Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Facile and highly chemoselective synthesis of benzil derivatives *via* oxidation of stilbenes in I_2/H_2O System

Xianghua Zeng,[a,b] Chengxia Miao,[a] Shoufeng Wang, Chungu Xia[a] and Wei Sun*[a]

[a] *State Key Laboratory for Oxo Synthesis and Selective Oxidation, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou, 730000 China*

E-mail: wsun@licp.cas.cn

[b] *Graduate School of the Chinese Academy of Sciences, Beijing, 100039 China*

Table of Contents

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1. General Information

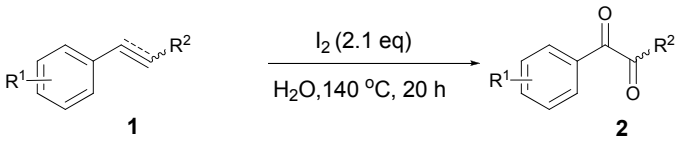
All reactions were conducted with teflon tubes. NMR spectra were recorded with a Bruker Avance III 400 MHz spectrometer. HRMS (ESI) was determined on a Bruker Daltonics micrOTOF-Q^{II} mass spectrometer. Gas chromatography–mass spectrometry (GC/MS) experiments were performed on Agilent 7890A/5975C. ^{1}H and ^{13}C NMR chemical shifts (δ) are given in ppm relative to TMS (δ = 0 ppm) and ppm are downfield from tetramethylsilane ($CDCl_3$: δ C = 77.0 ppm, residual $CHCl_3$ in $CDCl_3$: δ H = 7.26 ppm). Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. The substituted stilbenes were synthesized as following literature.[1]

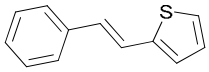
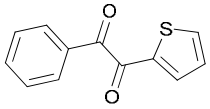
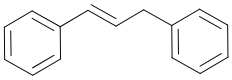
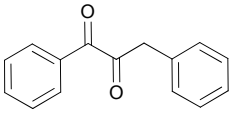
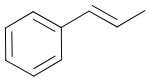
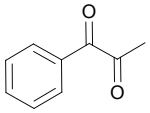
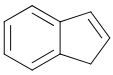
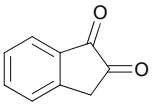
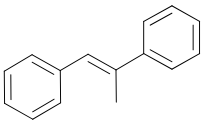
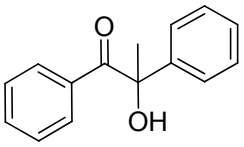
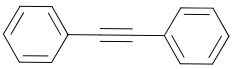
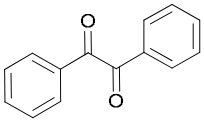
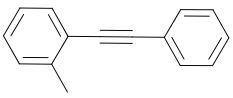
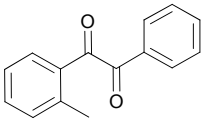
2. General procedure for the oxidation of stilbenes in I_2/H_2O system

A mixture of stilbenes (0.2 mmol), iodine (0.4 mmol), water (1.0 mL) and MeCN (25 μL) were allowed to react for 20 h at 140 °C under air conditions in 25 mL sealed tube. After that the reaction mixture was extracted with dichloromethane (5 mL) and aq saturated solution of sodium thiosulfate (0.5 mL). The organic layer was dried over anhydrous sodium sulfate and concentrated in vacuo. The crude product was chromatographed on a silica gel column with a petroleum ether / ethyl acetate (v/v = 5/1) mixture to afford diketone derivatives in good to excellent yields.

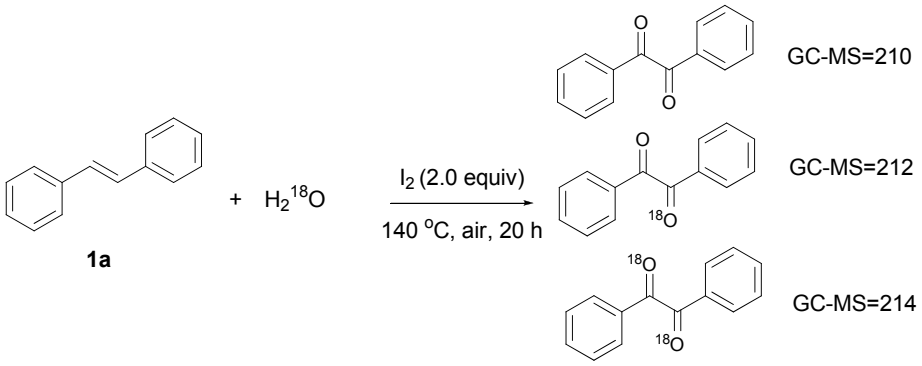
3. Supporting Table, Figures and Scheme

Table S1. Oxidation of a series of alkynes and alkenes in I_2/H_2O system[a]

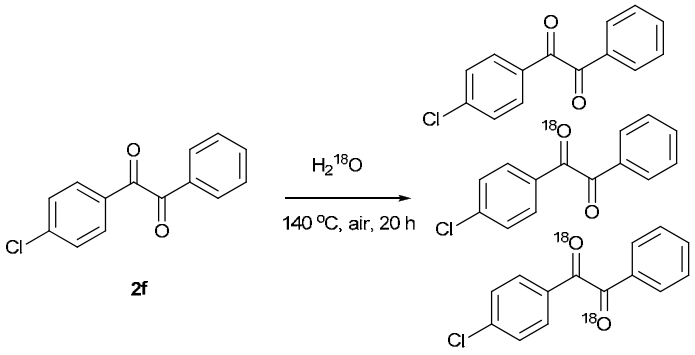


Entry	Substrate	Product	Yield(%)[b]
1			trace
2			NR[c]
3			NR[c]
4			NR[c]
5			NR[c]
6			92
7			95

[a] Unless otherwise noted, all reactions were run with **1** (0.2 mmol), I_2 (0.40 mmol), H_2O (1.0 mL) and MeCN (25 μL) at 140 °C for 20 h under air condition in sealed tubes. [b] Isolated yield. [c] NR= No Reaction.



Scheme S1. Isotopic labelling experiments of **1a** with $H_2{}^{18}O$.



Scheme S2. Isotopic labelling experiments of **2f** exchanging oxygen atom with $H_2{}^{18}O$.

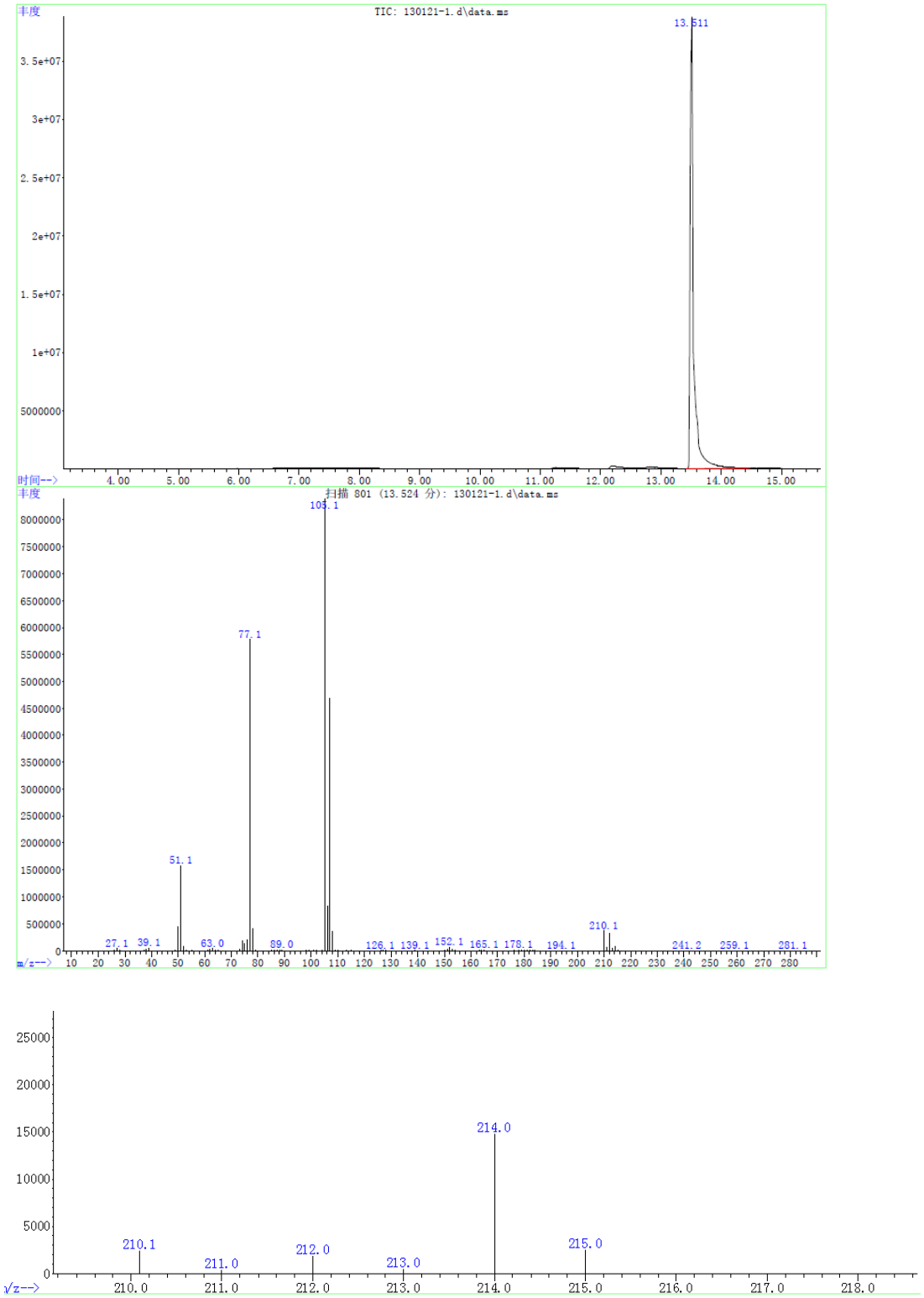


Figure S1. GC-MS Spectra of the product obtained in 97% $H_2{}^{18}O$.

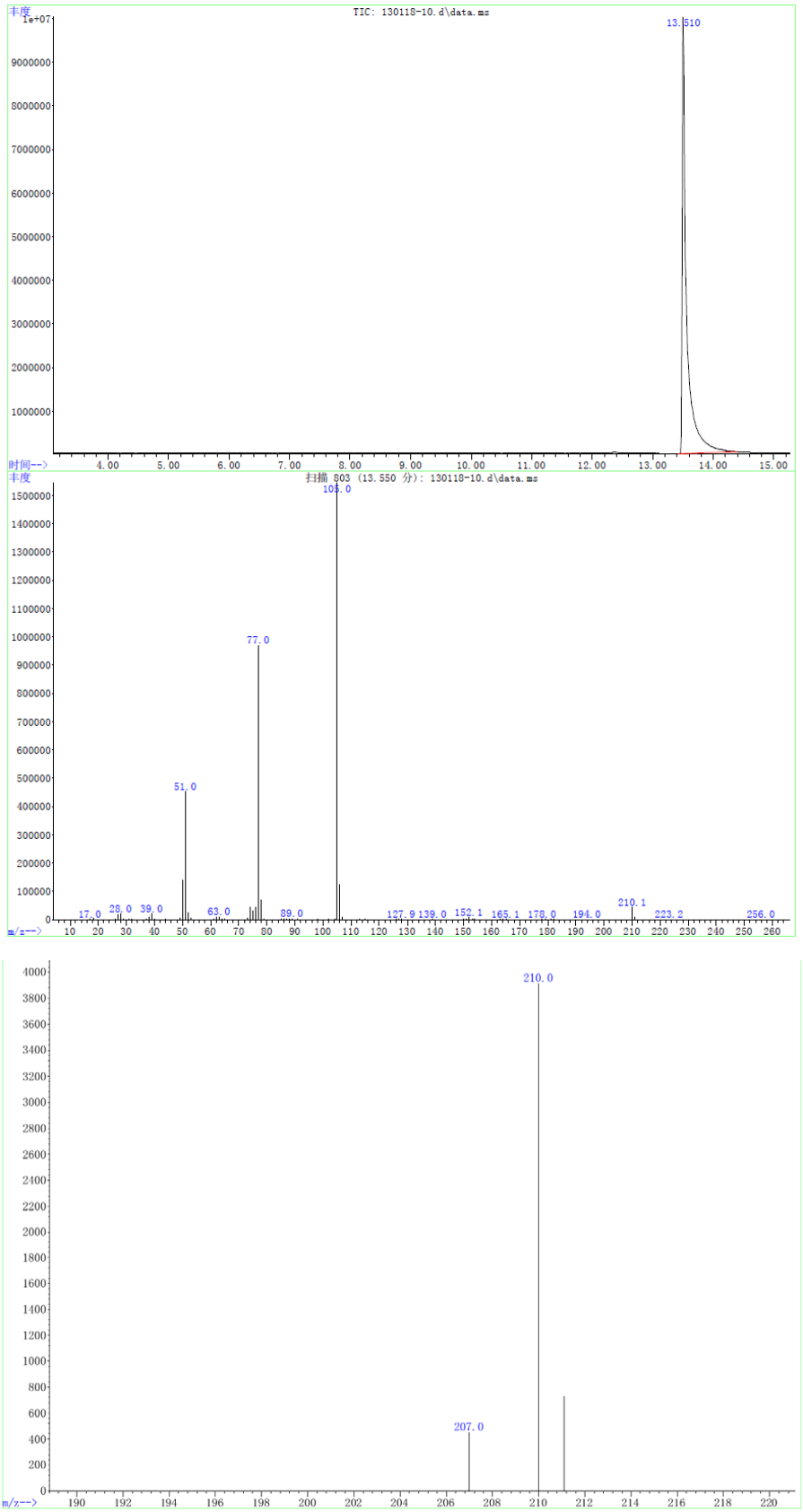


Figure S2. GC-MS Spectra of the product obtained in H_2O.

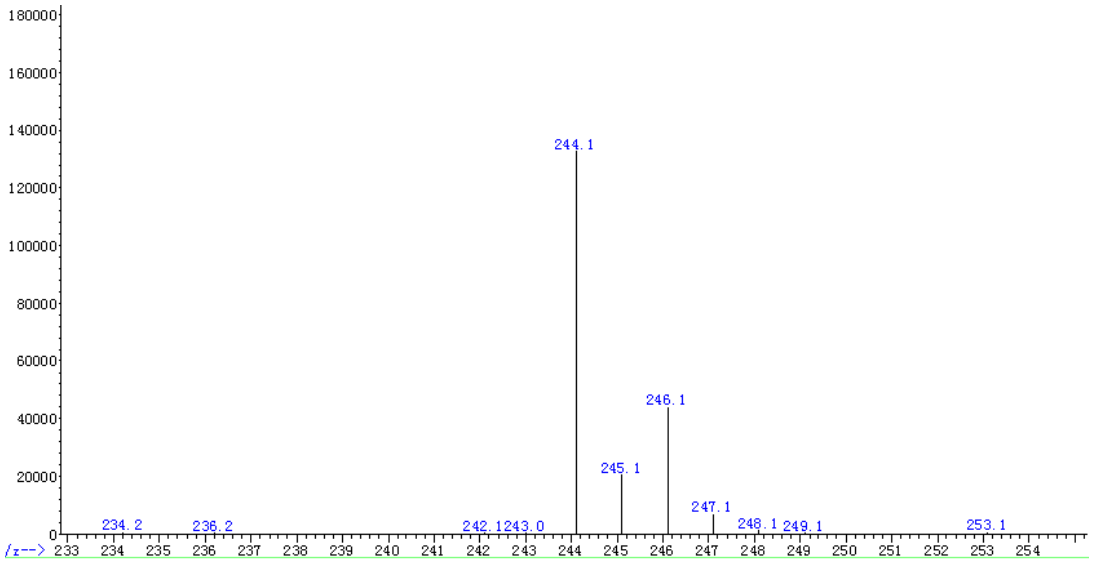


Figure S3. GC-MS spectra of **2f** obtained from the optimized reaction conditions.

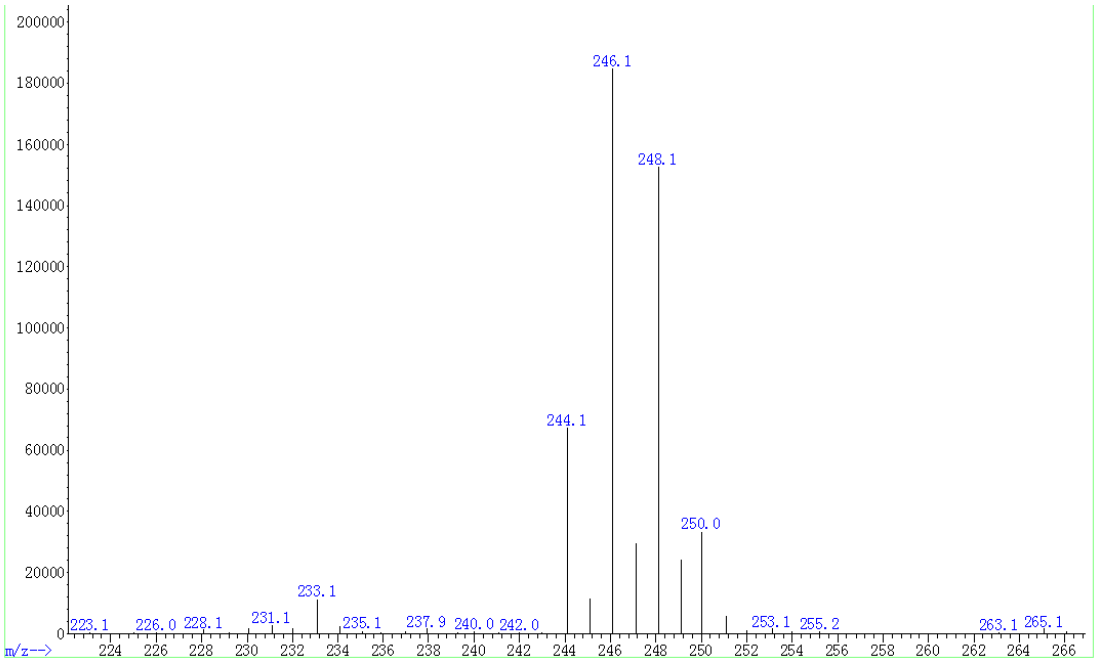


Figure S4. GC-MS spectra of **2f** obtained from the exchange oxygen atom in $H_2{}^{18}O$ under the optimized conditions.

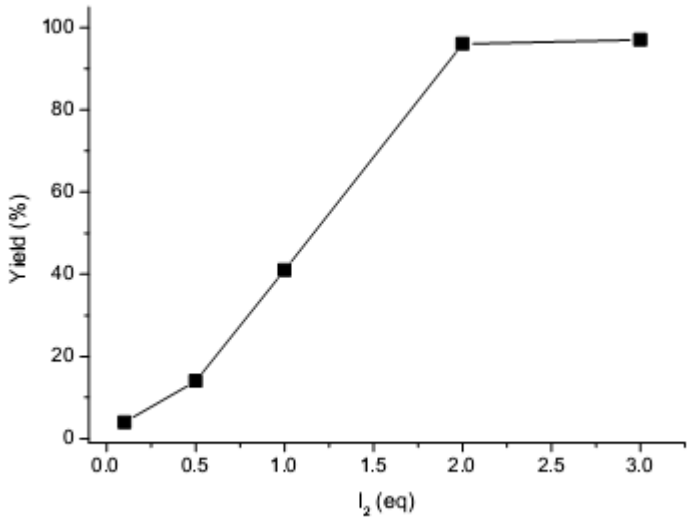
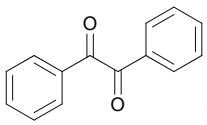


Figure S5. The influence of the amount of iodine on the yield.

