Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Copper Catalyzed α-C-H Acyloxylation of Carbonyl Compounds with Terminal Alkynes

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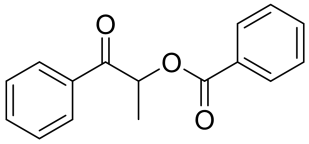
Experimental:

^{1}H and ^{13}CNMR spectra were recorded in $CDCl_3$ on a Bruker AV-400 spectrometer. Chemical shifts for ^{1}H NMR spectra are reported in ppm relative to residual $CDCl_3$ as internal reference (δ 7.26 ppm for ^{1}H) downfield from TMS, chemical shifts for ^{13}C NMR spectra are reported in ppm relative to internal $CDCl_3$ (δ 77.16 ppm for ^{13}C). Coupling constants (J) are given in Hertz (Hz). The terms m, s, d, t, q refer to multiplet, singlet, doublet, triplet, quartlet respectively; br refers to a broad signal.Reagents and solvents used were mostly AR grade. Silica gel coated plates were used for TLC.

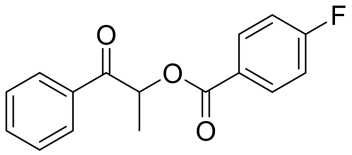
Typical Procedure.

The mixture of carbonyl compounds (0.4 mmol), terminal alkynes (0.2 mmol), $Cu(acac)_2$ (5 mol%), TBHP (4.0 eq) and chlorobenzene (1 ml) was stirred at 120 °C for 12 h. After cooling to r.t., the reaction mixture was washed with aq. $Na_2S_2O_3$ (10 ml), and extracted by ethyl acetate for three times. The obtained top organic layer was dried with anhydrous $MgSO_4$. The mixture was concentrated in vacuo and the residue was purified by column chromatography on silica gel (EA/n-Hexane=5%) to afford pure product.

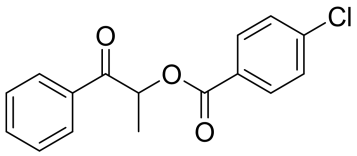
Characteristic Data.



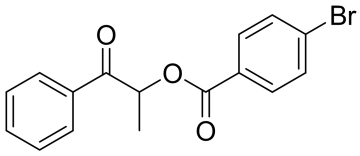
1-oxo-1-phenylpropan-2-yl benzoate (**3aa**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.5 Hz, 2 H), 8.00 (d, *J* = 7.5 Hz, 2 H), 7.58 (q, *J* = 7.2 Hz, 2 H), 7.46 (dt, *J* = 15.8, 7.8 Hz, 4 H), 6.21 (q, *J* = 6.9 Hz, 1 H), 1.67 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR(100 MHz, $CDCl_3$) δ 196.66, 165.92, 134.43, 133.53, 133.18, 129.81, 129.44, 128.74, 128.45, 128.33,, 71.84, 17.09.



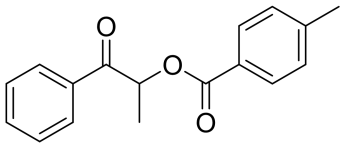
1-oxo-1-phenylpropan-2-yl 4-fluorobenzoate (**3ab**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.05 (m, 2 H), 8.05 – 7.90 (m, 2 H), 7.66 – 7.55 (m, 1 H), 7.49 (t, *J* = 7.6 Hz, 2 H), 7.11 (t, *J* = 8.6 Hz, 2 H), 6.20 (q, *J* = 6.9 Hz, 1 H), 1.67 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, CDCl3) δ 196.72, 167.37, 165.12, 164.84, 134.53, 133.77, 132.64, 132.55, 128.96, 128.62, 125.92, 125.89, 115.82, 115.60, 72.12, 17.34.



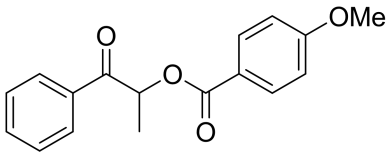
1-oxo-1-phenylpropan-2-yl 4-chlorobenzoate (**3ac**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (q, *J* = 8.0 Hz, 4 H), 7.57 (t, *J* = 7.4 Hz, 1 H), 7.47 (t, *J* = 7.5 Hz, 2 H), 7.40 (d, J = 7.6 Hz, 2 H), 6.19 (q, *J* = 6.9 Hz, 1 H), 1.66 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ196.38, 164.98, 139.63, 134.23, 133.56, 131.15, 128.73, 128.65, 128.37, 72.30, 17.09.



1-oxo-1-phenylpropan-2-yl 4-bromobenzoate (**3ad**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.93 (m, 4 H), 7.57 (d, *J* = 7.4 Hz, 3 H), 7.46 (t, *J* = 7.6 Hz, 2 H), 6.19 (q, *J* = 6.9 Hz, 1 H), 1.65 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, CDCl3) δ 196.40, 165.12, 134.27, 133.63, 131.70, 131.32, 128.79, 128.43, 128.41, 128.35, 72.10, 17.12.

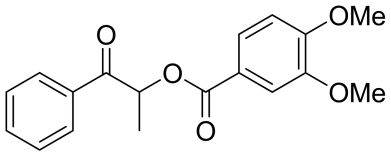


1-oxo-1-phenylpropan-2-yl 4-methylbenzoate (**3ae**). ^{1}H NMR (400 MHz, $CDCl_3$) δ7.99 (t, *J* = 6.9 Hz, 4 H), 7.55 (t, *J* = 7.6 Hz, 1 H), 7.45 (t, *J* = 7.4 Hz, 2 H), 7.21 (d, *J* = 8.4 Hz, 2 H), 6.17 (q, *J* = 6.9 Hz, 1 H), 2.37 (s, 3 H), 1.64 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.76, 165.94, 143.95, 134.42, 133.47, 129.83, 129.23, 128.90, 128.61, 126.88, 71.70, 22.56, 17.11.

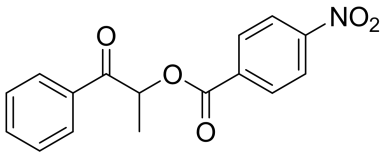


1-oxo-1-phenylpropan-2-yl 4-methoxybenzoate (**3af**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (q, *J* = 8.0 Hz, 4 H), 7.55 (t, *J* = 7.0 Hz, 1 H), 7.45 (t, *J* = 7.8 Hz, 2 H), 6.90 (d, *J* = 8.6 Hz, 2 H), 6.16 (q, *J* = 7.0 Hz, 1 H), 3.81 (s, 3 H), 1.64 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, CDCl3) δ 196.92, 165.57, 163.58, 134.45, 133.43, 131.84, 128.69, 128.41, 121.78, 113.59,

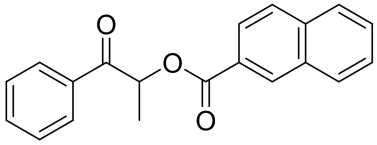
71.55, 55.32, 17.09.



1-oxo-1-phenylpropan-2-yl 3,4-dimethoxybenzoate (**3ag**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.92 (m, 2 H), 7.73 (dd, *J* = 8.4, 1.9 Hz, 1 H), 7.64 – 7.34 (m, 4 H), 6.87 (d, *J* = 8.5 Hz, 1 H), 6.16 (q, *J* = 7.0 Hz, 1 H), 3.91 (s, 3 H), 3.89 (s, 3 H), 1.64 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.96, 165.74, 153.29, 148.61, 134.52, 133.51, 128.75, 128.48, 124.02, 121.90, 112.13, 110.25, 71.72, 56.01, 55.96, 17.16.

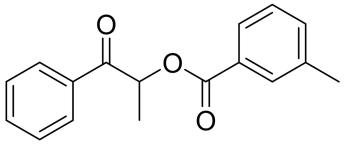


1-oxo-1-phenylpropan-2-yl 4-nitrobenzoate (**3ah**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.15 (m, 4 H), 7.99 (d, *J* = 7.8 Hz, 2 H), 7.62 (t, *J* = 7.4 Hz, 1 H), 7.50 (t, *J* = 7.6 Hz, 2 H), 6.25 (q, *J* = 7.0 Hz, 1 H), 1.70 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.94, 164.09, 150.70, 134.90, 134.11, 133.84, 130.96, 130.96, 128.90, 128.45, 123.53, 72.78, 17.25.

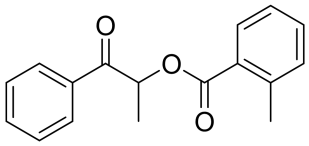


1-oxo-1-phenylpropan-2-yl 2-naphthoate (**3ai**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1 H), 8.17 – 7.77 (m, 6 H), 7.68 – 7.38 (m, 5 H), 6.27 (q, *J* = 6.9 Hz, 1 H), 1.72 (d, *J* = 7.0

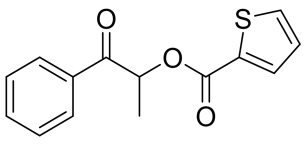
Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.79, 166.12, 135.68, 134.50, 133.58, 132.43, 131.50, 129.41, 128.80, 128.65, 128.53, 128.38, 128.19, 127.76, 126.72, 126.66, 125.30 , 72.01, 17.27.



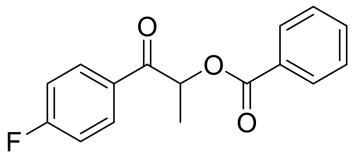
1-oxo-1-phenylpropan-2-yl 3-methylbenzoate (**3aj**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 2 H), 7.89 (d, *J* = 8.8 Hz, 2 H), 7.55 (t, *J* = 7.2 Hz, 1 H), 7.45 (t, *J* = 7.6 Hz, 2 H), 7.37 – 7.29 (m, 2 H), 6.19 (q, *J* = 6.9 Hz, 1 H), 2.37 (s, 3 H), 1.66 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.70, 166.05, 138.11, 134.42, 133.96, 133.50, 130.27, 129.38, 128.70, 128.42, 128.23, 126.94, 71.82, 21.12, 17.10.



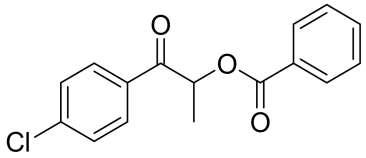
1-oxo-1-phenylpropan-2-yl 2-methylbenzoate (**3ak**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (t, *J* = 7.2 Hz, 3 H), 7.56 (t, *J* = 7.2 Hz, 1 H), 7.46 (t, *J* = 7.4 Hz, 2 H), 7.38 (t, *J* = 7.6 Hz, 1 H), 7.23 (t, *J* = 9.2 Hz, 2 H), 6.19 (q, *J* = 6.9 Hz, 1 H), 2.59 (s, 3 H), 1.64 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.83, 166.85, 140.41, 134.41, 133.55, 132.36, 131.63, 130.85, 128.88, 128.79, 128.44, 125.73, 71.70, 21.65, 17.13.



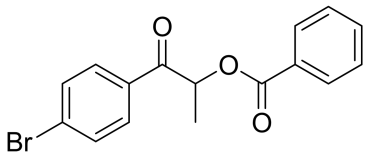
1-oxo-1-phenylpropan-2-yl thiophene-2-carboxylate (**3al**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.91 (m, 2 H), 7.91 – 7.75 (m, 1 H), 7.69 – 7.51 (m, 2 H), 7.46 (t, *J* = 7.6 Hz, 2 H), 7.14 – 7.02 (m, 1 H), 6.14 (q, *J* = 7.0 Hz, 1 H), 1.64 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.48, 161.52, 134.37, 134.10, 133.58, 132.87, 129.00, 128.78, 128.51, 127.81, 77.39, 77.07, 76.75, 72.13, 17.18.



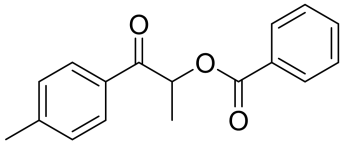
1-(4-fluorophenyl)-1-oxopropan-2-yl benzoate (**3ba**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 - 8.04 (m, 4 H), 7.60 (t, *J* = 7.2 Hz, 1 H), 7.47 (t, *J* = 7.6 Hz, 2 H), 7.18 (t, *J* = 8.0 Hz, 2 H), 6.17 (q, *J* = 7.0 Hz, 1 H), 1.69 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.22, 167.15, 165.97, 164.67, 133.35, 131.27, 131.17, 130.86, 130.83, 129.84, 129.37, 128.41, 116.09, 115.89, 71.75, 17.10.



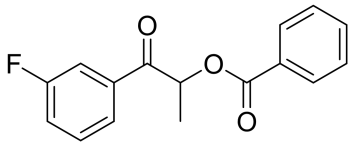
1-(4-chlorophenyl)-1-oxopropan-2-yl benzoate (**3ca**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.8 Hz, 2 H), 7.95 (d, *J* = 8.0 Hz, 2 H), 7.58 (t, *J* = 7.2 Hz, 1 H), 7.45 (t, *J* = 7.0 Hz, 4 H), 6.14 (q, *J* = 6.9 Hz, 1 H), 1.66 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.69, 165.94, 139.97, 133.37, 132.73, 129.94, 129.80, 129.31, 128.39, 71.84, 17.01.



1-(4-bromophenyl)-1-oxopropan-2-yl benzoate (**3da**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.0 Hz, 2 H), 7.86 (d, *J* = 7.8 Hz, 2 H), 7.67 - 7.55 (m, 3 H), 7.45 (t, *J* = 7.6 Hz, 2 H), 6.12 (q, *J* = 6.9 Hz, 1 H), 1.66 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.82, 165.90, 133.40, 133.18, 132.12, 130.00, 129.84, 129.31, 128.44, 71.83, 17.04.

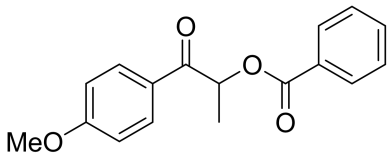


1-oxo-1-(p-tolyl)propan-2-yl benzoate (**3ea**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.8 Hz, 2 H), 7.93 (d, *J* = 7.6 Hz, 2 H), 7.60 (t, *J* = 7.6 Hz, 1 H), 7.46 (t, *J* = 7.8 Hz, 2 H), 7.30 (d, *J* = 7.9 Hz, 2 H), 6.21 (q, *J* = 6.9 Hz, 1 H), 2.43 (s, 3 H), 1.68 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.13, 165.94, 144.37, 133.16, 131.80, 129.79, 129.53, 129.41, 128.57, 128.29, 71.83, 21.60, 17.18.

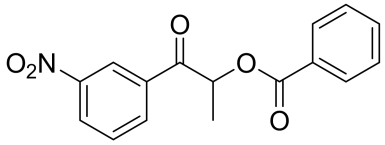


1-(3-fluorophenyl)-1-oxopropan-2-yl benzoate (**3ga**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.8 Hz, 2 H), 7.80 (d, *J* = 7.8 Hz, 1 H), 7.71 (d, *J* = 9.6 Hz, 1 H), 7.60 (t, *J* = 7.6 Hz, 1 H), 7.49 - 7.45 (m, 3 H), 7.34 - 7.28 (m, 1 H), 6.14 (q, *J* = 6.9 Hz, 1 H), 1.68 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.71, 165.94, 164.07, 161.63, 161.21,

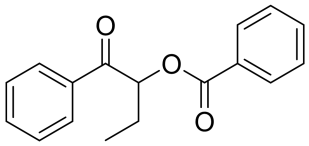
133.34, 130.57, 130.48, 129.84, 129.26, 128.37, 124.20, 120.48, 115.45, 115.21, 71.87, 17.08.



1-(4-methoxyphenyl)-1-oxopropan-2-yl benzoate (**3fa**). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.09 – 8.10 (m, 2 H), 7.99 (d, *J* = 6.4 Hz, 2 H), 7.57 (t, *J* = 4.8 Hz, 1 H), 7.44 (t, *J* = 4.8 Hz, 1 H), 6.95 (t, *J* = 6.0 Hz, 2 H), 6.18 (q, *J* = 4.8 Hz, 1 H), 3.87 (s, 3 H), 1.66 (d, *J* = 4.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.11, 165.96, 163.95, 133.27, 130.85, 129.86,129.63, 128.38, 127.22, 114.06, 71.79, 55.51, 17.41.

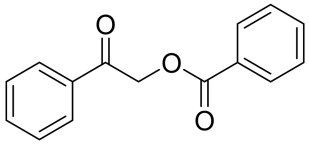


1-(3-nitrophenyl)-1-oxopropan-2-yl benzoate (**3ha**). ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1 H), 8.45 (d, *J* = 8.1 Hz, 1 H), 8.32 (d, *J* = 7.8 Hz, 1 H), 8.08 (d, *J* = 7.8 Hz, 2 H), 7.71 (t, *J* = 7.9 Hz, 1 H), 7.60 (t, *J* = 7.4 Hz, 1 H), 7.46 (t, *J* = 7.2 Hz, 2 H), 6.13 (q, *J* = 6.9 Hz, 1 H), 1.71 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.08, 165.98, 133.57, 130.05, 129.87, 129.69, 128.97, 128.44, 127.70, 123.30, 72.10, 16.99.

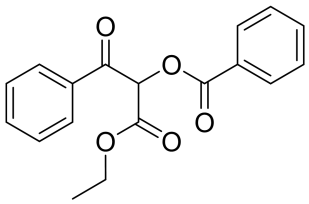


1-oxo-1-phenylbutan-2-yl benzoate (**3ia**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 7.4 Hz, 2 H), 8.00 (d, *J* = 7.8 Hz, 2 H), 7.59 - 7.56 (m, 2 H), 7.49 - 7.42 (m, 4 H), 6.06 (t,

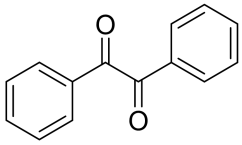
J = 5.4 Hz, 1 H), 2.14 - 1.99 (m, 2 H), 1.11 (t, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.33, 166.14, 134.90, 133.52, 133.25, 129.80, 129.01, 128.79, 128.40, 128.37, 24.91, 9.93.



2-oxo-2-phenylethyl benzoate (**3ja**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 - 8.12 (m, 2 H), 7.99 – 7.97 (m, 2 H), 7.66 - 7.58 (m, 2 H), 7.54 - 7.46 (m, 4 H), 5.59 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.28, 166.26, 134.04, 133.53, 130.45, 130.15, 129.05, 128.76, 128.65, 127.98, 66.65.

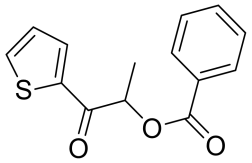


1-ethoxy-1,3-dioxo-3-phenylpropan-2-yl benzoate (**3ka**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (t, *J* = 9.0 Hz, 4 H), 7.67 - 7.60 (m, 2 H), 7.55 - 7.45 (m, 4 H), 6.55 (s, 1 H), 4.31 (q, *J* = 6.9 Hz, 2 H), 1.27 (t, *J* = 7.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.77, 165.24, 165.12, 134.31, 134.21, 133.80, 130.24, 129.31, 128.83, 128.57, 128.47, 74.90, 62.51, 13.95.

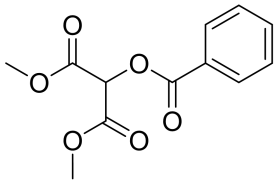


benzil (**3la'**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.89 (m, 2 H), 7.65 (t, *J* = 7.4 Hz, 1

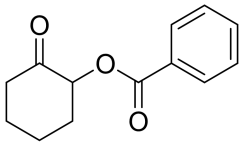
H), 7.50 (t, *J* = 7.7 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.55, 134.87, 132.97, 129.87, 129.00, 129.00, 77.33, 77.01, 76.69.



