Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

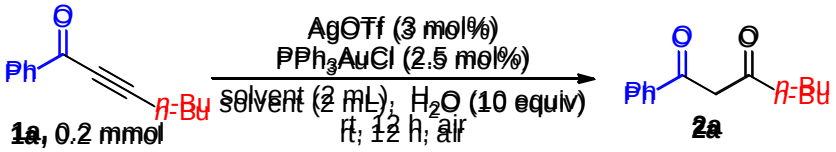
Facile Access to 1,3-Diketones by Gold(I)-Catalyzed Regioselective Hydration of Ynones

1. General Information

All commercially available reagents were used without further purification. Analytical TLC was performed on glass-backed plates pre-coated with silica gel, which were visualized by UV fluorescence (λmax = 254 nm) and/or by staining with 1% *w*/*v* $KMnO_4$ in 0.5 M aqueous K_2CO_3. ^1H NMR and ^{13}C NMR spectra were measured on a 500 MHz spectrometer (^1H: 500 MHz, ^{13}C: 125 MHz), using $CDCl_3$ or d^6-DMSO as the solvent with tetramethylsilane (TMS) as an internal standard at room temperature. All ^1H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals at 7.26 ppm ($CHCl_3$) or the signals at 0.00 ppm (TMS). All ^{13}C NMR spectra were reported in ppm relative to residual $CHCl_3$ (77.0 ppm) and were obtained with ^1H-decoupling. Data for ^1H NMR are described as following: chemical shift (δ in ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; quin, quintet; sep, septet; m, multiplet; br, broad signal), coupling constant (Hz), integration. Data for ^{13}C NMR are described in terms of chemical shift (δ in ppm). High resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Melting points were measured on X4 melting point apparatus and uncorrected.

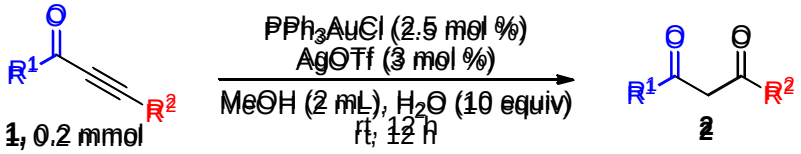
Ynones are prepared from known literature procedure[1].

2. **Table S1** Optimization of solvent for the synthesis of 1,3-diketone **2a**



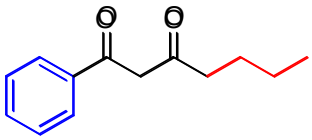
Entry	solvent	Isolated yield of **2a**
1	MeOH	98%
2	DCM	Not detected
3	1,4-dioxane	90%
4	CH_3CN	Not detected

3. General procedure for the Gold(I)-Catalyzed Synthesis of 1,3-Diketones

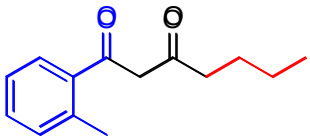


To a 10 mL Schlenk tube equipped with a stirring bar was charged with PPh_3AuCl (0.005 mmol), AgOTf (0.006 mmol), ynone **1** (0.2 mmol), methanol (2 mL), and H_2O (2 mmol) sequentially without any protection. The reaction was then stirred at room temperature for 12h (open to the air, monitored by TLC). Upon completion the solvent was removed under reduced pressure and the crude product was purified by column chromatography (eluent: PE / EA) to afford the 1,3-diketone products **2**.

All the 1,3-diketone products are in keto-enol equilibrium, and the enol forms are contained as the majority as indicated in the parentheses. Characterization data of enol form of each product are shown below.
From the copies of the NMR spectra we could observe very small amount of the keto forms in all cases, which are in very low ratio and some of the peaks are overlapped with those of the enol forms. According to suggestions of the reviewer and editor, we have indicated signals of the minor keto form with asterisk. For the same compound prepared from different precursors, the names of the precursors are given in corresponding spectra.