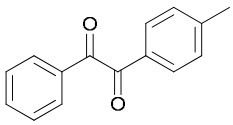
4. Characterization data of the diones 2a-w

benzil (2a)[2]



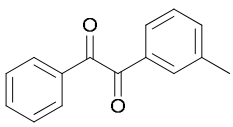
Yellow solid, (39.1 mg, 93%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.97-7.99 (m, 4H), 7.65-7.69 (m, 2H), 7.50-7.54 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.6, 135.0, 133.0, 129.9, 129.0. GC/MS (EI-MS) m/z: 210.0. HRMS m/z: $[M+Na]^+$ Calcd for $C_{14}H_{10}O_2Na$ 233.0573; Found 233.0575.

1-phenyl-2-*p*-tolylethane-1,2-dione (2b)[2]



Yellow solid, (42.1 mg, 94%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-7.98 (dd, J = 8.4, 1.2 Hz, 2H), 7.87 (d, J = 8.4 Hz, 2H), 7.62-7.66 (m, 1H), 7.48-7.52 (m, 2H), 7.30 (d, J = 8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.8, 194.3, 146.3, 134.8, 133.1, 130.6, 130.0, 129.9, 129.8, 129.0, 22.0. GC/MS (EI-MS) m/z: 224.1.

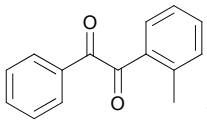
1-phenyl-2-*m*-tolylethane-1,2-dione (2c)[4]



Yellow solid, (43.4 mg, 97%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-7.98 (m, 2H),

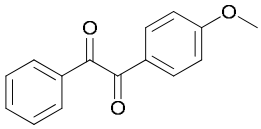
7.76-7.78 (m, 2H), 7.63-7.68 (m, 1H), 7.46-7.53 (m, 3H), 7.39 (t, J=7.6 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.9, 194.7, 139.0, 135.6, 134.9, 133.1, 133.0, 130.2, 129.9, 129.0, 128.9, 127.3, 21.3. GC/MS (EI-MS) m/z: 224.1.

1-phenyl-2-*o*-tolylethane-1,2-dione (2d)[2]



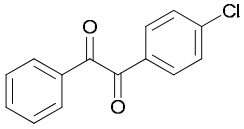
Yellow solid, (43.4 mg, 97%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-7.98 (m, 2H), 7.63-7.67 (m, 2H), 7.46-7.53 (m, 3H), 7.34 (d, J = 7.6 Hz, 1H), 7.25-7.28 (m, 3H), 2.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 196.8, 194.9, 141.4, 134.7, 133.8, 133.2, 133.1, 132.6, 131.8, 130.0, 129.0, 126.1, 21.9. GC/MS (EI-MS) m/z: 224.1.

1-(4-methoxyphenyl)-2-phenylethane-1,2-dione (2e)[2]



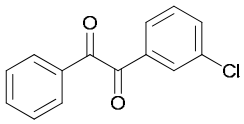
Yellow solid, (26.9 mg, 56%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.87-7.91 (m, 4H), 7.56-7.60 (m, 1H), 7.42-7.46 (m, 2H), 6.91 (d, J = 9.2 Hz, 2H), 2.82 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.8, 192.1, 164.0, 133.7, 132.2, 131.4, 28.9, 127.9, 15.1, 113.4, 54.6. GC/MS (EI-MS) m/z: 240.1.

1-(4-chlorophenyl)-2-phenylethane-1,2-dione (2f)[5]



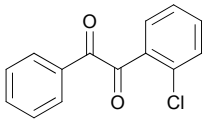
Yellow solid, (47.8 mg, 98%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.91-7.97 (m, 4H), 7.66-7.69(m, 1H), 7.48-7.54 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.9, 193.1, 141.6, 135.1, 132.8, 131.4, 131.3, 130.0, 129.5, 129.1. GC/MS (EI-MS) m/z: 244.1.

1-(3-chlorophenyl)-2-phenylethane-1,2-dione (2g)[1]



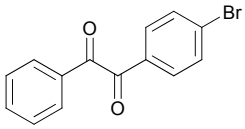
Yellow solid, (46.8 mg, 96%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-7.98 (m, 2H), 7.84 (d, J=8.0 Hz, 1H), 7.62-7.70 (m, 2H), 7.44-7.55 (m, 3H), 7.35-7.39 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.6, 193.0, 139.3, 135.2, 134.8, 130.4, 130.0, 129.6, 129.1, 128.2, 126.7, 124.8. GC/MS (EI-MS) m/z: 243.9.

1-(2-chlorophenyl)-2-phenylethane-1,2-dione (2h)[1]



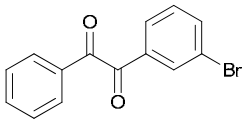
Yellow solid, (44.4 mg, 91%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.03-8.05 (m, 2H), 7.90-7.93 (m, 2H), 7.65-7.69 (m, 1H), 7.52-7.57 (m, 3H), 7.43-7.47 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.7, 192.1, 134.6, 134.5, 134.0, 133.9, 132.5, 132.2, 130.5, 130.3, 128.9, 127.4. GC/MS (EI-MS) m/z:244.0.

1-(4-bromophenyl)-2-phenylethane-1,2-dione (2i)[2]



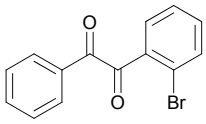
Yellow solid, (51.3 mg, 89%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.95-7.97 (m, 2H), 7.83-7.85 (m, 2H), 7.65-7.69 (m, 3H), 7.50-7.54 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.9, 193.3, 135.1, 132.8, 132.5, 131.8, 131.3, 130.5, 130.0, 129.1. GC/MS (EI-MS) m/z: 290.0.

1-(3-bromophenyl)-2-phenylethane-1,2-dione (2j)[6]



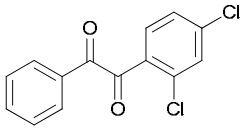
Yellow solid, (53.0 mg, 92%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.12-8.13 (m, 1H), 7.95-7.98 (m, 2H), 7.87-7.89 (m, 1H), 7.76-7.79 (m, 1H), 7.65-7.70 (m, 1H), 7.50-7.54 (m, 2H), 7.39 (d, J = 8.0 Hz, 1H), ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.6, 192.9, 137.7, 135.2, 134.7, 132.7, 132.5, 130.6, 130.0, 129.1, 128.6, 123.4. GC/MS (EI-MS) m/z: 290.0.

1-(2-bromophenyl)-2-phenylethane-1,2-dione (2k)[7]



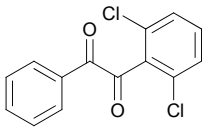
Yellow solid, (50.7 mg, 88%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.06-8.09 (m, 2H), 7.81-7.83 (m, 1H), 7.62-7.69 (m, 2H), 7.42-7.54 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.2, 191.5, 136.0, 134.5, 134.4, 133.8, 132.7, 132.6, 130.4, 128.9, 127.9, 121.8. GC/MS (EI-MS) m/z:290.0.

1-(2,4-dichlorophenyl)-2-phenylethane-1,2-dione (2l)[7]



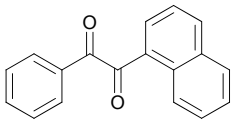
Yellow solid, (50.0 mg, 90%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.00-8.03 (m, 2H), 7.86 (d, J = 8.4 Hz, 1H), 7.65-7.69 (m, 1H), 7.52-7.56 (m, 2H), 7.41-7.46 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.5, 191.7, 140.6, 134.9, 134.7, 133.1, 132.3, 132.2, 130.5, 130.2, 129.0, 128.0. GC/MS (EI-MS) m/z: 278.0.

1-(2,6-dichlorophenyl)-2-phenylethane-1,2-dione (2m)



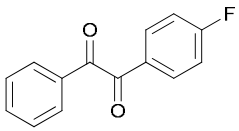
Yellow solid, (43.4 mg, 78%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.07-8.09 (m, 2H), 7.56-7.60 (m, 1H), 7.42-7.46 (m, 2H), 7.15-7.25 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 190.0, 188.3, 134.7, 134.7, 133.0, 132.1, 130.8, 130.1, 128.8, 128.4, 127.4. GC/MS m/z, Calcd: 278.0, Found: 278.0. HRMS m/z: $[M+Na]^+$ Calcd for $C_{14}H_8Cl_2O_2Na$ 300.9794; Found 300.9797.

1-(naphthalen-1-yl)-2-phenylethane-1,2-dione (2n)[8]



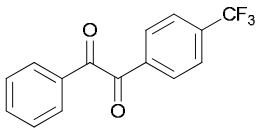
Yellow solid, (46.8 mg, 90%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 9.33 (d, J=8.8 Hz, 1H), 8.12 (d, J=8.0 Hz, 1H), 8.04-7.06 (m, 2H), 7.92-7.96 (m, 2H), 7.74-7.78 (m, 1H), 7.62-7.69 (m, 2H), 7.47-7.55 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 197.2, 194.6, 136.0, 135.1, 134.8, 134.1, 133.4, 131.0, 130.1, 129.5, 129.1, 128.8, 128.7, 127.2, 126.0, 124.5. GC/MS (EI-MS) m/z: 260.1.

1-(4-fluorophenyl)-2-phenylethane-1,2-dione (2o)[4]



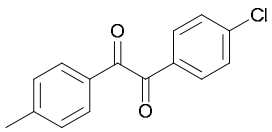
Yellow solid, (44.7 mg, 98%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-8.05 (m, 4H), 7.65-7.69 (m, 1H), 7.50-7.54 (m, 2H), 7.16-7.22 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.1, 192.8, 171.1(d, J = 257.0 Hz), 135.0, 132.9, 132.7(d, J = 11.0 Hz), 130.0, 129.5(d, J = 3.0 Hz), 129.1, 116.4 (d, J = 22.0 Hz). GC/MS (EI-MS) m/z: 228.1.

1-phenyl-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2p)[1]



Yellow solid, (50.6 mg, 91%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.10 (d, J = 8.0 Hz, 2H), 7.97-7.99 (m, 2H), 7.78 (d, J = 8.0 Hz, 2H), 7.67-7.71 (m, 1H), 7.52-7.56 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 193.5, 193.0, 136.0, 135.6 (d, J = 8.0 Hz), 133.9 (d, J = 264.0 Hz), 130.2, 130.0, 129.2, 126.1 (q, J = 4.0 Hz), 124.7, 122.0. GC/MS (EI-MS) m/z: 278.1.

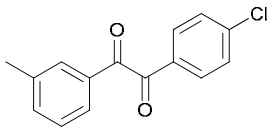
1-(4-chlorophenyl)-2-p-tolylethane-1,2-dione (2q)[9]



Yellow solid, (49.5 mg, 96%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.91 (dd, J=6.8, 2.0

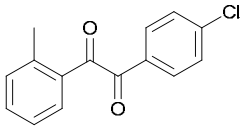
Hz, 2H), 7.85(dd, *J*=6.8, 1.6 Hz, 2H), 7.47(dd, *J*=6.8, 2.0 Hz, 2H), 7.31 (d, *J*=8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.6, 192.2, 145.4, 140.4, 130.4, 130.2, 129.4, 129.0, 128.8, 128.4, 20.9. GC/MS (EI-MS) m/z: 258.1.

1-(4-chlorophenyl)-2-m-tolylethane-1,2-dione (2r)



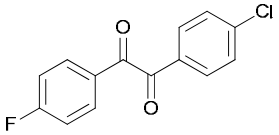
Yellow solid, (49.5 mg, 96%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.90-7.93 (m, 2H), 7.74-7.77 (m, 2H), 7.47-7.50 (m, 3H), 7.40 (t, J = 7.6 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 194.2, 193.2, 141.6, 139.1, 136.0, 132.9, 131.4, 130.3, 129.4, 129.0, 127.3, 21.3. GC/MS m/z, Calcd: 258.0, Found: 258.1. HRMS m/z: $[M+Na]^+$ Calcd for $C_{15}H_{11}ClO_2Na$ 281.0340; Found 281.0346.

1-(4-chlorophenyl)-2-o-tolylethane-1,2-dione (2s)



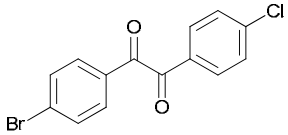
Yellow solid, (49.0 mg, 95%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.90-7.94 (m, 2H), 7.61 (d, *J*=7.6 Hz, 1H), 7.48-7.52 (m, 3H), 7.34-7.36 (m, 1H), 7.27-7.29 (m, 1H), 2.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 196.2, 193.4, 141.5, 141.4, 134.0, 133.0, 132.7, 131.6, 131.5, 131.3, 129.5, 126.1, 21.9. GC/MS m/z, Calcd: 258.0, Found: 258.1. HRMS m/z: $[M+Na]^+$ Calcd for $C_{15}H_{11}ClO_2Na$ 281.0340; Found 281.0344.

1-(4-chlorophenyl)-2-(4-fluorophenyl)ethane-1,2-dione (2t)[10]



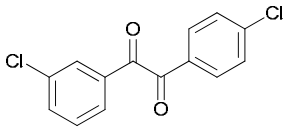
Yellow solid, (48.8 mg, 93%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.99-8.03 (m, 2H), 7.90-7.94 (m, 2H), 7.48-7.51 (m, 2H), 7.17-7.21 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.6, 192.0, 166.8 (d, J = 257.0 Hz), 141.8, 132.7 (d, J = 9.0 Hz), 131.3, 131.2, 129.5, 129.2 (d, J = 3.0 Hz), 116.5 (d, J = 23.0 Hz). GC/MS (EI-MS) m/z: 262.1.

1-(4-bromophenyl)-2-(4-chlorophenyl)ethane-1,2-dione (2u)[10]



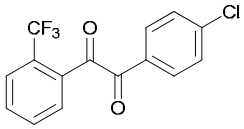
Yellow solid, (50.4 mg, 78%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.91-7.93 (m, 2H), 7.83 (dd, J = 6.8, 1.6 Hz, 2H), 7.64-7.68 (m, 2H), 7.50 (dd, J = 6.8, 2.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.6, 192.3, 141.9, 132.5, 131.5, 131.3, 131.1, 130.8, 129.5, 128.8. GC/MS (EI-MS) m/z: 324.0.

1-(3-chlorophenyl)-2-(4-chlorophenyl)ethane-1,2-dione (2v)[11]



Yellow solid, (54.0 mg, 97%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 7.96-7.97 (m, 1H), 7.91-7.94 (m, 2H), 7.83 (d, J = 8.0 Hz, 2H), 7.63-7.65 (m, 1H), 7.45-7.52 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.3, 192.1, 141.9, 135.5, 135.0, 134.3, 131.3, 131.0, 130.4, 129.7, 129.6, 128.2. GC/MS (EI-MS) m/z: 278.0.

1-(4-chlorophenyl)-2-(2-(trifluoromethyl)phenyl)ethane-1,2-dione (2w)



Yellow solid, (50.7 mg, 81%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 8.03-8.07 (m, 2H), 7.79-7.81 (m, 1H), 7.68-7.74 (m, 3H), 7.50-7.54 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ = 192.7, 189.3, 141.6, 166.8(d, J = 257.0 Hz), 141.8, 134.4, 132.4, 132.0, 131.8, 130.7, 129.4, 127.0 (d, J = 6.0 Hz), 124.8, 122.1. GC/MS m/z, Calcd: 312.0, Found: 311.9. HRMS m/z: $[M+Na]^+$ Calcd for $C_{15}H_8ClF_3O_2Na$ 335.0057; Found 335.0063.

