Supporting Information for

Intramolecular Oxidative Coupling: I_2/TBHP/NaN_3-Mediated Synthesis of Benzofuran Derivatives

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1 General information

All reactions were performed in air. ^{1}H and ^{13}C NMR spectra were determined in $CDCl_3$ or DMSO-d_6 on a Varian-Inova 400MHz, 500MHz or 600 MHz spectrometer and chemical shifts were reported in ppm from internal TMS (δ). Column chromatography was performed with 300-400 mesh silica gel using column techniques. All of the reagents were used directly as obtained commercially unless otherwise noted.

2 General experimental procedure

General experimental procedure for the synthesis of trans-2-hydroxychalcones

To a solution of aromatic methyl ketones (40 mmol) and salicyl-aldehyde (6.10 g, 50 mmol) in EtOH (50 mL) was added 40% KOH (10 mL) aqueous solution dropwise and the reaction was carried out at 60 °C (or room temperature) for 2–4 h until the disappearance of starting material (monitored by thin layer chromatography). The solution/suspension was poured into cold H_2O and the mixture was neutralized with 2M HCl to a pH in the range of 2–3. The resulting precipitate was collected, washed with H_2O and recrystallized from EtOH.

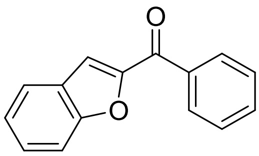
General experimental procedure of the oxidative coupling reaction

To a solution of trans-2-hydroxychalcones (0.25 mmol), NaN_3 (0.05 mmol) and iodine (0.025 mmol) in EtOH (4 mL) was added TBHP (0.5mmol) aqueous solution and the reaction was carried out at 80 °C for 6–16 h until the disappearance of starting material (monitored by thin layer chromatography). The solvent was evaporated under reduced pressure and the crude mixture was purified by silica gel column chromatography for pure product.

3 Compounds characterization data

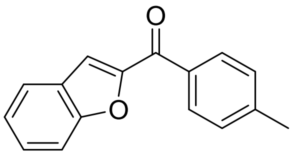
-------^{1}HNMR , ^{13}CNMR and Unknown Compounds' HRMS data

2a benzofuran-2-yl(phenyl)methanone[1]



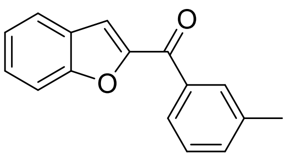
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.65 (t, *J* = 8.4 Hz, 2H), 7.57 – 7.53 (m, 3H), 7.53 – 7.49 (m, 1H), 7.34 (t, *J* = 7.5 Hz, 1H).^{13}C NMR (151 MHz, $CDCl_3$) δ 184.42, 156.00, 152.18, 137.23, 132.94, 129.46, 128.57, 128.43, 127.01, 124.02, 123.36, 116.64, 112.57.

2b benzofuran-2-yl(p-tolyl)methanone[1]



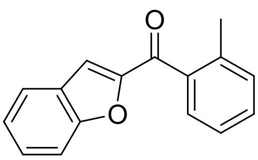
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.2 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.63 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.53 – 7.45 (m, 2H), 7.33 (d, *J* = 7.7 Hz, 3H), 2.45 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 184.12, 155.92, 152.38, 143.88, 134.57, 129.67, 129.29, 128.26, 127.05, 123.96, 123.30, 116.21, 112.56, 21.77.

2c benzofuran-2-yl(m-tolyl)methanone



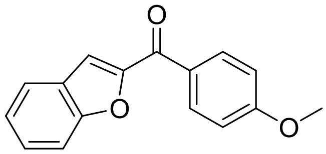
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 6.4 Hz, 2H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.63 (m, 1H), 7.54 – 7.48 (m, 2H), 7.45 (dd, *J* = 10.7, 7.7 Hz, 2H), 7.37 – 7.32 (m, 1H), 2.47 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 184.65, 156.01, 152.28, 138.48, 137.31, 133.72, 129.87, 128.39, 128.35, 127.05, 126.69, 123.98, 123.33, 116.52, 112.57, 21.42. HRMS (ESI$^+$): calcd for $C_{16}H_{12}NaO_2$ $[M+Na]^+$ 259.0735, found 259.0724.

2d benzofuran-2-yl(o-tolyl)methanone[2]

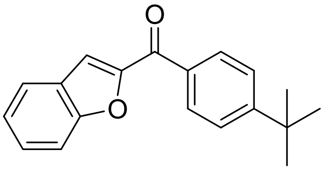


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.9 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.46 (td, *J* = 7.6, 1.0 Hz, 1H), 7.33 (dd, *J* = 14.1, 6.3 Hz, 4H), 2.47 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 186.94, 156.27, 152.73, 137.44, 137.42, 131.30, 130.96, 128.63, 128.61, 127.07, 125.28, 124.01, 123.44, 117.37, 112.67, 19.77.

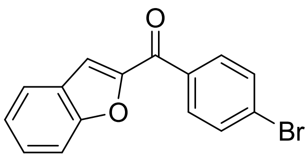
2e benzofuran-2-yl(4-methoxyphenyl)methanone[1]


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 – 8.08 (m, 2H), 7.72 (d, J = 7.9 Hz, 1H), 7.67 – 7.61 (m, 1H), 7.54 – 7.44 (m, 1H), 7.35 – 7.29 (m, 1H), 7.02 (d, J = 8.9 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ182.87, 163.62, 155.81, 152.66, 131.99, 129.82, 128.05, 127.06, 123.91, 123.19, 115.59, 113.87, 112.50, 55.57.

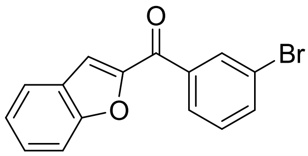
2f benzofuran-2-yl(4-(tert-butyl)phenyl)methanone[3]


^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 – 8.01 (m, 2H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.66 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.59 – 7.55 (m, 3H), 7.51 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.37 – 7.32 (m, 1H), 1.41 (s, 9H).^{13}C NMR (126 MHz, $CDCl_3$) δ 184.03, 156.76, 155.95, 152.51, 134.55, 129.52, 128.21, 127.09, 125.55, 123.93, 123.27, 116.13, 112.55, 35.19, 31.15.

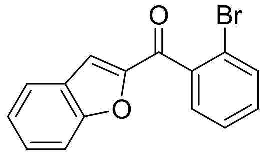
2g benzofuran-2-yl(4-bromophenyl)methanone[1]


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.94 (m, 2H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.68 (m, 2H), 7.65 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.57 (d, *J* = 0.8 Hz, 1H), 7.53 (ddd, *J* = 8.4, 7.3, 1.2 Hz, 1H), 7.38 – 7.34 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 183.09, 156.04, 152.08, 135.85, 131.89, 131.04, 128.59, 128.11, 126.92, 124.14, 123.38, 116.50, 112.58.

2h benzofuran-2-yl(3-bromophenyl)methanone[4]

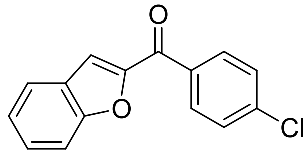

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (s, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.76 (t, *J* = 7.0 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.57 (s, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 182.67, 156.11, 151.81, 138.91, 135.78, 132.33, 130.14, 128.73, 128.03, 126.89, 124.18, 123.46, 122.78, 116.91, 112.62.

2i benzofuran-2-yl(2-bromophenyl)methanone[4]



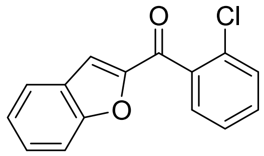
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (t, *J* = 1.7 Hz, 1H), 8.01 – 7.95 (m, 1H), 7.79 – 7.72 (m, 2H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 0.6 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.35 (dd, *J* = 11.1, 3.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 182.75, 156.11, 151.73, 138.89, 135.81, 132.32, 130.17, 128.78, 128.04, 126.88, 124.20, 123.49, 122.79, 117.04, 112.64.

2j benzofuran-2-yl(4-chlorophenyl)methanone[1]



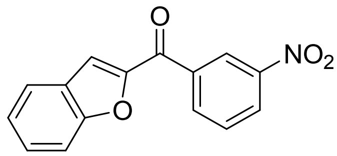
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 2H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 0.6 Hz, 1H), 7.55 – 7.51 (m, 3H), 7.37 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 182.92, 156.04, 152.13, 139.46, 135.42, 130.95, 128.91, 128.57, 126.93, 124.13, 123.37, 116.45, 112.57.

2k benzofuran-2-yl(2-chlorophenyl)methanone[5]



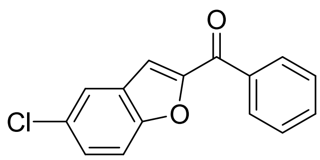
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.9 Hz, 1H), 7.64 (dd, *J* = 8.5, 0.7 Hz, 1H), 7.57 – 7.48 (m, 4H), 7.42 (td, *J* = 7.3, 1.7 Hz, 1H), 7.38 – 7.31 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 183.90, 156.43, 151.98, 137.43, 131.83, 131.79, 130.40, 129.37, 128.97, 127.01, 126.65, 124.13, 123.56, 117.73, 112.72.

2l benzofuran-2-yl(3-nitrophenyl)methanone[6]



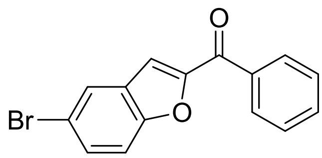
^{1}H NMR (500 MHz, DMSO) δ 8.71 – 8.64 (m, 1H), 8.53 (ddd, *J* = 8.3, 2.3, 1.0 Hz, 1H), 8.45 – 8.39 (m, 1H), 7.94 – 7.86 (m, 3H), 7.78 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.61 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.44 – 7.39 (m, 1H). ^{13}C NMR (126 MHz, DMSO) δ 181.99, 155.98, 151.37, 148.27, 138.34, 135.74, 131.03, 129.63, 127.66, 127.24, 124.81, 124.52, 124.24, 118.51, 112.82.

2m (5-chlorobenzofuran-2-yl)(phenyl)methanone[1]



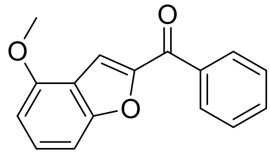
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.70 (d, *J* = 2.0 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.56 (dd, *J* = 15.4, 7.9 Hz, 3H), 7.49 – 7.44 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 184.08, 154.22, 153.31, 136.85, 133.19, 129.62, 129.48, 128.67, 128.64, 128.22, 122.63, 115.49, 113.67.

2n (5-bromobenzofuran-2-yl)(phenyl)methanone[7]



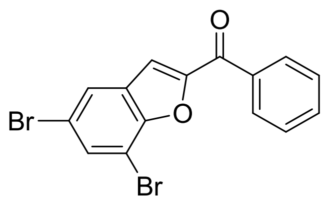
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.86 (d, *J* = 1.8 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.61 – 7.51 (m, 4H), 7.47 (s, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 184.01, 154.59, 153.20, 136.86, 133.19, 131.29, 129.49, 128.87, 128.64, 125.76, 117.05, 115.22, 114.08.

2o (4-methoxybenzofuran-2-yl)(phenyl)methanone[8]



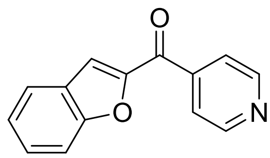
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 2H), 7.67 – 7.63 (m, 1H), 7.58 – 7.53 (m, 3H), 7.51 (s, 1H), 7.48 (d, J = 0.6 Hz, 1H), 7.33 (dd, J = 6.8, 1.2 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 184.42, 154.59, 152.41, 137.36, 133.63, 132.83, 130.03, 129.46, 128.53, 127.14, 122.75, 116.38, 112.09, 21.34.

2p (5,7-dibromobenzofuran-2-yl)(phenyl)methanone[9]



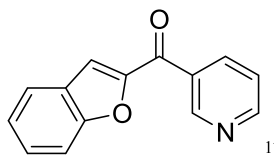
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 1H), 8.14 (d, *J* = 1.2 Hz, 1H), 7.83 (d, *J* = 1.7 Hz, 1H), 7.80 (d, *J* = 1.7 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.58 (dd, *J* = 9.9, 5.4 Hz, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 183.20, 154.01, 152.10, 136.42, 133.45, 133.28, 129.74, 129.38, 128.70, 124.80, 117.13, 115.05, 106.02.

2q benzofuran-2-yl(pyridin-4-yl)methanone



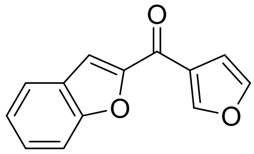
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (dd, *J* = 4.4, 1.6 Hz, 2H), 7.84 (dd, *J* = 4.4, 1.6 Hz, 2H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.64 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.60 (d, *J* = 0.8 Hz, 1H), 7.54 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.38 – 7.33 (m, 1H).^{13}C NMR (126 MHz, $CDCl_3$) δ 182.84, 156.26, 151.47, 150.59, 143.50, 129.16, 126.78, 124.36, 123.60, 122.48, 117.49, 112.64. HRMS (ESI$^+$): calcd for $C_{14}H_{10}NO_2$ $[M+H]^+$ 224.0706, found 224.0732.

2r benzofuran-2-yl(pyridin-3-yl)methanone



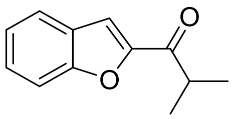
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.30 (d, *J* = 1.8 Hz, 1H), 8.84 (dd, *J* = 4.8, 1.3 Hz, 1H), 8.34 (dt, *J* = 7.9, 1.7 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.56 – 7.47 (m, 2H), 7.35 (t, J = 7.5 Hz, 1H).^{13}C NMR (151 MHz, $CDCl_3$) δ 182.37, 156.11, 153.25, 151.89, 150.40, 136.87, 132.77, 128.90, 126.82, 124.27, 123.57, 123.52, 116.89, 112.59. HRMS (ESI$^+$): calcd for $C_{14}H_{10}NO_2$ $[M+H]^+$ 224.0706, found 224.0726.

2s benzofuran-2-yl(furan-3-yl)methanone



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (d, J = 0.7 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.72 – 7.68 (m, 1H), 7.64 (dd, J = 8.4, 0.5 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.33 (dd, J = 11.2, 3.9 Hz, 1H), 6.67 (dd, J = 3.6, 1.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.05, 155.73, 151.62, 151.50, 147.18, 128.34, 127.14, 124.00, 123.38, 120.37, 115.46, 112.63, 112.41. HRMS (ESI$^+$): calcd for $C_{13}H_8NaNO_3$ $[M+Na]^+$ 235.0371, found 235.0394.

2t 1-(benzofuran-2-yl)-2-methylpropan-1-one[10]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, J = 8.0 Hz, 1H), 7.60 (dd, J = 8.4, 0.7 Hz, 1H), 7.53 (d, J = 0.8 Hz, 1H), 7.48 (ddd, J = 8.4, 7.3, 1.2 Hz, 1H), 7.35 – 7.30 (m, 1H), 3.54 – 3.46 (m, 1H), 1.30 (d, J = 6.9 Hz, 6H).^{13}C NMR (126 MHz, $CDCl_3$) δ 195.50, 155.63, 152.11, 128.07, 127.10, 123.83, 123.20, 112.80, 112.45, 36.70, 18.79.

