Supporting information

Chemoselective photocatalytic oxidation of alcohols to aldehydes and ketones by nitromethane on titanium dioxide under violet 400 nm LED light irradiation

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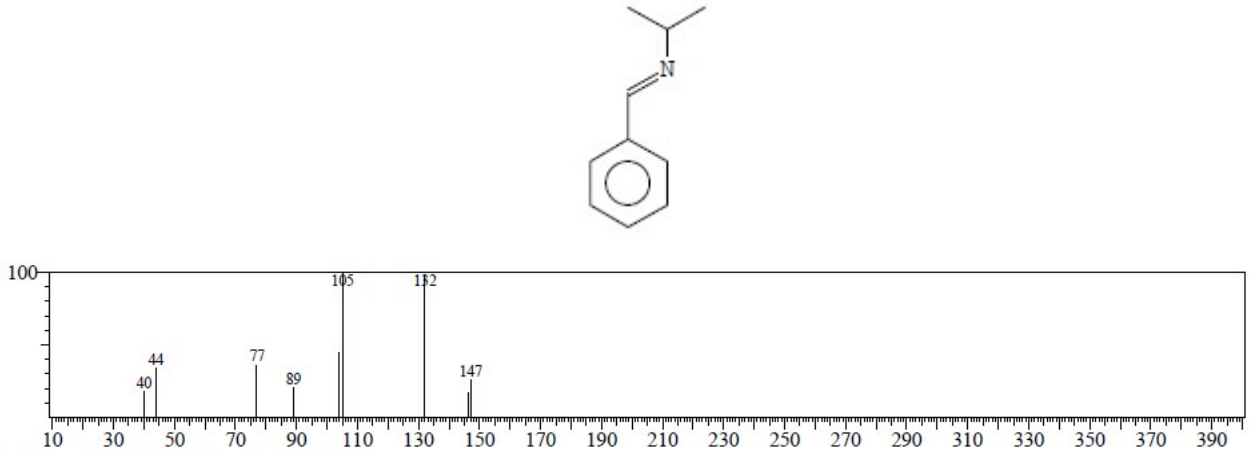
1.mass spectrum

a)



b)

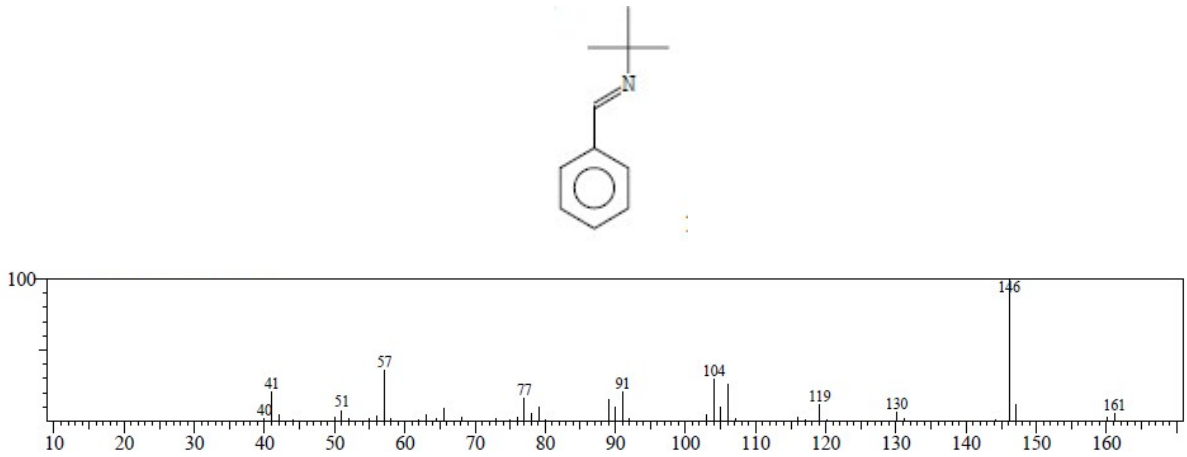
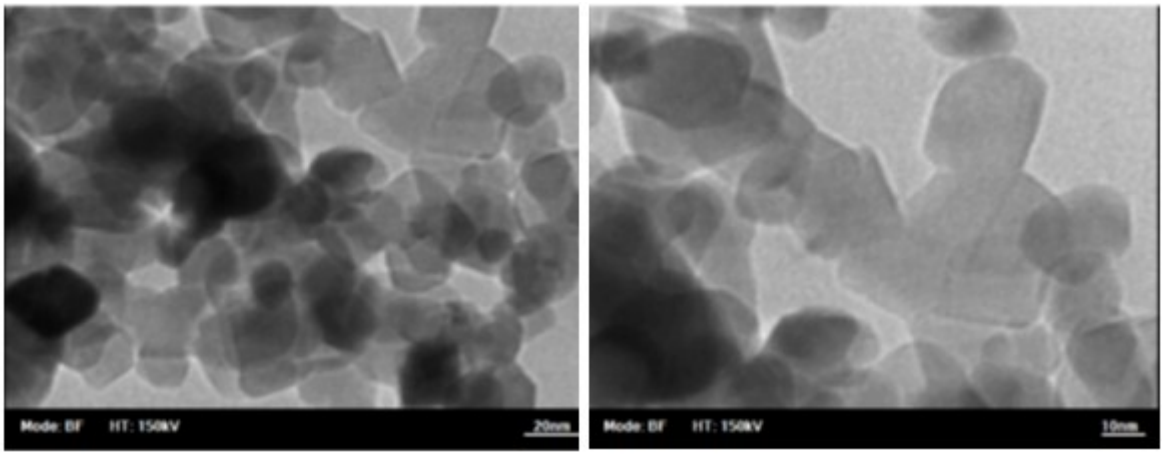


Figure S1: The mass spectrum of the eimines obtained in the reaction of benzaldehyde in the presence of a) 2-nitropropane and b) 2-methyl-2-nitropropane

2. TEM

a)



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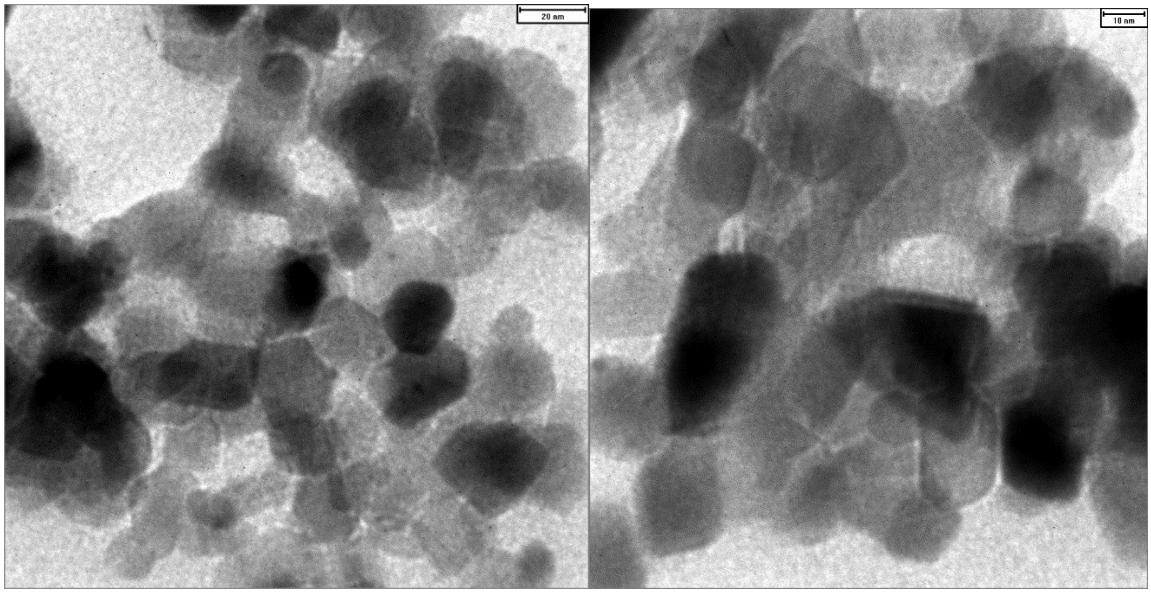


Figure S2: TEM images of TiO_2 - P25 before (a) and after the reaction (b)

3.TGA

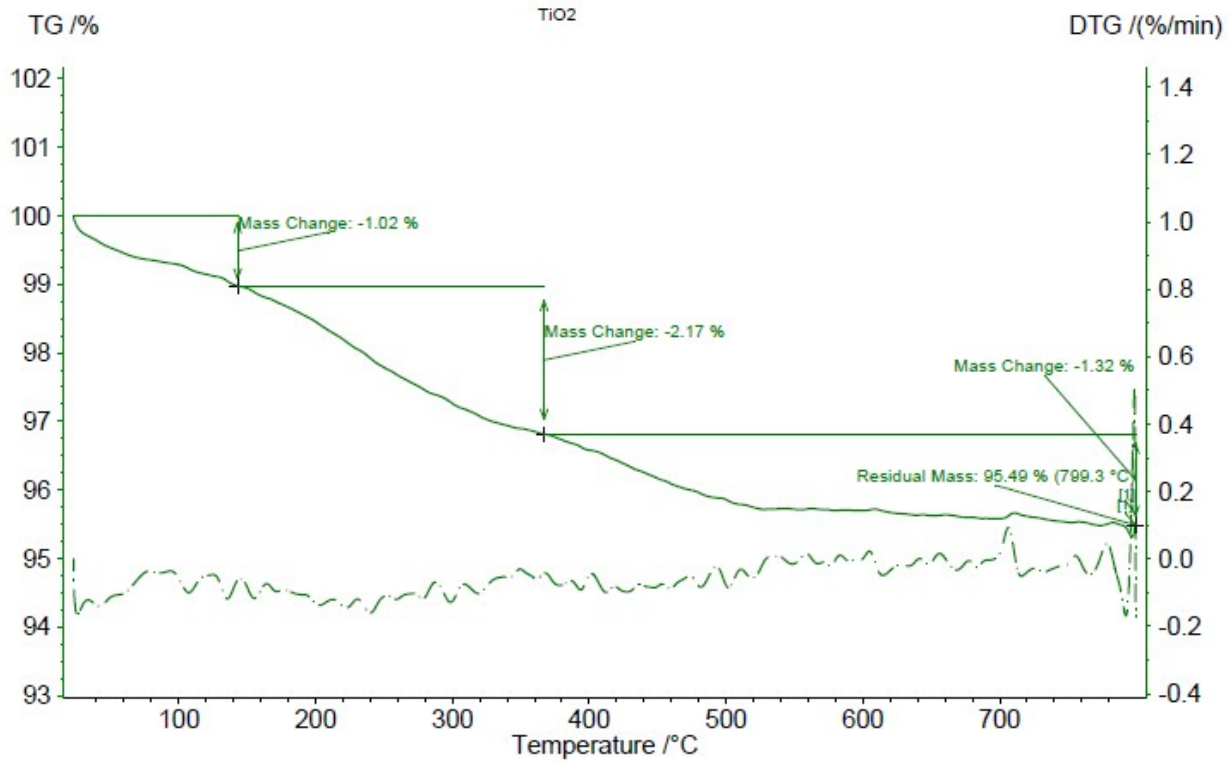


Figure S3. TG/DTG analysis of TiO_2- P25 after the reaction

4. BET

Table S1: Physical Properties of the Catalyst

catalyst	BET(m^2/g)	Pore volume
TiO_2 P25 before the reaction	70	0.6
TiO_2 P25 after the reaction	49.4	0.41

a) **b)**

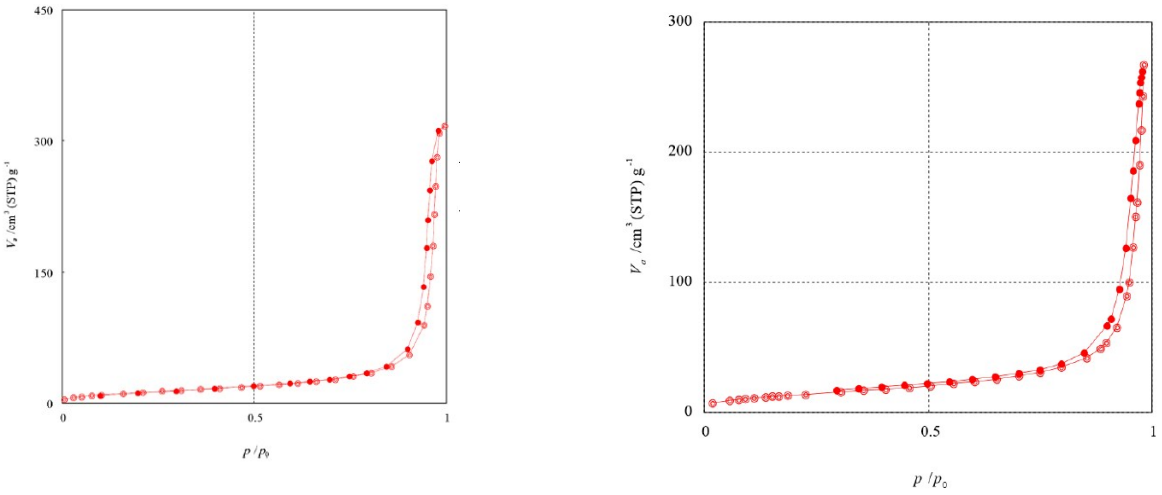


Figure S4. N_2 Adsorption / desorption isotherm of TiO_2 P25 before (a) and after the reaction (b)