1-oxo-1-(thiophen-2-yl)propan-2-yl benzoate (**3ma**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.2 Hz, 2 H), 7.87 (t, *J* = 3.6 Hz, 1 H), 7.69 (t, *J* = 4.8 Hz, 1 H), 7.60- 7.56 (m, 1 H), 7.44 (t, *J* = 7.6 Hz, 2 H), 7.16 – 7.15 (m, 1 H), 5.97 (q, *J* = 7.2 Hz, 1 H), 1.71 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.75, 165.99, 140.57, 134.56, 133.47, 132.87, 130.03, 128.60, 127.94, 126.30, 72.94, 17.75.

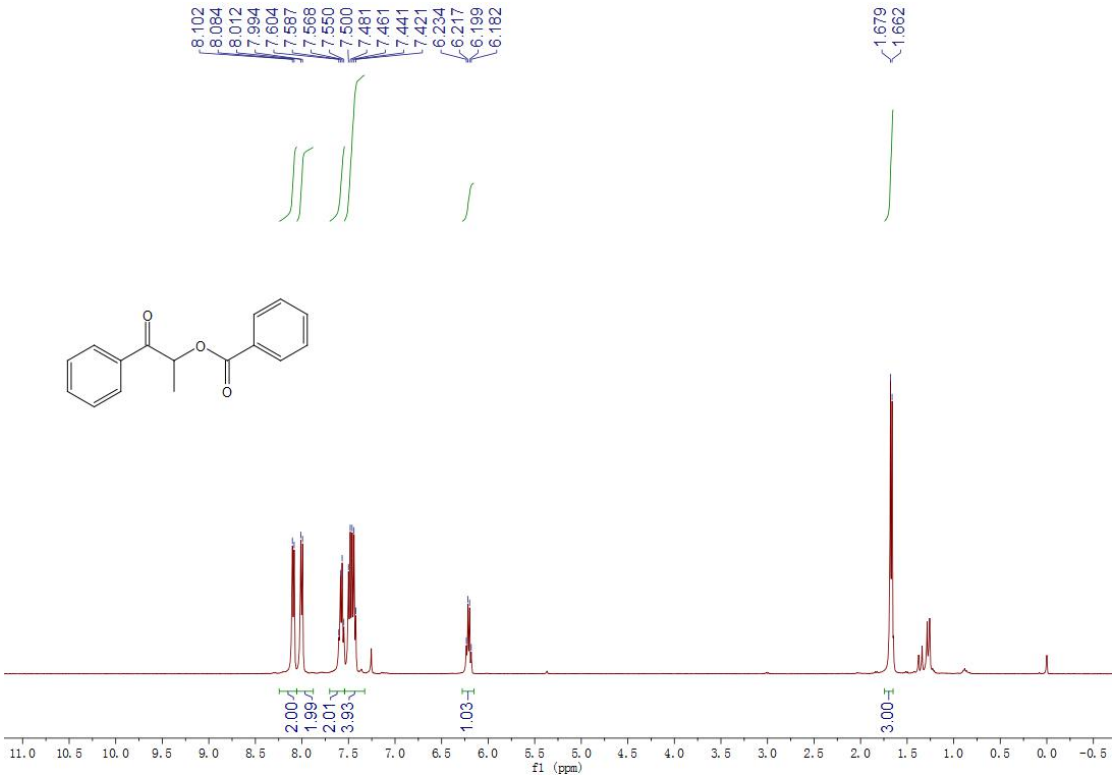


dimethyl 2-(benzoyloxy)malonate (**3na**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.0 Hz, 2 H), 7.62 (t, *J* = 7.2 Hz, 1 H), 7.48 (t, *J* = 7.2 Hz, 2 H), 5.81 (s, 1 H), 3.88 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.07, 164.92, 133.91, 130.24, 128.51, 128.31, 71.84, 53.35.



2-oxocyclohexyl benzoate (**3oa**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.8 Hz, 2 H), 7.57 (t, *J* = 7.4 Hz, 1 H), 7.45 (t, *J* = 7.4 Hz, 2 H), 5.41 (q, *J* = 8.6 Hz, 1 H), 2.57 (d, *J* = 12.0 Hz, 1 H), 2.51 - 2.41 (m, 2 H), 2.15 - 2.11 (m, 1 H), 2.04 (d, *J* = 13.2 Hz, 1 H),