5. References

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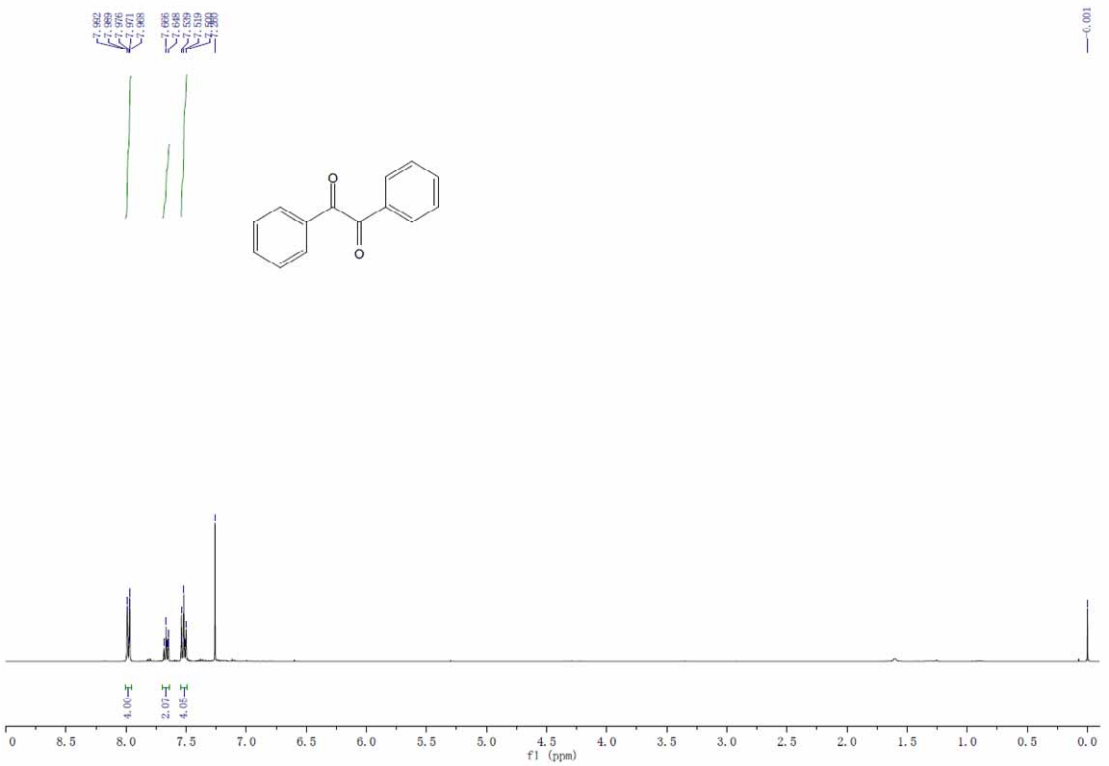
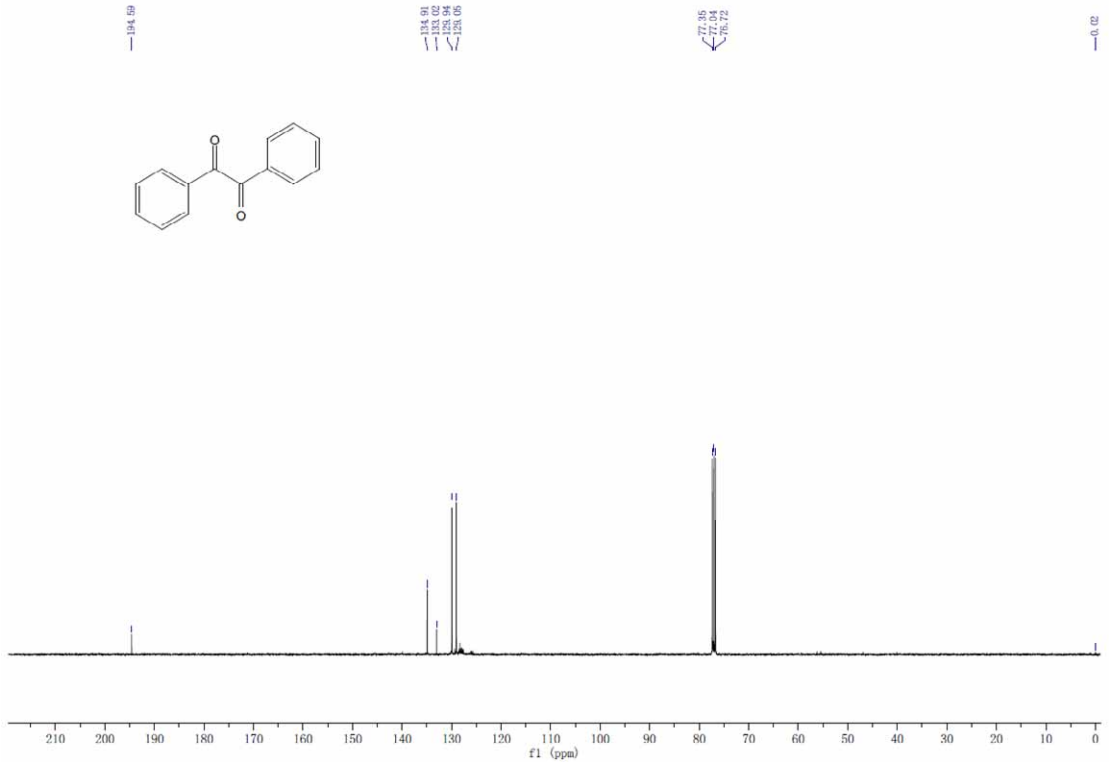
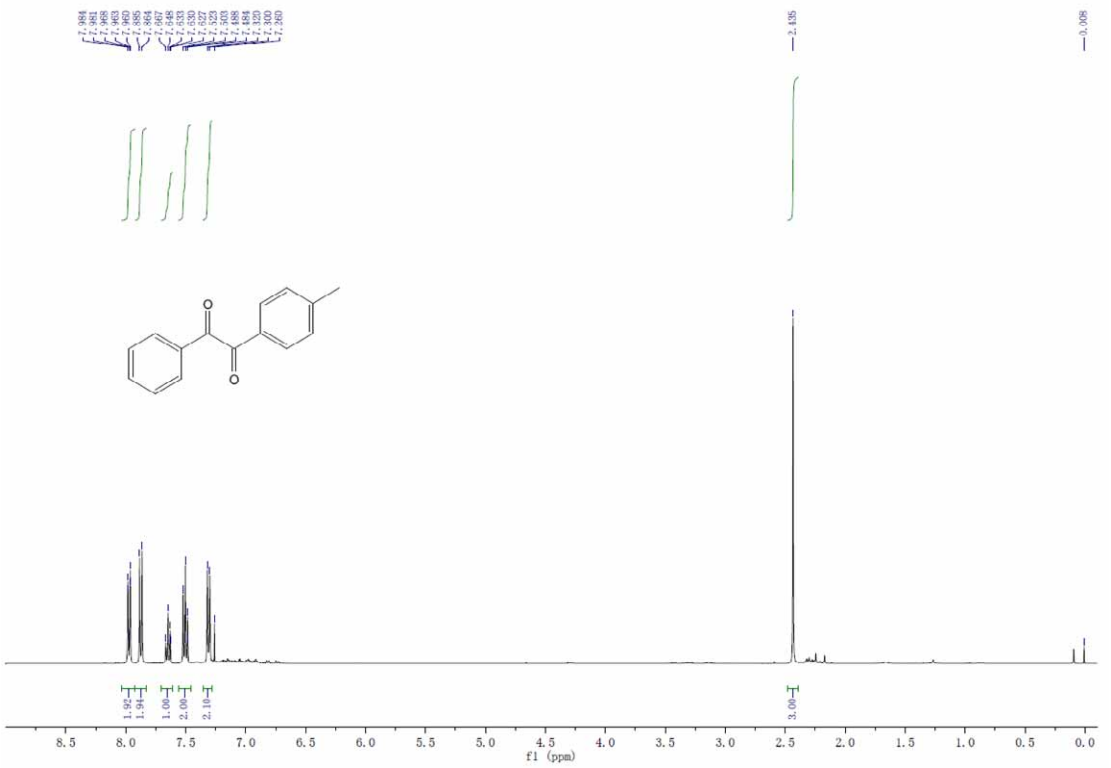
6. Copies of the diones 2a-w ^{1}H and ^{13}C NMR spectra

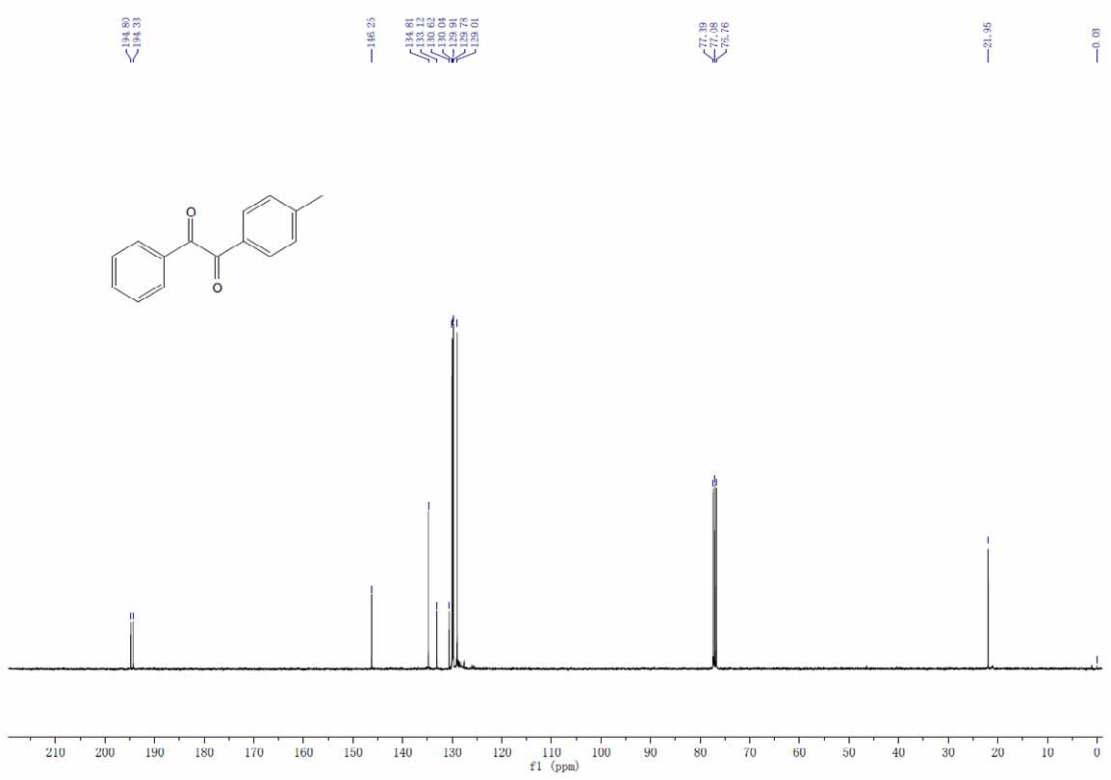
2a





2b





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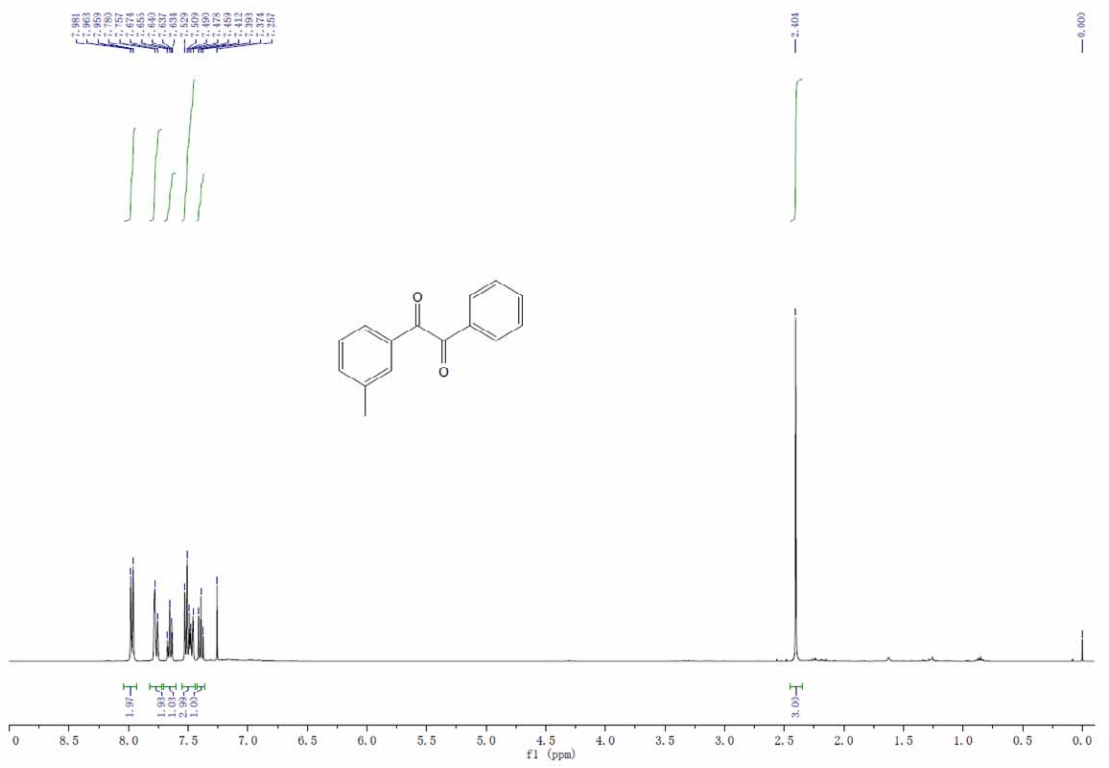

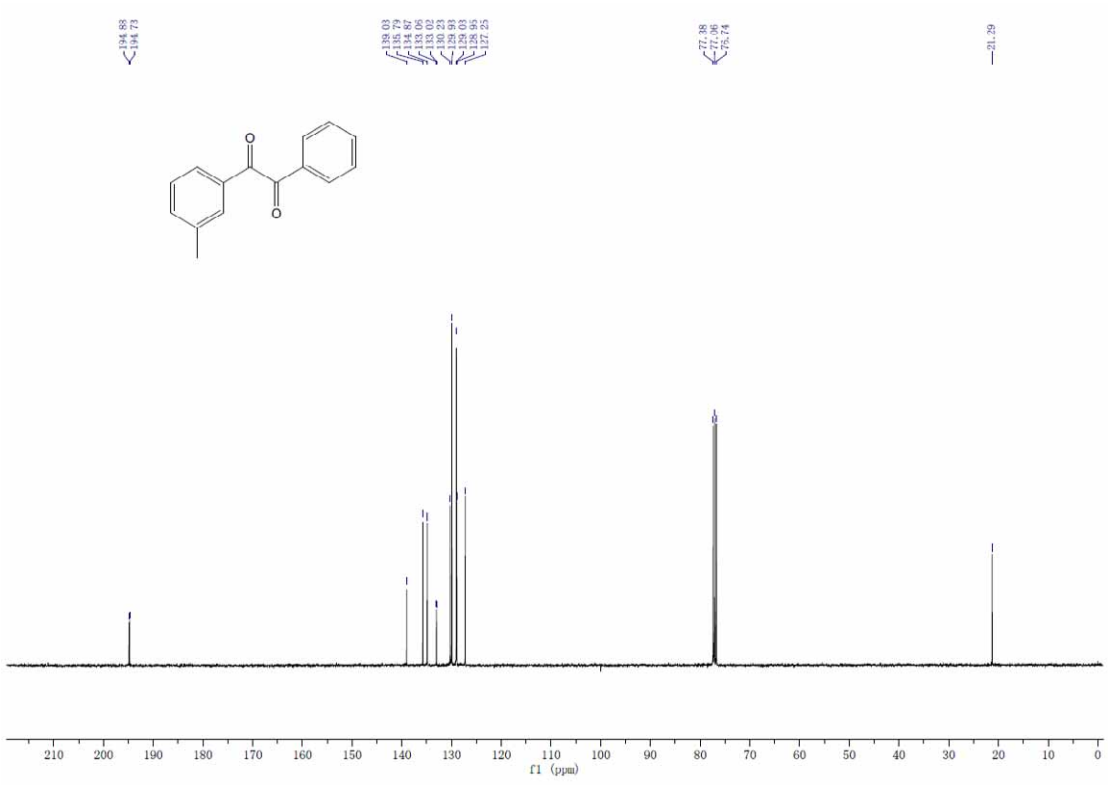

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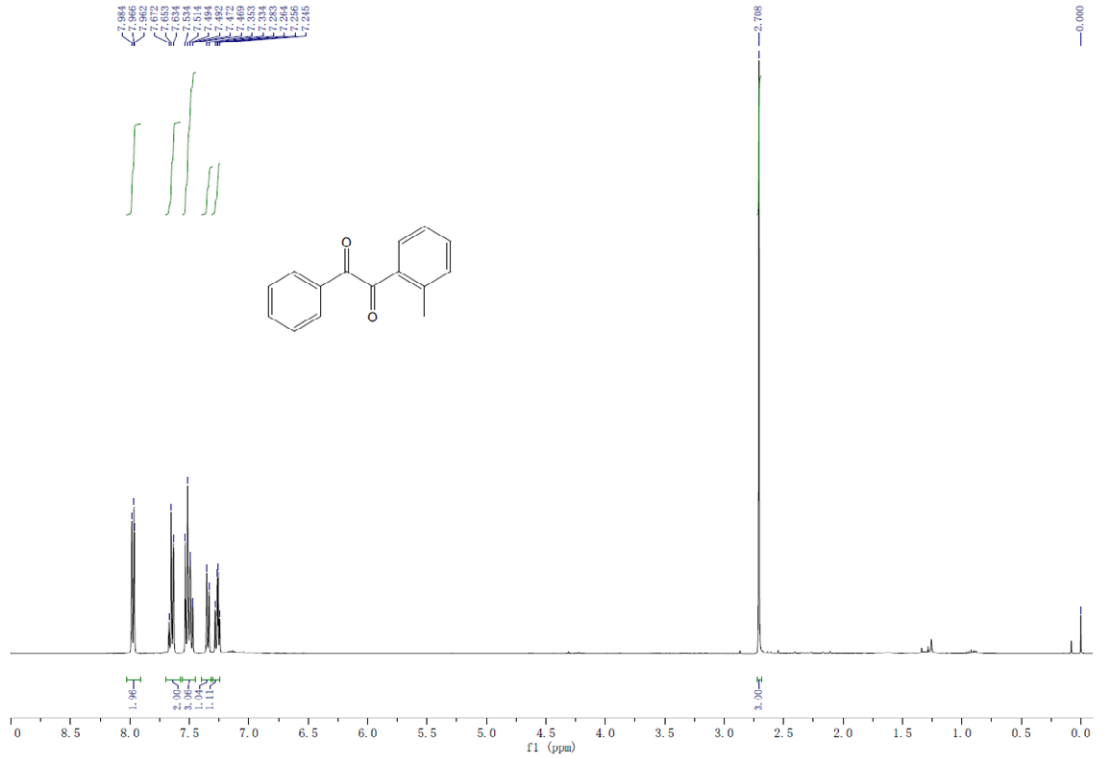

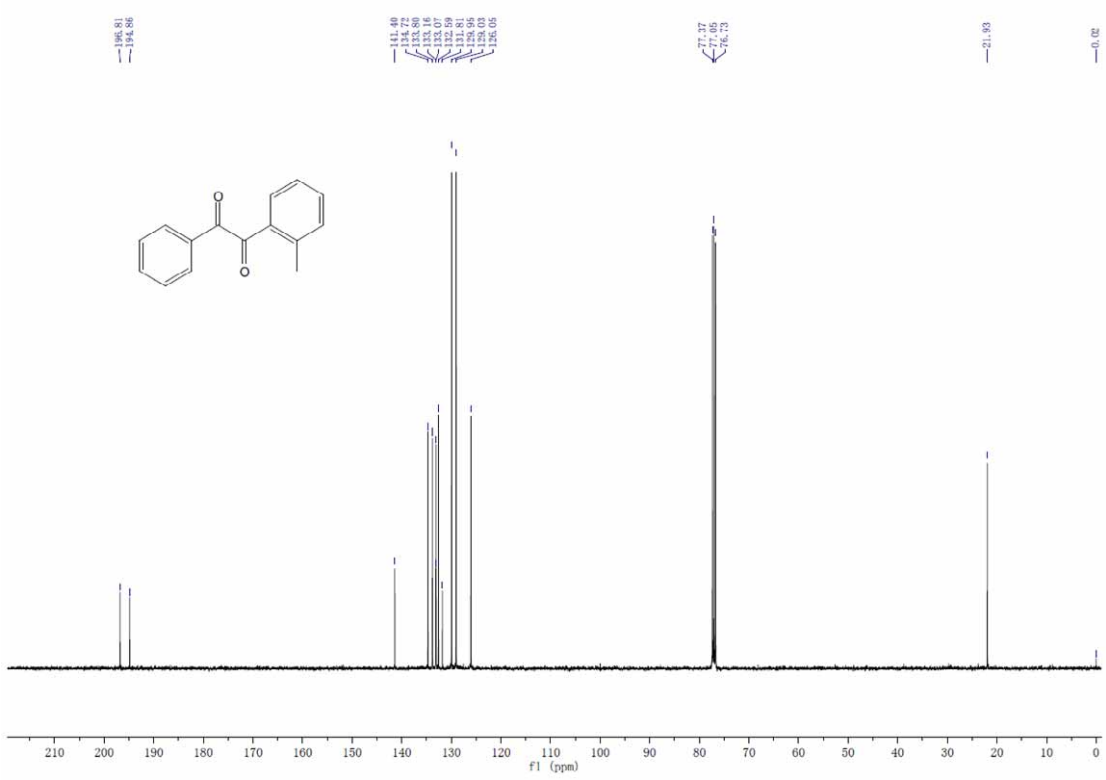

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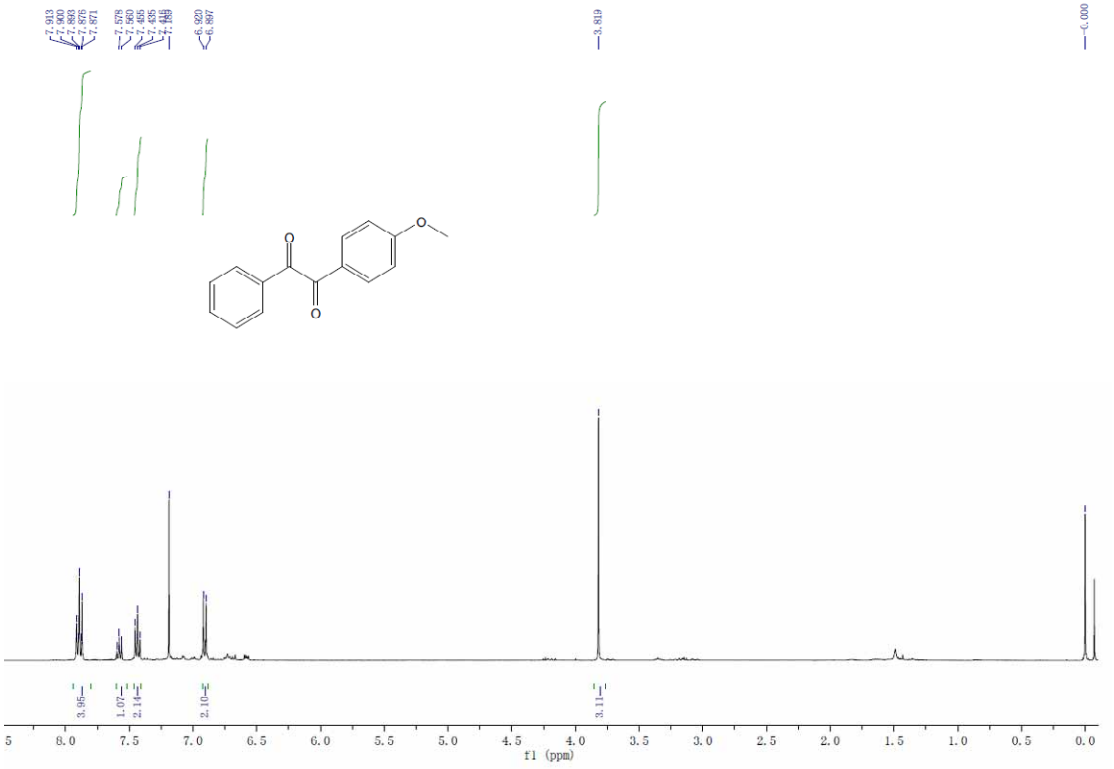

