Supplementary Information

NBS/DBU mediated one-pot synthesis of α-acyloxyketones from benzylic secondary alcohols and carboxylic acids

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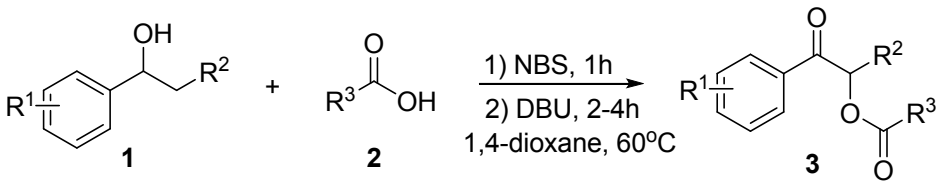
1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Beijing Ouhe Chemical Company and used as received without further purification unless otherwise stated. ^{1}H NMR, ^{13}C NMR and ^{31}P NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 spectrometer with TMS as internal standard (400 MHz ^{1}H, 100 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh).

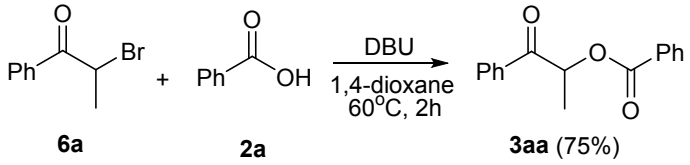
2. General procedure for NBS/DBU mediated one-pot synthesis of α-acyloxyketones from benzylic secondary alcohols and carboxylic acids



In a tube (25ml), alcohol **1** (0.25 mmol), carboxylic acid **2** (0.5 mmol), NBS (0.5 mmol), and 1,4-dioxane (2 mL) were added. Subsequently, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h, then DBU (0.5 mmol) was added to reaction system. After another 2-4 hours, the reaction was stopped and the solution was concentrated under vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3**.

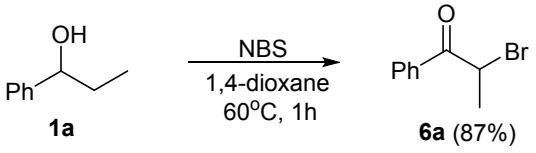
3. Preliminary mechanistic studies.

(1) The reaction of **6a** and **2a** in the presence of DBU.



In a sealed tube (25ml), α-bromo ketone **6a** (0.25 mmol), benzoic acid **2a** (0.25 mmol), and 1,4-dioxane (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 2 h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3aa** in 75% yield.

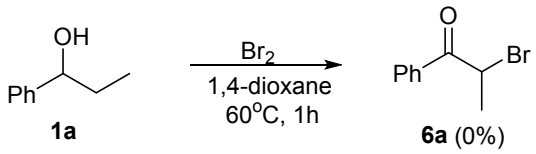
(2) The reaction of 1-phenylpropan-1-ol **1a** with NBS



In a tube (25ml), 1-phenylpropan-1-ol **1a** (0.25 mmol), NBS (0.5 mmol), and 1,4-

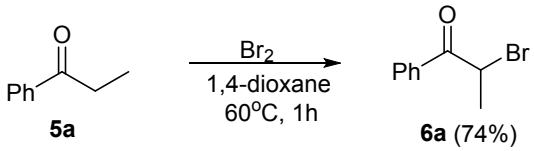
dioxane (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired α-bromo ketone **6a** in 87% yield.

(3) The reaction of 1-phenylpropan-1-ol **1a** with Br_2



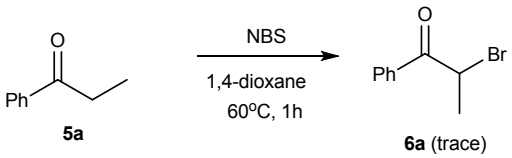
In a tube (25ml), 1-phenylpropan-1-ol **1a** (0.25 mmol), Br_2 (0.5 mmol), and 1,4-dioxane (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h. After the reaction, the solution was concentrated in vacuum. None of the desired desired α-bromo ketone **6a** was detected.

(4) The reaction of propiophenone **5a** with Br_2



In a tube (25ml), propiophenone **5a** (0.25 mmol), Br_2 (0.5 mmol), and 1,4-dioxane (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired α-bromo ketone **6a** in 74% yield.

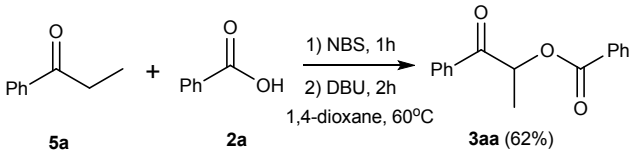
(4) The reaction of propiophenone **5a** with NBS



In a tube (25ml), propiophenone **5a** (0.25 mmol), NBS (0.5 mmol), and 1,4-

dioxane (2 mL) were added. Then, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h. After the reaction, the solution was concentrated in vacuum. Only a trace amount of the desired α-bromo ketone **6a** was detected.

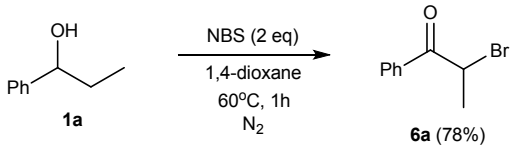
(5) The reaction of propiophenone **5a** with benzoic acid **2a** under the standard conditions.



5a **2a** **3aa** (62%)

In a tube (25ml), propiophenone **5a** (0.25 mmol), benzoic acid **2a** (0.375 mmol), NBS (0.5 mmol), and 1,4-dioxane (2 mL) were added. Subsequently, the tube was sealed and the reaction vessel was allowed to stir at 60 °C for 1 h, then DBU (0.5 mmol) was added to reaction system. After another 2 hours, the reaction was stopped and the solution was concentrated under vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3aa** in 62% yield.

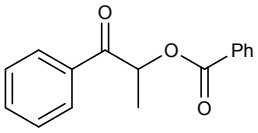
(6) The reaction of 1-phenylpropan-1-ol **1a** with NBS under N_2.



1a **6a** (78%)

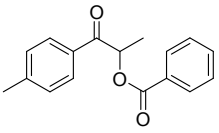
An oven-dried Schlenk tube was charged with a magnetic stir-bar, 1-phenylpropan-1-ol **1a** (0.25 mmol) and NBS (0.5 mmol). The tube was then evacuated and backfill with nitrogen. The evacuated/backfill sequence was repeated two additional times. Under a counter-flow of nitrogen, 1,4-dioxane (2 mL) was added. Then, the reaction vessel was allowed to stir at 60 °C for 1 h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired α-bromo ketone **6a** in 78% yield.

4. Characterization data of products



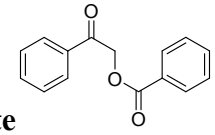
1-oxo-1-phenylpropan-2-yl benzoate

Compound **3aa** was obtained in 99% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.12 (d, J = 7.1 Hz, 2H), 8.03 (d, J = 7.1 Hz, 2H), 7.63-7.58 (m, 2H), 7.53-7.45 (m, 4H), 6.24 (q, J = 7.0 Hz, 3H), 1.70 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.7, 166.0, 134.5, 133.6, 133.3, 129.9, 129.5, 128.8, 128.5, 128.4, 71.9, 17.2; HRMS calc. for $C_{16}H_{14}O_3Na$ $(M+Na)^+$, 277.0841; found, 277.0846.



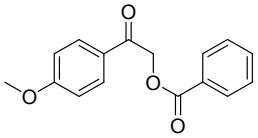
1-oxo-1-p-tolylpropan-2-yl benzoate

Compound **3ba** was obtained in 89% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.11 (d, J = 7.0 Hz, 2H), 7.93 (d, J = 8.2 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.9 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 6.22 (q, J= 7.0 Hz, 1H), 2.44 (s, 3H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.2, 166.0, 144.5, 133.2, 132.0, 129.9, 129.6, 129.5, 128.7, 128.4, 71.8, 21.7, 17.3; HRMS calc. for $C_{17}H_{16}O_3Na$ $(M+Na)^+$, 291.0997; found, 291.0999.



2-oxo-2-phenylethyl benzoate

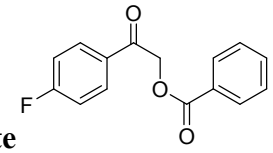
Compound **3ca** was obtained in 88% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.17 (d, J = 7.1 Hz, 2H), 8.00 (d, J = 7.1 Hz, 2H), 7.66-7.61 (m, 2H), 7.56-7.48 (m, 4H), 5.61 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 192.3, 166.0, 134.4, 133.9, 133.3, 130.0, 128.9, 128.5, 127.9, 66.5; HRMS calc. for $C_{15}H_{12}O_3Na$ $(M+Na)^+$, 263.0684; found, 263.0685.



2-(4-methoxyphenyl)-2-oxoethyl benzoate

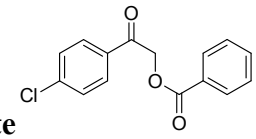
Compound **3da** was obtained in 85% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.17 (d, J = 7.1 Hz, 2H), 7.98 (d, J = 6.9 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.00 (d, J = 6.9 Hz, 2H), 5.57 (s, 2H),

3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 190.6, 166.1, 164.1, 133.3, 130.2, 130.0, 129.6, 128.4, 127.4, 114.1, 66.2, 55.5; HRMS calc. for $C_{16}H_{14}O_4Na$ $(M+Na)^+$, 293.0790; found, 293.0791.



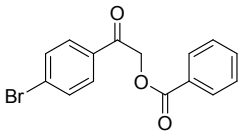
2-(4-fluorophenyl)-2-oxoethyl benzoate

Compound **3ea** was obtained in 69% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.16 (d, J = 7.1 Hz, 2H), 8.06-8.02 (m, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.50 (t, J = 7.9 Hz, 2H), 7.21 (t, J = 8.6 Hz, 2H), 5.57 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 190.7, 166.2 (d, J = 254.5 Hz), 166.1, 133.4, 130.8 (d, J = 2.9 Hz), 130.6 (d, J = 9.4 Hz), 130.0, 129.3, 128.5, 116.1 (d, J = 21.9 Hz), 66.3; HRMS calc. for $C_{15}H_{11}O_3FNa$ $(M+Na)^+$, 281.0590; found, 281.0593.



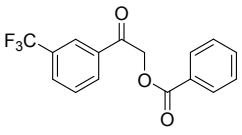
2-(4-chlorophenyl)-2-oxoethyl benzoate

Compound **3fa** was obtained in 85% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.16 (d, J = 7.1 Hz, 2H), 7.94 (d, J = 8.6 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.52-7.48 (m, 3H), 5.56 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 191.1, 166.0 140.4, 133.4, 132.7, 130.0, 129.3, 129.2, 128.5, 66.3; HRMS calc. for $C_{15}H_{11}O_3ClNa$ $(M+Na)^+$, 297.0294; found, 297.0291.



2-(4-bromophenyl)-2-oxoethyl benzoate

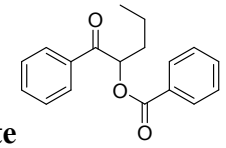
Compound **3ga** was obtained in 66% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.17-8.15 (m, 2H), 7.86 (d, J = 8.6 Hz, 2H), 7.68 (d, J = 8.6 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.9 Hz, 2H), 5.55 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 191.3, 166.0, 133.4, 133.1, 132.3, 130.0, 129.3, 129.3, 129.2, 128.5, 66.3; HRMS calc. for $C_{15}H_{11}O_3BrNa$ $(M+Na)^+$, 340.9789; found, 340.9791.



2-oxo-2-(3-(trifluoromethyl)phenyl)ethyl benzoate

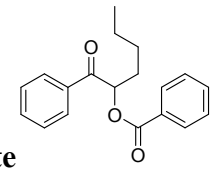
Compound **3ha** was obtained in 55% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.26 (s, 1H), 8.19-8.14 (m, 3H), 7.91 (d, J = 7.8 Hz,

1H), 7.69 (t, J = 7.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.51 (t, J = 7.9 Hz, 2H), 5.60 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 191.2, 166.0, 134.9, 133.5, 131.6 (d, J = 33.0 Hz), 131.0, 130.3 (q, J = 3.4 Hz, Hz), 130.0, 129.6, 129.2, 128.5, 128.4, 124.8 (d, J = 4.1 Hz), 66.4; HRMS calc. for $C_{16}H_{11}O_3F_3Na$ $(M+Na)^+$, 331.0558; found, 331.0561.



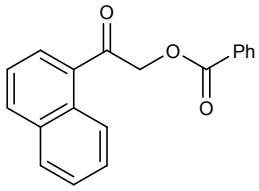
1-oxo-1-phenylpentan-2-yl benzoate

Compound **3ia** was obtained in 92% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.13 (d, J = 7.1 Hz, 2H), 8.03 (J = 7.2 Hz, 2H), 7.62-7.59 (m, 2H), 7.54-7.46 (m, 4H), 6.14 (dd, J_1 = 5.4 Hz, J_2 = 7.9 Hz, 1H), 2.04-1.99 (m, 2H), 1.66-1.59 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.5, 166.2, 134.9, 133.5, 133.2, 129.9, 129.6, 128.8, 128.5, 128.4, 75.6, 33.5, 19.0, 13.8; HRMS calc. for $C_{18}H_{18}O_3Na$ $(M+Na)^+$, 305.1154; found, 305.1155.



1-oxo-1-phenylhexan-2-yl benzoate

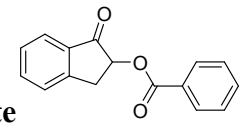
Compound **3ja** was obtained in 91% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.13 (d, J = 7.1 Hz, 2H), 8.03 (d, J = 7.1 Hz, 2H), 7.64-7.59 (m, 2H), 7.54-7.47 (m, 4H), 6.12 (t, J = 6.2 Hz, 1H), 2.06-2.01 (m, 2H), 1.59-1.53(m, 2H), 1.46-1.39 (m, 2H), 0.95 (t, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.5, 166.2, 135.0, 133.5, 133.2, 129.9, 129.6, 128.8, 128.5, 128.4, 75.8, 31.2, 27.7, 22.4, 13.8; HRMS calc. for $C_{19}H_{20}O_3Na$ $(M+Na)^+$, 319.1310; found, 319.1311.



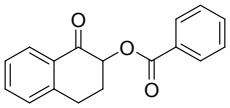
2-(naphthalen-2-yl)-2-oxoethyl benzoate

Compound **3ka** was obtained in 70% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.71 (d, J = 8.6 Hz, 1H), 8.18 (t, J = 7.1 Hz, 2H), 8.07 (d, J = 8.3 Hz, 1H), 7.98 (dd, J_1 = 0.9 Hz, J_2 = 7.2 Hz, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.65-7.61 (m, 2H), 7.59-7.56 (m, 2H), 7.50 (t, J = 7.8 Hz, 1H), 5.59 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.0, 166.1, 134.0, 133.5, 133.4, 132.5, 130.3,

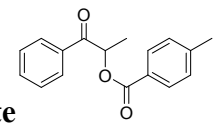
130.2, 130.0, 129.5, 128.5, 128.4, 127.5, 126.8, 125.7, 124.3, 67.9; HRMS calc. for $C_{19}H_{14}O_3Na$ $(M+Na)^+$, 313.0841; found, 313.0844.

1-oxo-2,3-dihydro-1H-inden-2-yl benzoate 

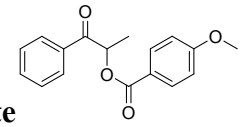
Compound **3la** was obtained in 88% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.12 (d, J = 7.1 Hz, 2H), 7.87 (d, J = 7.7 Hz, 1H), 7.70 (dt, J_1 = 1.1 Hz, J_2 = 7.6 Hz, 1H), 7.63-7.59 (m, 1H), 7.52-7.46 (m, 4H), 5.67 (dd, J_1 = 4.8 Hz, J_2 = 8.0 Hz, 1H), 3.80 (dd, J_1 = 8.0 Hz, J_2 = 17.0 Hz, 1H), 3.23 (dd, J_1 = 4.8 Hz, J_2 = 17.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 200.4, 166.1, 150.4, 135.9, 134.7, 133.4, 130.0, 129.4, 128.4, 128.2, 126.7, 124.6, 74.5, 33.6; HRMS calc. for $C_{16}H_{12}O_3Na$ $(M+Na)^+$, 275.0684; found, 275.0685.

1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl benzoate 

Compound **3ma** was obtained in 92% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.19-8.16 (m, 2H), 8.09 (dd, J_1 = 1.1 Hz, J_2 = 7.8 Hz, 1H), 7.64-7.59 (m, 1H), 7.56 (dt, J_1 = 1.4 Hz, J_2 = 7.5 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.38 (t, J = 7.6 Hz, 1H), 7.32 (d, J = 7.7 Hz, 1H), 5.83 (dd, J_1 = 5.2 Hz, J_2 = 13.2 Hz, 1H), 3.36-3.28 (m, 1H), 3.21-3.15 (m, 1H), 2.60-2.54 (m, 1H), 2.52-2.41 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 192.8, 165.8, 143.1, 133.9, 133.2, 131.7, 129.9, 129.8, 128.7, 128.4, 127.9, 127.0, 75.0, 29.3, 28.0; HRMS calc. for $C_{17}H_{14}O_3Na$ $(M+Na)^+$, 289.0841; found, 289.0845.

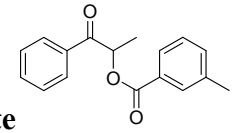
1-oxo-1-phenylpropan-2-yl 4-methylbenzoate 

Compound **3ab** was obtained in 90% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.04-7.99 (m, 4H), 7.61 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 6.21 (q, J = 7.0 Hz, 1H), 2.44 (s, 3H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.9, 166.1, 144.1, 134.5, 133.6, 129.9, 129.1, 128.8, 128.6, 126.7, 71.7, 21.7, 17.2; HRMS calc. for $C_{17}H_{16}O_3Na$ $(M+Na)^+$, 291.0997; found, 291.0993.



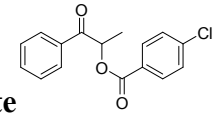
1-oxo-1-phenylpropan-2-yl 4-methoxybenzoate

Compound **3ac** was obtained in 91% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.08-8.01 (m, 4H), 7.61 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 6.94 (d, J = 9.0 Hz, 2H), 6.20 (q, J = 7.0 Hz, 1H), 3.89 (s, 3H), 1.68 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 197.0, 165.7, 163.7, 134.6, 133.5, 132.0, 128.8, 128.6, 121.9, 113.7, 71.6, 55.5, 17.2; HRMS calc. for $C_{17}H_{16}O_4Na$ $(M+Na)^+$, 307.0946; found, 307.0944.



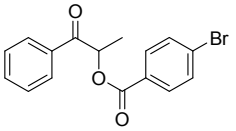
1-oxo-1-phenylpropan-2-yl 3-methylbenzoate

Compound **3ad** was obtained in 93% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (d, J = 7.8 Hz, 2H), 7.92 (d, J = 9.0 Hz, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.41 (d, J = 7.6 Hz, 1H), 7.36 (t, J = 7.5 Hz, 1H), 6.23 (q, J = 7.0 Hz, 1H), 2.43 (s, 3H), 1.70 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.8, 166.2, 138.2, 134.5, 134.1, 133.6, 130.4, 129.4, 128.8, 128.6, 128.3, 127.1, 71.8, 21.3, 17.2; HRMS calc. for $C_{17}H_{16}O_3Na$ $(M+Na)^+$, 291.0997; found, 291.0991.



1-oxo-1-phenylpropan-2-yl 4-chlorobenzoate

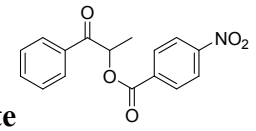
Compound **3ae** was obtained in 92% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.07-8.01 (m, 4H), 7.63 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.45 (d, J = 8.6 Hz, 2H), 6.22 (q, J = 7.0 Hz, 1H), 1.70 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.5, 165.1, 139.8, 134.3, 133.7, 131.3, 128.9, 128.8, 128.5, 128.0, 72.1, 17.2; HRMS calc. for $C_{16}H_{13}O_3ClNa$ $(M+Na)^+$, 311.0451; found, 311.0453.



1-oxo-1-phenylpropan-2-yl 4-bromobenzoate

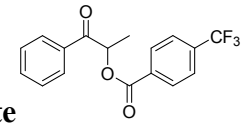
Compound **3af** was obtained in 90% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02-7.97 (m, 4H), 7.64-7.60 (m, 3H), 7.52 (t, J = 7.9 Hz, 2H), 6.22 (q, J = 7.0 Hz, 1H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100

MHz, ppm): δ 196.5, 165.3, 134.3, 133.7, 131.8, 131.4, 128.9, 128.5, 128.4, 72.1, 17.3; HRMS calc. for $C_{16}H_{13}O_3BrNa$ $(M+Na)^+$, 354.9946; found, 354.9949.



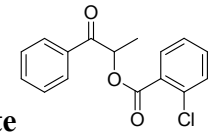
1-oxo-1-phenylpropan-2-yl 4-nitrobenzoate

Compound **3ag** was obtained in 92% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.35-8.29 (m, 4H), 8.01 (t, J = 7.2 Hz, 2H), 7.66 (t, J = 7.4 Hz, 1H), 7.54 (t, J = 7.9 Hz, 2H), 6.28 (q, J = 7.0 Hz, 1H), 1.74 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.0, 164.2, 150.8, 135.0, 134.2, 133.9, 131.0, 129.0, 128.5, 123.6, 72.8, 17.3; HRMS calc. for $C_{16}H_{13}NO_5Na$ $(M+Na)^+$, 322.0691, found, 322.0693.



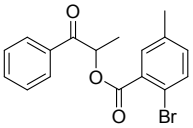
1-oxo-1-phenylpropan-2-yl 4-(trifluoromethyl)benzoate

Compound **3ah** was obtained in 72% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.24 (d, J = 8.0 Hz, 2H), 8.01 (d, J = 7.2 Hz, 2H), 7.74 (d, J = 8.2 Hz, 2H), 7.64 (t, J = 7.3 Hz, 1H), 7.53 (t, J = 7.8 Hz, 2H), 6.26 (q, J = 7.0 Hz, 1H), 1.72 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.3, 164.8, 134.7(d, J = 32.5 Hz), 134.3, 133.8, 132.8, 130.3, 128.9, 128.5, 125.5 (q, J = 3.7 Hz), 123.6 (d, J = 271.1 Hz), 72.4, 17.3; HRMS calc. for $C_{17}H_{13}O_3F_3Na$ $(M+Na)^+$, 345.0714; found, 345.0717.



1-oxo-1-phenylpropan-2-yl 2-chlorobenzoate

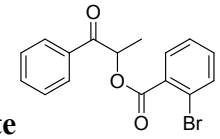
Compound **3ai** was obtained in 93% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (t, J = 7.4 Hz, 2H), 7.98 (d, J = 7.1 Hz, 1H), 7.64 (t, J = 7.3 Hz, 1H), 7.53 (t, J = 7.9 Hz, 2H), 7.50-7.44 (m, 2H), 7.38-7.34 (m, 1H), 6.27 (q, J = 7.0 Hz, 1H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.4, 164.9, 134.1, 133.6, 132.8, 131.8, 131.1, 129.4, 128.8, 128.5, 126.6, 72.3, 17.1; HRMS calc. for $C_{16}H_{13}O_3ClNa$ $(M+Na)^+$, 311.0451; found, 311.0553.



1-oxo-1-phenylpropan-2-yl 2-bromo-5-methylbenzoate

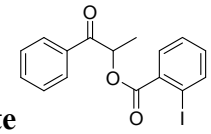
Compound **3aj** was obtained in 88% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (d, J = 7.7 Hz, 2H), 7.76 (d, J = 1.9 Hz, 1H),

7.63 (t, J = 7.2 Hz, 1H), 7.56-7.51 (m, 3H), 7.18 (dd, J_1 = 2.2 Hz, J_2 = 8.2 Hz, 1H), 6.27 (q, J = 7.0 Hz, 1H), 2.37 (s, 3H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.5, 165.6, 137.4, 134.4, 134.1, 133.8, 133.7, 132.3, 131.0, 128.8, 128.6, 118.5, 72.3, 20.8, 17.2; HRMS calc. for $C_{17}H_{15}O_3BrNa$ $(M+Na)^+$, 369.0102; found, 369.0104.