1.96 - 1.83 (m, 2 H), 1.75 – 1.61 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.33, 165.57, 133.14, 129.86, 129.68, 128.32, 76.68, 40.74,33.19, 27.19, 23.77.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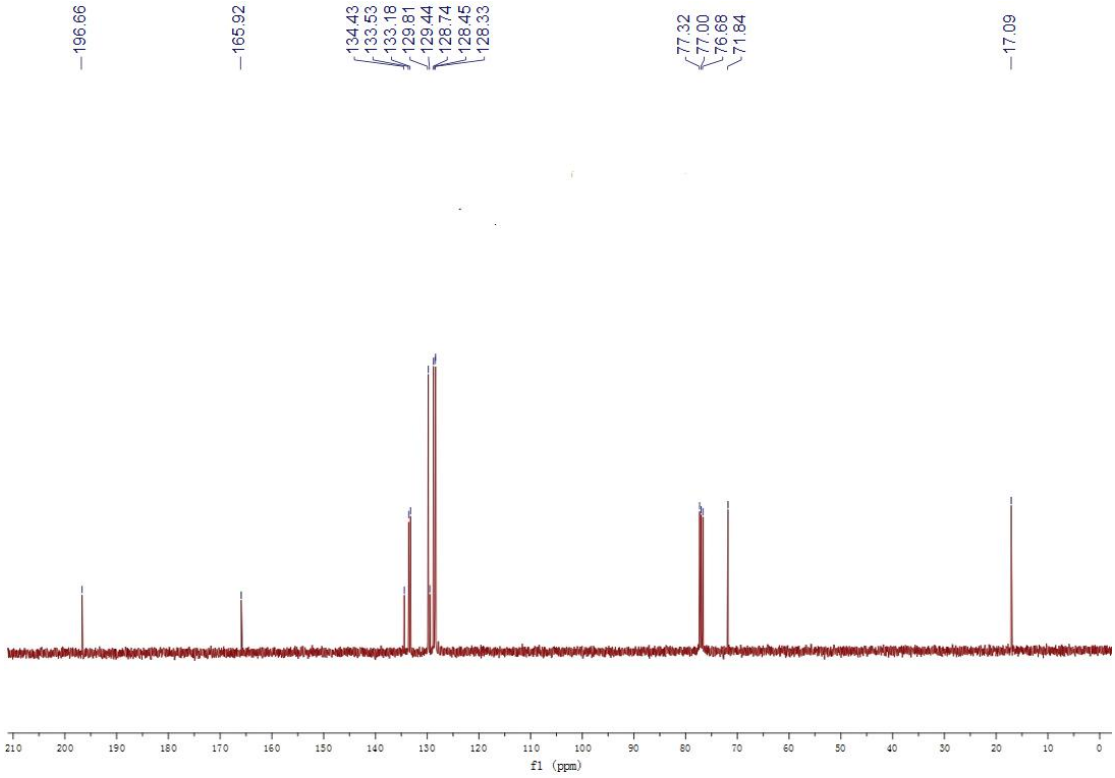
3.00
f1 (ppm)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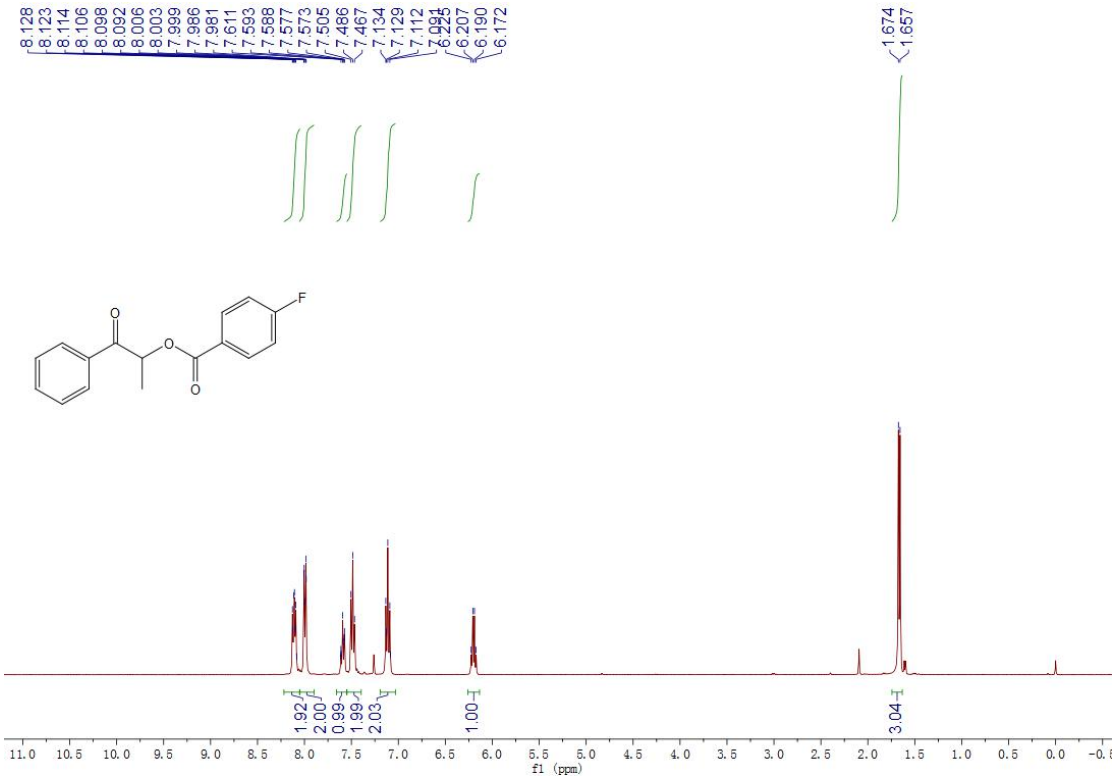
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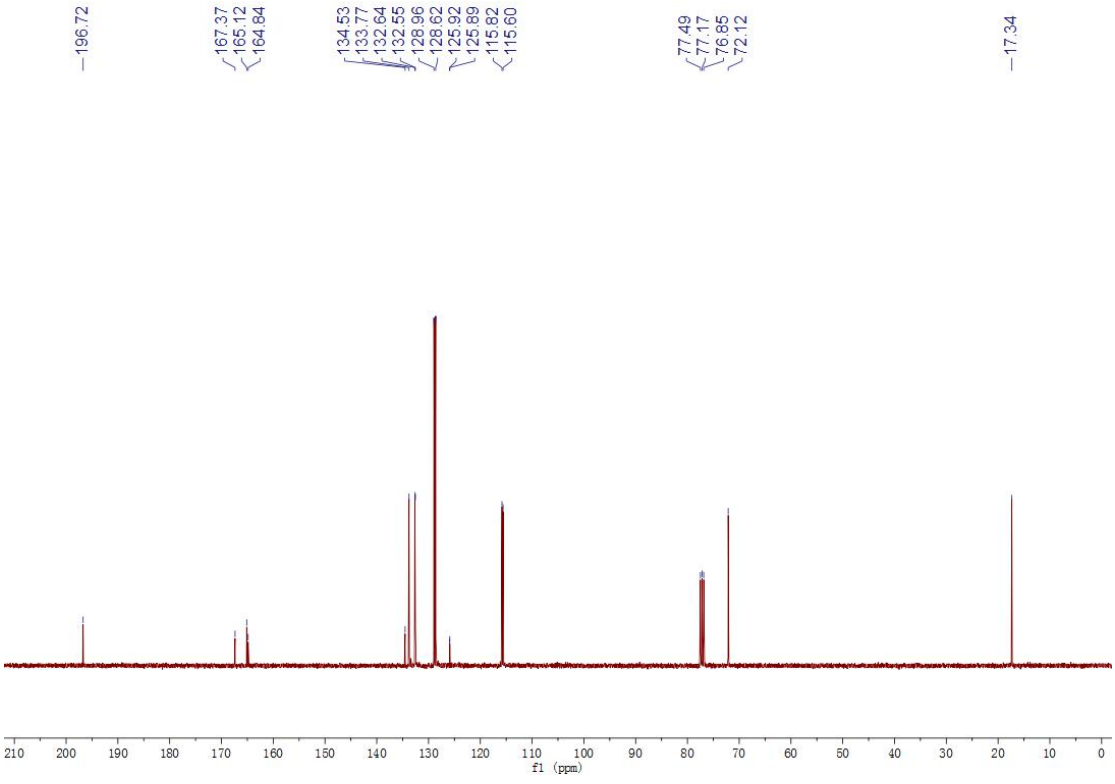
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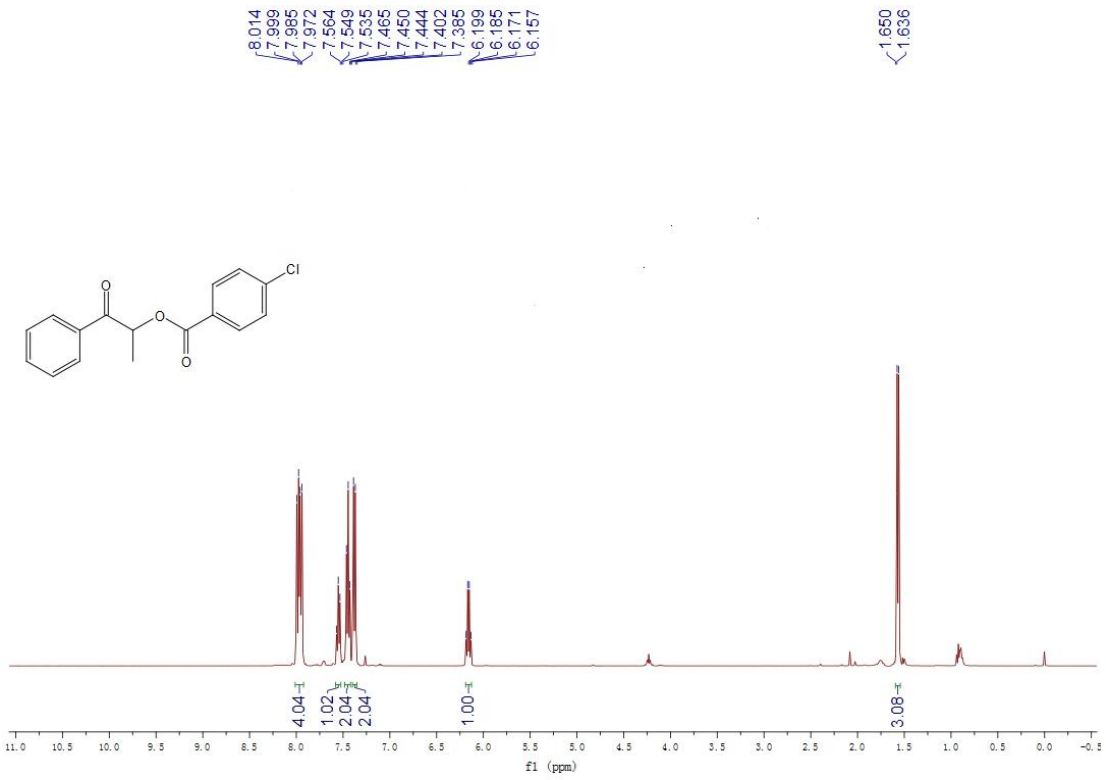
17.34
f1 (ppm)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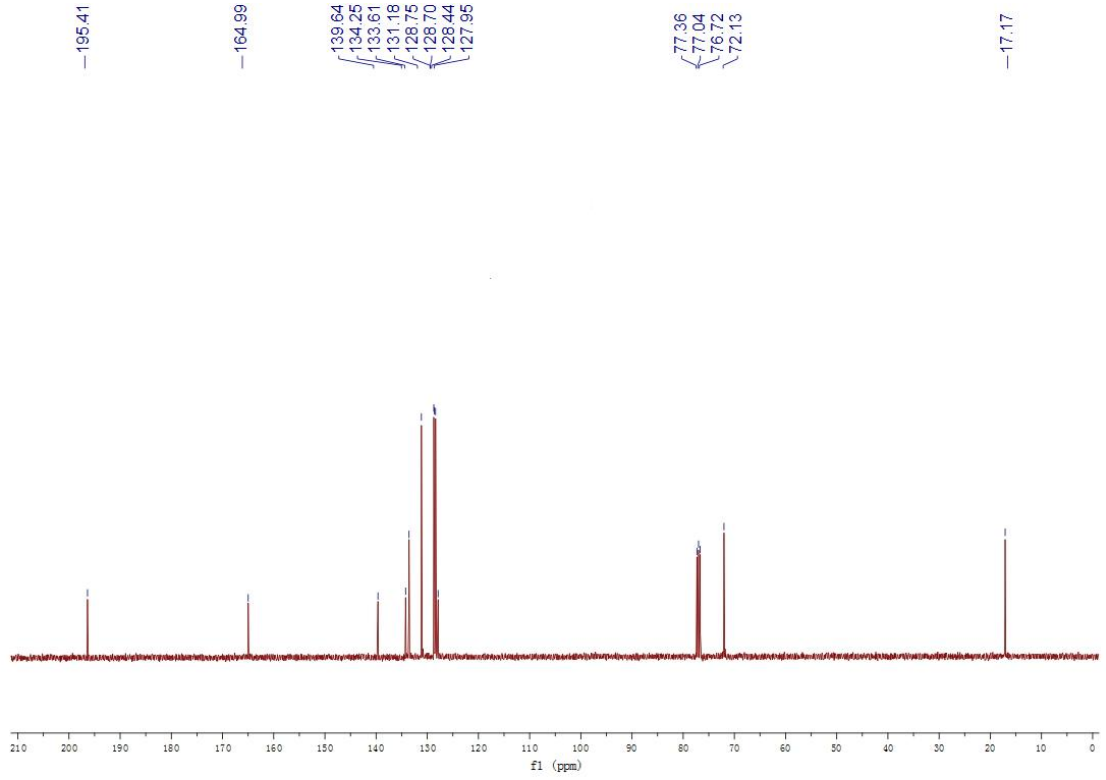
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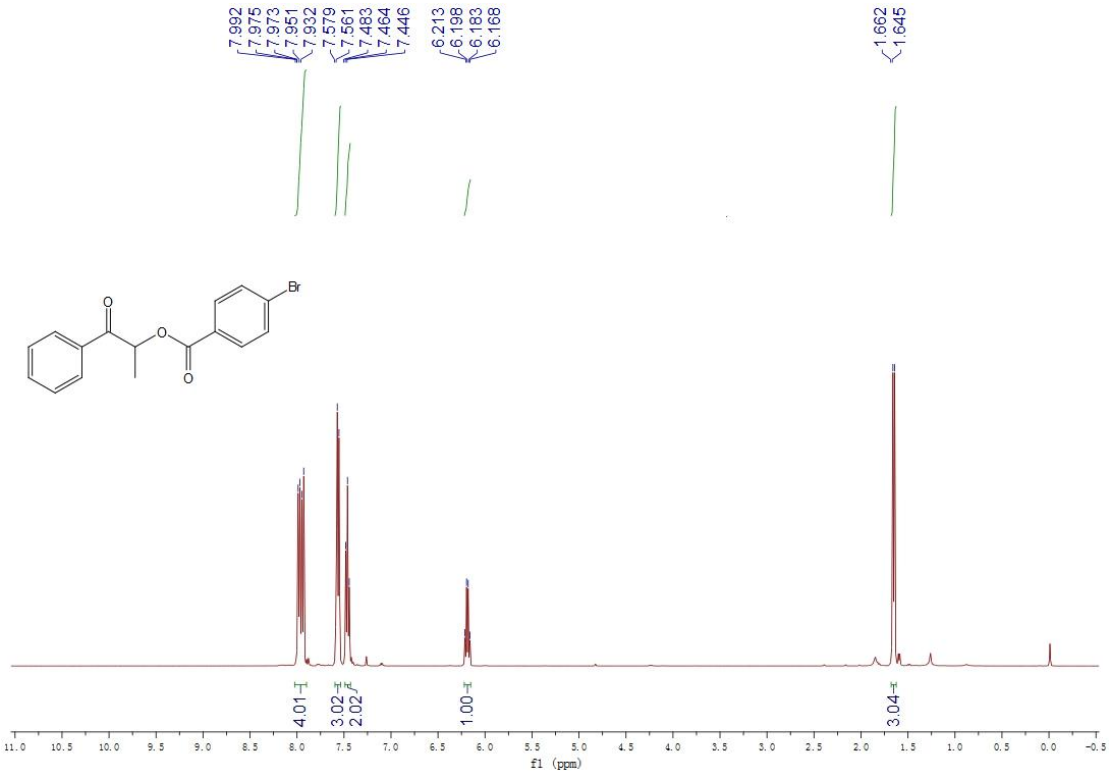
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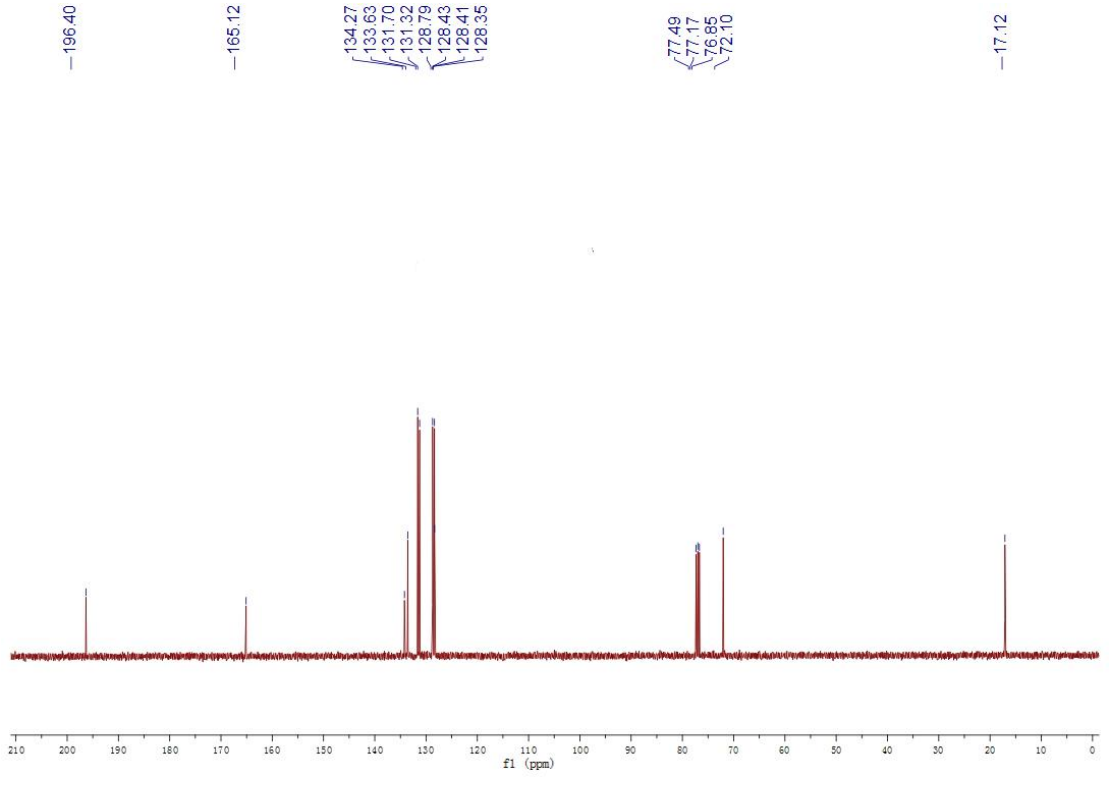
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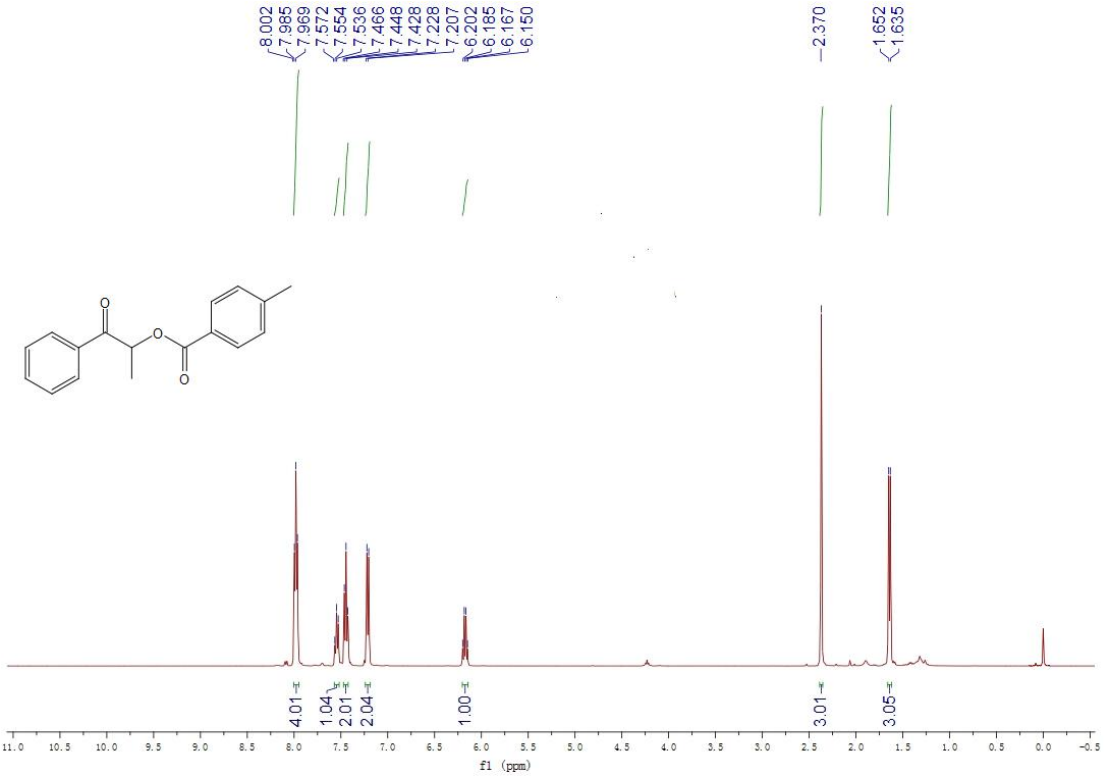
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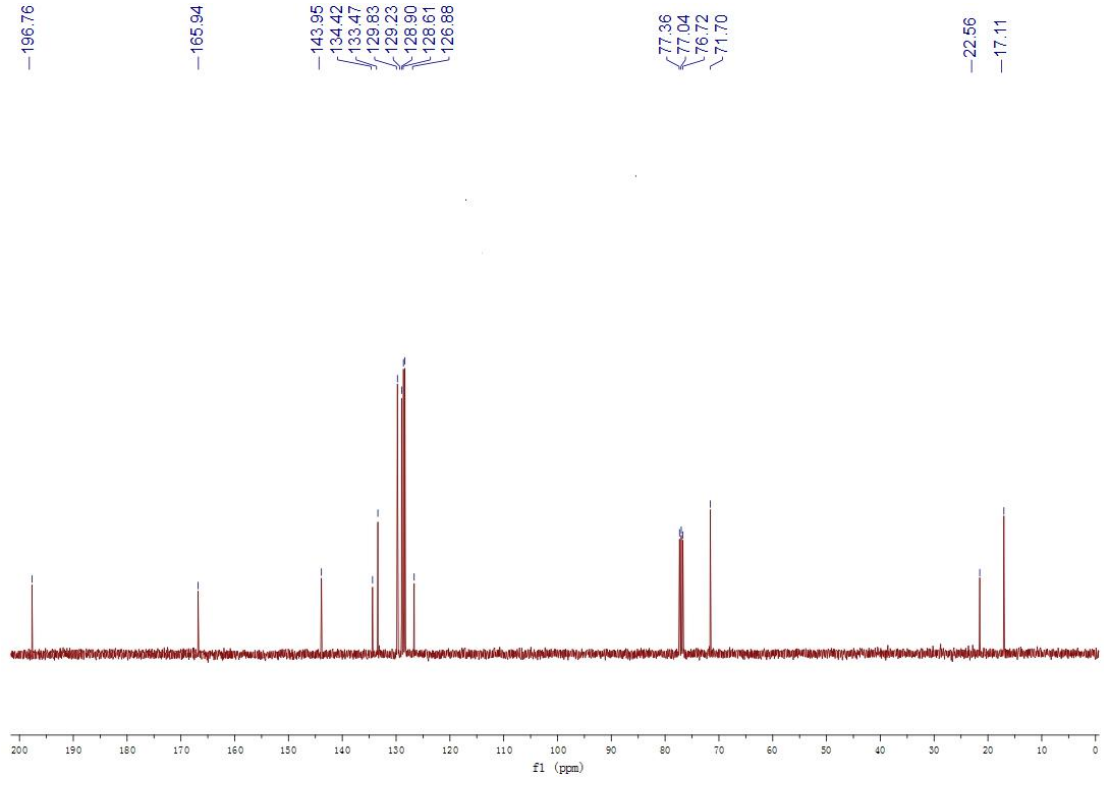
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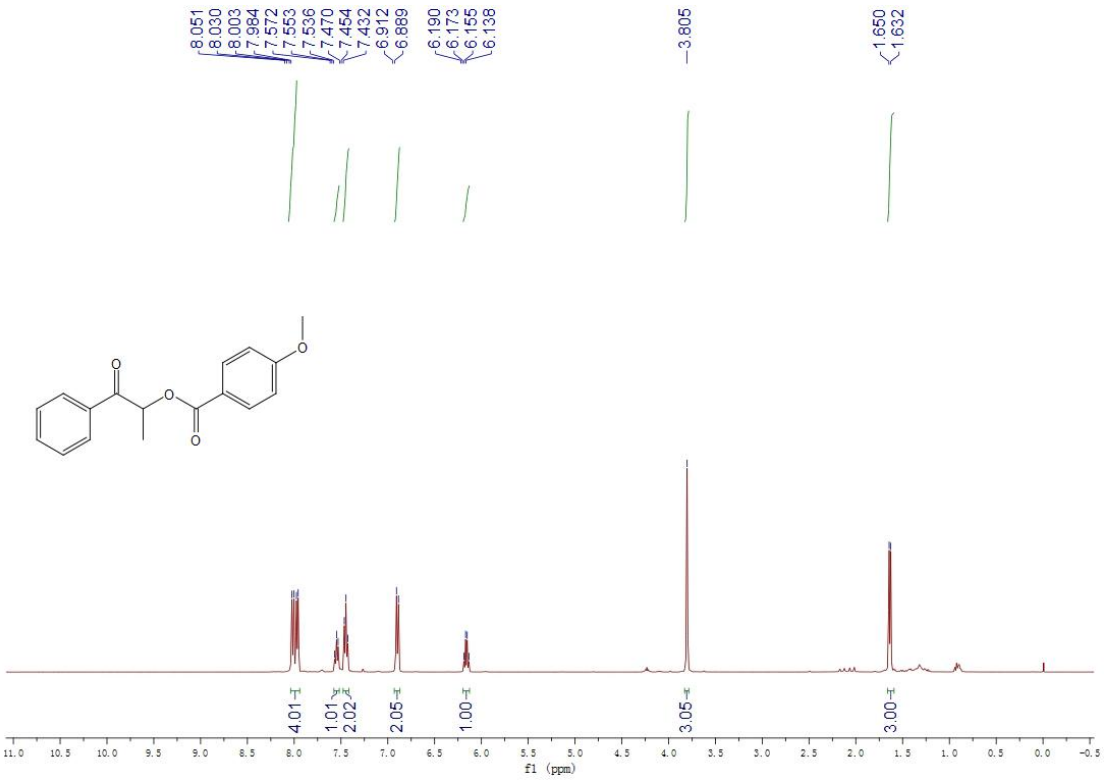
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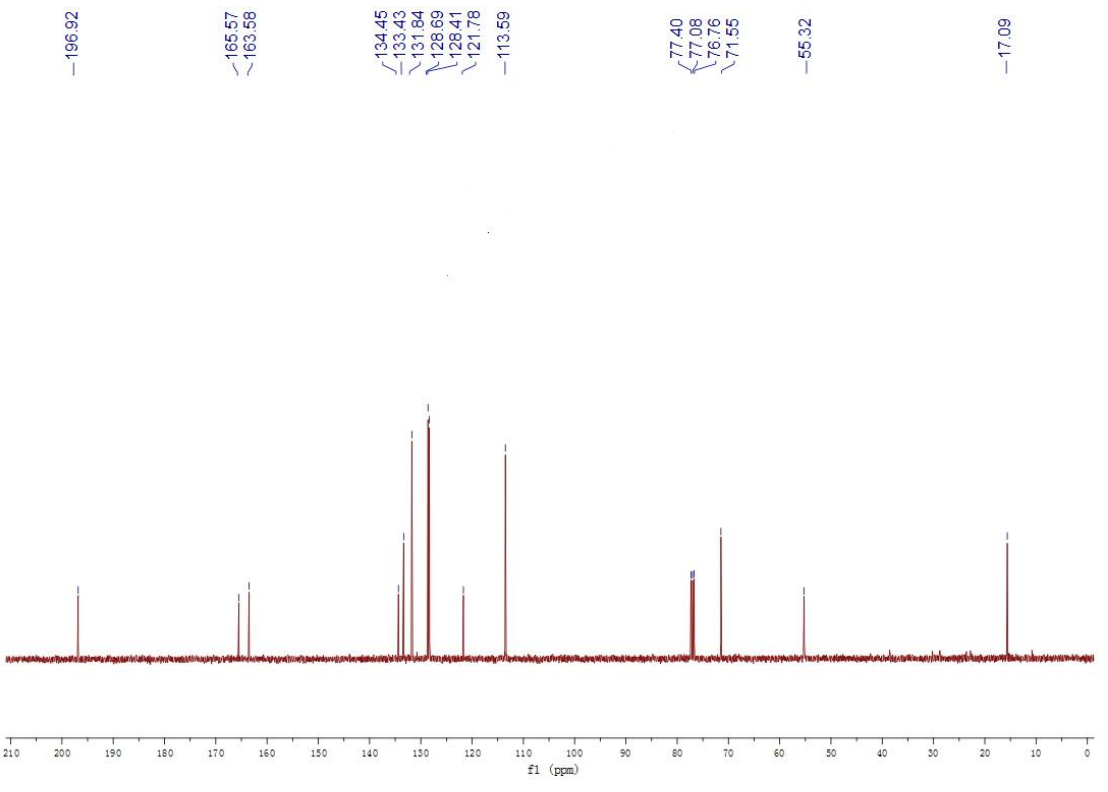
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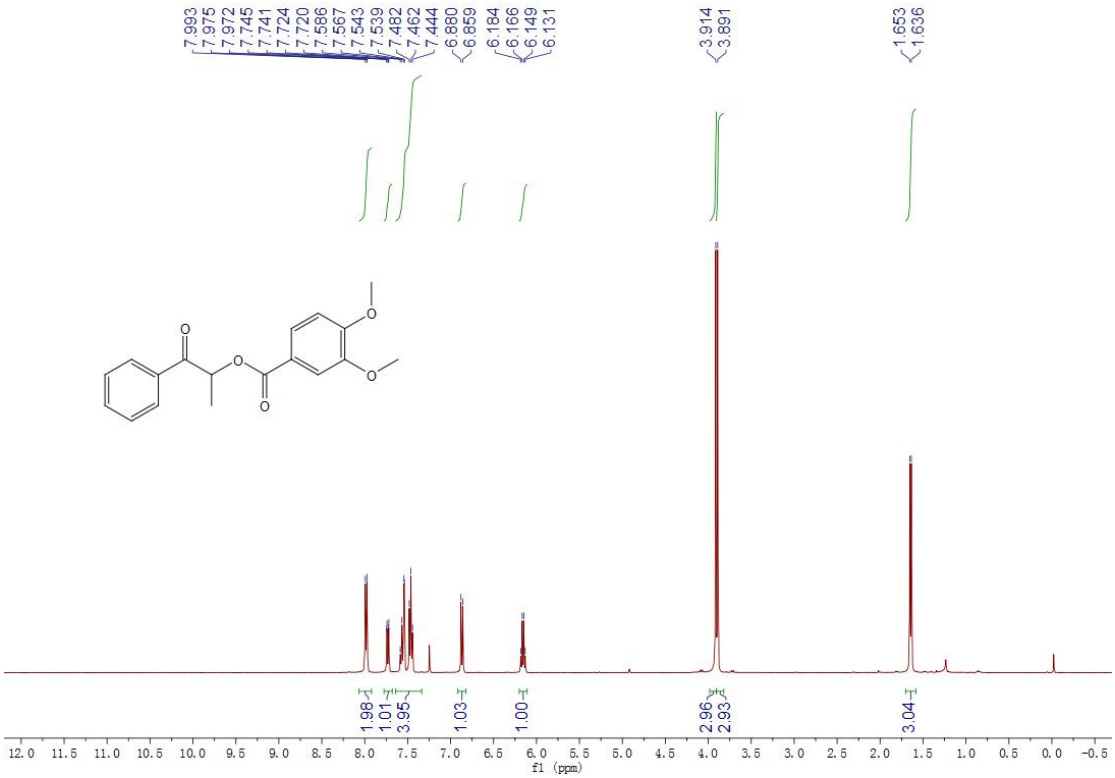