5. Reusability of the catalyst

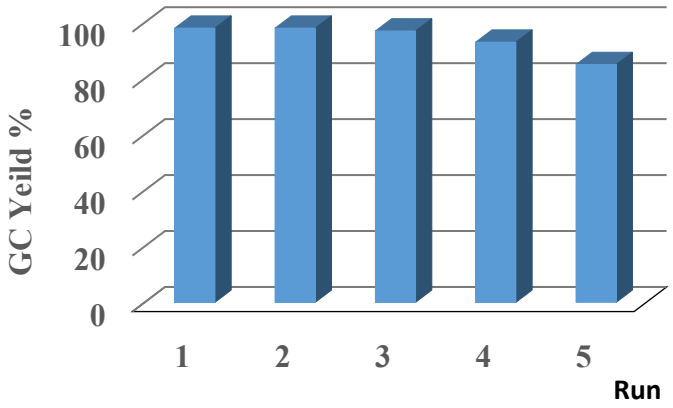


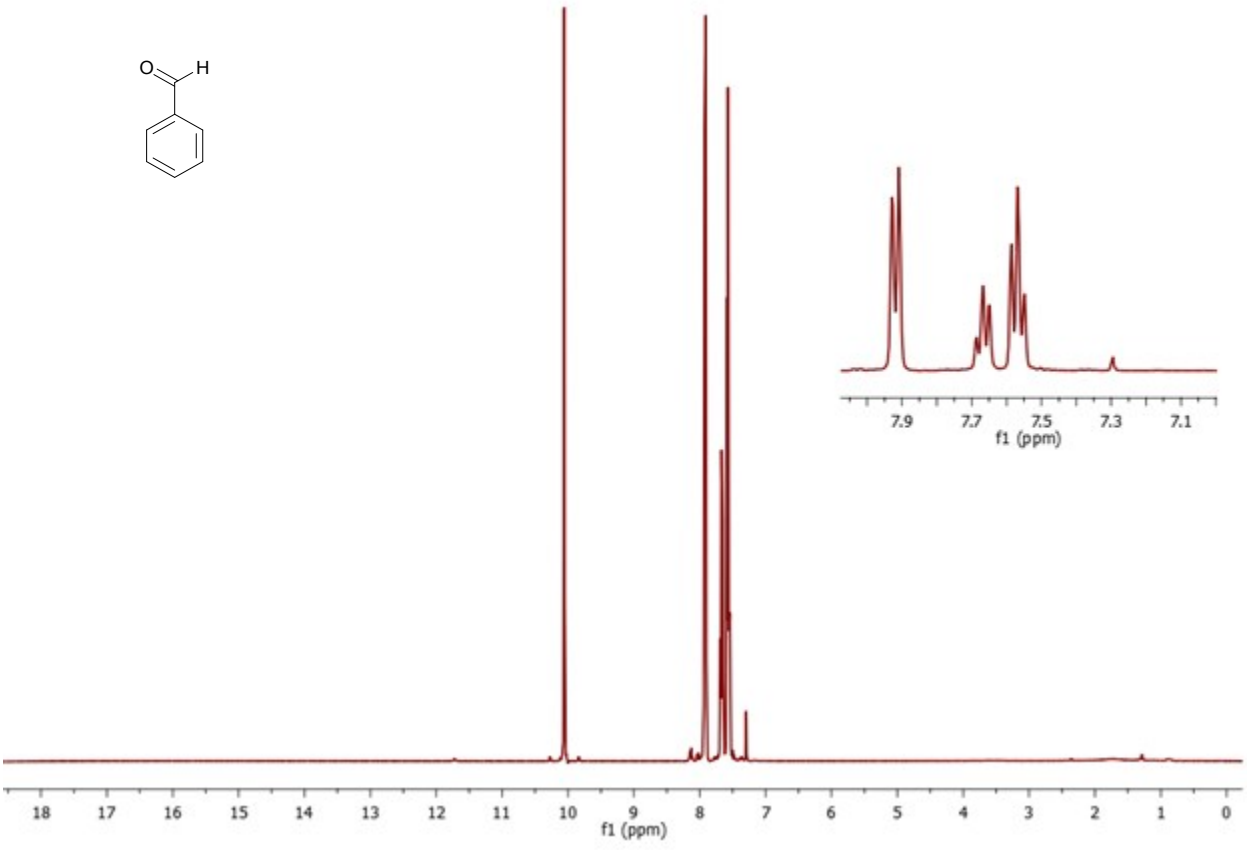
Figure S5. Reusability of the catalyst in the photocatalytic oxidation of 4-methoxybenzyl alcohol under light irradiation

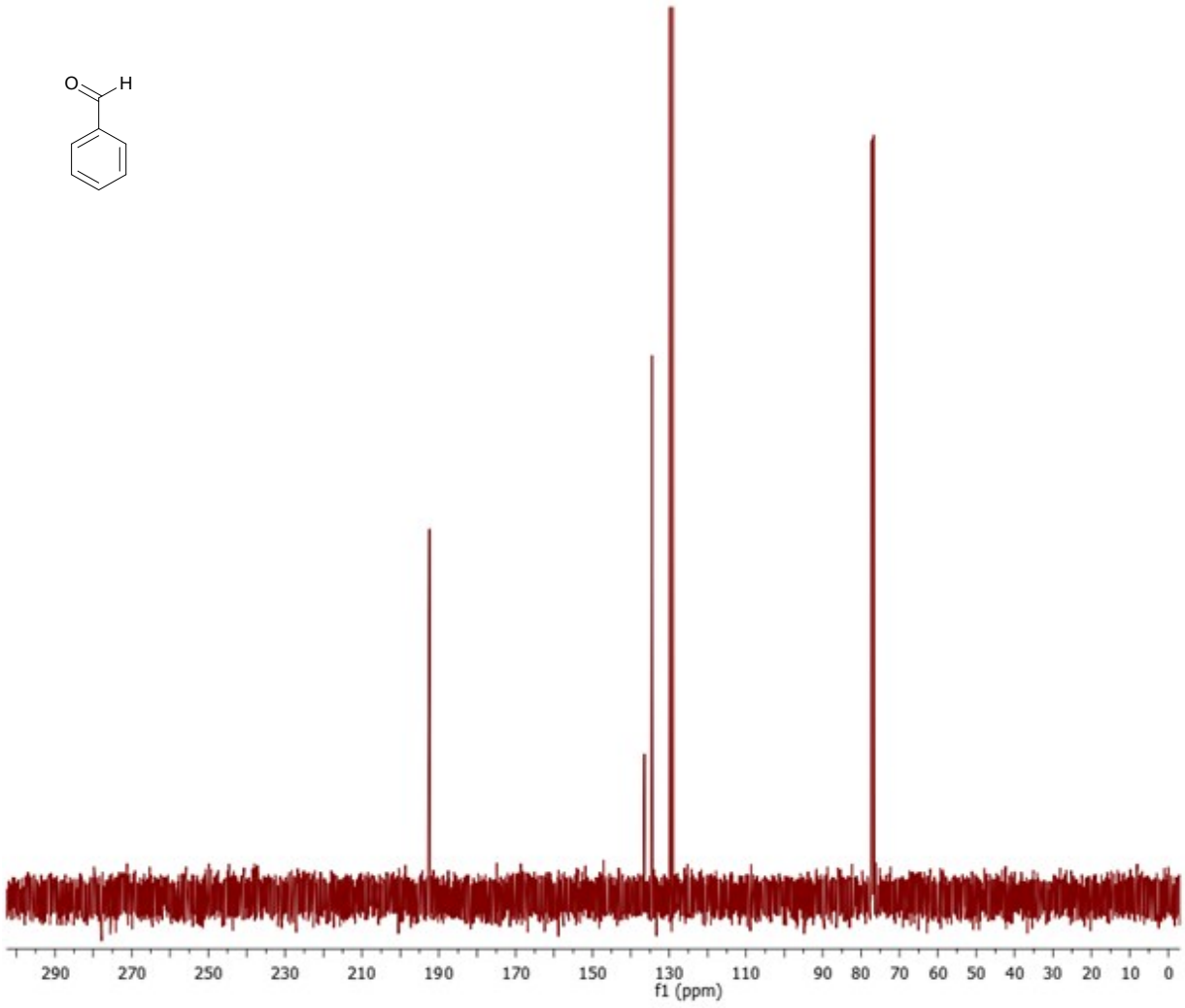
6. ^{13}C NMR and ^{1}H NMR spectra of products

Synthesized compounds are known compounds. [1-8] The spectrum of NMR products is as follows:

Benzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.06 (s, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.70 – 7.64 (m, 1H), 7.57 (t, J = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 192.40, 136.44, 134.48, 129.76, 129.02.

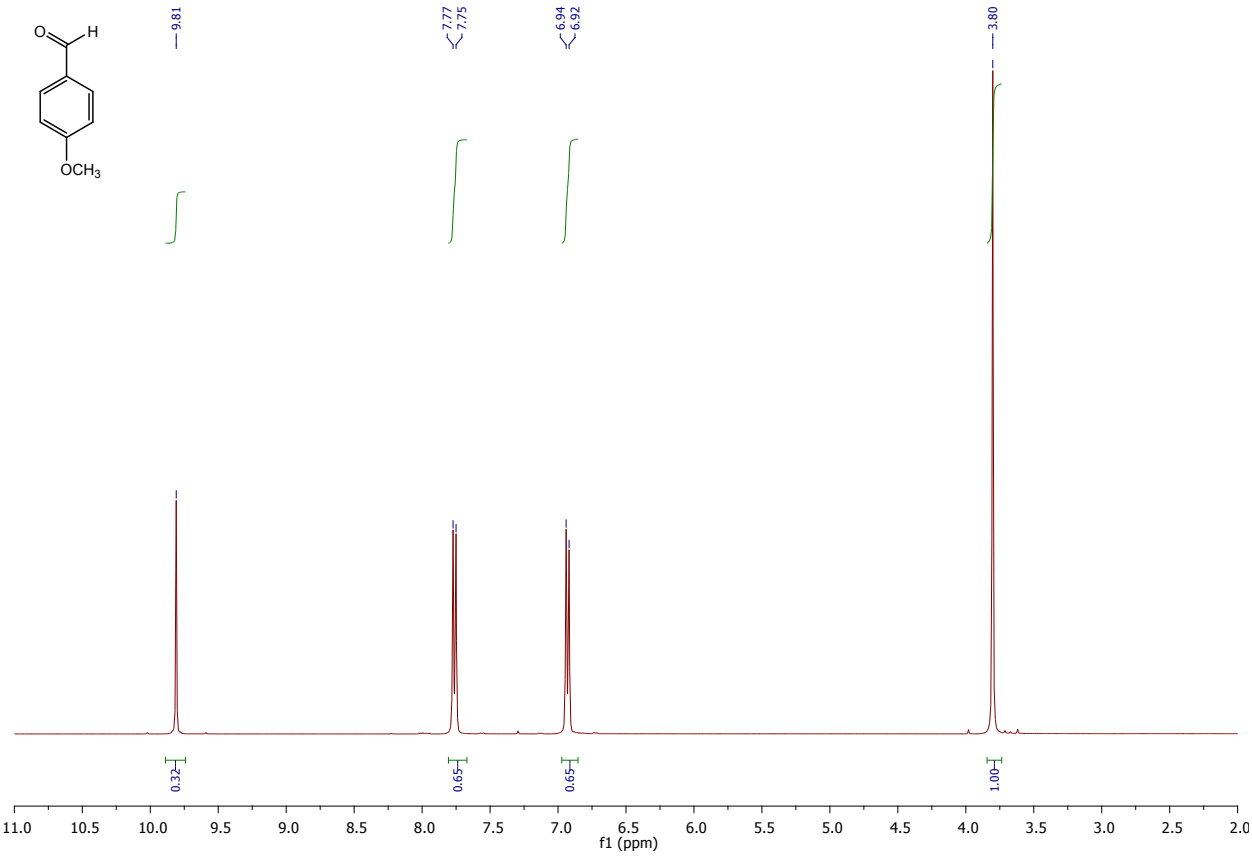


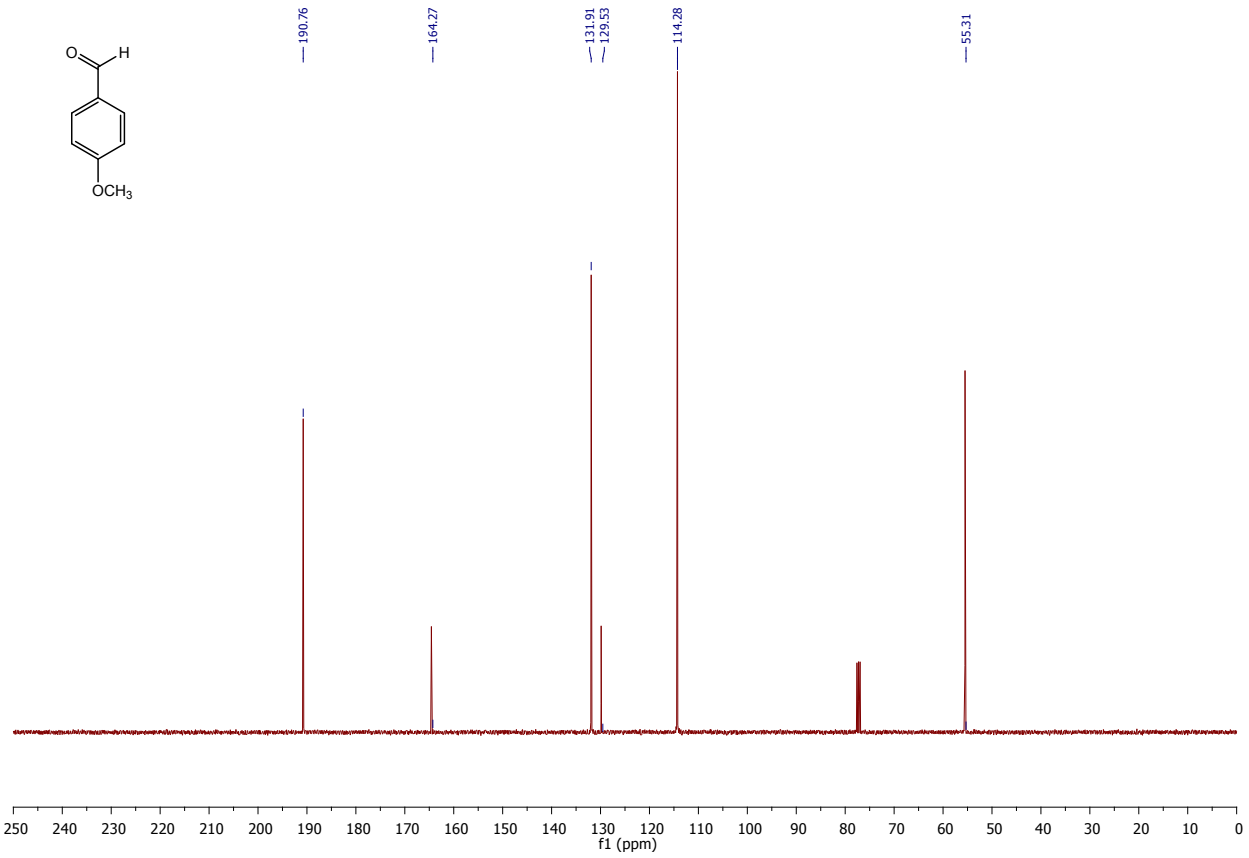

O
H
290
270
250
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4-Methoxybenzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.81 (s, 1H), 7.76 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 3.80 (s, 3H).

