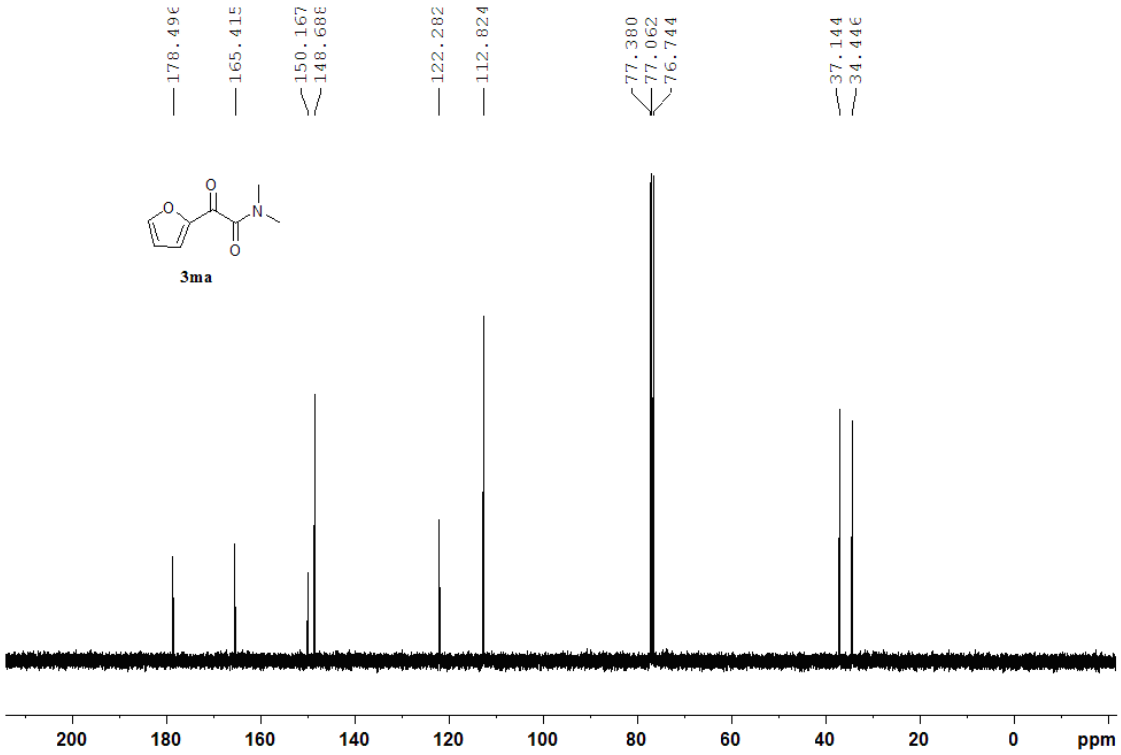
160
140
120
100
80
60
40
20
0
ppm


7.694
7.345
7.337
7.272
6.589
6.586
6.581
3.054
3.006
3ma
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.01
3.00
3.00


178.496
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150.167
148.688
122.282
112.824
77.380
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37.144
34.446
3ma
200
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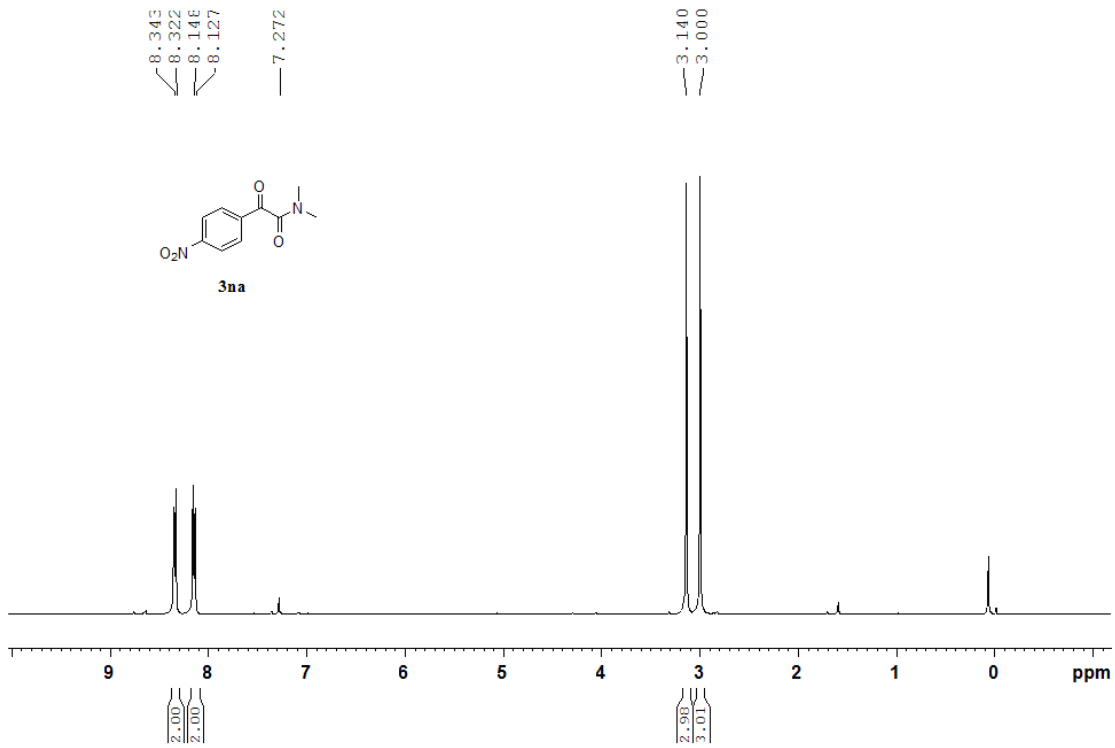
120
100
80
60
40
20
0
ppm