f1 (ppm)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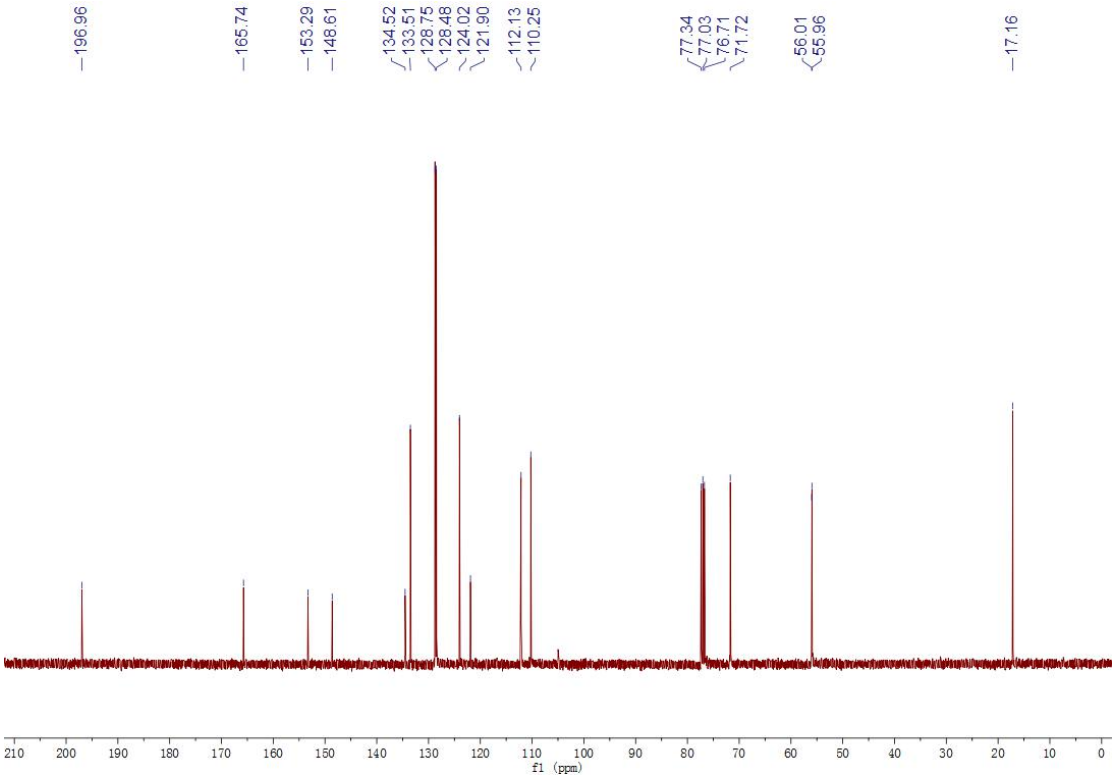
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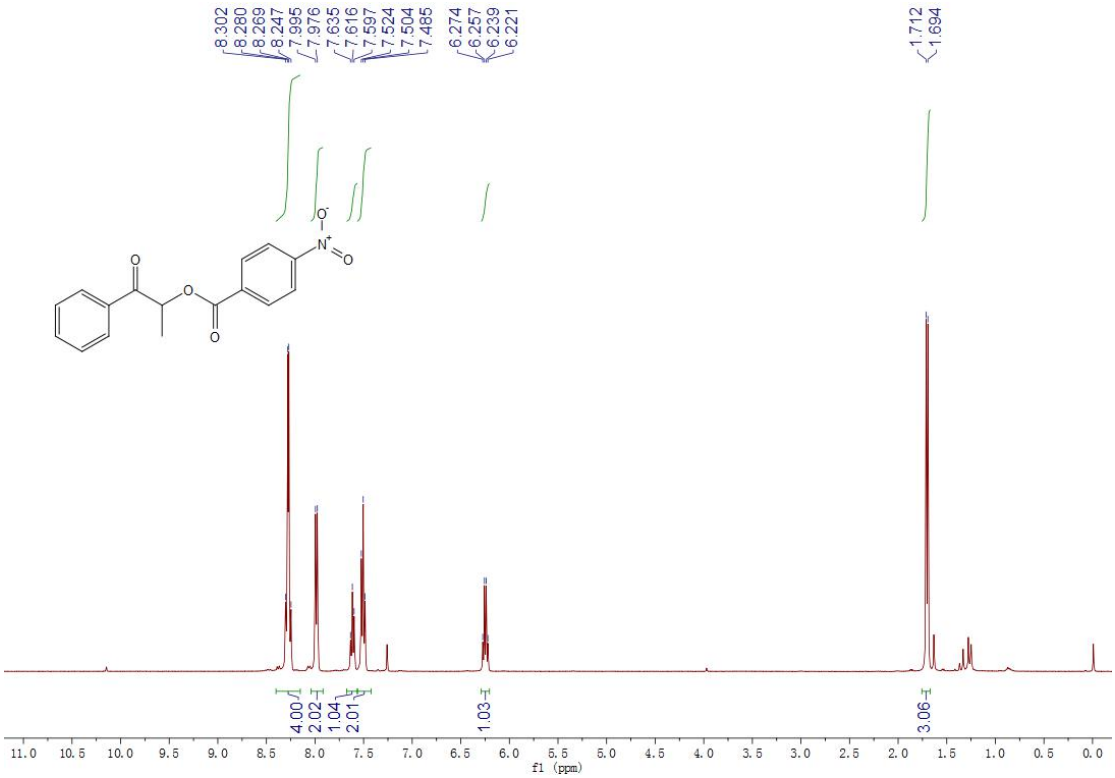
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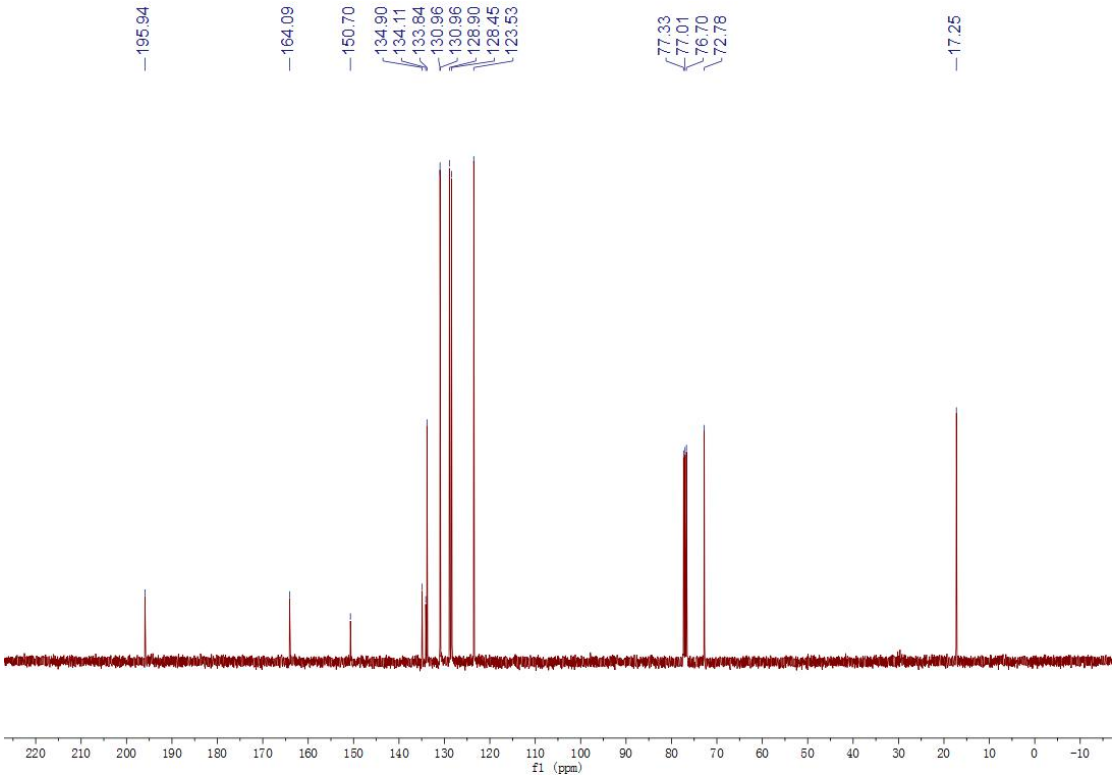
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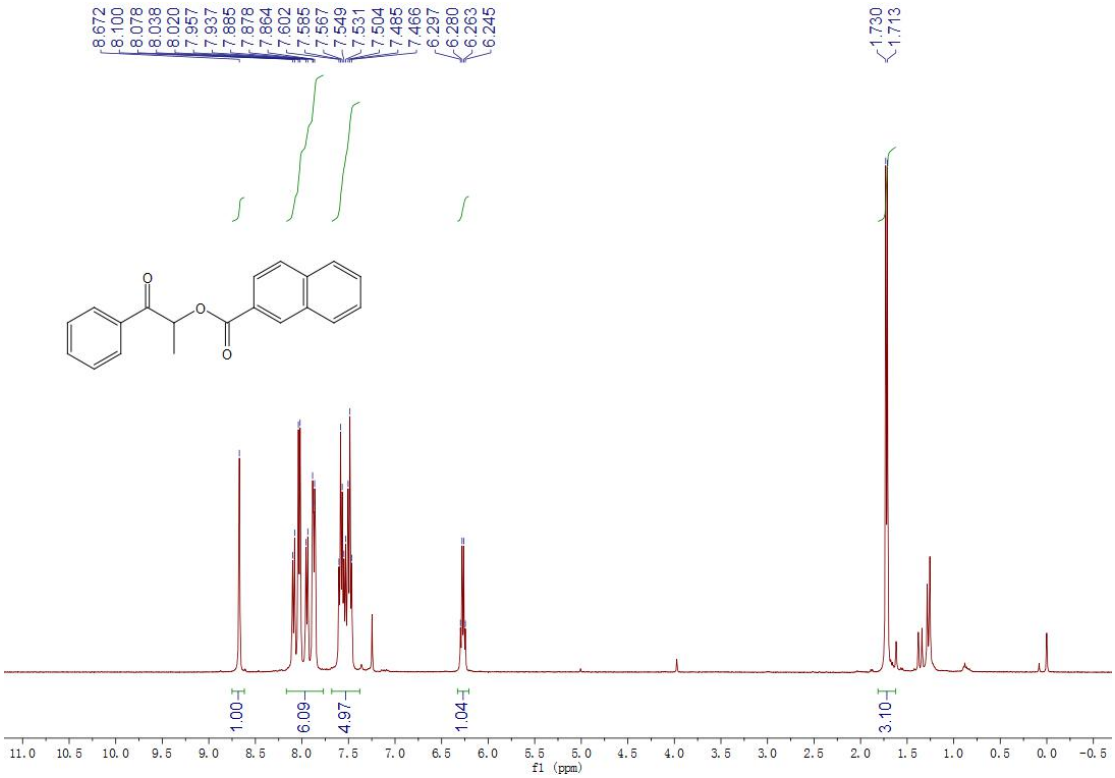
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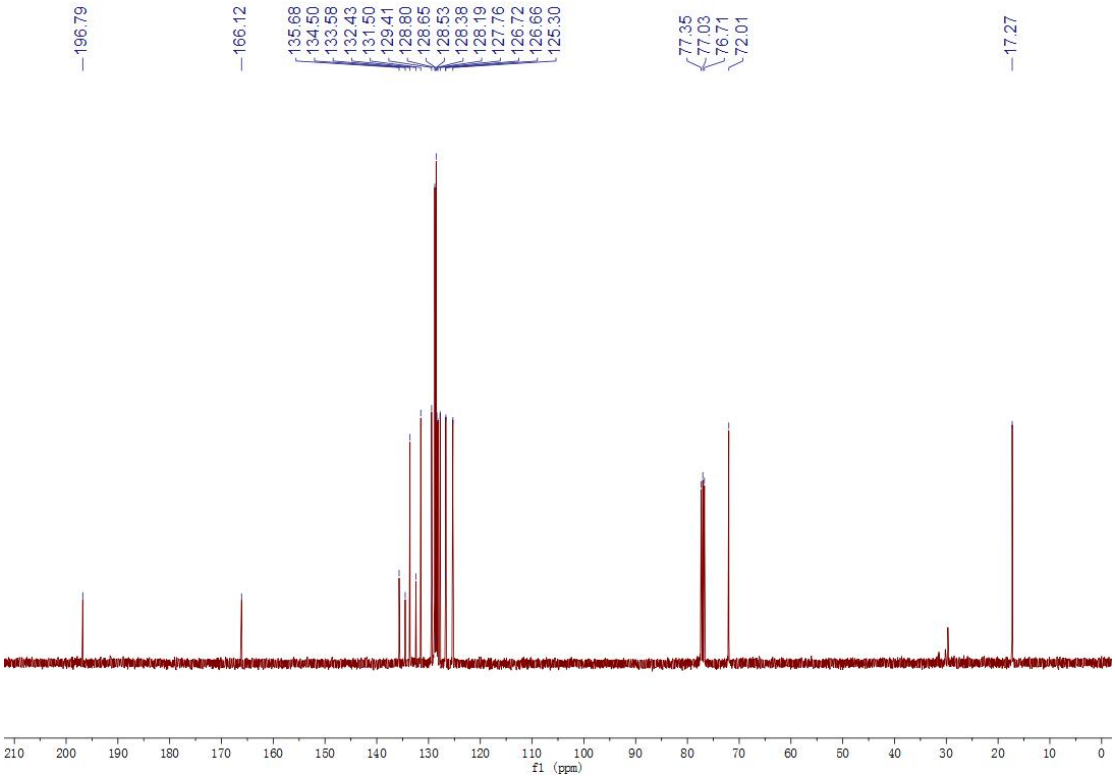
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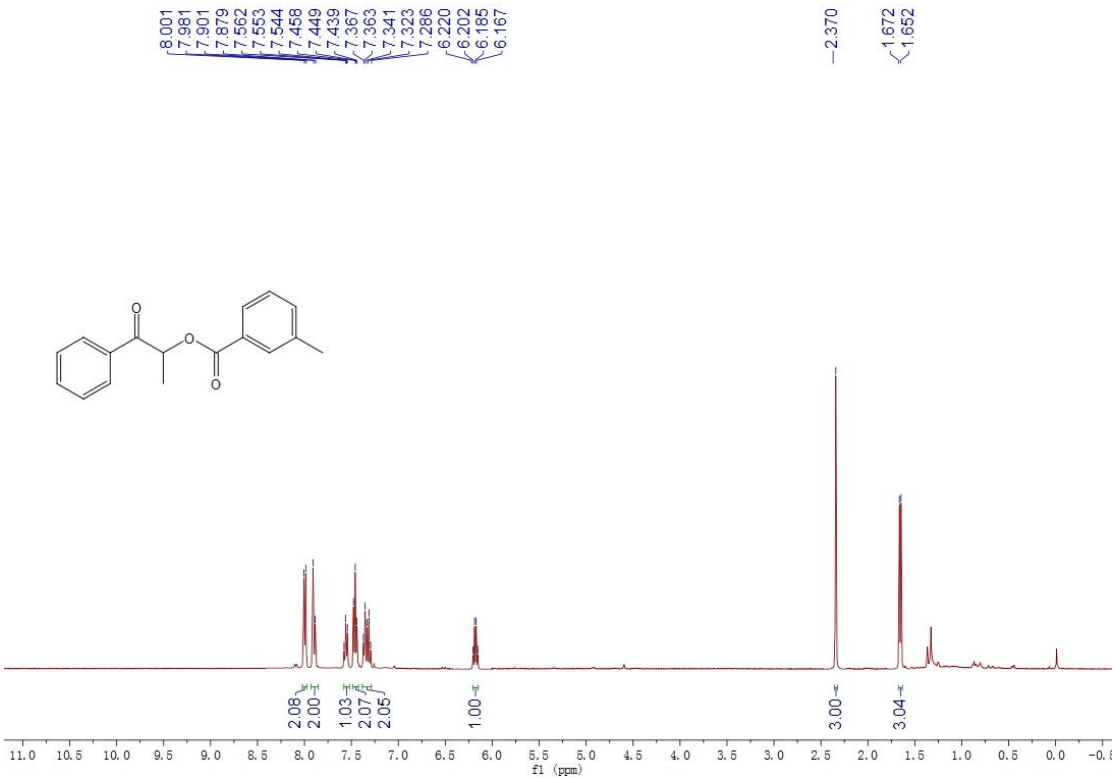
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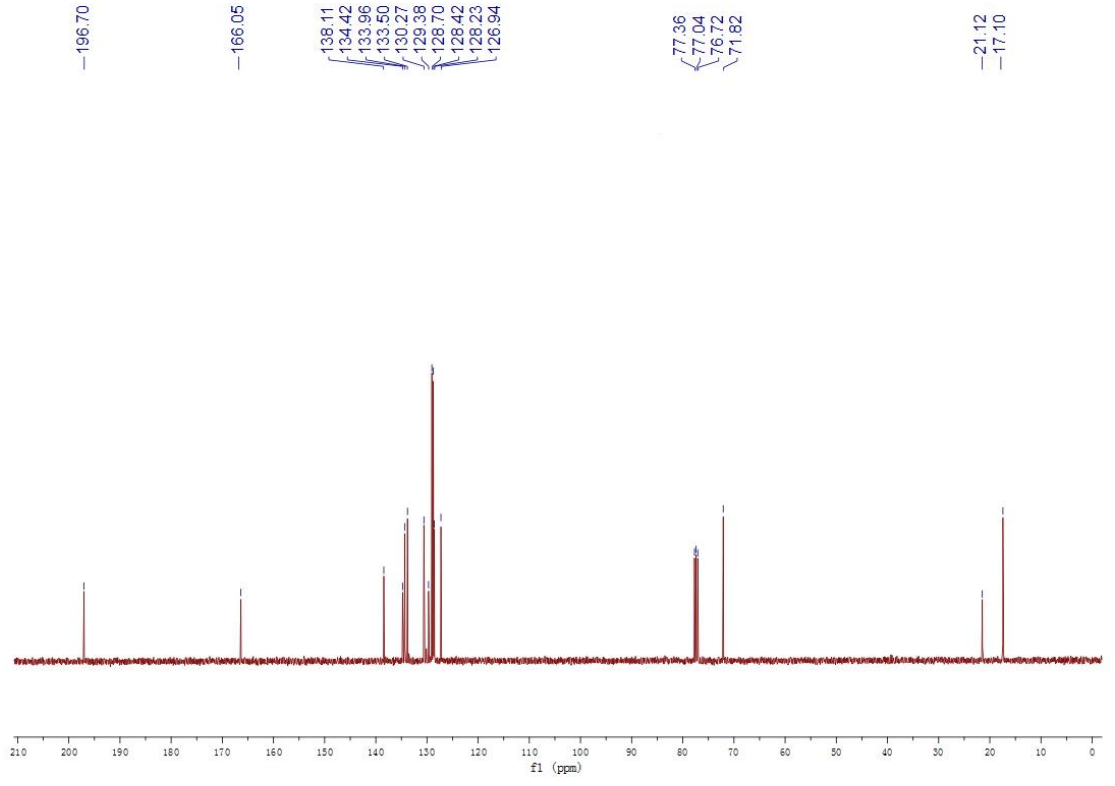
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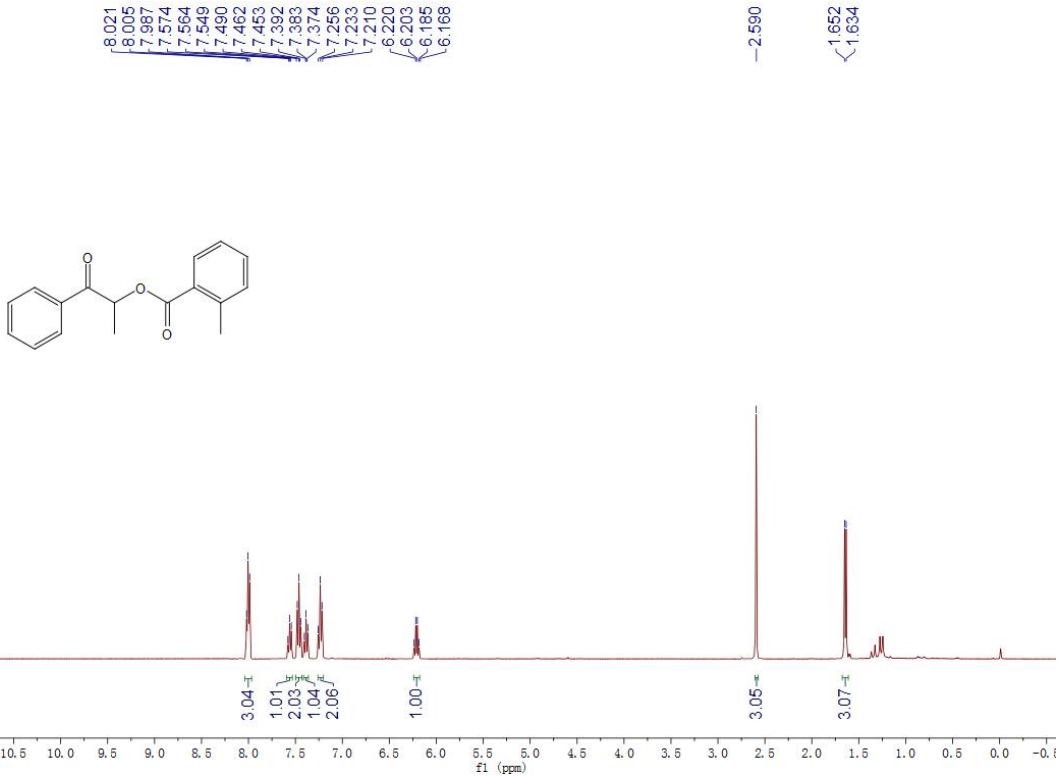
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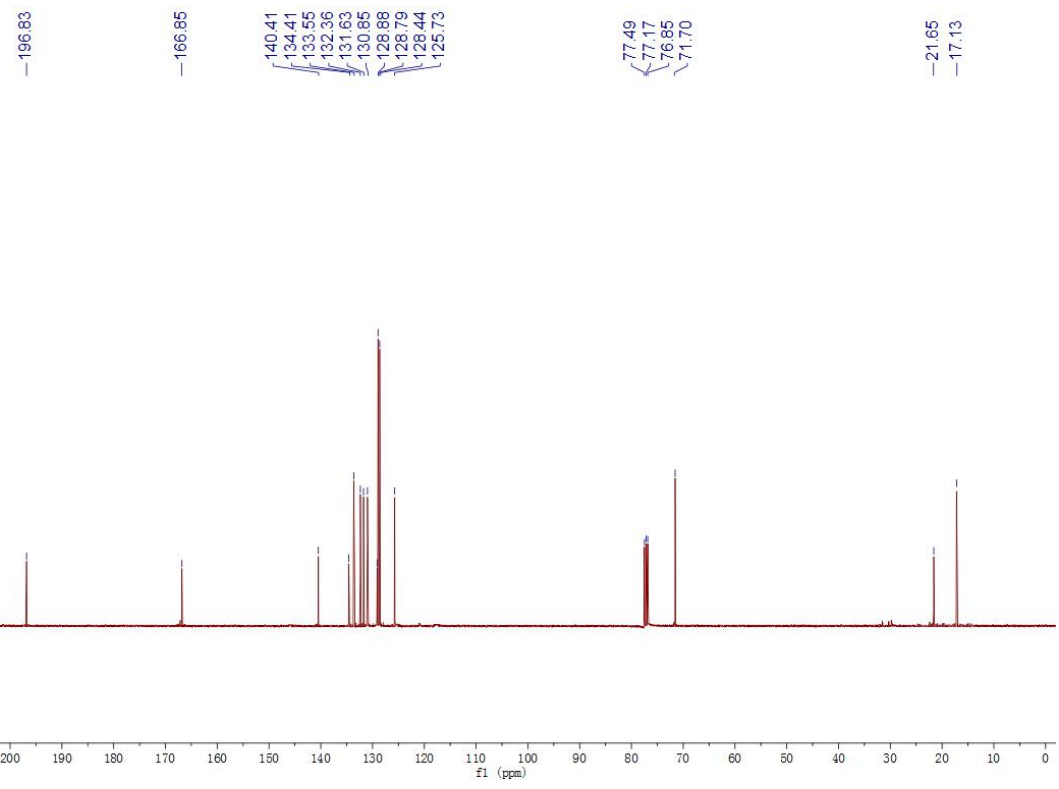
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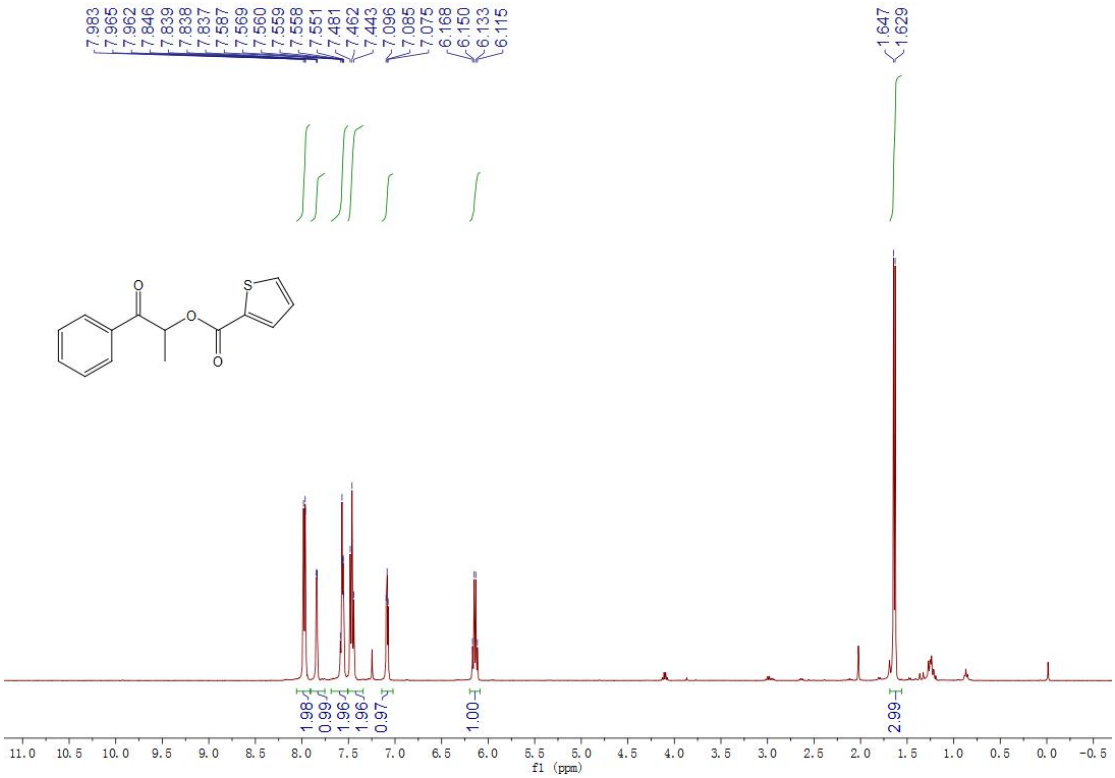
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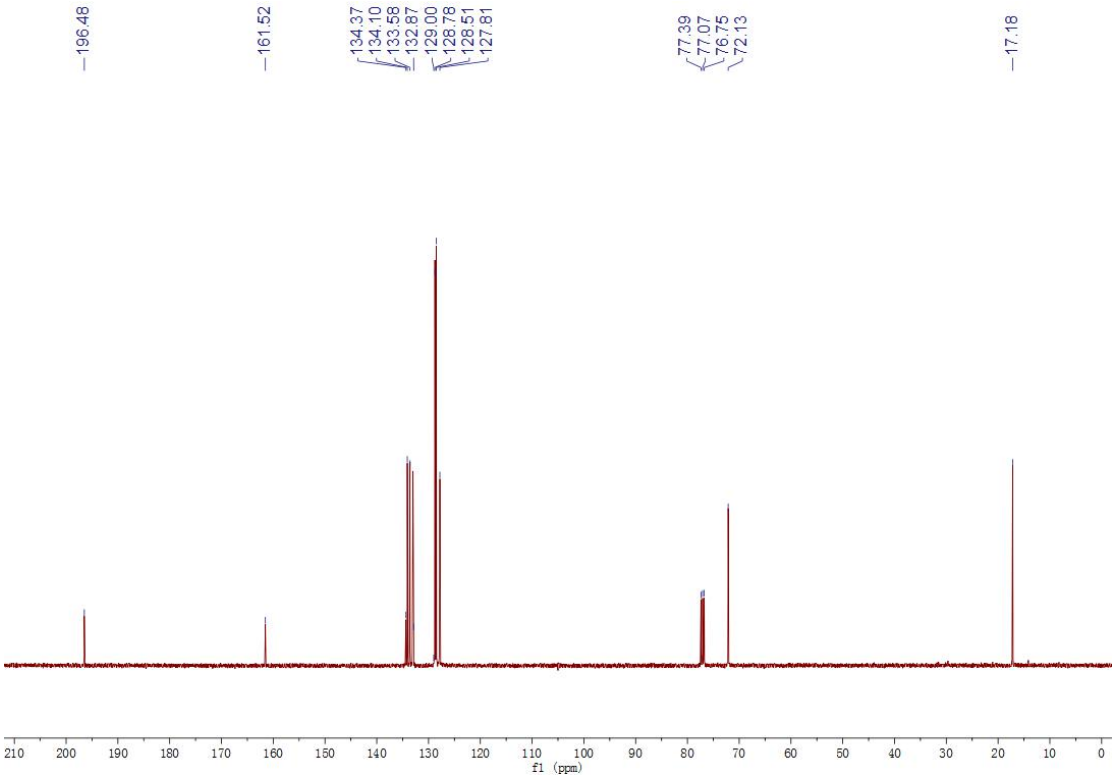
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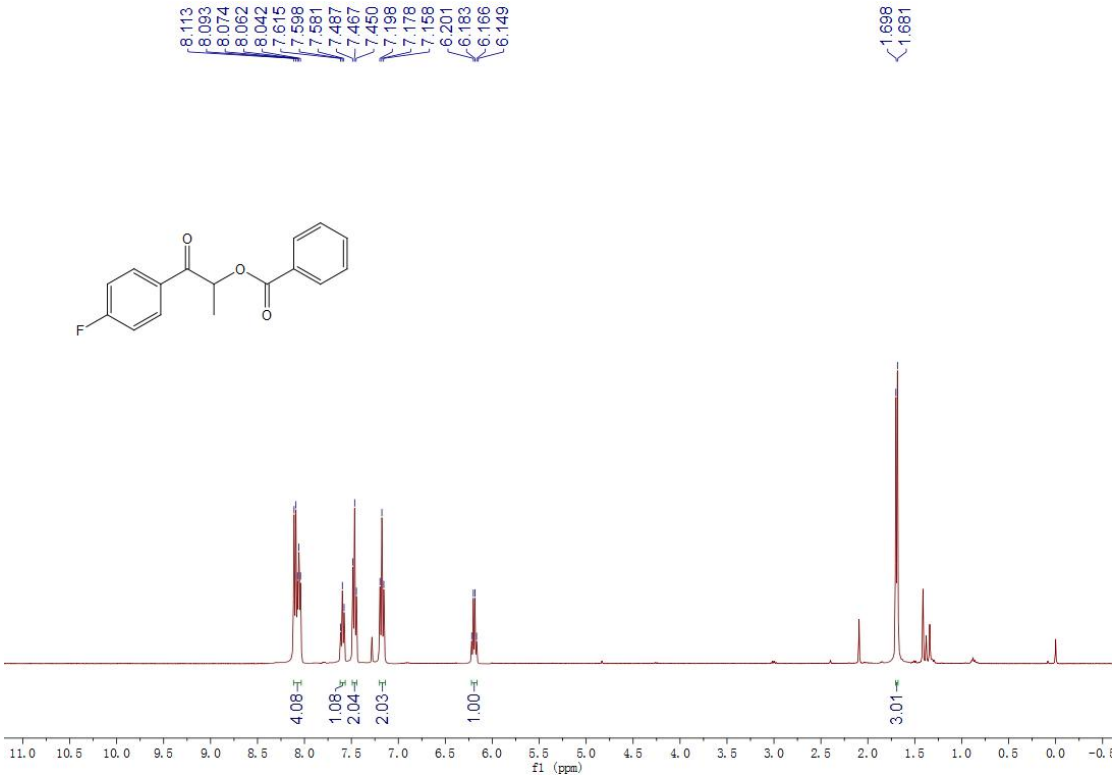
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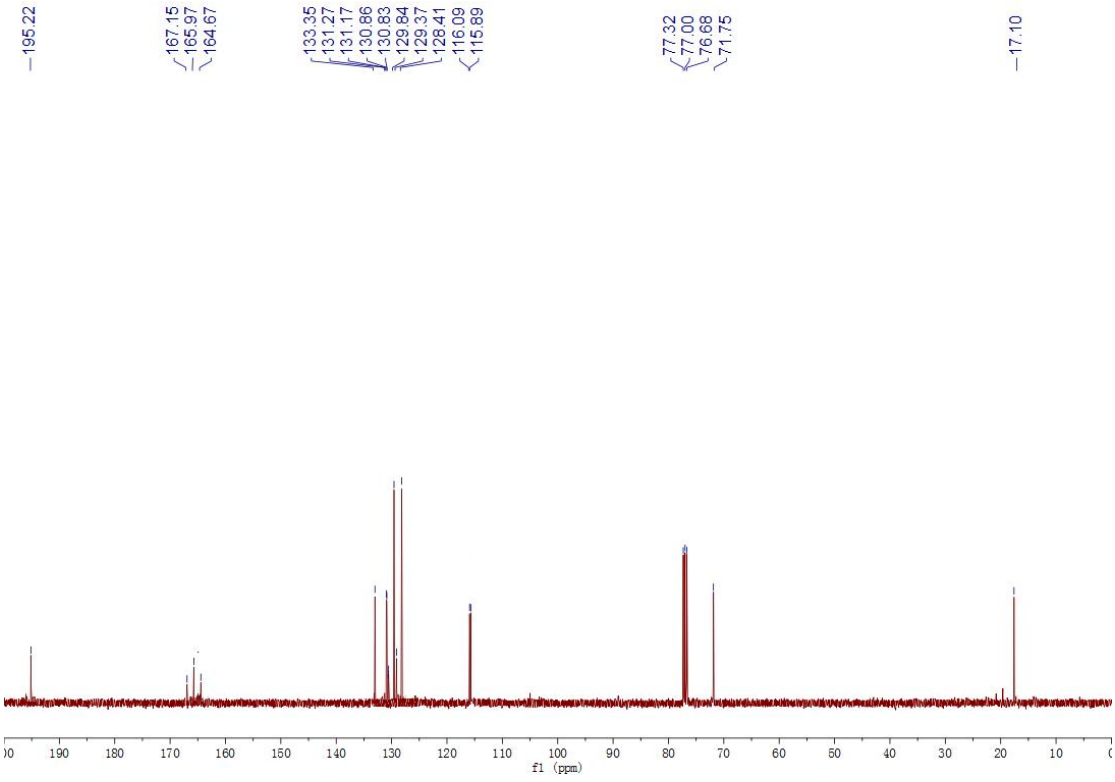
6.201
6.183
6.166
6.149
1.698
1.681
O
O
O
F
4.08
1.08
2.04
2.03
1.00
3.01
f1 (ppm)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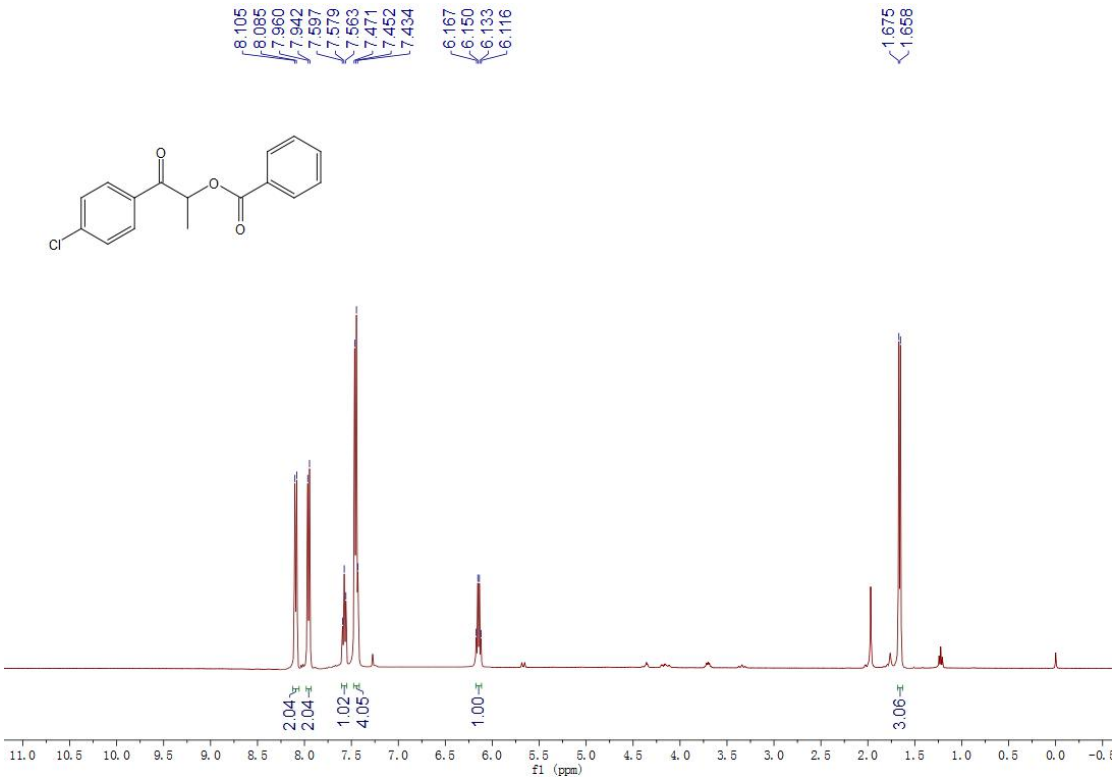