4 References

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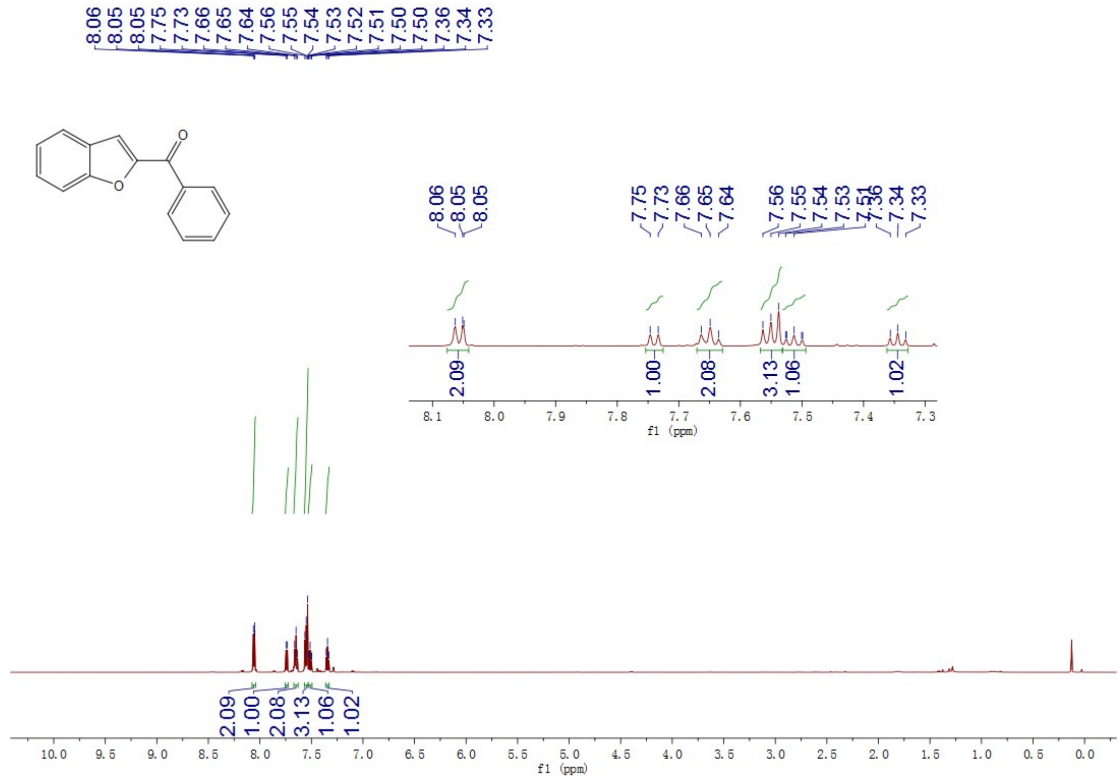
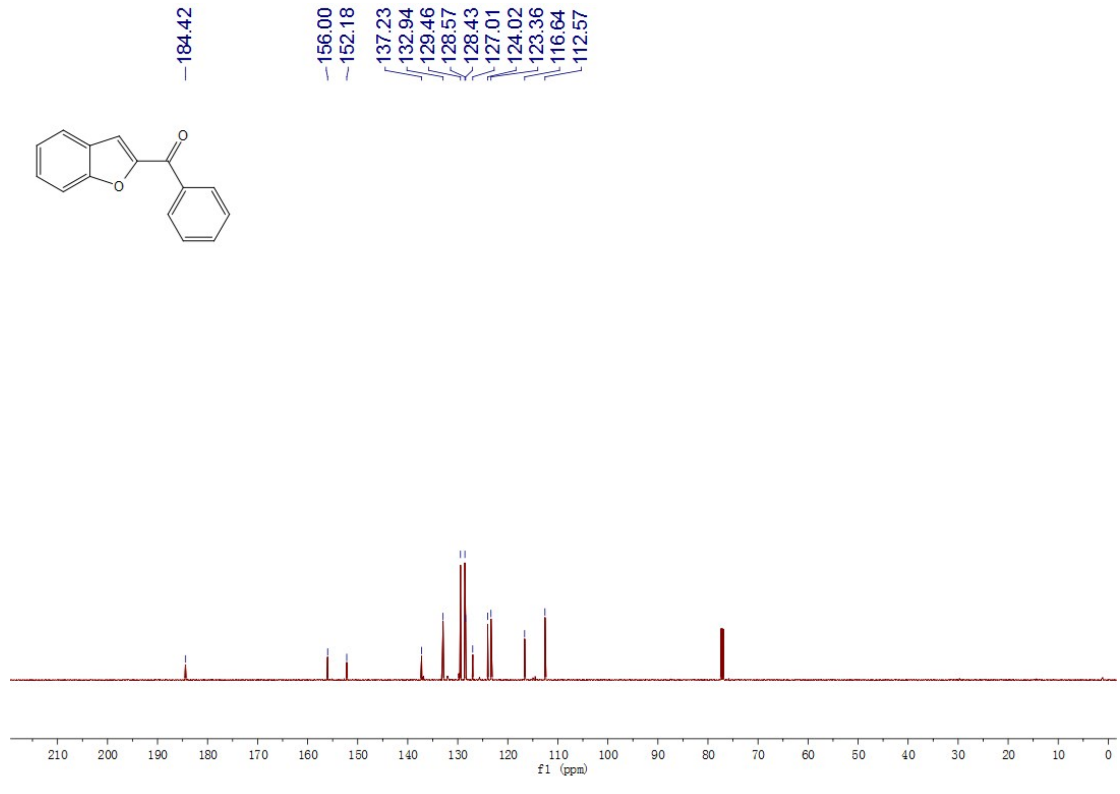
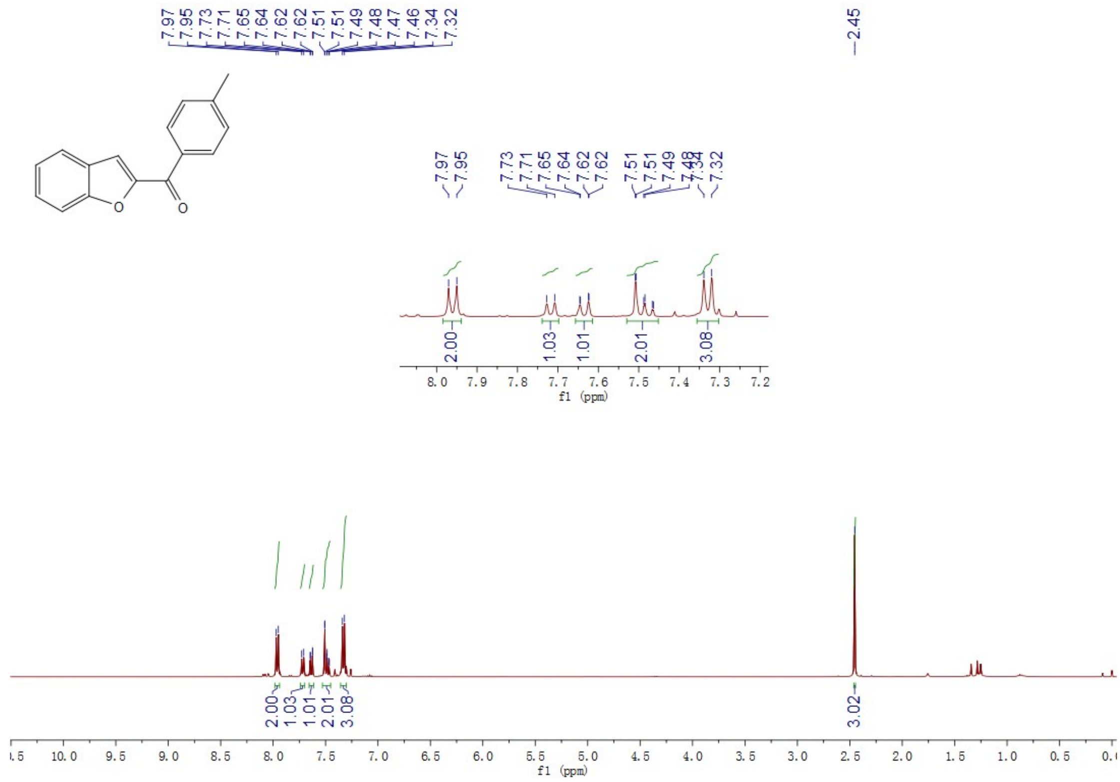
5 ^{1}H and ^{13}C NMR Spectra

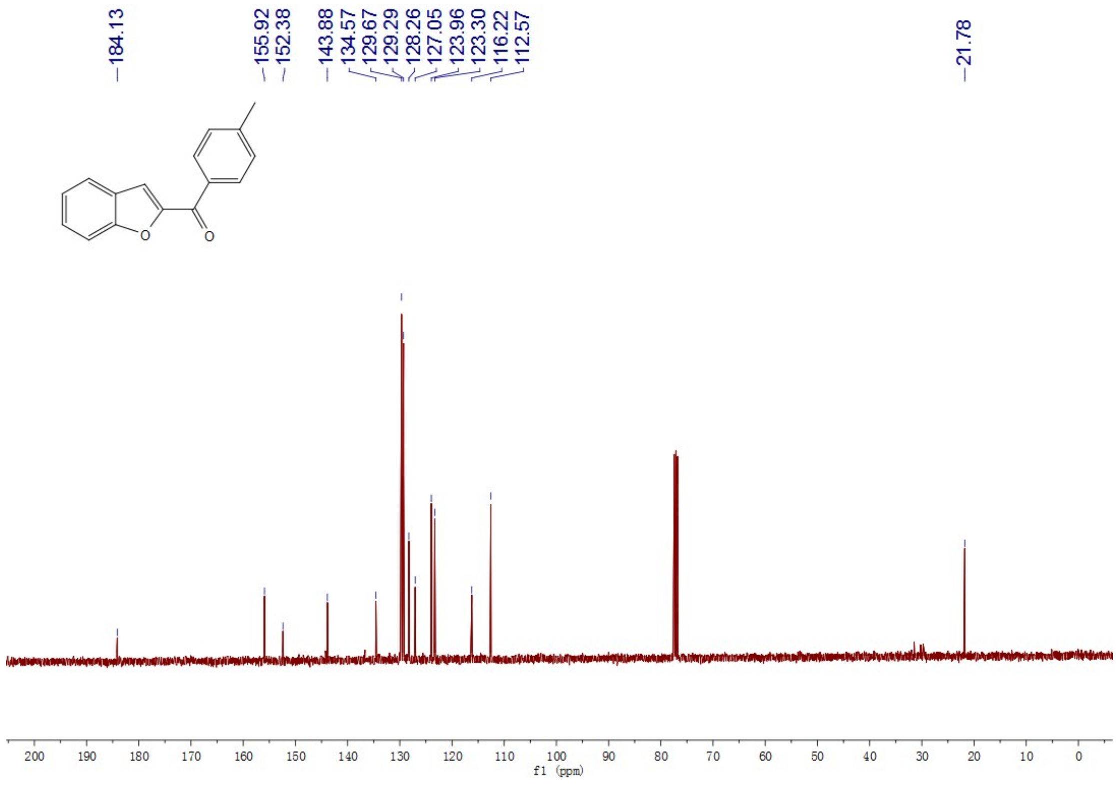
2a



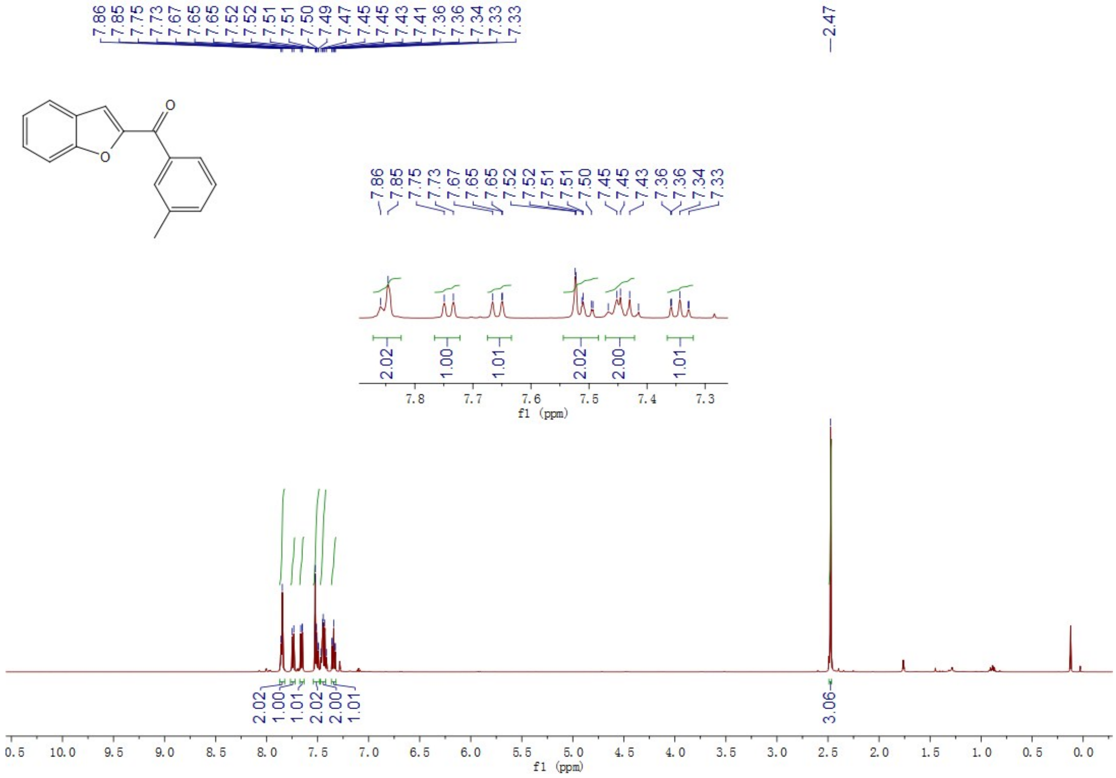


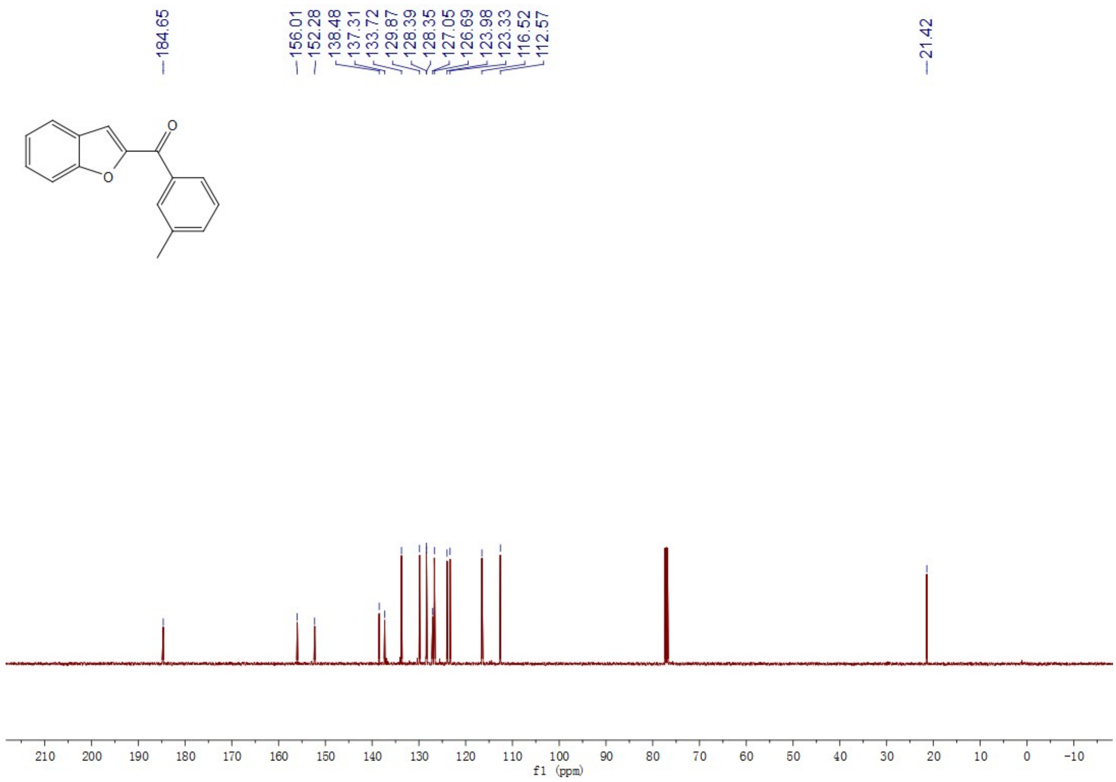
2b


7.97 7.95 7.73 7.71 7.65 7.64 7.62 7.62 7.51 7.51 7.49 7.48 7.47 7.46 7.34 7.32
2.45
2.00 1.03 1.01 2.01 3.08
3.02
f1 (ppm)


184.13
155.92 152.38
143.88 134.57 129.67 129.29 128.26 127.05 123.96 123.30 116.22 112.57
21.78
f1 (ppm)

