Electronic Supplementary Material (ESI) for ChemComm.

Visible Light Mediated Efficient Oxidative Benzylic sp^3 C–H to Ketone Derivatives under Mild Conditions using O_2

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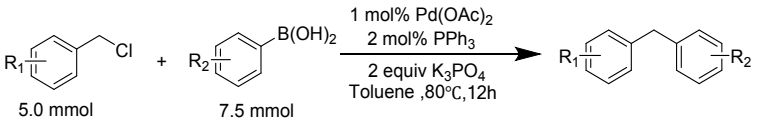
1. General Information

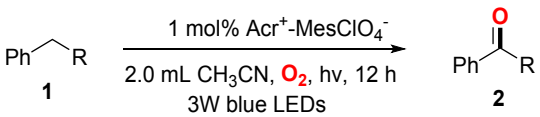
All manipulations were carried out by standard Schlenk techniques. Unless otherwise noted, analytical grade solvents and commercially available reagents were used to conduct the reactions. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (boiling point is between 60-90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient using petroleum ether and ethyl acetate. The known compounds were characterized by ^{1}H NMR and ^{13}C NMR. GC-MS spectra were recorded on a Varian GC-MS 3900-2100T. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer with tetramethylsilane as an internal standard. The chemical shifts (δ) were given in part per million relative to internal tetramethyl silane (TMS, 0 ppm for ^{1}H), $CDCl_3$ (77.3 ppm for ^{13}C).

2. General Procedures for Synthesizing Phenylmethane Derivatives



To a 50 mL schlenk flask, benzyl chloride (5.0 mmol), arylboronic acid (7.5 mmol), $Pd(OAc)_2$ (0.05 mmol), triphenylphosphine (0.1 mmol) and K_3PO_4 (10.0 mmol) was added into 20 mL toluene under N_2 atmoshphere, the mixture was stirred for 12 h at 80℃. After completion of the reaction, the mixture was cooled to room temperature and filterred through diatomite. As indicated by TLC and GC-MS, the organic mixture was purified by flash column chromatography on silica gel using petroleum ether and ethyl acetate to afford phenylmethane derivatives.

3. General Procedures for Synthesizing Ketone Derivatives



In a dried schlenk tube, phenylmethane (0.5 mmol), and $Acr^{+}MesClO_4^{-}$ (1 mol%, 0.005 mmol) was stirred in 2.0 mL acetonitrile for 12 hours at room temperature under an atmospheric pressure oxygen atmosphere. After completion of the reaction, as indicated by TLC and GC-MS, the mixture

was diluted by ethyl acetate. The pure product was obtained by flash column chromatography on silica gel using petroleum ether and ethyl acetate.

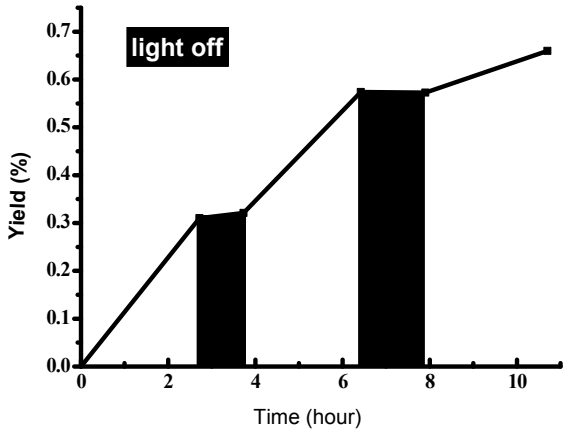
4. Mechanism Study

4.1 Radical Trapping Experiment

Phenylmethane (0.5 mmol)，$Acr^+MesClO_4^-$ (1 mol%, 0.005 mmol) and 2.0 equivalent TEMPO (1.0 mmol) was stirred under O_2 atmosphere in 2.0 mL acetonitrile under 3W blue LEDs at room temperature for 12 h. The result was detected by GC-MS.

4.2 Time Profile of Photocatalytic Reaction with and without Visible Light.

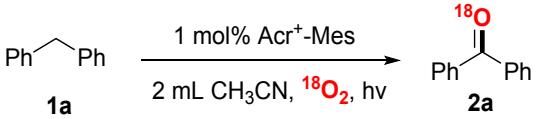
We use in-situ IR to monitor the reaction. Phenylmethane (0.5 mmol) and Acr^+-$MesClO_4^-$(3.0 mol%, 0.015 mmol) was stirred in an IR tube under O_2 atmosphere in 3.0 mL acetonitrile under 3W blue LEDs at room temperature. The yield was detected by GC using diphenyl as internal standard.

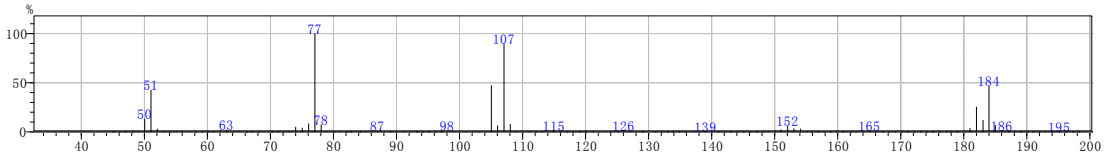


4.3 Labelling Experiment

4.3.1 $^{18}O_2$ labelling experiment using phenylmethane mediated by visible light

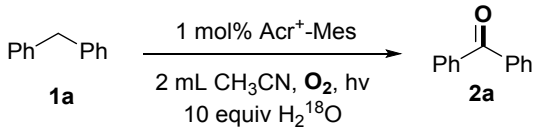
In a schlenk tube with stirrer, phenylmethane (0.5 mmol) and Acr^+-$MesClO_4^-$(1 mol%, 0.005 mmol) was mixed in 2.0 mL acetonitrile under N_2 atmosphere. Then the tube was frozen by liquid nirtrogen, afer this, the tube was pumped into vacuum and $^{18}O_2$ gas was injected into the system. The system was stirred under 3W blue LEDs for 10 h. The ratio of ^{16}O and ^{18}O was detected by MS.

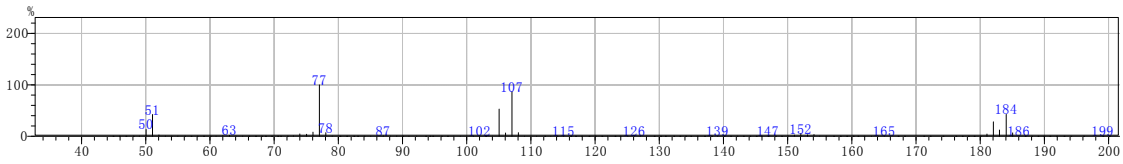


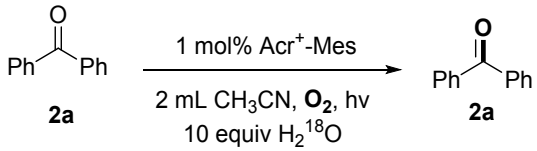


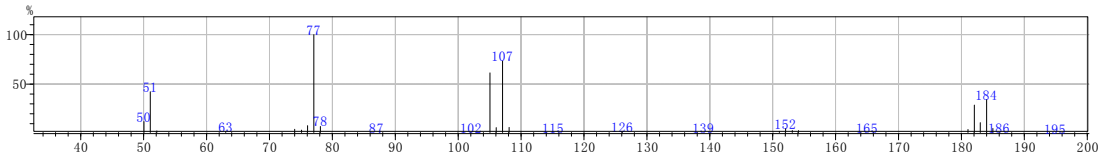
4.3.2 $H_2{}^{18}O$ Labelling Experiment using phenylmethane or benzophenone mediated by visible light

In a dried schlenk tube, phenylmethane or benzophenone (0.5 mmol), Acr^+-$MesClO_4^-$(1 mol%, 0.005 mmol) and 10 equivlent $H_2{}^{18}O$ (2.0 mmol) was stirred in 2.0 mL acetonitrile at room temperature under an atmospheric pressure oxygen atmosphere. The system was stirred under 3W blue LEDs for 10 h. The ratio of ^{16}O and ^{18}O was detected by MS.



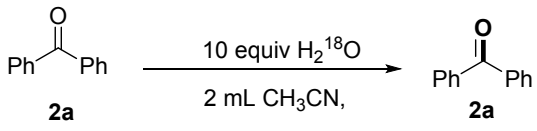


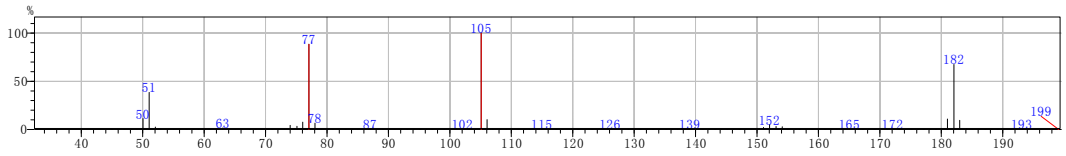




4.3.3 $H_2{}^{18}O$ Labelling Experiment using benzophenone without visible light and photocatalyst

In a dried schlenk tube, phenylmethane or benzophenone (0.5 mmol), and 10 equivlent $H_2{}^{18}O$ (2.0 mmol) was stirred in 2.0 mL acetonitrile for 10 hours at room temperature under an atmospheric pressure nitrogen atmosphere. The ratio of ^{16}O and ^{18}O was detected by MS.

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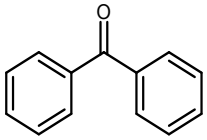
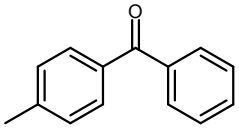
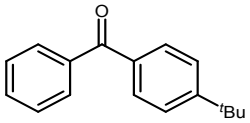
5. Characterization of Products



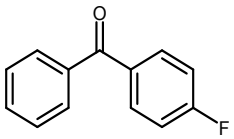
Benzophenone **(2a)**[1]: 0.5 mmol scale, 69.8 mg (77%), white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 - 7.79 (m, 4H), 7.60 - 7.56 (m, 2H), 7.49 - 7.45 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 197.1, 137.8, 132.7 , 130.3, 128.6.



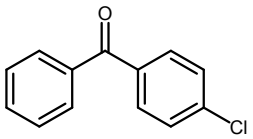
Phenyl(p-tolyl)methanone **(2b)**[1]: 0.5 mmol scale, 62.7 mg (64%), white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 - 7.76 (m, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.60 - 7.54 (m, 1H), 7.48 - 7.43 (m, 2H), 7.28 - 7.24 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 196.7, 143.5, 138.1, 135.0, 132.4, 130.5, 130.1, 129.2, 128.4, 21.9.



(4-(*tert*-Butyl)phenyl)(phenyl)methanone **(2c)**[2]: 0.5 mmol scale, 73.0 mg (61%), white solid; ^{1}H NMR (400 MHz, DMSO-d6) δ = 7.73 - 7.64 (m, 5H), 7.59 - 7.53 (m, 4H), 1.31 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d6) δ = 195.4, 155.8, 137.3, 134.3, 132.5, 129.8, 129.6, 128.6, 125.4, 34.9, 30.9.