167.15
165.97
164.67
133.35
131.27
131.17
130.86
130.83
129.84
129.37
128.41
116.09
115.89
77.32
77.00
76.68
71.75
17.10
f1 (ppm)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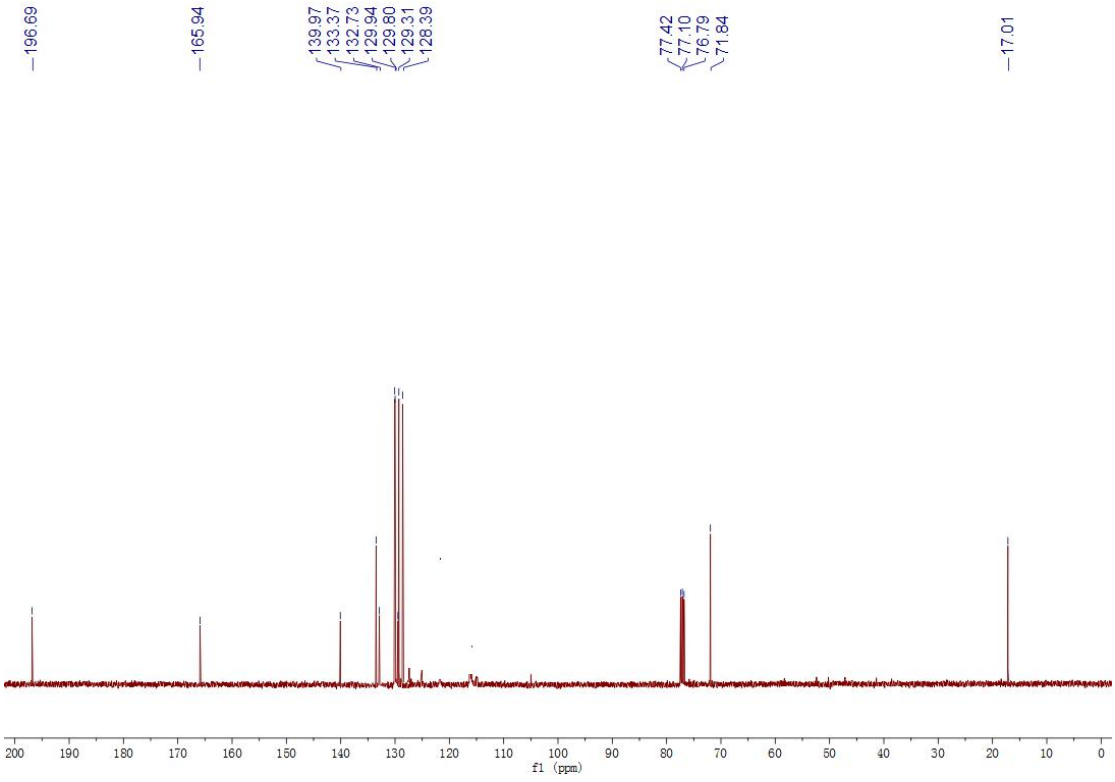
8.085
7.960
7.942
7.597
7.579
7.563
7.471
7.452
7.434
6.167
6.150
6.133
6.116
1.675
1.658
O
O
O
Cl
2.04
2.04
1.02
4.05
1.00
3.06
f1 (ppm)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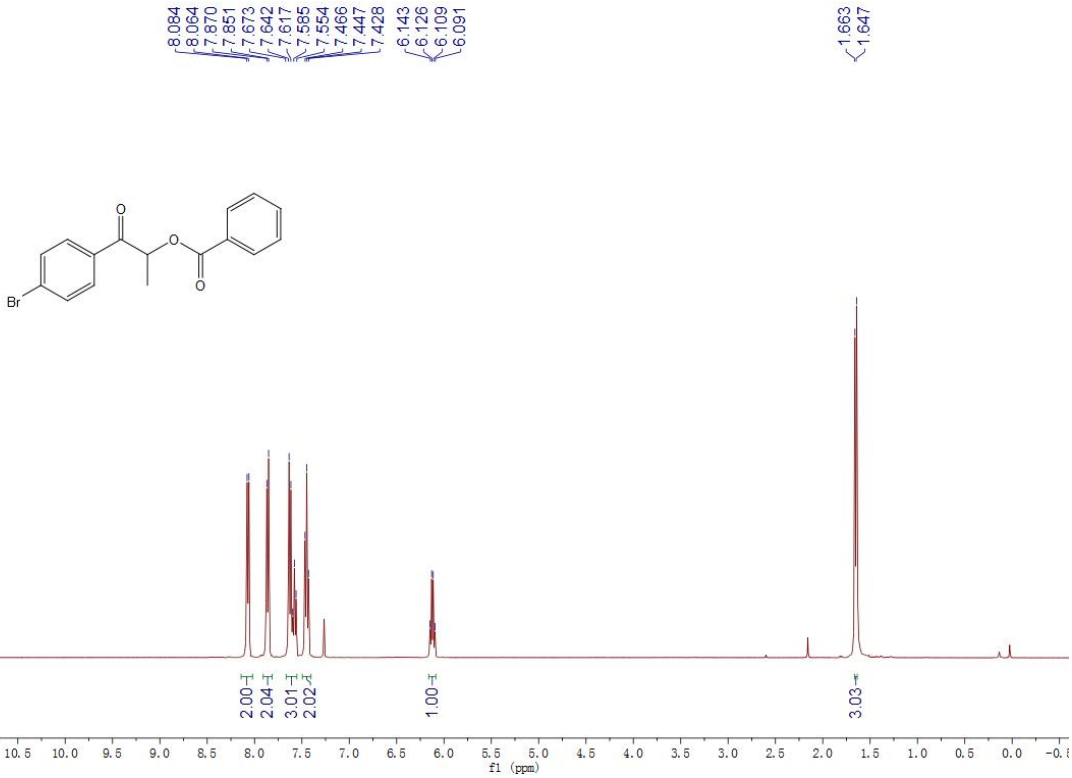
165.94
139.97
133.37
132.73
129.94
129.80
129.31
128.39
77.42
77.10
76.79
71.84
17.01
f1 (ppm)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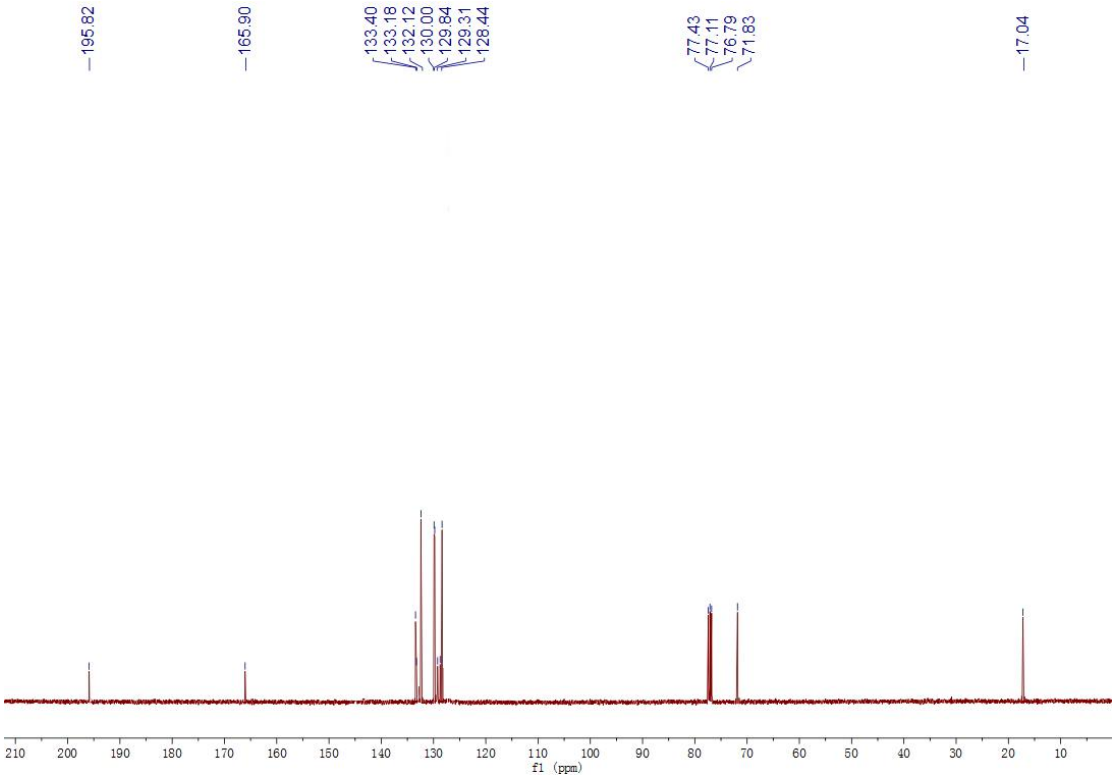
8.064
7.870
7.851
7.673
7.642
7.617
7.585
7.554
7.466
7.447
7.428
6.143
6.126
6.109
6.091
1.663
1.647
O
O
O
Br
2.00
2.04
3.01
2.02
1.00
3.03
f1 (ppm)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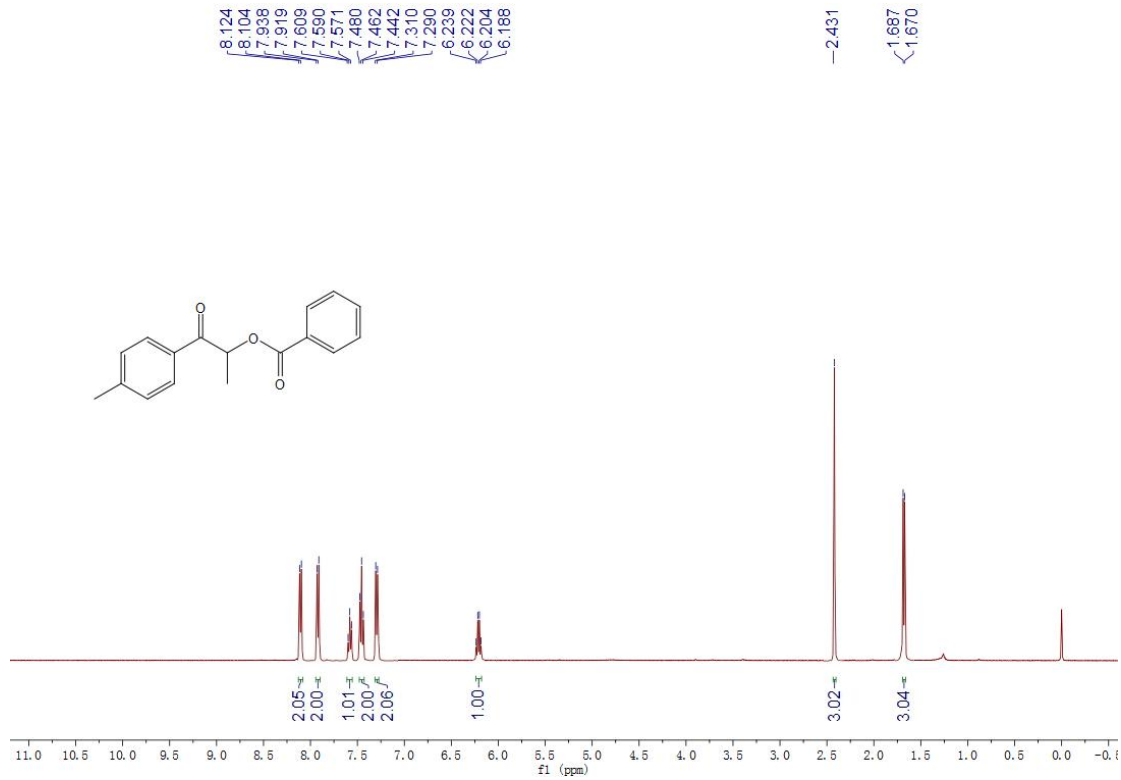
165.90
133.40
133.18
132.12
130.00
129.84
129.31
128.44
77.43
77.11
76.79
71.83
17.04
f1 (ppm)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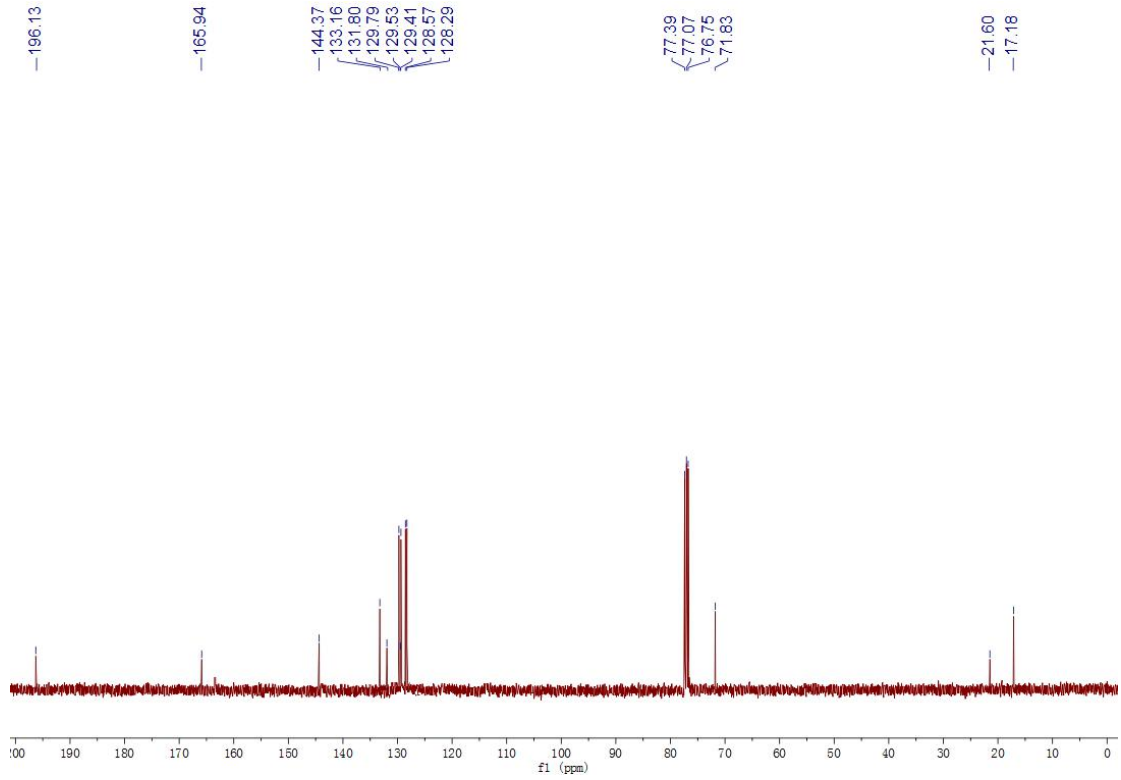
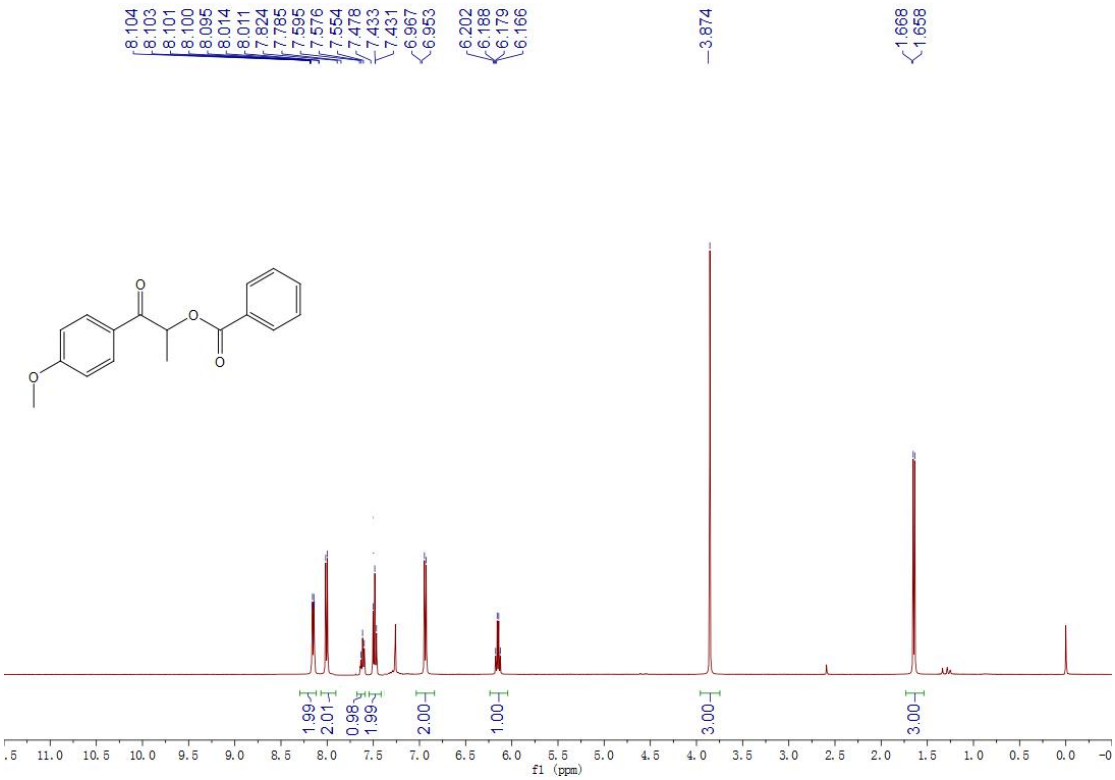
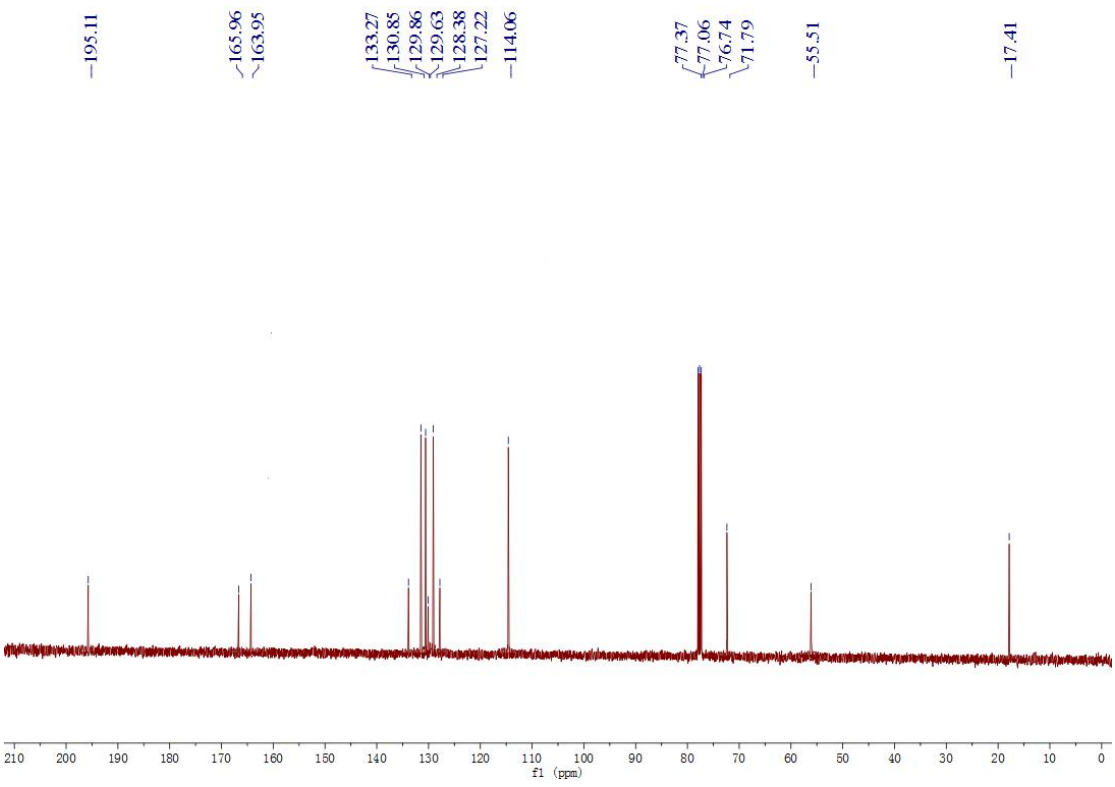
8.104
7.938
7.919
7.609
7.590
7.571
7.480
7.462
7.442
7.310
7.290
6.239
6.222
6.204
6.188
2.431
1.687
1.670
O
O
O
2.05
2.00
1.01
2.00
2.06
1.00
3.02
3.04
f1 (ppm)