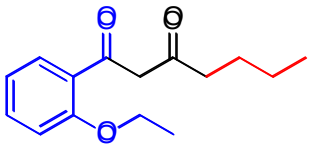


1-phenylheptane-1,3-dione(2a)[2]**:** Light brown oil (39.4 mg, 98%). (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.95 (t, *J* = 7.5 Hz, 3H), 1.36 – 1.46 (m, 2H), 1.63 – 1.73 (m, 2H), 2.43 (t, *J* = 7.5 Hz, 2H), 6.17 (s, 1H), 7.42 - 7.48 (m, 2H), 7.51 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.85 – 7.91 (m, 2H), 16.19 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 27.9, 39.0, 96.1, 127.0, 128.6, 132.2, 135.2, 183.5, 196.9 ppm;
HRMS (ESI): calcd for $C_{13}H_{17}O_2$ $[M+H]^+$ 205.1229, found 205.1219.

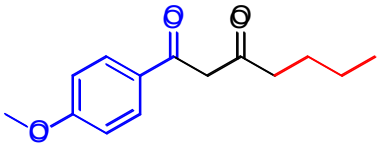


1-o-tolylheptane-1,3-dione(2b): Light brown oil (41.3 mg, 98%). (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)** δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.35 – 1.45 (m, 2H), 1.63 – 1.69 (m, 2H), 2.39 (t, *J* = 7.5 Hz, 2H), 2.49 (s, 3H), 5.84 (s, 1H), 7.22 (d, *J* = 7.0 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H) 7.30 – 7.35 (m, 1H), 7.44 – 7.48 (m, 1H), 16.00 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 20.6, 22.4, 27.9, 38.7, 100.1, 125.7, 128.2, 130.5, 131.3, 136.2, 137.0, 188.2, 196.2 ppm.

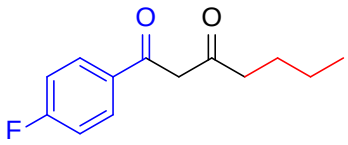
HRMS (ESI): calcd for $C_{14}H_{19}O_2$ $[M+H]^+$ 219.1385, found 219.1376.



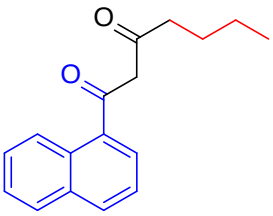
1-(2-ethoxyphenyl)heptane-1,3-dione (**2c**)**:** White solid (47.0 mg, 93%). Mp: 39-41℃. (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.36 – 1.44 (m, 2H), 1.49 (t, *J* = 7.0 Hz, 3H), 1.62 – 1.71 (m, 2H), 2.40 (t, *J* = 7.5 Hz, 2H), 4.12 (q, *J* = 7.0 Hz, 2H), 6.56 (s, 1H), 6.93 (d, *J* = 8.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 1H), 16.21 (br, 1H) ppm; **^{13}C NMR (125 MHz, $CDCl_3$)**: δ = 13.8, 14.7, 22.3, 27.9, 39.2, 64.3, 101.3, 112.5, 120.6, 124.4, 130.2, 132.7, 157.8, 181.2, 197.5 ppm;
HRMS (ESI): calcd for $C_{15}H_{21}O_3$ $[M+H]^+$ 249.1491, found 249.1485.



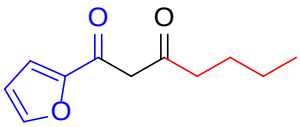
1-(4-methoxyphenyl)heptane-1,3-dione(2d): colorless oil (47.5 mg, 99%). (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.35 – 1.44 (m, 2H), 1.61 – 1.71 (m, 2H), 2.39 (t, *J* = 7.5 Hz, 2H), 3.85 (s, 3H), 6.10 (s, 1H), 6.93 (d, *J* = 9.0 Hz, 2H), 7.86 (d, *J* = 9.0 Hz, 2H), 16.35 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$) δ = 13.8, 22.4, 28.1, 38.4, 55.4, 95.1, 113.9, 129.1, 131.1, 163.0, 184.3, 194.8 ppm;
HRMS (ESI): calcd for $C_{14}H_{19}O_3$ $[M+H]^+$ 235.1334, found 235.1326.