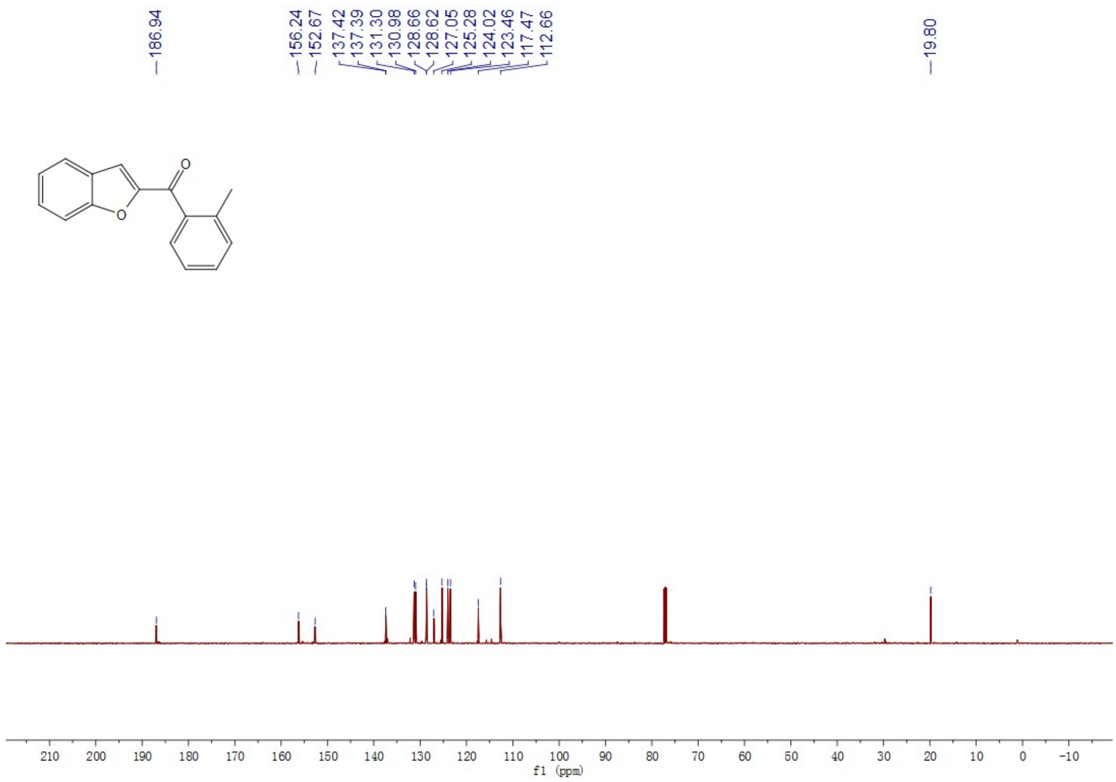
2c


7.86 7.85 7.75 7.73 7.67 7.65 7.65 7.52 7.52 7.51 7.51 7.50 7.49 7.47 7.45 7.45 7.43 7.41 7.36 7.36 7.34 7.33 7.33
2.47
O
O
2.02 1.00 1.01 2.02 2.00 1.01
3.06
f1 (ppm)


184.65
156.01 152.28 138.48 137.31 133.72 129.87 128.39 128.35 127.05 126.69 123.98 123.33 116.52 112.57
21.42
O
O
f1 (ppm)

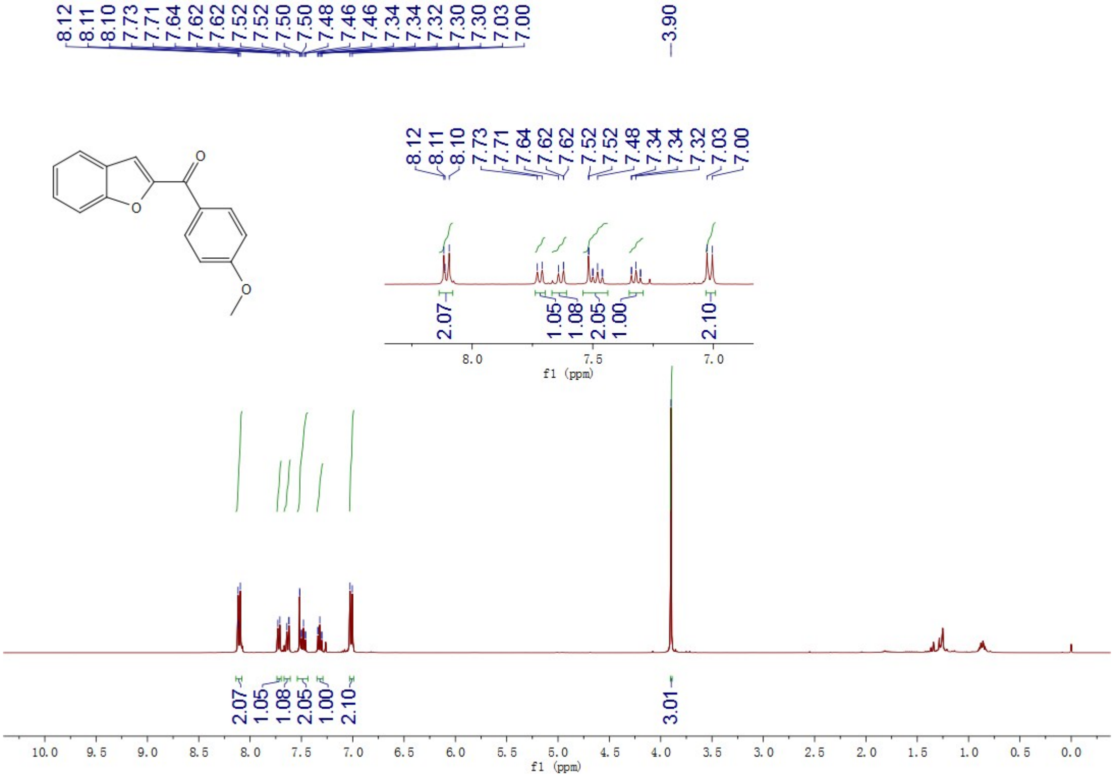
2d

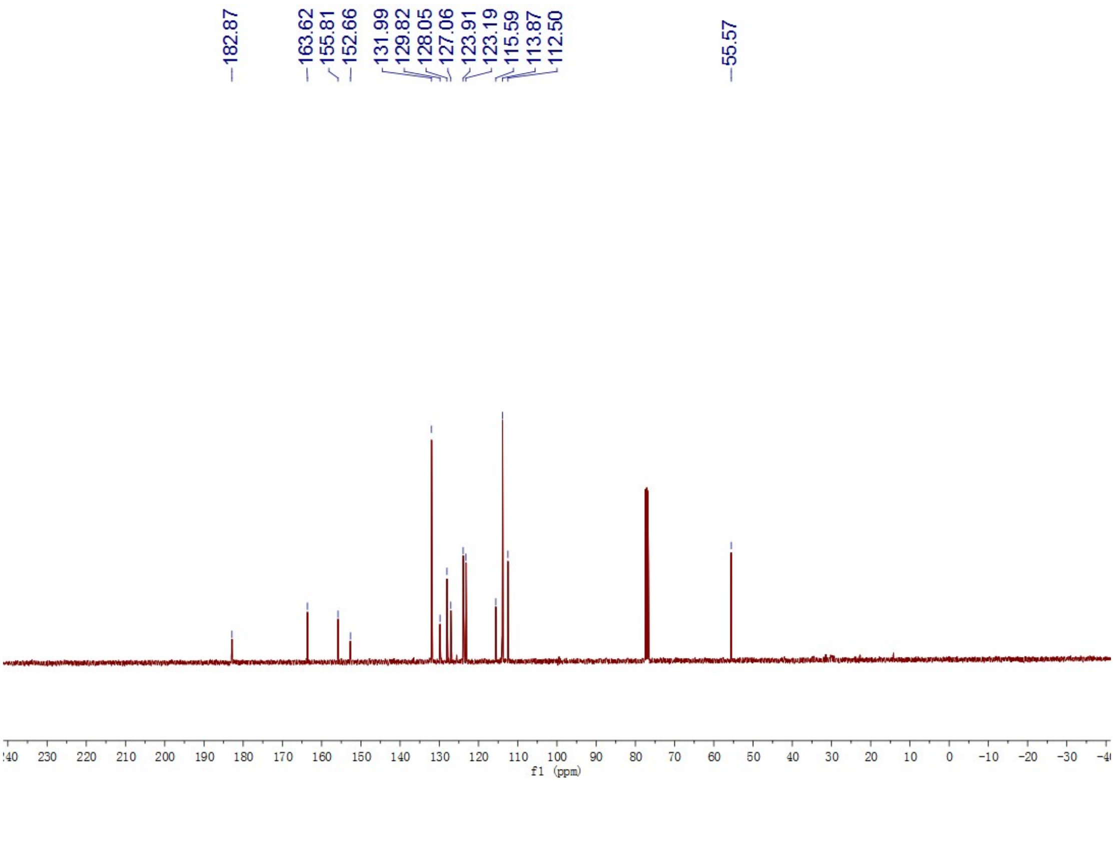
7.71 7.69 7.66 7.64 7.60 7.58 7.53 7.53 7.52 7.50 7.50 7.48 7.47 7.46 7.46 7.45 7.44 7.35 7.34 7.32 7.31
2.47
O
CH3
7.71 7.69 7.66 7.64 7.60 7.58 7.53 7.52 7.50 7.50 7.46 7.46 7.45 7.44 7.35 7.34 7.32 7.31
0.95 0.98 0.99 1.01 1.12 4.12
7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)
0.95 0.98 0.99 1.01 1.12 4.12
3.00
10.5 10.0 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)



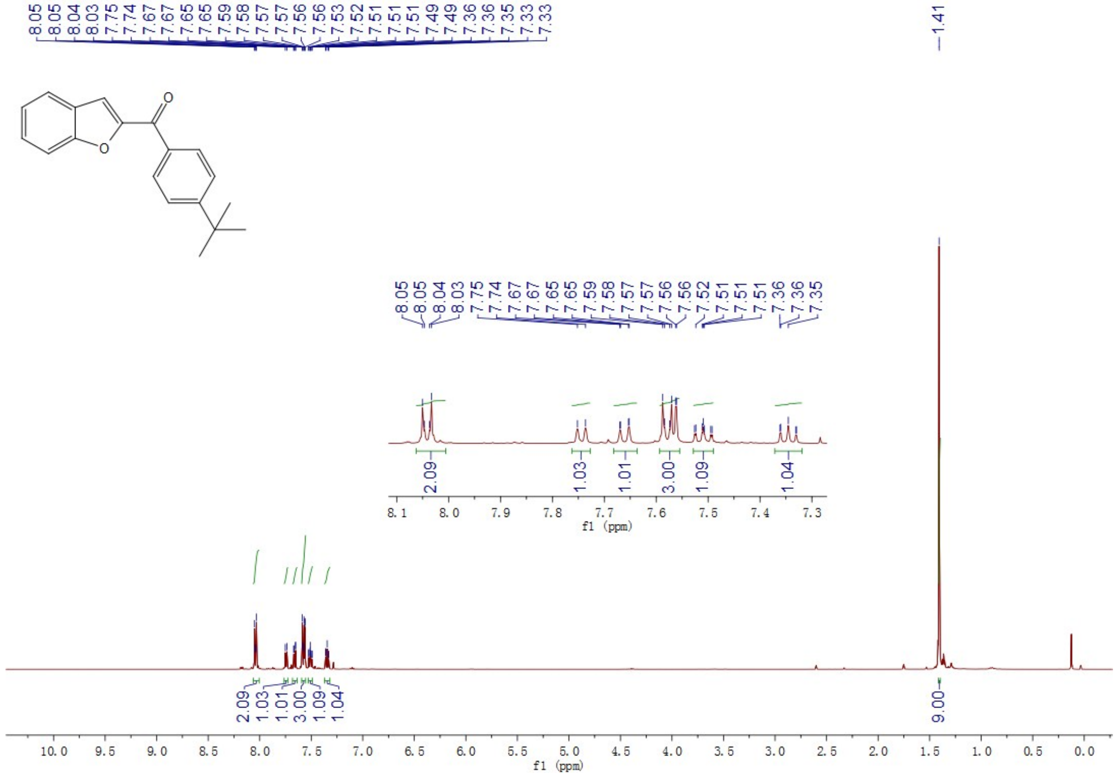
186.94
156.24 152.67 137.42 137.39 131.30 130.98 128.66 128.62 127.05 125.28 124.02 123.46 117.47 112.66
19.80
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

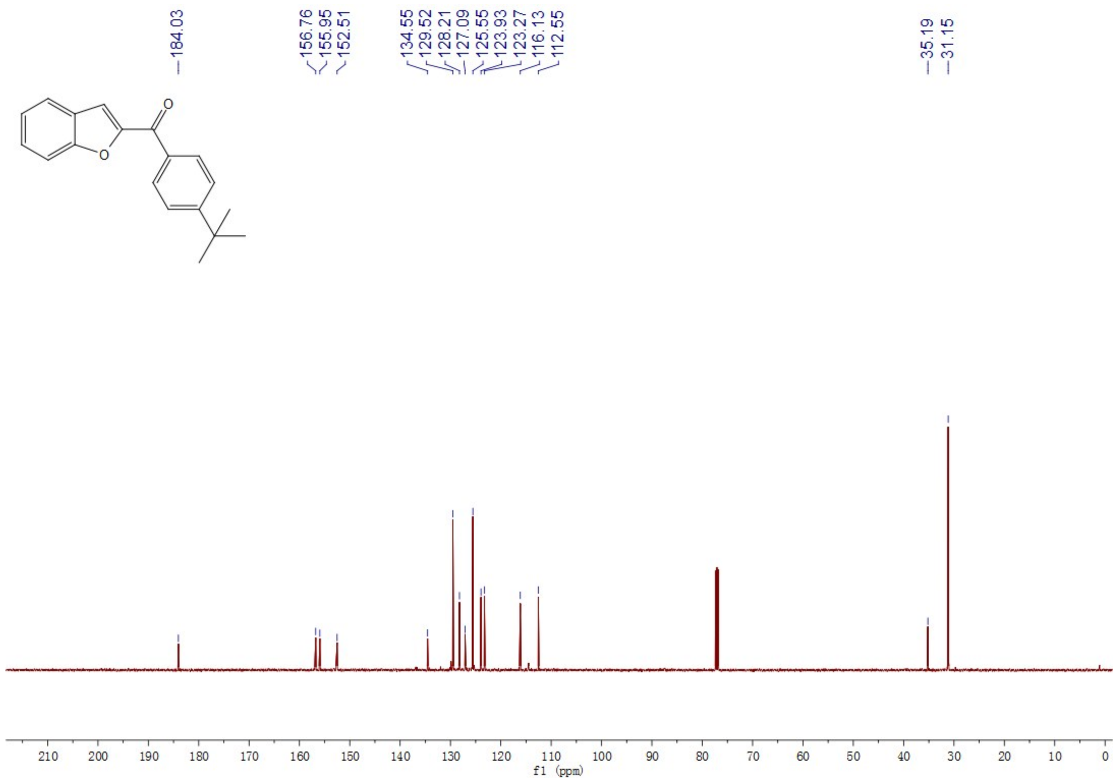
2e


8.12
8.11
8.10
7.73
7.71
7.64
7.62
7.52
7.52
7.50
7.48
7.46
7.46
7.34
7.32
7.30
7.30
7.03
7.00
3.90
2.07
1.05
1.08
2.05
1.00
2.10
3.01
f1 (ppm)

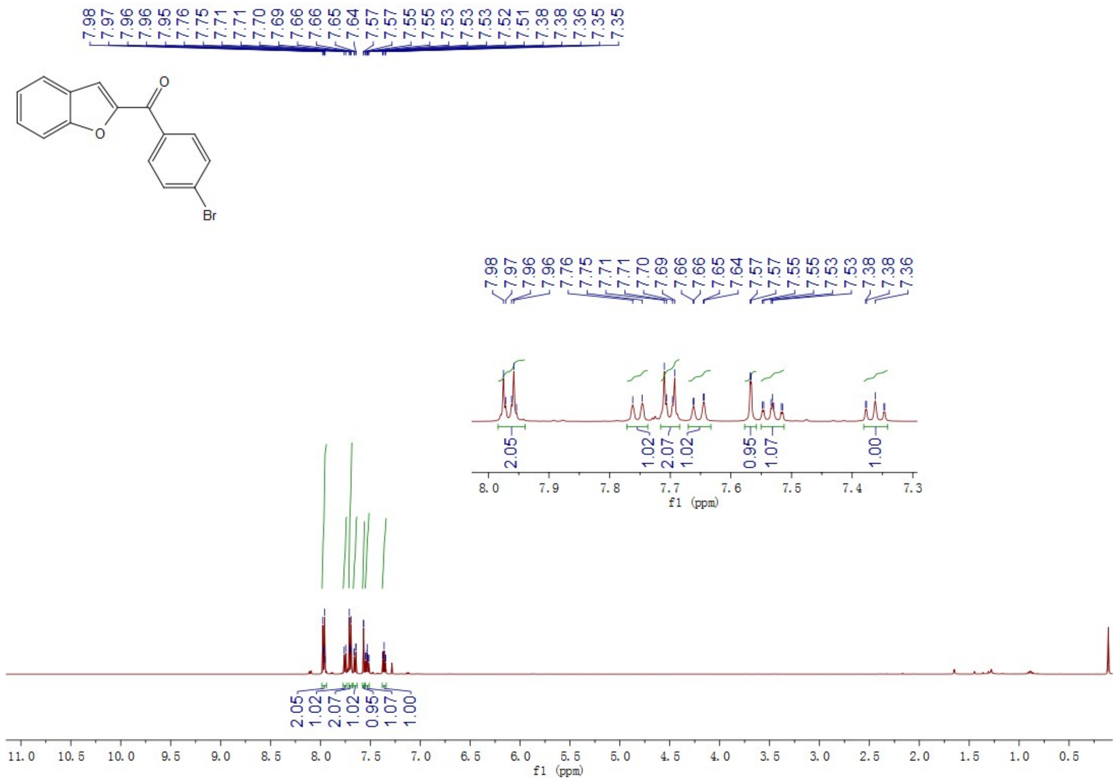

182.87
163.62
155.81
152.66
131.99
129.82
128.05
127.06
123.91
123.19
115.59
113.87
112.50
55.57
f1 (ppm)