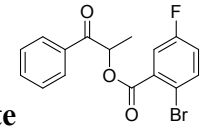
1-oxo-1-phenylpropan-2-yl 2-bromobenzoate

Compound **3ak** was obtained in 84% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm):δ 8.01 (d, J = 7.2 Hz, 2H), 7.97 (dd, J_1 = 2.0 Hz, J_2 = 7.6 Hz, 1H), 7.69 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.43-7.37 (m, 2H), 6.27 (q, J = 7.0 Hz, 1H), 1.69 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.4, 165.4, 134.4, 134.4, 133.7, 132.8, 131.8, 131.4, 128.8, 128.5, 127.2, 121.9, 72.4, 17.1; HRMS calc. for $C_{16}H_{13}O_3BrNa$ $(M+Na)^+$, 354.9946; found, 354.9949.



1-oxo-1-phenylpropan-2-yl 2-iodobenzoate

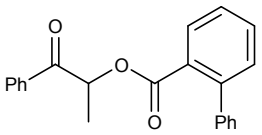
Compound **3al** was obtained in 78% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.2 Hz, 3H), 7.99 (dd, J_1 = 1.7 Hz, J_2 = 7.8 Hz, 1H), 7.66-7.61 (m, 1H), 7.53 (t, J = 7.8 Hz, 2H), 7.45 (dt, J_1 = 1.1 Hz, J_2 = 7.6 Hz, 1H), 7.20 (dt, J_1 = 1.7 Hz, J_2 = 7.7 Hz, 1H), 6.28 (q, J = 7.0 Hz, 1H), 1.70 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.4, 165.8, 141.4, 134.3, 134.2, 133.7, 133.0, 131.6, 128.9, 128.6, 128.0, 94.3, 72.5, 17.2; HRMS calc. for $C_{16}H_{13}O_3INa$ $(M+Na)^+$, 402.9807; found, 402.9809 .



1-oxo-1-phenylpropan-2-yl 2-bromo-5-fluorobenzoate

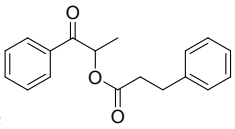
Compound **3am** was obtained in 78% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 7.1 Hz, 2H), 7.71 (dd, J_1 = 3.1 Hz, J_2 = 8.6 Hz, 1H), 7.67-7.62 (m, 2H), 7.53 (t, J = 7.9 Hz, 2H), 7.14-7.09 (m, 1H), 6.26 (q, J = 7.0 Hz, 1H), 1.70 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.1, 164.3, 161.2 (d, J = 245.7 Hz), 135.8 (d, J = 7.5 Hz), 134.2, 133.8, 132.7 (d, J = 7.4

Hz), 128.9, 128.5, 120.3 (d, J = 22.1 Hz), 119.0 (d, J = 24.5 Hz), 116.3 (d, J = 3.6 Hz), 72.7, 17.2; HRMS calc. for $C_{16}H_{12}O_3BrFNa$ $(M+Na)^+$, 372.9852; found, 372.9857.



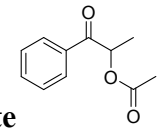
1-oxo-1-phenylpropan-2-yl biphenyl-2-carboxylate

Compound **3an** was obtained in 82% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.97-7.92 (m, 3H), 7.61-7.55 (m, 2H), 7.50-7.45 (m, 3H), 7.41-7.35(m, 6H), 5.96 (q, J = 7.0 Hz, 1H), 1.32 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.5, 167.6, 143.0, 141.4, 134.4, 133.5, 131.6, 130.8, 130.4, 130.0, 128.7, 128.6, 128.5, 128.0, 127.2, 127.2, 72.0, 16.8; HRMS calc. for $C_{22}H_{18}O_3Na$ $(M+Na)^+$, 353.1154; found, 353.1151.



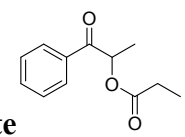
1-oxo-1-phenylpropan-2-yl 3-phenylpropanoate

Compound **3ao** was obtained in 93% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.96 (d, J = 7.2 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.9 Hz, 2H), 7.31 (t, J = 7.6 Hz, 2H), 7.24-7.22 (m, 3H), 6.00 (q, J = 7.0 Hz, 1H), 3.00 (t, J = 7.9 Hz, 2H), 2.80-2.75 (m, 2H), 1.54 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.9, 172.3, 140.4, 134.4, 133.6, 128.8, 128.5, 128.5, 128.3, 126.3, 71.4, 35.5, 30.8, 17.1; HRMS calc. for $C_{18}H_{18}O_3Na$ $(M+Na)^+$, 305.1154; found, 305.1157.



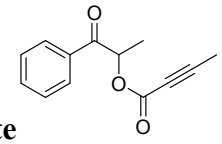
1-oxo-1-phenylpropan-2-yl acetate

Compound **3ap** was obtained in 84% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.97 (d, J = 7.2 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 5.99 (q, J = 7.0 Hz, 1H), 2.17 (s, 3H), 1.56 (d, J = 7.1 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 196.9, 170.4, 134.5, 133.5, 128.8, 128.5, 71.4, 20.7, 17.1; HRMS calc. for $C_{11}H_{12}O_3Na$ $(M+Na)^+$, 215.0684; found, 215.0682.



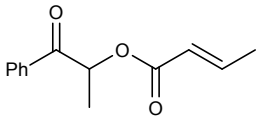
1-oxo-1-phenylpropan-2-yl propionate

Compound **3aq** was obtained in 85% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.97 (d, J = 7.7 Hz, 2H), 7.61 (t, J = 7.3 Hz, 1H), 7.50 (t, J = 7.8 Hz, 2H), 6.00 (q, J = 7.0 Hz, 1H), 2.47-2.43 (m, 2H), 1.55 (d, J = 7.0 Hz, 3H), 1.18 (t, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 197.1, 173.9, 134.6, 133.5, 128.7, 128.4, 71.2, 27.3, 17.1, 8.9; HRMS calc. for $C_{12}H_{14}O_3Na$ $(M+Na)^+$, 229.0841; found, 229.0845.



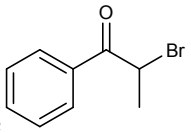
1-oxo-1-phenylpropan-2-yl but-2-ynoate

Compound **3ar** was obtained in 90% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.96 (d, J = 8.1 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.9 Hz, 2H), 6.05 (q, J = 7.0 Hz, 1H), 2.03 (s, 3H), 1.60 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 195.7, 152.8, 134.1, 133.7, 128.8, 128.5, 87.1, 72.7, 71.9, 17.1, 3.9; HRMS calc. for $C_{13}H_{12}O_3Na$ $(M+Na)^+$, 239.0684; found, 239.0687.



(*E*)-1-oxo-1-phenylpropan-2-yl but-2-enoate

Compound **3as** was obtained in 50% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 500 MHz, ppm): δ 7.98 (d, J = 7.2 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.9 Hz, 2H), 7.11-7.04 (m, 1H), 6.05(q, J = 7.0 Hz, 1H), 5.96 (dq, J_1 = 1.6 Hz, J_2 = 15.6 Hz, 1H), 1.91 (dd, J_1 = 1.7 Hz, J_2 = 7.0 Hz, 3H), 1.58 (d, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm): δ 197.0, 165.7, 146.1, 134.5, 133.5, 128.8, 128.5, 121.9, 71.1, 18.1, 17.1; HRMS calc. for $C_{13}H_{14}O_3Na$ $(M+Na)^+$, 241.0841; found, 241.0845.

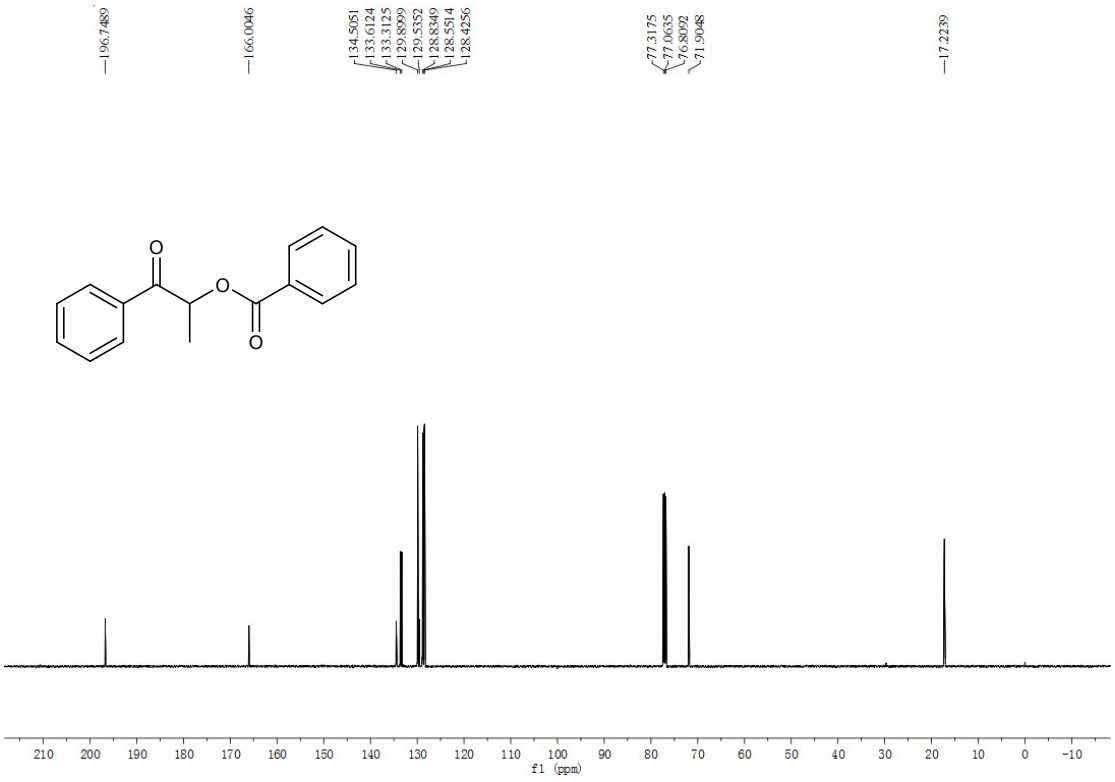


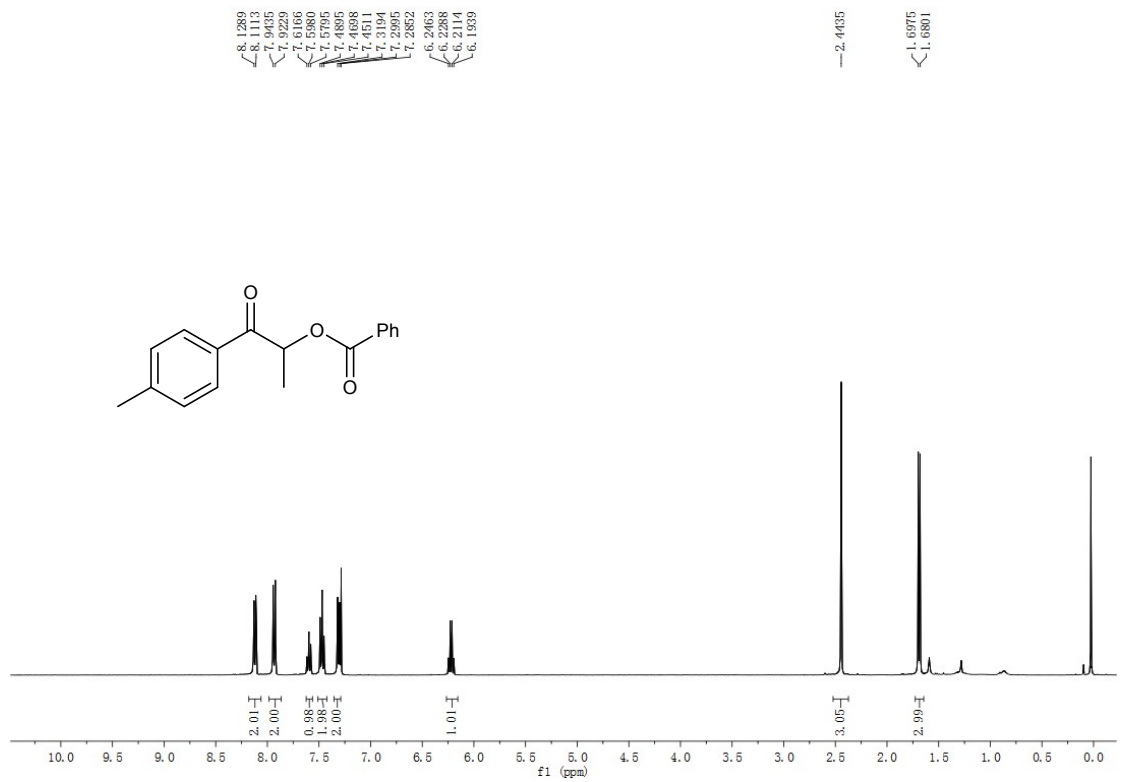
2-bromo-1-phenylpropan-1-one

^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.05 (t, J = 7.2 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.8 Hz, 2H), 5.3 (q, J = 6.6 Hz, 1H), 1.93 (d, J = 6.6 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 193.3, 134.1, 133.6, 128.9, 128.7, 41.5, 20.1.

HRMS calc. for C_9H_9BrONa $(M+Na)^+$, 234.9734; found, 234.9729.