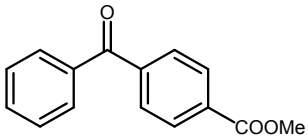


(4-Fluorophenyl)(phenyl)methanone **(2d)**[1]: 0.5 mmol scale, 70.5 mg (71%), white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.87 - 7.82 (m, 2H), 7.78 - 7.75 (m, 2H), 7.61 - 7.57 (m, 1H), 7.50 - 7.46 (m, 2H), 7.18 - 7.12 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.5, 165.5 (d, *J* = 253.0 Hz), 137.6, 134.0 (d, *J* = 3.0 Hz), 132.9 (d, *J* = 9.0 Hz), 132.7, 130.1, 128.6, 115.7 (d, *J* = 22.0 Hz).

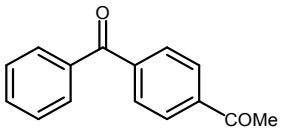


(4-Chlorophenyl)(phenyl)methanone **(2e)**[1]: 0.5 mmol scale, 81.2 mg (75%), white solid; ^{1}H NMR

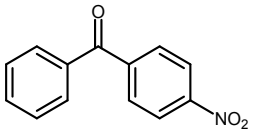
(400 MHz, $CDCl_3$) δ = 7.79 - 7.75 (m, 4H), 7.63 - 7.58 (m, 1H), 7.51 - 7.45 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.7, 139.2, 137.5, 136.1, 132.9, 131.7, 130.2, 128.9, 128.7.



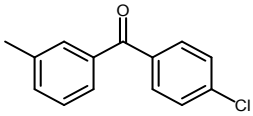
Methyl 4-benzoylbenzoate **(2f)**[2]: 0.5 mmol scale, 70.1 mg (58%), white solid; ^1H NMR (400 MHz, $CDCl_3$) δ = 8.15 (d, *J* = 8.0 Hz, 2H), 7.85 - 7.79 (m, 4H), 7.64 - 7.61 (m, 1H), 7.52 - 7.48 (m, 2H), 3.96 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 196.2, 166.5, 141.5, 137.1, 133.4, 133.2, 130.3, 130.0, 129.7, 128.7, 52.7.



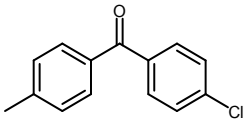
1-(4-Benzoylphenly)ethan-1-one **(2g)**[3]: 0.5 mmol scale, 77.5 mg (69%), light yellow liquid; ^1H NMR (400 MHz, $CDCl_3$) δ = 8.07 - 8.05 (m, 2H), 7.84 (dd, *J* = 24.0, 7.7 Hz, 4H), 7.64 - 7.61 (m, 1H), 7.52 - 7.48 (m, 2H), 2.67 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 197.9, 196.2, 141.5, 139.7, 137.1, 133.3, 130.3, 130.2(8), 128.7, 128.4, 27.2.



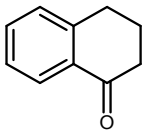
(4-Nitrophenyl)(phenyl)methanone **(2h)**[4]: 0.5 mmol scale, 31.9 mg (28%), white solid; ^1H NMR (400 MHz, $CDCl_3$) δ = 8.36 - 8.33 (m, 2H), 7.96 - 7.93 (m, 2H), 7.82 - 7.80 (m, 2H), 7.69 - 7.64 (m, 1H), 7.55 - 7.51 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.0, 150.1, 143.1, 136.5, 133.7, 130.9, 130.3, 128.9, 123.8.



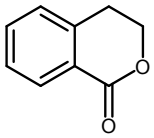
(4-Chlorophenly)(m-tolyl)methanone **(2i)**[5]: 0.5 mmol scale, 58.8 mg (51%), white solid; ^1H NMR (400 MHz, $CDCl_3$) δ = 7.76 - 7.73 (m, 2H), 7.59 (s, 1H), 7.55 - 7.53 (m, 1H), 7.46 - 7.44 (m, 2H), 7.42 - 7.34 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 196.0, 139.0, 138.5, 137.5, 136.2, 133.7, 131.7, 130.6, 128.8, 128.4, 127.5, 21.6.



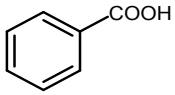
(4-Chlorophenly)(p-tolyl)methanone **(2j)**[6]: 0.5 mmol scale, 58.9 mg (51%), white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.74 - 7.72 (m, 2H), 7.70 - 7.68 (m, 2H), 7.46 - 7.43 (m, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 195.5, 143.8, 138.8, 136.4, 134.7, 131.6, 130.4, 129.3, 128.8, 21.9.



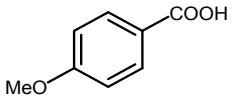
3,4-Dihydronaphthalen-1(2H)-one **(2k)**[7]: 0.5 mmol scale, 46.9mg (64%), light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.06 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.51 - 7.47 (m, 1H), 7.35 - 7.27 (m, 2H), 2.99 (t, *J* = 6.1 Hz, 2H), 2.68 (t, *J* = 6.7Hz, 2H), 2.19 - 2.13 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 198.7, 144.7, 133.6, 132.8, 129.0, 127.4, 126.8, 39.4, 29.9, 23.5.



Isochroman-1-one **(2l)**[7]: 0.5 mmol scale, 47.5mg (64%), light yellow liquid; ^{1}H NMR (400 MHz, DMSO-d6) δ = 7.94 (dd, *J* = 7.7, 0.8 Hz, 1H), 7.63 (td, *J* = 7.5, 1.3 Hz, 1H), 7.47 - 7.41 (m, 2H), 4.51 (t, *J* = 6.0 Hz, 2H), 3.07 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ = 169.6, 145.5, 138.9, 134.6, 132.9, 132.6, 130.2, 72.4, 32.2.



Benzoic acid **(4a)**[8]: 0.5 mmol scale, 52.2 mg (54%), white solid; ^{1}H NMR (400 MHz, DMSO-d6) δ = 13.01 (br, 1H), 7.97 - 7.95 (m, 2H), 7.65 - 7.61 (m, 1H), 7.53 - 7.49 (m, 2H); ^{13}C NMR (101 MHz, DMSO-d6) δ = 167.4, 132.9, 130.8, 129.4, 128.6.



4-methoxybenzoic acid **(4b)**[8]: 0.5 mmol scale, 94.3 mg (62%), white solid; ^{1}H NMR (400 MHz, DMS-d6) δ = 12.66 (br, 1H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d6) δ = 167.2, 163.0, 131.5, 123.1, 113.9, 55.5.

6. Reference

(1) He, C.; Zhang, X.; Huang, R.; Pan, J.; Li, J.; Ling, X.; Xiong, Y.; Zhu, X. *Tetrahedron Letters* **2014**, *55*, 4458.