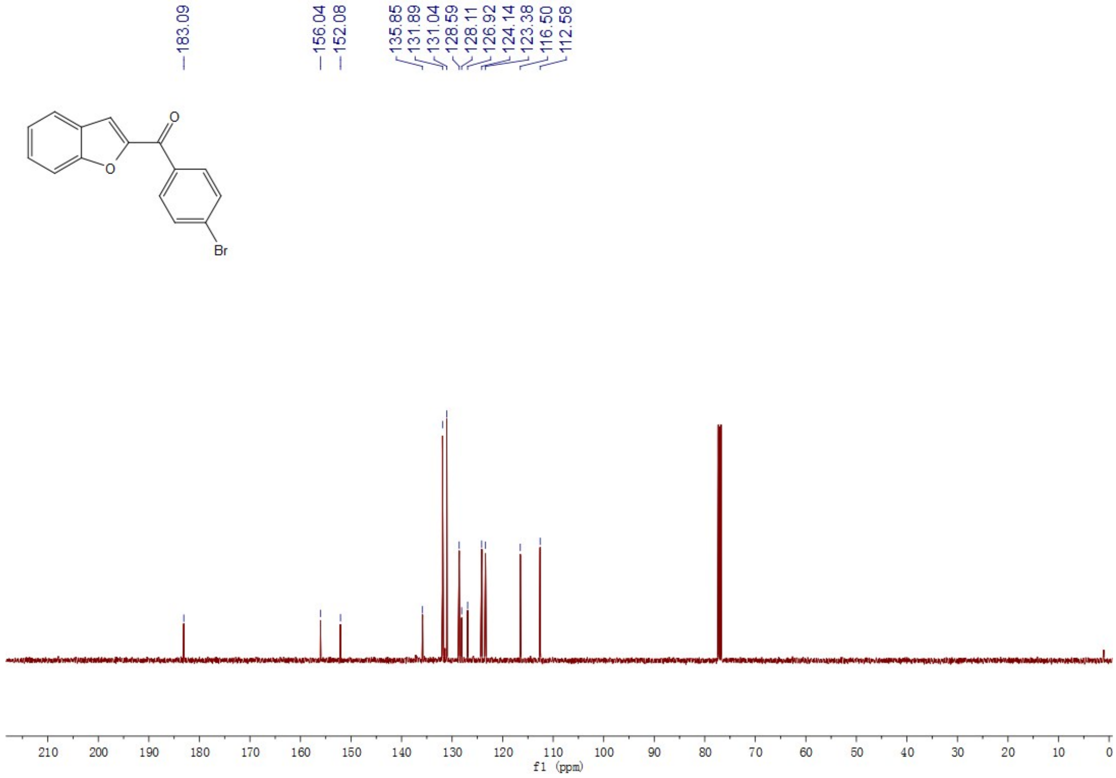
2f


8.05 8.05 8.04 8.03 7.75 7.74 7.67 7.67 7.65 7.65 7.59 7.58 7.57 7.57 7.56 7.56 7.53 7.52 7.51 7.51 7.51 7.49 7.49 7.36 7.36 7.35 7.33 7.33
1.41
O
2.09 1.03 1.01 3.00 1.09 1.04
9.00
f1 (ppm)

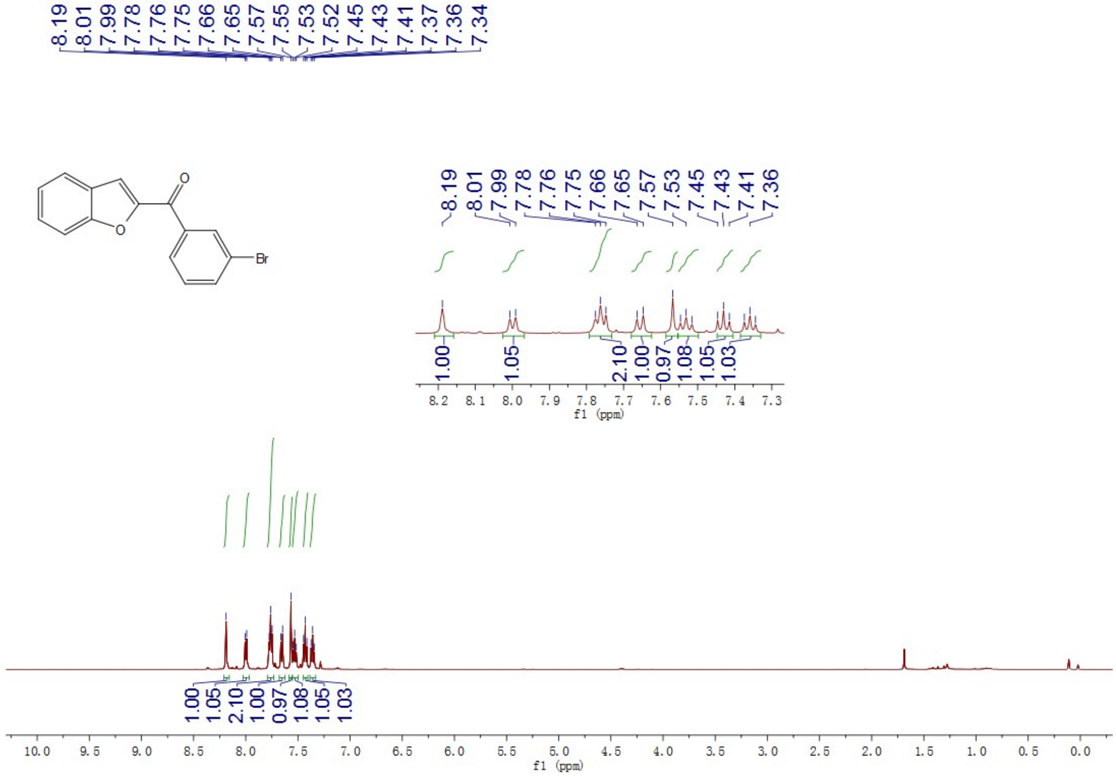

184.03
156.76 155.95 152.51
134.55 129.52 128.21 127.09 125.55 123.93 123.27 116.13 112.55
35.19 31.15
O
f1 (ppm)

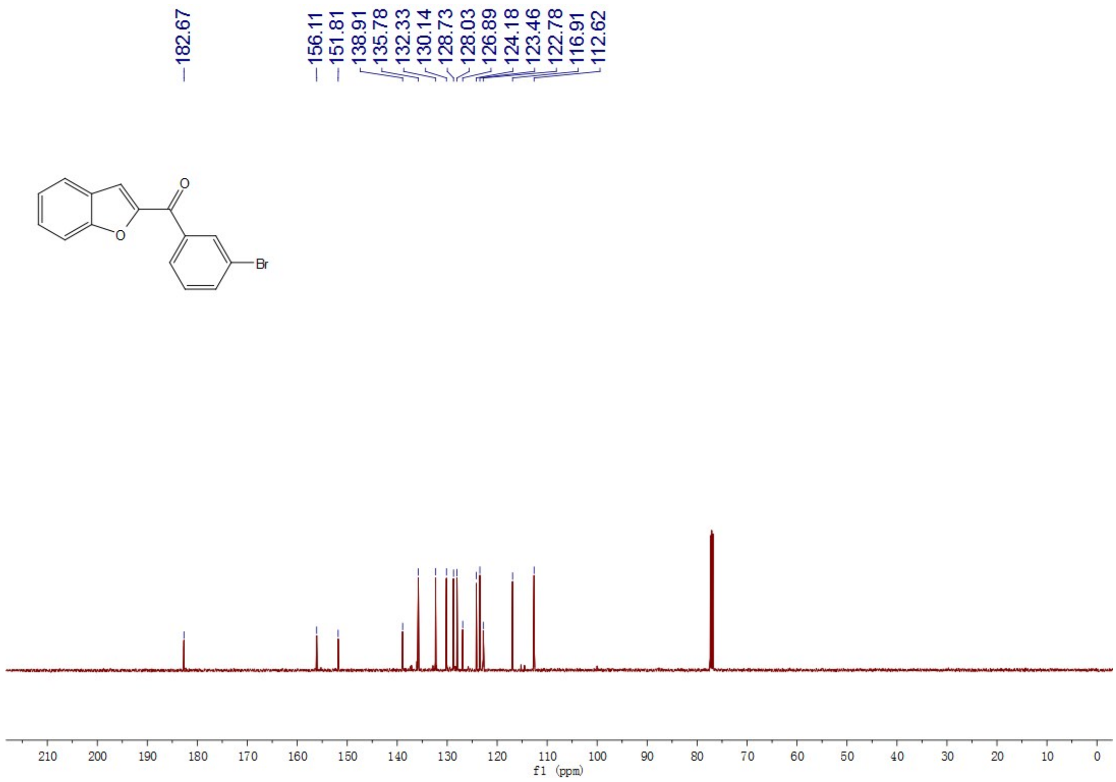
2g


7.98 7.97 7.96 7.95 7.76 7.75 7.71 7.71 7.70 7.69 7.66 7.66 7.65 7.64 7.57 7.57 7.55 7.55 7.53 7.53 7.52 7.51 7.38 7.38 7.36 7.35 7.35
O
O
Br
7.98 7.97 7.96 7.96 7.76 7.75 7.71 7.71 7.70 7.69 7.66 7.66 7.65 7.64 7.57 7.57 7.55 7.55 7.53 7.53 7.38 7.38 7.36
2.05 1.02 2.07 1.02 0.95 1.07 1.00
f1 (ppm)
2.05 1.02 2.07 1.02 0.95 1.07 1.00
f1 (ppm)

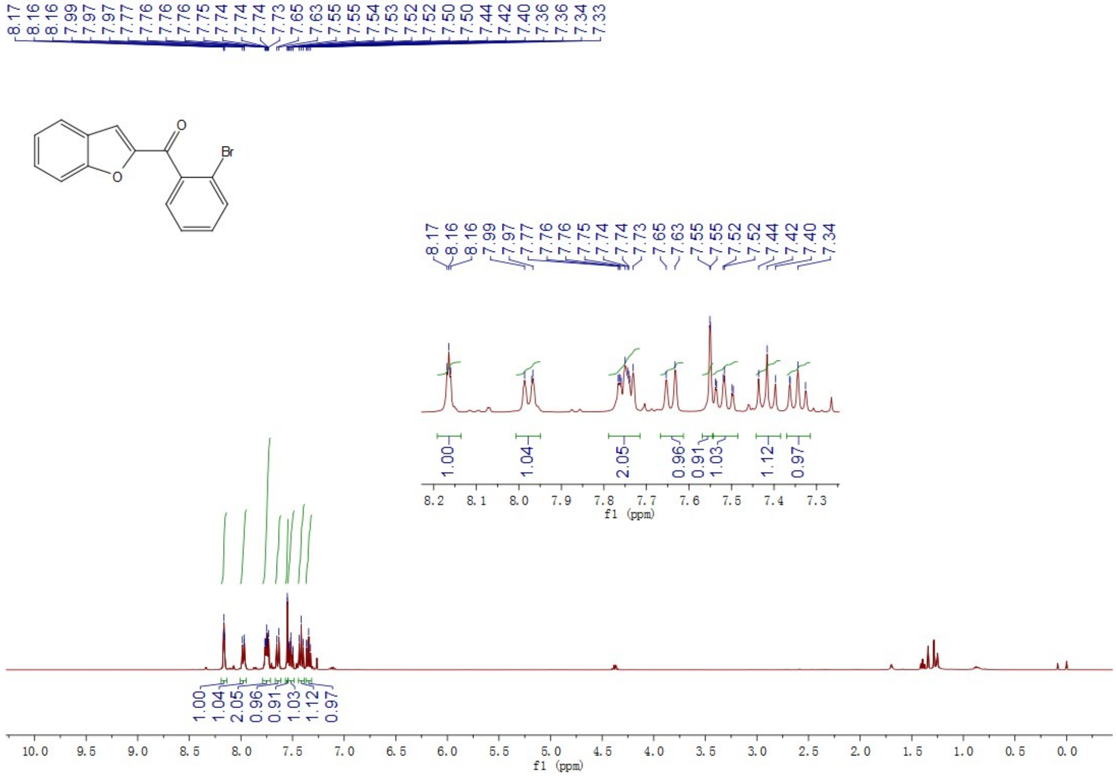

183.09
156.04 152.08
135.85 131.89 131.04 128.59 128.11 126.92 124.14 123.38 116.50 112.58
O
O
Br
f1 (ppm)

2h

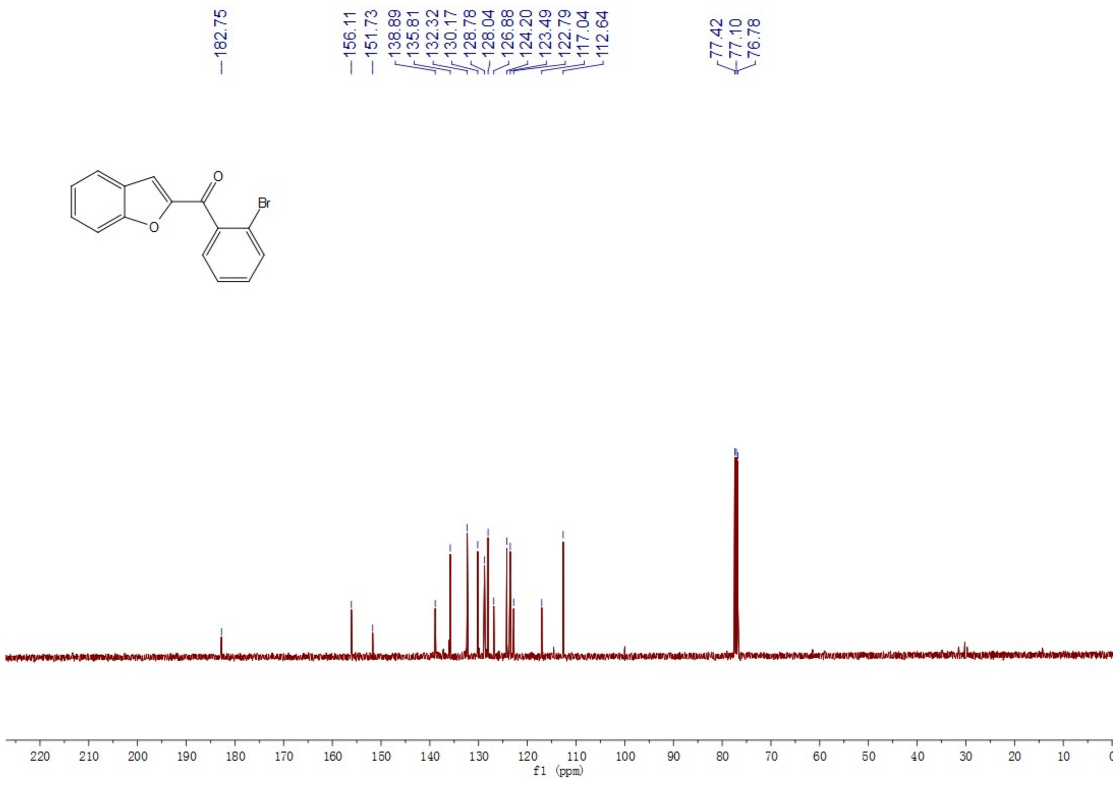

8.19 8.01 7.99 7.78 7.76 7.75 7.66 7.65 7.57 7.55 7.53 7.52 7.45 7.43 7.41 7.37 7.36 7.34
O
O
Br
8.19 8.01 7.99 7.78 7.76 7.75 7.66 7.65 7.57 7.53 7.45 7.43 7.41 7.36
1.00 1.05 2.10 1.00 0.97 1.08 1.05 1.03
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.00 1.05 2.10 1.00 0.97 1.08 1.05 1.03
10.0 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)