5. Copies of NMR spectra for 3aa−3as, 6a

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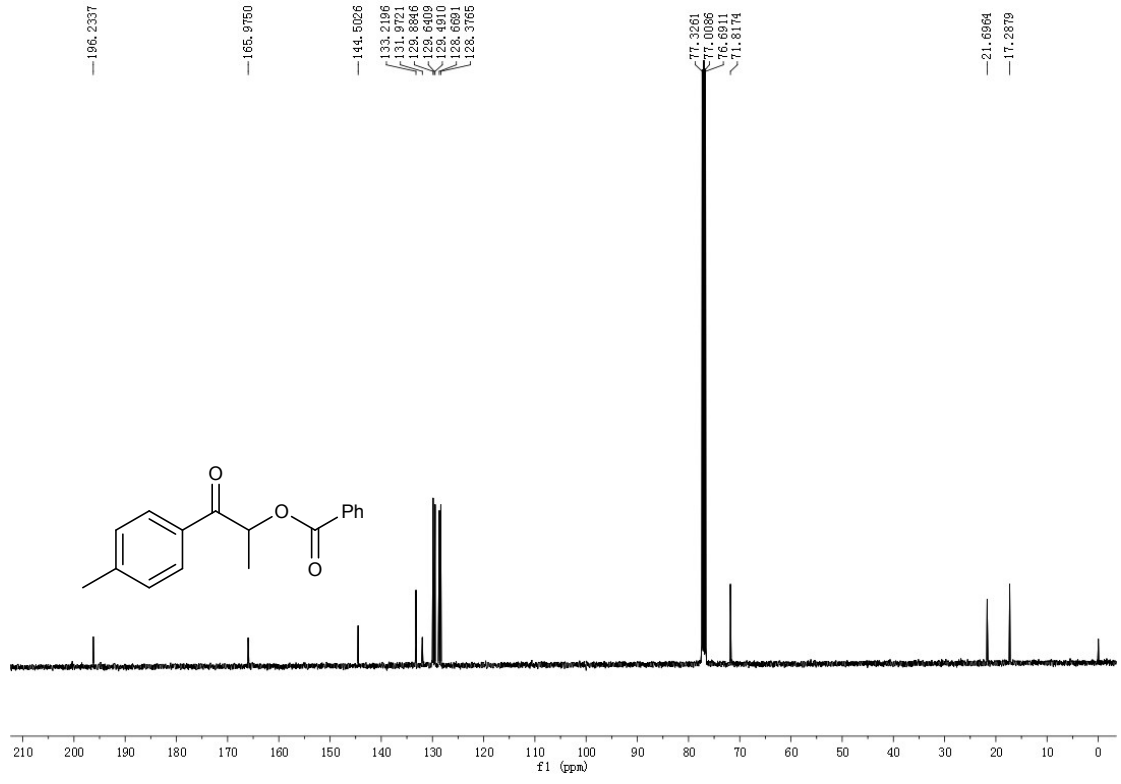
7.3194
7.2995
7.2852
6.2463
6.2288
6.2114
6.1939
2.4435
1.6975
1.6801
O
O
Ph
O
2.01
2.00
0.98
1.98
2.00
1.01
3.05
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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144.5026
133.2196
131.9721
128.8846
128.6969
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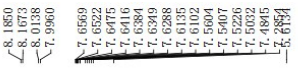
128.4691
128.3765
77.3261
77.0086
76.6911
71.8174
21.6964
17.2879
O
O
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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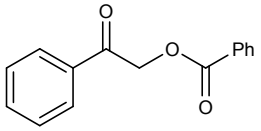
7.5032
7.4845
7.2854
5.6194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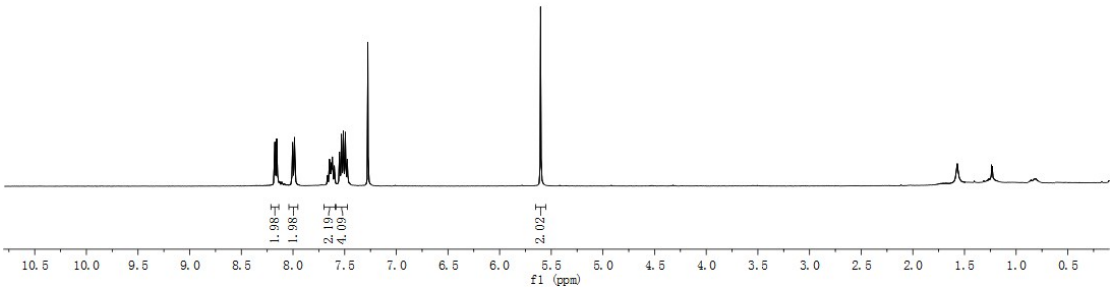
Ph
O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2.19
4.09
2.02
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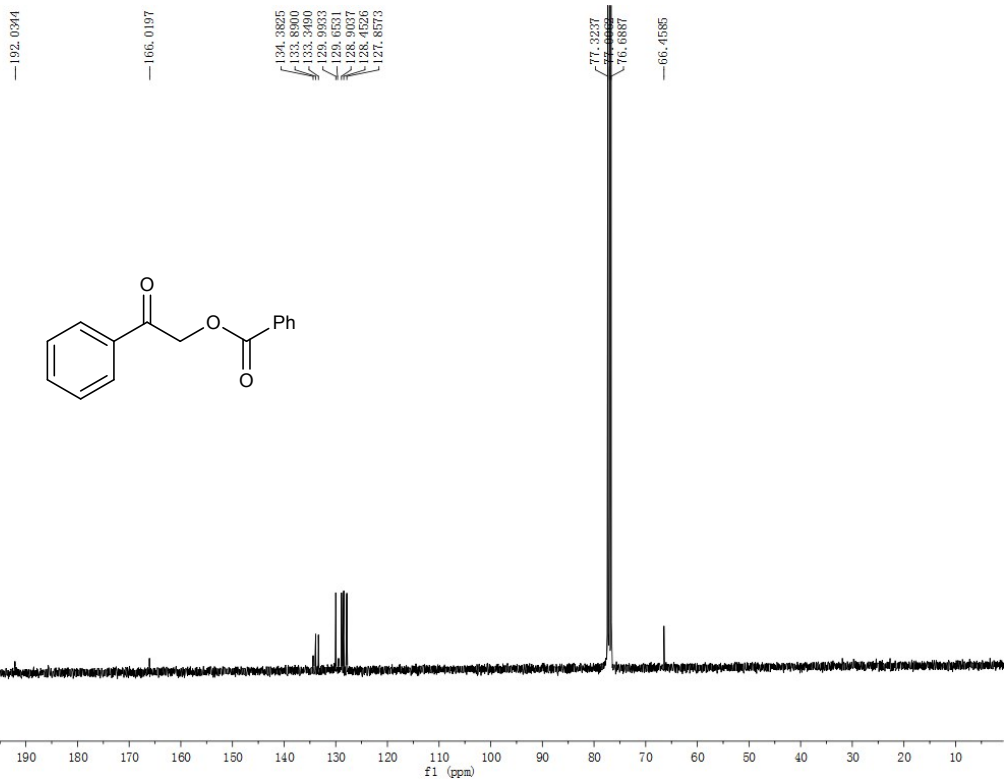
f1 (ppm)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133.3490
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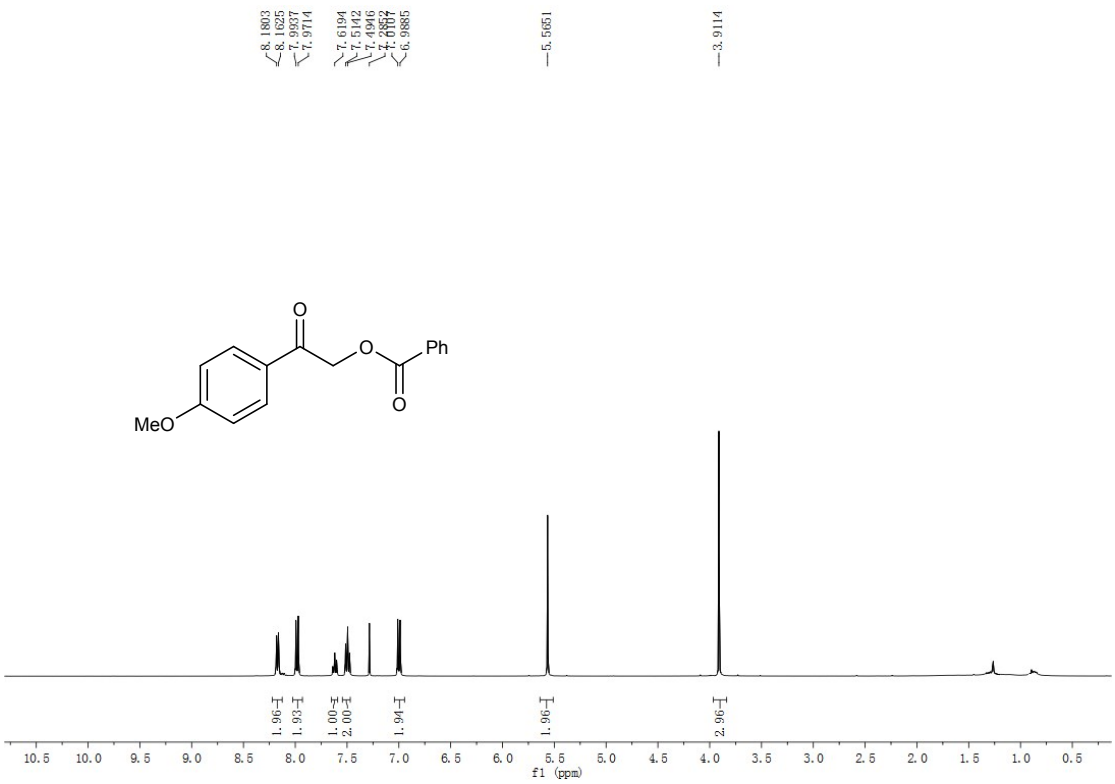
76.6887
66.4585
O
O
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.6194
7.5142
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5.5651
3.9114
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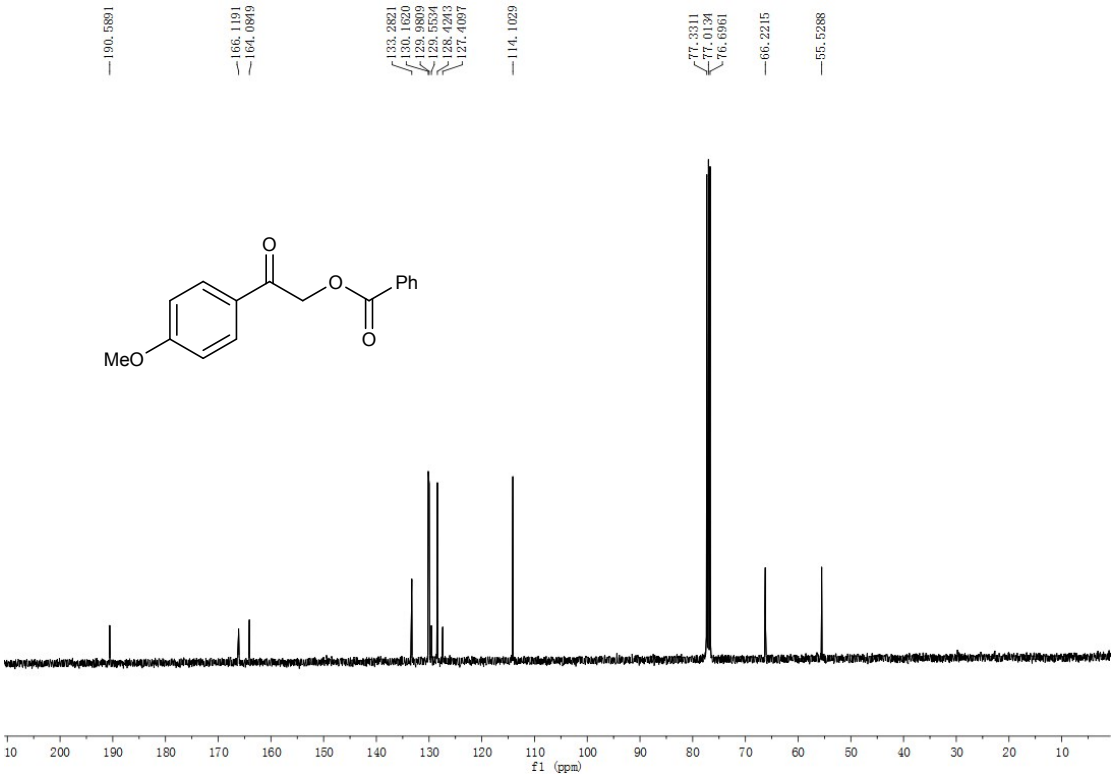
O
Ph
O
MeO
1.96
1.93
1.00
2.00
1.94
1.96
2.96
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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130.1620
129.9809
129.5534
128.4243
127.4097
114.1029
77.3311
77.0134
76.6961
66.2215
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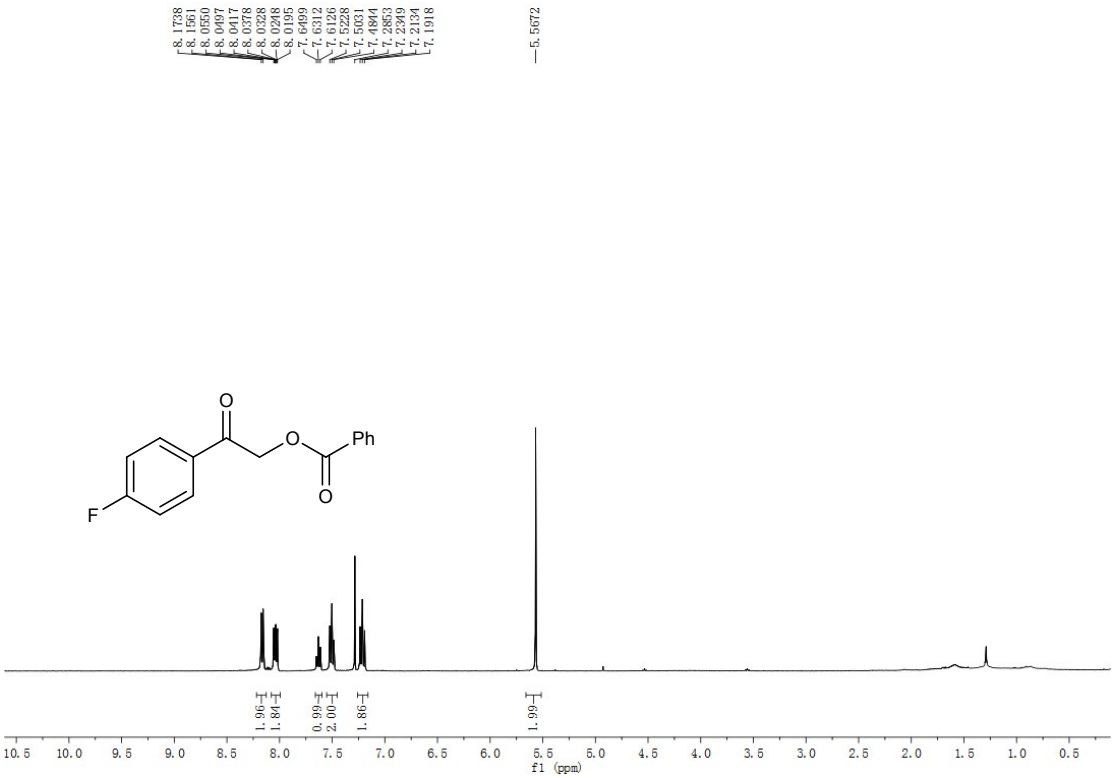
O
O
Ph
O
MeO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.0195
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7.6126
7.5228
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7.4894
7.2853
7.2349
7.2134
7.1918
5.5672
O
O
Ph
O
F
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1.84
0.99
2.00
1.86
1.99
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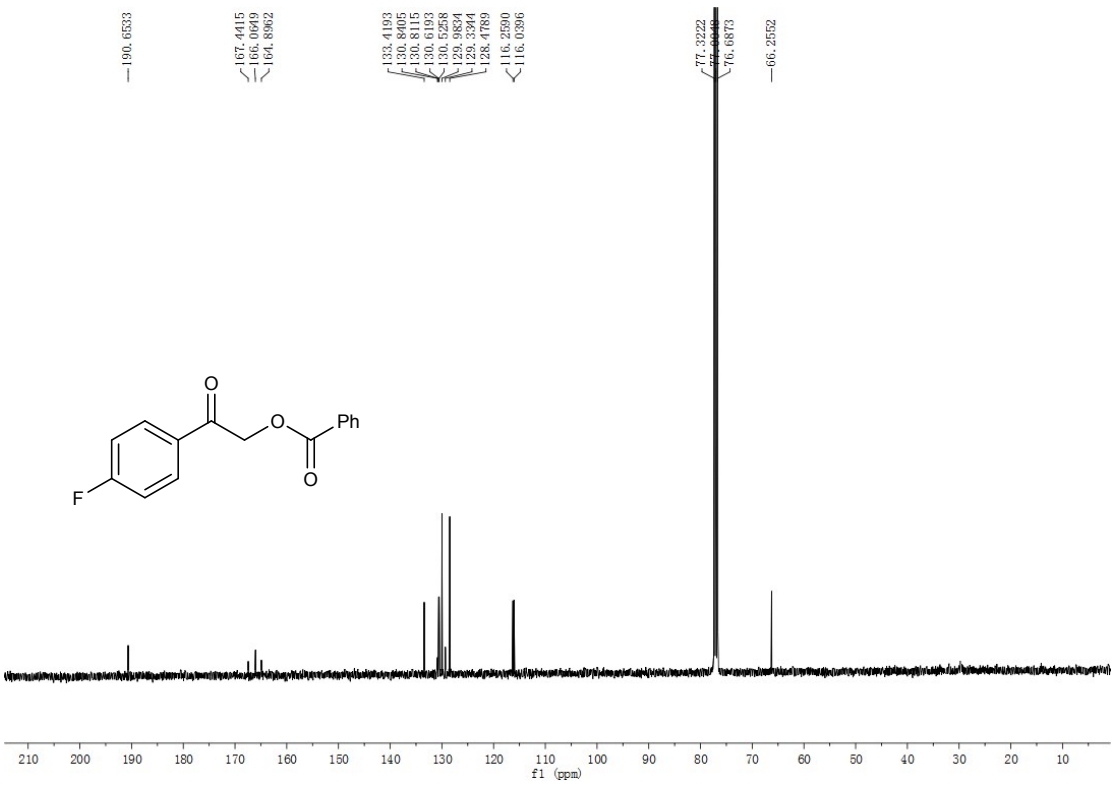
f1 (ppm)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130.8405
130.8115
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129.3344
128.4789
116.2590
116.0396
77.3222
76.6873
66.2552
O
O
Ph
O
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.1688
8.1511
7.9524
7.9310
7.6501
7.6315
7.6129
7.5232
7.5021
7.4835
7.2851
5.5599
O
O
Ph
O
Cl
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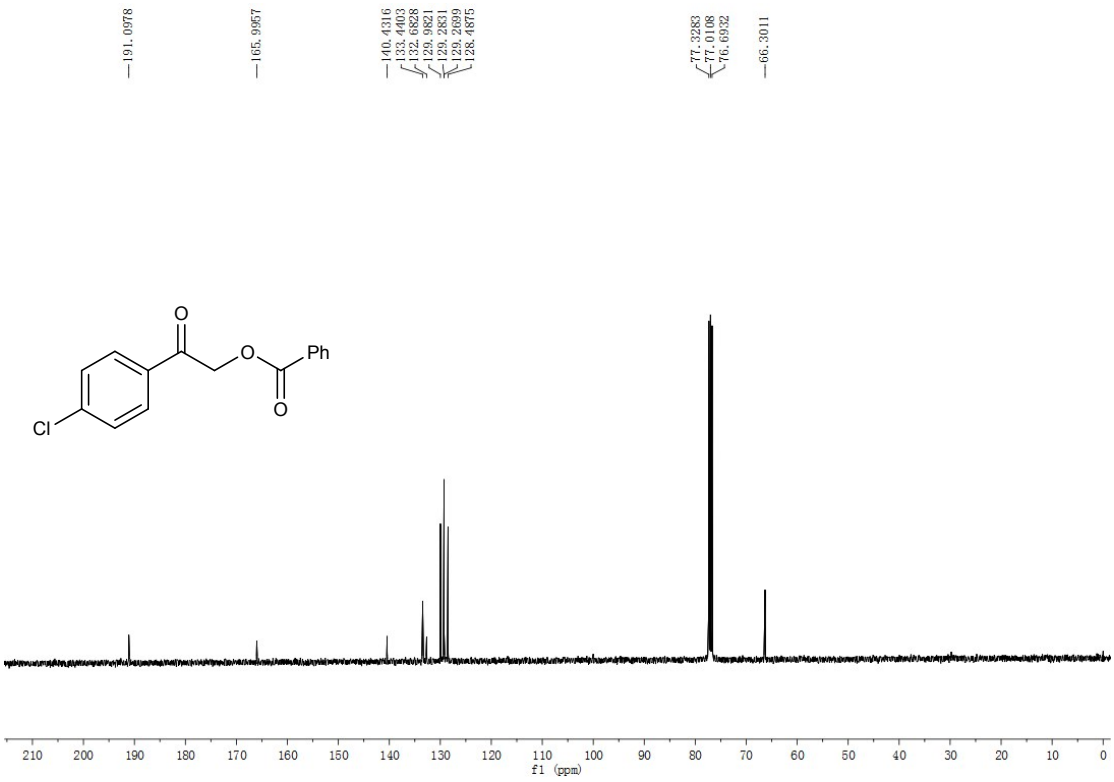
1.95
1.00
3.80
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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77.0108
76.6932
66.3011
O
O
Ph
O
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.1702
8.1672
8.1542
8.1496
8.1461
7.8742