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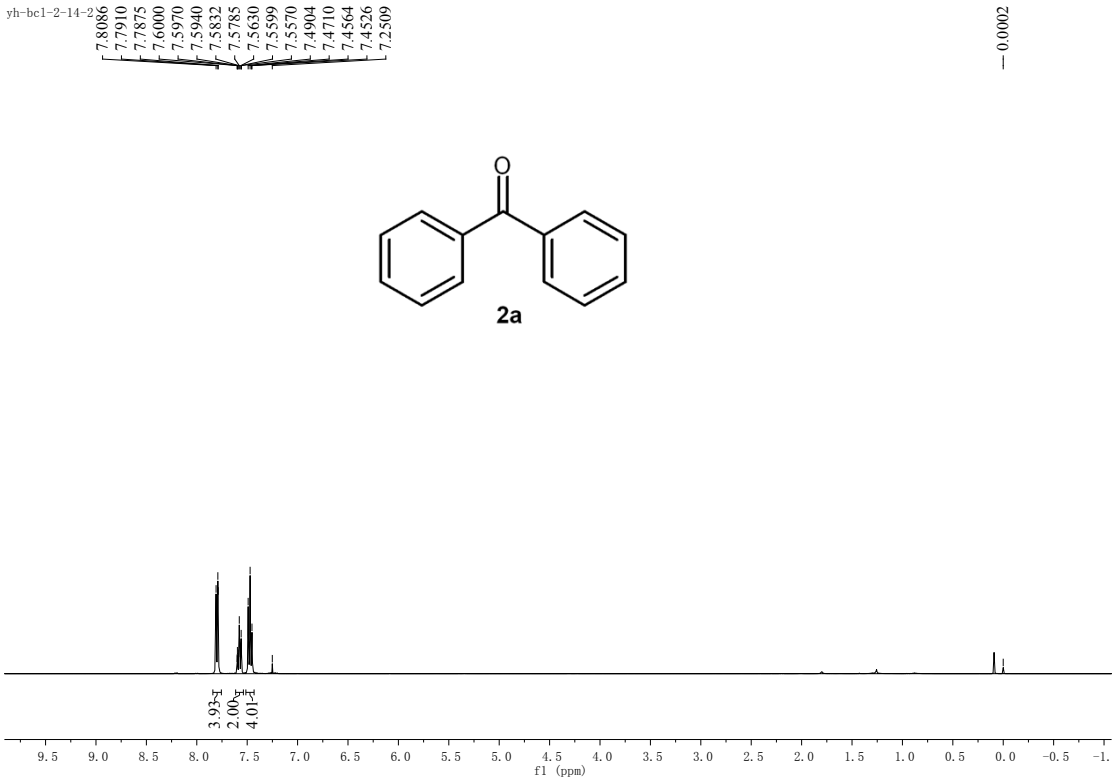
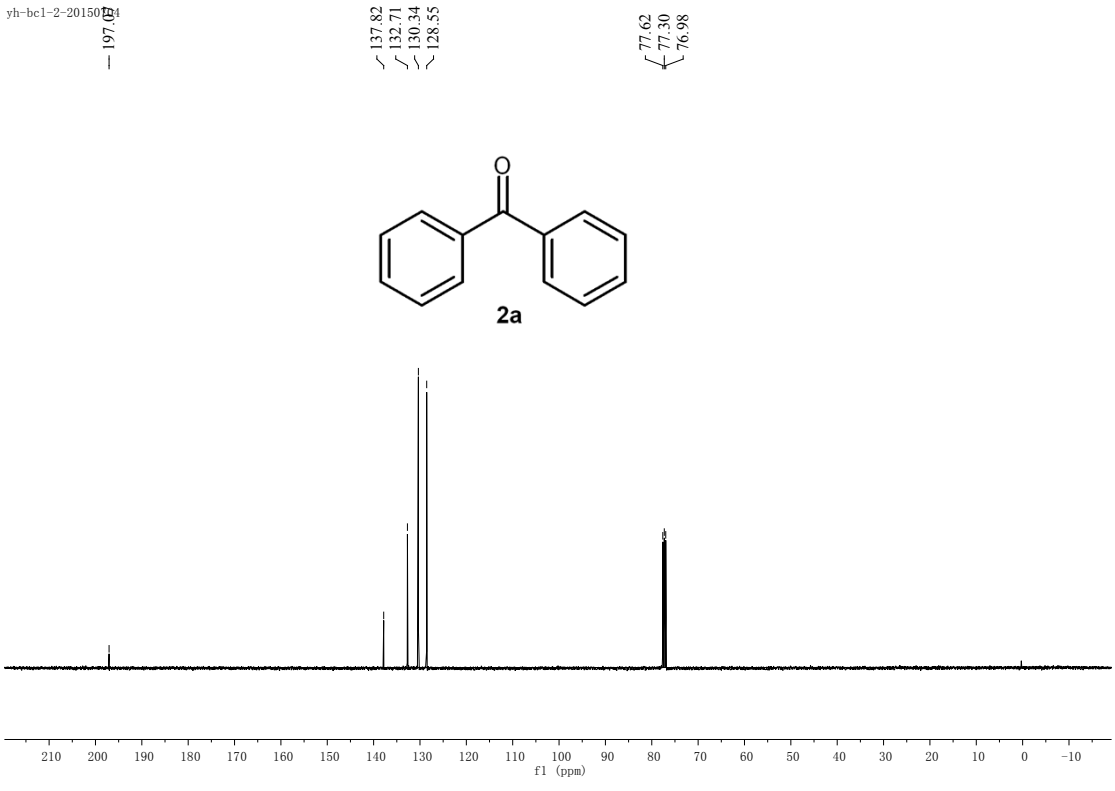
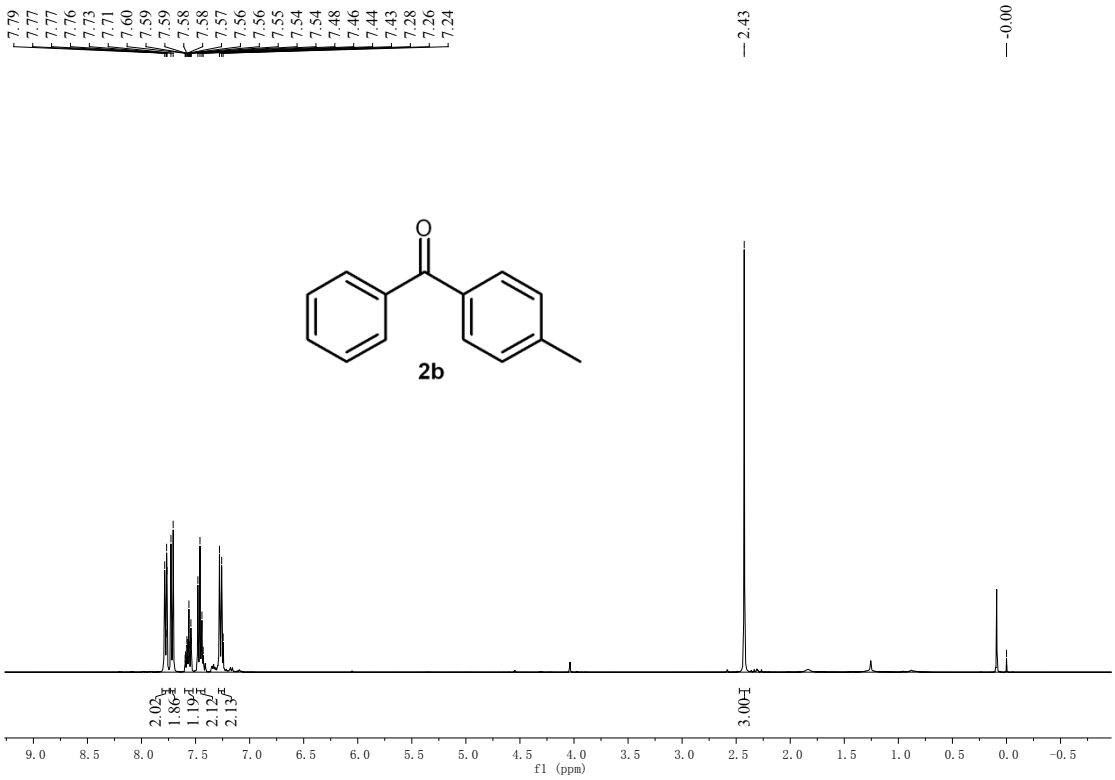
7. NMR Spectra of Product



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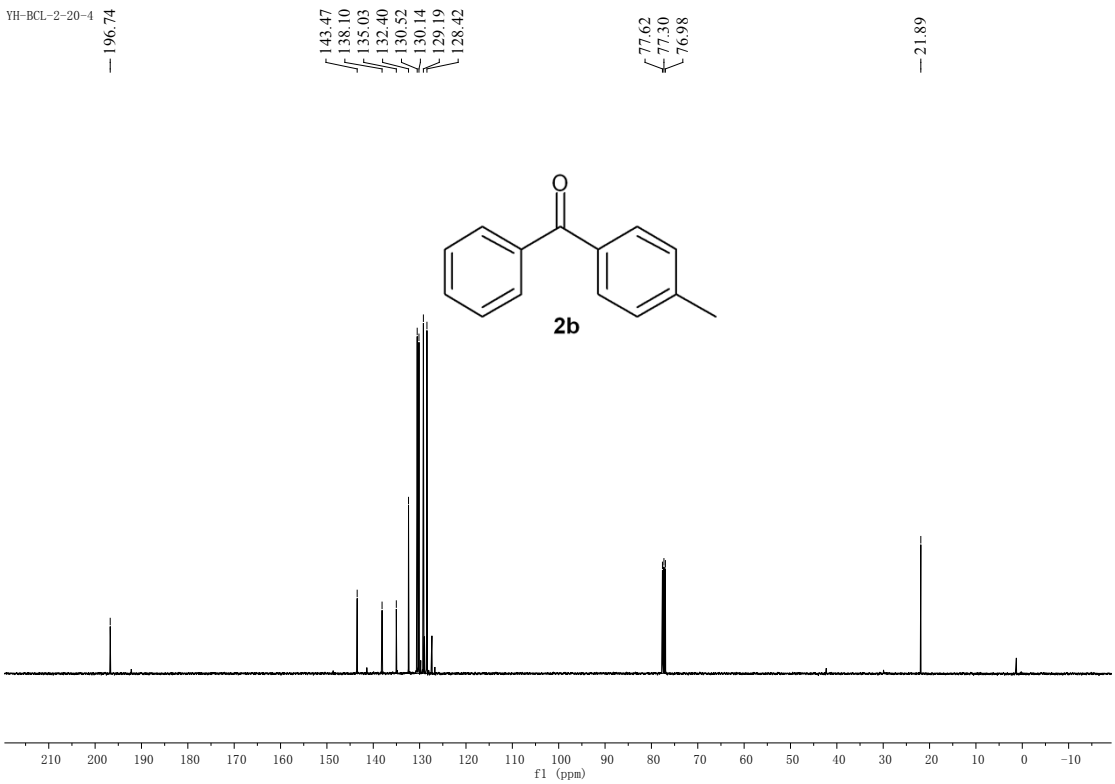
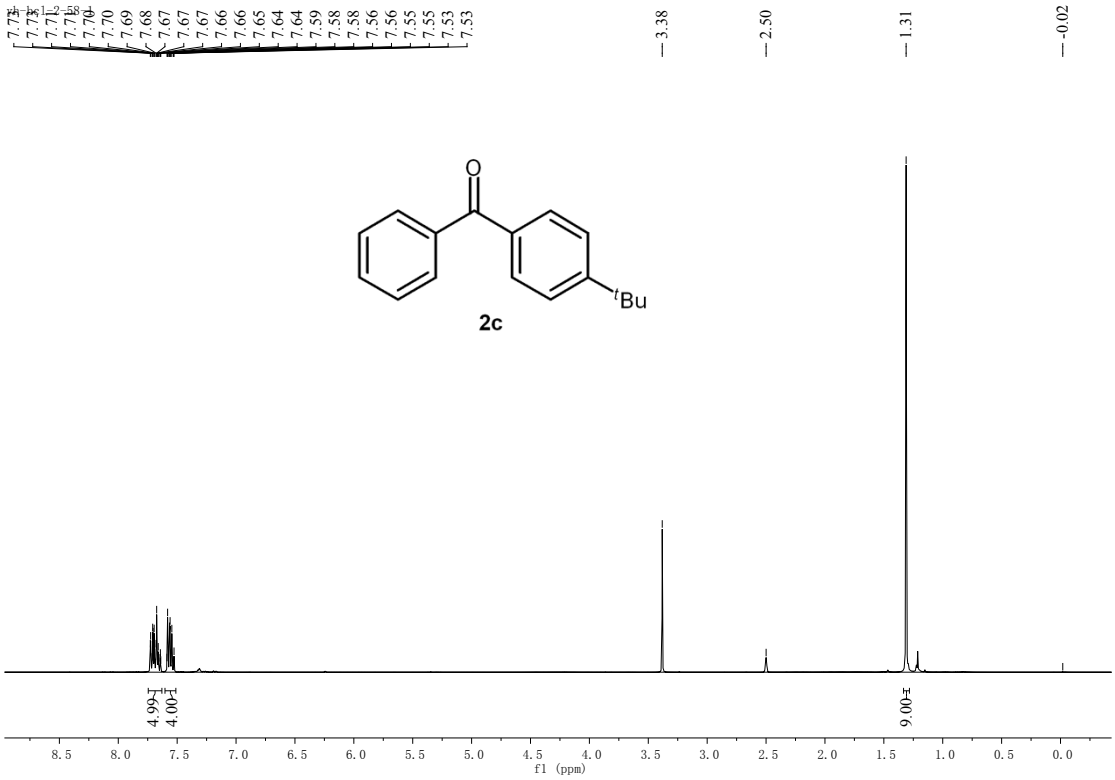
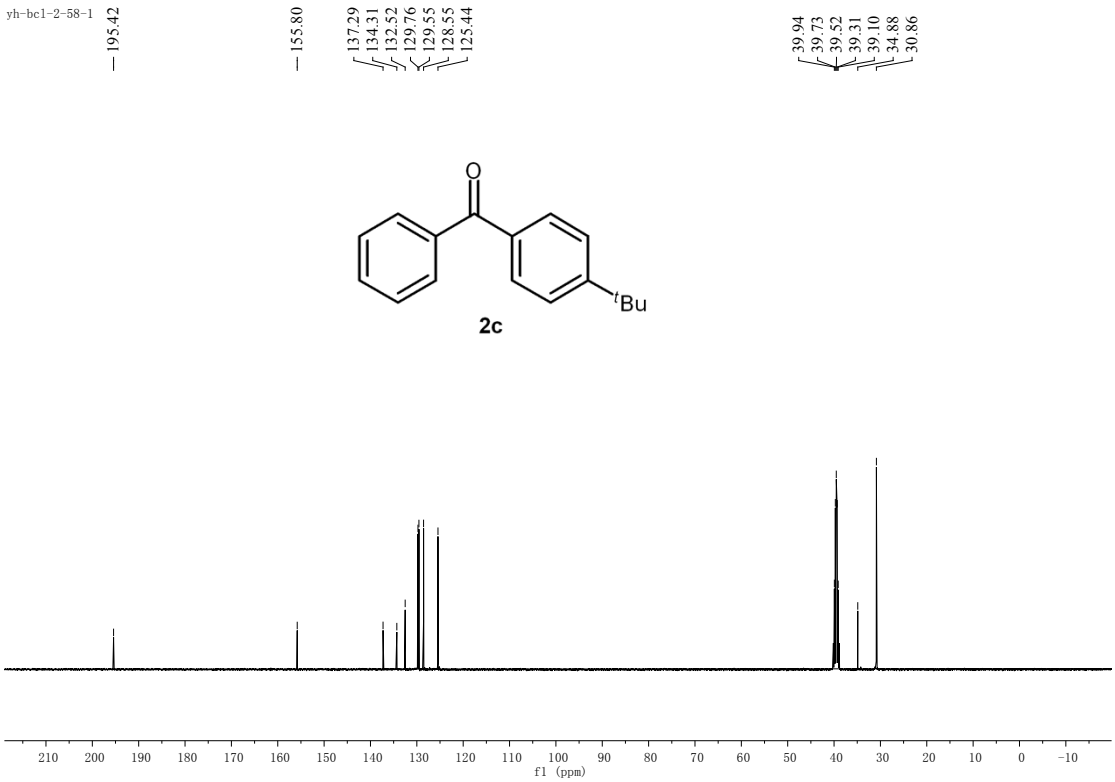
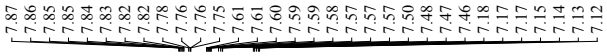
3.00
f1 (ppm)