182.67
156.11 151.81 138.91 135.78 132.33 130.14 128.73 128.03 126.89 124.18 123.46 122.78 116.91 112.62
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

2i

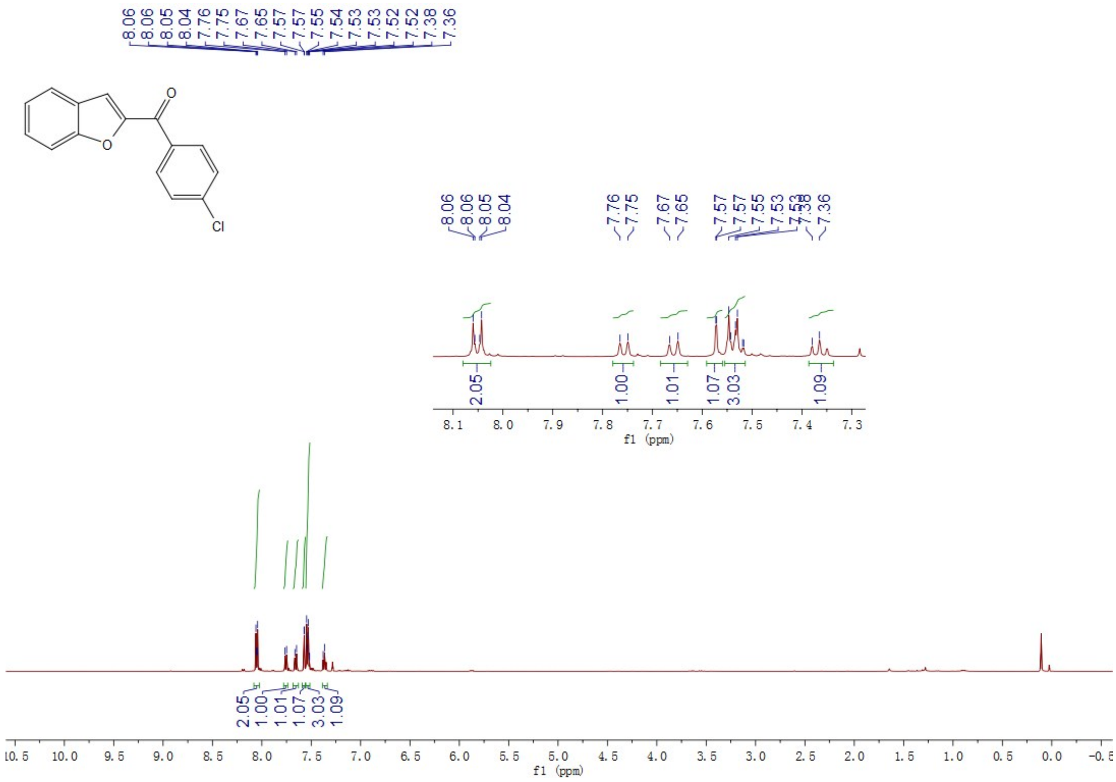


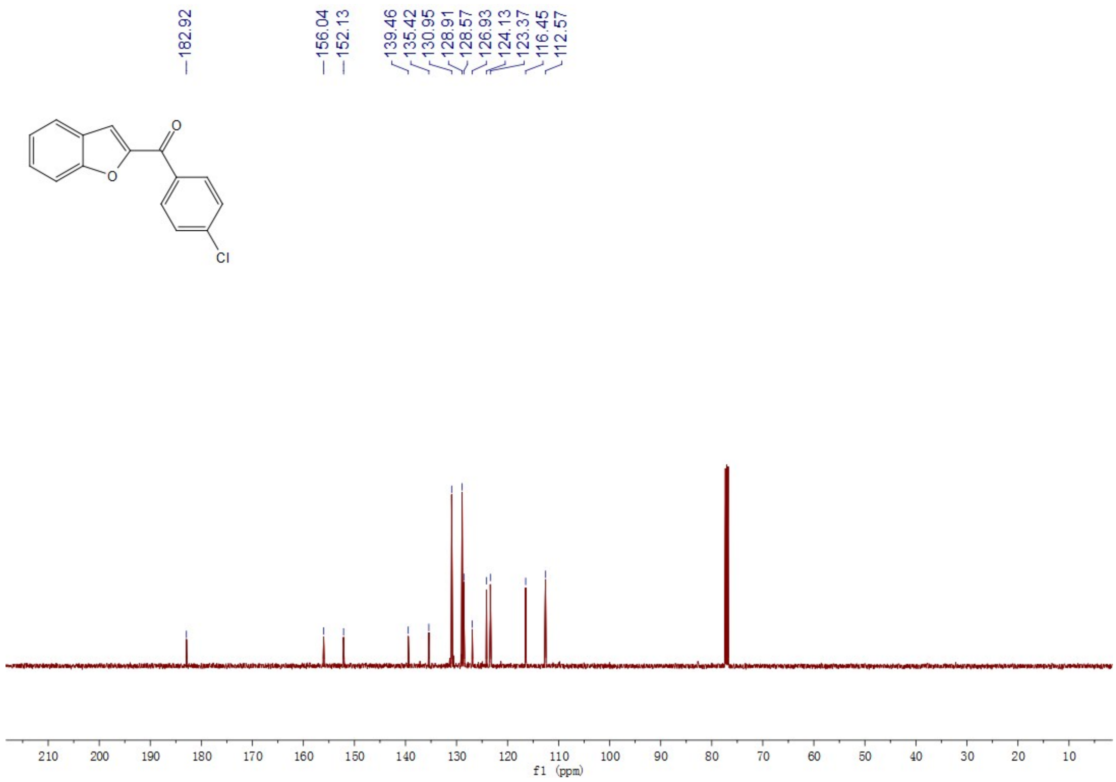
8.17 8.16 8.16 7.99 7.97 7.77 7.76 7.76 7.75 7.74 7.74 7.74 7.73 7.65 7.63 7.55 7.55 7.54 7.53 7.52 7.52 7.50 7.50 7.44 7.42 7.40 7.36 7.36 7.34 7.33
Br
O
1.00 1.04 2.05 0.96 0.91 1.03 1.12 0.97
f1 (ppm)



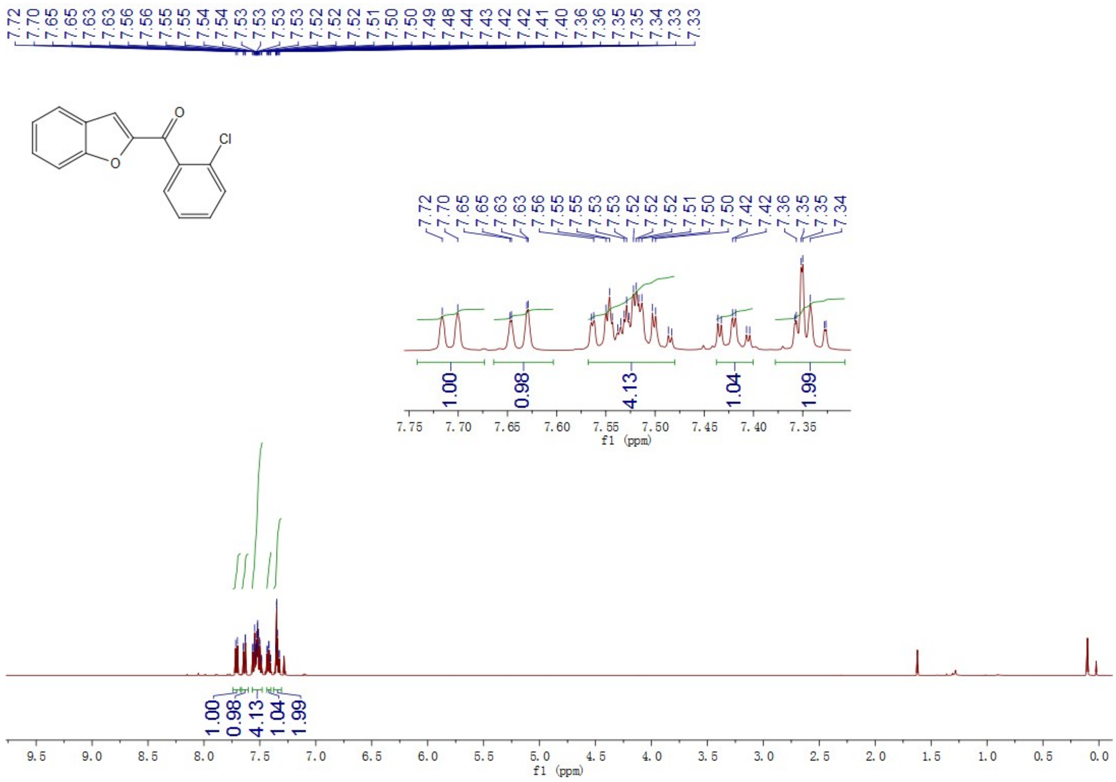
182.75
156.11 151.73 138.89 135.81 132.32 130.17 128.78 128.04 126.88 124.20 123.49 122.79 117.04 112.64
77.42 77.10 76.78
Br
O
f1 (ppm)

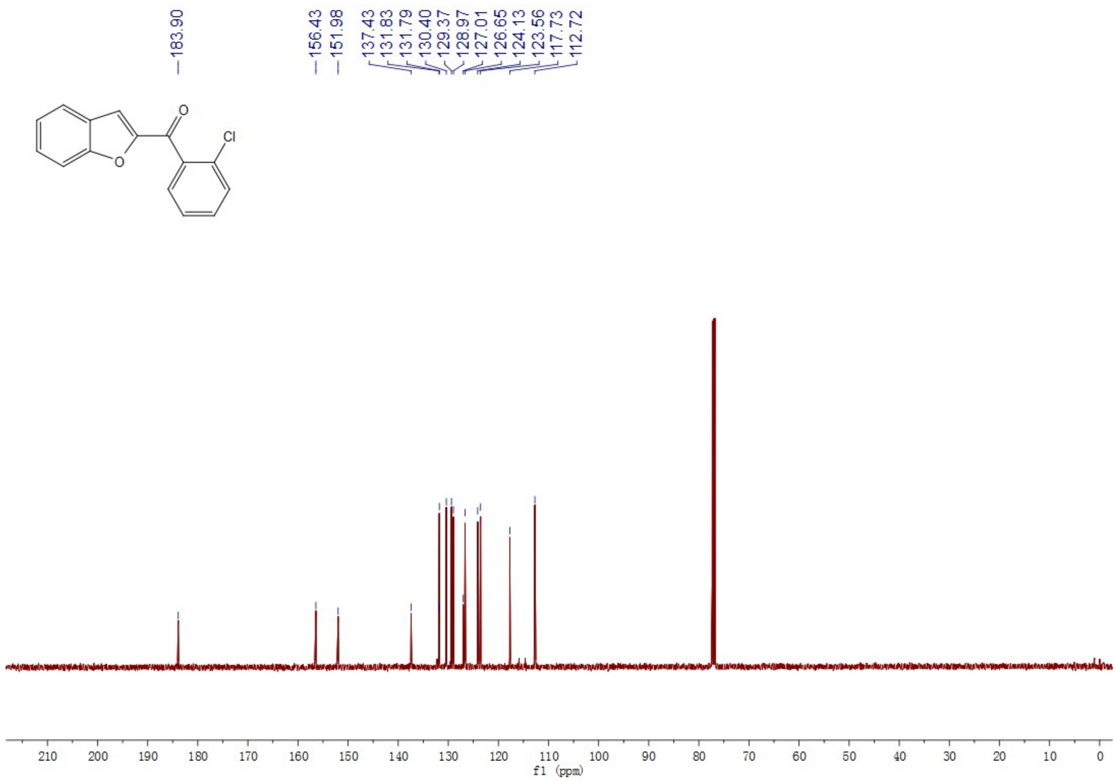
2j


8.06
8.06
8.05
8.04
7.76
7.75
7.67
7.65
7.57
7.57
7.55
7.54
7.53
7.53
7.52
7.38
7.36
O
O
Cl
2.05
1.00
1.01
1.07
3.03
1.09
f1 (ppm)

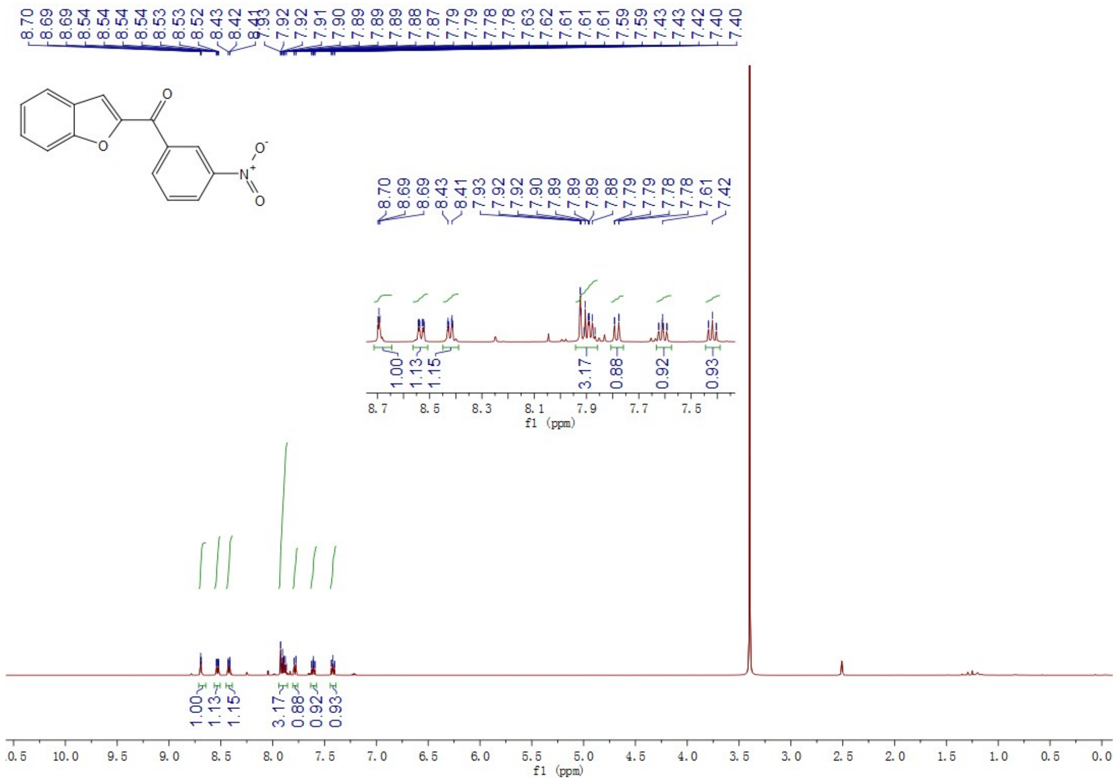

182.92
156.04
152.13
139.46
135.42
130.95
128.91
128.57
126.93
124.13
123.37
116.45
112.57
O
O
Cl
f1 (ppm)