7.8527
7.6931
7.6716
7.6498
7.6312
7.6126
7.5218
7.5021
7.4833
7.2852
5.5514
O
O
Ph
O
Br
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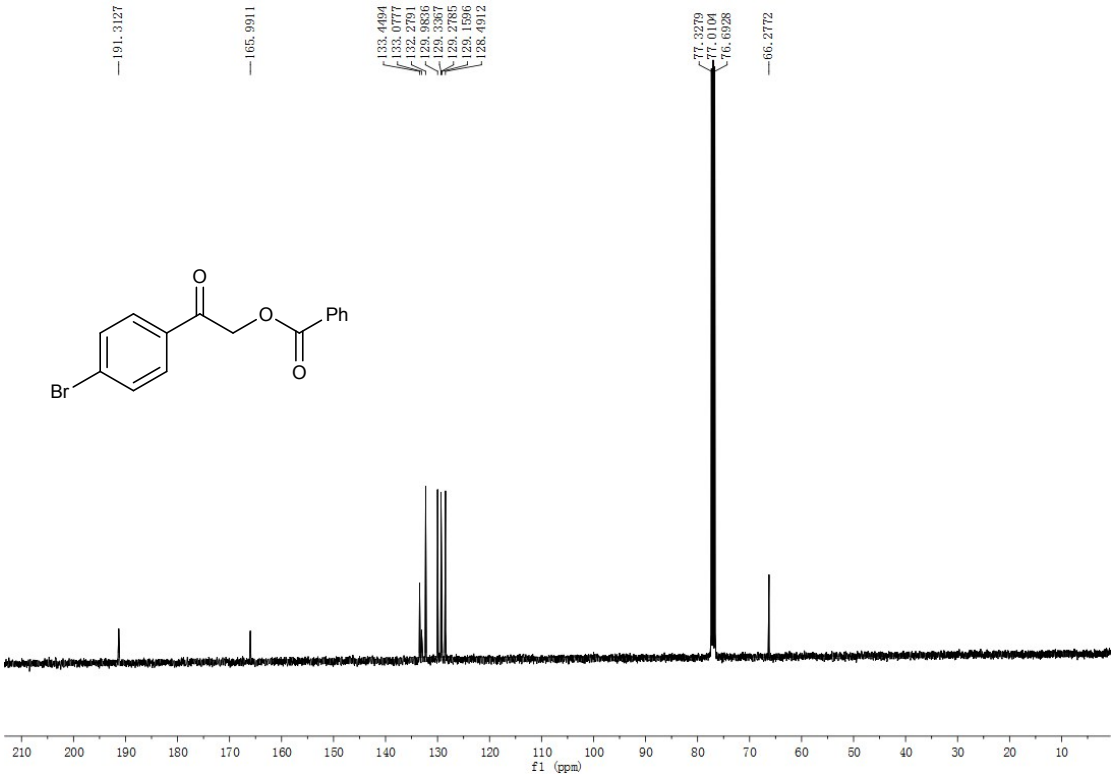
2.00
1.83
1.00
1.95
1.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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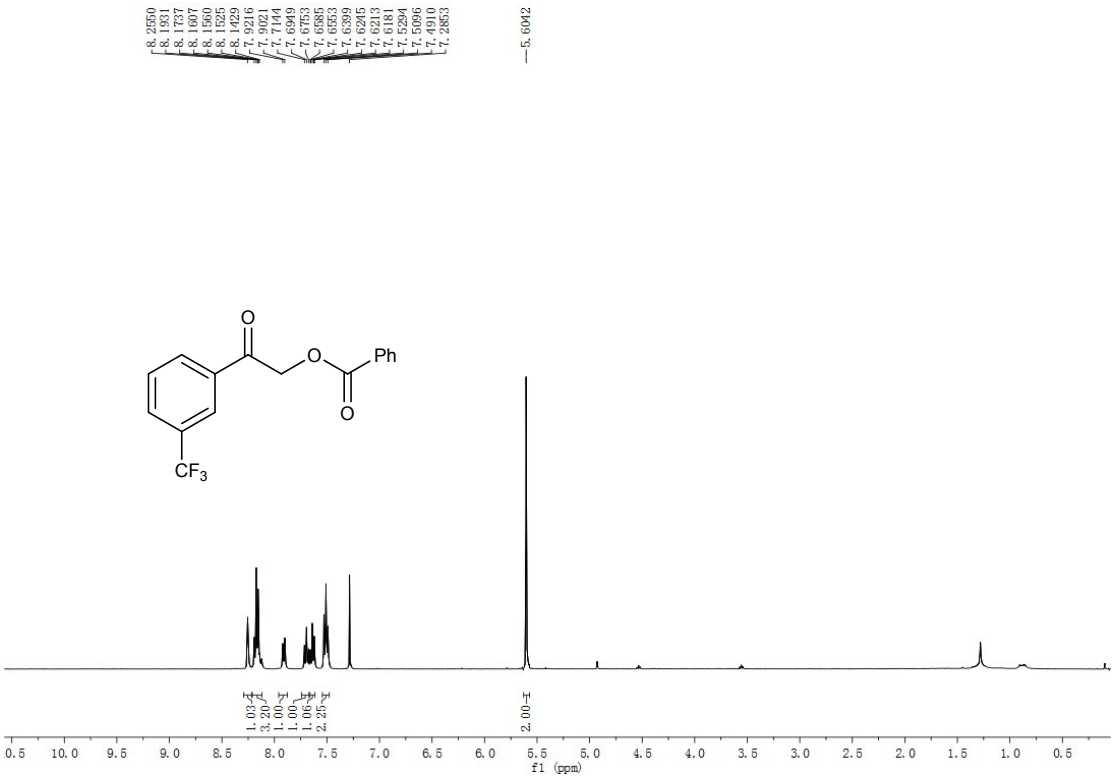
O
O
Ph
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.6753
7.6585
7.6553
7.6399
7.6245
7.6213
7.6181
7.5294
7.5096
7.4910
7.2853
5.6042
O
O
Ph
O
CF3
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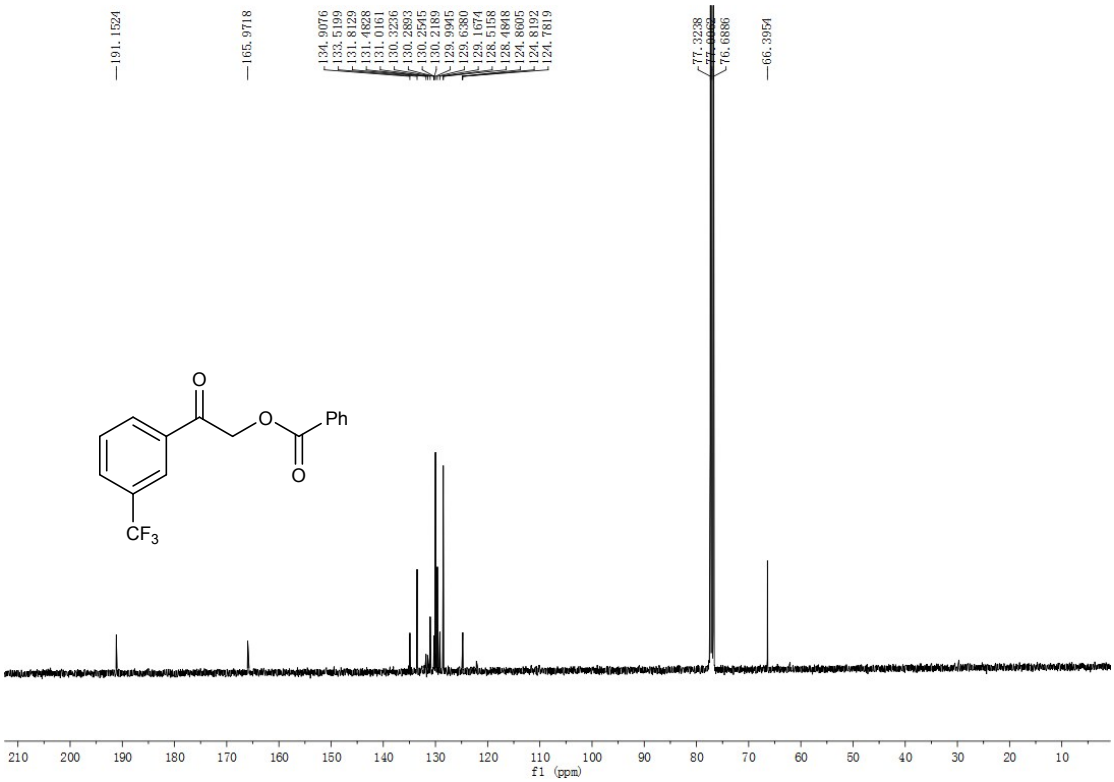
3.20
1.00
1.00
1.06
2.25
2.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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129.6780
129.1674
128.5158
128.4948
124.8605
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O
O
Ph
O
CF3
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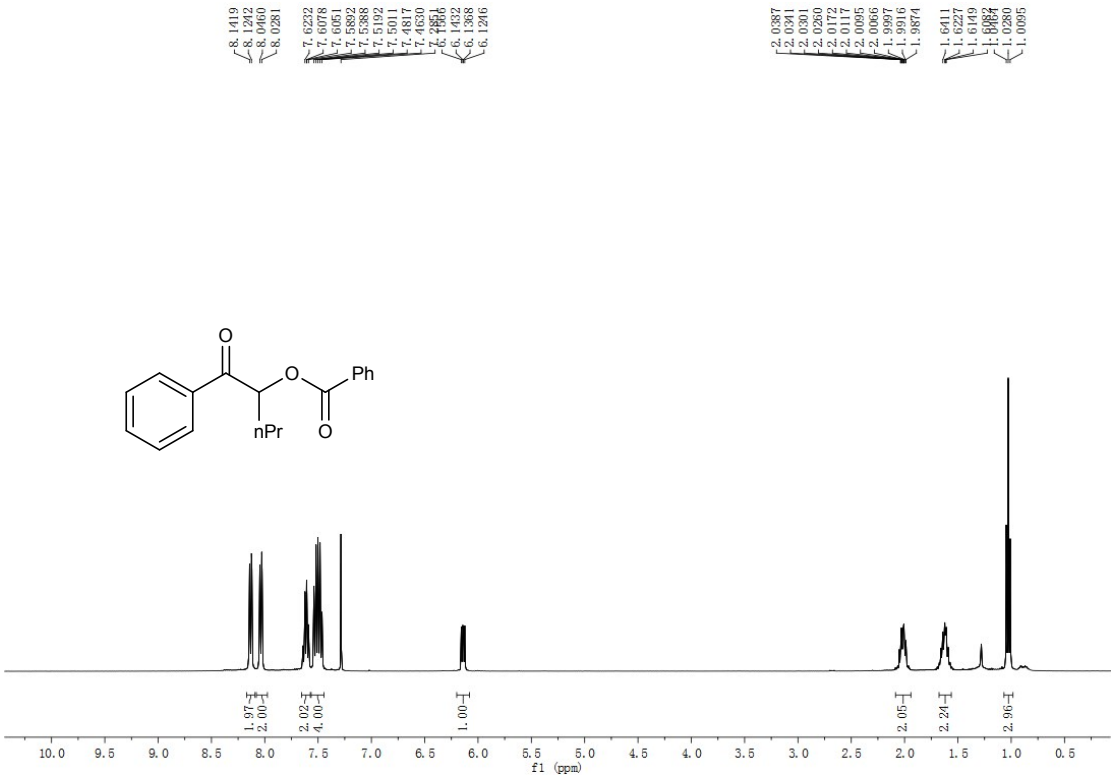
f1 (ppm)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O
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4.00
1.00
2.05
2.24
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10.0
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9.0
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7.0
6.5
6.0
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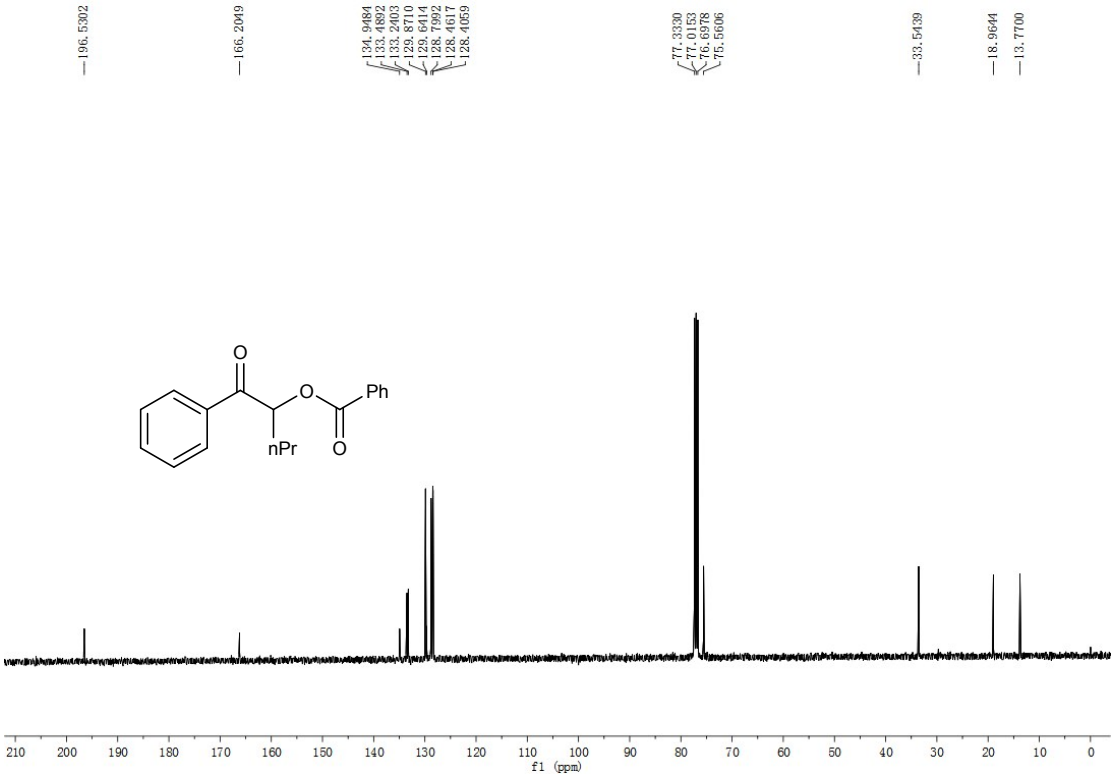
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200
190
180
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120
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90
80
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50
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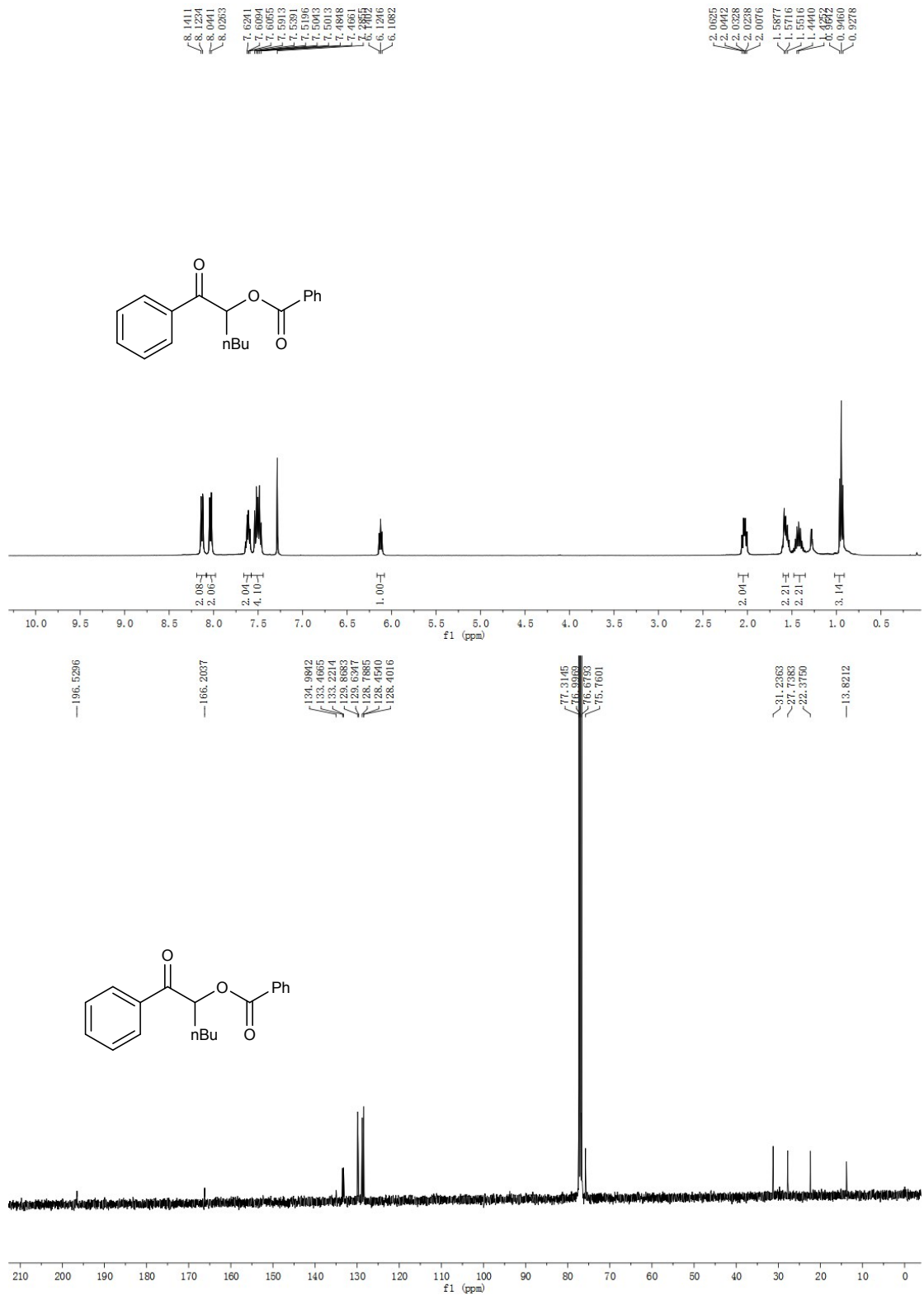
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O
Ph
nBu
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2.06
2.04
4.10
1.00
2.04
2.21
2.21
3.14
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27.7383
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Ph
nBu
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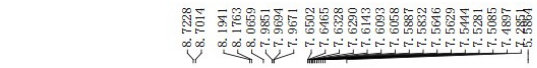
f1 (ppm)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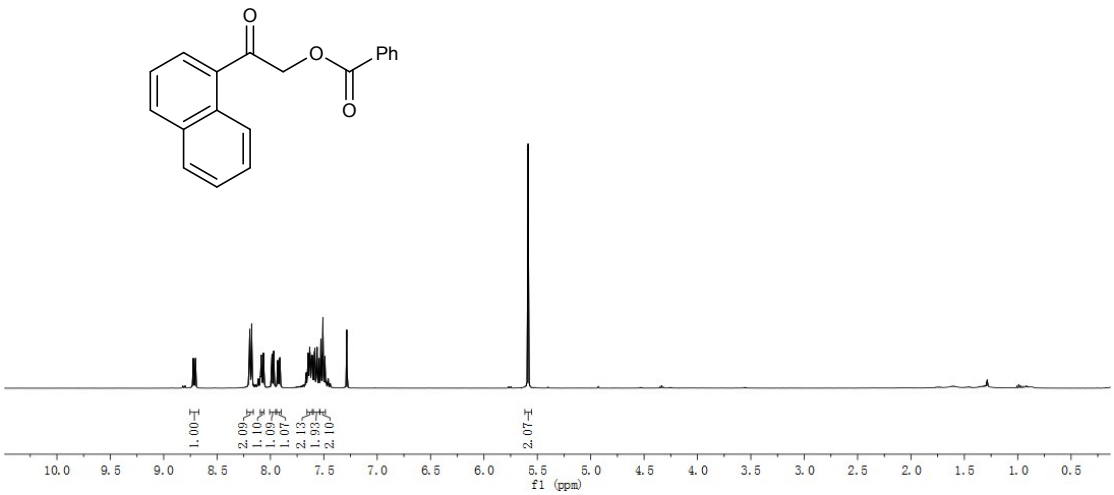
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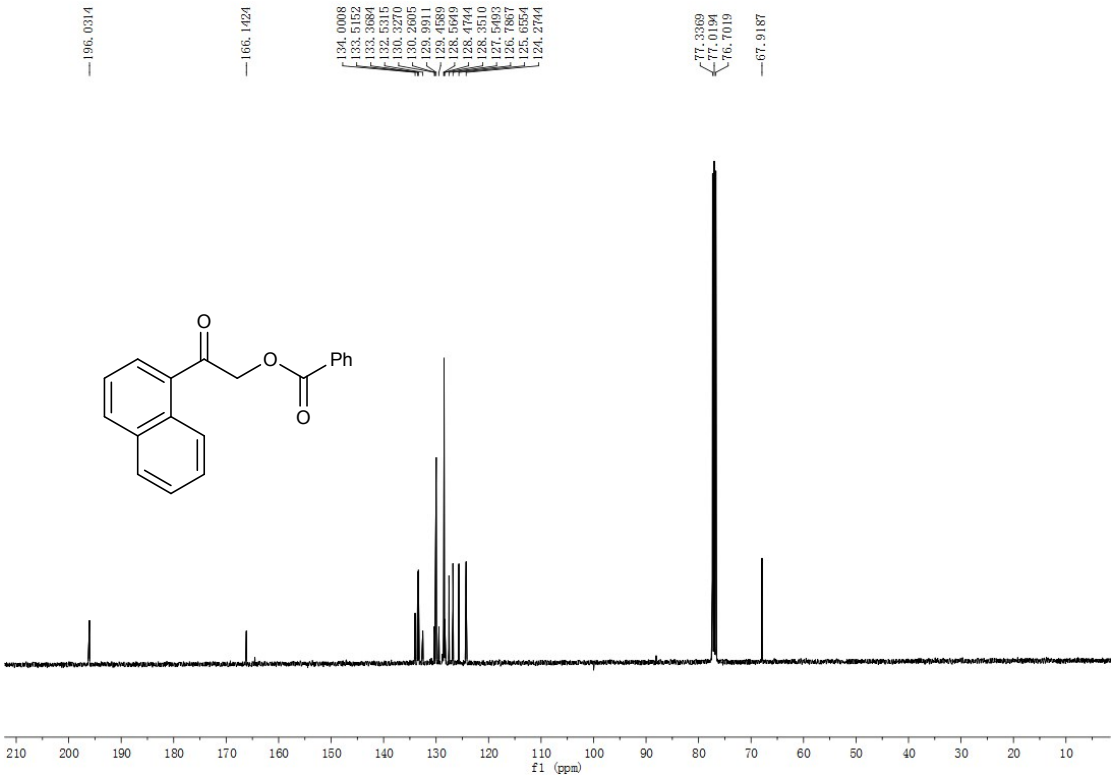
f1 (ppm)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125.6854
124.2744
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O
Ph
O
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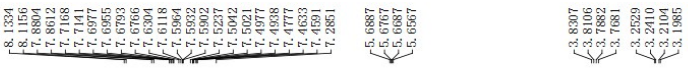
f1 (ppm)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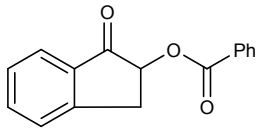
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Ph
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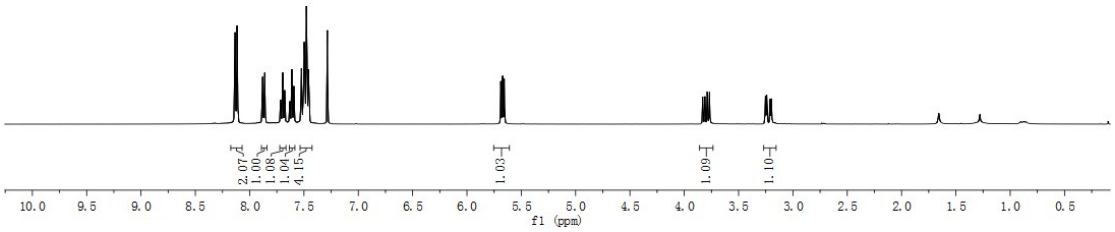
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1.09
1.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