196.13
165.94
144.37
133.16
131.80
129.79
129.53
129.41
128.57
128.29
77.39
77.07
76.75
71.83
21.60
17.18
f1 (ppm)


8.104
8.103
8.101
8.100
8.095
8.014
8.011
7.824
7.785
7.595
7.576
7.554
7.478
7.433
7.431
6.967
6.953
6.202
6.188
6.179
6.166
3.874
1.668
1.658
1.99
2.01
0.98
1.99
2.00
1.00
3.00
3.00
f1 (ppm)


195.11
165.96
163.95
133.27
130.85
129.86
129.63
128.38
127.22
114.06
77.37
77.06
76.74
71.79
55.51
17.41
f1 (ppm)


8.114
8.095
7.792
7.773
7.726
7.700
7.620
7.602
7.584
7.490
7.487
7.475
7.469
7.452
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7.310
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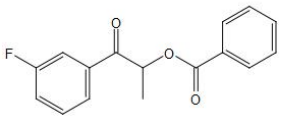
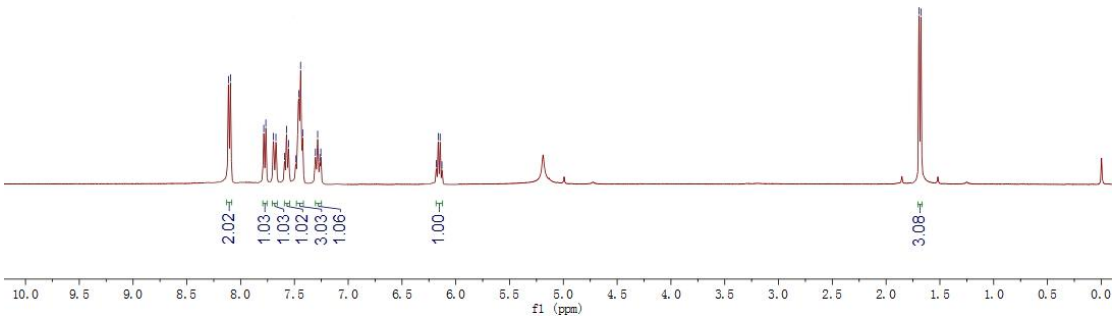
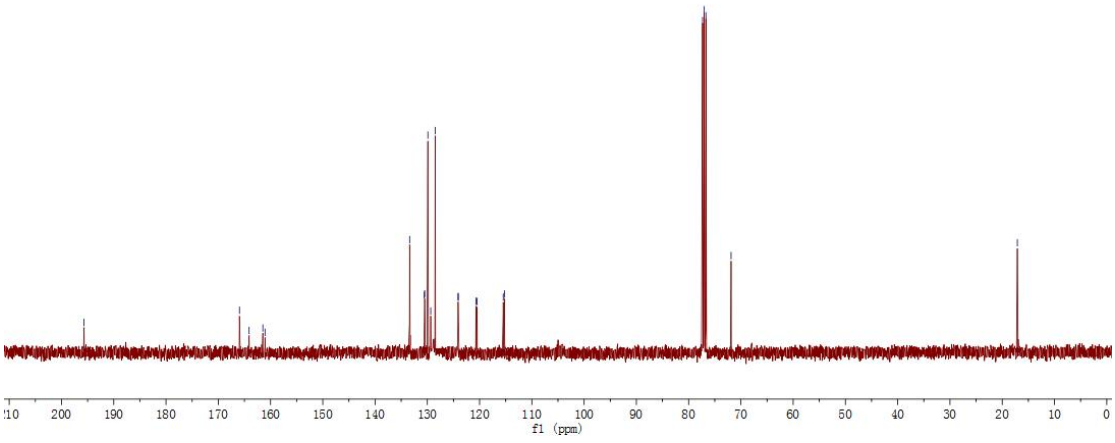
7.281
6.168
6.150
6.133
6.116