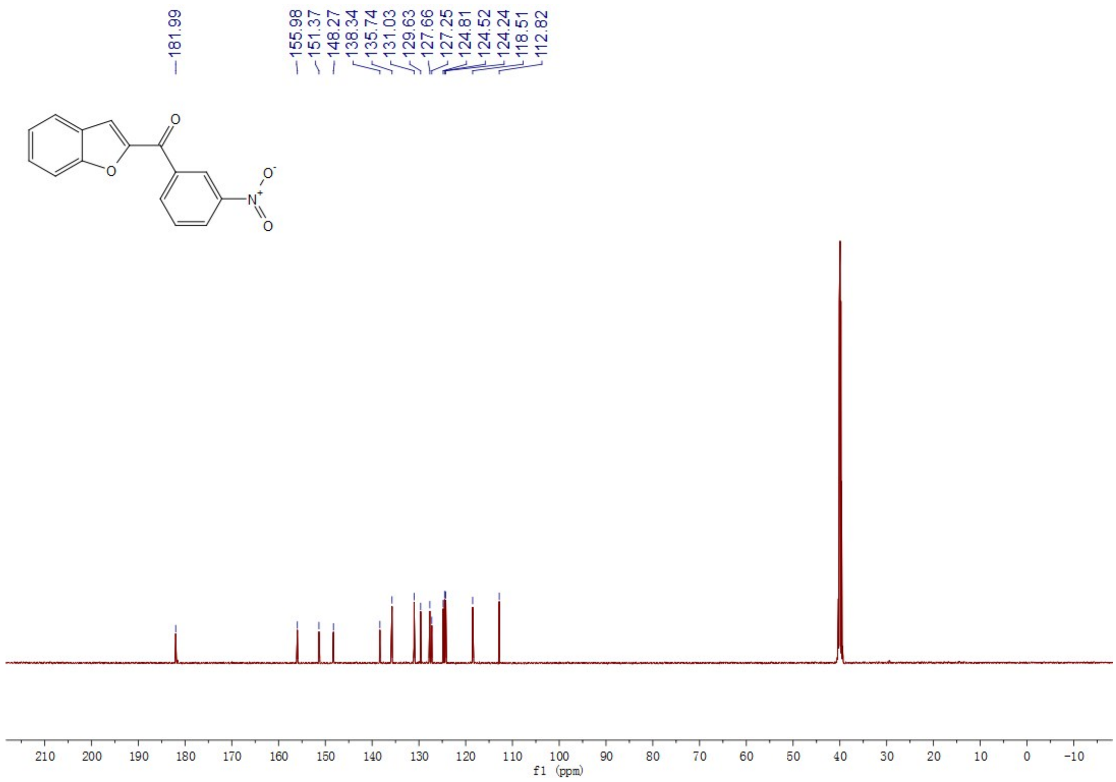
2k


7.72 7.70 7.65 7.65 7.63 7.63 7.56 7.56 7.55 7.55 7.54 7.54 7.53 7.53 7.53 7.53 7.52 7.52 7.52 7.52 7.51 7.50 7.50 7.49 7.48 7.44 7.43 7.42 7.42 7.41 7.40 7.36 7.36 7.35 7.35 7.34 7.33 7.33
O
Cl
O
1.00
0.98
4.13
1.04
1.99
f1 (ppm)

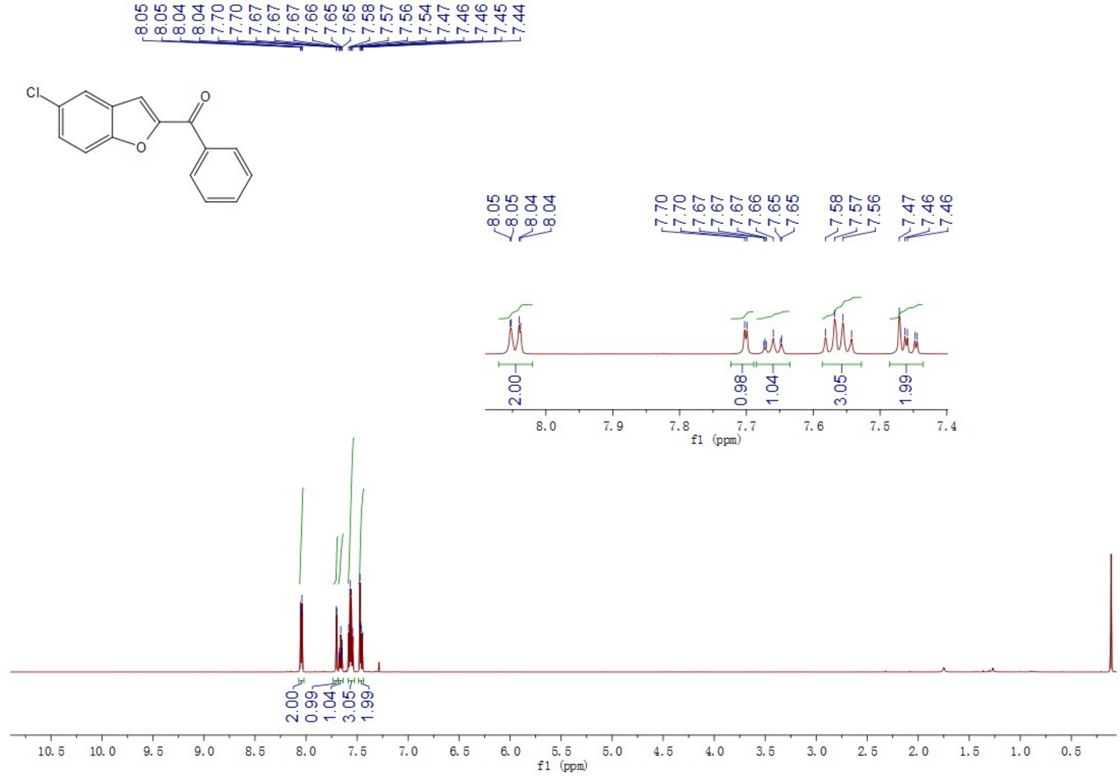

183.90
156.43
151.98
137.43 131.83 131.79 130.40 129.37 128.97 127.01 126.65 124.13 123.56 117.73 112.72
O
Cl
O
f1 (ppm)

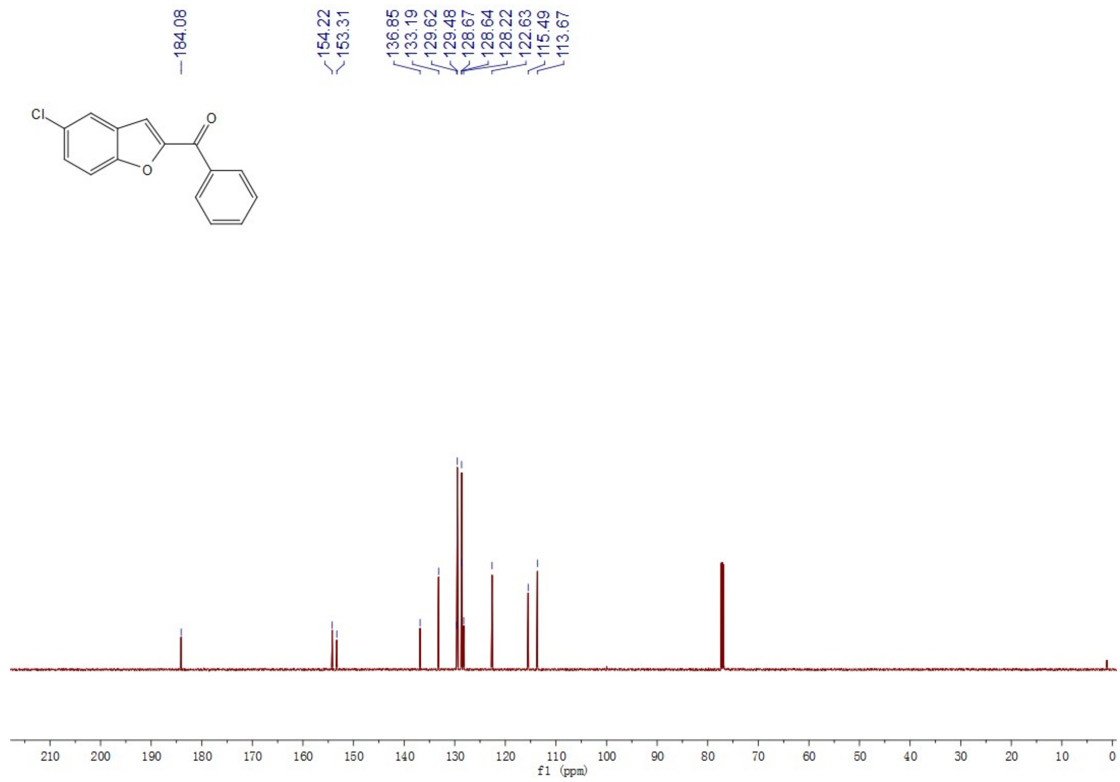
2l



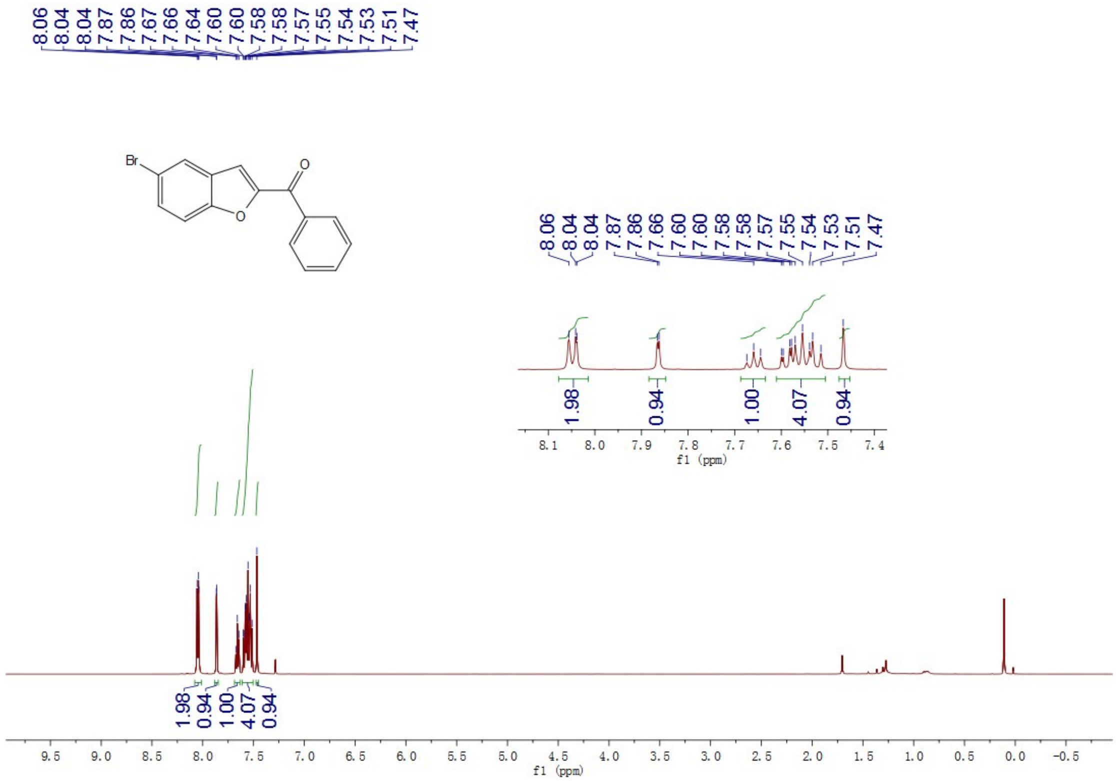


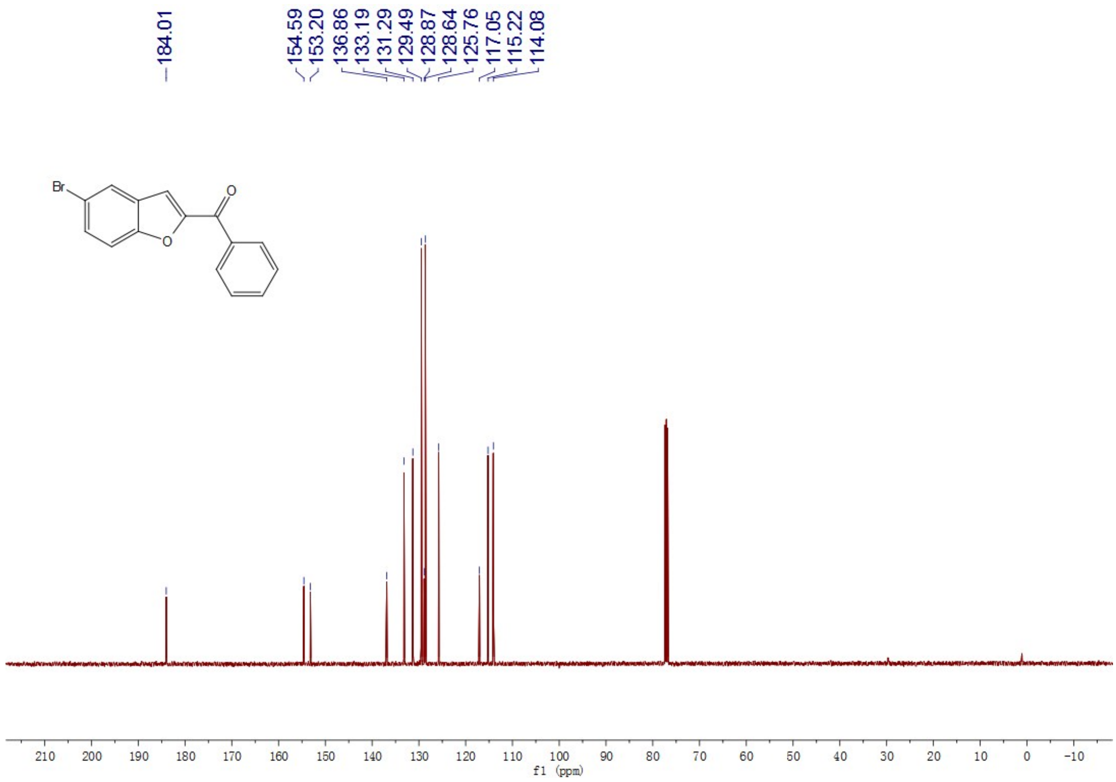
2m


8.05 8.05 8.04 8.04 7.70 7.70 7.67 7.67 7.67 7.66 7.65 7.65 7.58 7.57 7.56 7.54 7.47 7.46 7.46 7.45 7.44
Cl
O
O
2.00 0.98 1.04 3.05 1.99
2.00 0.99 1.04 3.05 1.99
f1 (ppm)

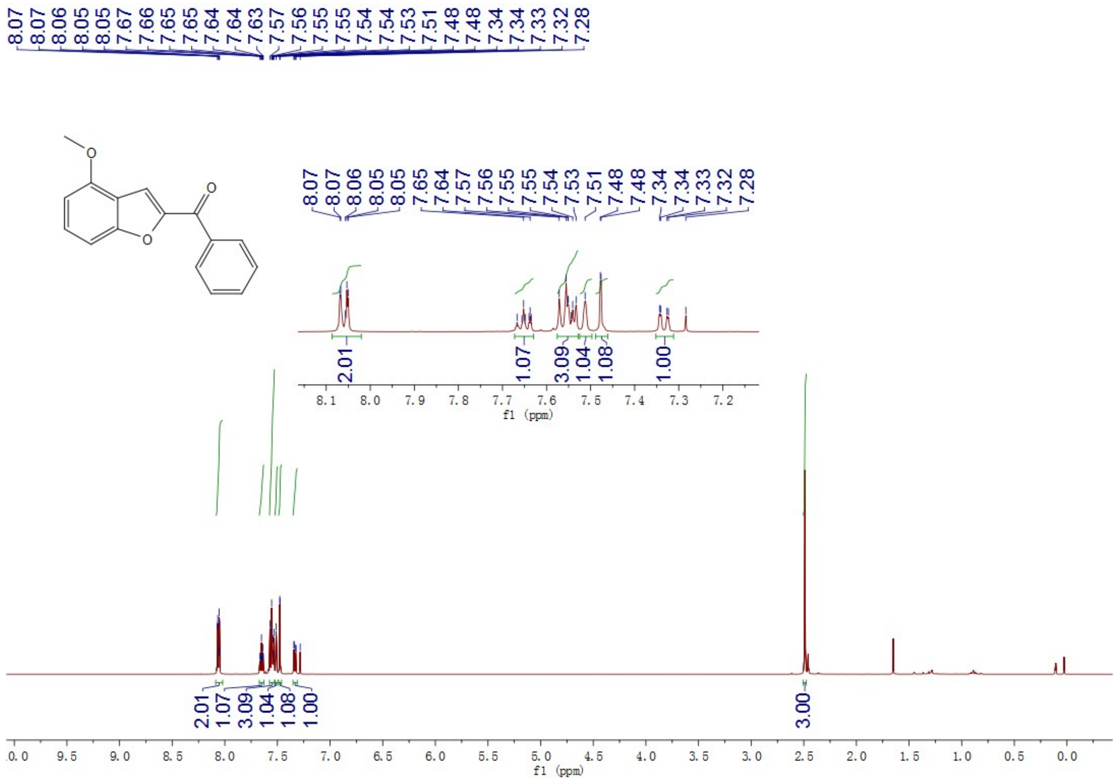

184.08
154.22 153.31
136.85 133.19 129.62 129.48 128.67 128.64 128.22 122.63 115.49 113.67
Cl
O
O
f1 (ppm)