YH-BCL-2-20-4
196.74
143.47
138.10
135.03
132.40
130.52
130.14
129.19
128.42
77.62
77.30
76.98
21.89
O
2b
f1 (ppm)


7.73
7.73
7.71
7.71
7.70
7.70
7.69
7.68
7.67
7.67
7.67
7.66
7.66
7.65
7.64
7.64
7.59
7.58
7.58
7.56
7.56
7.55
7.55
7.53
7.53
3.38
2.50
1.31
-0.02
O
tBu
2c
4.99
4.00
9.00
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)


yh-bc1-2-58-1
195.42
155.80
137.29
134.31
132.52
129.76
129.55
128.55
125.44
39.94
39.73
39.52
39.31
39.10
34.88
30.86
O
tBu
2c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.87
7.86
7.85
7.85
7.84
7.83
7.82
7.82
7.78
7.76
7.76
7.75
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.57
7.57
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7.47
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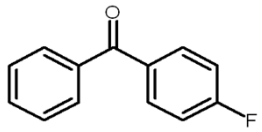
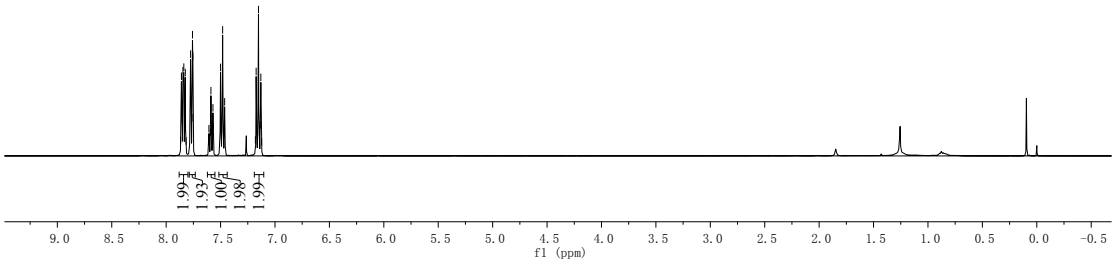
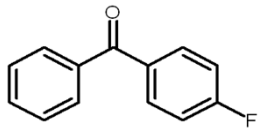
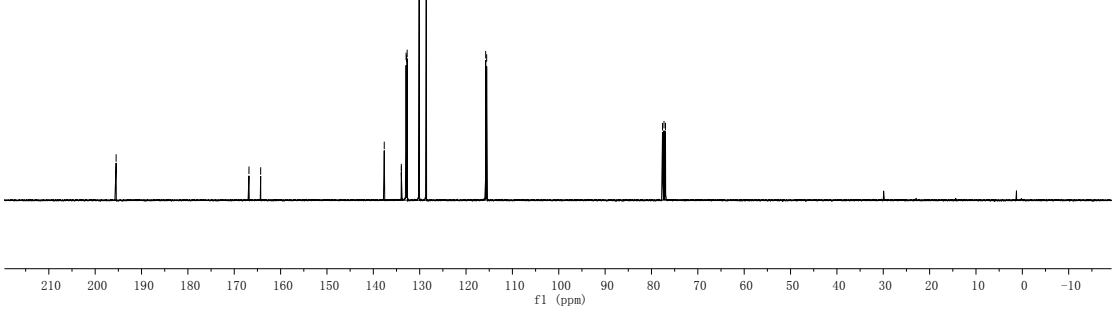
7.17
7.17
7.15
7.14
7.13
7.12

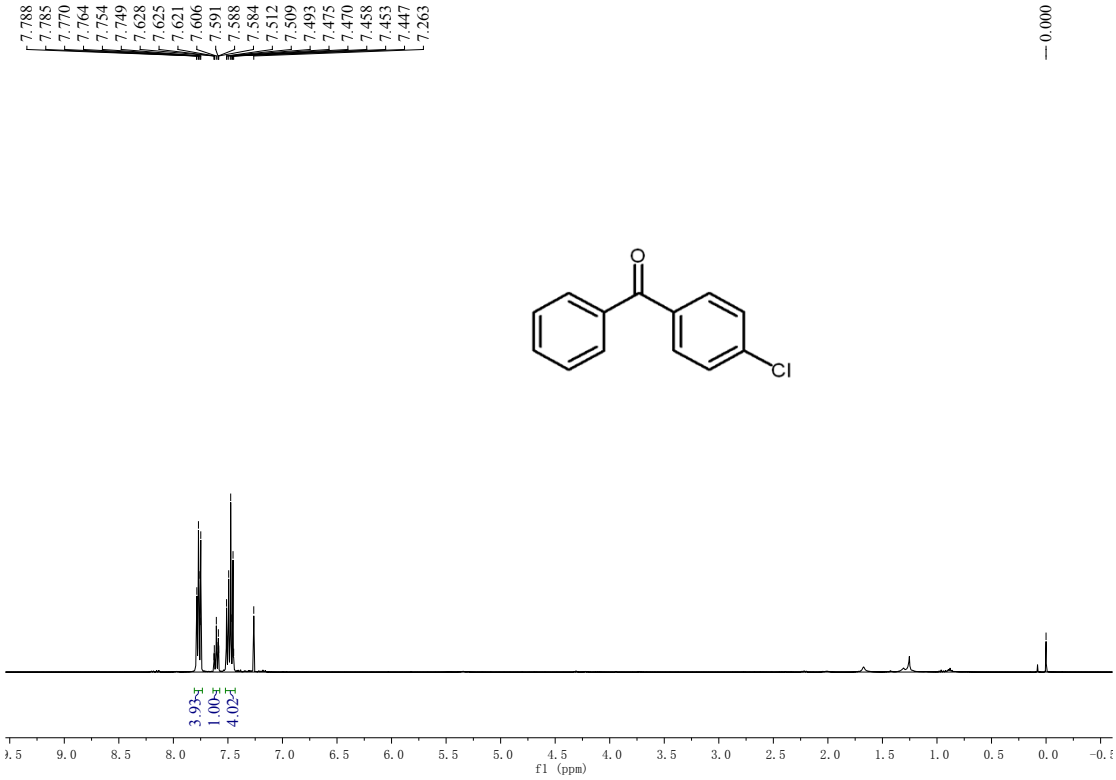

O
F

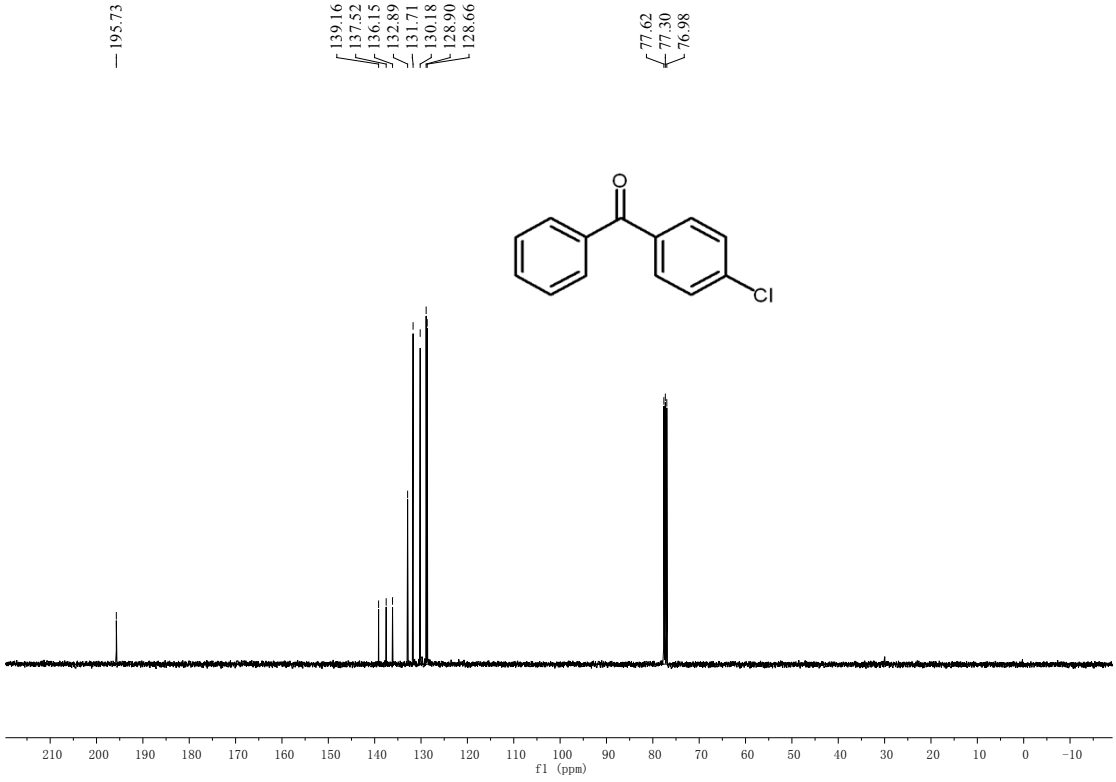

1.99
1.93
1.00
1.98
1.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


YH-BCL-2-20-3
195.48
166.83
164.30
137.64
133.97
133.94
132.93
132.84
132.70
130.09
128.57
115.77
115.55
77.62
77.30
76.98