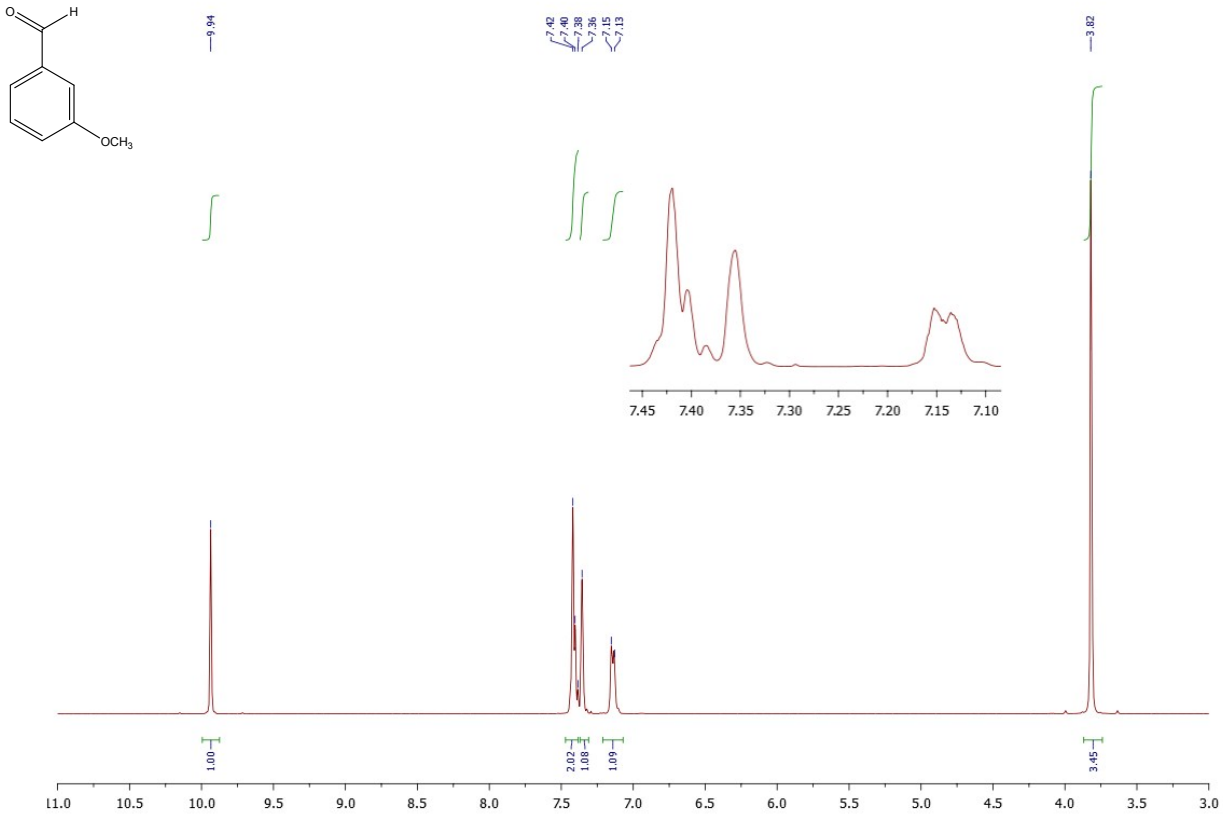
^{13}C NMR (101 MHz, $CDCl_3$) δ 190.76 (s), 164.27 (s), 131.91 (s), 129.87 (s), 114.28 (s), 55.31 (s).

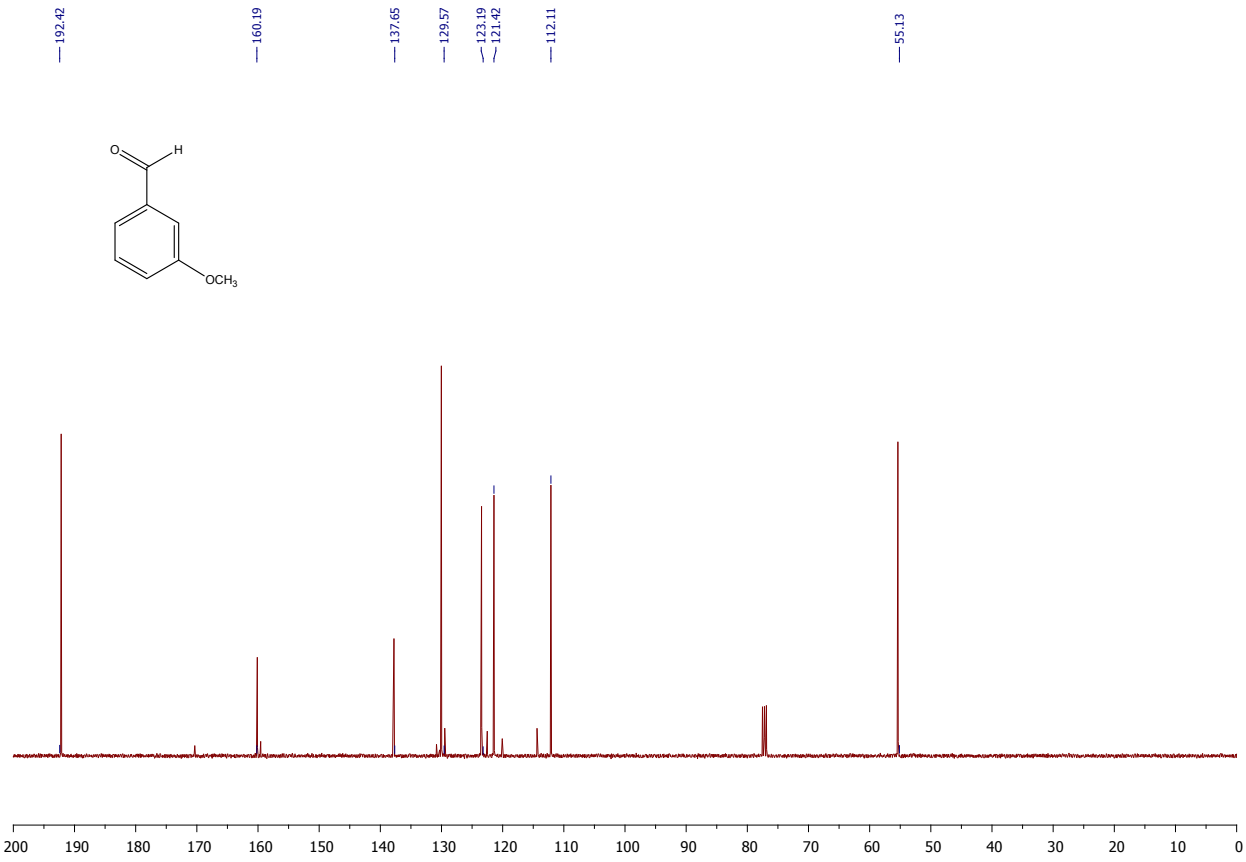



O
H
OCH3
190.76
164.27
131.91
129.53
114.28
55.31
250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3-Methoxybenzaldehyde

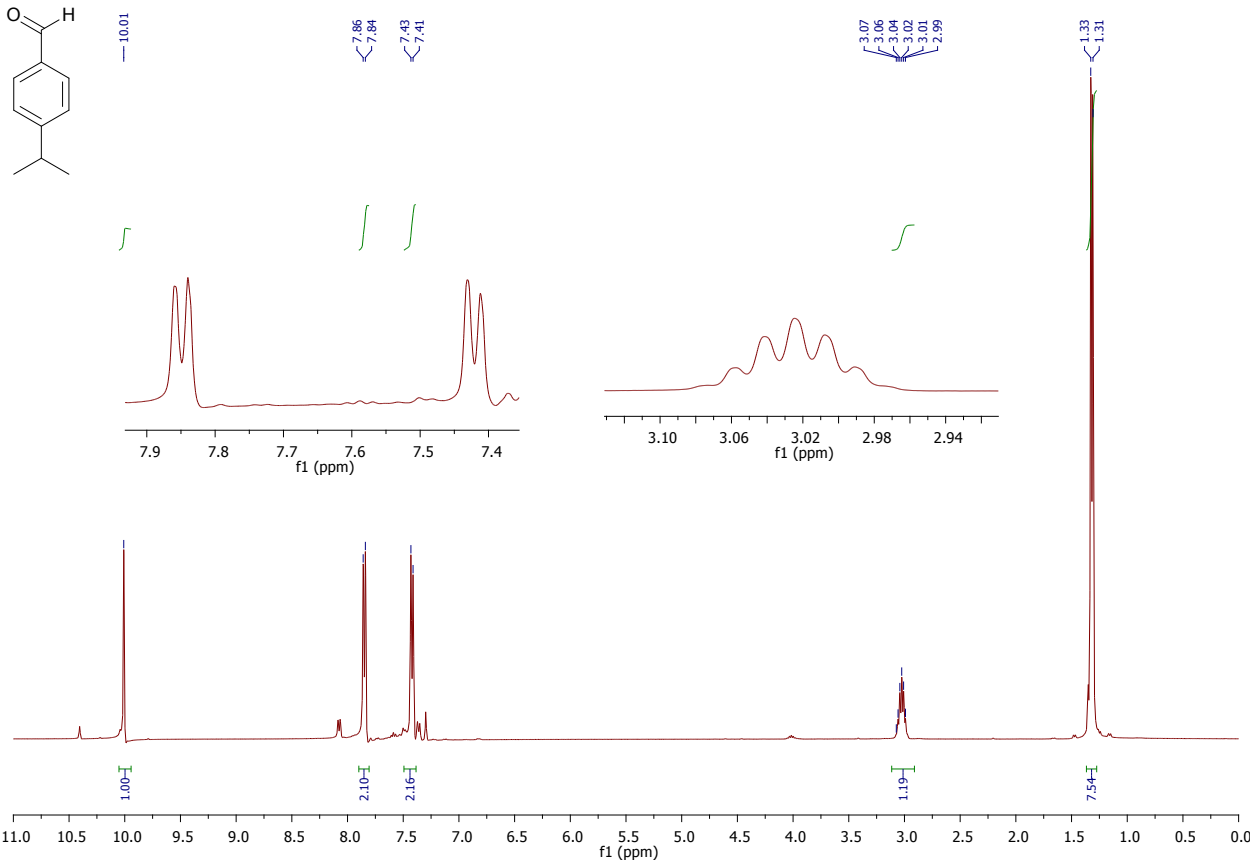
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 7.47 – 7.38 (m, 2H), 7.36 (s, 1H), 7.14 (d, *J* = 9.1 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.42, 160.19,137.65,129.57, 123.19, 121.42, 112.11, 55.13.

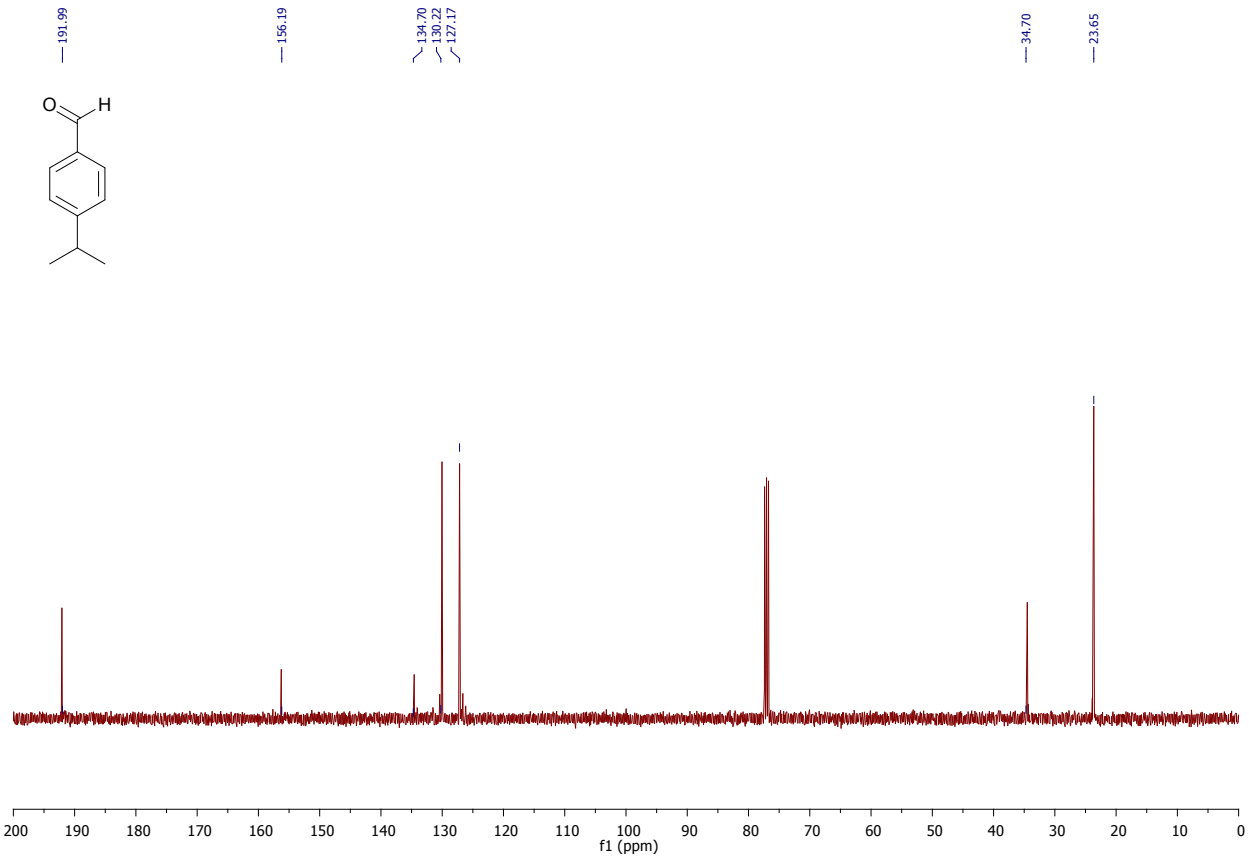



192.42
160.19
137.65
129.57
123.19
121.42
112.11
55.13
O
H
OCH3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

4-Isopropyl benzaldehyde

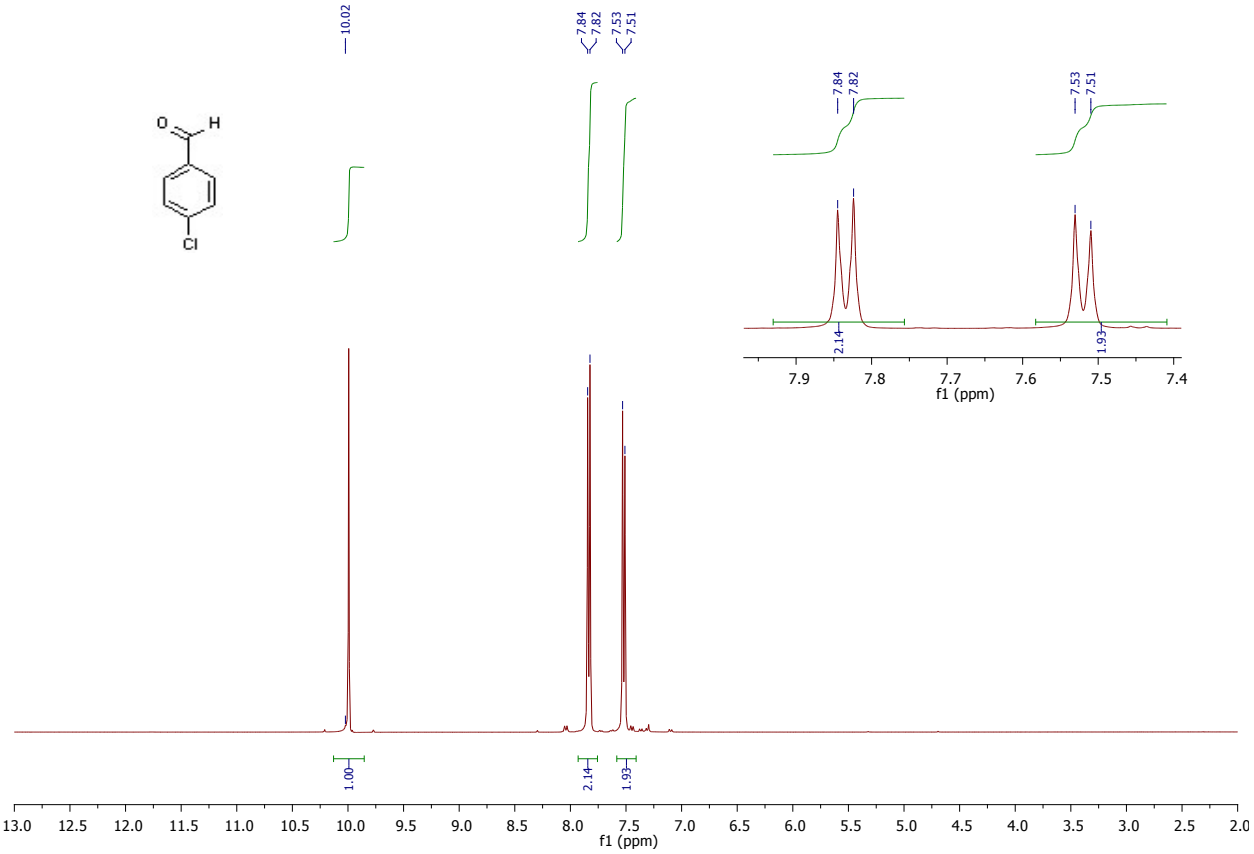
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 7.85 (d, *J* = 7.9 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 2H), 3.37 – 2.84 (m, 1H), 1.32 (d, *J* = 8.1 Hz, 7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.99, 156.19, 130.22, 127.17, 34.42, 23.65.