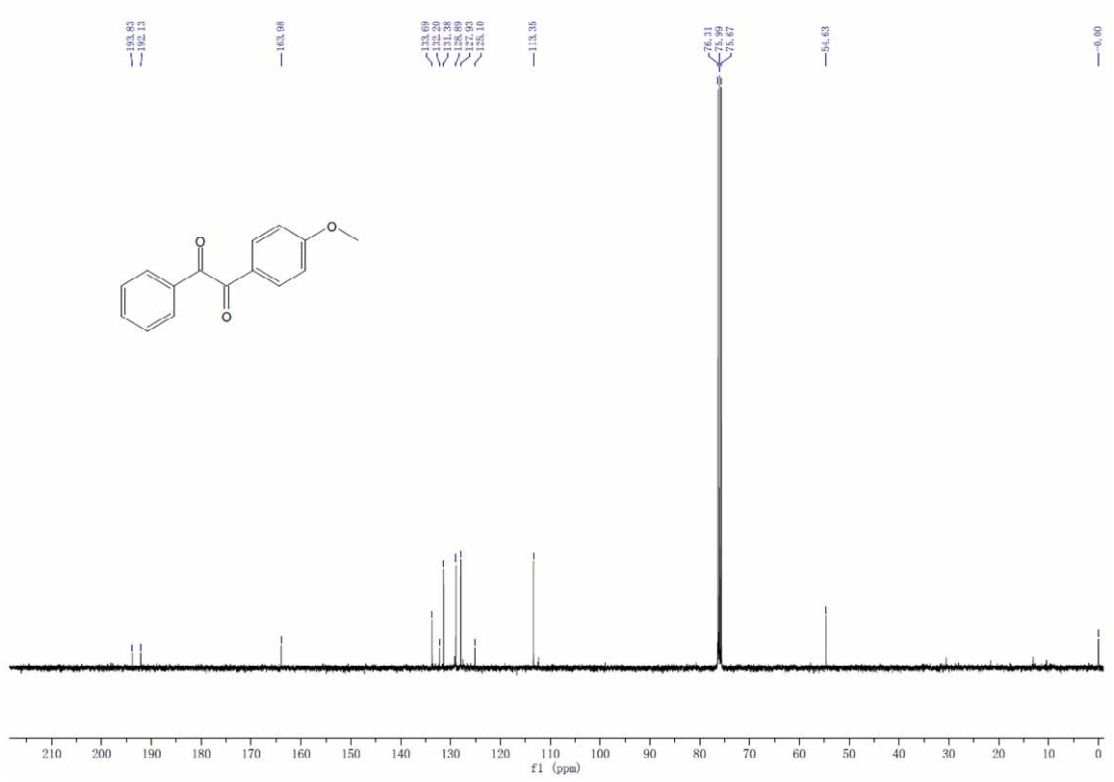

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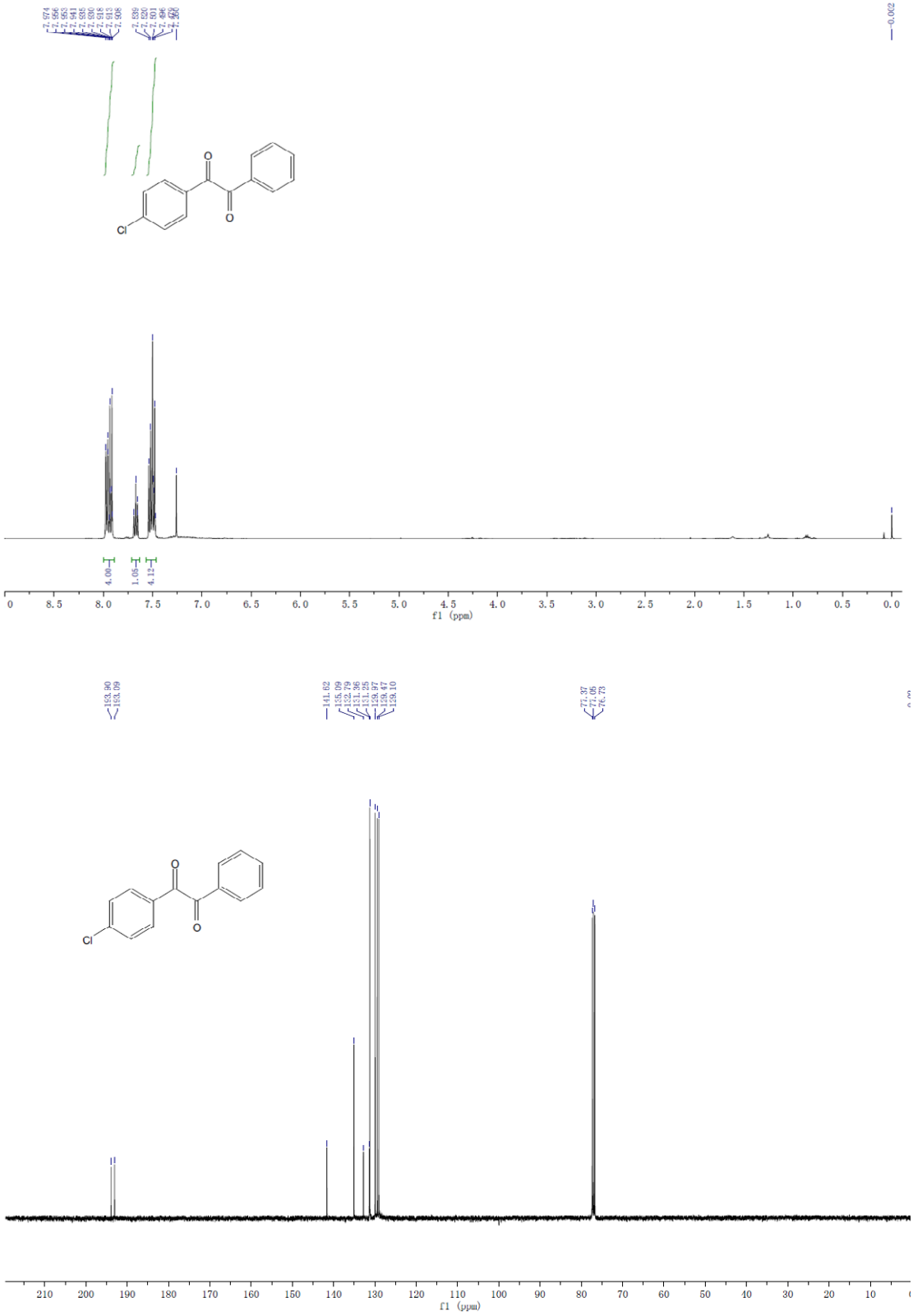

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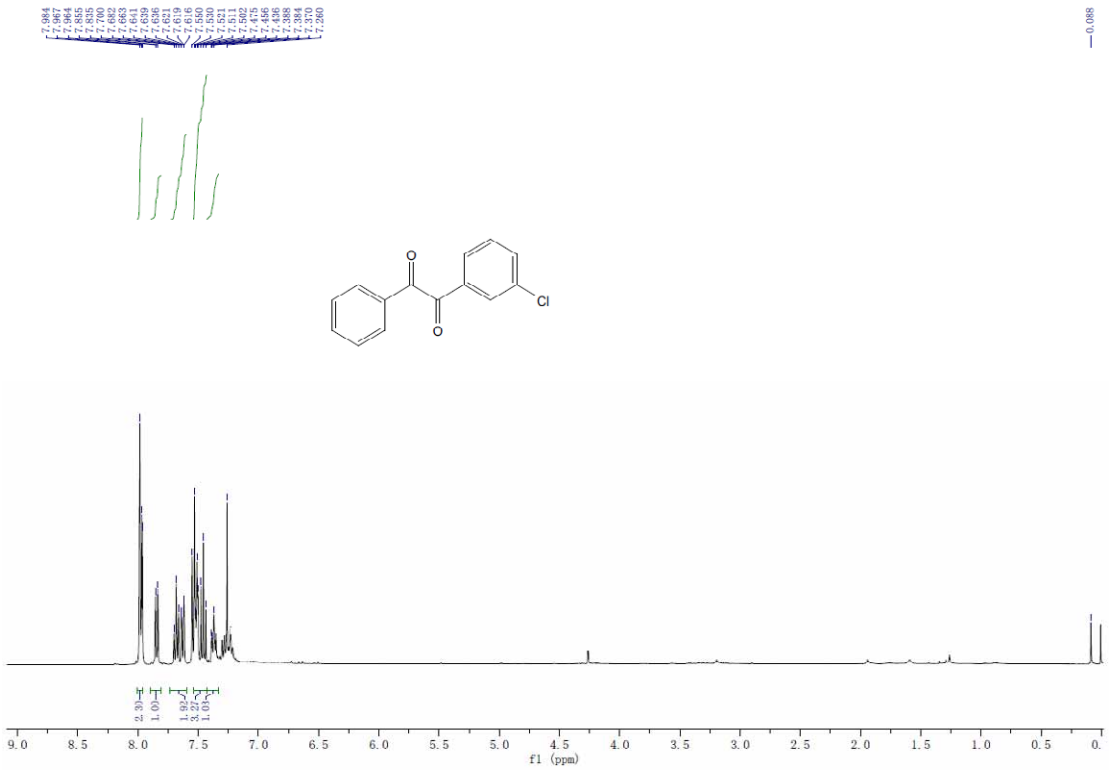

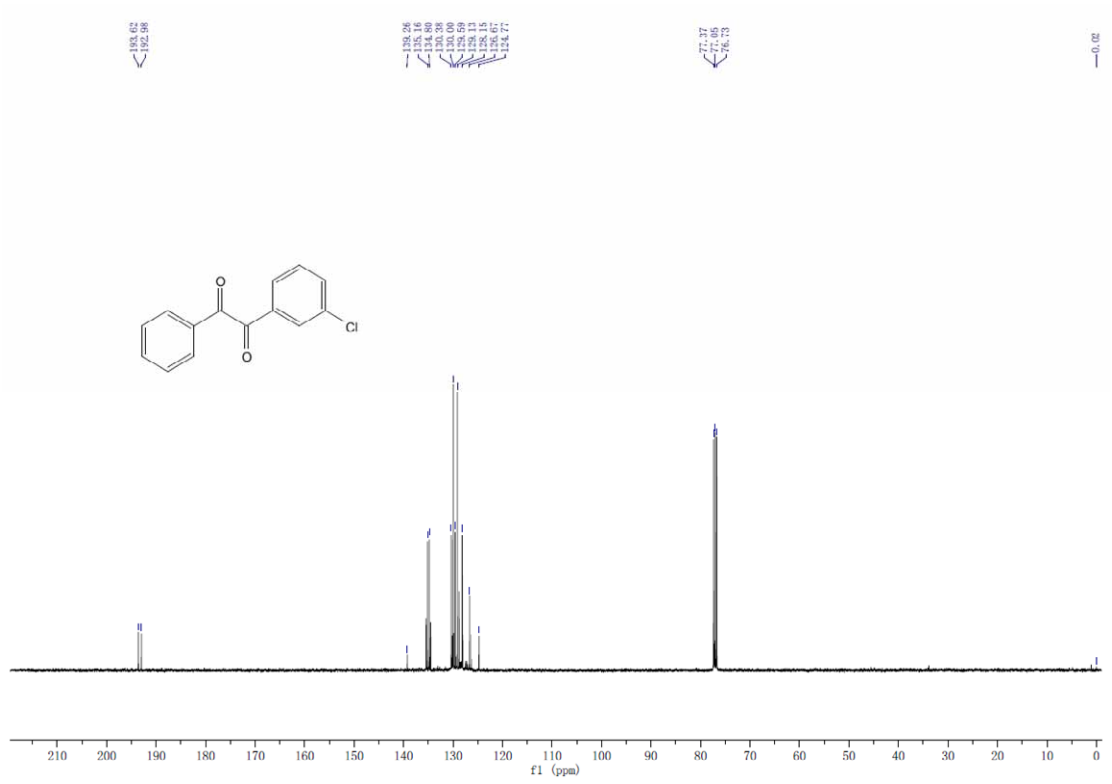

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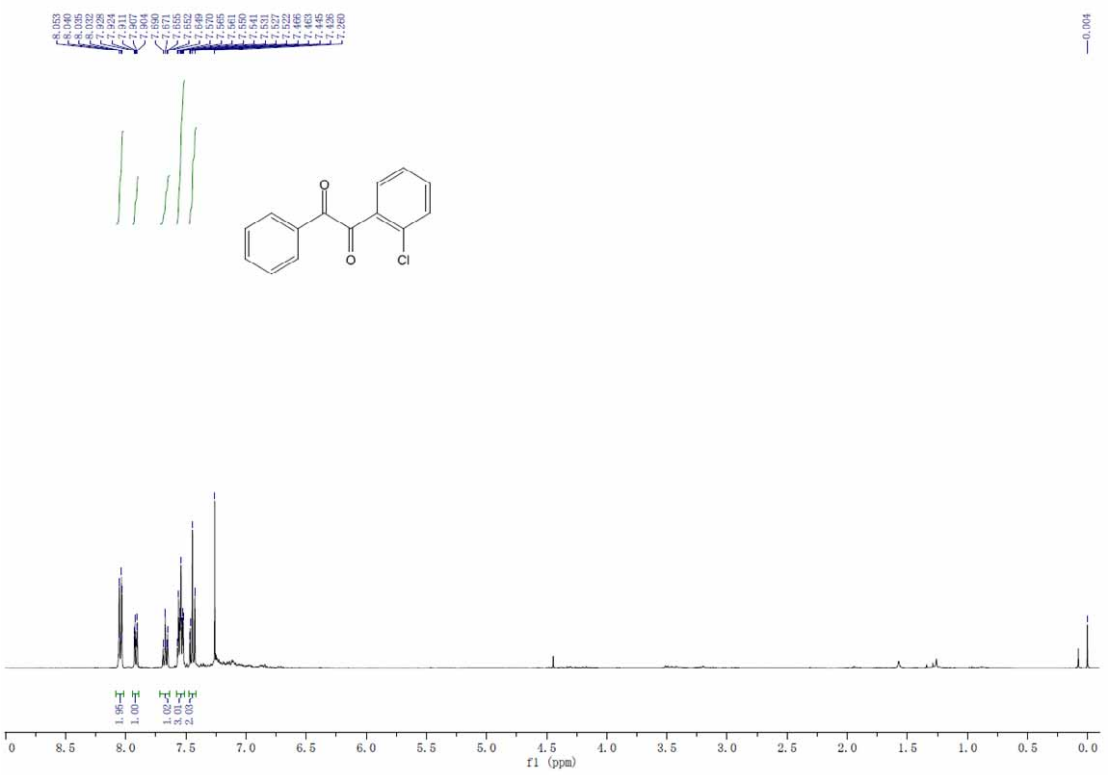