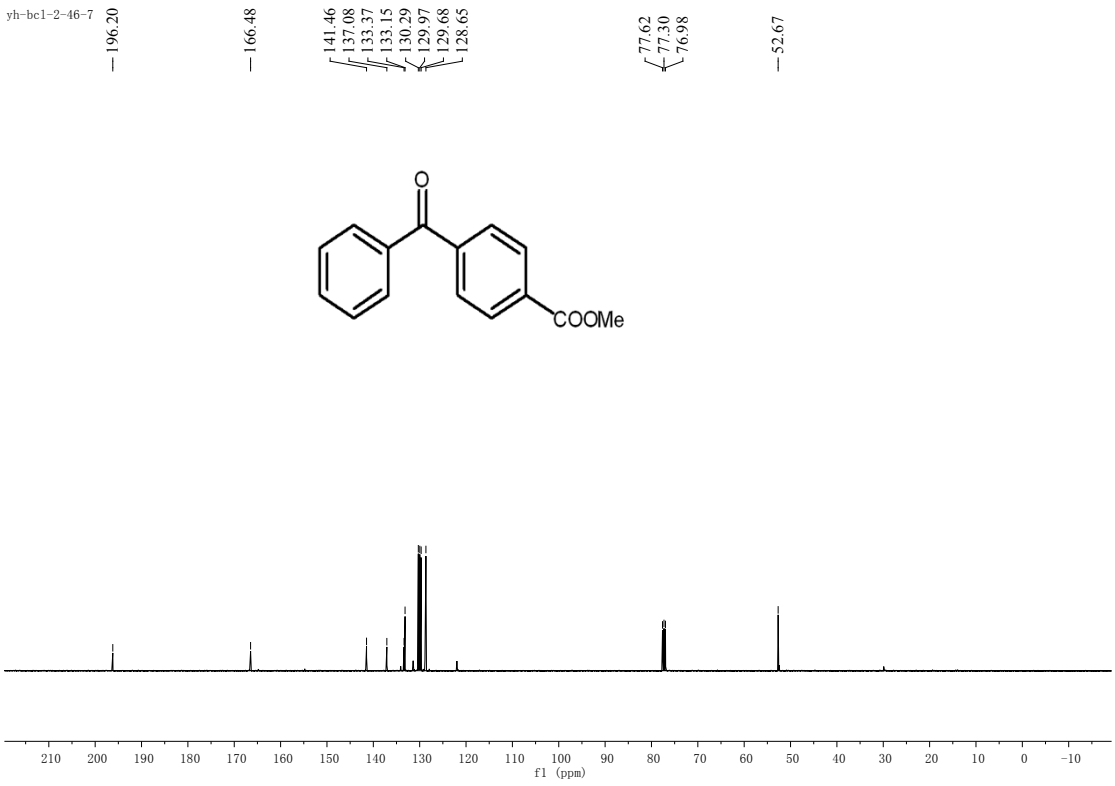

O
F

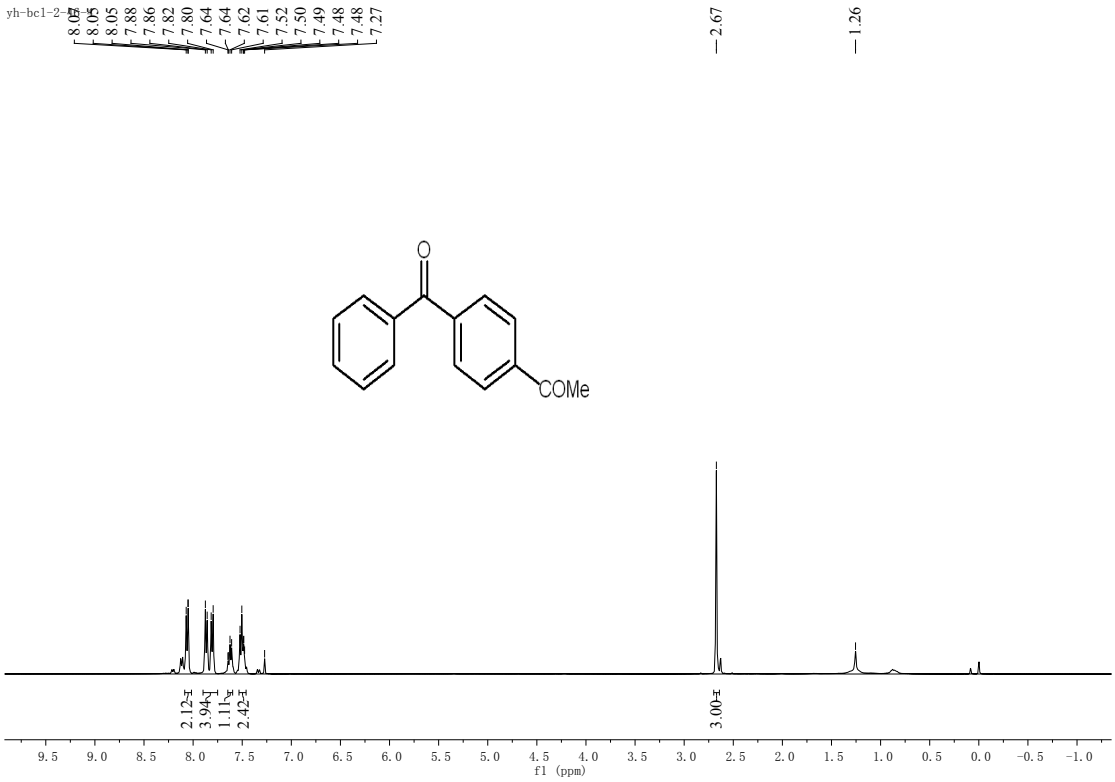

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

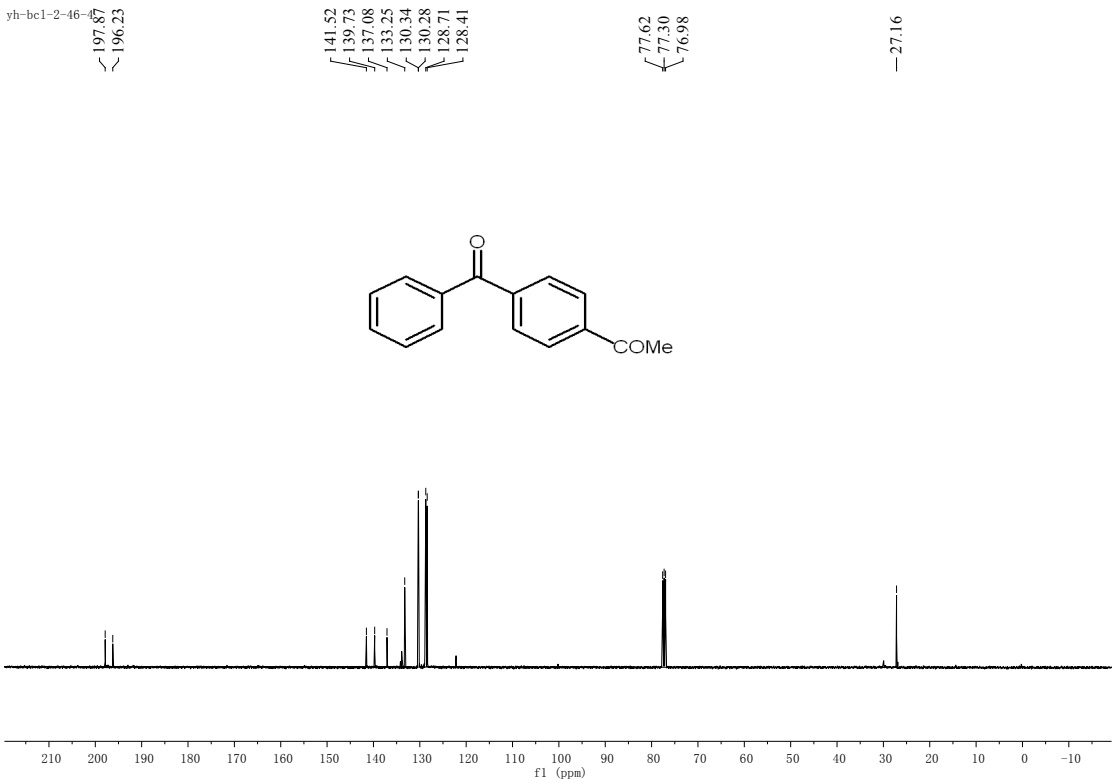

7.788
7.785
7.770
7.764
7.754
7.749
7.628
7.625
7.621
7.606
7.591
7.588
7.584
7.512
7.509
7.493
7.475
7.470
7.458
7.453
7.447
7.263
0.000
O
Cl
3.93
1.00
4.02
f1 (ppm)

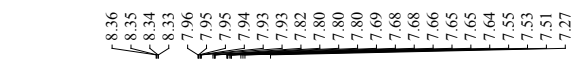

195.73
139.16
137.52
136.15
132.89
131.71
130.18
128.90
128.66
77.62
77.30
76.98
O
Cl
f1 (ppm)


yh-bcl-2-46-7
8.157
8.137
7.848
7.828
7.812
7.792
7.633
7.615
7.597
7.515
7.496
7.478
3.960
0.000
COOMe
2.02
3.98
1.06
2.11
3.00
f1 (ppm)


yh-bcl-2-46-7
196.20
166.48
141.46
137.08
133.37
133.15
130.29
129.97
129.68
128.65
77.62
77.30
76.98
52.67
COOMe
f1 (ppm)


8.05
8.05
7.88
7.86
7.82
7.80
7.64
7.64
7.62
7.61
7.52
7.50
7.49
7.48
7.27
2.67
1.26
O
COMe
2.12
3.94
1.11
2.42
3.00
f1 (ppm)


197.87
196.23
141.52
139.73
137.08
133.25
130.34
130.28
128.71
128.41
77.62
77.30
76.98
27.16
O
COMe
f1 (ppm)


8.36
8.35
8.34
8.33
7.96
7.95
7.95
7.94
7.93
7.93
7.82
7.80
7.80
7.80
7.69
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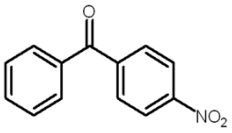
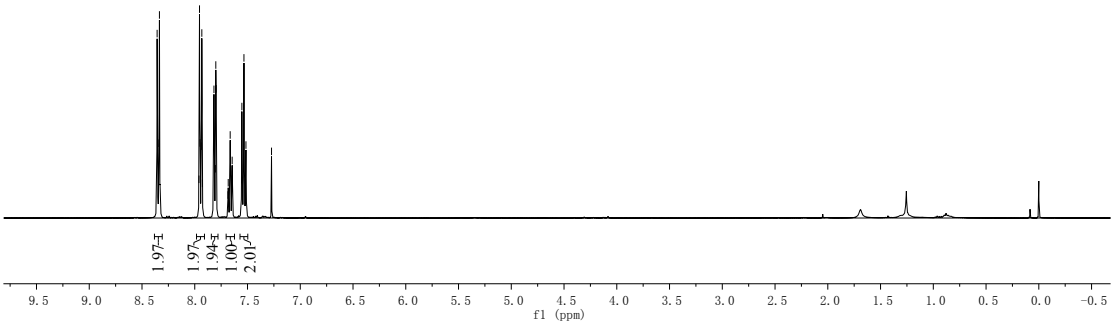
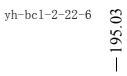
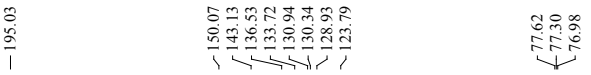
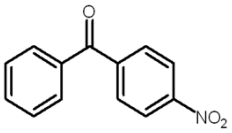
7.68
7.66
7.65
7.65
7.64
7.55
7.53
7.51
7.27