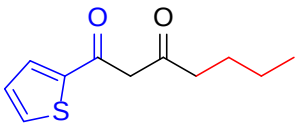
1-(4-fluorophenyl)heptane-1,3-dione(2e): Pale yellow oil (40.8 mg, 90%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.95 (t, *J* = 7.5 Hz, 3H), 1.35 – 1.46 (m, 2H), 1.62 – 1.72 (m, 2H), 2.42 (t, *J* = 7.5 Hz, 2H), 6.12 (s, 1H), 7.07 – 7.16 (m, 2H), 7.86 – 7.93 (m, 2H), 16.19 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 28.0, 38.7, 95.7, 115.7 (d, *J* = 21.8 Hz), 129.4 (d, *J* = 9.0 Hz), 131.5 (d, *J* = 3.0 Hz), 165.3 (d, *J* = 252.0 Hz), 183.1, 196.1 ppm;
^{19}F NMR (471 MHz, $CDCl_3$): δ = -106.7 ppm;
HRMS (ESI): calcd for $C_{13}H_{16}FO_2$ $[M+H]^+$ 223.1134, found 223.1123.



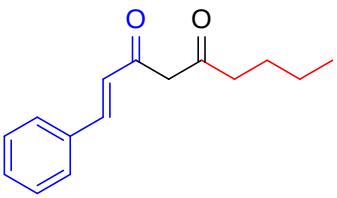
1-(naphthalen-1-yl)heptane-1,3-dione (2f): Light brown oil (52.0 mg, > 99%). (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.95 (t, *J* = 7.5 Hz, 3H), 1.38 – 1.46 (m, 2H), 1.65 – 1.71 (m, 2H), 2.43 (t, *J* = 7.5 Hz, 2H), 6.02 (s, 1H), 7.46 – 7.70 (m, 3H), 7.71 (dd, *J* = 7.0, 1.0 Hz, 1H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 8.46 (d, *J* = 8.0 Hz, 1H), 16.15 (s, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4 27.9, 38.5, 101.0, 124.7, 125.6, 126.3, 126.9, 127.1, 128.5, 130.2, 131.5, 133.8, 134.5, 188.4, 195.7 ppm;
HRMS (ESI): calcd for $C_{17}H_{19}O_2$ $[M+H]^+$ 255.1385, found 255.1380.



1-(furan-2-yl)heptane-1,3-dione (2g): Pale yellow oil (29.6 mg, 76%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.34 – 1.43 (m, 2H), 1.62 - 1.68 (m, 2H), 2.42 (t, *J* = 7.5 Hz, 2H), 6.07 (s, 1H), 6.54 (dd, *J* = 3.5, 1.5 Hz, 1H), 7.15 (d, *J* = 3.5 Hz, 1H), 7.56 (d, *J* = 1.0 Hz, 1H), 15.56 (s, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.3, 28.1, 37.7, 95.4, 112.4, 115.4, 145.8, 150.7, 176.2, 193.0 ppm;
HRMS (ESI): calcd for $C_{11}H_{15}O_3$ $[M+H]^+$ 195.1021, found 195.1018.

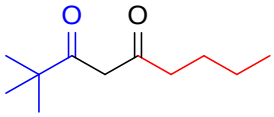


1-(thiophen-2-yl)heptane-1,3-dione (2h): Light brown oil (40.8 mg, 93%). (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.36 – 1.45 (m, 2H), 1.61 – 1.70 (m, 2H), 2.36 (t, *J* = 7.5 Hz, 2H), 6.01 (s, 1H), 7.12 (dd, *J* = 5.0, 4.0 Hz, 1H),7.59 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.69 (dd, *J* = 4.0, 1.0 Hz, 1H),15.69 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$) δ = 13.7, 22.3, 28.2, 37.2, 95.7, 128.1, 130.0, 132.1, 141.8, 181.8, 190.8 ppm;
HRMS (ESI): calcd for $C_{11}H_{15}O_2S$ $[M+H]^+$ 211.0793, found 211.0789.