200.4357
166.0685
150.4268
135.8904
134.6665
133.4050
129.9888
129.3819
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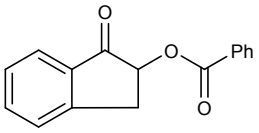
128.1859
126.7081
124.5535
77.3427
77.0251
76.7075
74.4705
33.6176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O
Ph
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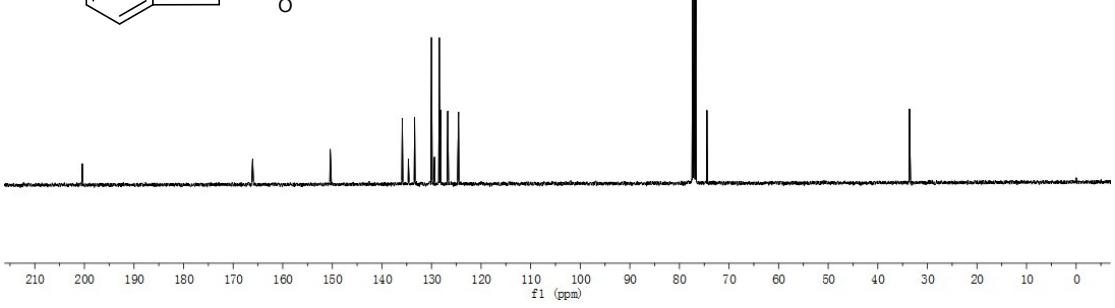
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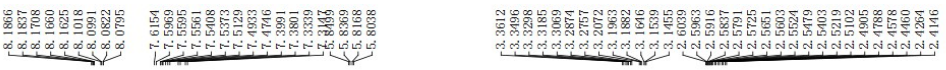
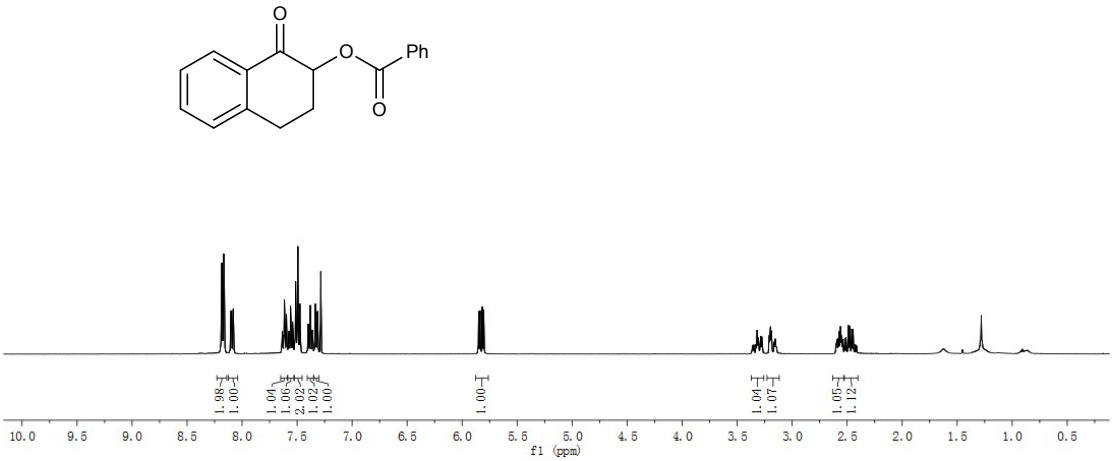
f1 (ppm)

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O
Ph
O
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1.04
1.06
2.02
1.02
1.00
1.00
1.04
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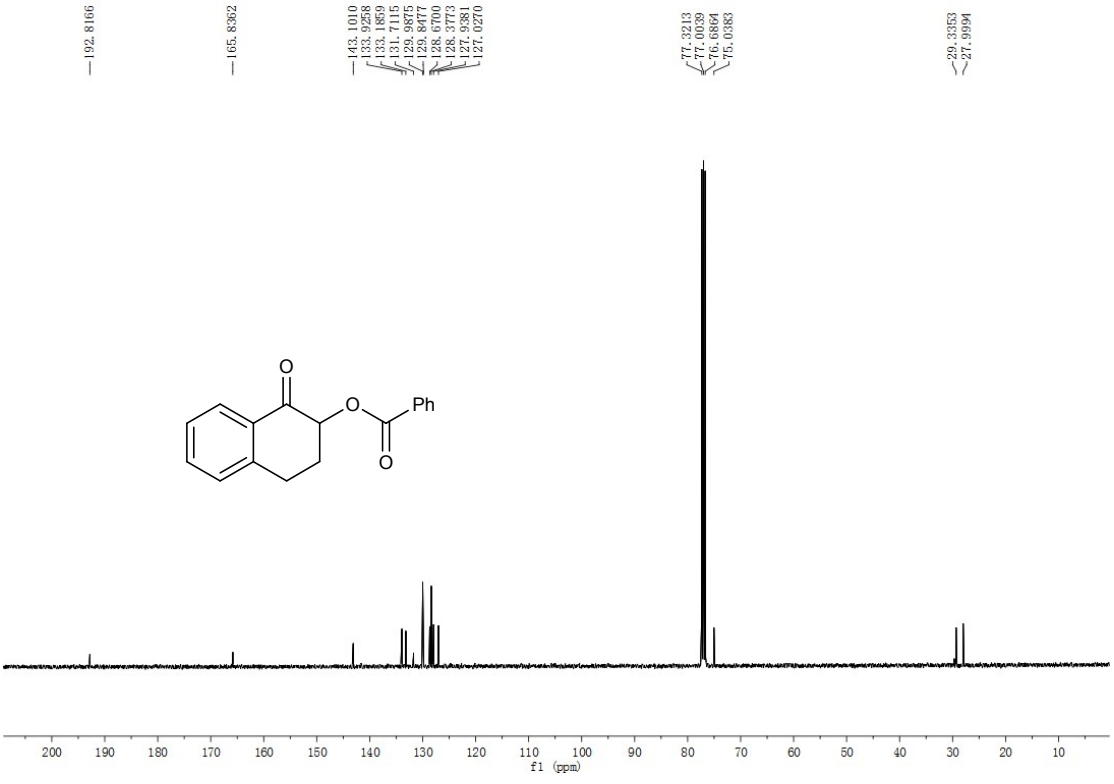
1.05
1.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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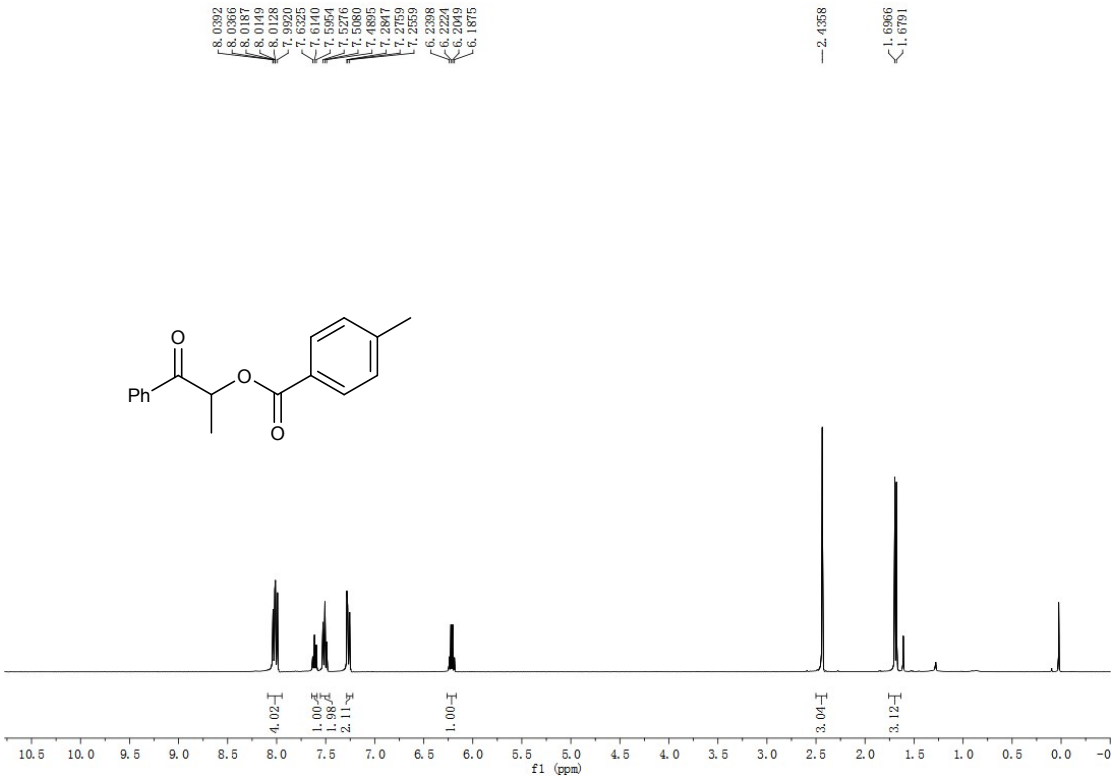
143.1010
133.9258
133.1859
131.7115
129.9875
129.8477
128.6700
128.3773
127.9381
127.0270
77.3213
77.0039
76.6864
75.0383
29.3353
27.9994
O
O
Ph
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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8.0366
8.0187
8.0149
8.0128
7.9920
7.6325
7.6140
7.5954
7.5276
7.5080
7.4895
7.2847
7.2759
7.2559
6.2398
6.2224
6.2049
6.1875
2.4358
1.6966
1.6791
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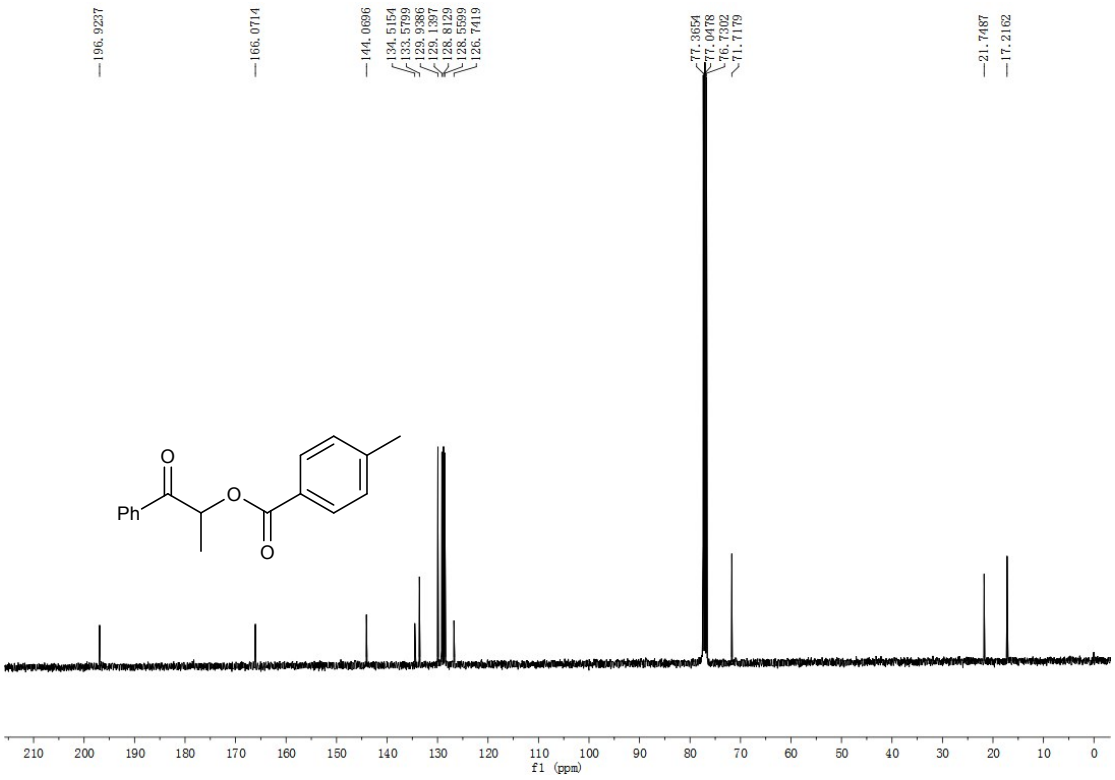
Ph
O
O
4.02
1.00
1.98
2.11
1.00
3.04
3.12
f1 (ppm)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144.0696
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129.9386
129.1397
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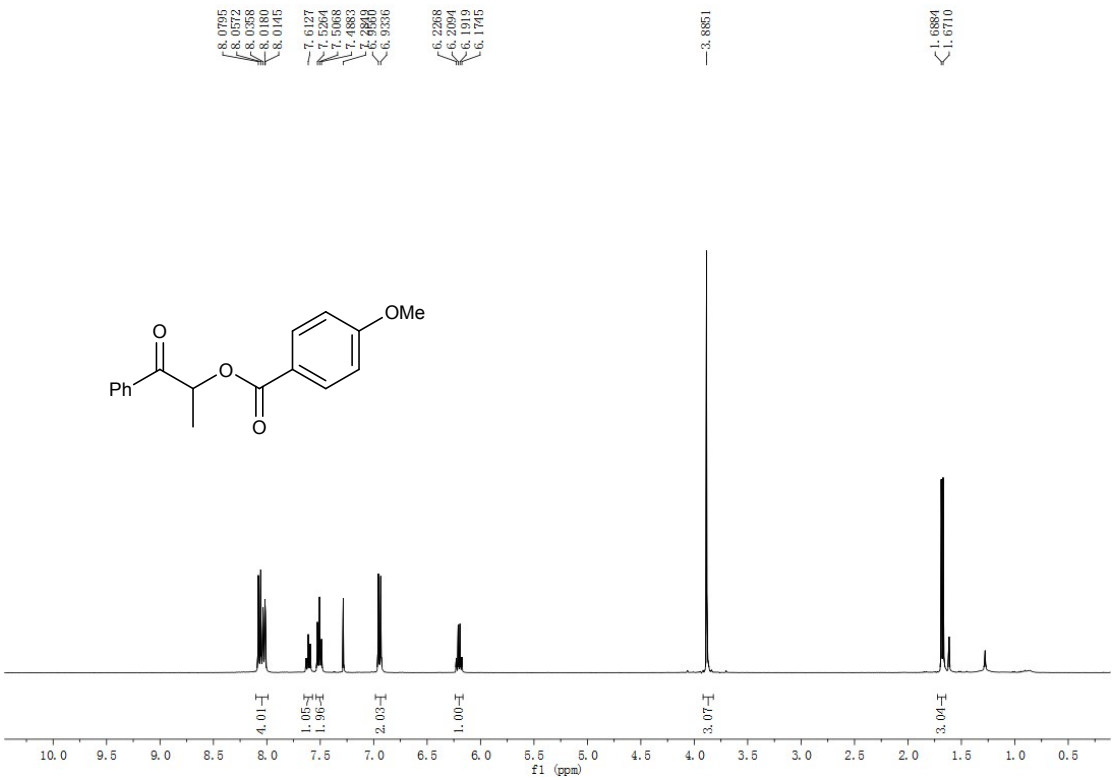
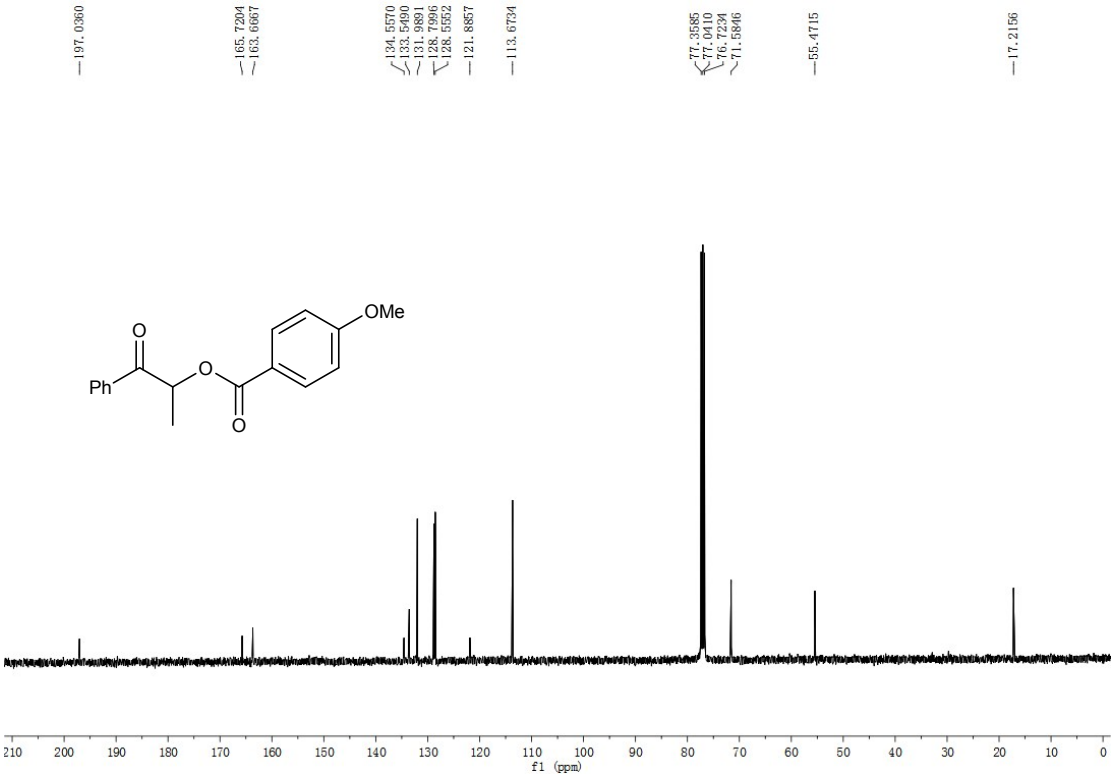
128.5599
126.7419
77.3654
77.0478
76.7302
71.7179
21.7487
17.2162
O
Ph
O
O
f1 (ppm)