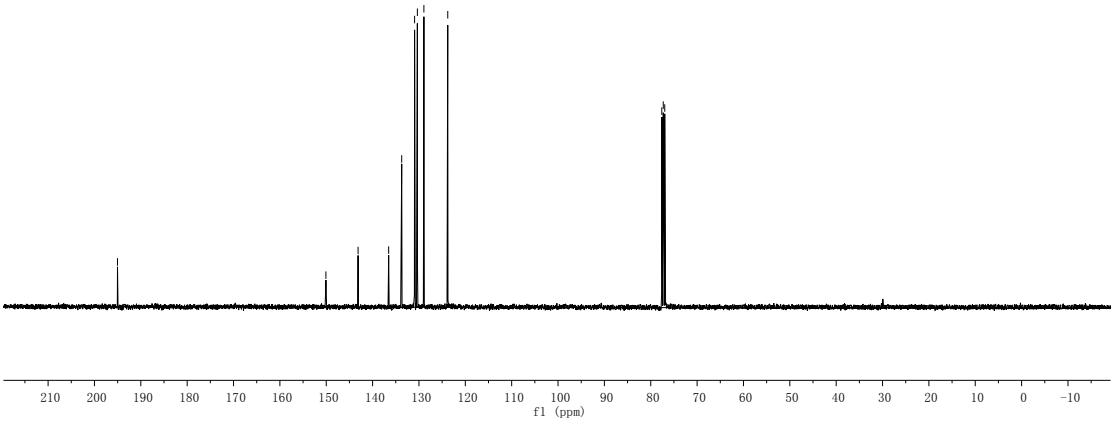

O
NO2

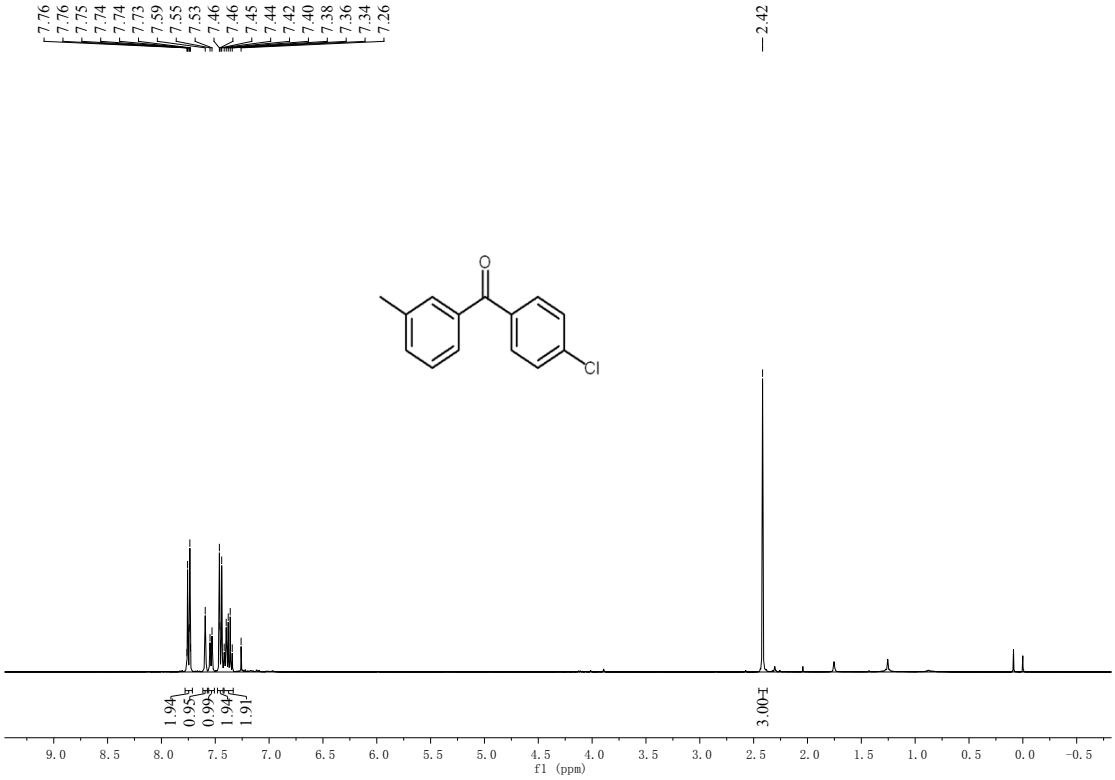

1.97
1.97
1.94
1.00
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

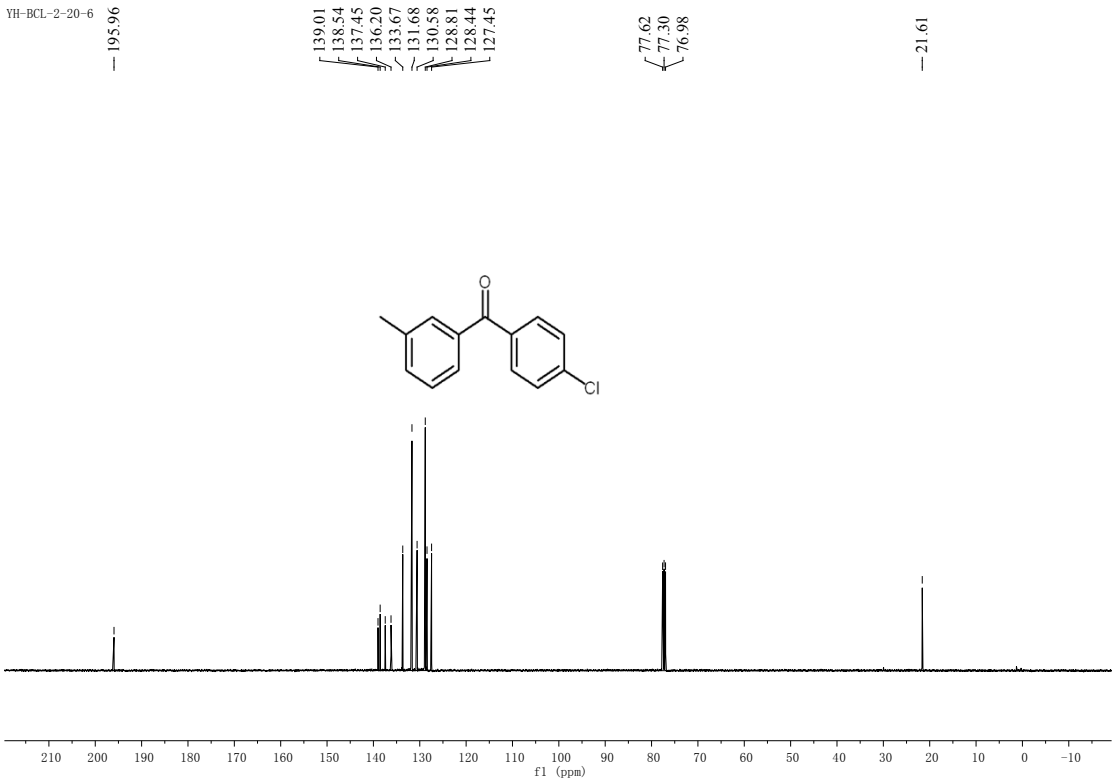

yh-bc1-2-22-6

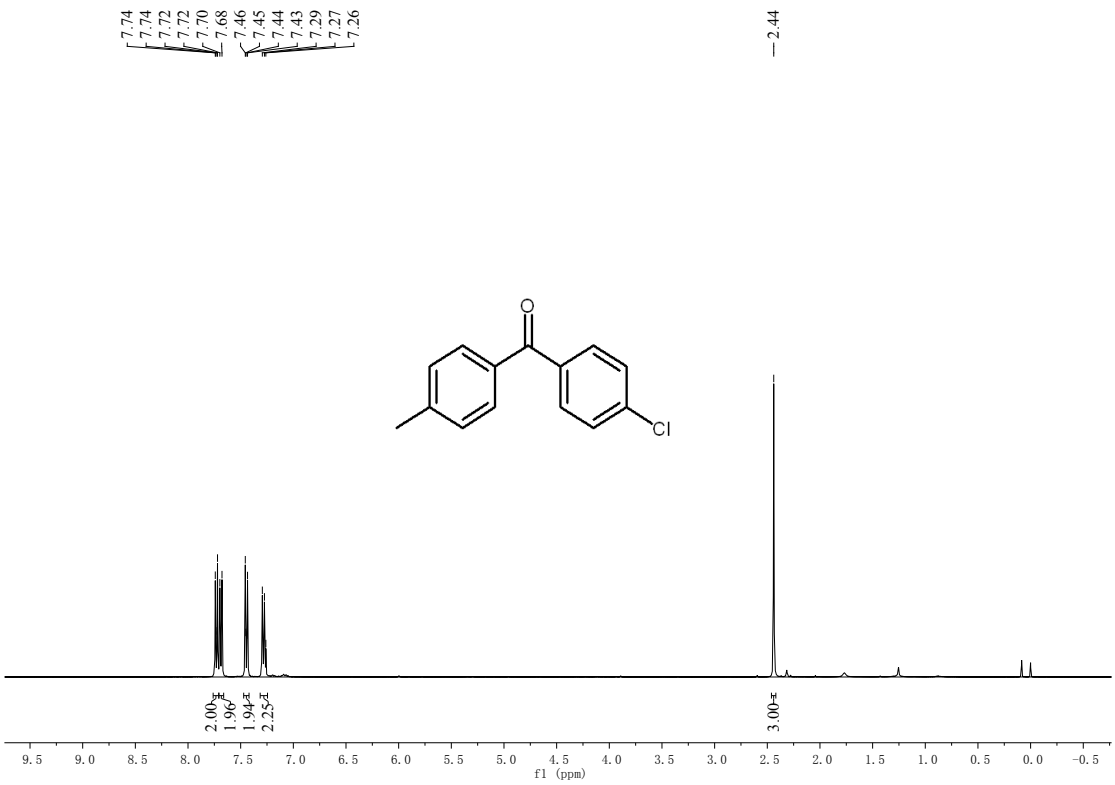

195.03
150.07
143.13
136.53
133.72
130.94
130.34
128.93
123.79
77.62
77.30
76.98


O
NO2


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


7.76
7.76
7.75
7.74
7.74
7.73
7.59
7.55
7.53
7.46
7.46
7.45
7.44
7.42
7.40
7.38
7.36
7.34
7.26
2.42
O
Cl
1.94
0.95
0.99
1.94
1.91
3.00
f1 (ppm)