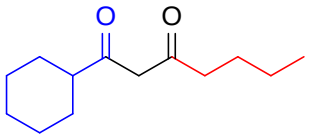


(*E*)-1-phenylnon-1-ene-3,5-dione (2i): Pale yellow solid (40.7 mg, 86%). Mp: 39-41℃. (PE/EA = 80/1)
(enol form) ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.94 (t, *J* = 7.5 Hz, 3H), 1.34 – 1.43 (m, 2H),1.60 –

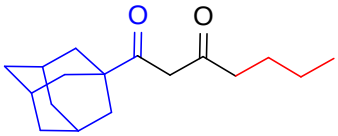
1.68 (m, 2H), 2.40 (t, *J* = 7.5, 2H), 5.65 (s, 1H), 6.48 (d, *J* = 16.0, Hz, 1H), 7.33 – 7.42 (m, 3H), 7.49 – 7.54 (m, 2H), 7.59 (d, *J* = 16.0 Hz, 1H), 15.41 (br, 1 H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 27.6, 40.03, 100.6, 123.0, 127.9, 128.9, 129.8, 135.1, 139.5, 177.0, 201.1 ppm;
HRMS (ESI): calcd for $C_{15}H_{19}O_2$ $[M+H]^+$ 231.1385, found 231.1387.



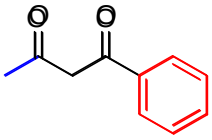
2,2-dimethylnonane-3,5-dione (2j): colorless oil (26.5 mg, 72%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.93 (t, *J* = 7.5 Hz, 3H), 1.17 (s, 9H), 1.31 – 1.40 (m, 2H), 1.56 – 1.63 (m, 2H), 2.31 (t, *J* = 7.5, 2H), 5.59 (s, 1H), 15.84 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 27.3, 27.9, 38.6, 39.1, 95.0, 195.6, 200.4 ppm;
HRMS (ESI): calcd for $C_{11}H_{21}O_2$ $[M+H]^+$ 185.1542, found 185.1536.



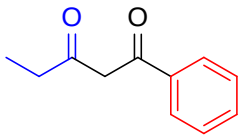
1-cyclohexylheptane-1,3-dione (2k): Light brown oil (34.9 mg, 86%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.92 (t, *J* = 7.5 Hz, 3H), 1.27– 1.39 (m, 6H), 1.55 – 1.62 (m, 2H), 1.66 – 1.87 (m, 6H), 2.16 (tt, *J* = 11.5, 3.5 Hz, 1H), 2.29 (t, *J* = 7.0 Hz, 2H), 5.48 (s, 1H), 15.65 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 25.8, 25.9, 27.9, 29.6, 38.4 , 46.5, 97.3, 195.4, 197.3 ppm.
HRMS (ESI): calcd for $C_{13}H_{23}O_2$ $[M+H]^+$ 211.1698, found 211.1699.



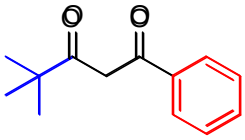
1-{(3r,5r,7r)-Adamantan-1-yl}heptane-1,3-dione (2l): Light brown oil(51.0 mg, 97%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.92 (t, *J* = 7.5 Hz, 3H), 1.32 – 1.40 (m, 2H), 1.56 – 1.63 (m, 2H), 1.65 – 1.76 (m, 6H), 1.82 (d, *J* = 2.5 Hz, 6H), 2.04 (s, 3H), 2.31 (t, *J* = 7.5 Hz, 2H), 5.54 (s, 1H), 15.92 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.8, 22.4, 27.9, 28.1, 36.6, 38.8, 39.0, 40.8, 94.8, 196.8, 198.8 ppm;
HRMS (ESI): calcd for $C_{17}H_{27}O_2$ $[M+H]^+$ 263.2011, found 263.2002.