8.0795
8.0572
8.0358
8.0180
8.0145
7.6127
7.5264
7.5068
7.4883
7.2843
6.9560
6.9336
6.2268
6.2094
6.1919
6.1745
3.8851
1.6884
1.6710
OMe
O
Ph
O
O
4.01
1.05
1.96
2.03
1.00
3.07
3.04
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
f1 (ppm)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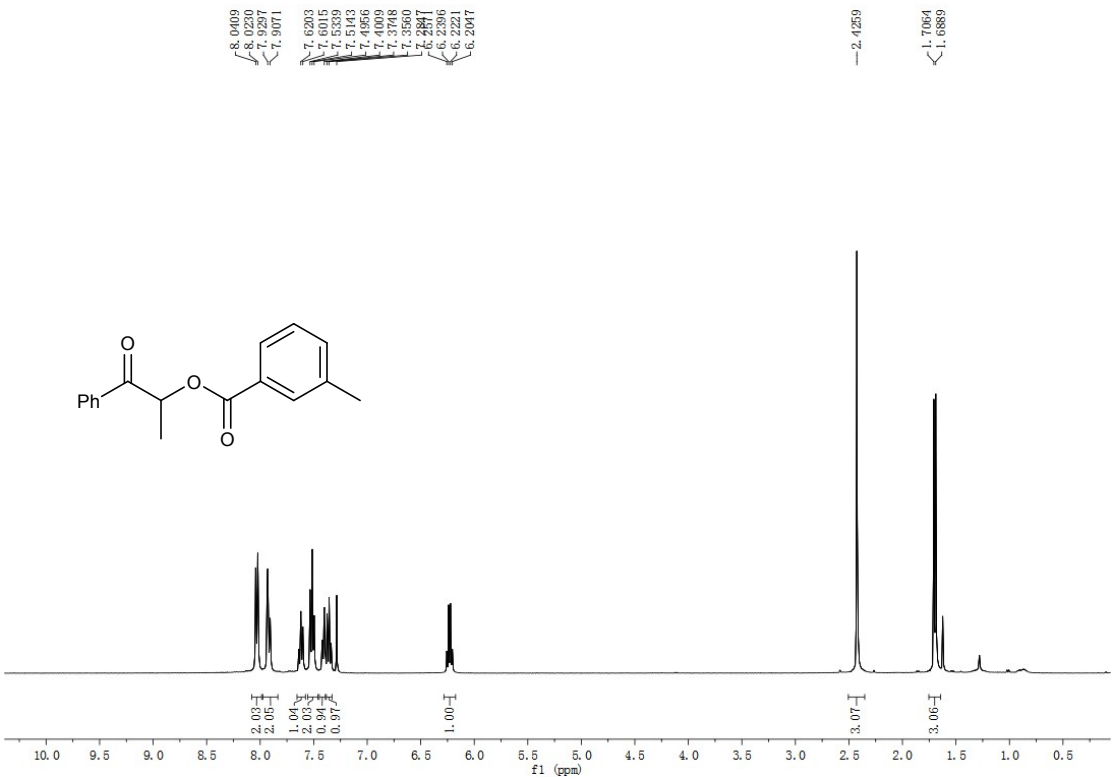
163.6667
134.5570
133.5490
131.9891
128.7996
128.5552
121.8857
113.6734
77.3585
77.0410
76.7234
71.5846
55.4715
17.2156
OMe
O
Ph
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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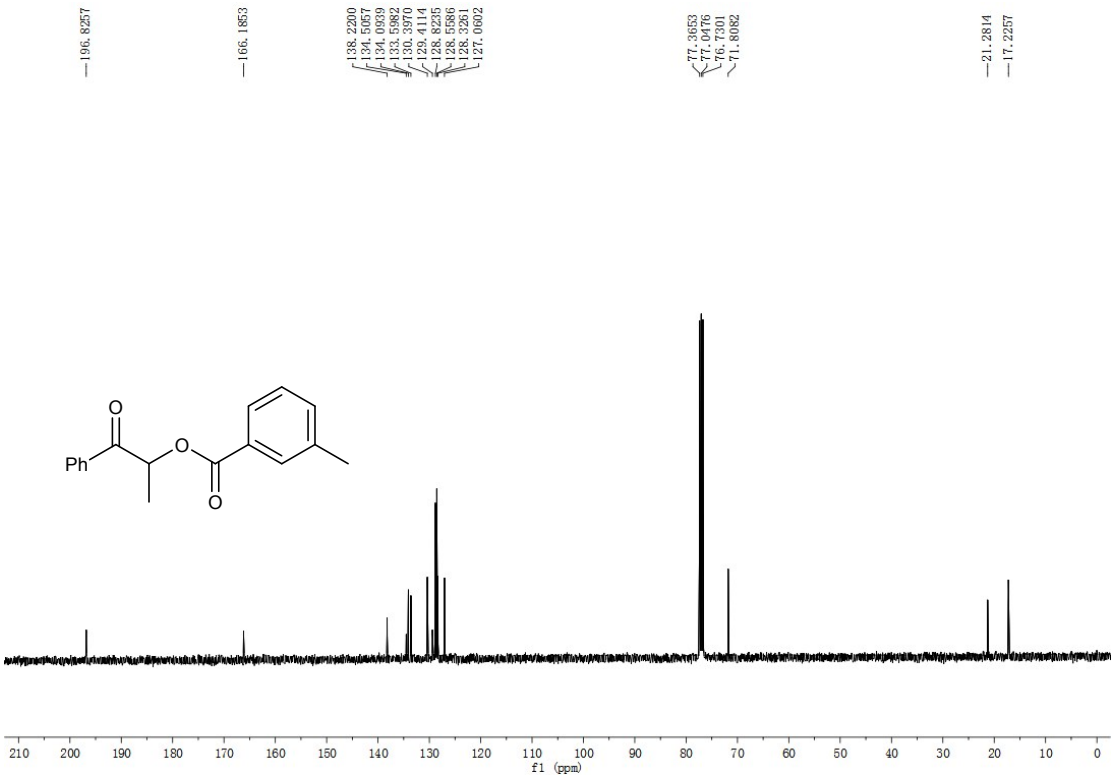
8.0230
7.9297
7.9071
7.6203
7.6015
7.5339
7.5143
7.4956
7.4009
7.3748
7.3560
7.2847
6.2396
6.2221
6.2047
2.4259
1.7064
1.6889
O
O
Ph
O
2.03
2.05
1.04
2.03
0.94
0.97
1.00
3.07
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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138.2200
134.5667
134.0939
133.5962
130.3970
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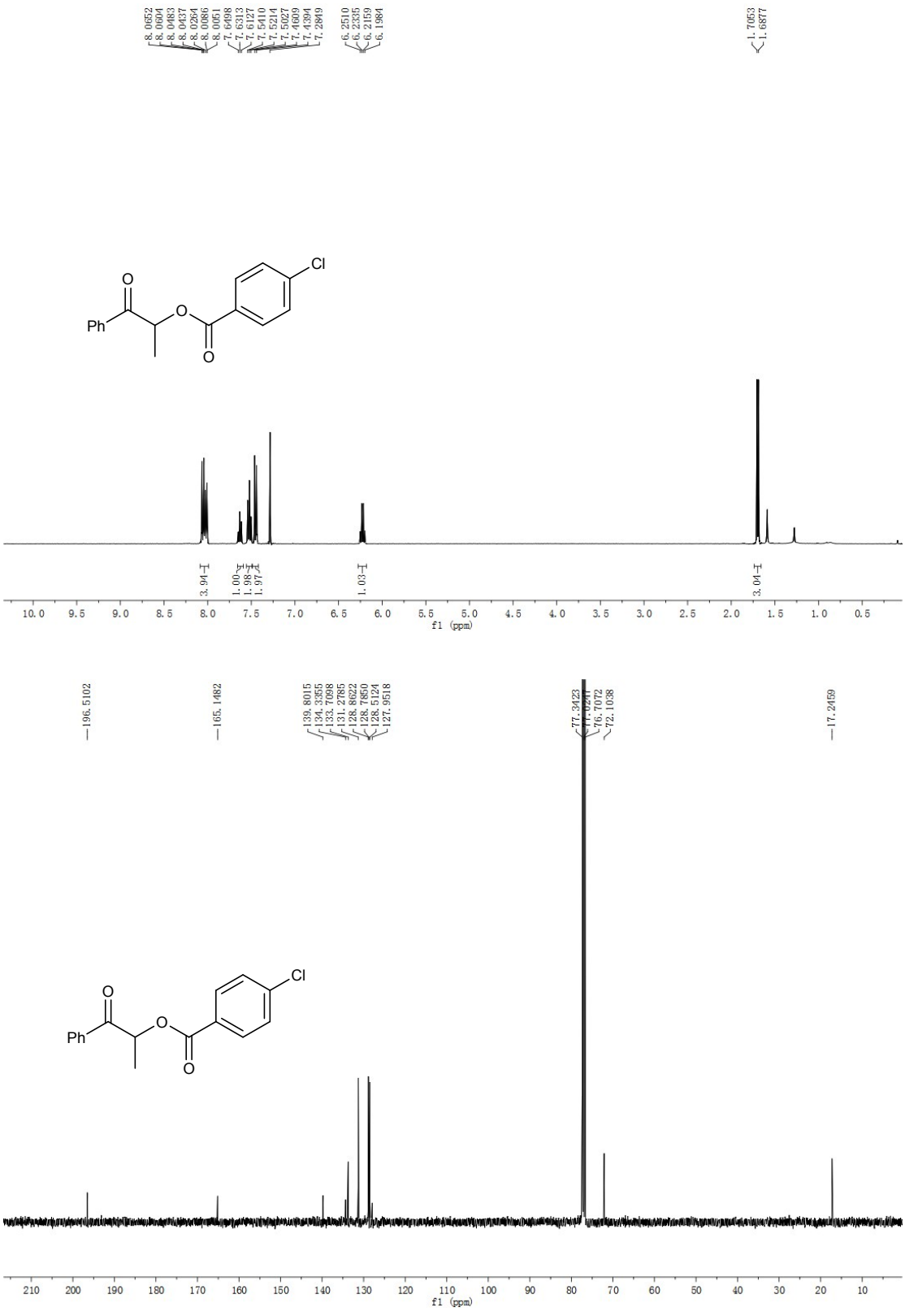
128.8235
128.5586
128.3251
127.0602
77.3653
77.0476
76.7301
71.8082
21.2814
17.2257
O
O
Ph
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.0604
8.0483
8.0437
8.0264
8.0086
8.0051
7.6498
7.6313
7.6127
7.5410
7.5214
7.5027
7.4609
7.4394
7.2849
6.2510
6.2335
6.2159
6.1984
1.7053
1.6877
Cl
O
O
Ph
O
3.94
1.00
1.98
1.97
1.03
3.04
f1 (ppm)
196.5102
165.1482
139.8015
134.3355
133.7098
131.2785
128.8622
128.7850
128.5124
127.9518
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77.0247
76.7072
72.1038
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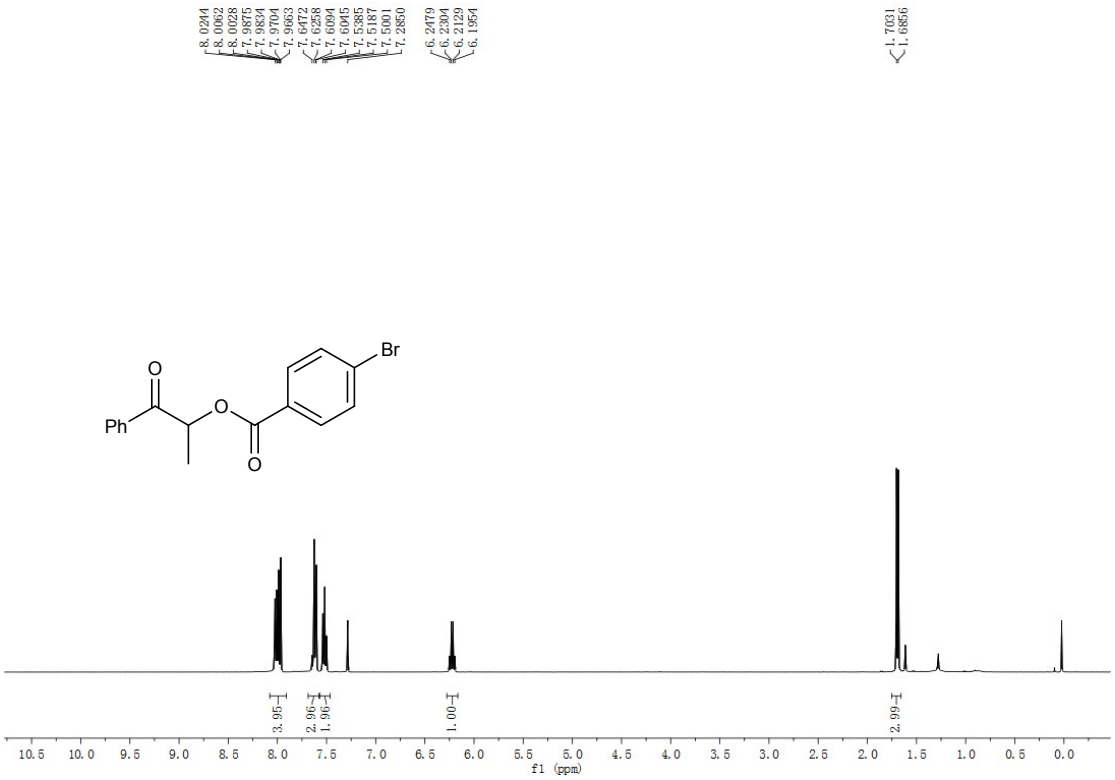
Cl
O
O
Ph
O
f1 (ppm)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8.0028
7.9875
7.9834
7.9704
7.9663
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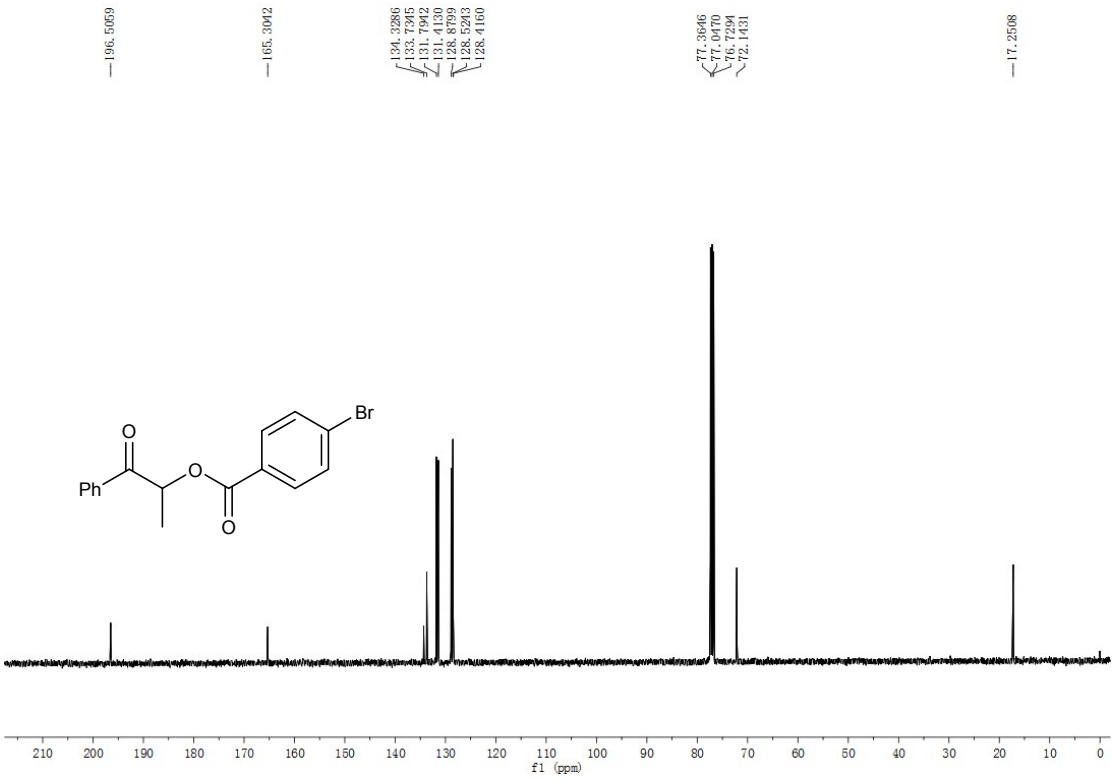
7.6258
7.6094
7.6045
7.5385
7.5187
7.5001
7.2850
6.2479
6.2304
6.2129
6.1954
1.7031
1.6856
Br
O
Ph
O
O
3.95
2.96
1.96
1.00
2.99
f1 (ppm)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134.3286
133.7945
131.7942
131.4130
128.8799
128.5243
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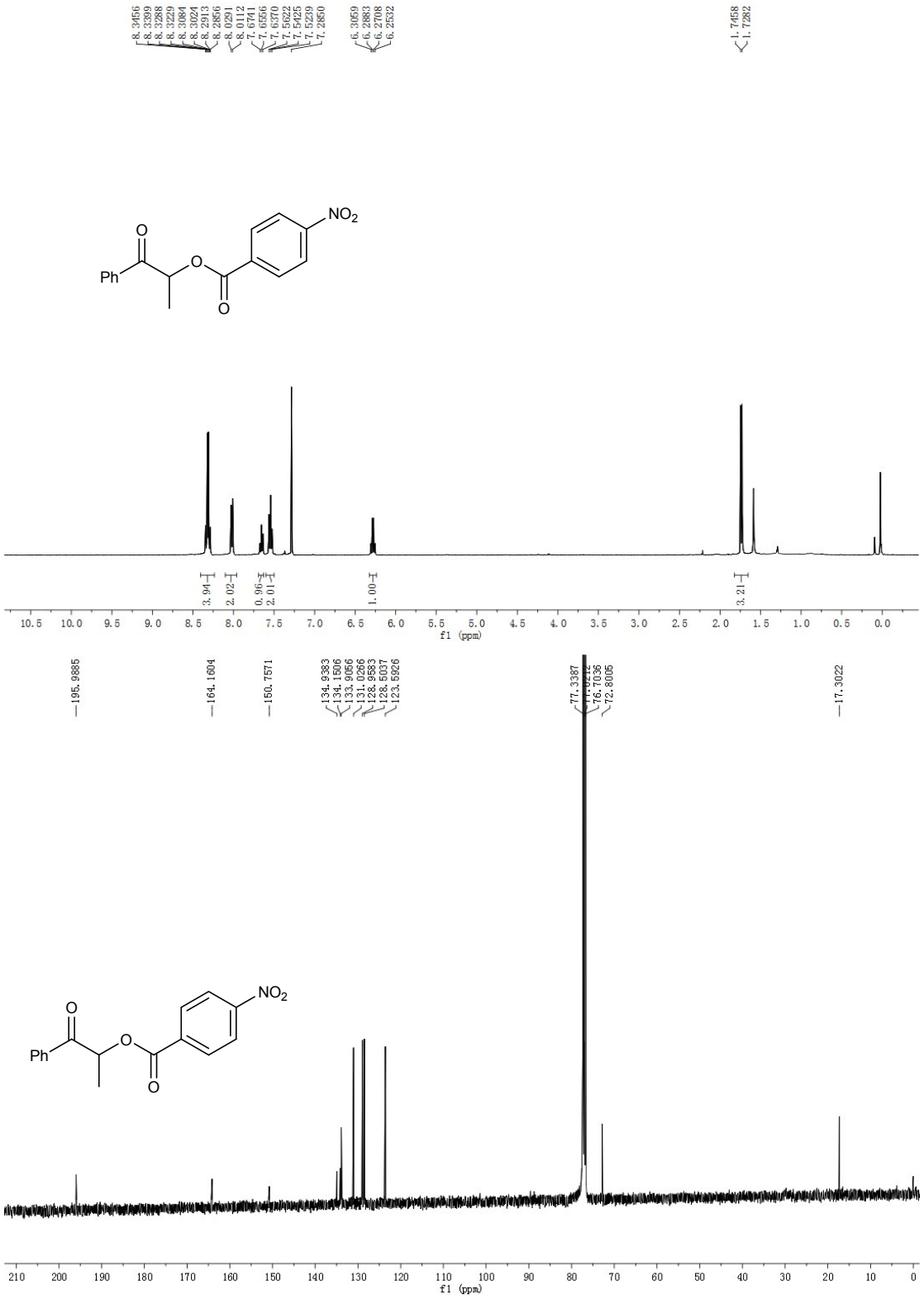
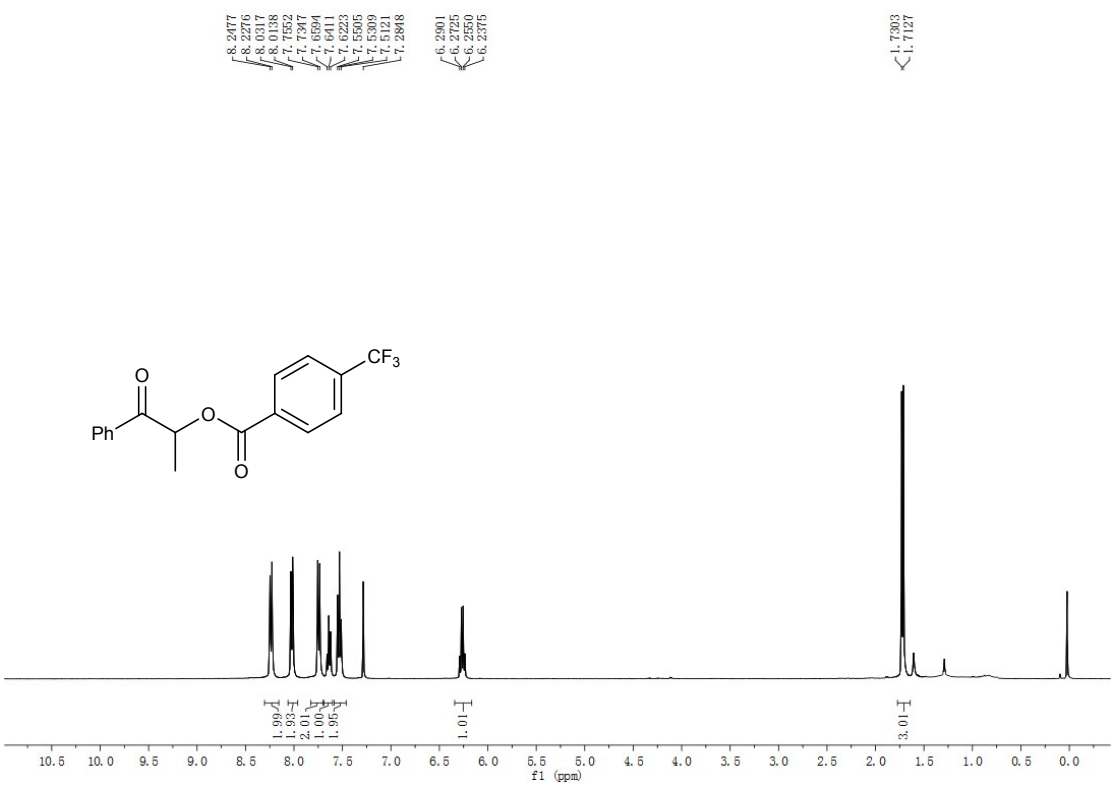
77.3646
77.0470
76.7294
72.1431
17.2508
Br
O
Ph
O
O
f1 (ppm)