1.689
1.671


F
O
O
O

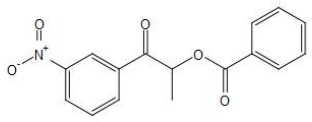

2.02
1.03
1.03
1.02
3.03
1.06
1.00
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

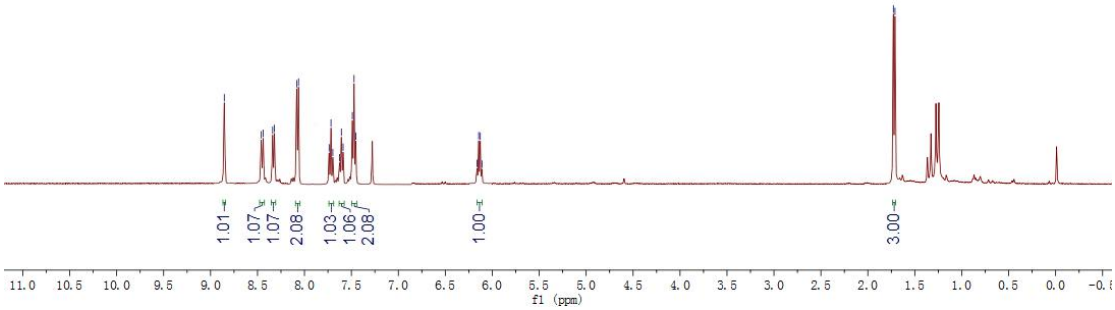

195.71
165.94
164.07
161.63
161.21
133.34
130.57
130.48
129.84
129.26
128.37
124.20
120.48
115.45
115.21
77.33
77.02
76.70
71.87
17.08


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

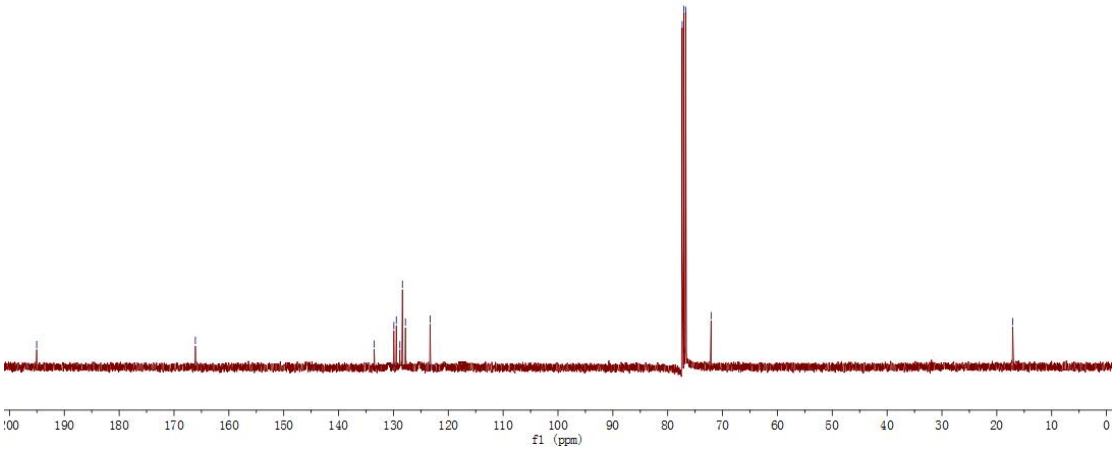

8.847
8.461
8.440
8.328
8.309
8.087
8.068
7.725
7.706
7.686
7.624
7.596
7.578
7.478
7.460
7.443
6.160
6.143
6.125
6.108

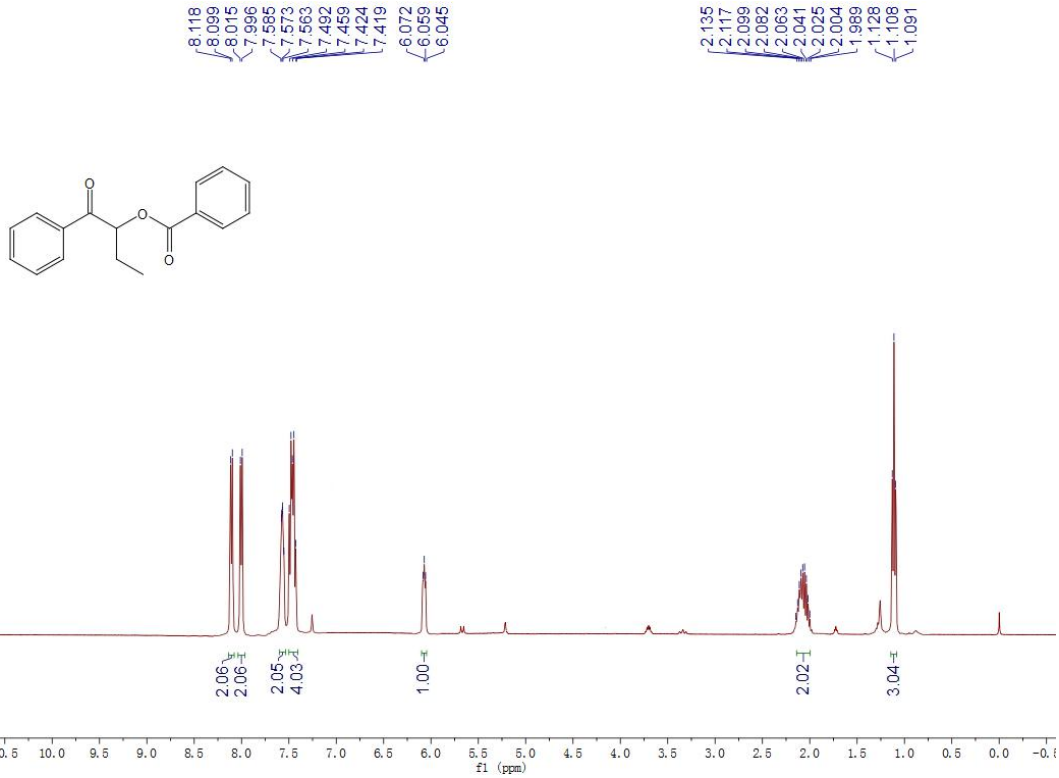

1.723
1.706

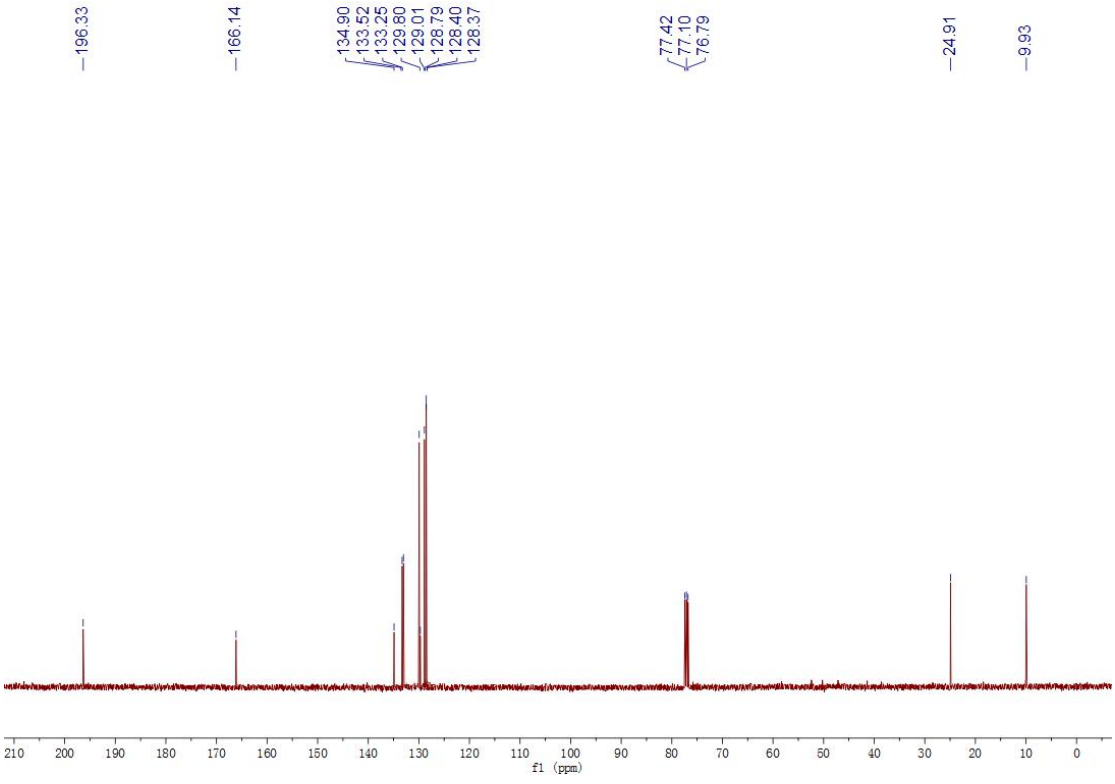

O
O
N+
O-
O
O


1.01
1.07
1.07
2.08
1.03
1.06
2.08
1.00
3.00
11.0 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)

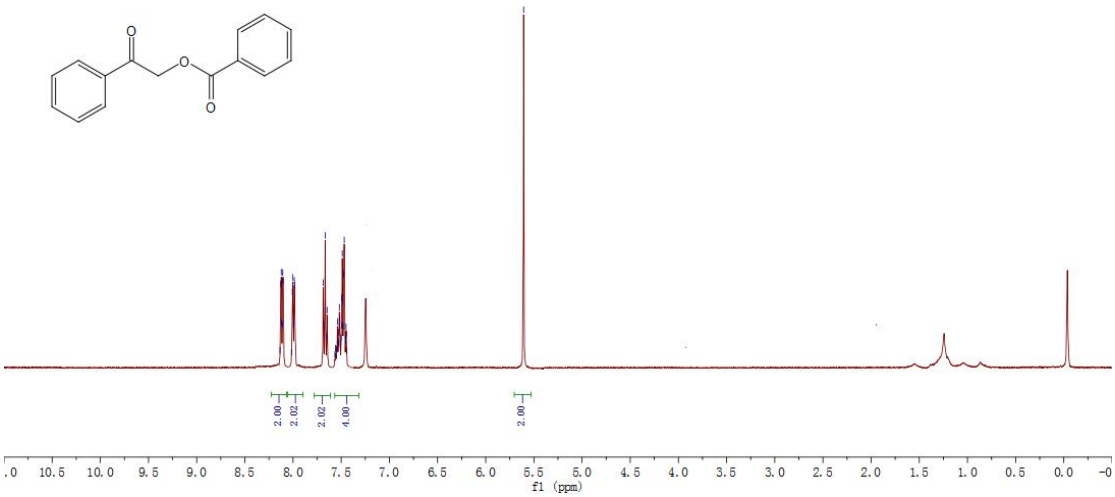

195.08
165.98
133.57
130.05
129.87
129.69
128.97
128.44
127.70
123.30
77.36
77.04
76.72
72.10
16.99

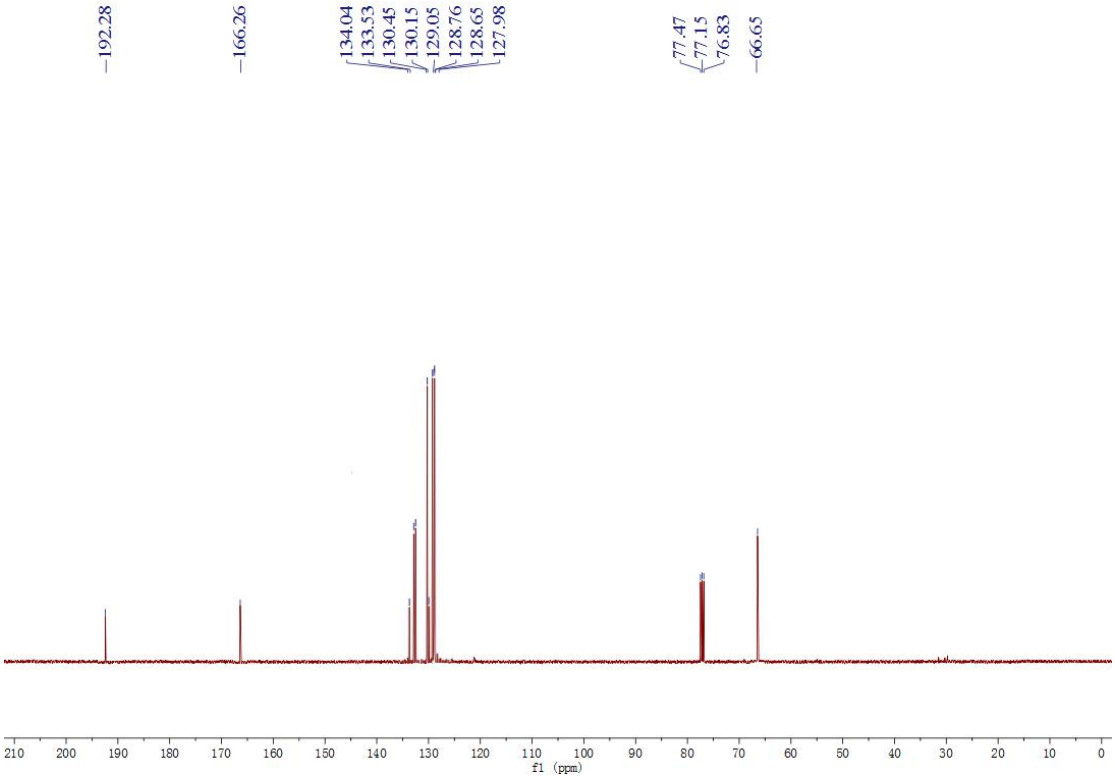

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

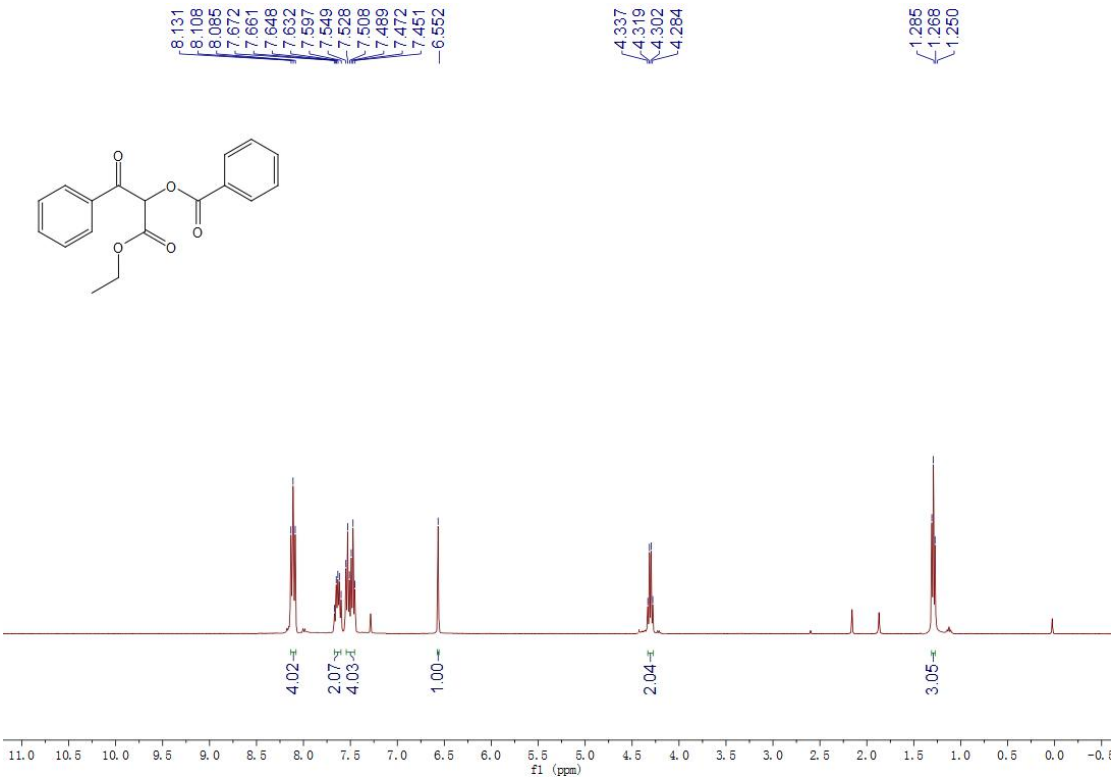

8.118
8.099
8.015
7.996
7.585
7.573
7.563
7.492
7.459
7.424
7.419
6.072
6.059
6.045
2.135
2.117
2.099
2.082
2.063
2.041
2.025
2.004
1.989
1.128
1.108
1.091
O
O
O
2.06
2.06
2.05
4.03
1.00
2.02
3.04
f1 (ppm)

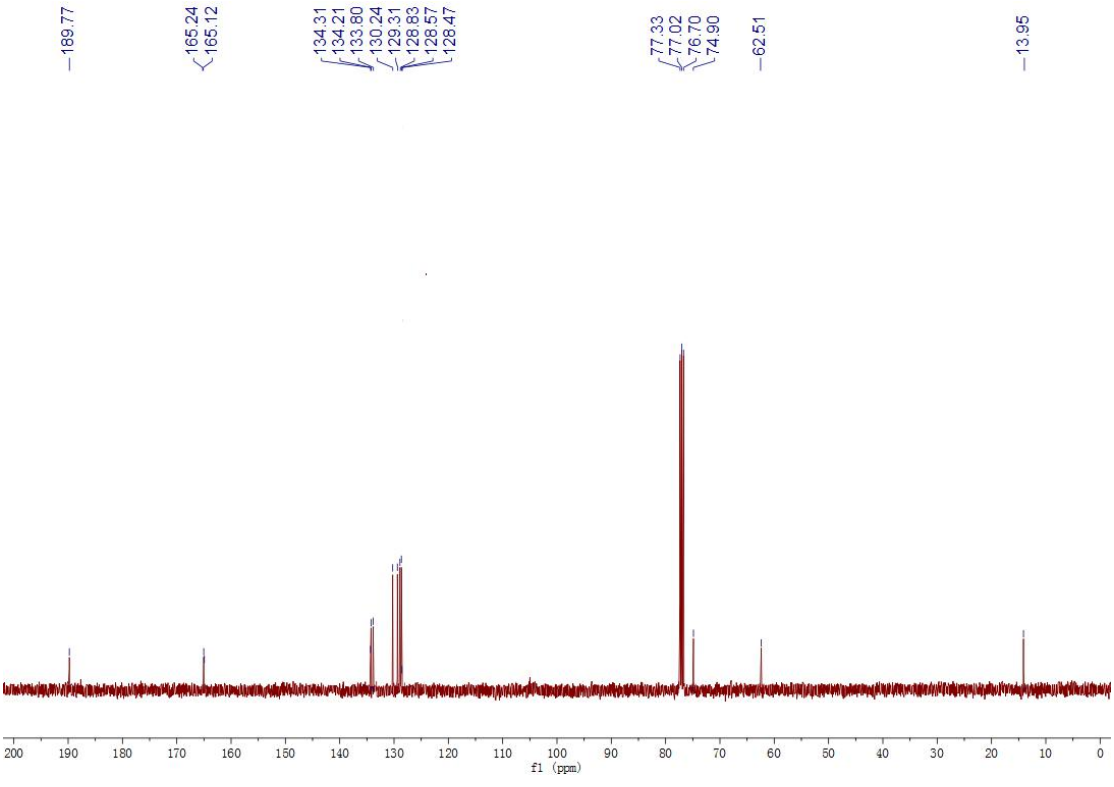

196.33
166.14
134.90
133.52
133.25
129.80
129.01
128.79
128.40
128.37
77.42
77.10
76.79
24.91
9.93
f1 (ppm)