YH-BCL-2-20-6
195.96
139.01
138.54
137.45
136.20
133.67
131.68
130.58
128.81
128.44
127.45
77.62
77.30
76.98
21.61
O
Cl
f1 (ppm)

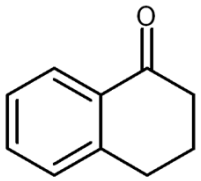

7.74
7.74
7.72
7.72
7.70
7.68
7.46
7.45
7.44
7.43
7.29
7.27
7.26
2.44
O
Cl
2.00
1.96
1.94
2.25
3.00
f1 (ppm)


YH-BCL-2-20-5
195.49
143.79
138.81
136.40
134.70
131.59
130.41
129.33
128.78
77.62
77.30
76.98
21.93
O
Cl
f1 (ppm)

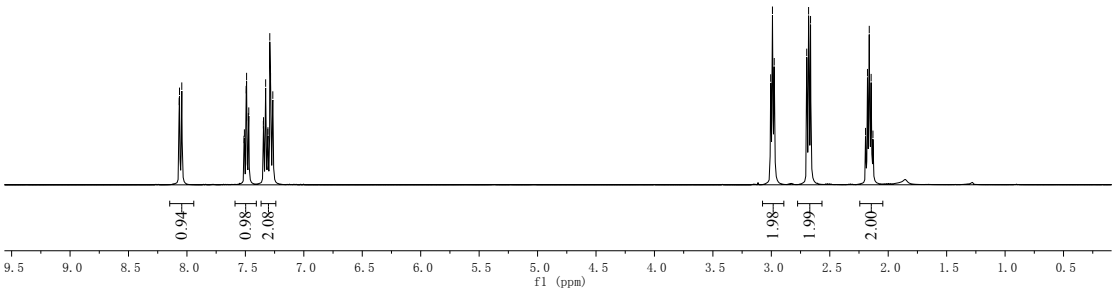
yh-bcl-2-46-5

8.07 8.06 8.05 8.04 7.51 7.51 7.49 7.49 7.47 7.47 7.35 7.34 7.33 7.31 7.31 7.29 7.28 7.27

3.01 2.99 2.98 2.70 2.68 2.66 2.19 2.18 2.16 2.15 2.13



2k



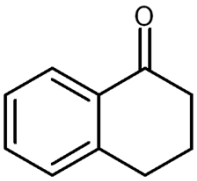
yh-bcl-2-46-5

198.71

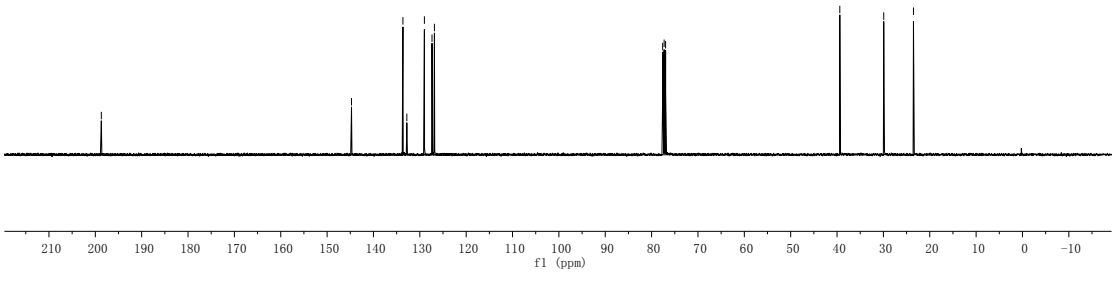
144.74 133.64 132.80 129.01 127.37 126.85