8.3456
8.3399
8.3288
8.3229
8.3084
8.3024
8.2913
8.2856
8.0291
8.0112
7.6741
7.6556
7.6370
7.5622
7.5425
7.5239
7.2850
6.3059
6.2883
6.2708
6.2532
1.7458
1.7282
NO2
O
Ph
O
O
3.94
2.02
0.96
2.01
1.00
3.21
f1 (ppm)
195.9885
164.1604
150.7571
134.9383
134.1506
133.9056
131.0266
128.9583
128.5037
123.5926
77.3387
76.7036
72.8006
17.3022
NO2
O
Ph
O
O
f1 (ppm)


8.2477
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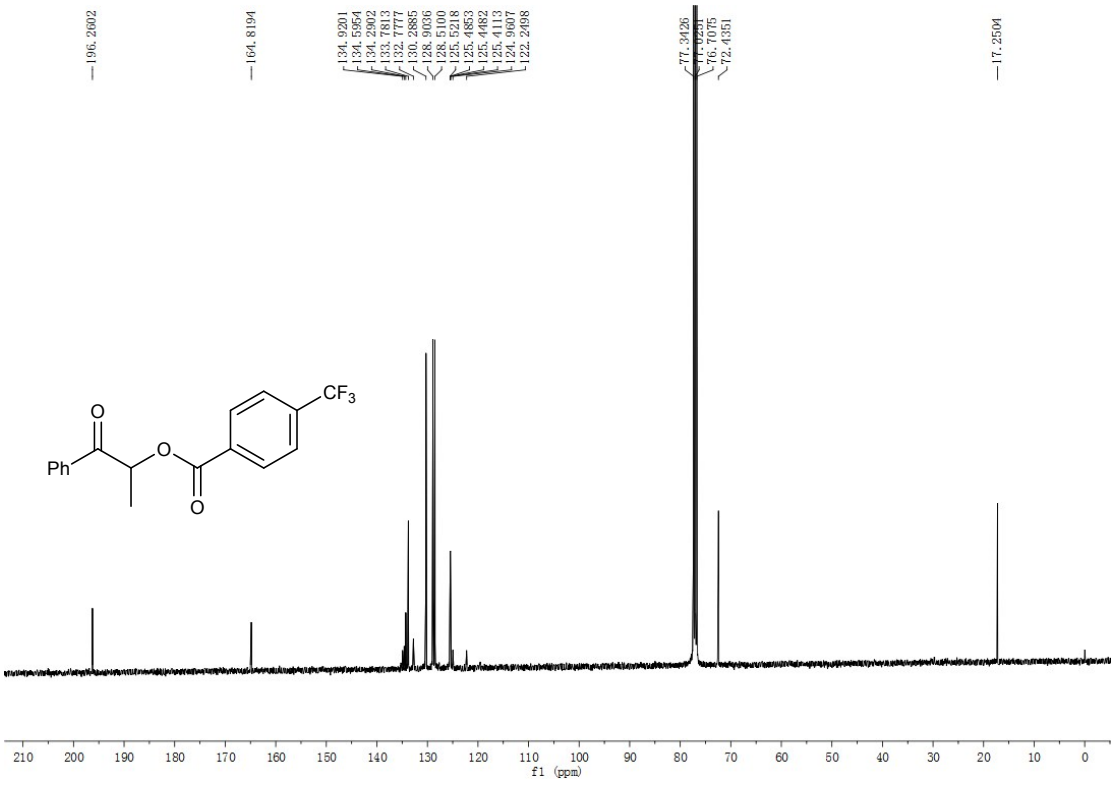
8.0317
8.0138
7.7552
7.7347
7.6594
7.6411
7.6223
7.5505
7.5309
7.5121
7.2848
6.2901
6.2725
6.2550
6.2375
1.7303
1.7127
CF3
O
Ph
O
O
1.99
1.93
2.01
1.00
1.95
1.01
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.5218
125.4853
125.4482
125.4113
124.9607
122.2498
77.3426
77.0251
76.7075
72.4351
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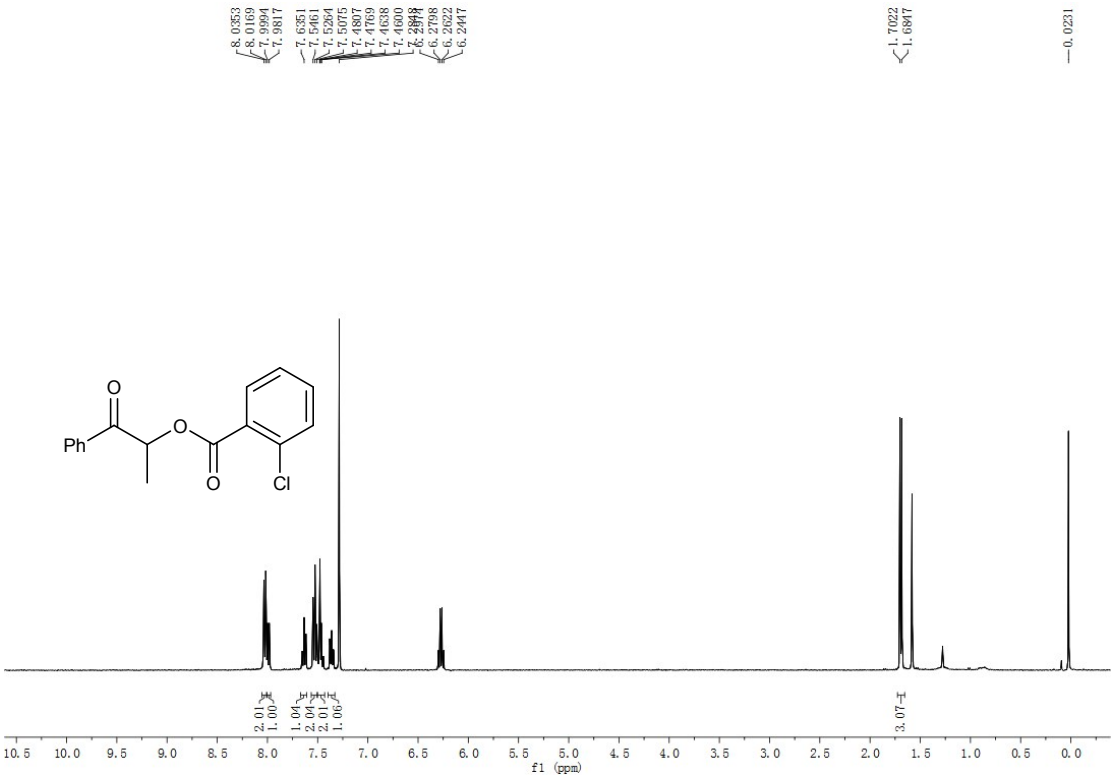
CF3
O
Ph
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4807
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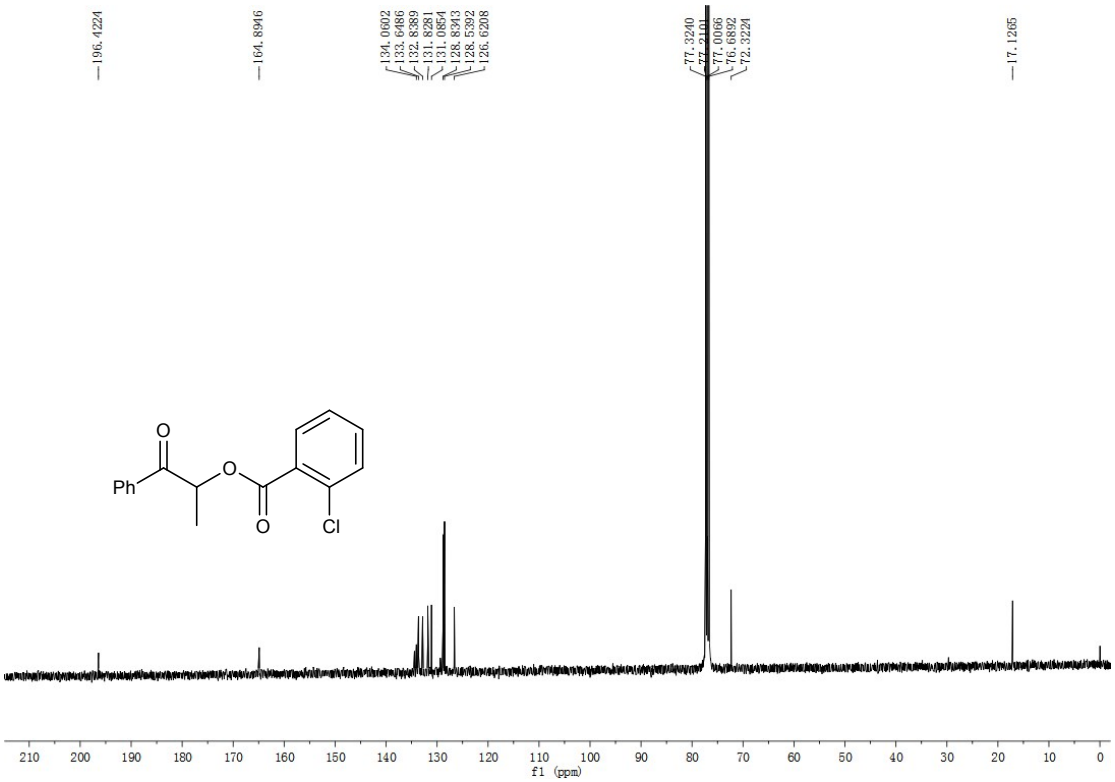
7.4638
7.4600
6.2798
6.2622
6.2447
1.7022
1.6847
0.0231
O
Ph
O
O
Cl
2.01
1.00
1.04
2.01
2.01
1.06
3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.0854
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128.5392
126.6208
77.3240
77.2401
77.0066
76.6892
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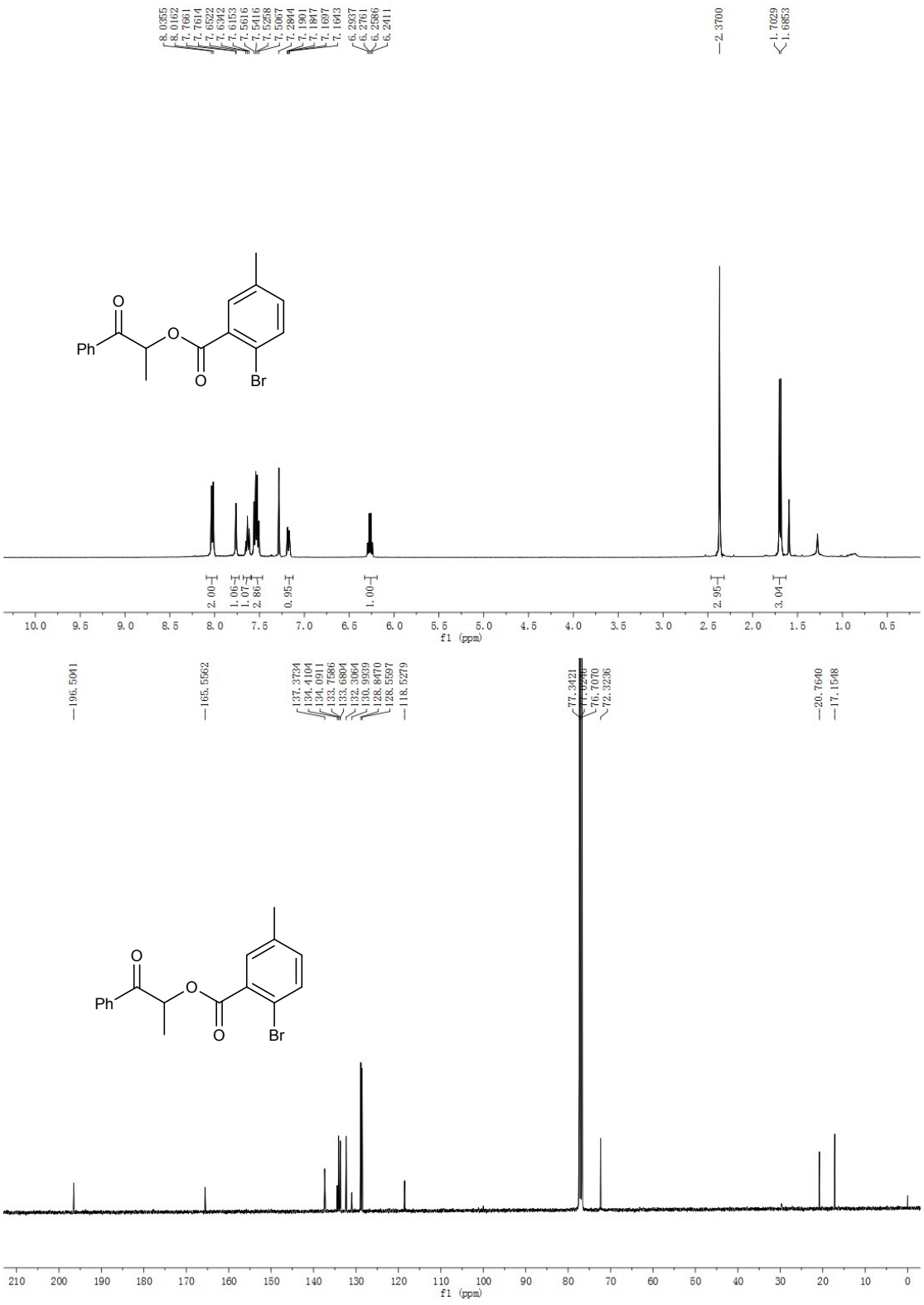
O
Ph
O
O
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5416
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7.5067
7.2894
7.1901
7.1847
7.1697
7.1043
6.2937
6.2761
6.2386
6.2411
2.3700
1.7029
1.6853
O
Ph
O
O
Br
2.00
1.06
1.07
2.86
0.95
1.00
2.95
3.04
f1 (ppm)
196.5041
165.5562
137.3734
134.4104
134.0911
133.7586
133.6804
132.3064
130.9939
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118.5279
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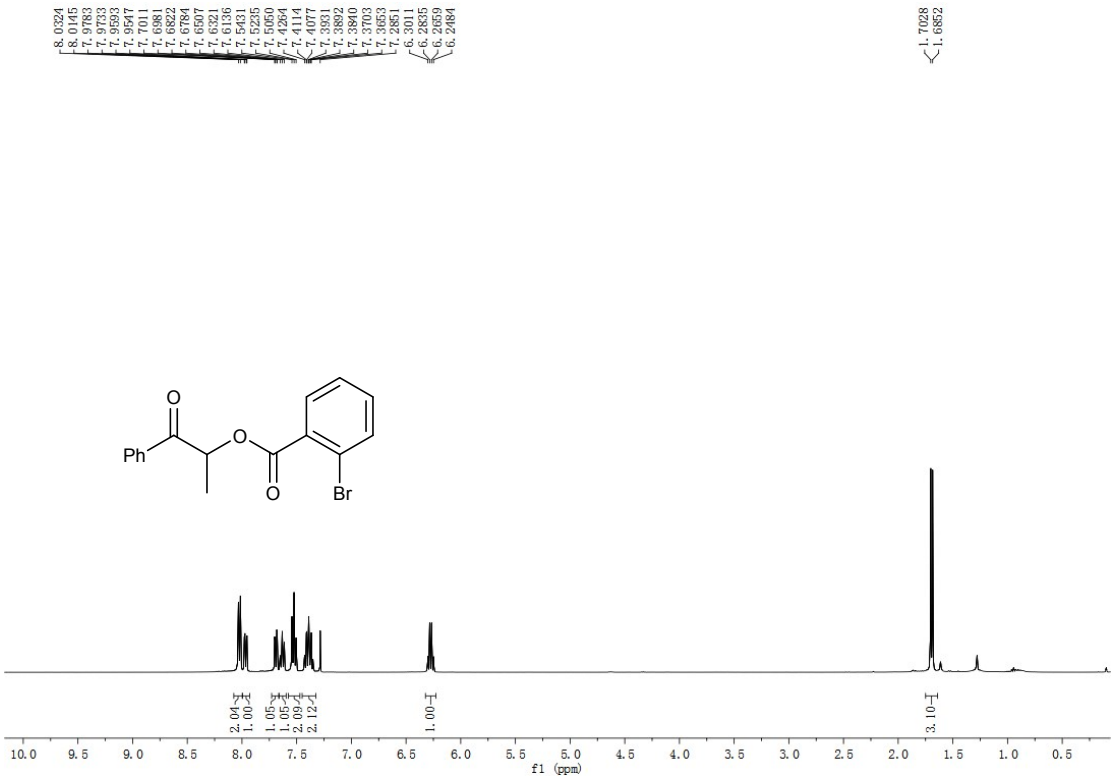
76.7070
72.3236
20.7640
17.1548
f1 (ppm)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7.9733
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7.6822
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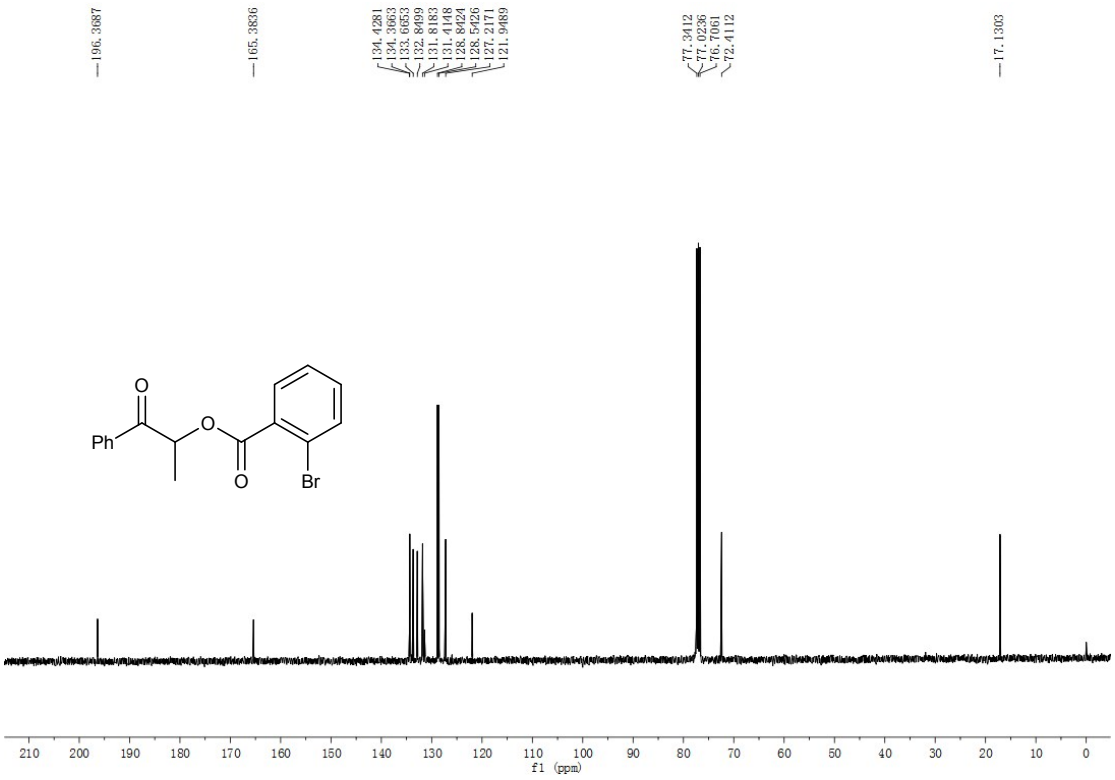
7.6507
7.6321
7.6136
7.5431
7.5235
7.5050
7.4264
7.4114
7.4077
7.3931
7.3892
7.3940
7.3703
7.3653
7.2851
6.3011
6.2835
6.2659
6.2484
1.7028
1.6852
O
Ph
O
O
Br
2.04
1.00
1.05
1.05
2.09
2.12
1.00
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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128.5426
127.2171
121.9489
77.3412
77.0236
76.7061
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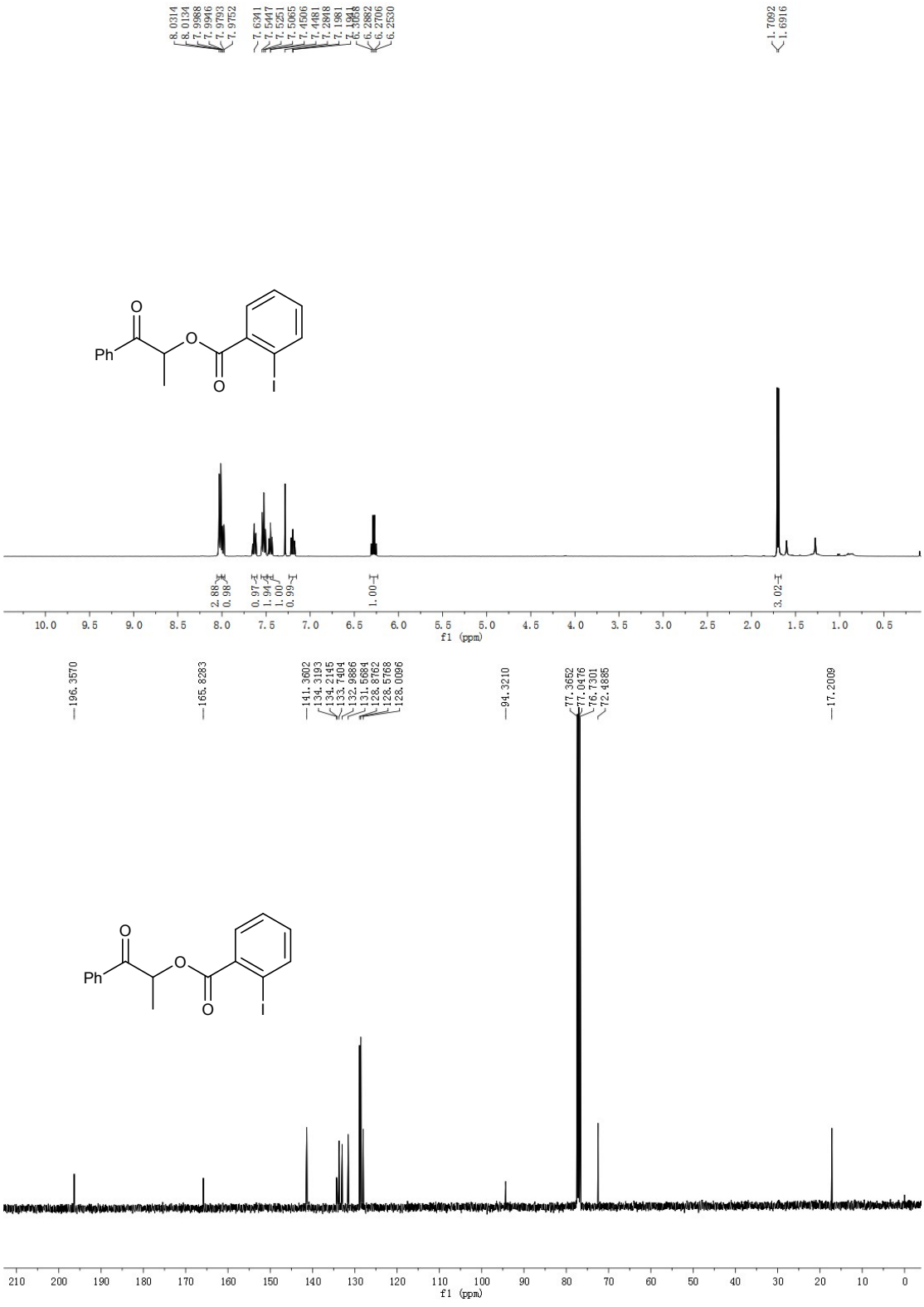
17.1303
O
Ph
O
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.0134
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7.9946
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7.9752
7.6241
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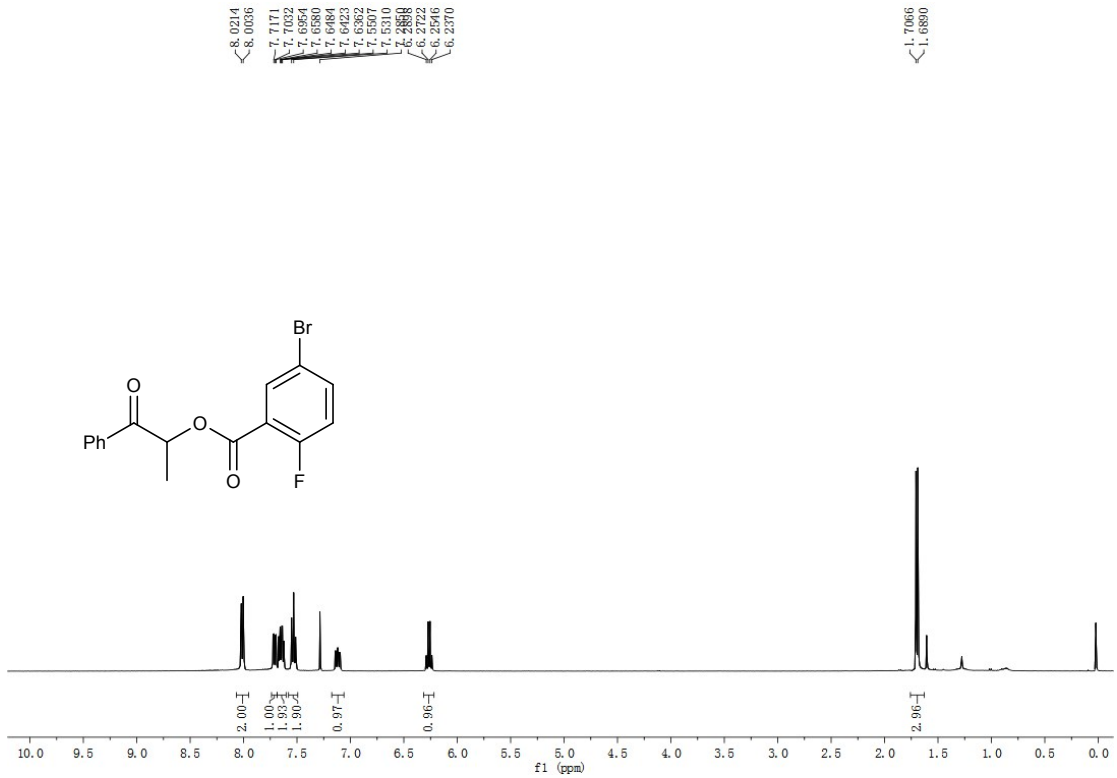
7.5251
7.5061
7.4506
7.4461
7.2648
7.1981
6.2882
6.2706
6.2530
1.7092
1.6916
O
O
Ph
O
I
2.88
0.98
0.97
1.94
1.00
0.99
1.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
196.3570
165.8283
141.3602
134.3193
134.2145
133.7404
132.9886
131.6684
128.8762
128.5768
128.0096
94.3210
77.3652
77.0476
76.7301
72.4885
17.2009
O
O
Ph
O
I
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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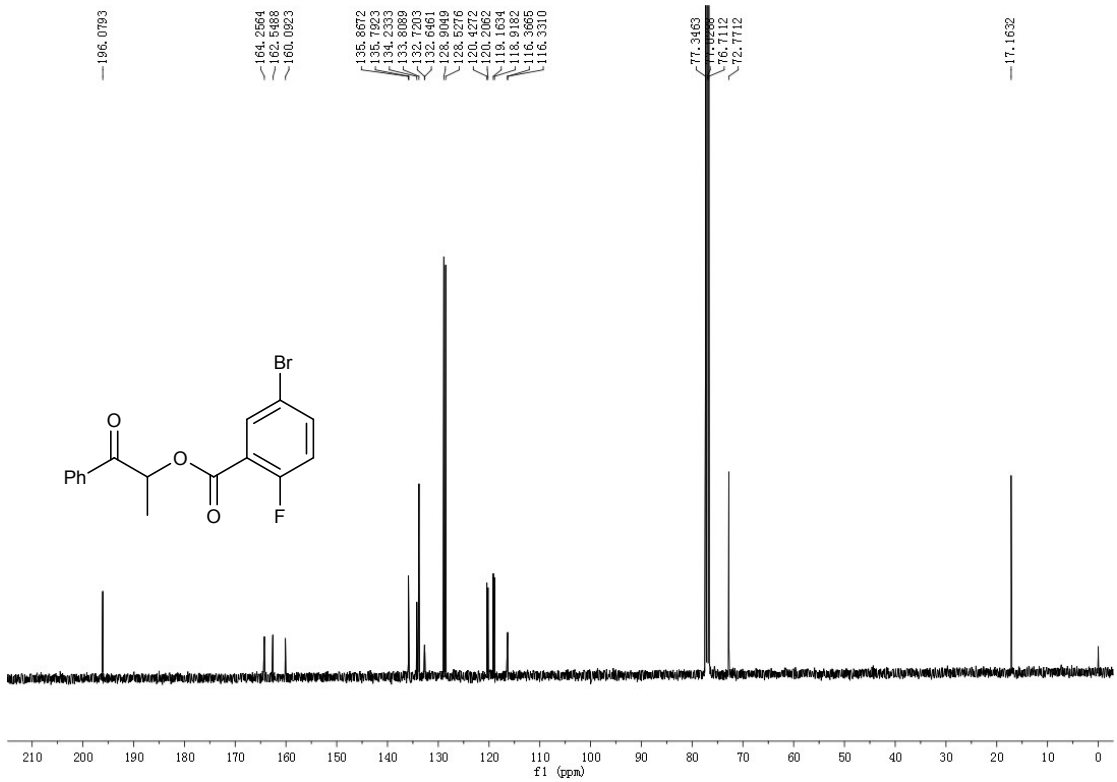
7.6362
7.5907
7.5310
6.2722
6.2546
6.2370
1.7066
1.6890
Br
O
Ph
O
O
F
2.00
1.00
1.93
1.90
0.97
0.96
2.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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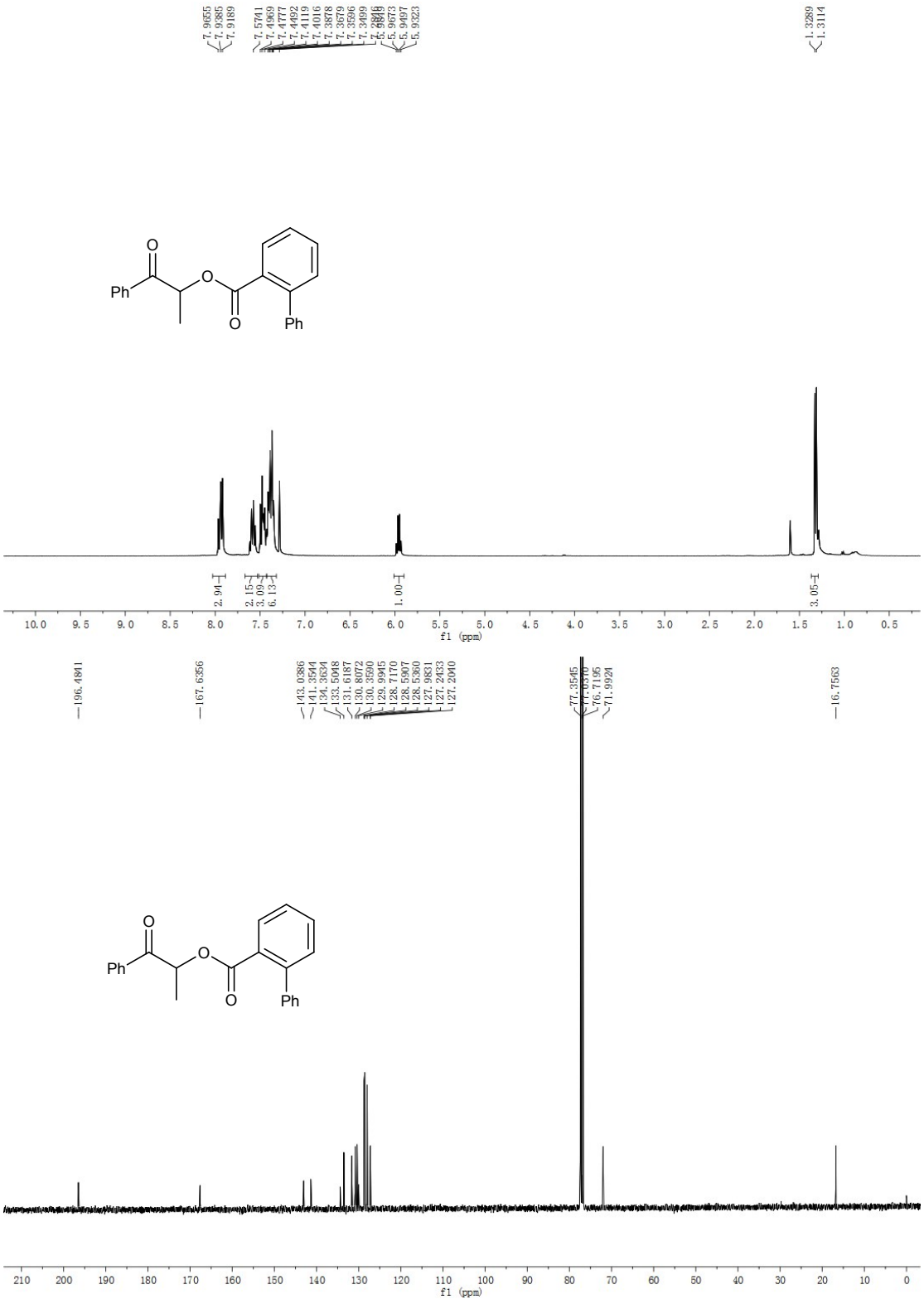
128.5276
120.4272
120.2062
119.1634
118.9182
116.3665
116.3310
77.3463
76.7112
72.7712
17.1632
Br
O
Ph
O
O
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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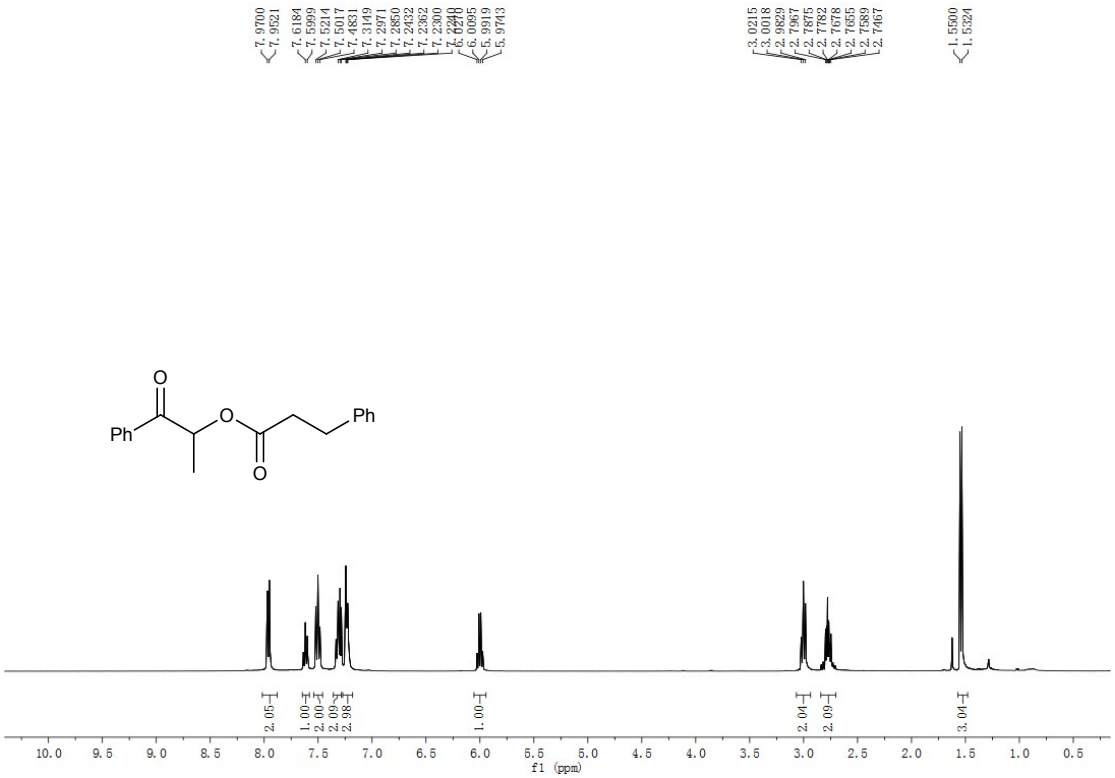
7.9189
7.5741
7.4969
7.4777
7.4492
7.4119
7.4016
7.3878
7.3679
7.3596
7.3499
5.9673
5.9497
5.9323
1.3289
1.3114
O
Ph
O
O
Ph
2.94
2.15
3.09
6.13
1.00
3.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
196.4841
167.6356
143.0386
141.3544
134.3634
133.5048
131.6187
130.8072
130.3590
129.9945
128.7170
128.5907
128.5360
127.9831
127.2433
127.2040
77.3545
77.0310
76.7195
71.9924
16.7563
O
Ph
O
O
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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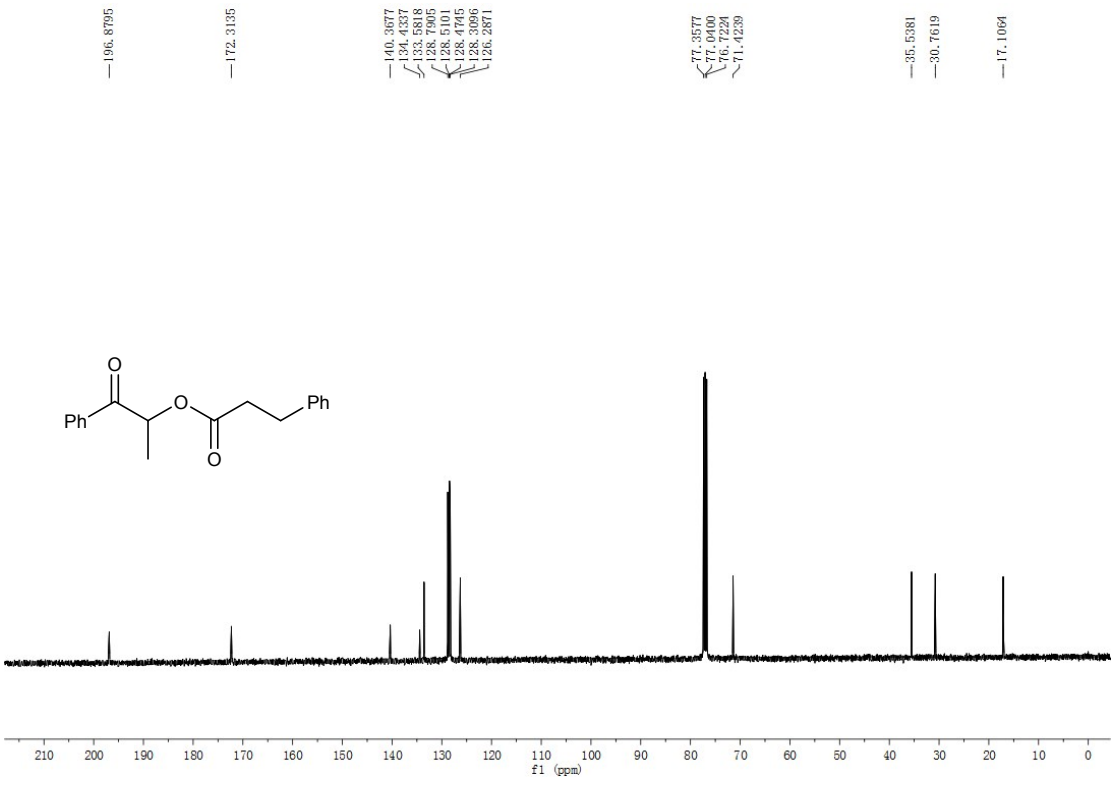
7.9521
7.6184
7.5999
7.5214
7.5017
7.4631
7.3149
7.2971
7.2850
7.2432
7.2362
7.2300
6.0095
5.9919
5.9743
3.0215
3.0018
2.9829
2.7967
2.7875
2.7782
2.7678
2.7655
2.7589
2.7467
1.5500
1.5324
O
Ph
O
O
Ph
2.05
1.00
2.00
2.09
2.98
1.00
2.04
2.09
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