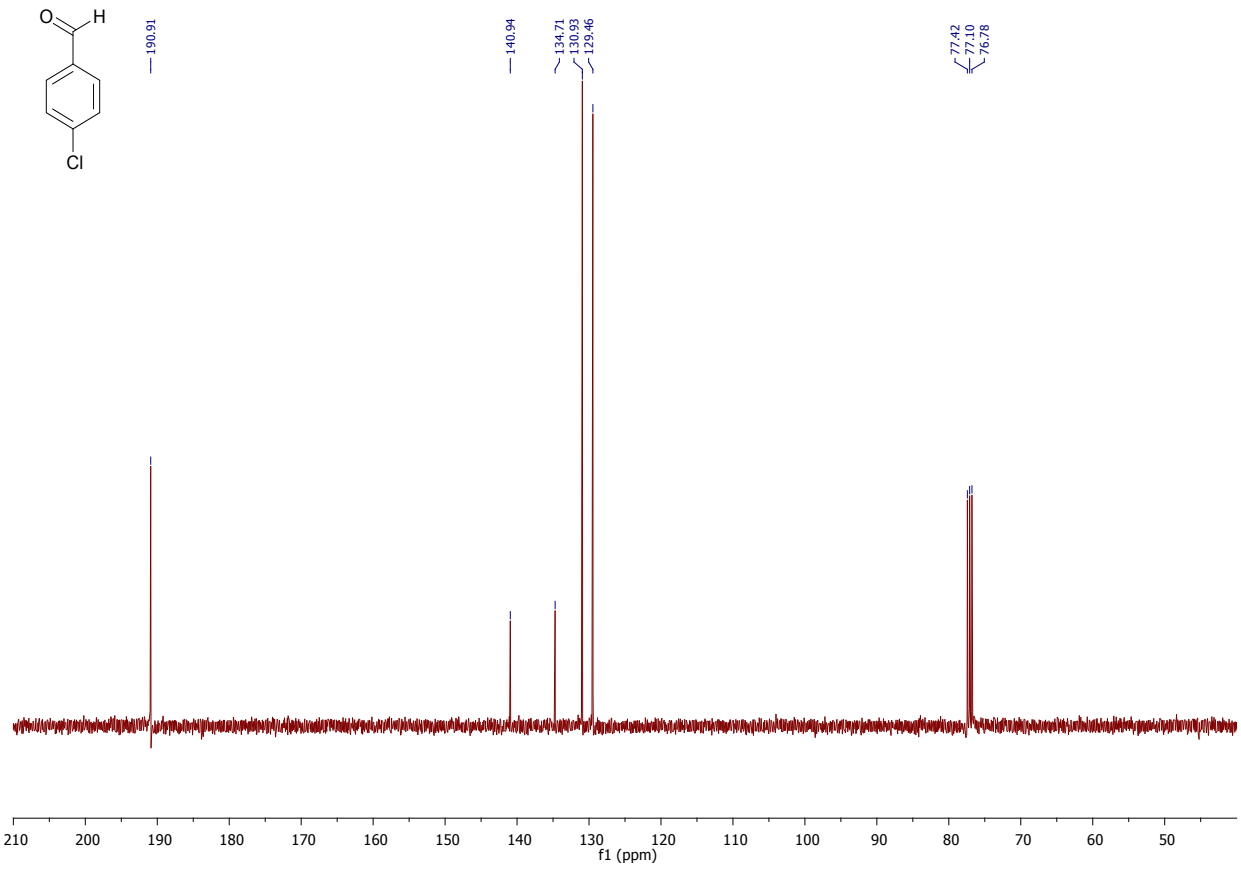



191.99
156.19
134.70
130.22
127.17
34.70
23.65
O
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4-Chlorobenzaldehyde

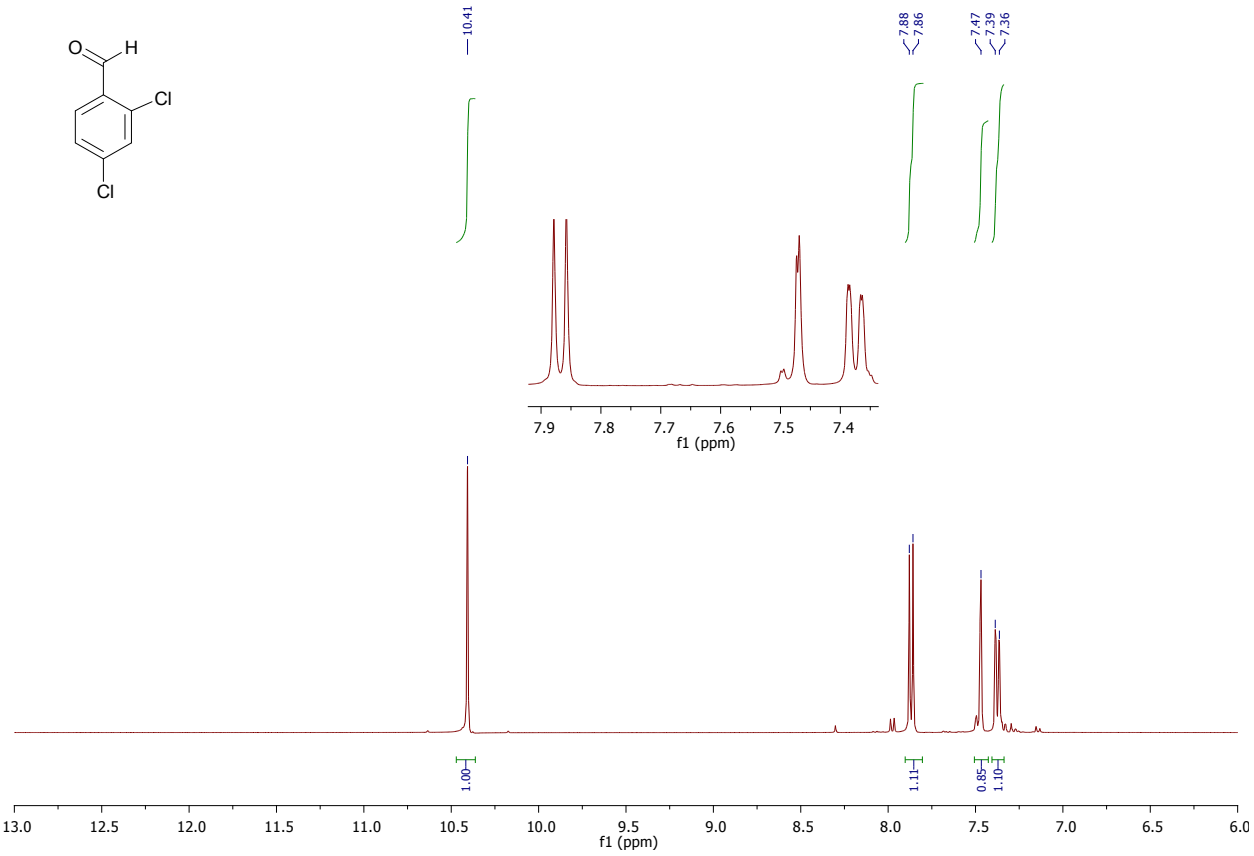
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.91, 140.94, 134.71, 130.93, 129.46.

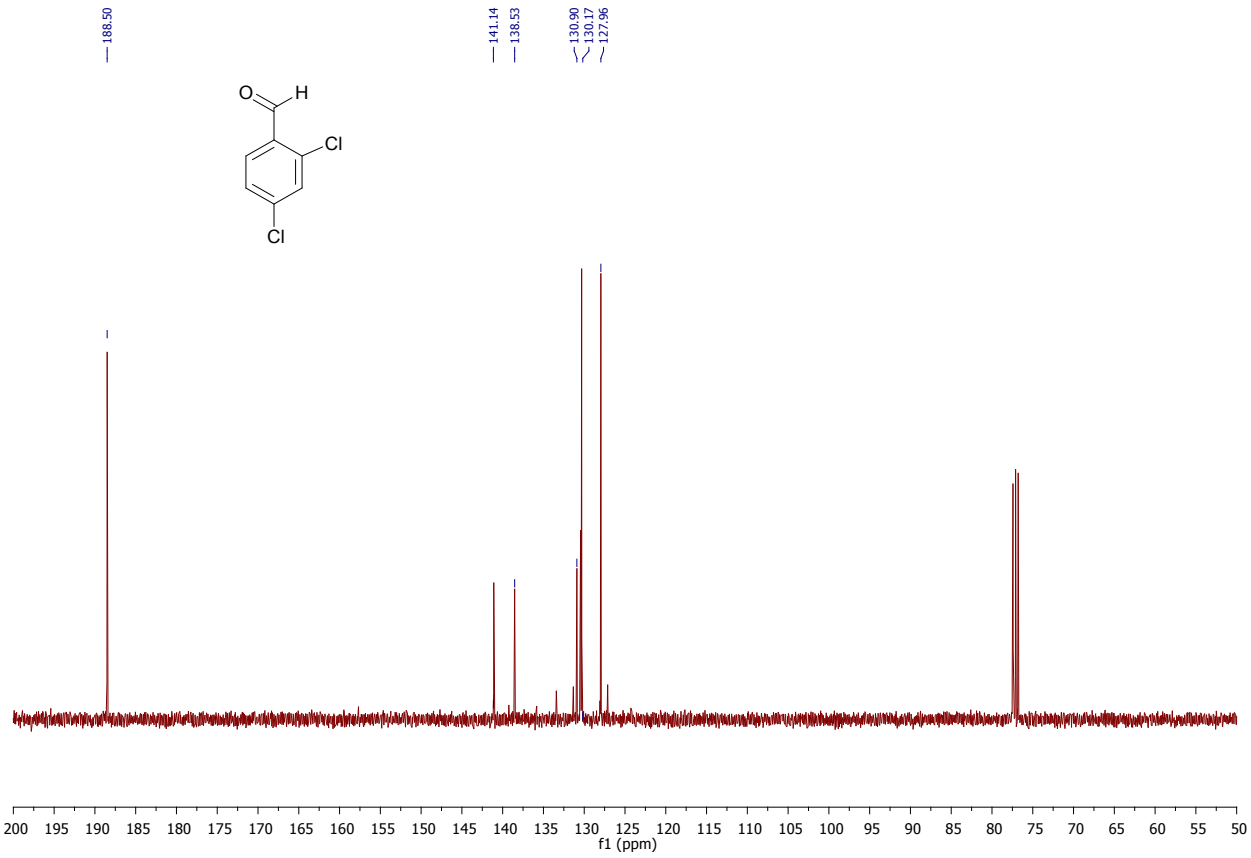



O
H
Cl
190.91
140.94
134.71
130.93
129.46
77.42
77.10
76.78
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

2,4-Dichlorobenzaldehyde

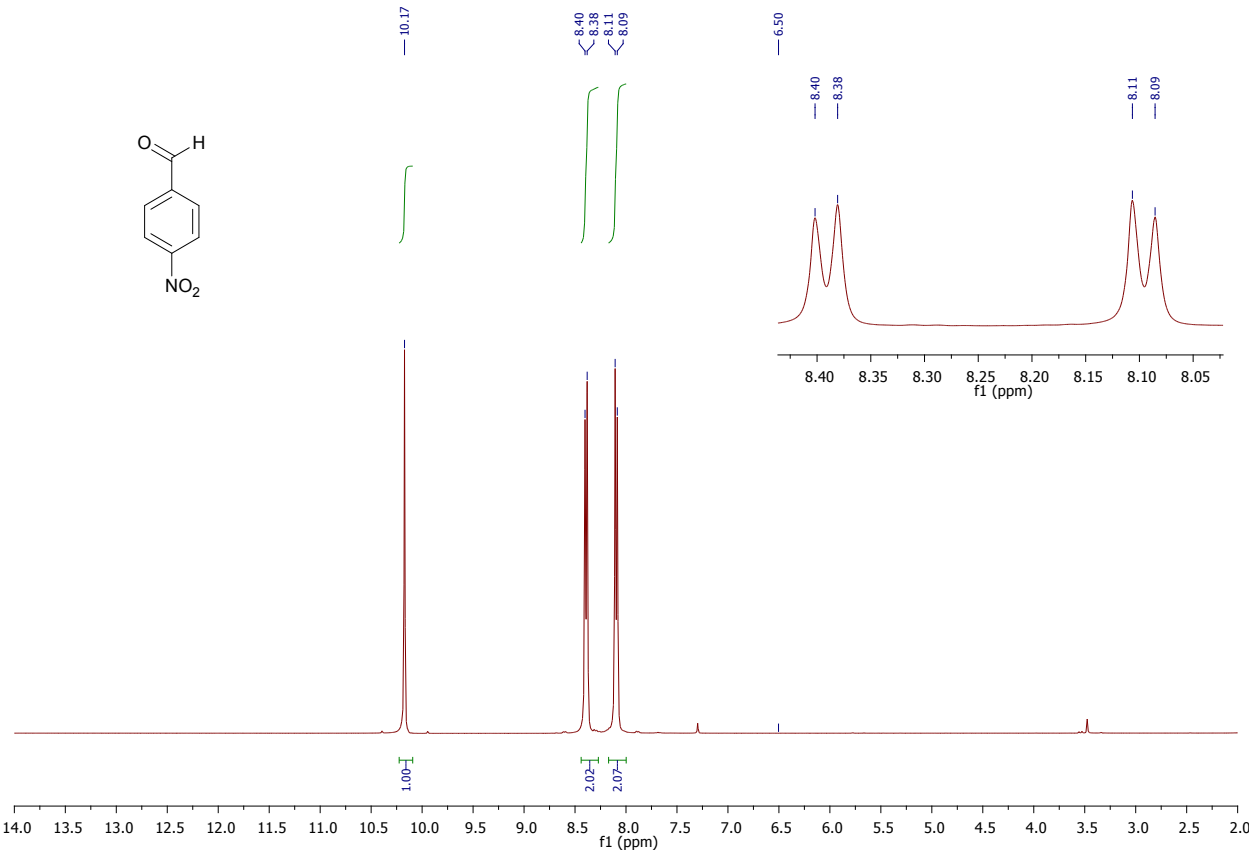
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.41 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.47 (s, 1H), 7.38 (d, *J* = 9.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.50, 141.14, 138.53, 130.90, 130.17, 127.96 .