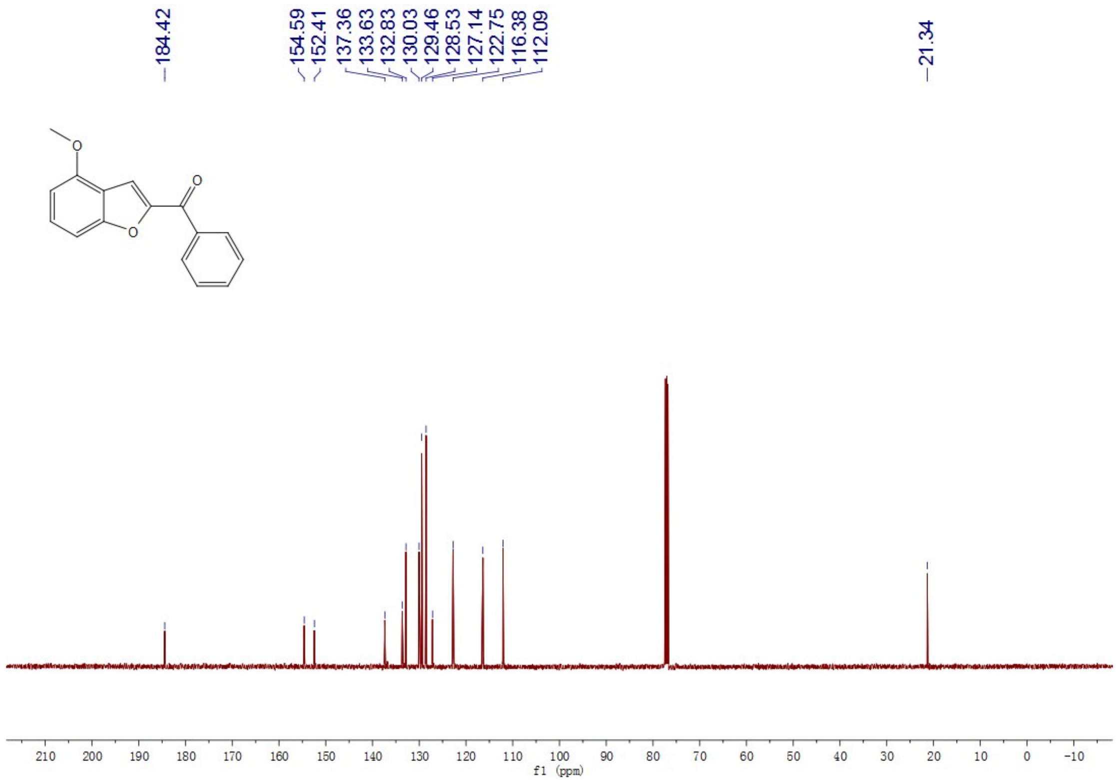
2n





2o





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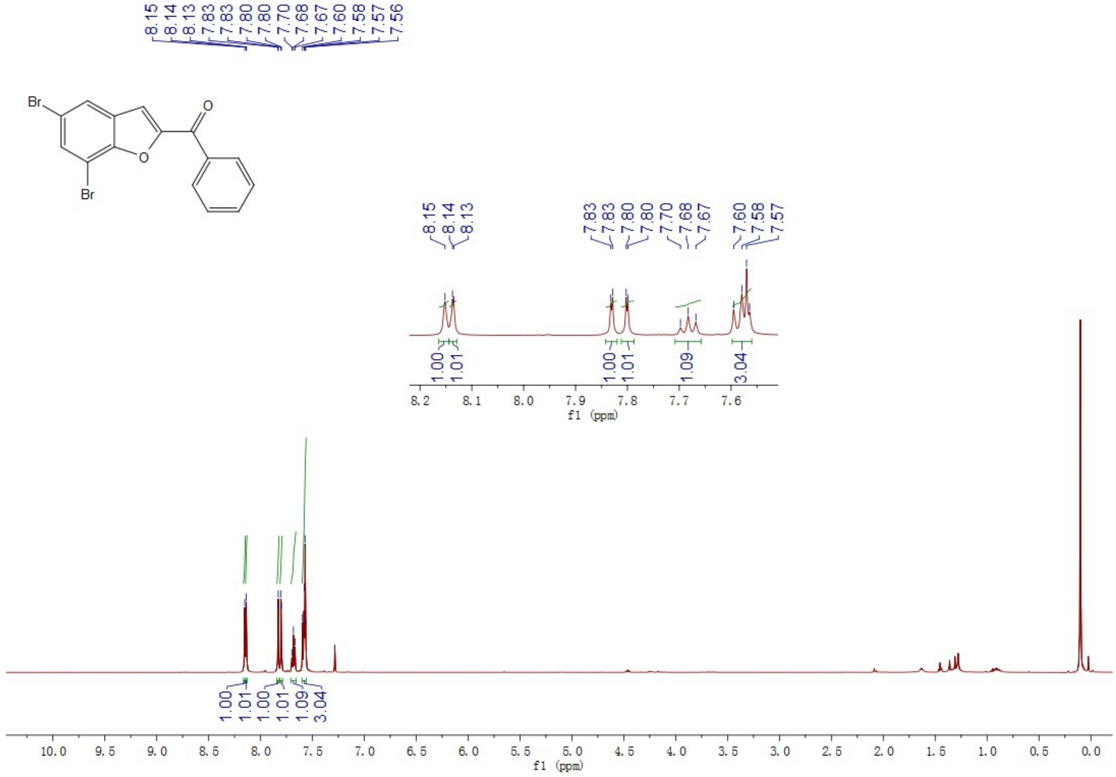
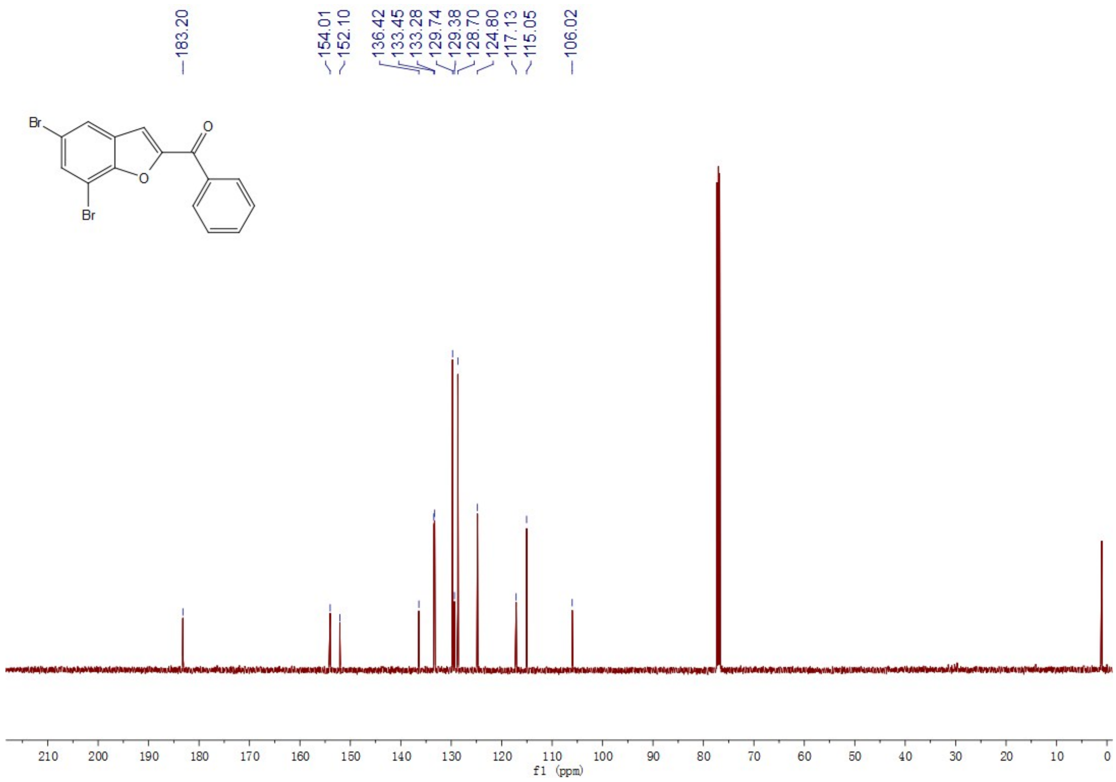


8.15
8.14
8.13
7.83
7.83
7.80
7.80
7.70
7.68
7.67
7.60
7.58
7.57
7.56
Br
O
O
Br
1.00
1.01
1.00
1.01
1.09
3.04
f1 (ppm)



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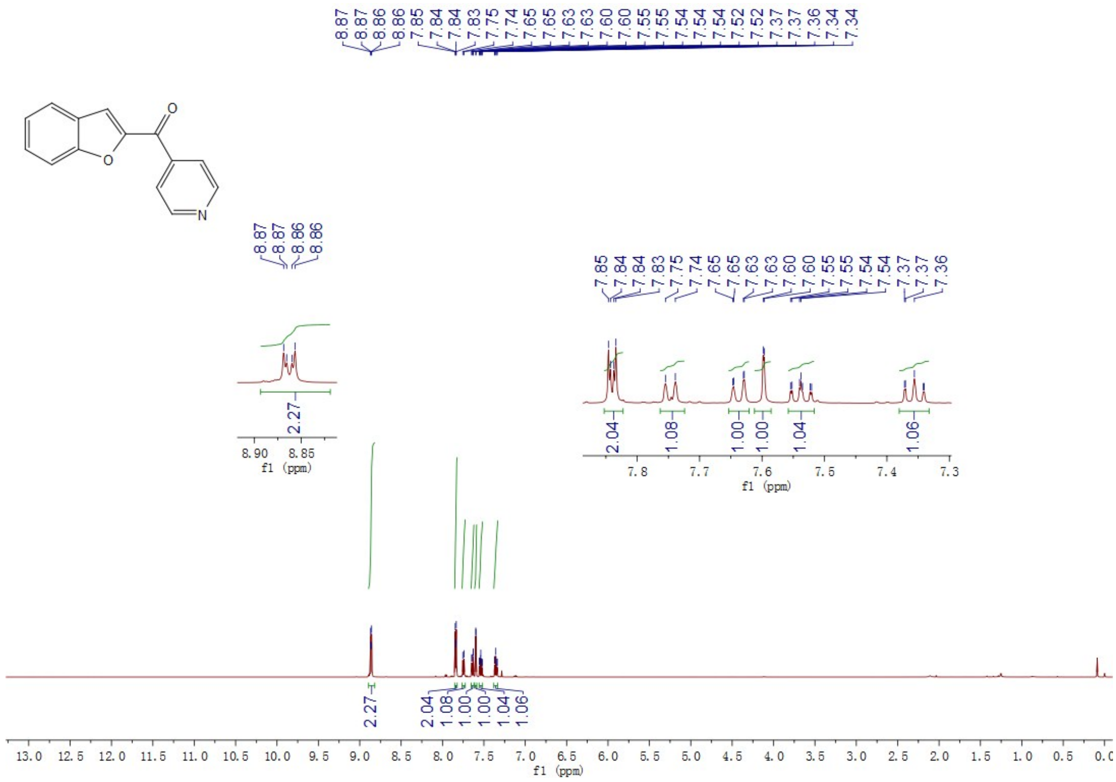
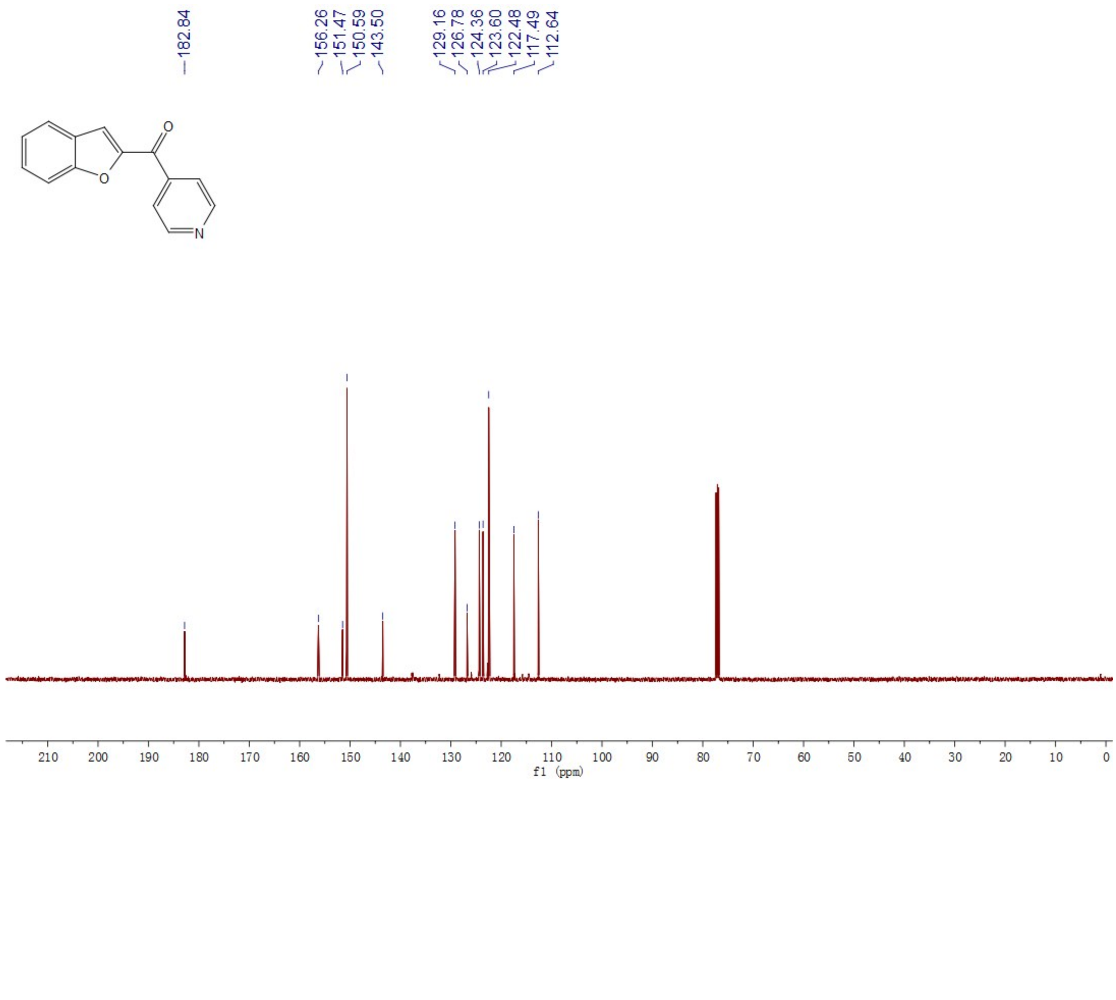
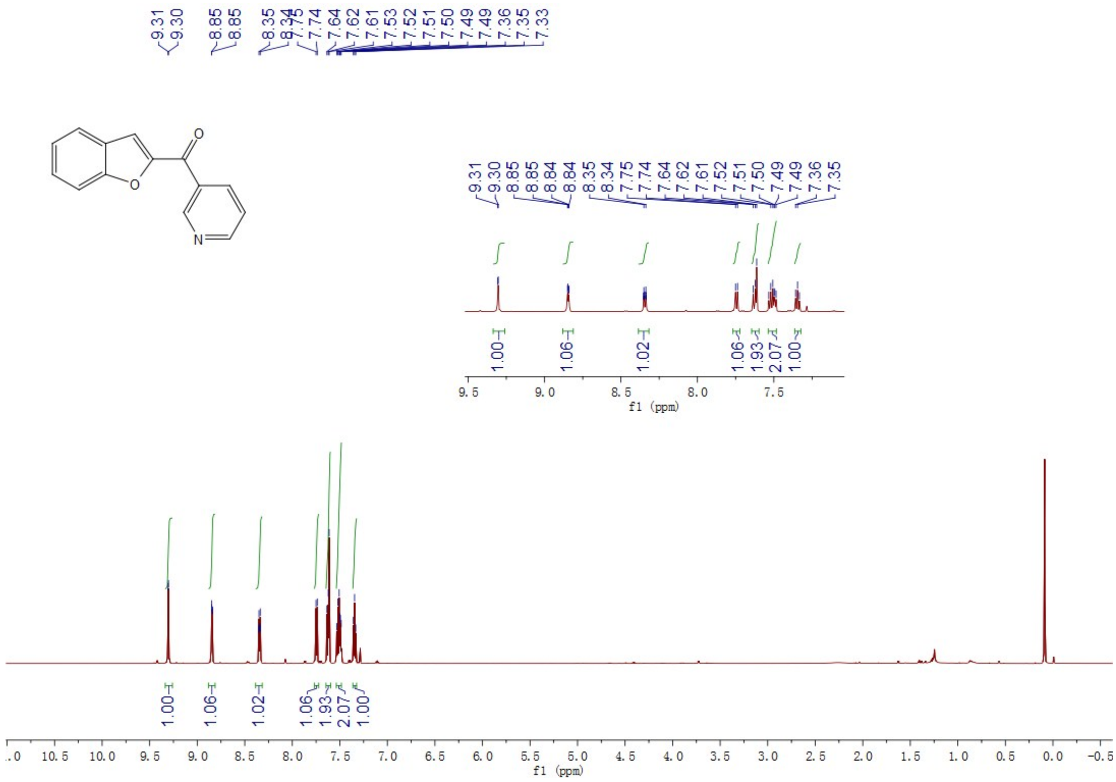
152.10
136.42
133.45
133.28
129.74
129.38
128.70
124.80
117.13
115.05
106.02
Br
O
O
Br
f1 (ppm)