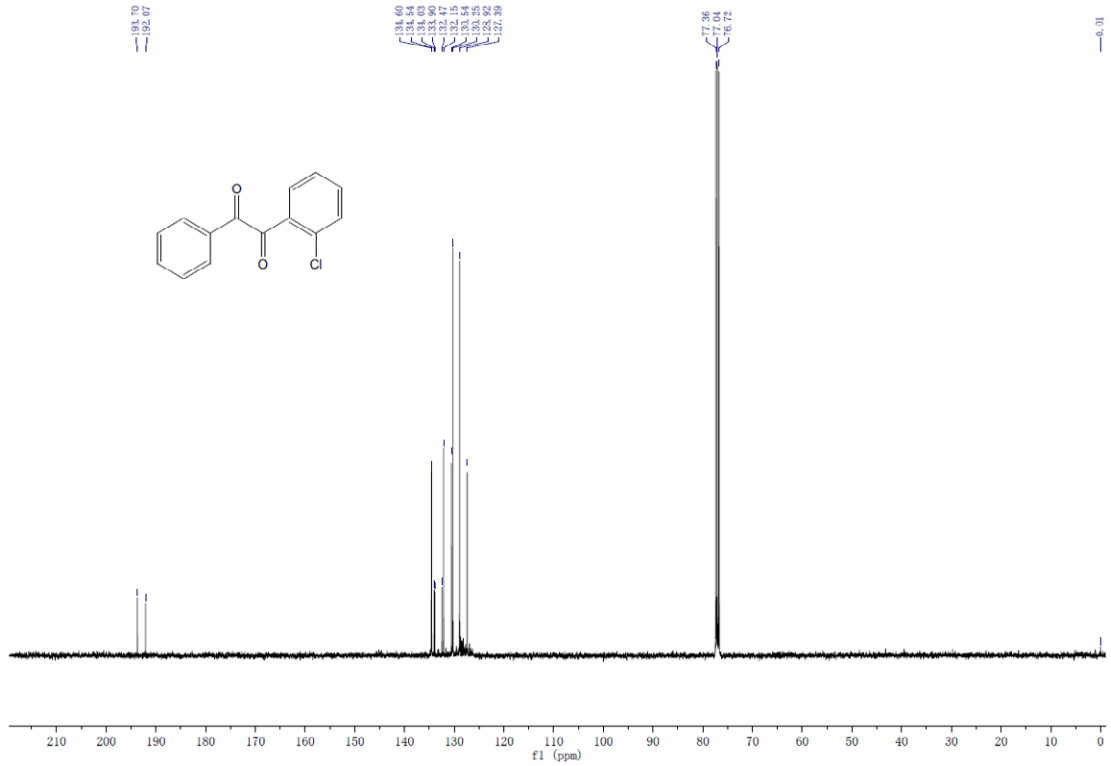

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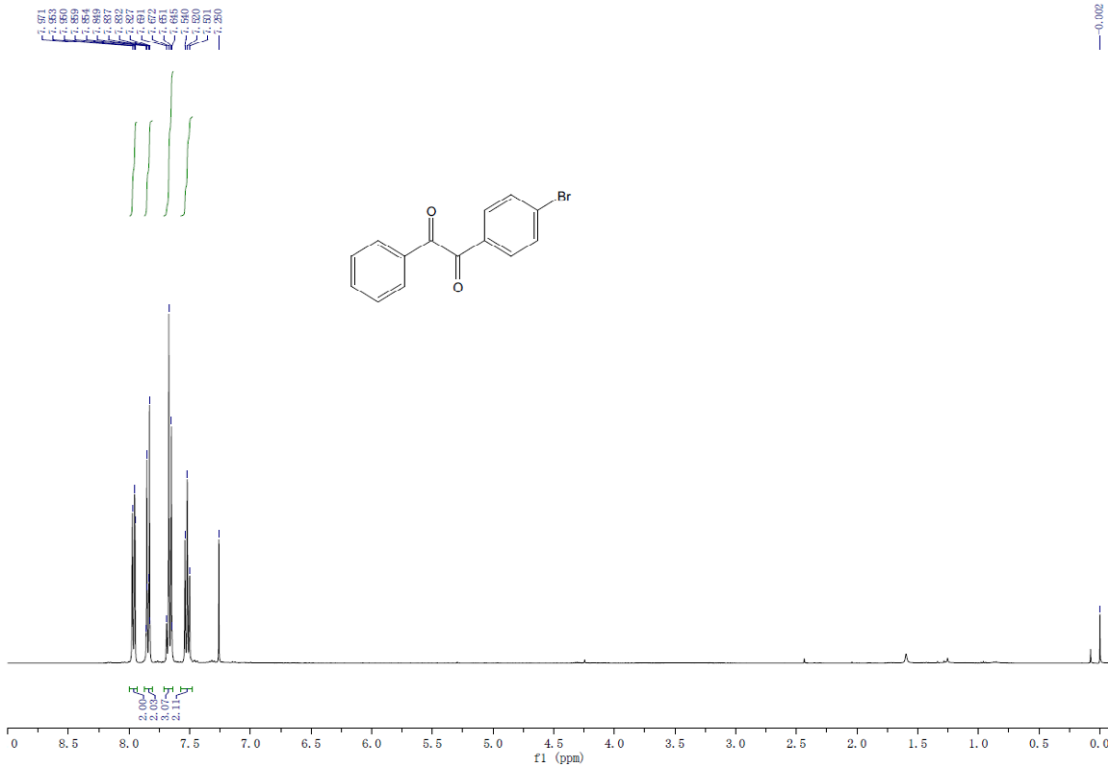

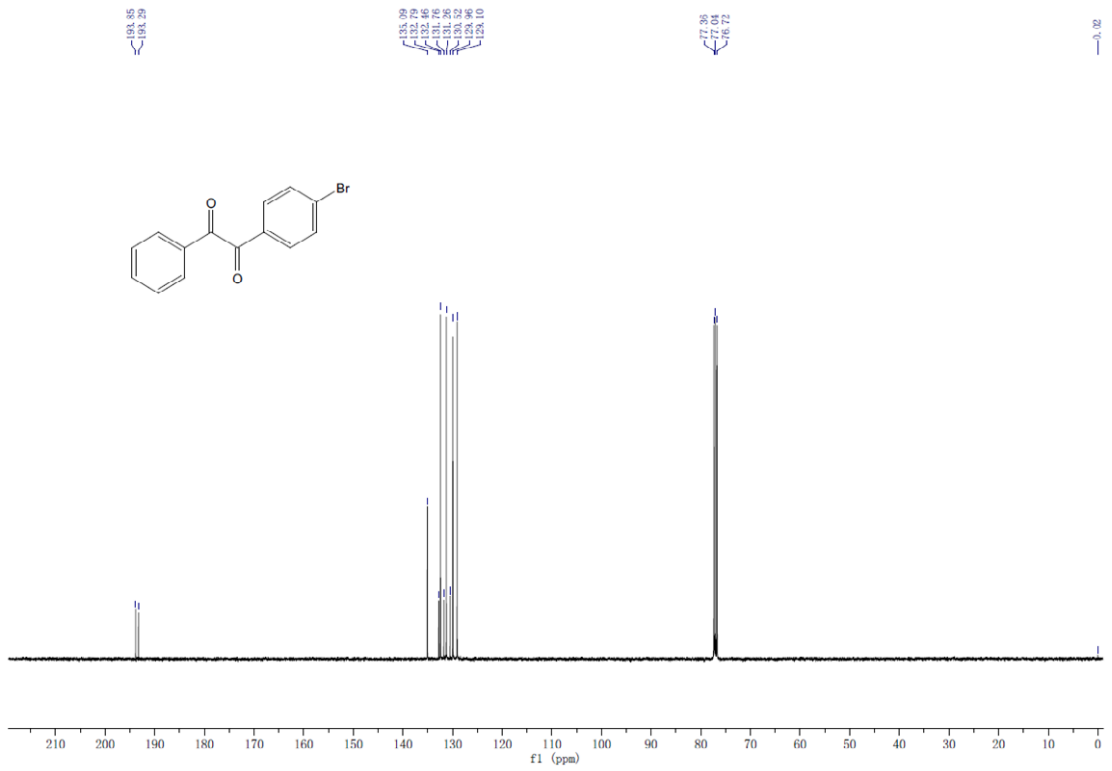

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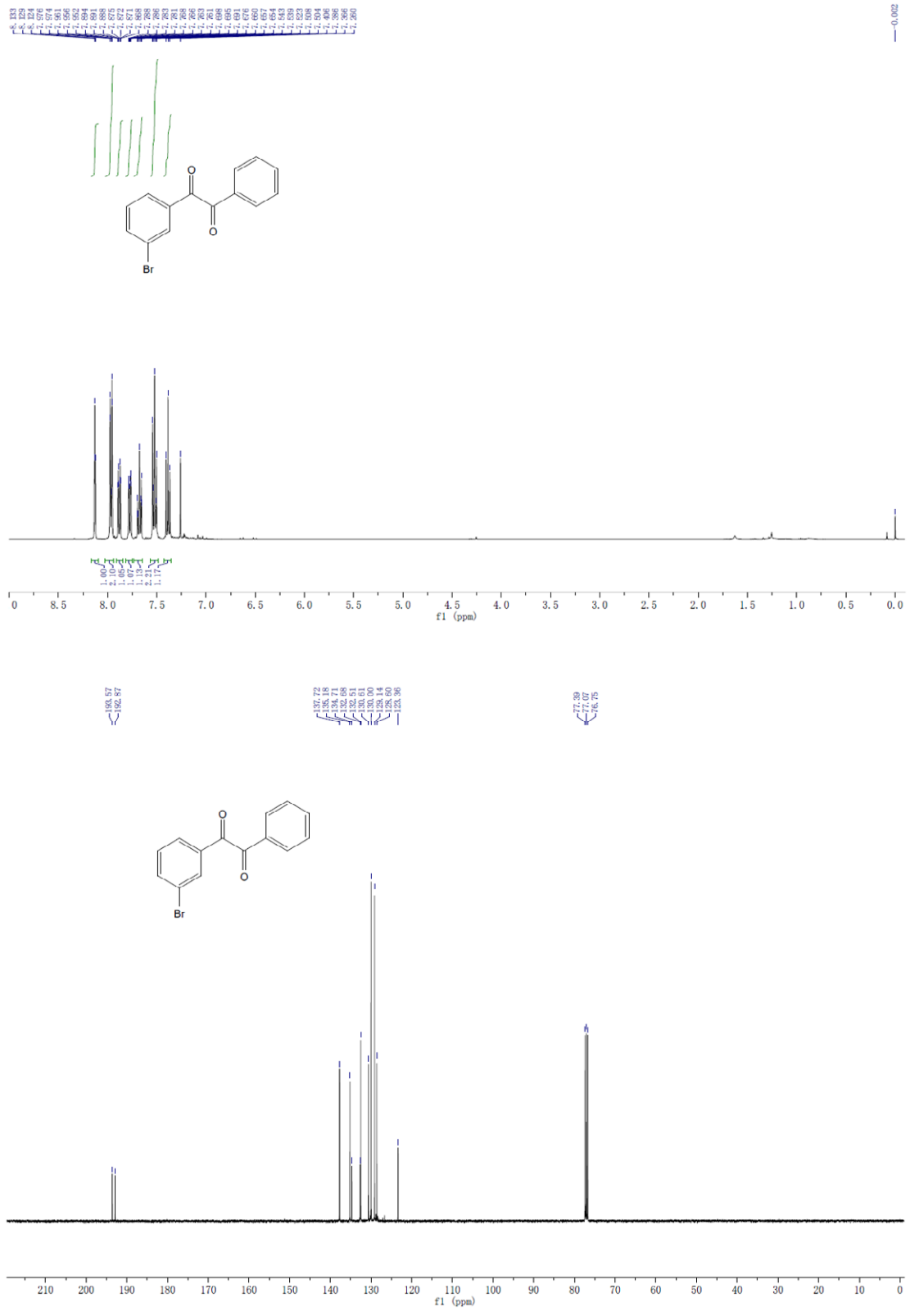

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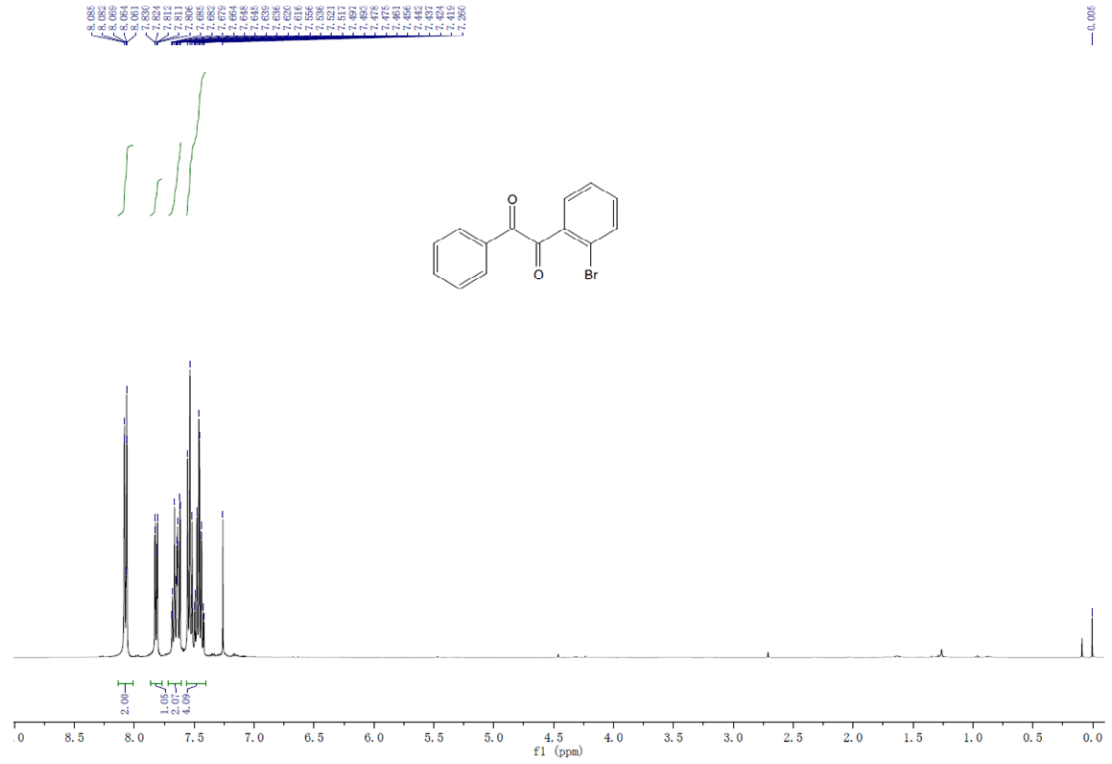

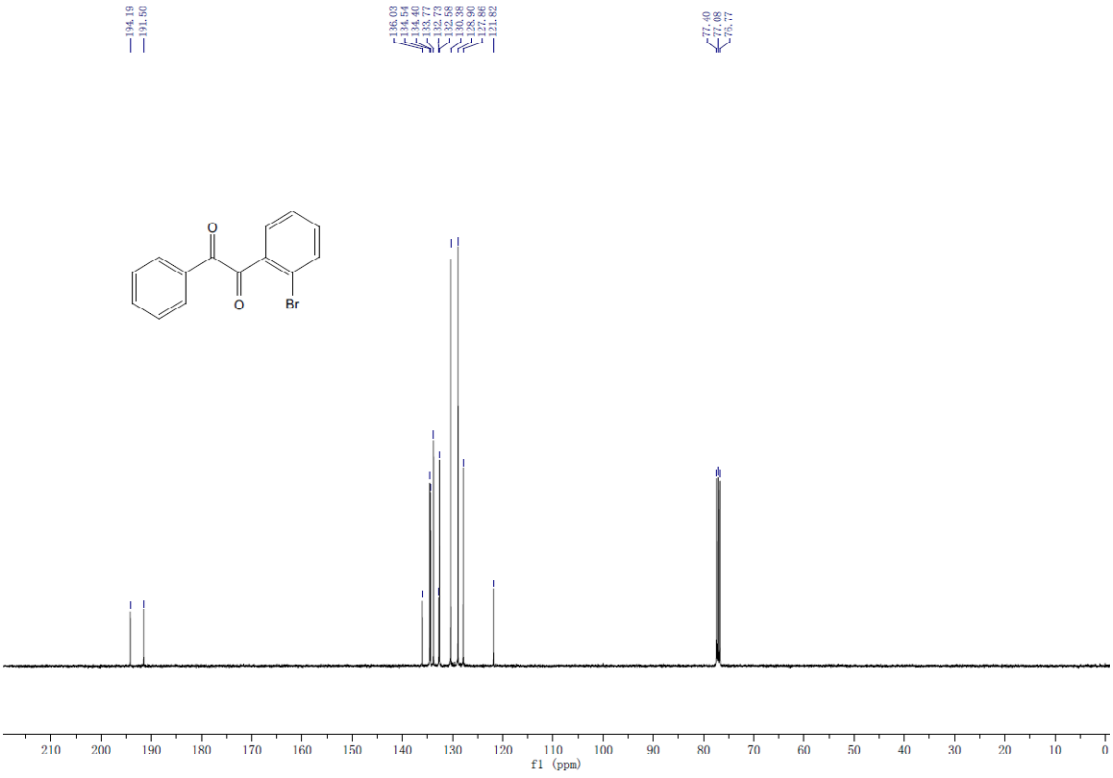

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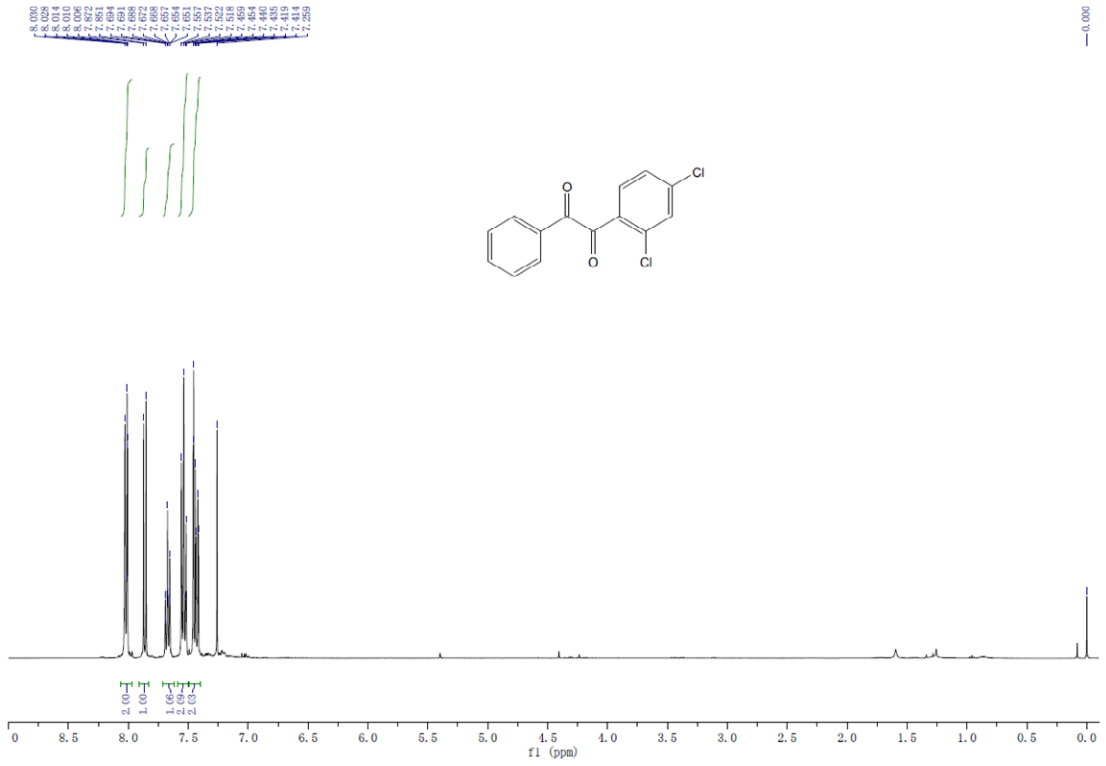