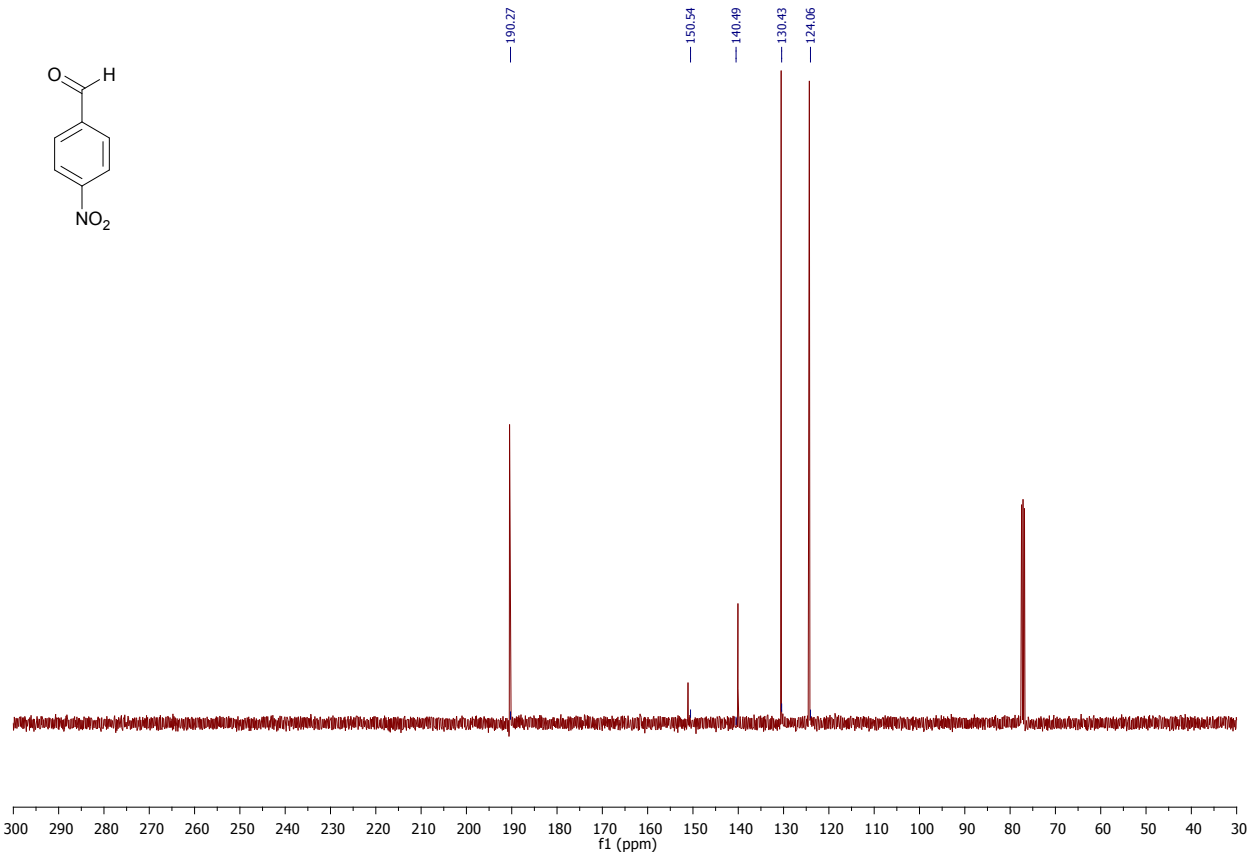



188.50
141.14
138.53
130.90
130.17
127.96
O
H
Cl
Cl
200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
f1 (ppm)

4-Nitrobenzaldehyde

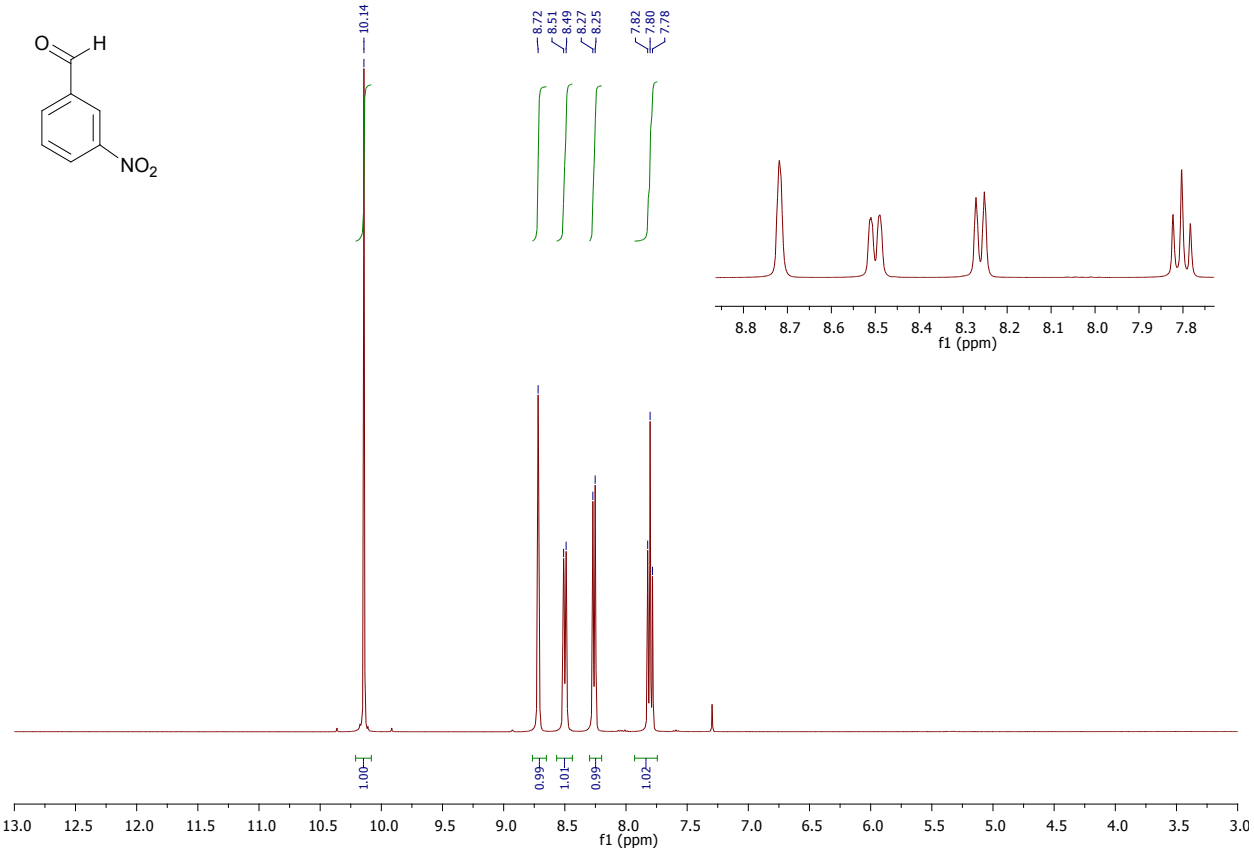
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.38 (s, 2H), 8.09 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.27, 150.54 , 130.43 , 124.06 .

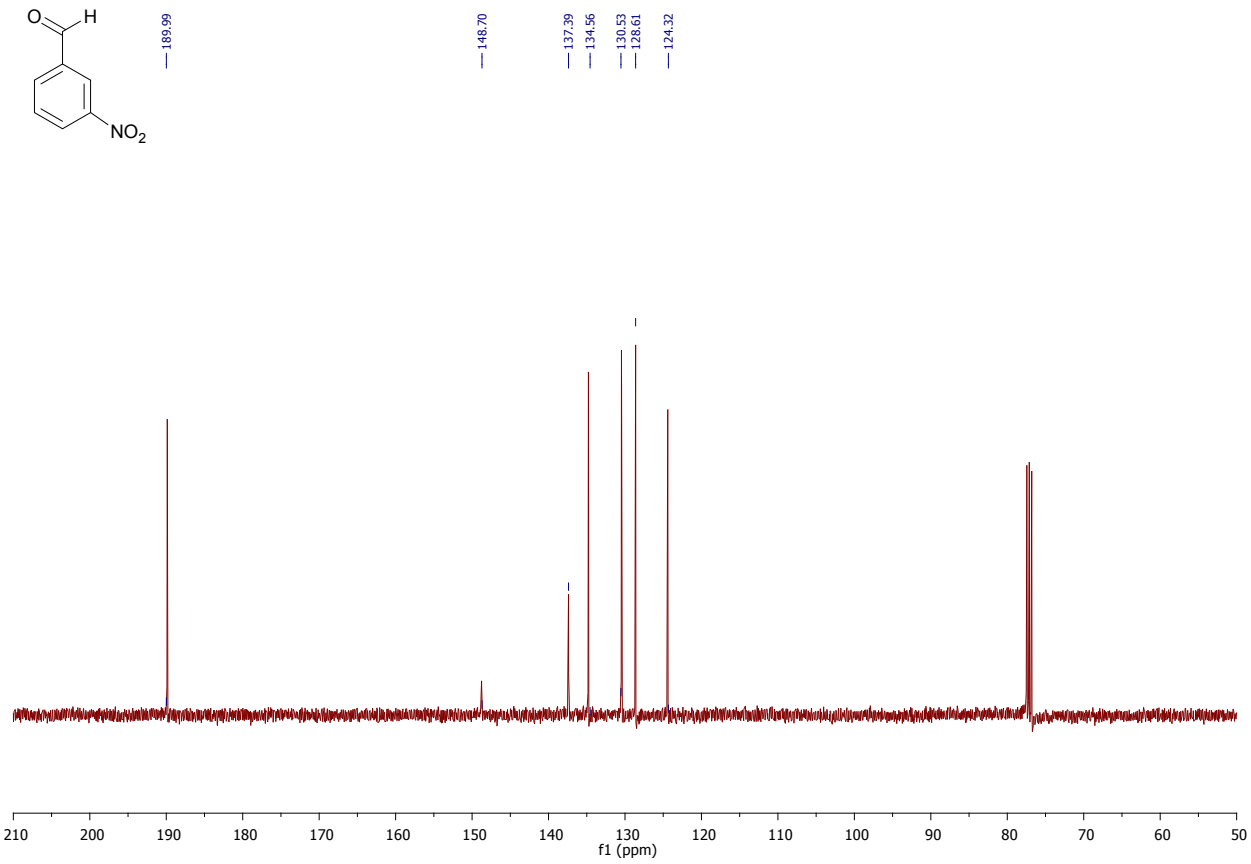



O
H
NO2
190.27
150.54
140.49
130.43
124.06
300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
f1 (ppm)

3-Nitrobenzaldehyde

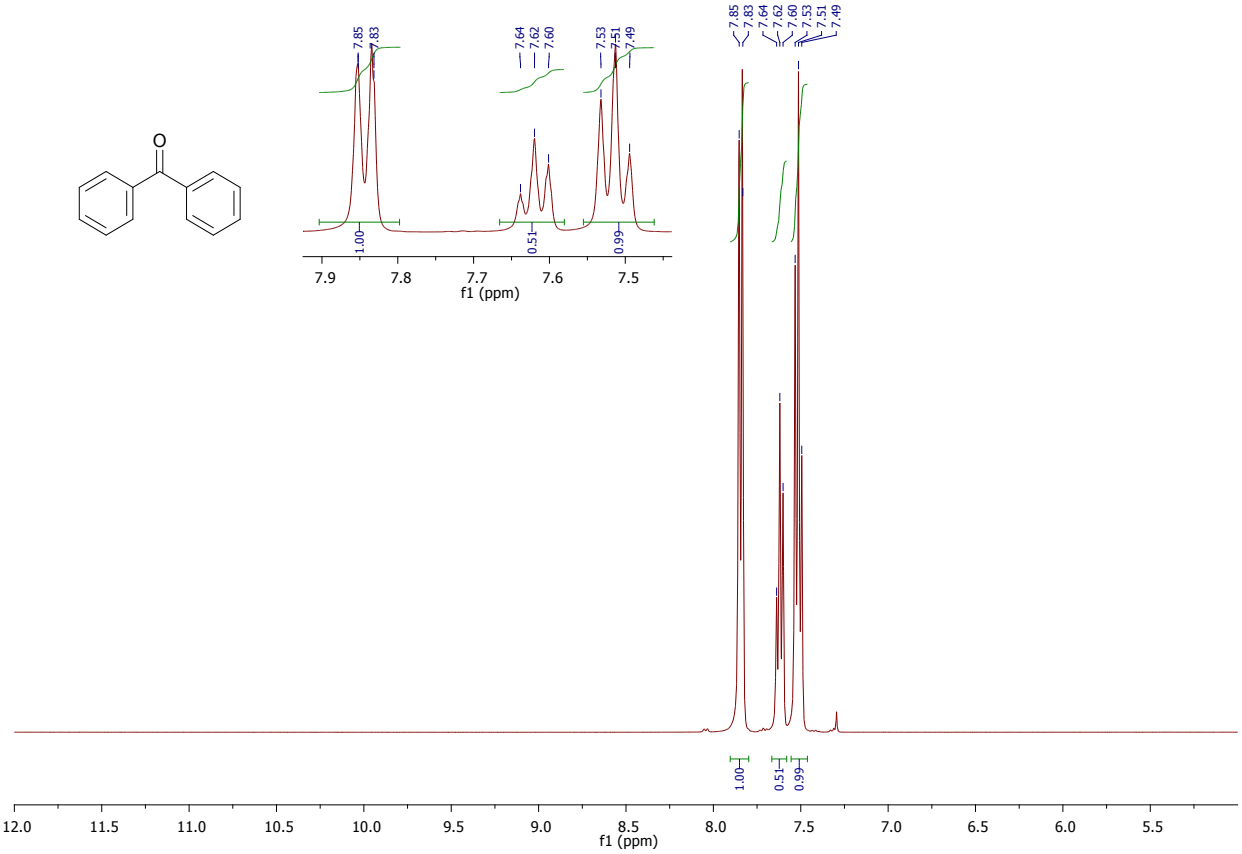
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.14 (s, 1H), 8.72 (s, 1H), 8.50 (d, *J* = 8.2 Hz, 1H), 8.26 (d, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 189.99 , 148.70, 137.39, 130.53, 128.61, 124.32 .