196.8795
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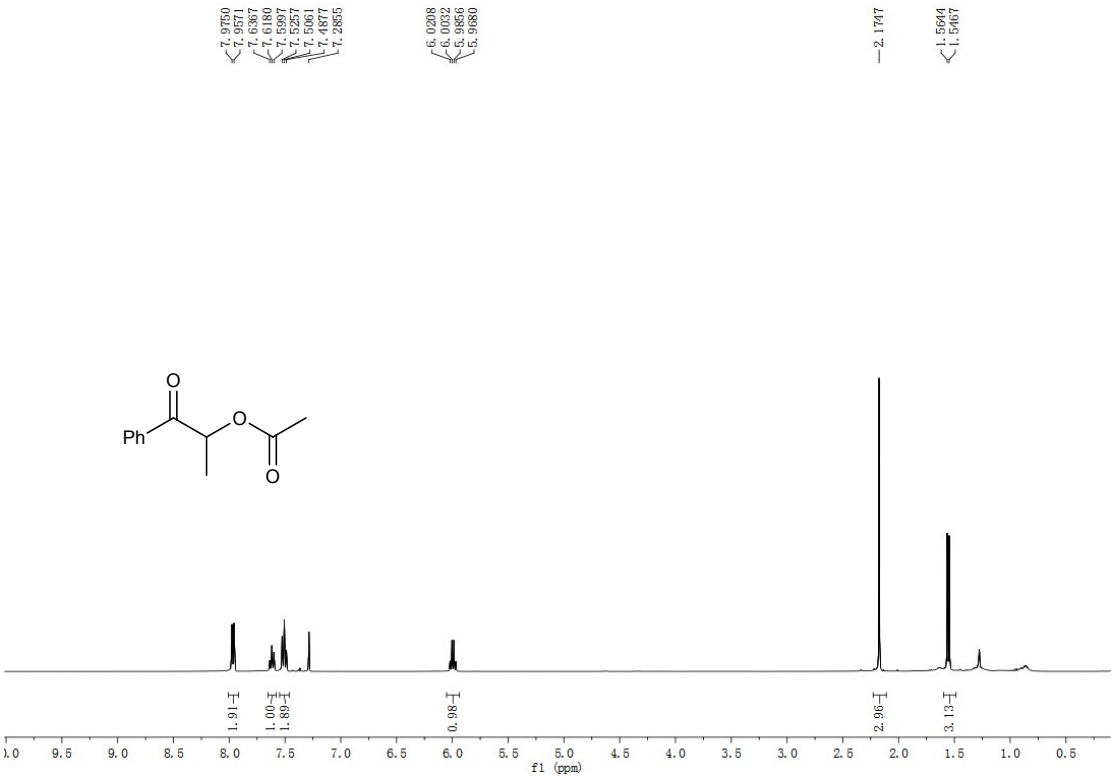
140.3677
134.4337
133.5818
128.7905
128.5101
128.4745
128.3096
126.2871
77.3577
77.0400
76.7224
71.4239
35.5381
30.7619
17.1064
O
Ph
O
O
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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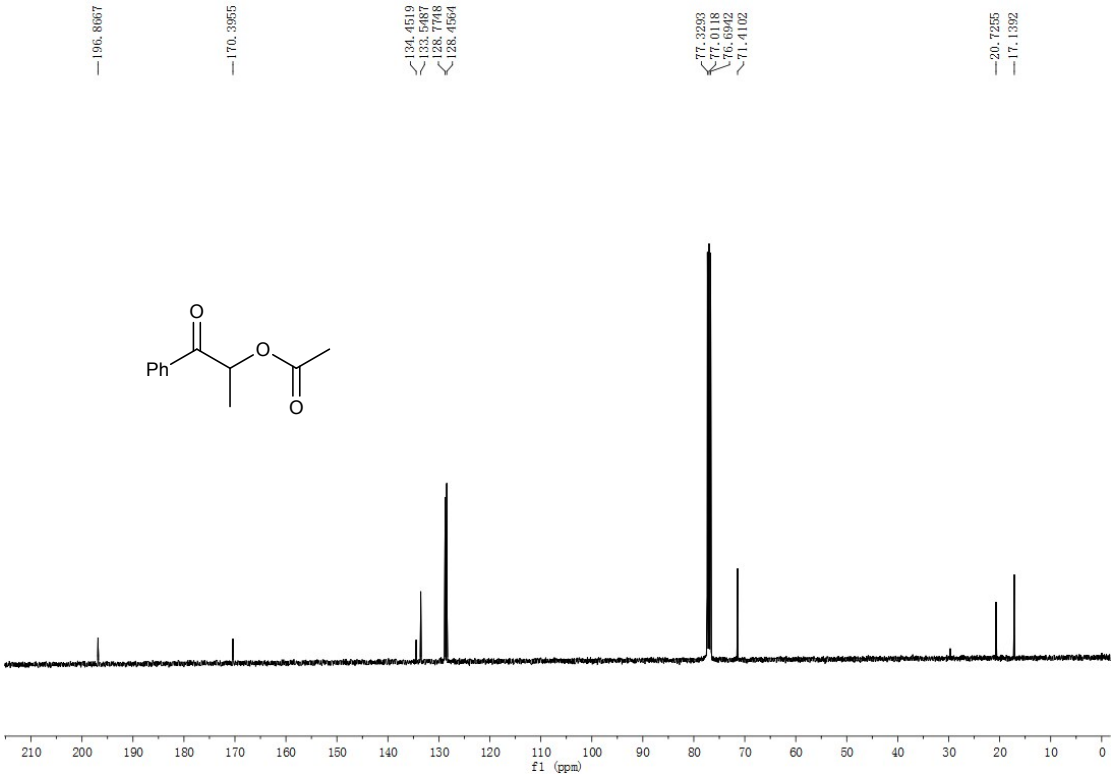
7.9571
7.6367
7.6180
7.5997
7.5257
7.5061
7.4877
7.2855
6.0208
6.0032
5.9856
5.9680
2.1747
1.5644
1.5467
O
Ph
O
O
1.91
1.00
1.89
0.98
2.96
3.13
f1 (ppm)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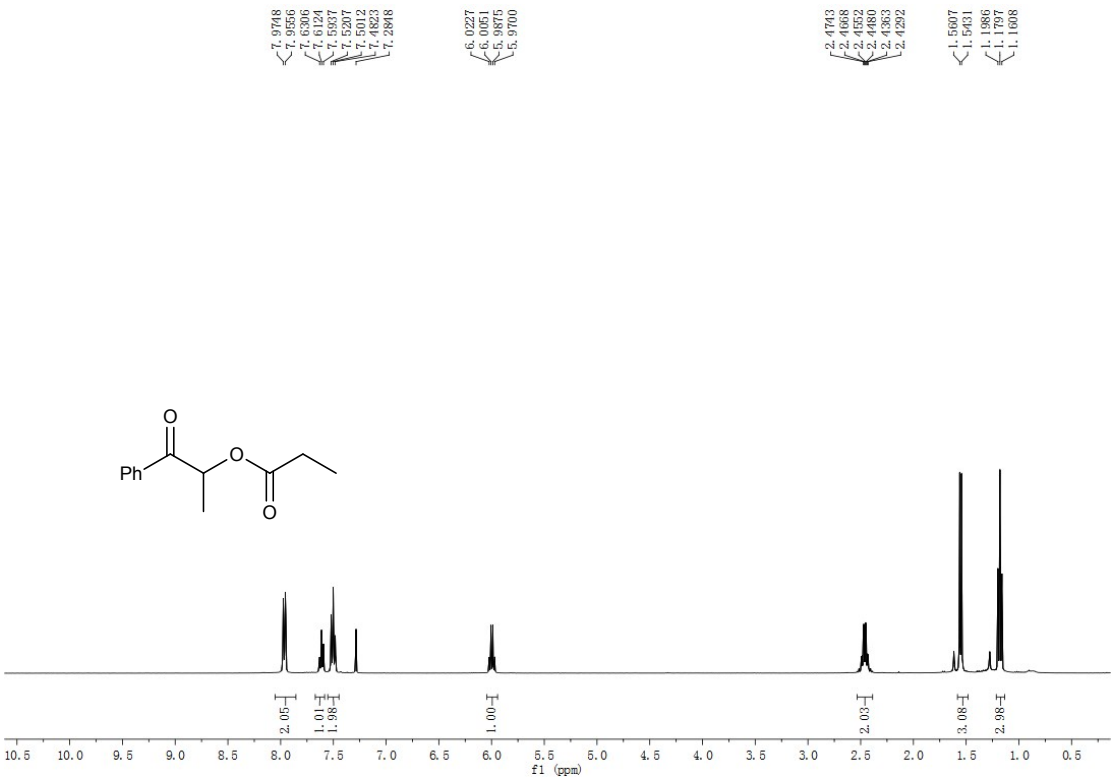
170.3955
134.4519
133.5687
128.7748
128.4564
77.3293
77.0118
76.6942
71.4102
20.7255
17.1392
O
Ph
O
O
f1 (ppm)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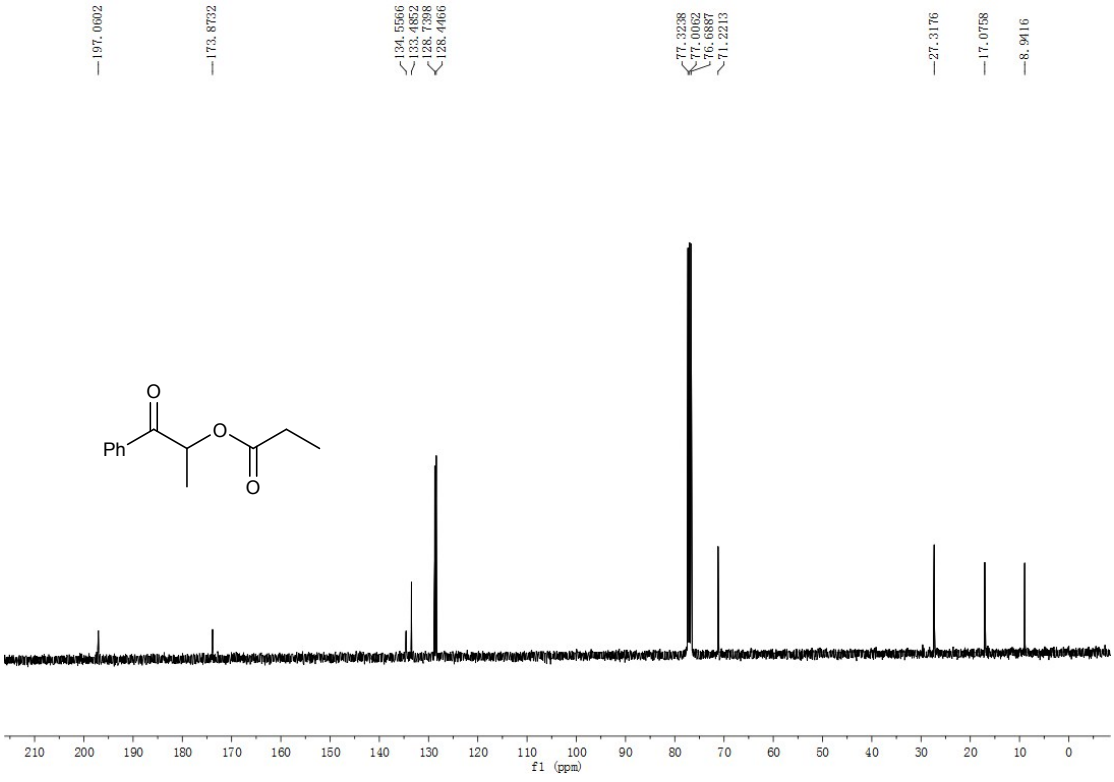
7.6306
7.6124
7.5937
7.5207
7.5012
7.4823
7.2848
6.0227
6.0051
5.9875
5.9700
2.4743
2.4668
2.4552
2.4480
2.4363
2.4292
1.5607
1.5431
1.1986
1.1797
1.1608
O
Ph
O
O
2.05
1.01
1.98
1.00
2.03
3.08
2.98
f1 (ppm)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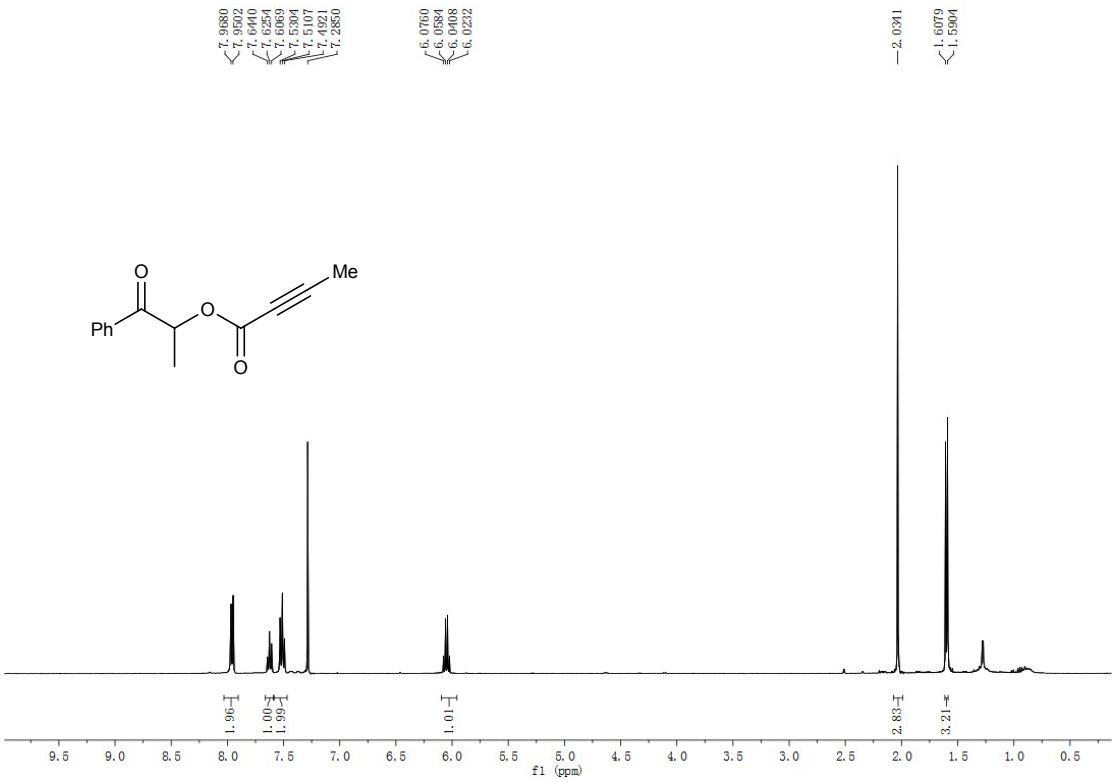
173.8732
134.5566
133.4852
128.7398
128.4466
77.3238
77.0062
76.6887
71.2213
27.3176
17.0758
8.9416
O
Ph
O
O
f1 (ppm)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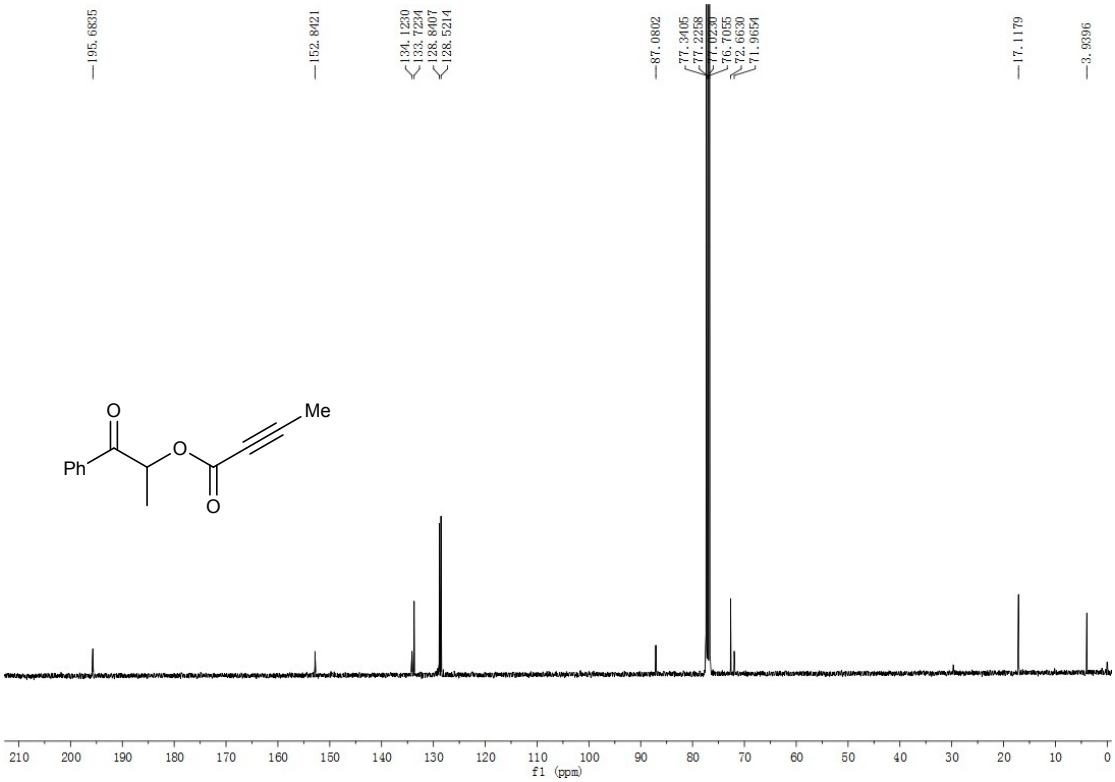
7.9502
7.6440
7.6254
7.6069
7.5304
7.5107
7.4921
7.2850
6.0760
6.0584
6.0408
6.0232
2.0341
1.6079
1.5904
O
Ph
O
O
Me
1.96
1.00
1.99
1.01
2.83
3.21
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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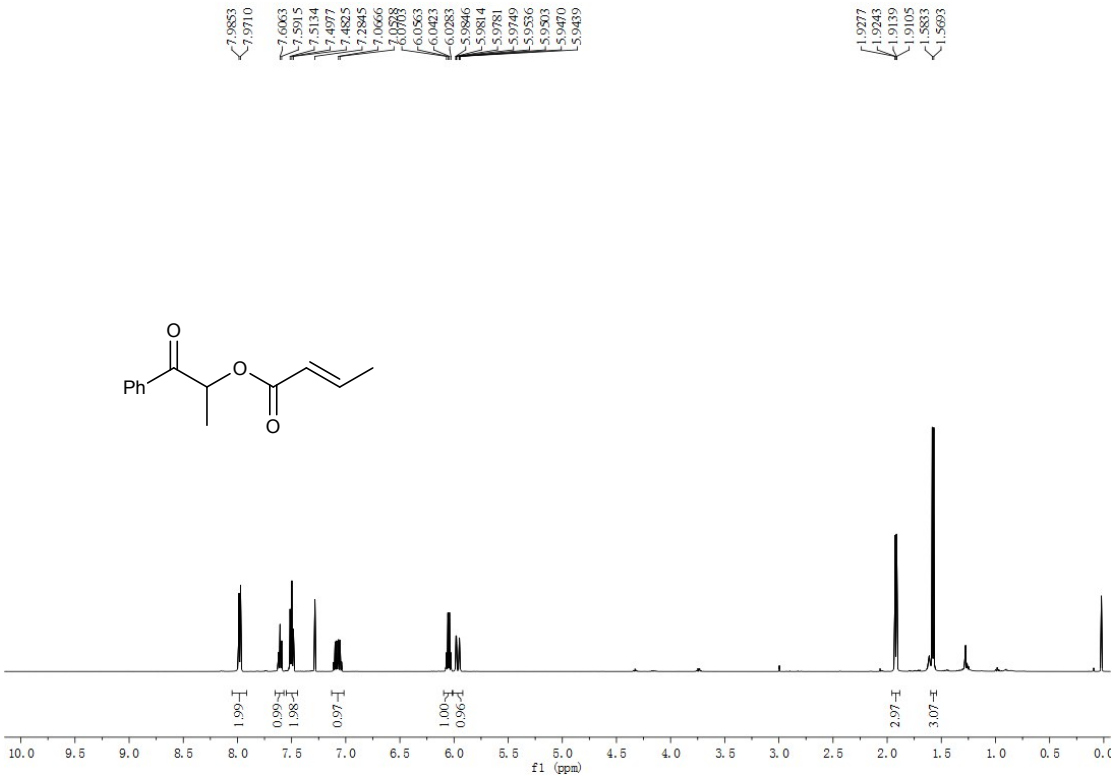
152.8421
134.1230
133.7234
128.8407
128.5214
87.0802
77.3405
77.2258
76.7055
72.6630
71.9654
17.1179
3.9396
O
Ph
O
O
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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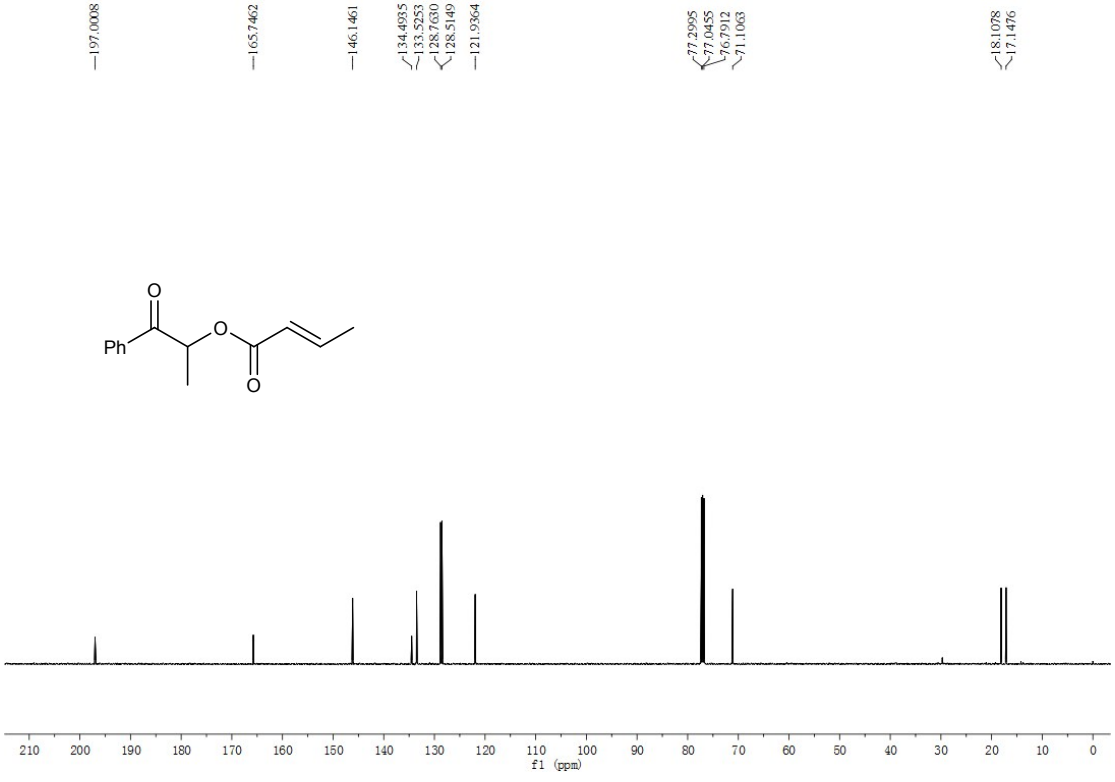
7.6063
7.5915
7.5134
7.4977
7.4825
7.2845
7.0666
6.0563
6.0423
6.0283
5.9846
5.9814
5.9781
5.9749
5.9536
5.9503
5.9470
5.9439
1.9277
1.9243
1.9139
1.9105
1.5833
1.5693
O
Ph
O
O
1.99
0.99
1.98
0.97
1.00
0.96
2.97
3.07
f1 (ppm)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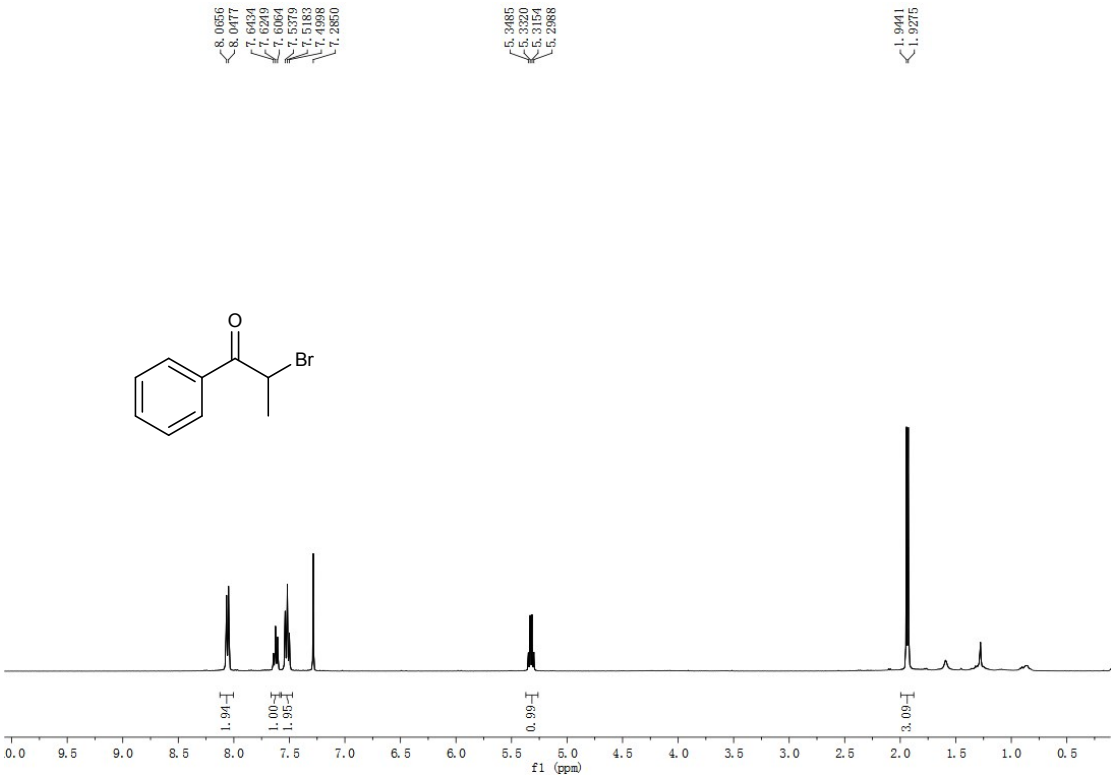
146.1461
134.4935
133.5253
128.7630
128.5149
121.9364
77.2995
77.0455
76.7912
71.1063
18.1078
17.1476
O
Ph
O
O
f1 (ppm)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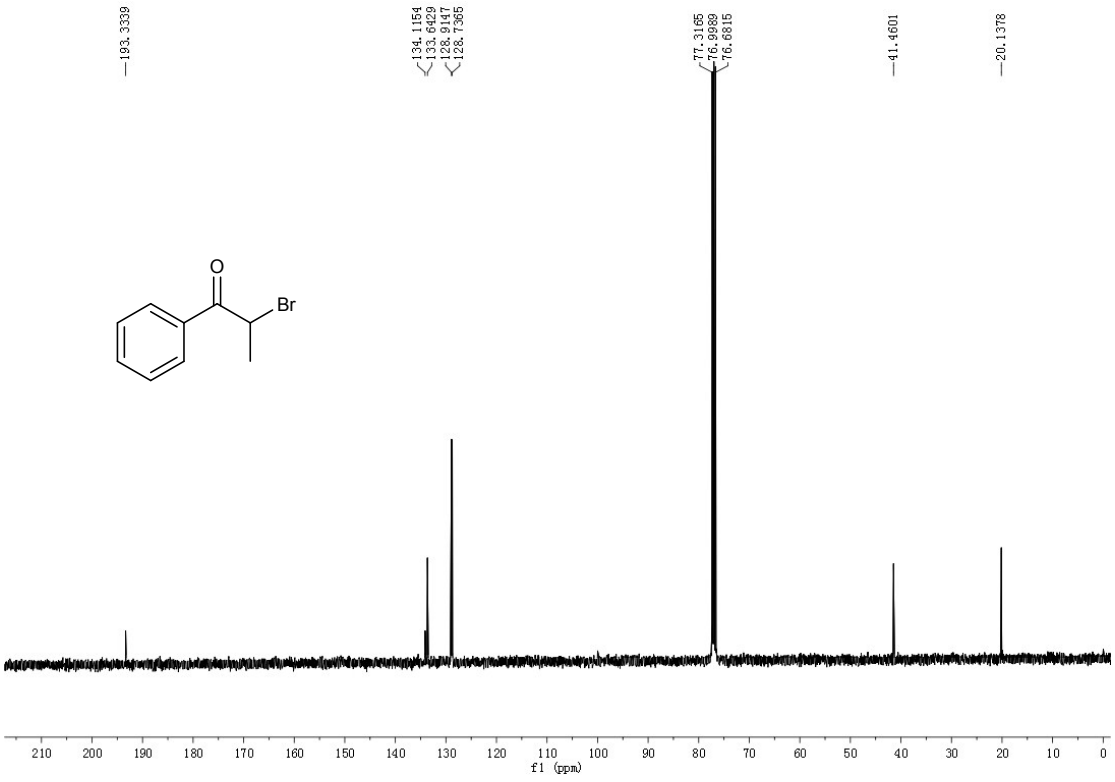
7.6434
7.6249
7.6064
7.5379
7.5183
7.4998
7.2850
5.3485
5.3320
5.3154
5.2988
1.9441
1.9275
O
Br
1.94
1.00
1.95
0.99
3.09
f1 (ppm)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133.6429
128.9147
128.7365
77.3165
76.9989
76.6815
41.4601
20.1378
O
Br
f1 (ppm)