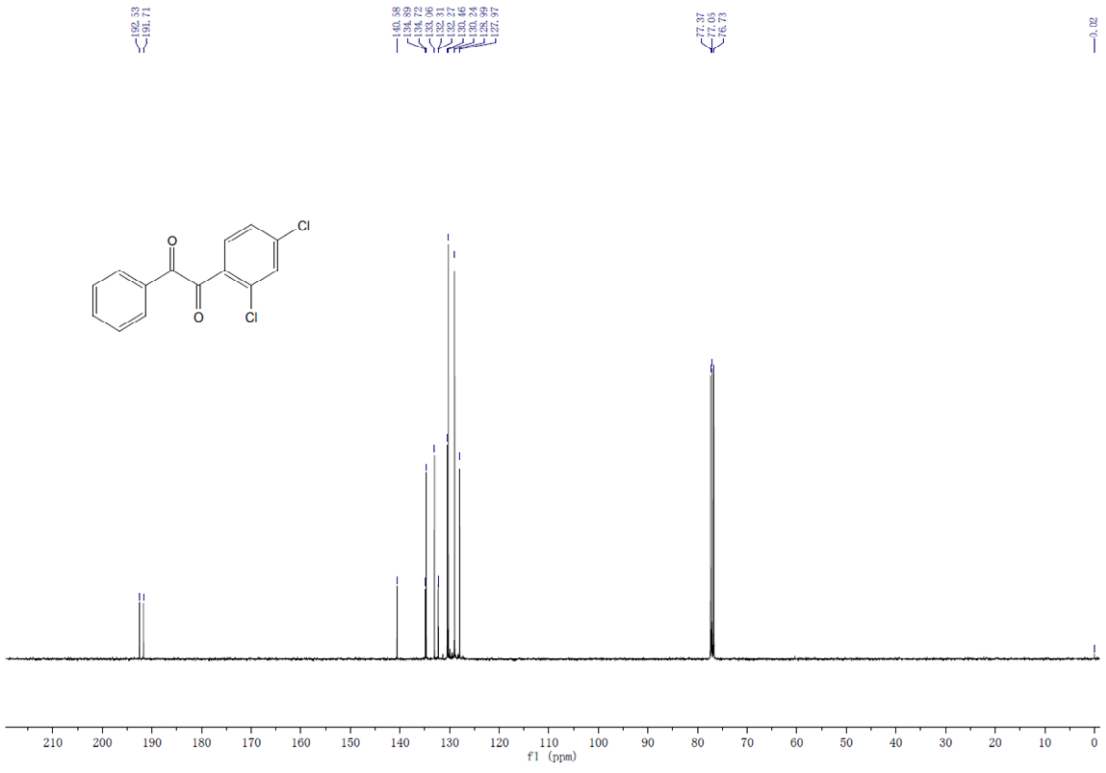

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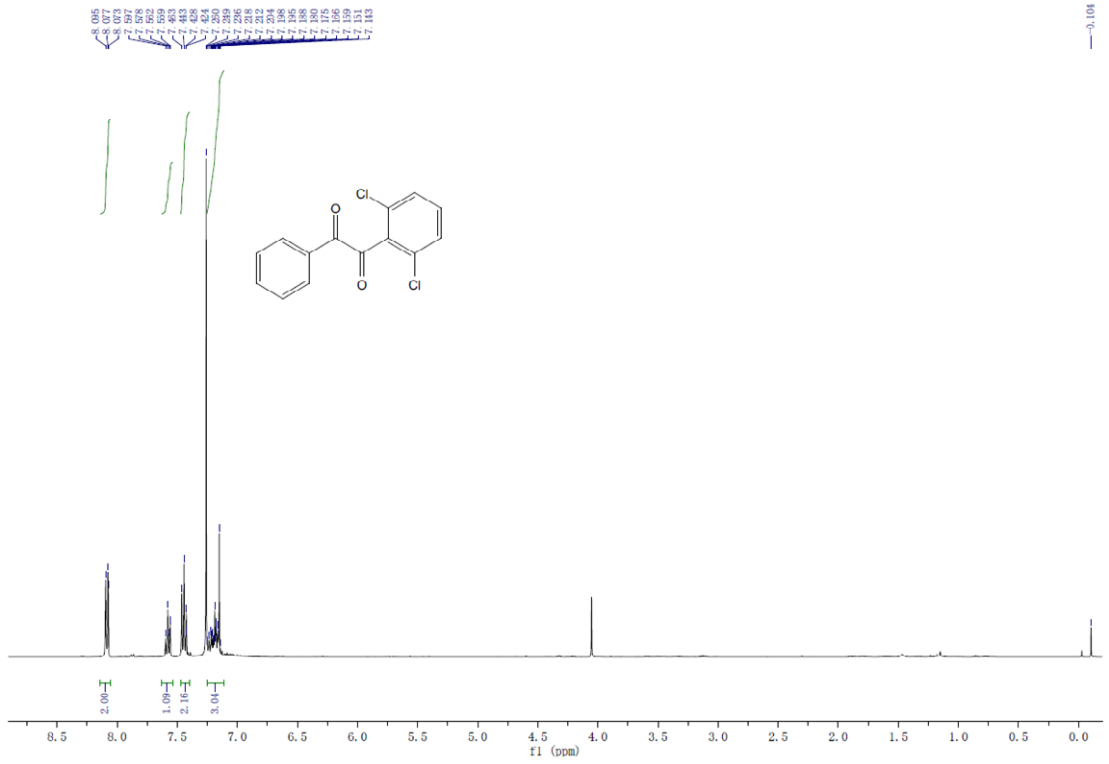

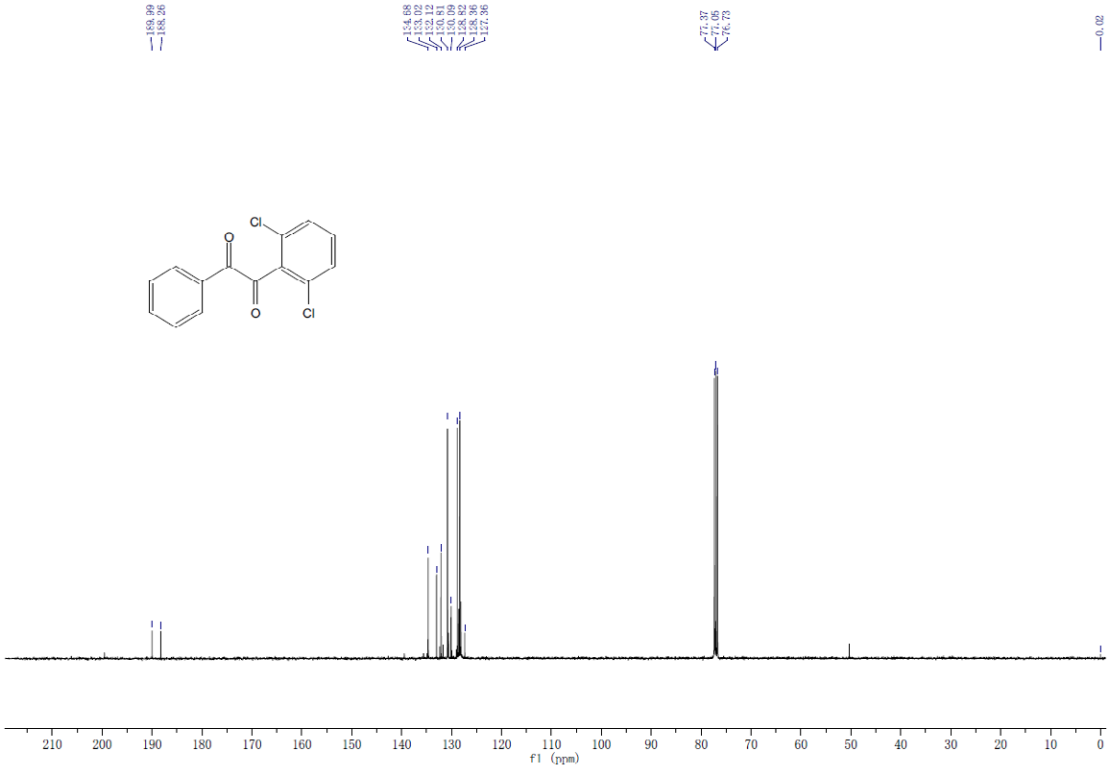

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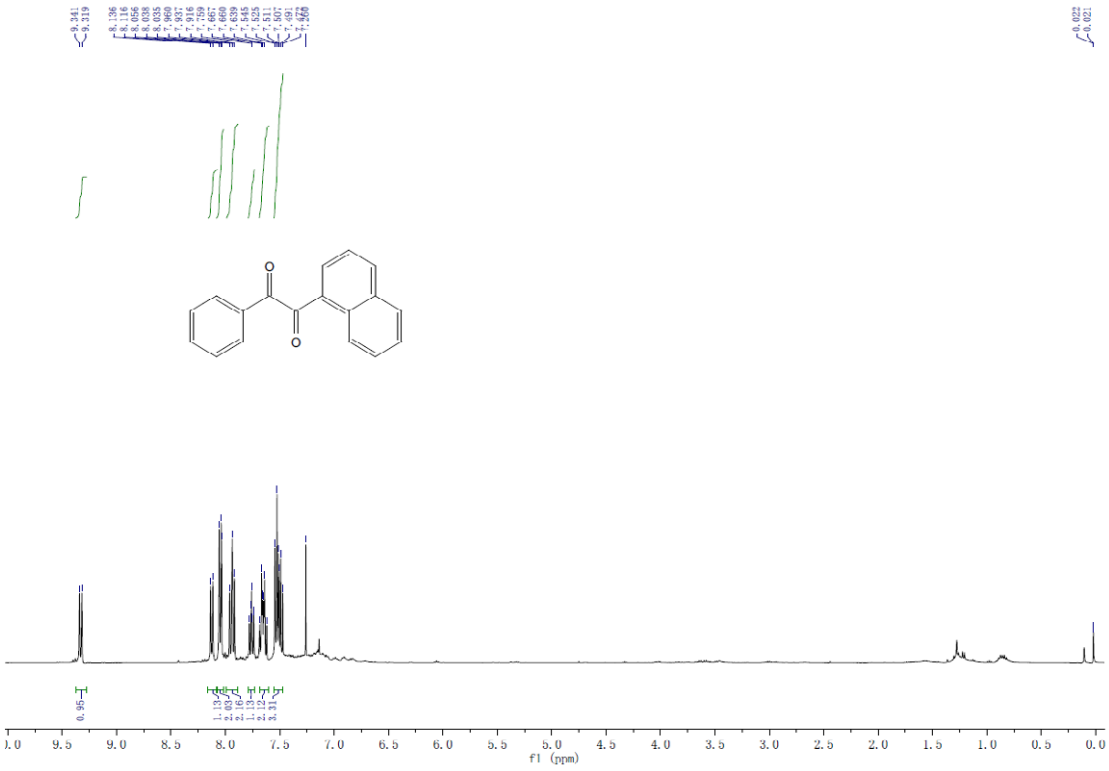

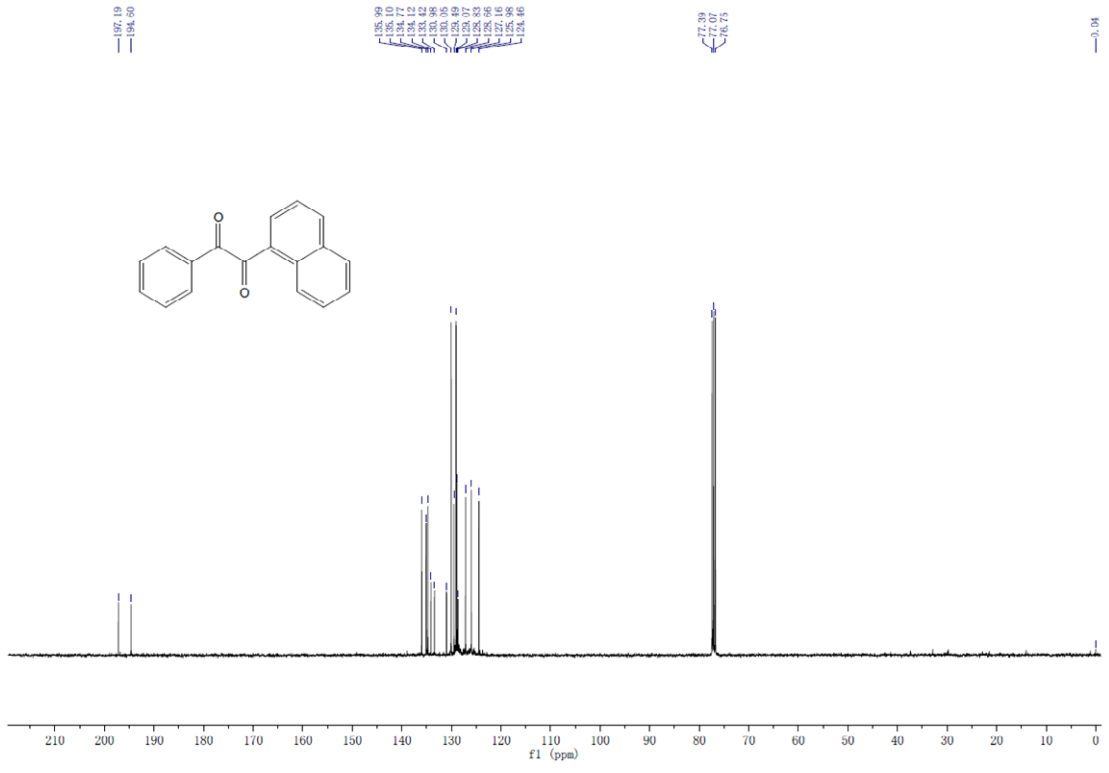

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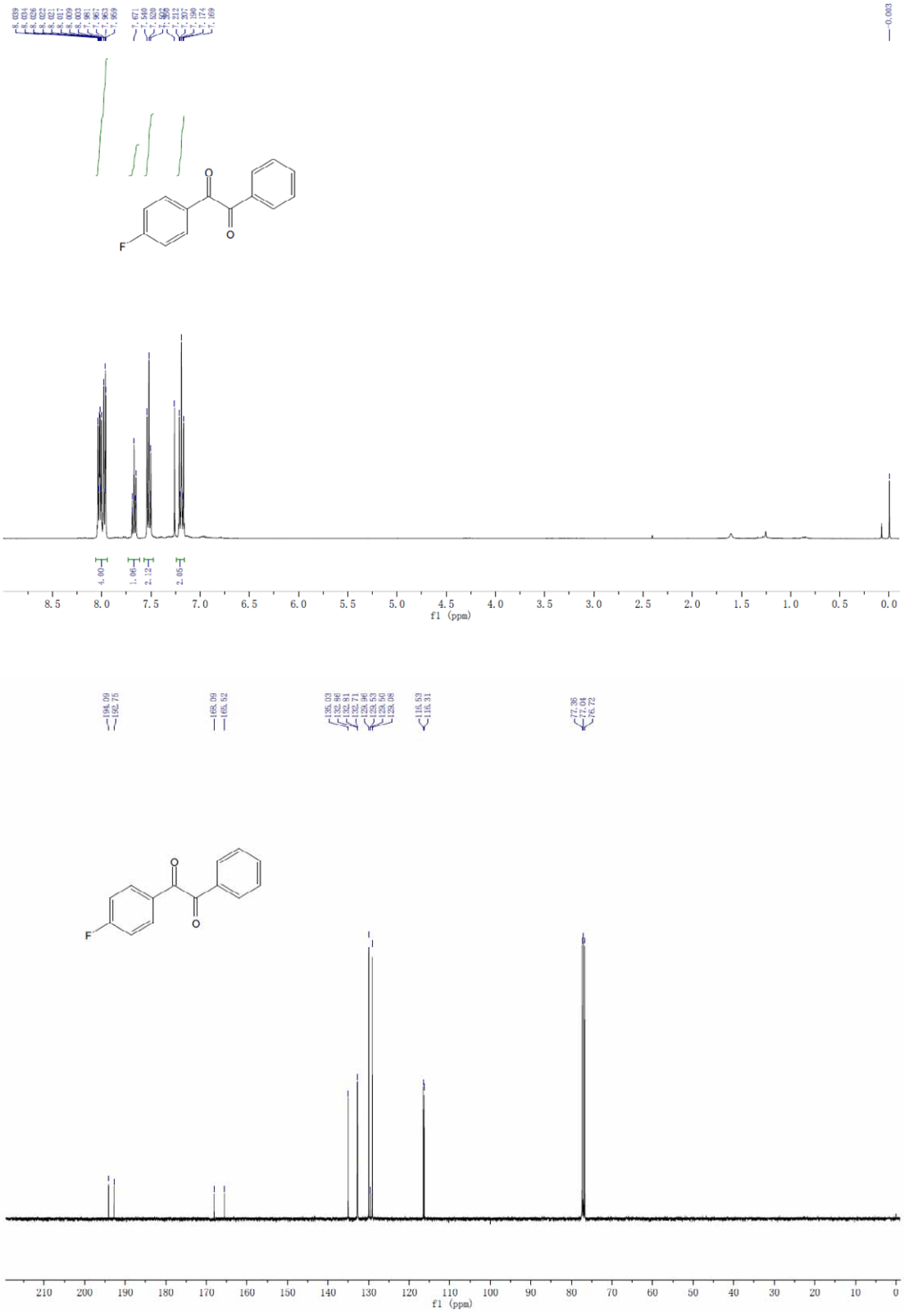