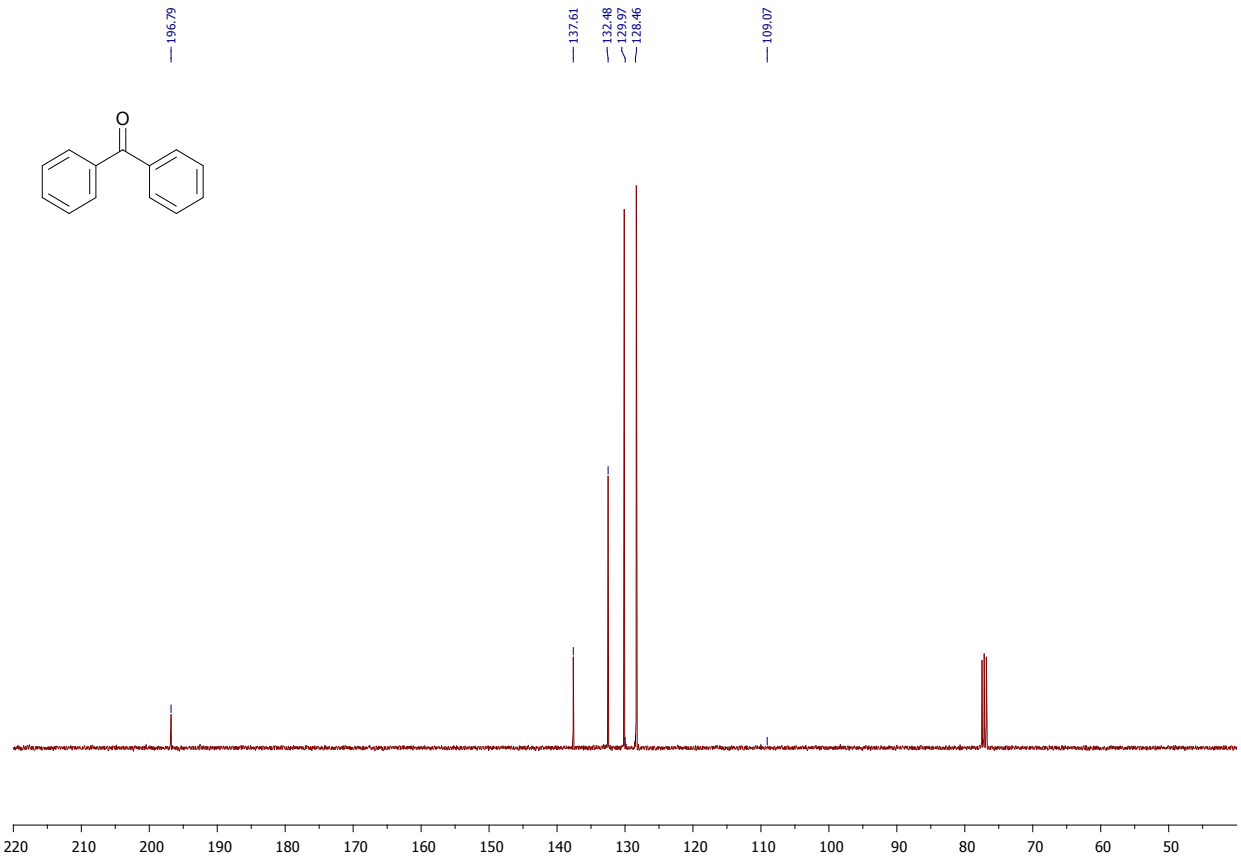



O
H
NO2
189.99
148.70
137.39
134.56
130.53
128.61
124.32
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
f1 (ppm)

Benzophenone

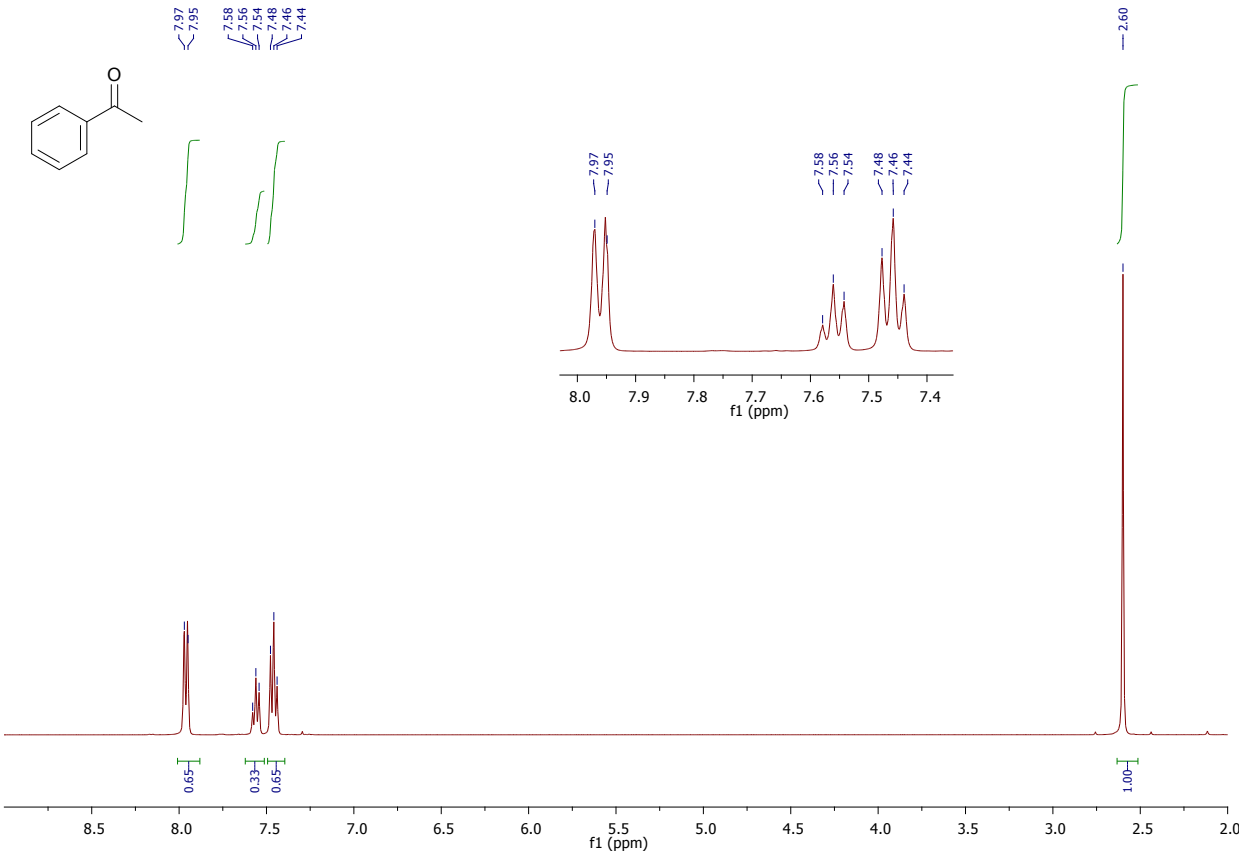
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.1 Hz, 4H), 7.62 (t, *J* = 7.4 Hz, 2H), 7.51 (t, *J* = 7.6 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.79, 137.61, 132.48, 129.97, 128.46.

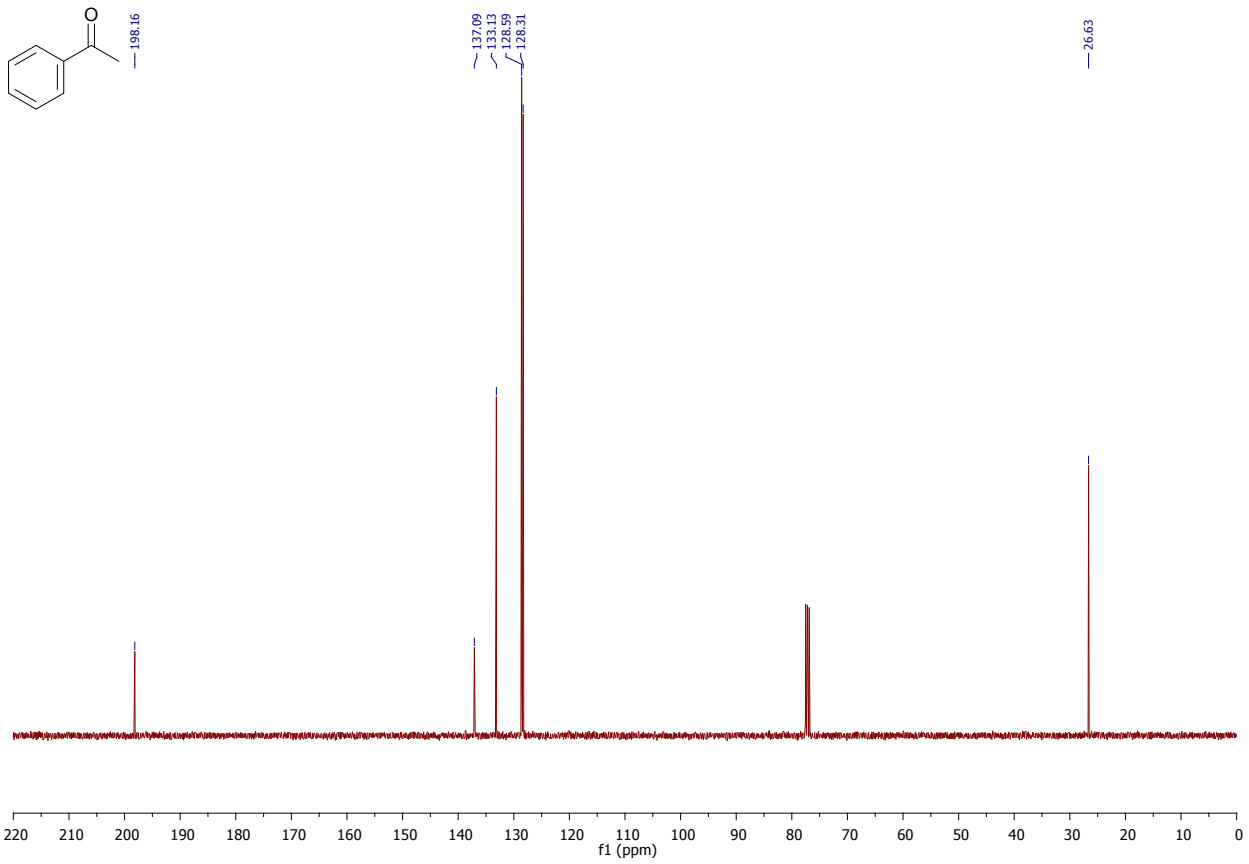



196.79
137.61
132.48
129.97
128.46
109.07
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50

Acetophenone

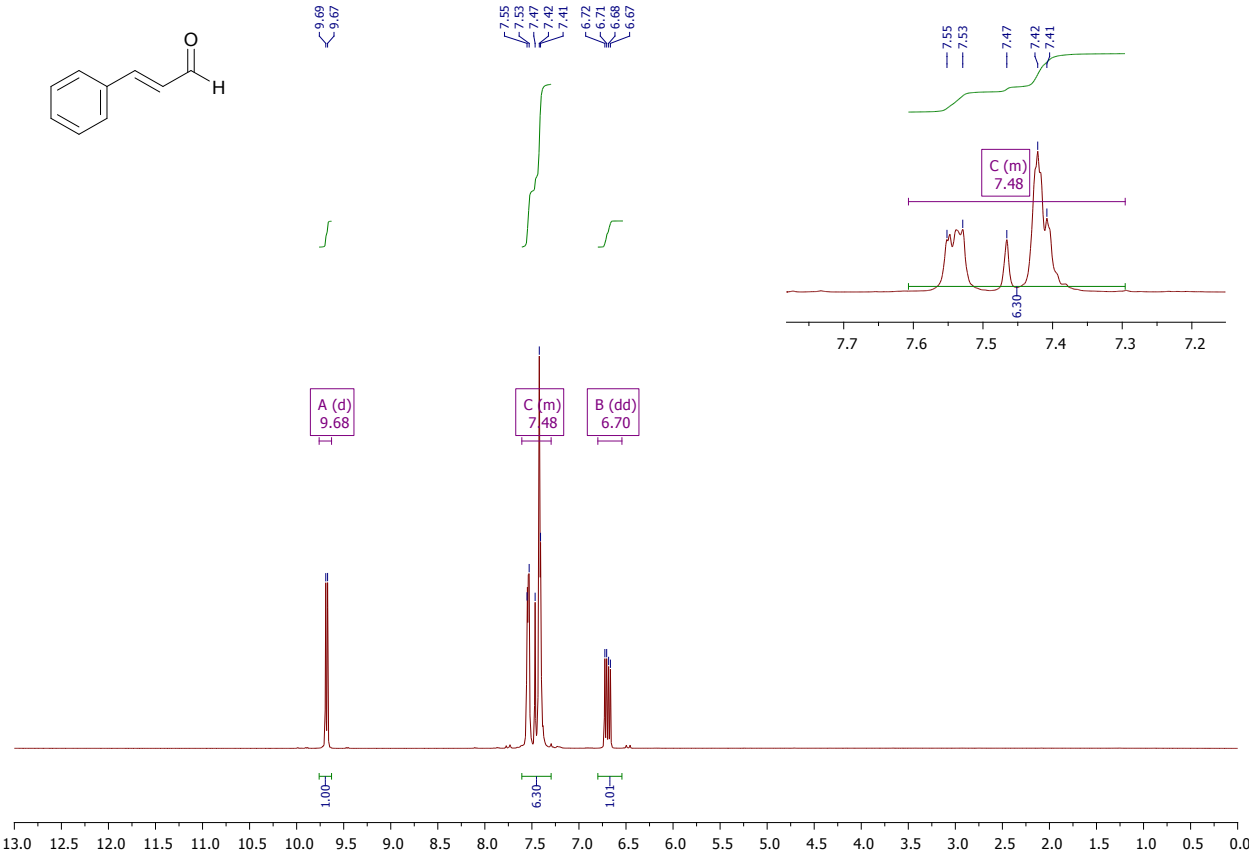
^{13}C NMR (101 MHz, $CDCl_3$) δ 198.16 (s), 137.09 (s), 133.13 (s), 128.59 (s), 128.31 (s), 26.63 (s).