8.343
8.322
8.148
8.127
7.272
3.140
3.000
3na
9
8
7
6
5
4
3
2
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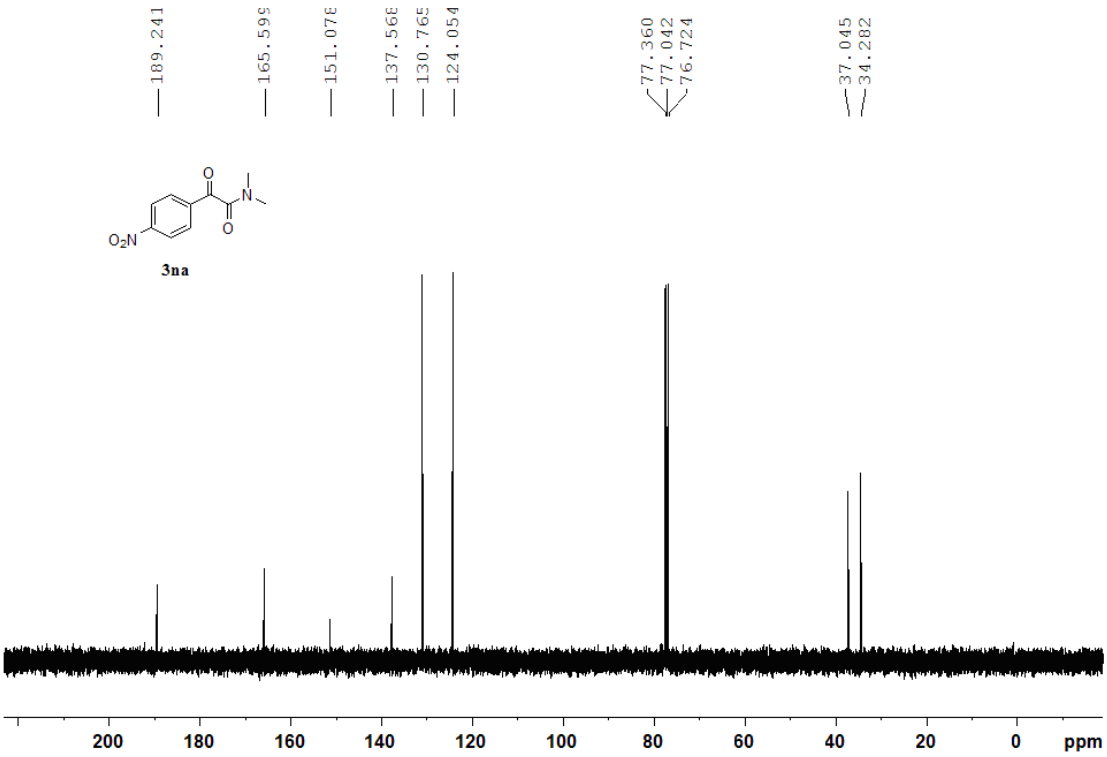
0
ppm
2.00
2.00
2.98
3.01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137.568
130.765
124.054
77.360
77.042
76.724
37.045
34.282
3na
200
180
160
140
120
100
80
60
40
20
0
ppm