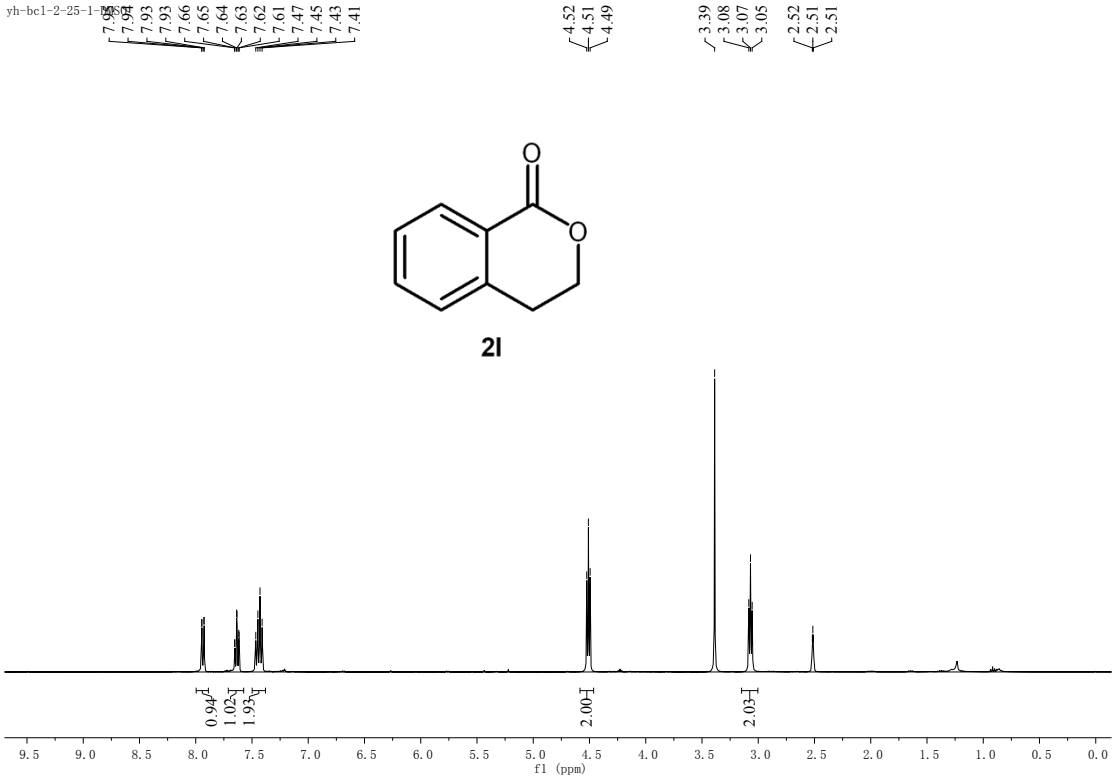
77.62 77.30 76.98

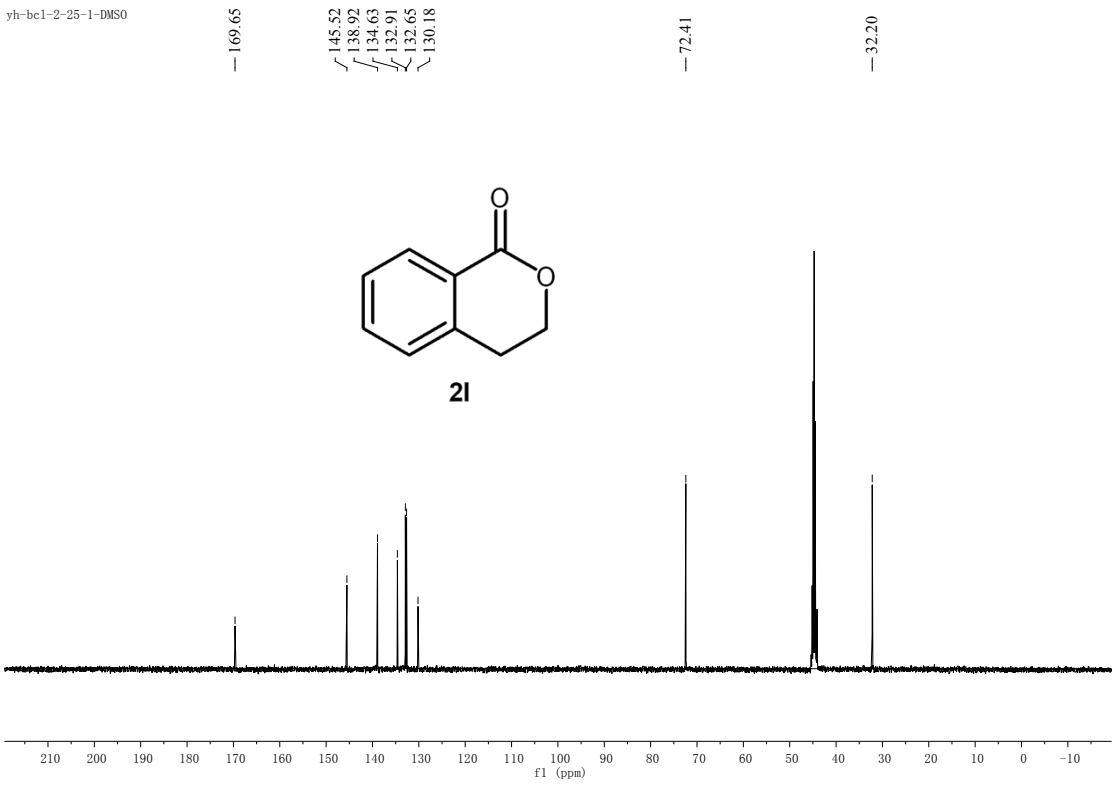
39.40 29.93 23.51

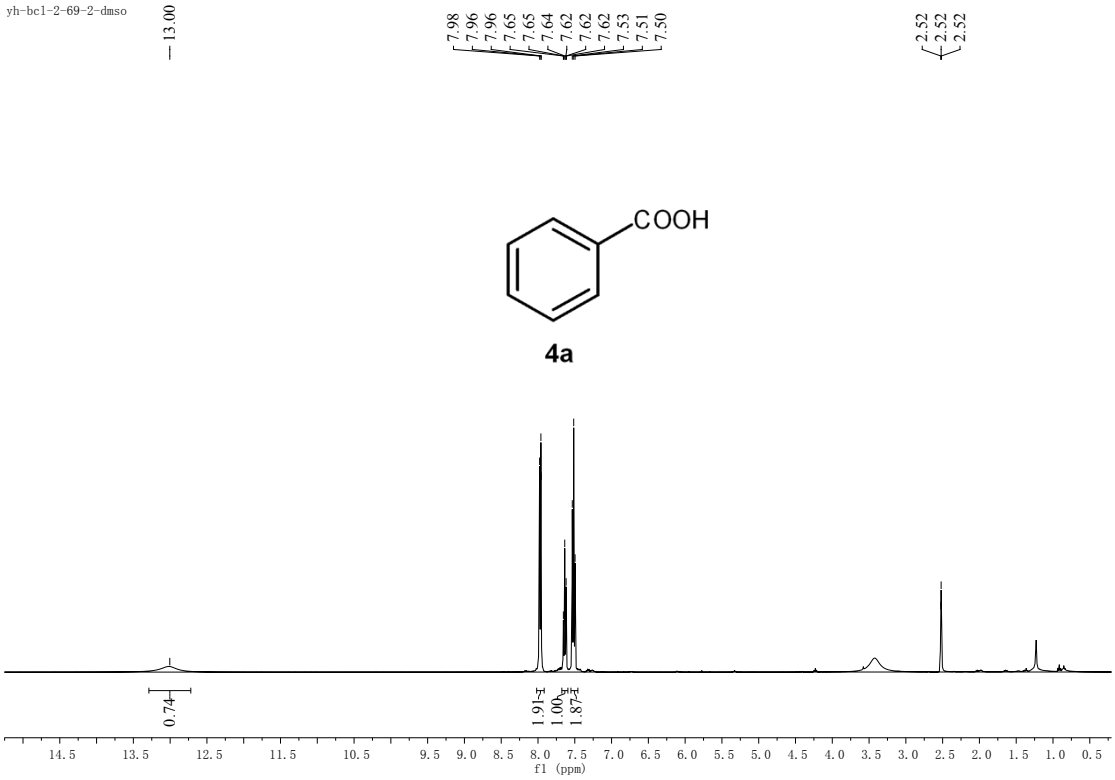


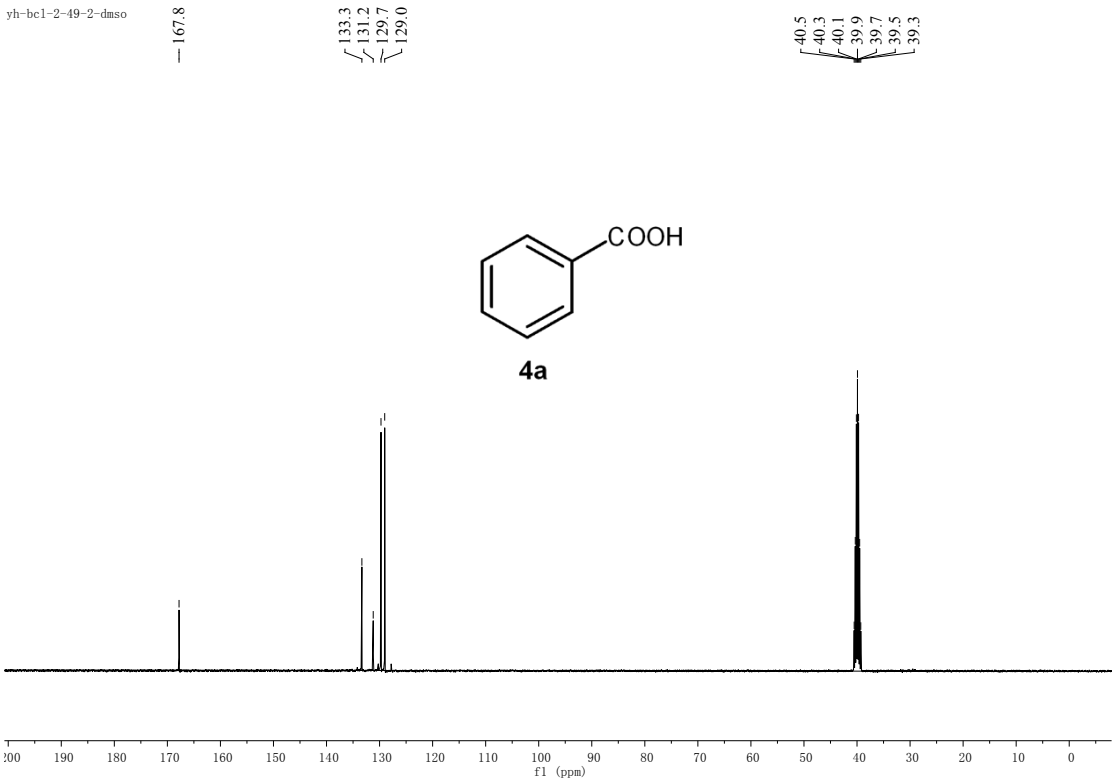
2k

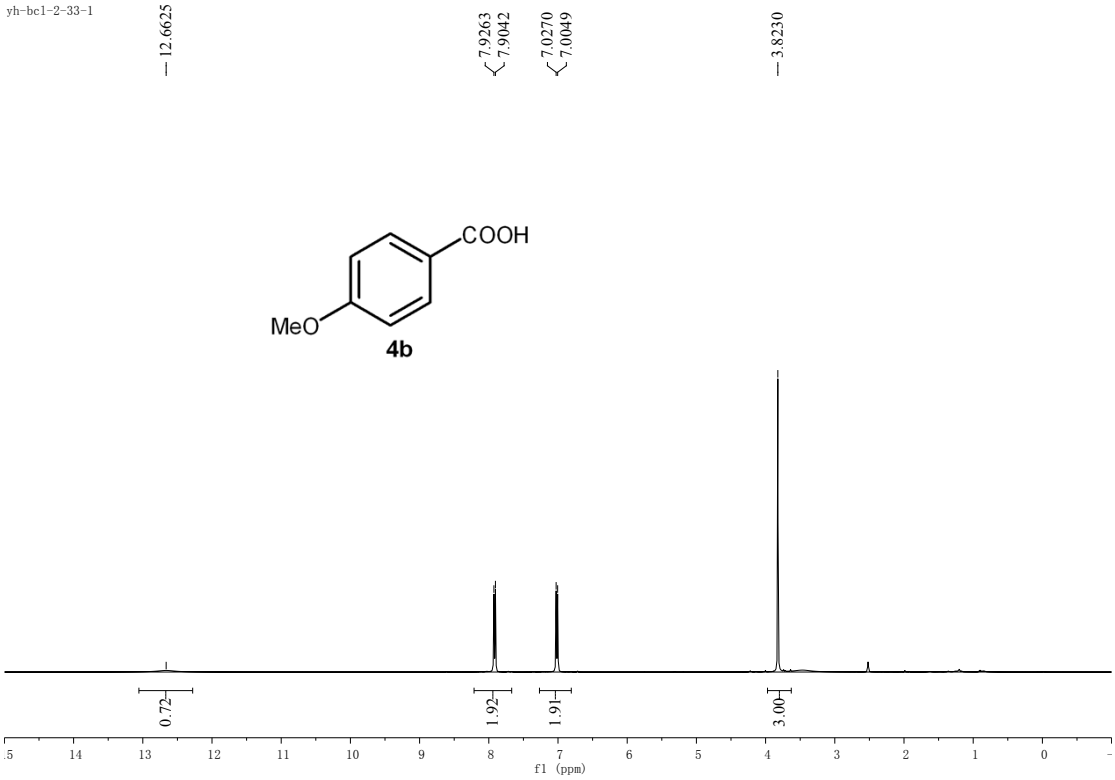


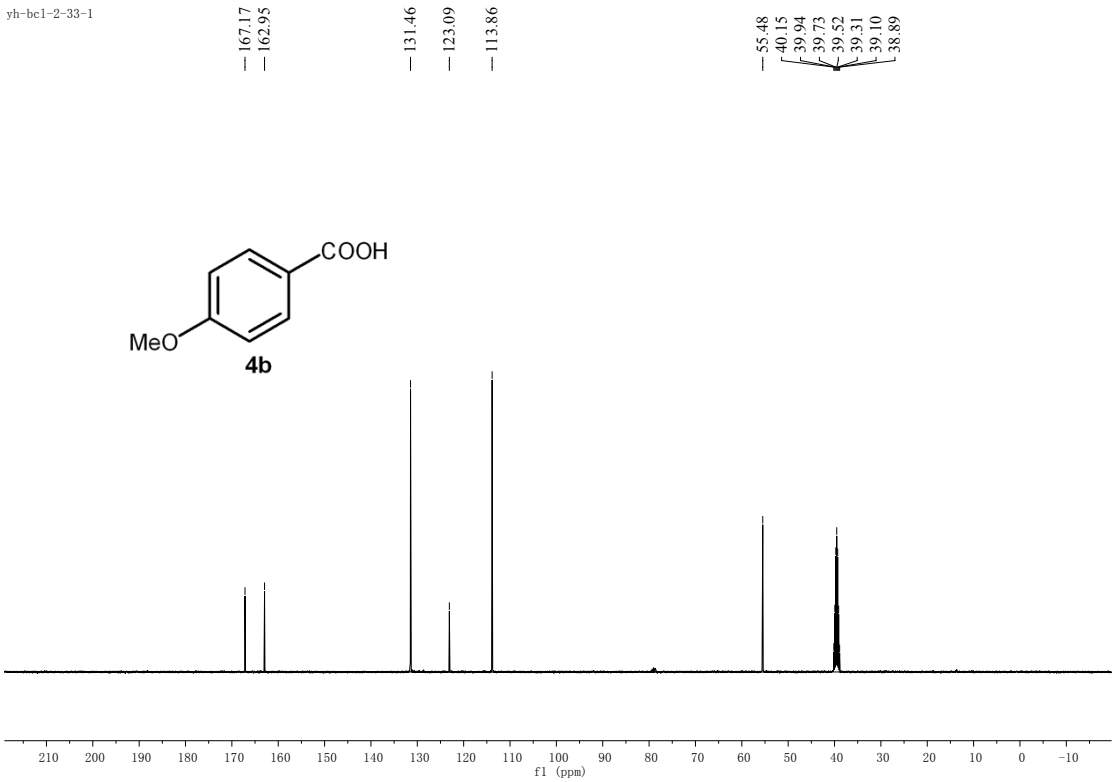

yh-bcl-2-25-1-DMSO
7.95
7.94
7.93
7.93
7.66
7.65
7.64
7.63
7.62
7.61
7.47
7.45
7.43
7.41
4.52
4.51
4.49
3.39
3.08
3.07
3.05
2.52
2.51
2.51
O
O
2l
0.94
1.02
1.93
2.00
2.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


yh-bcl-2-25-1-DMSO
169.65
145.52
138.92
134.63
132.91
132.65
130.18
72.41
32.20
O
O
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


yh-bc1-2-69-2-dmso
13.00
7.98
7.96
7.96
7.65
7.65
7.64
7.62
7.62
7.62
7.53
7.51
7.50
2.52
2.52
2.52
COOH
4a
0.74
1.91
1.00
1.87
14.5
13.5
12.5
11.5
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
f1 (ppm)


yh-bc1-2-49-2-dmso
167.8
133.3
131.2
129.7
129.0
40.5
40.3
40.1
39.9
39.7
39.5
39.3
COOH
4a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


yh-bc1-2-33-1
12.6625
7.9263
7.9042
7.0270
7.0049
3.8230
COOH
MeO
4b
0.72
1.92
1.91
3.00
f1 (ppm)


yh-bc1-2-33-1
167.17
162.95
131.46
123.09
113.86
55.48
40.15
39.94
39.73
39.52
39.31
39.10
38.89
COOH
MeO
4b
f1 (ppm)