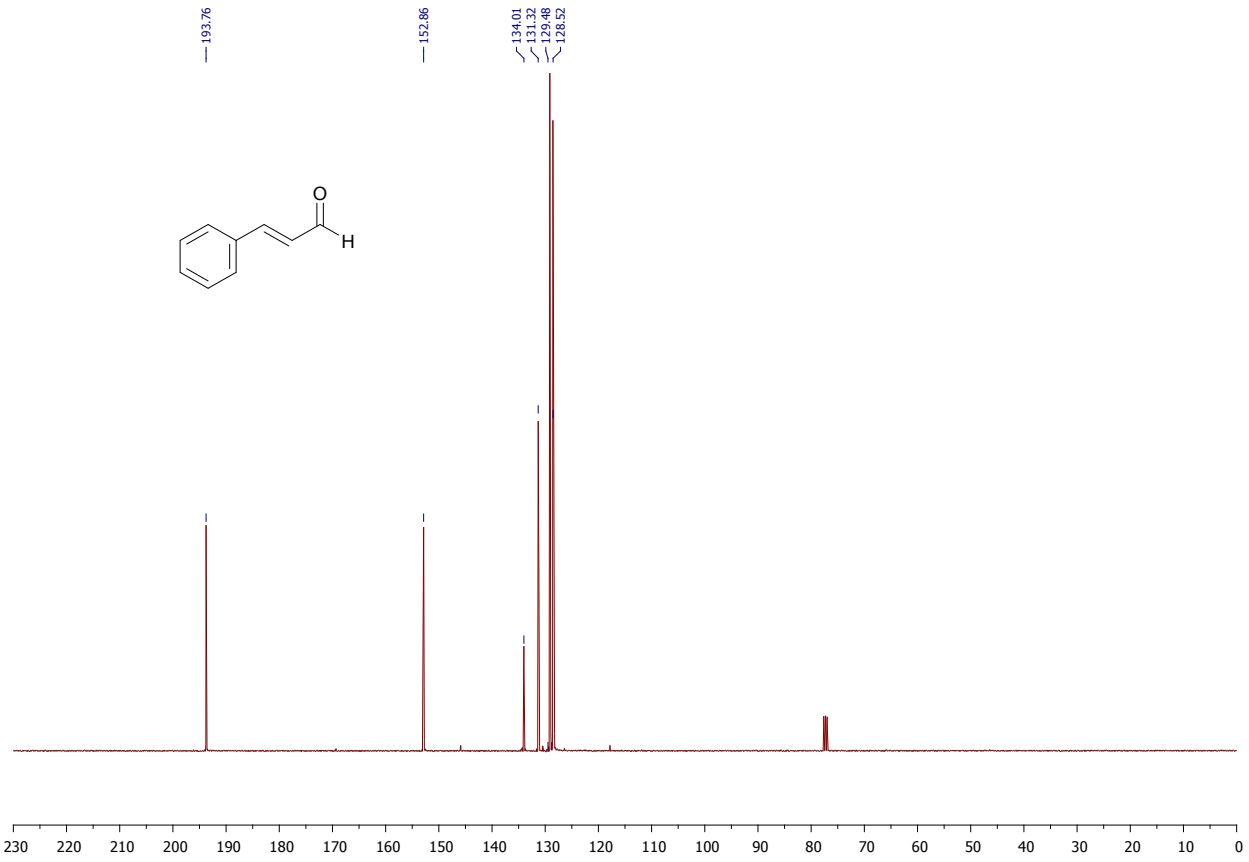



O
198.16
137.09
133.13
128.59
128.31
26.63
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Cinnamaldehyde

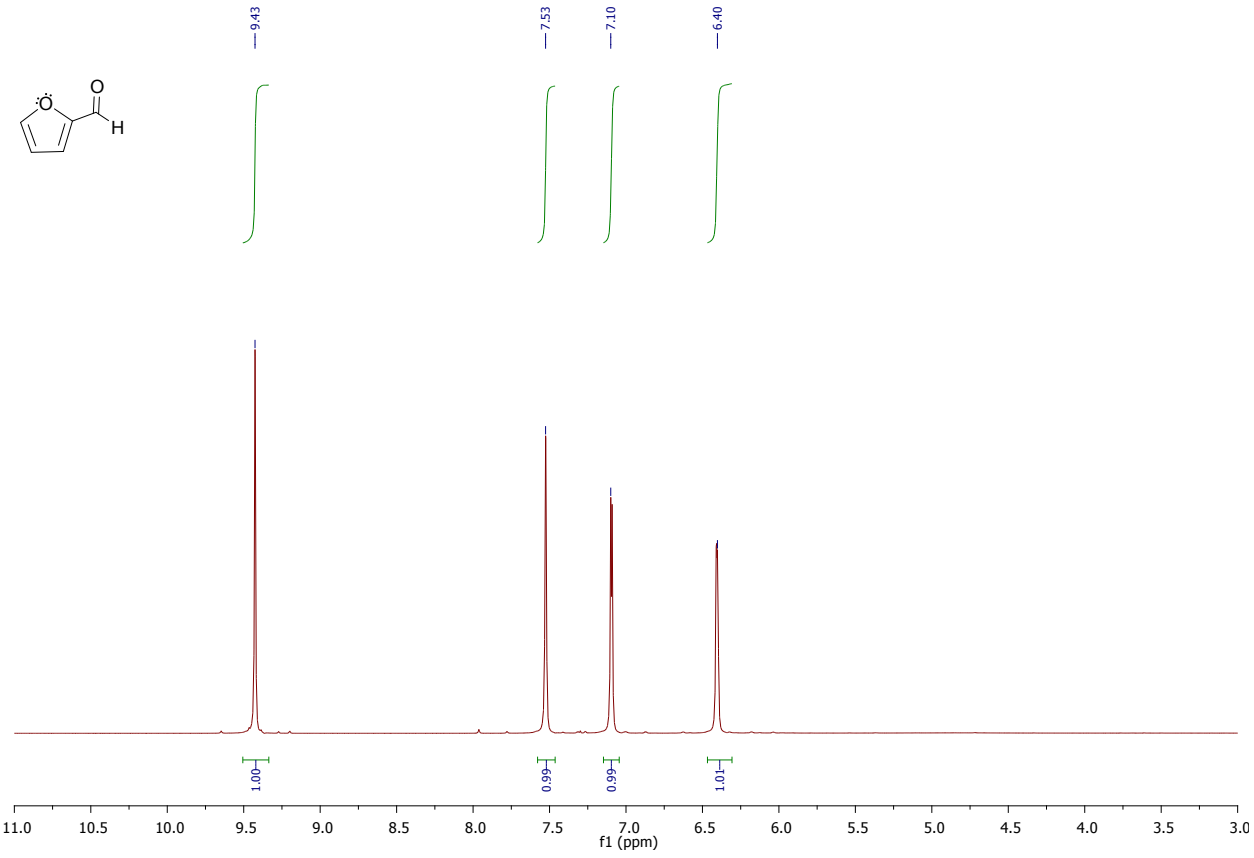
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (d, *J* = 7.7 Hz, 1H), 7.61 – 7.30 (m, 6H), 6.70 (dd, *J* = 15.9, 7.7 Hz, 1H). ^{3}C NMR (101 MHz, $CDCl_3$) δ 193.76 (s), 152.86 (s), 134.01 (s), 131.32 (s), 128.52 (s).

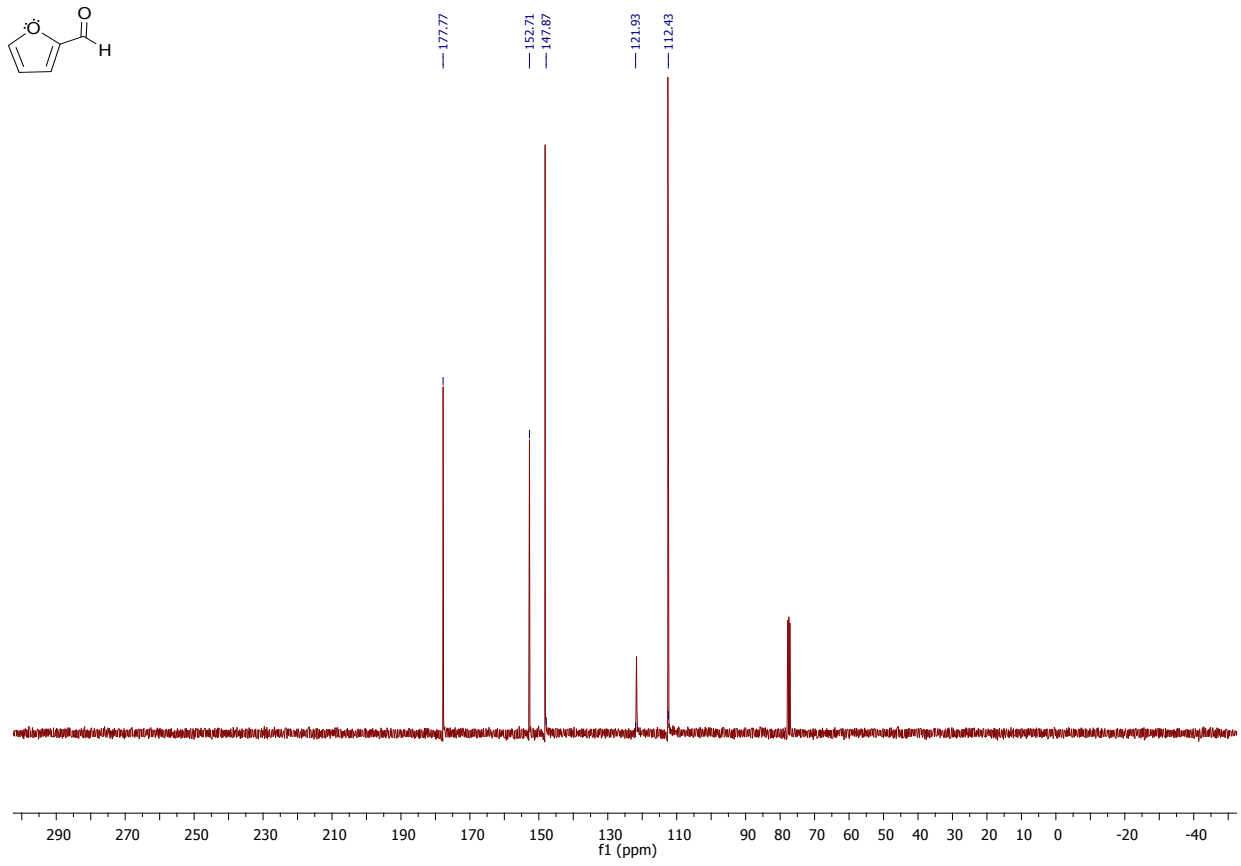



193.76
152.86
134.01
131.32
129.48
128.52
O
H
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Furfural

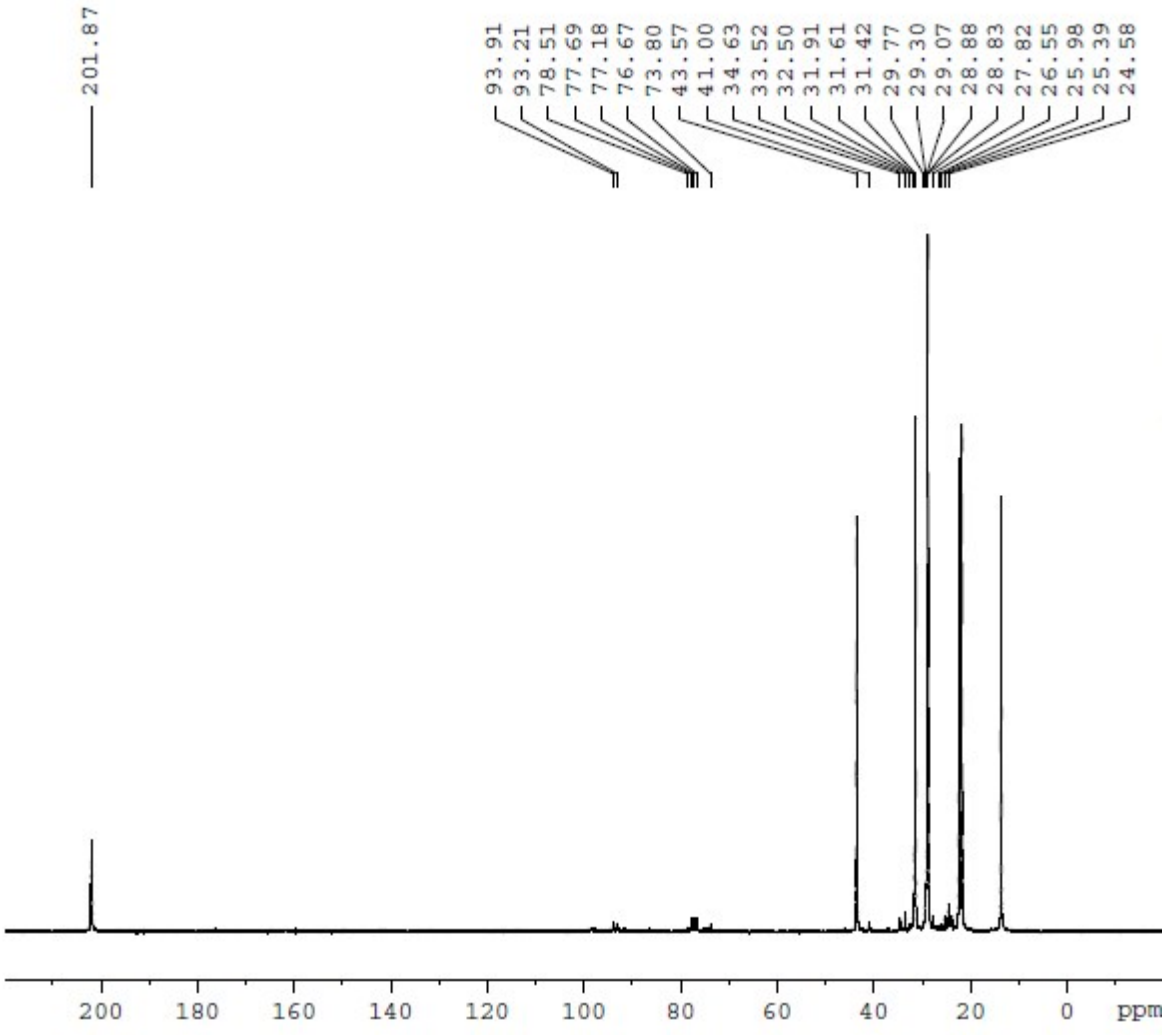
^{1}H NMR (400 MHz, CDCl3) δ 9.43 (s, 1H), 7.53 (s, 1H), 7.10 (d, J = 3.6 Hz, 1H), 6.41 (s, 1H).^{13}C NMR (101 MHz, CDCl3): δ 177.77, 152.71, 147.87, 121.93, 112.43.