2q





2r


9.31
9.30
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8.85
8.35
8.34
7.75
7.74
7.64
7.62
7.61
7.53
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7.51
7.50
7.49
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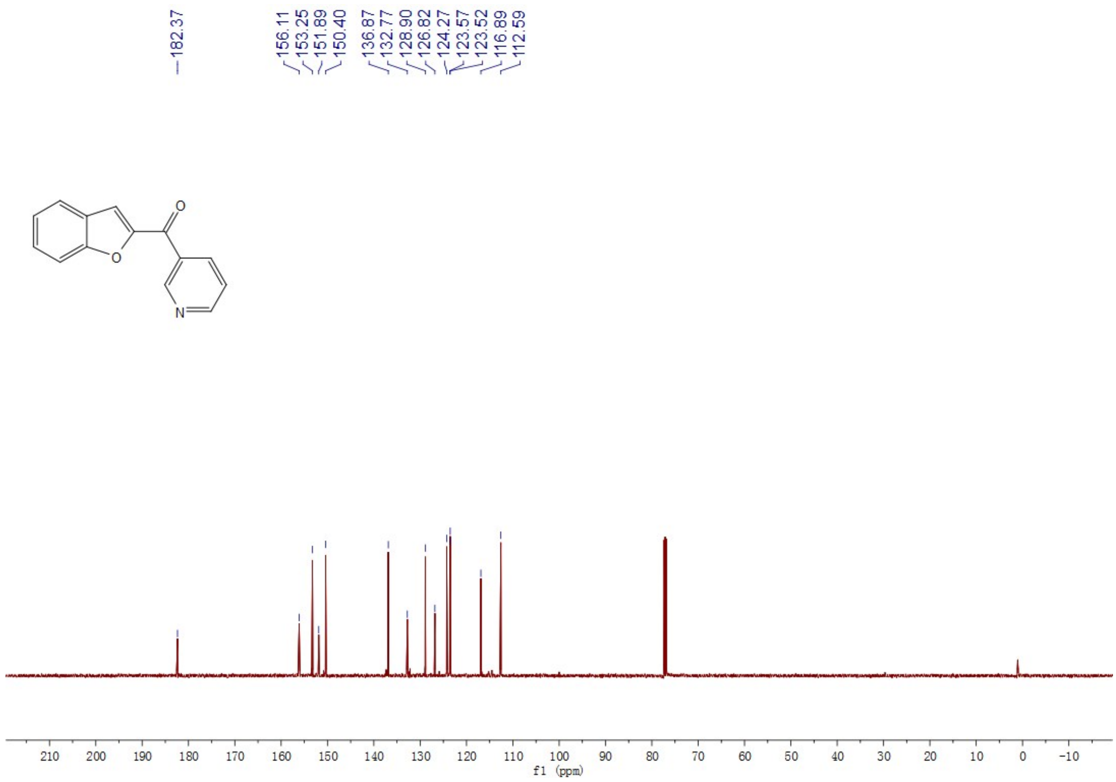
2.07
1.00
f1 (ppm)


182.37
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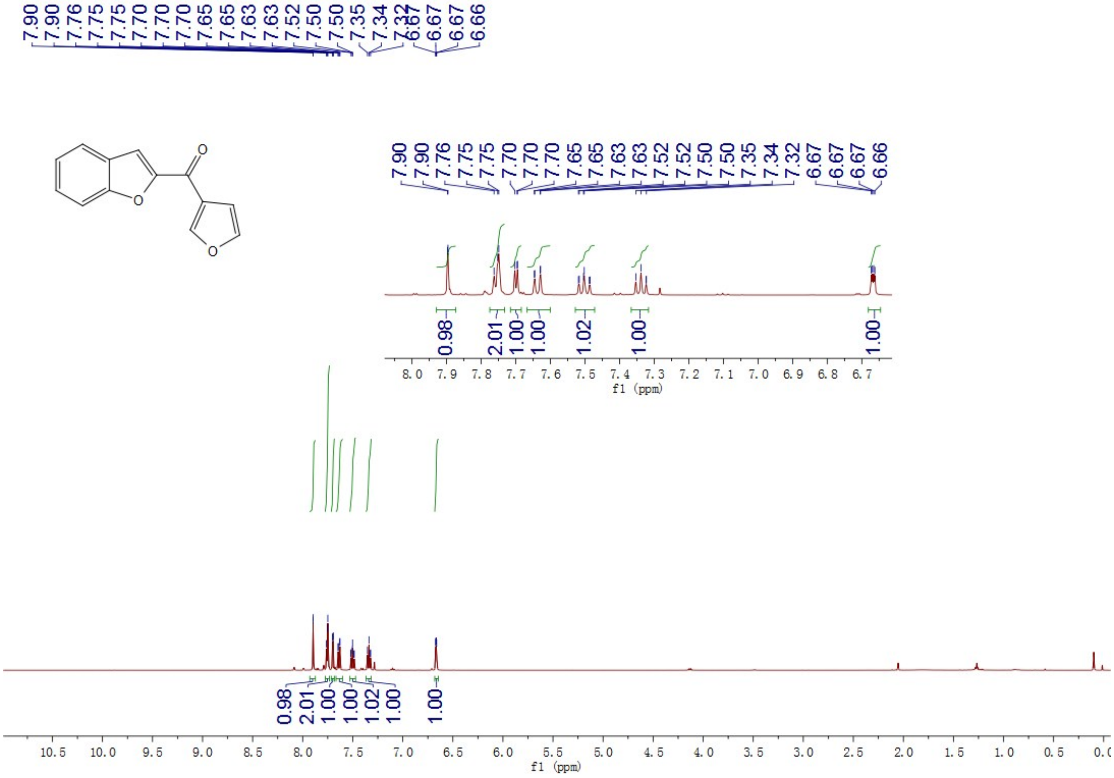
151.89
150.40
136.87
132.77
128.90
126.82
124.27
123.57
123.52
116.89
112.59
f1 (ppm)

2s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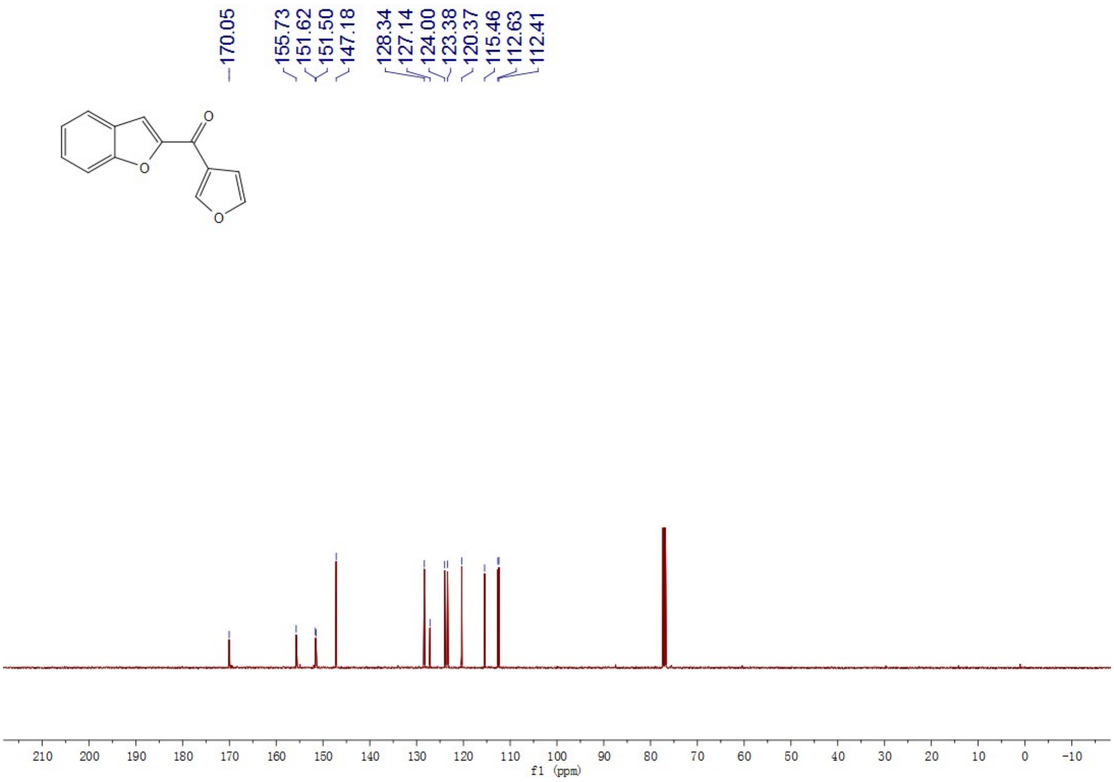
7.90
7.76
7.75
7.75
7.70
7.70
7.65
7.65
7.63
7.63
7.52
7.50
7.50
7.35
7.34
7.32
6.67
6.67
6.66
0.98
2.01
1.00
1.00
1.02
1.00
1.00
f1 (ppm)


170.05
155.73
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151.50
147.18
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127.14
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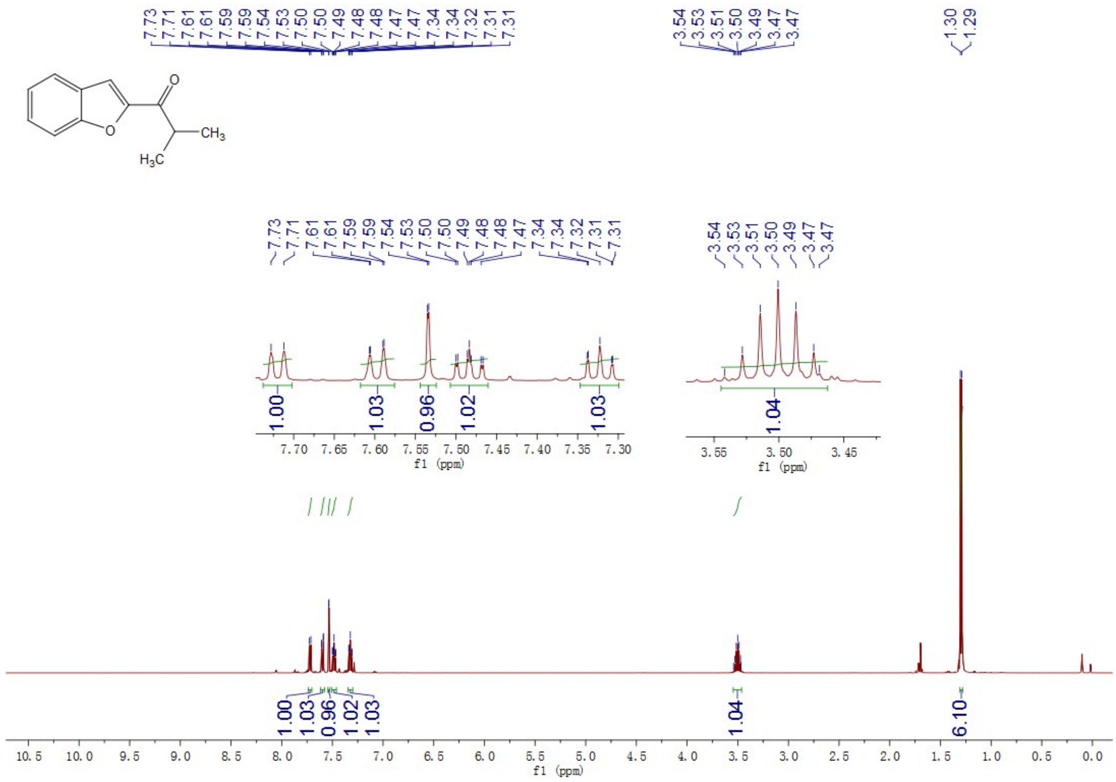
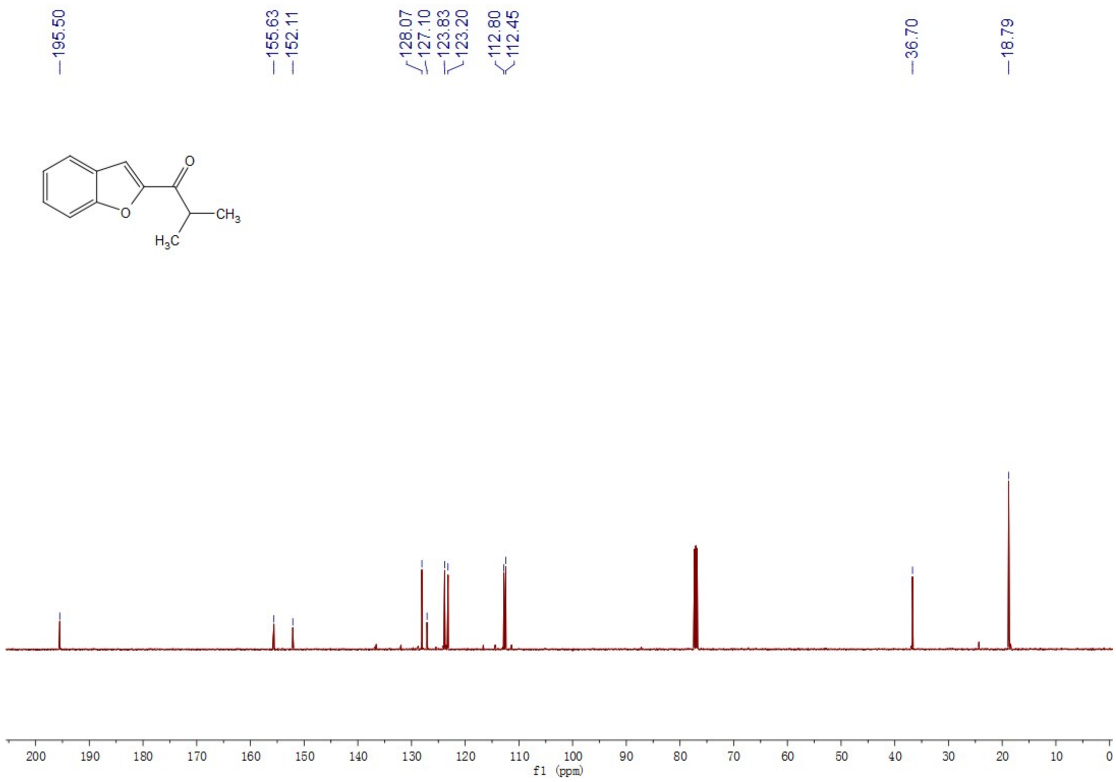
120.37
115.46
112.63
112.41
f1 (ppm)

2t


7.73 7.71 7.61 7.61 7.59 7.59 7.54 7.53 7.50 7.50 7.49 7.48 7.48 7.47 7.47 7.34 7.34 7.32 7.31 7.31
3.54 3.53 3.51 3.50 3.49 3.47 3.47
1.30 1.29
O
CH3
H3C
O
1.00 1.03 0.96 1.02 1.03
1.04
6.10
f1 (ppm)


195.50
155.63 152.11
128.07 127.10 123.83 123.20
112.80 112.45
36.70
18.79
O
CH3
H3C
O
f1 (ppm)