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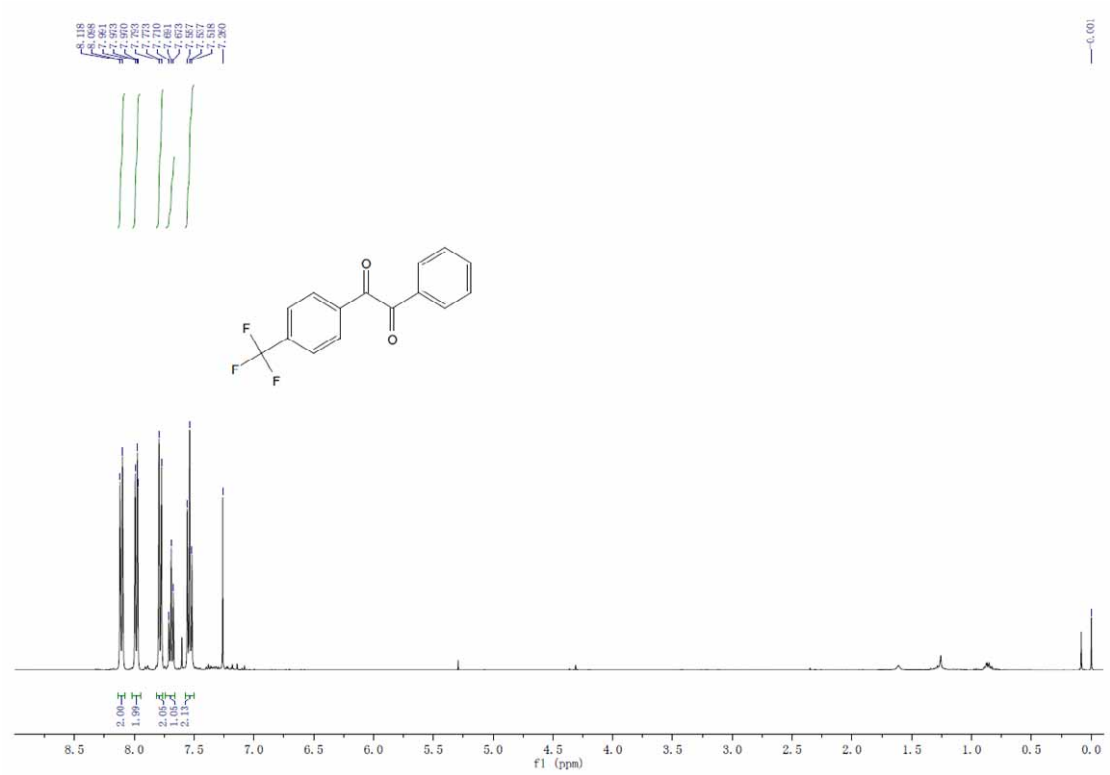
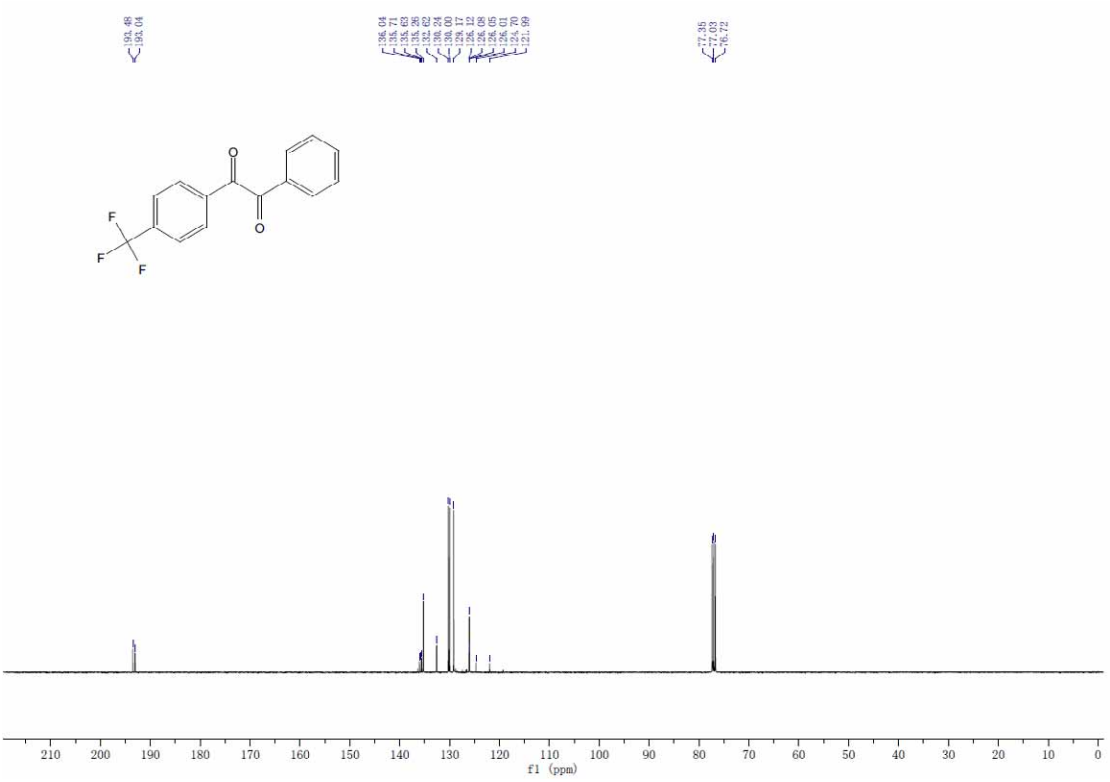
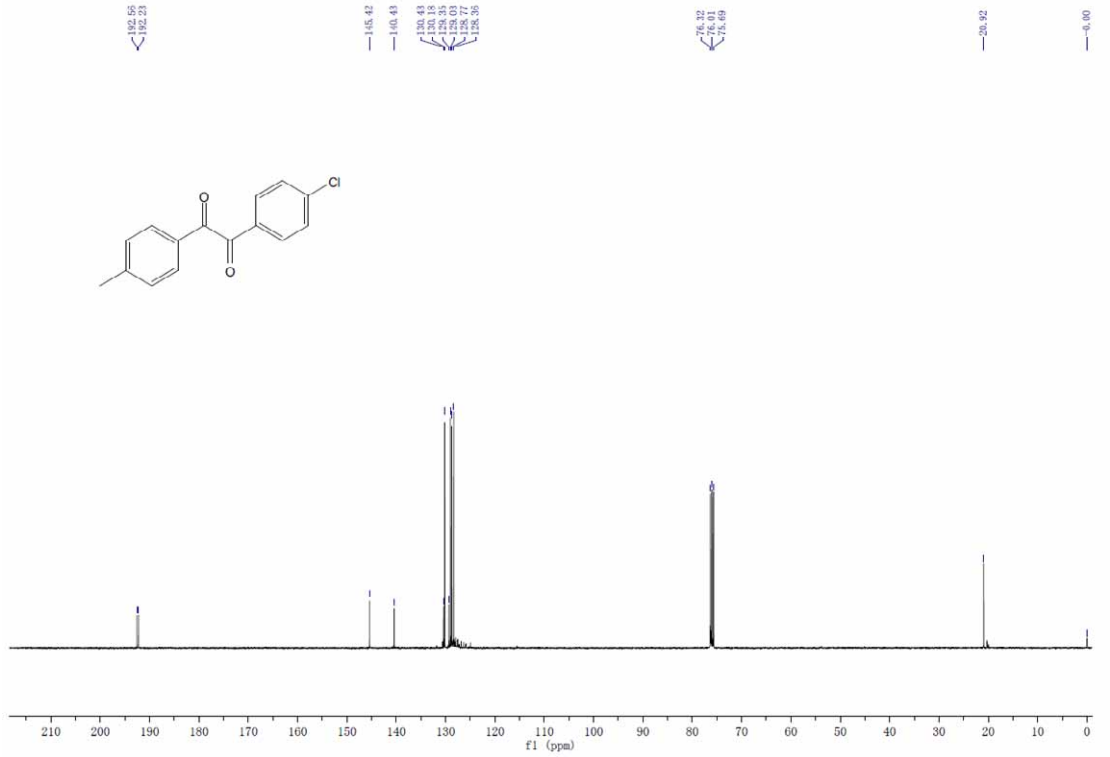




2q



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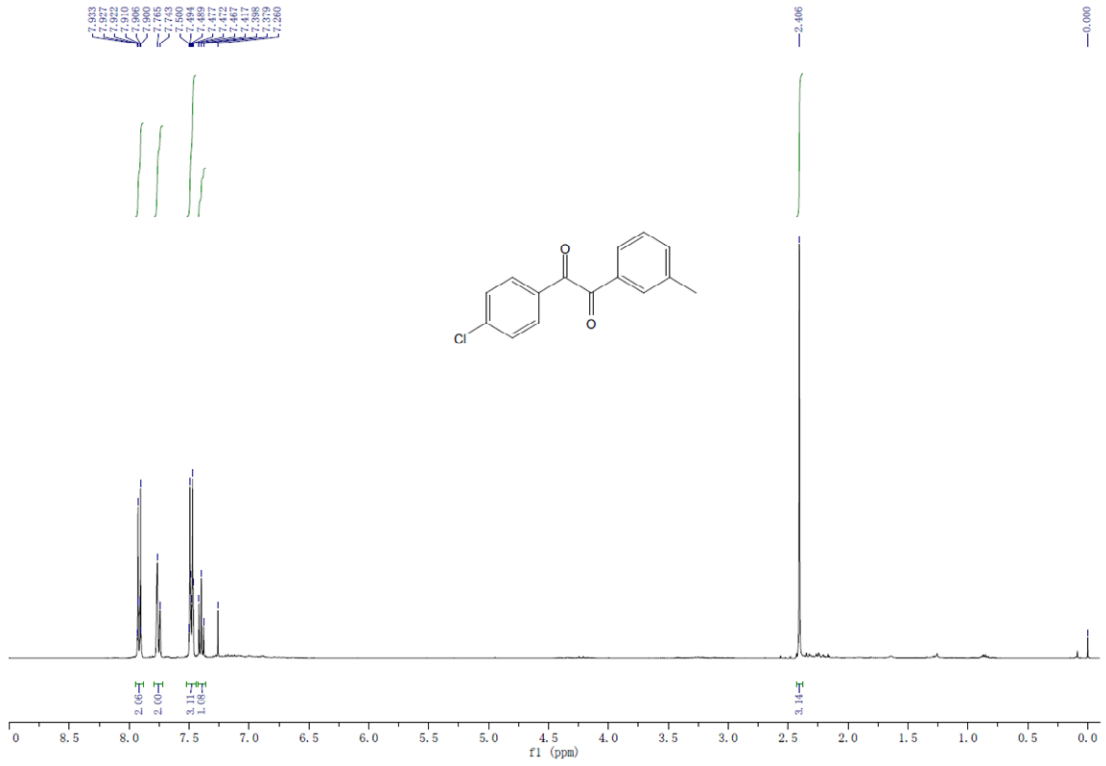

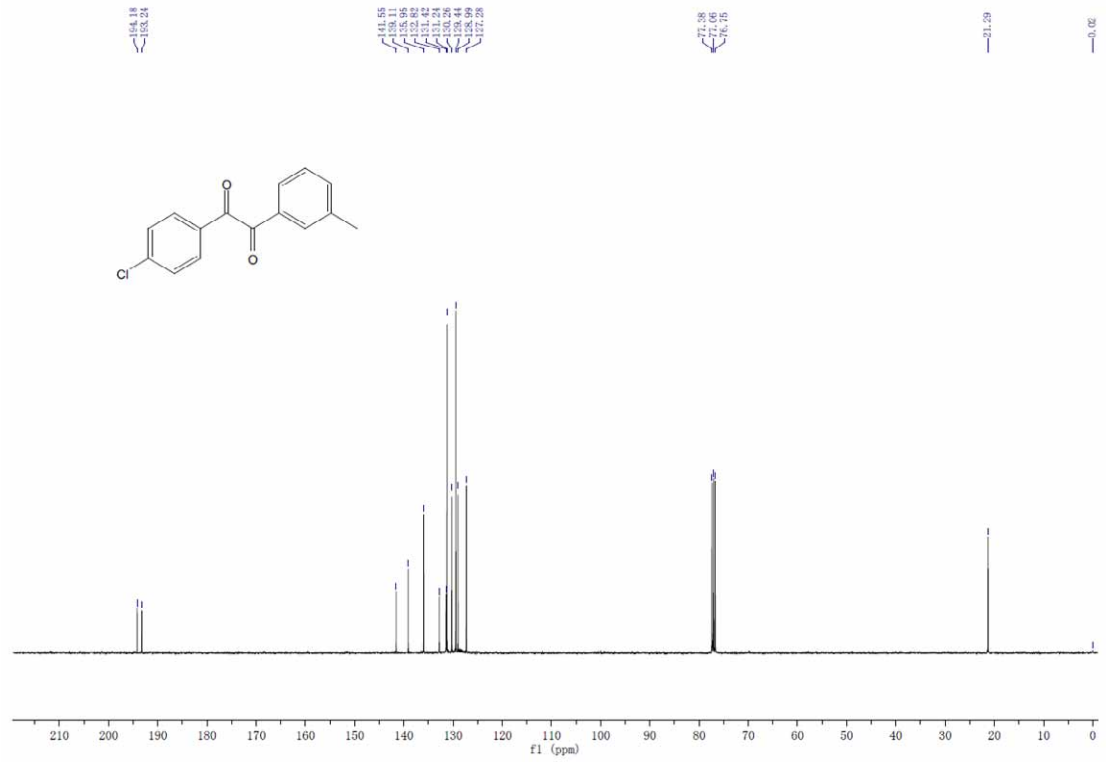

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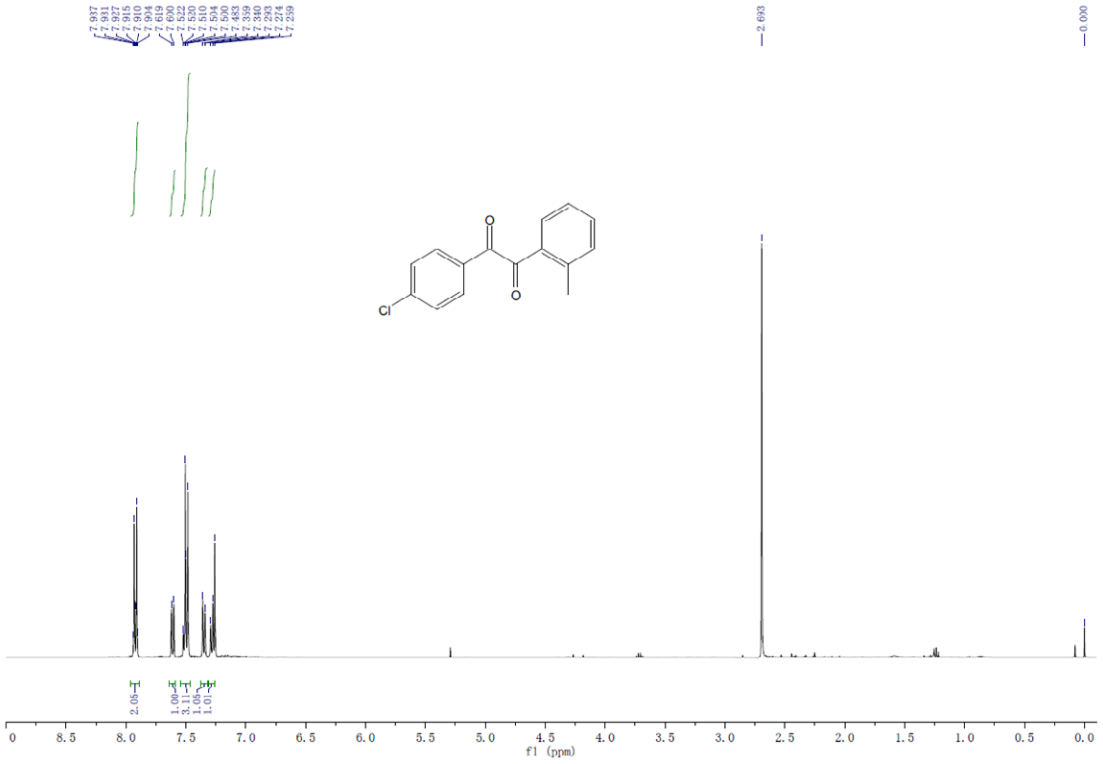

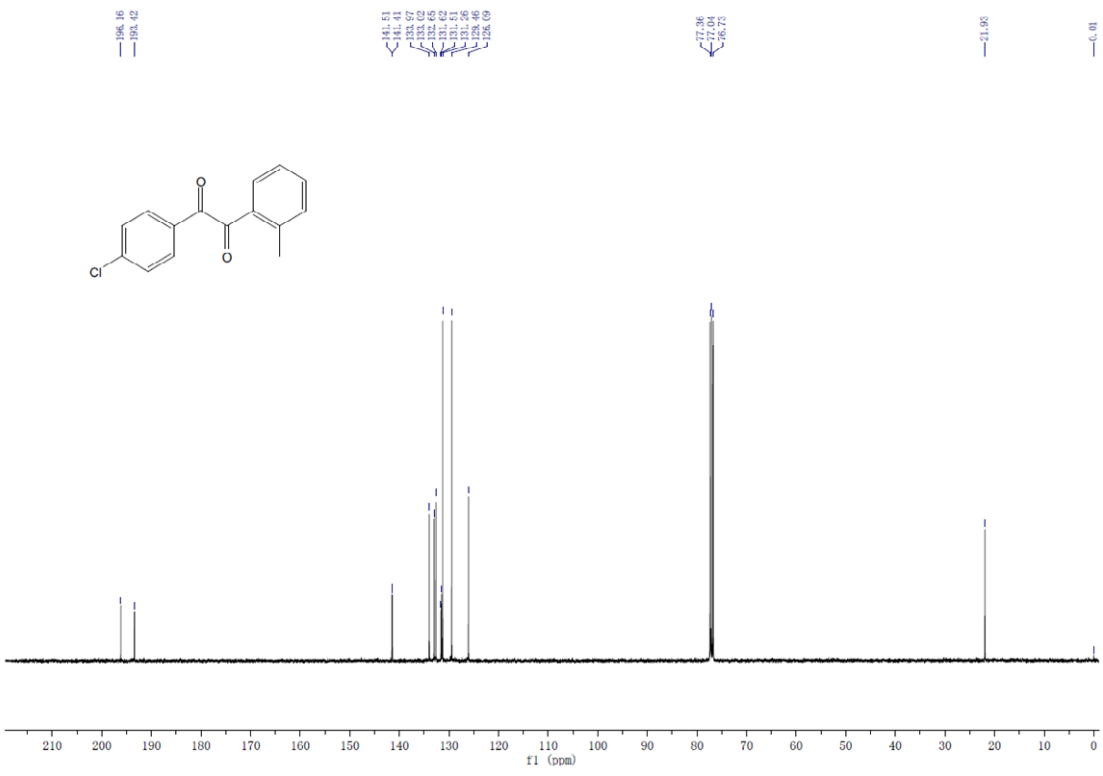

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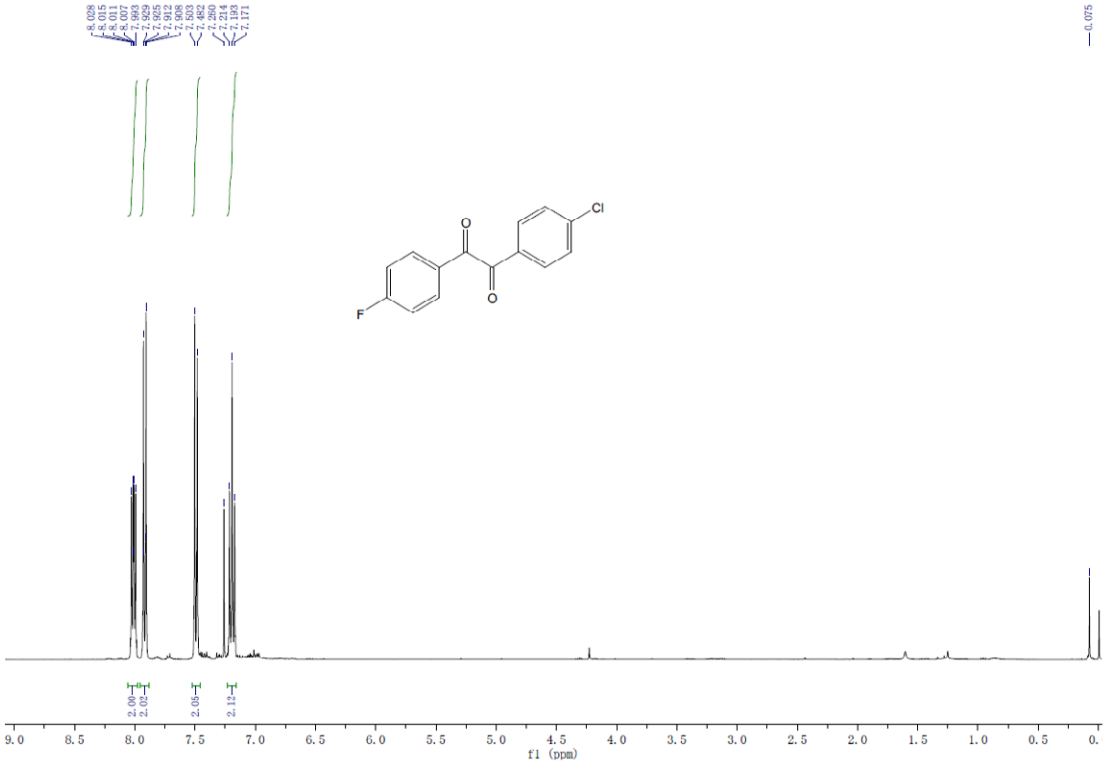