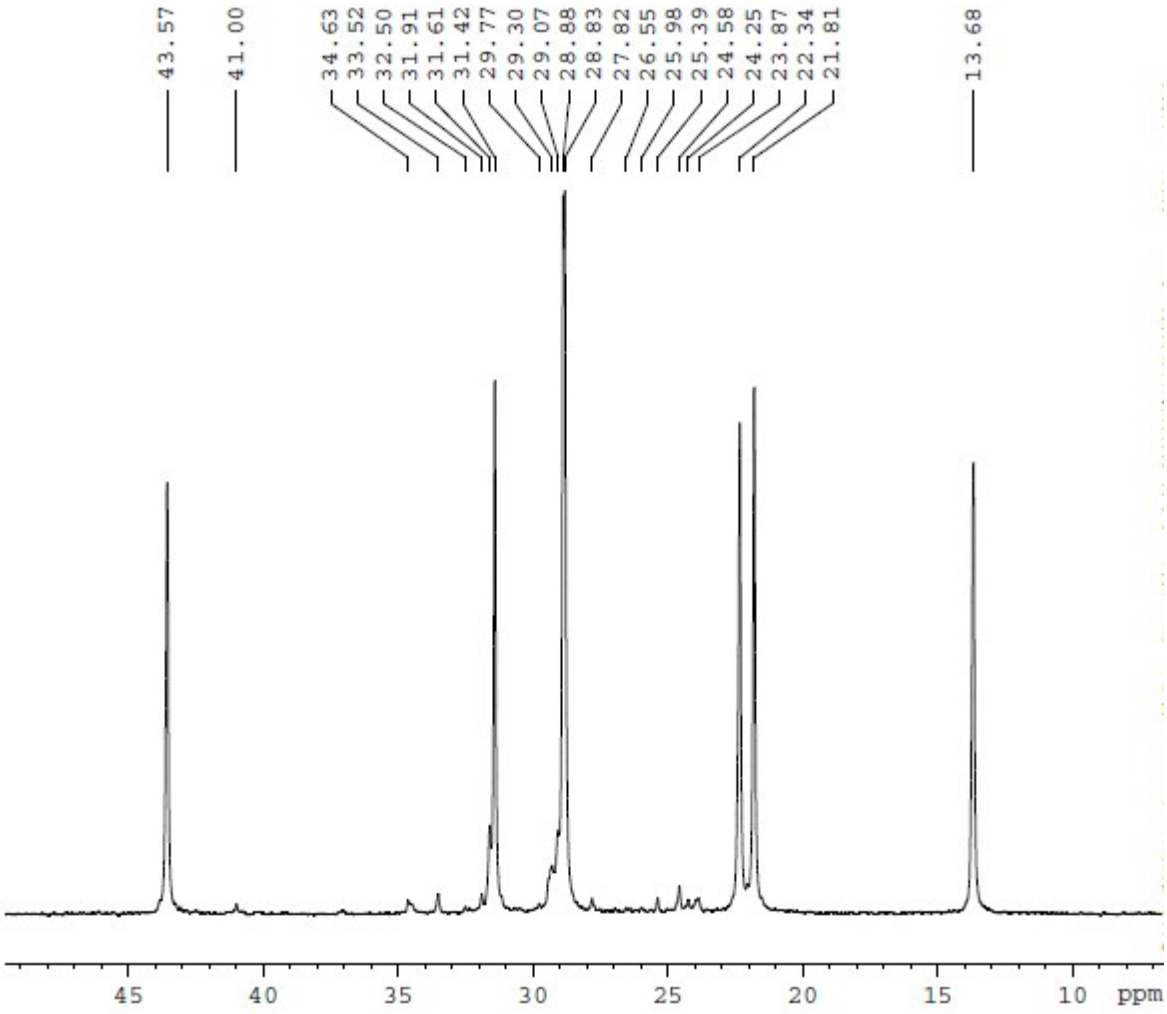


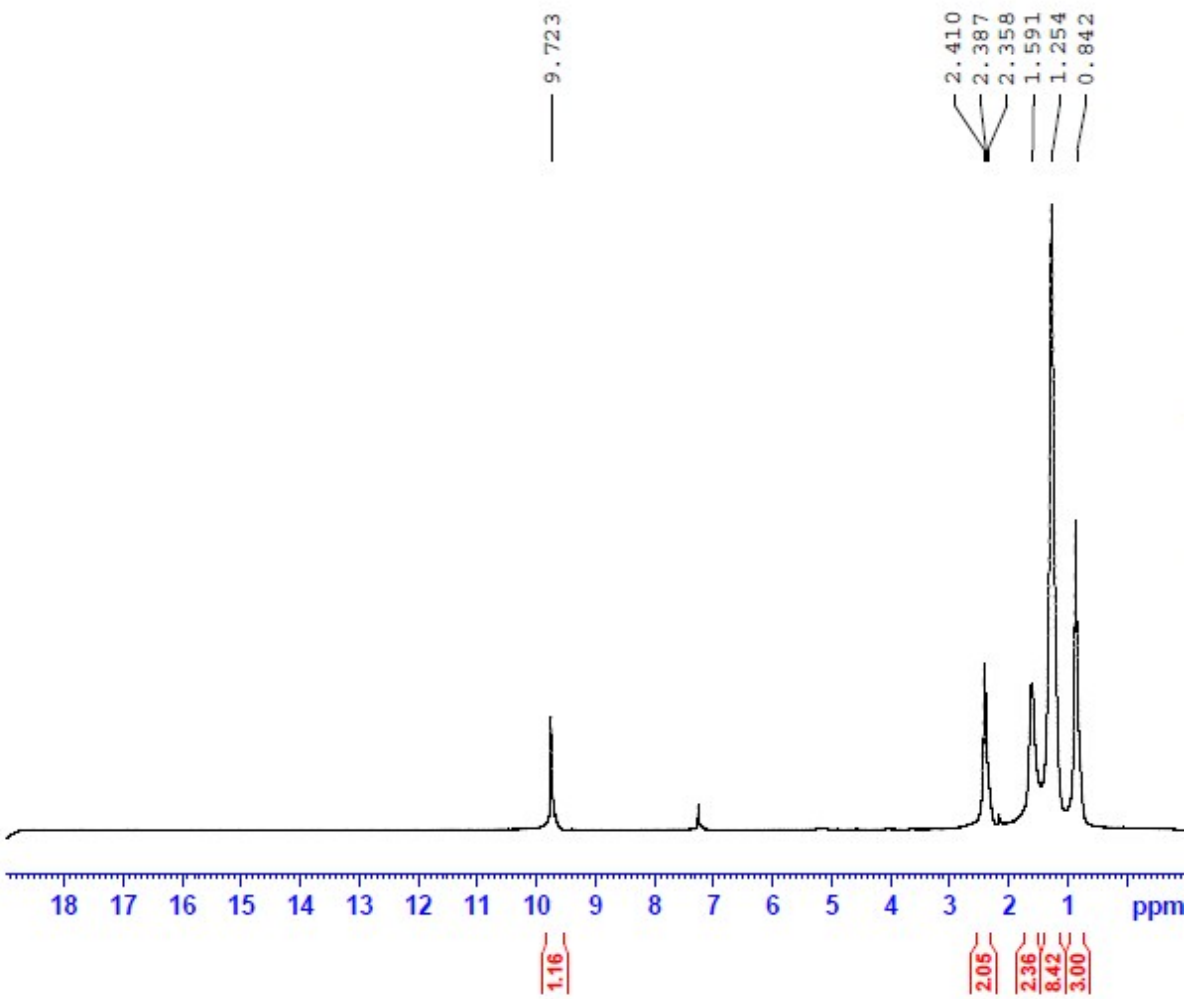

O
H
177.77
152.71
147.87
121.93
112.43
290
270
250
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-20
-40
f1 (ppm)

1-Octanal

^{1}H NMR (250 MHz, $CDCl_3$) δ 9.723 (s, 1H), 2.387 (t, *J* = 8.1 Hz, 2H), 1.591 (s, 2H), 1.254 (m, 8H), 0.842 (d, *J* = 6.6 Hz, 3H).
^{13}C NMR (63 MHz, $CDCl_3$) δ 201.87, 43.57 , 31.42 , 28.83, 22.88, 22.34, 21.81, 13.68.

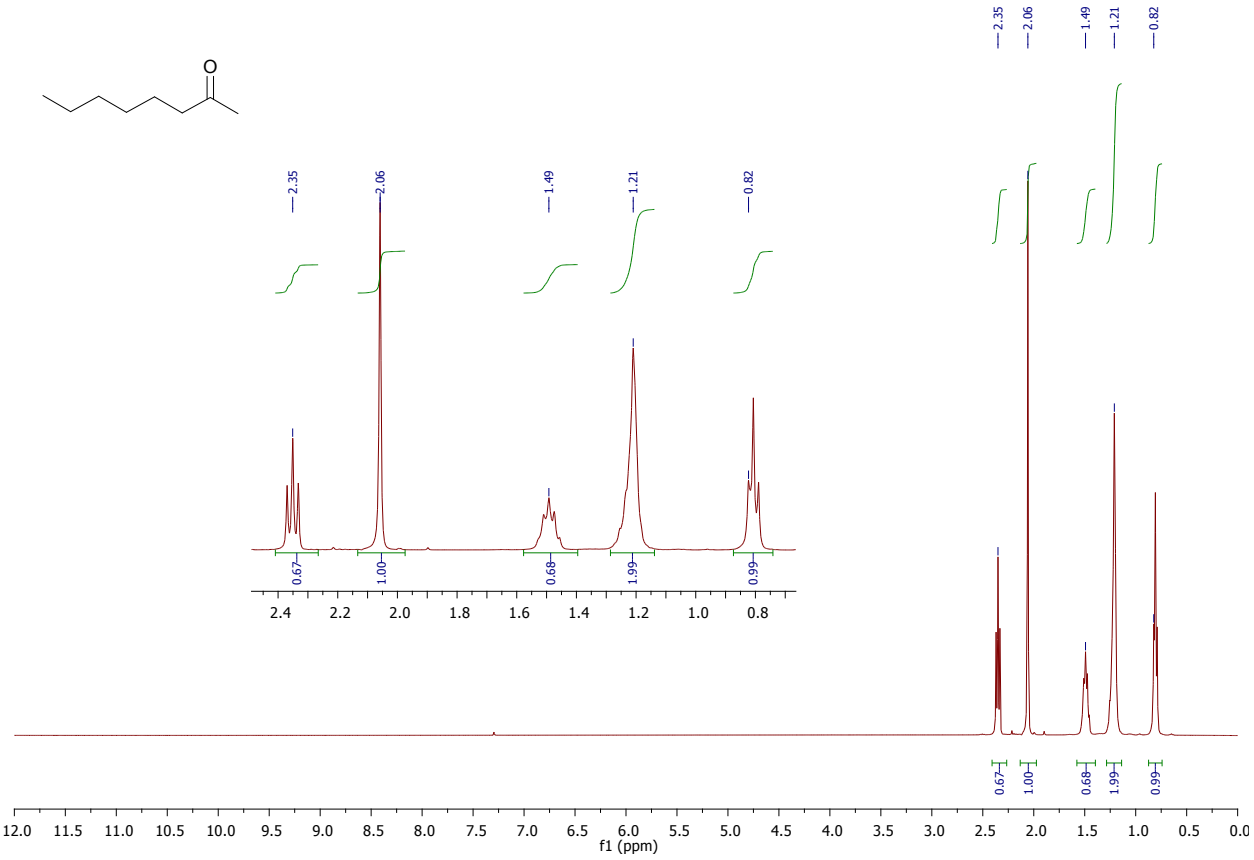


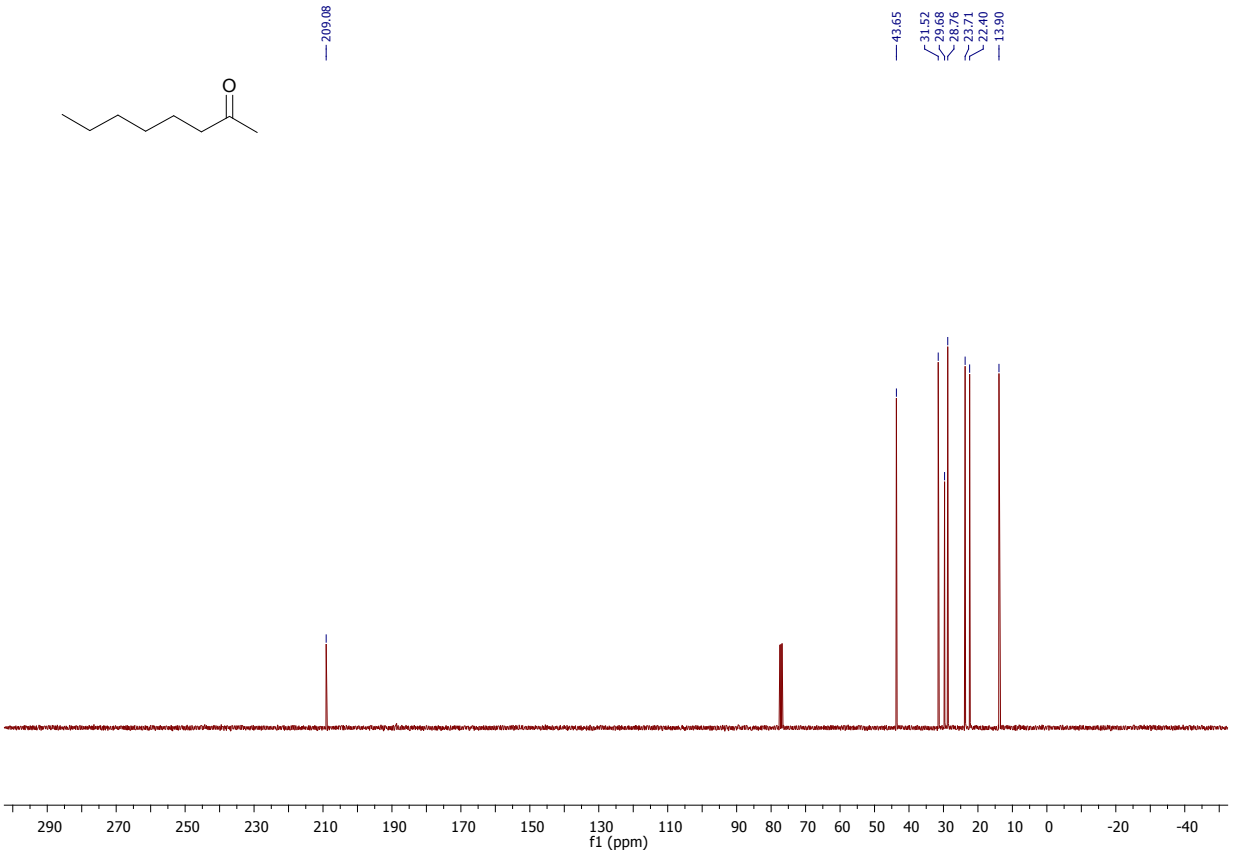

43.57
41.00
34.63
33.52
32.50
31.91
31.61
31.42
29.77
29.30
29.07
28.88
28.83
27.82
26.55
25.98
25.39
24.58
24.25
23.87
22.34
21.81
13.68
45
40
35
30
25
20
15
10
ppm


9.723
2.410
2.387
2.358
1.591
1.254
0.842
18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.16
2.05
2.36
8.42
3.00

2-Octanone

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 2H), 2.06 (s, 3H), 1.49 (s, 2H), 1.21 (s, 6H), 0.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.08, 43.65, 31.52, 29.68, 28.76, 23.71, 22.40, 13.90.





Refrence

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