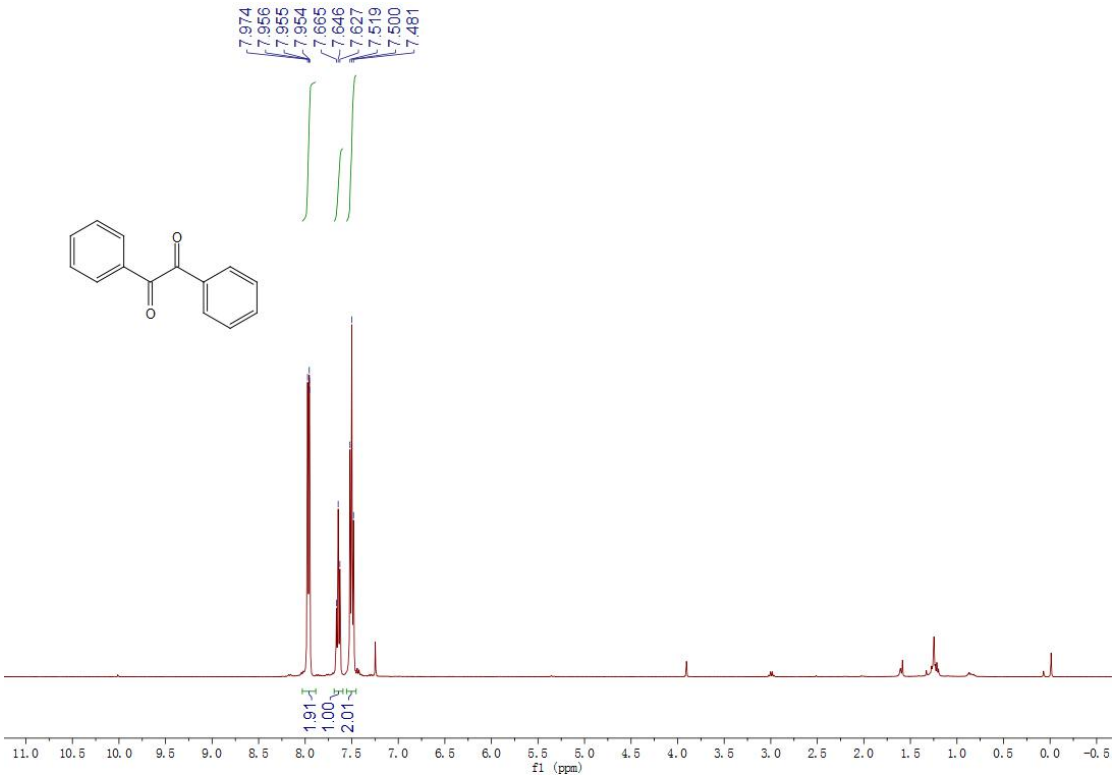

8.164
8.157
8.141
8.133
8.124
8.005
7.990
7.988
7.984
7.970
7.966
7.654
7.649
7.646
7.636
7.631
7.626
7.621
7.615
7.612
7.601
7.599
7.597
7.580
7.578
7.577
7.575
7.535
7.532
7.509
7.507
7.501
7.498
7.496
7.488
7.461
7.460
7.458
7.456
5.587

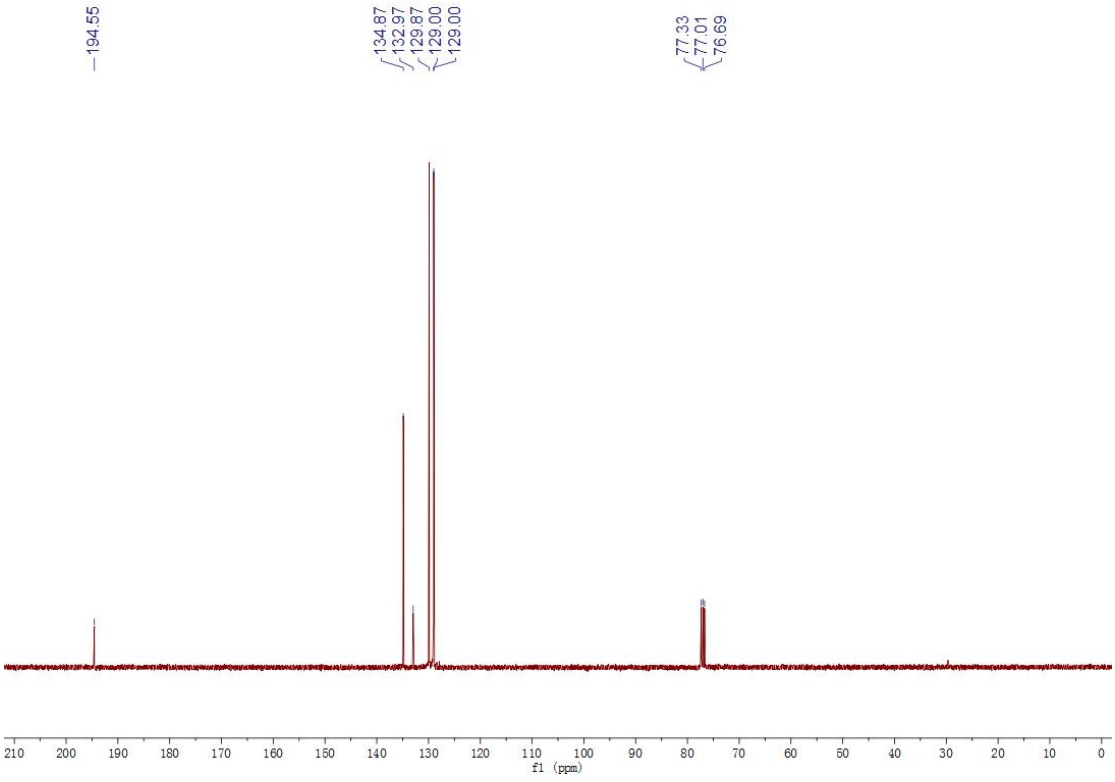

O
O
O
2.00
2.02
2.02
4.00
2.00
f1 (ppm)


192.28
166.26
134.04
133.53
130.45
130.15
129.05
128.76
128.65
127.98
77.47
77.15
76.83
66.65
f1 (ppm)

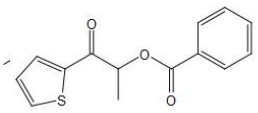

8.131
8.108
8.085
7.672
7.661
7.648
7.632
7.597
7.549
7.528
7.508
7.489
7.472
7.451
6.552
4.337
4.319
4.302
4.284
1.285
1.268
1.250
4.02
2.07
4.03
1.00
2.04
3.05
f1 (ppm)

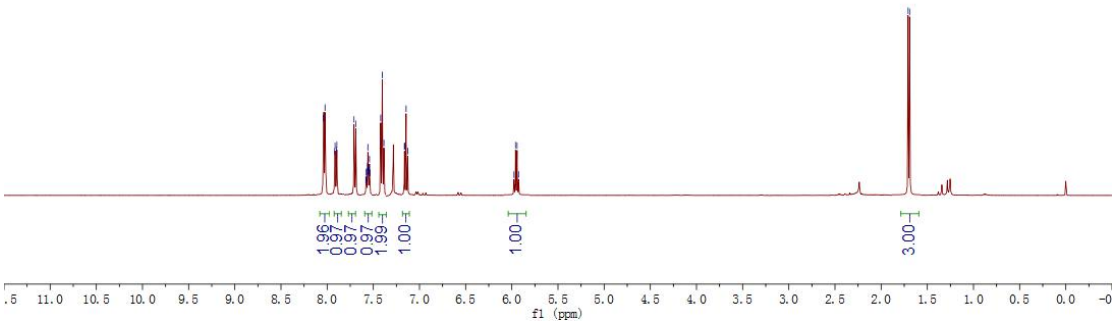

189.77
165.24
165.12
134.31
134.21
133.80
130.24
129.31
128.83
128.57
128.47
77.33
77.02
76.70
74.90
62.51
13.95
f1 (ppm)


7.974
7.956
7.955
7.954
7.665
7.646
7.627
7.519
7.500
7.481
O
O
1.91
1.00
2.01
f1 (ppm)

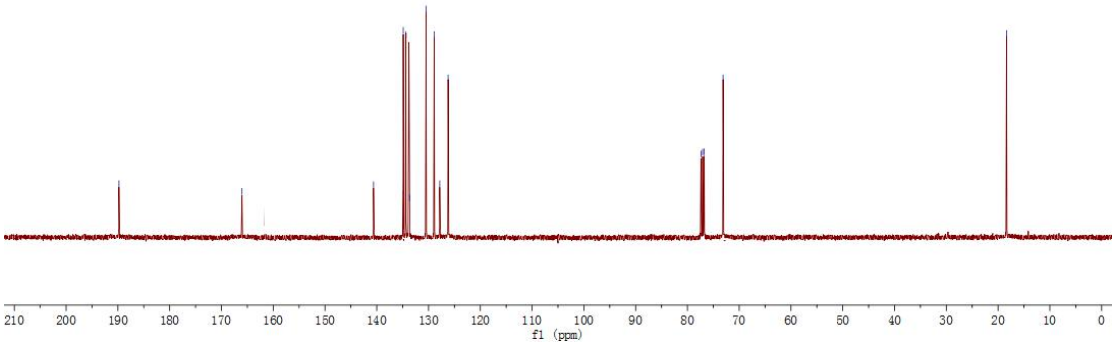

194.55
134.87
132.97
129.87
129.00
129.00
77.33
77.01
76.69
f1 (ppm)

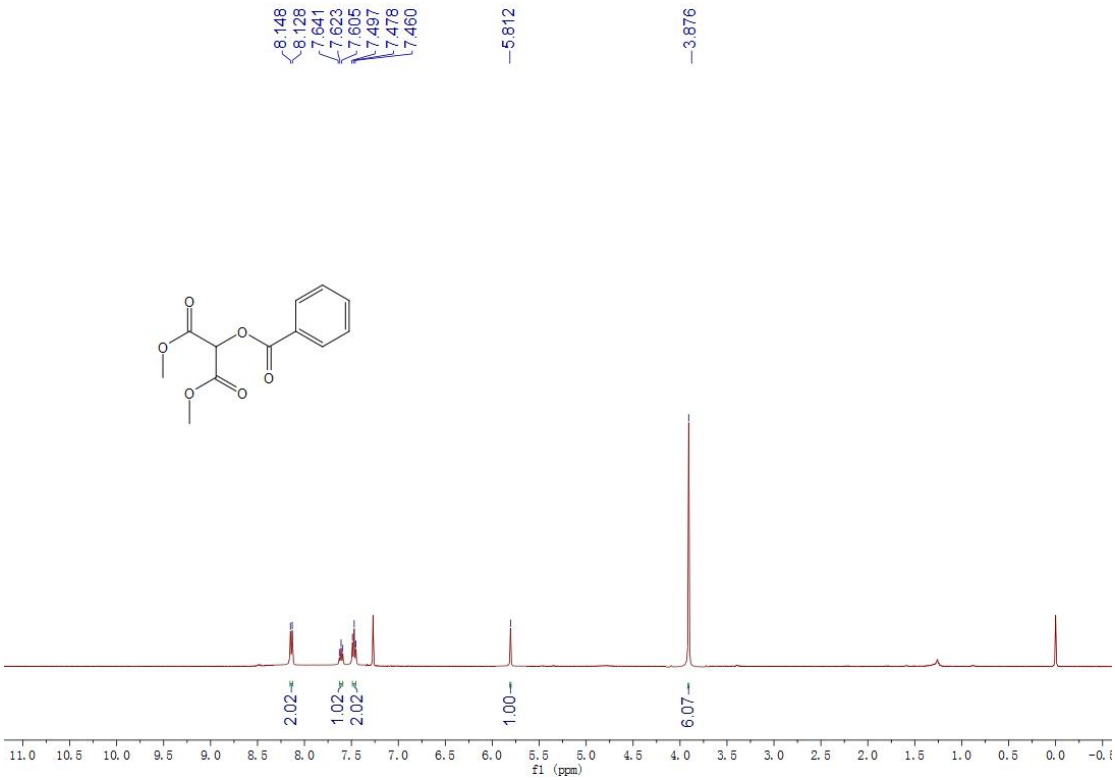

8.111
8.093
7.899
7.869
7.699
7.687
7.602
7.597
7.578
7.576
7.560
7.461
7.430
7.423
7.160
7.158
7.152
7.145
5.996
5.980
5.964
5.946
1.723
1.705

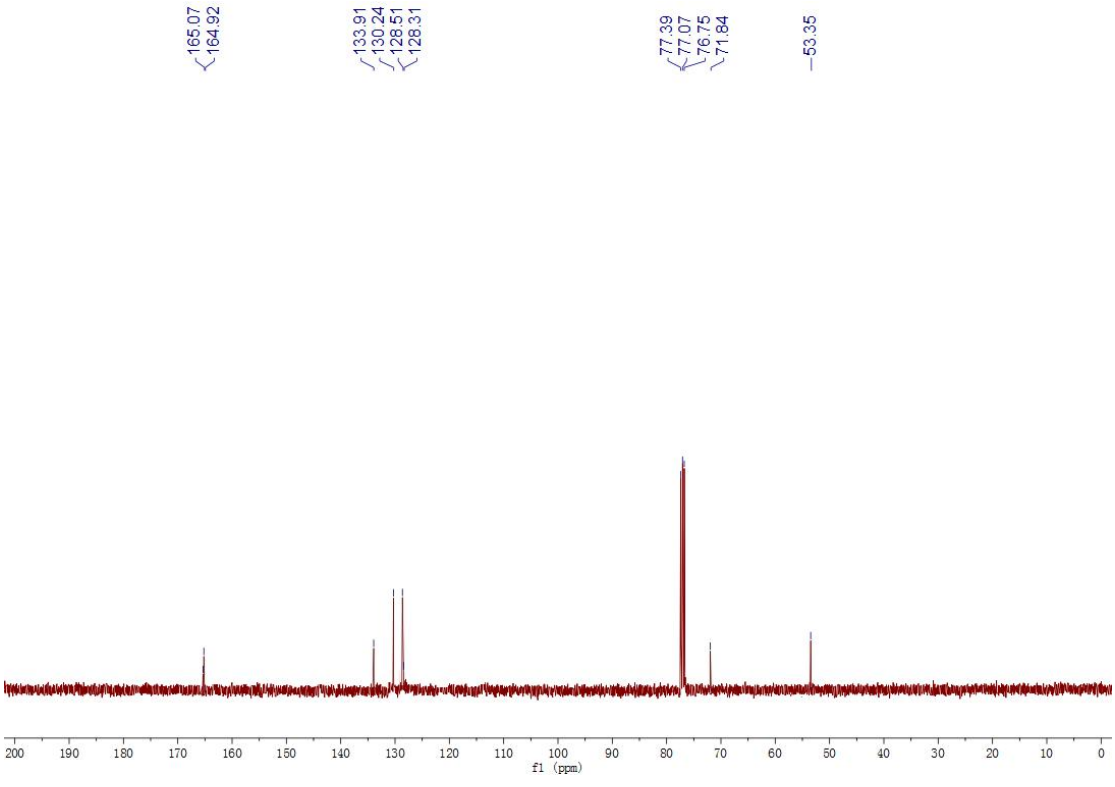

O
O
S
O


1.96
0.97
0.97
0.97
1.99
1.00
1.00
3.00
f1 (ppm)


189.75
165.99
140.57
134.56
133.47
132.87
130.03
128.60
127.94
126.30
77.39
77.07
76.75
72.94
17.75


f1 (ppm)


8.148
8.128
7.641
7.623
7.605
7.497
7.478
7.460
5.812
3.876
2.02
1.02
2.02
1.00
6.07
f1 (ppm)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164.92
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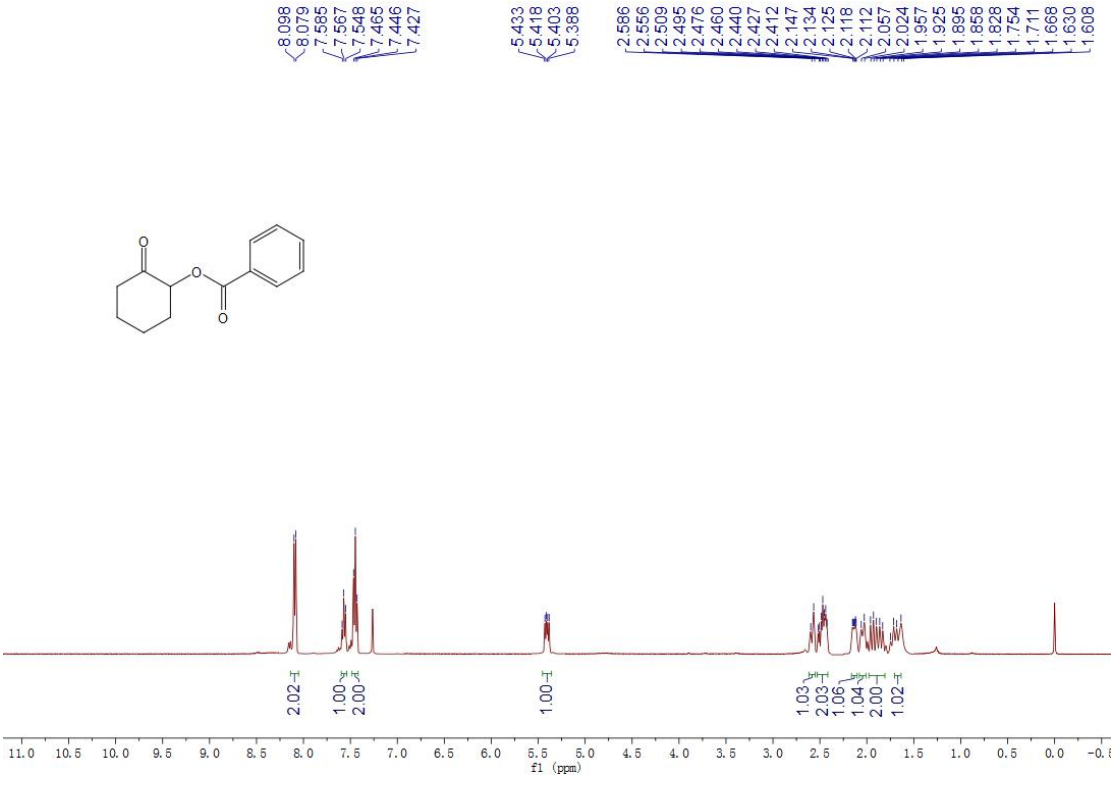
130.24
128.51
128.31
77.39
77.07
76.75
71.84
53.35
f1 (ppm)


8.098
8.079
7.585
7.567
7.548
7.465
7.446
7.427
5.433
5.418
5.403
5.388
2.586
2.556
2.509
2.495
2.476
2.460
2.440
2.427
2.412
2.147
2.134
2.125
2.118
2.112
2.057
2.024
1.957
1.925
1.895
1.858
1.828
1.754
1.711
1.668
1.630
1.608
O
O
O
2.02
1.00
2.00
1.00
1.03
2.03
1.06
1.04
2.00
1.02
f1 (ppm)
204.33
165.57
133.14
129.86
129.68
128.32
77.32
77.00
76.97
76.68
40.74
33.19
27.19
23.77
f1 (ppm)