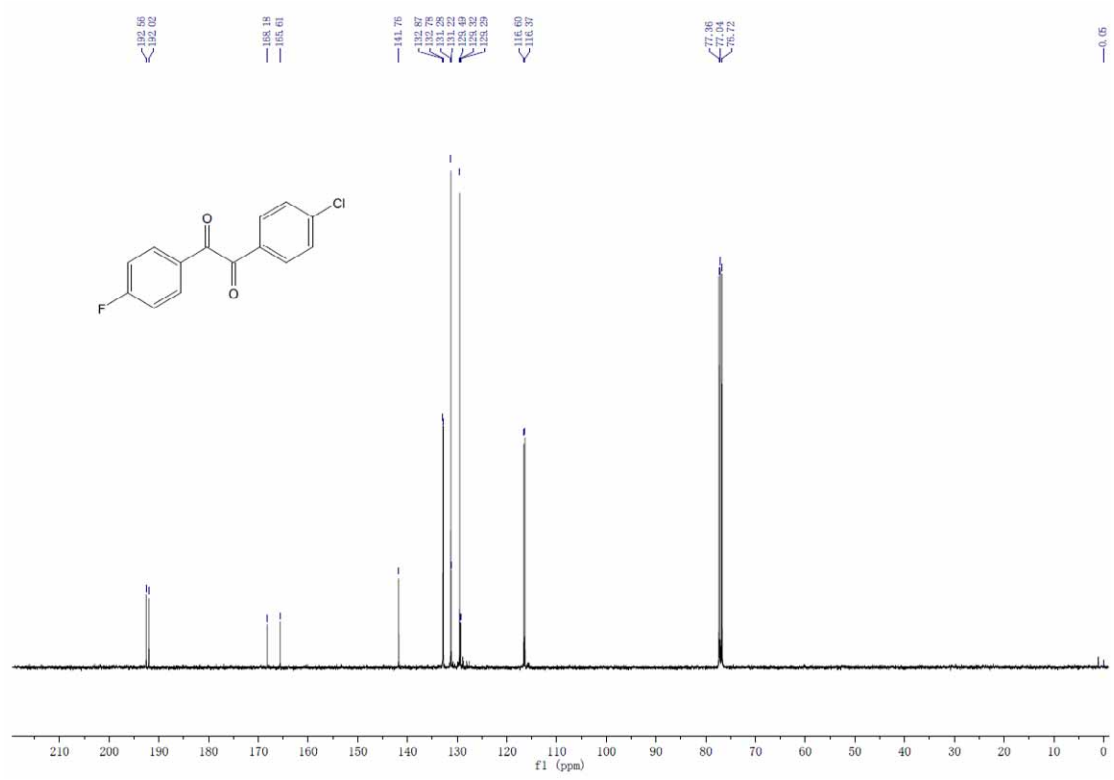

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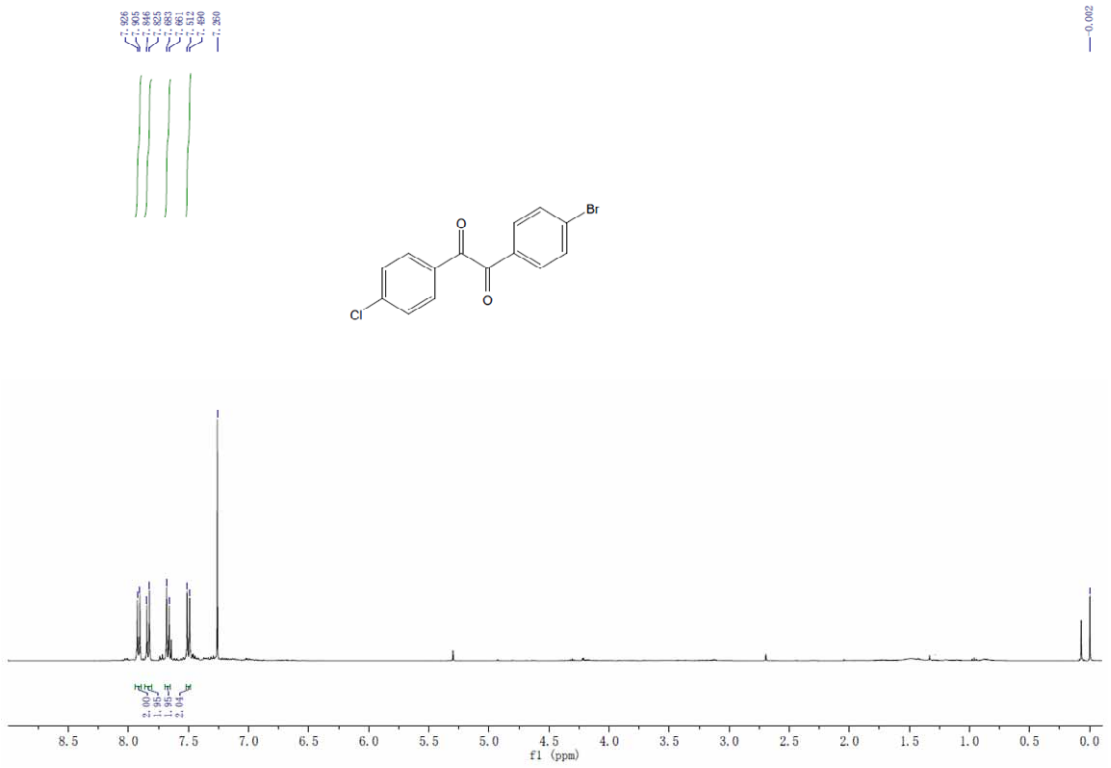
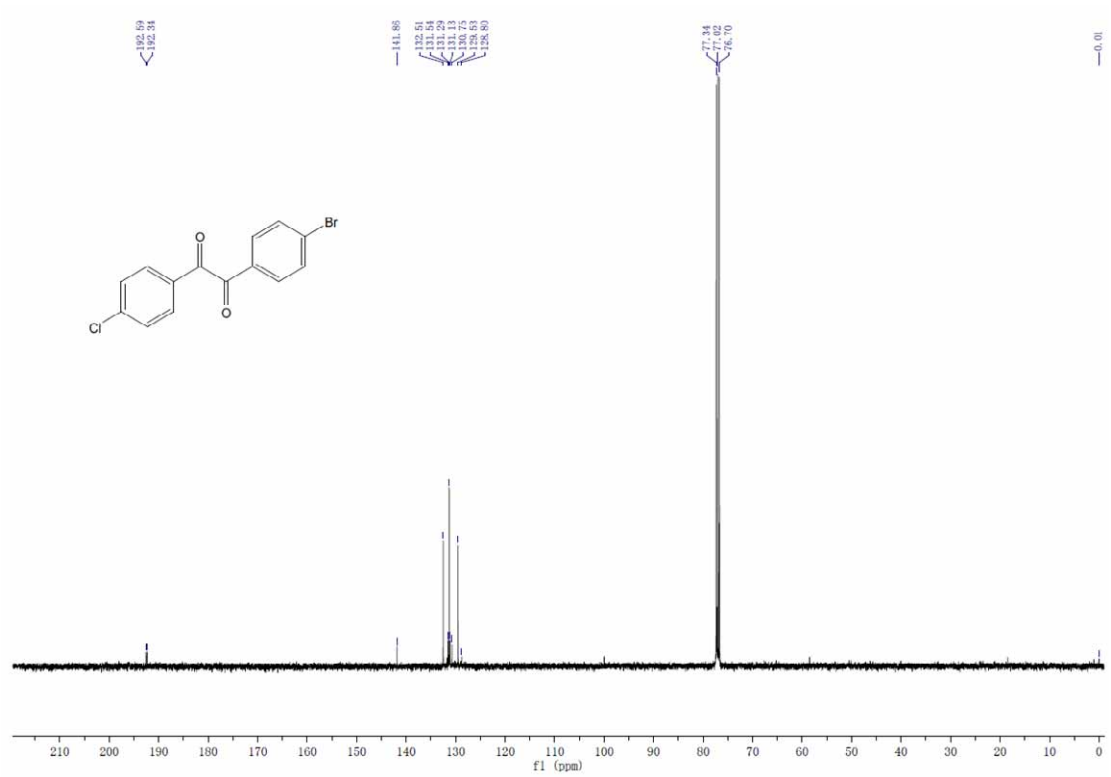
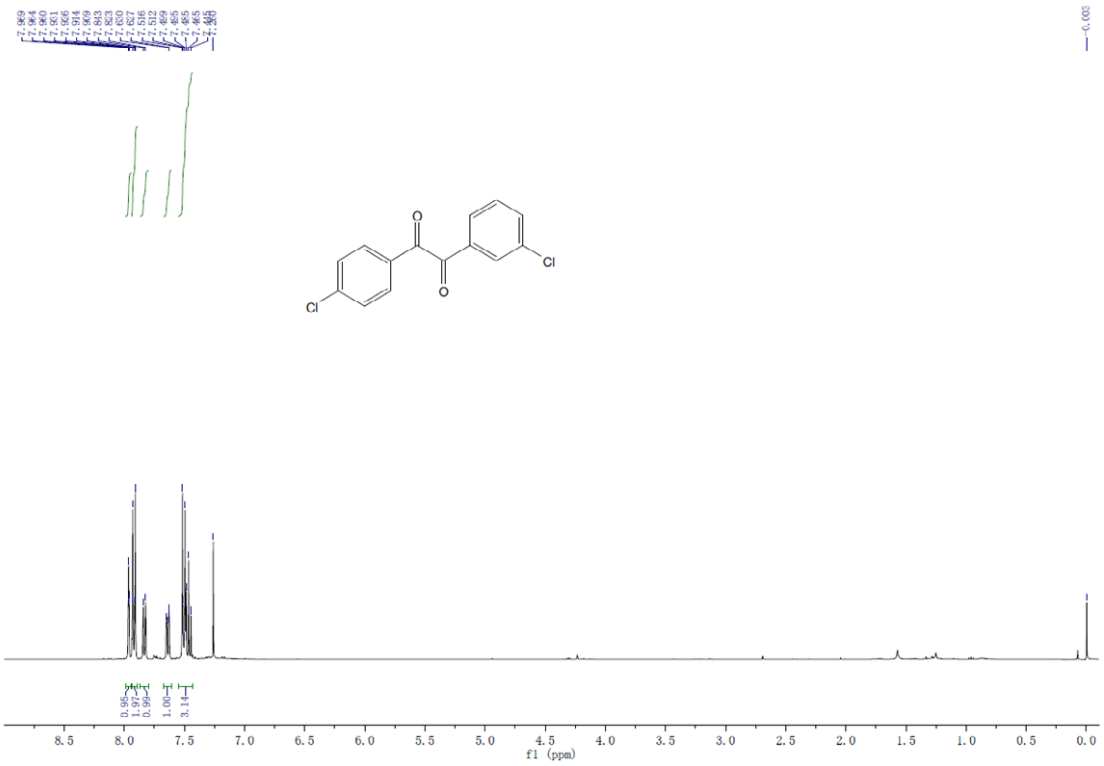




2v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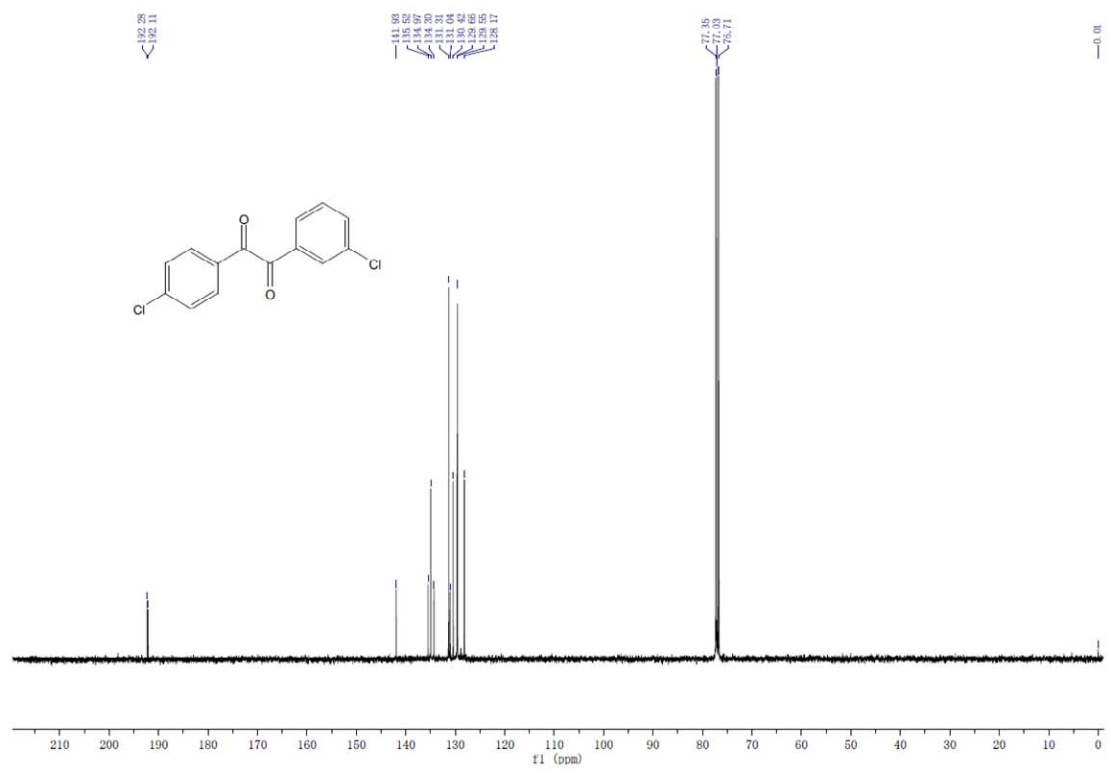
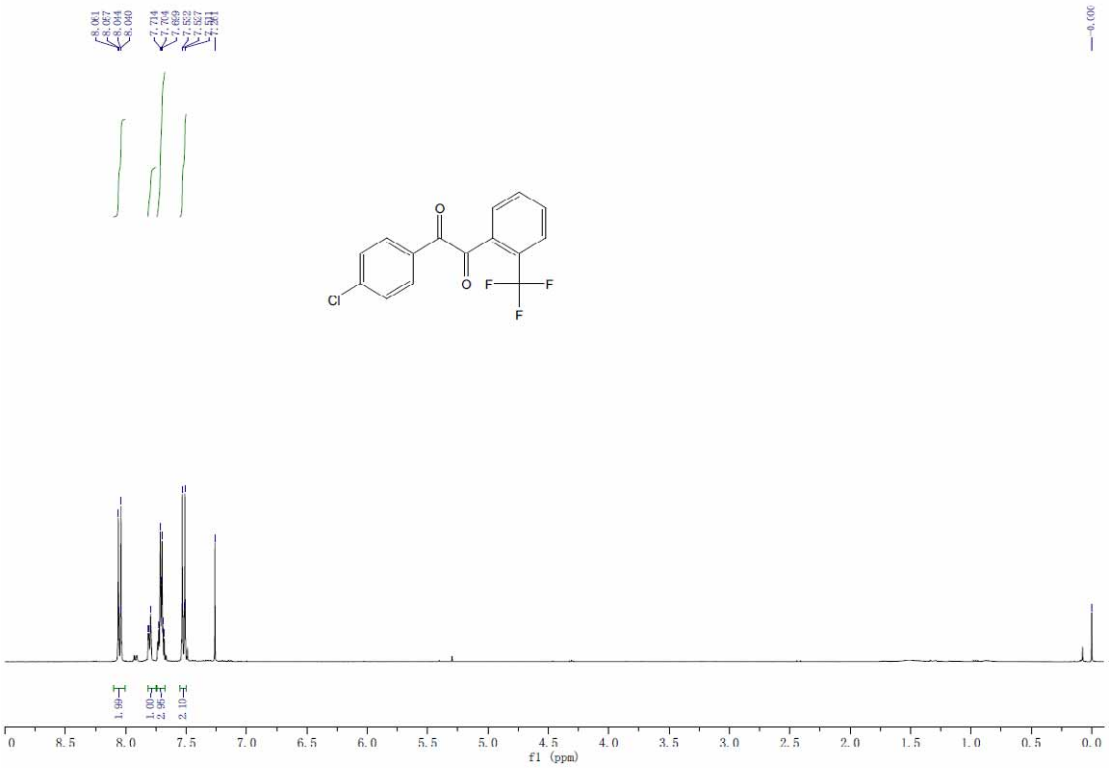
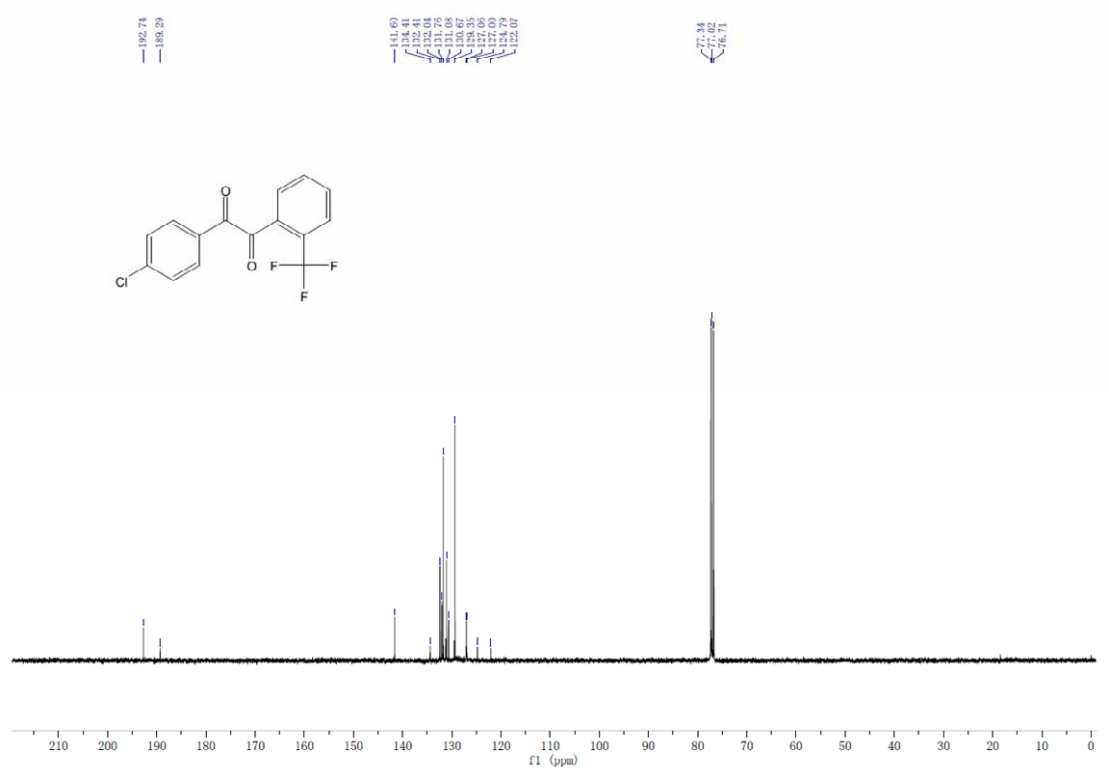
7.964
7.960
7.951
7.926
7.914
7.909
7.863
7.850
7.627
7.516
7.512
7.469
7.465
7.465
6.003
O
O
Cl
Cl
0.95
1.97
0.98
1.00
3.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


192.28
192.11
141.93
135.62
134.97
134.30
131.31
131.04
130.42
129.65
129.55
128.17
77.35
77.03
76.71
0.01
O
O
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2w


8.061
8.057
8.044
8.040
7.714
7.704
7.689
7.552
7.527
7.511
7.501
0.000
O
O
Cl
F
F
F
1.99
1.00
2.96
2.10
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)


192.74
189.29
141.60
135.41
134.44
132.04
131.75
131.08
130.67
129.35
127.06
127.00
125.79
122.07
77.84
77.42
77.00
76.71
O
O
Cl
F
F
F
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)