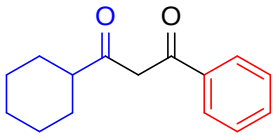
1-phenylbutane-1,3-dione (2m): White solid. From **4-phenylbut-3-yn-2-one** (29.5 mg, 0.20 mmol), (14.2 mg, 43%), or from **1-phenylbut-2-yn-1-one** (26.1 mg, 0.18 mmol), (23.5 mg, 80%). Mp: 57-59°C. (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 2.20 (s, 3H), 6.18 (s, 1H), 7.42 - 7.48 (m, 2H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.86 – 7.90 (m, 2H), 16.15 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 25.8, 96.7, 127.0, 128.6, 132.2, 134.9 , 183.4, 193.7 ppm;
HRMS (ESI): calcd for $C_{10}H_{13}O_2$ $[M+H]^+$ 163.0759, found 163.0756.



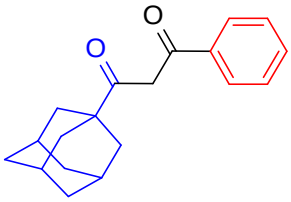
1-phenylpentane-1,3-dione(2n): colorless oil (26.4 mg, 74%). (PE/EA = 100/1)
(enol form) ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.22 (t, *J* = 7.5 Hz, 3H), 2.47 (q, *J* = 7.5 Hz, 2H), 6.18 (s, 1H), 7.41 – 7.48 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.85 – 7.91 (m, 2H), 16.12 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 9.7, 32.4, 95.4, 126.9, 128.7, 132.1, 135.1, 183.1, 198.0 ppm;
HRMS (ESI): calcd for $C_{11}H_{13}O_2$ $[M+H]^+$ 177.0916, found 177.0908.



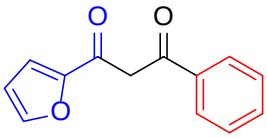
4,4-Dimethyl-1-phenylpentane-1,3-dione (2o)[3]: Light brown oil. From **4,4-dimethyl-1-phenylpent-2-yn-1-one** (36.6 mg, 0.20 mmol), (38.6 mg, 96%), or from **4,4-dimethyl-1-phenylpent-1-yn-3-one** (36.7 mg, 0.20 mmol), (26.7 mg, 66%). (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.26 (s, 9H), 6.30 (s, 1H), 7.42 – 7.48 (m, 2H), 7.52 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.87 – 7.91 (m, 2H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.4, 39.9, 92.1, 127.0, 128.6, 132.1, 135.6, 184.6, 202.9 ppm;
HRMS (ESI): calcd for $C_{13}H_{17}O_2$ $[M+H]^+$ 205.1229, found 205.1229.



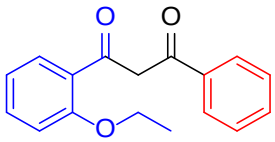
1-cyclohexyl-3-phenylpropane-1,3-dione (2p): White solid (41.2 mg, 89%). Mp: 48-49°C. (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.19 – 1.37 (m, 4H), 1.42 – 1.50 (m, 2H), 1.80 – 1.96 (m, 4H), 2.32 (tt, *J* = 11.5, 3.5 Hz, 1H), 6.18 (s, 1H), 7.40 – 7.46 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.84 – 7.90 (m, 2H), 16.30 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 25.8, 25.8, 29.6, 47.3, 94.4, 127.0, 128.5, 132.1, 135.4, 184.3, 199.8 ppm;
HRMS (ESI): calcd for $C_{15}H_{19}O_2$ $[M+H]^+$ 231.1380, found 231.1355.



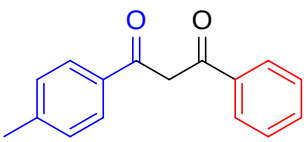
1-{(3r,5r,7r)-Adamantan-1-yl}-3-phenylpropane-1,3-dione (2q): White solid (46.9 mg, 90%). M.p.: 48-50℃. (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.76 (q, *J* = 12.5 Hz, 6H), 1.91 (d, *J* = 2.5 Hz, 6H), 2.08 (s, 3H), 6.26 (s, 1H), 7.41 – 7.48 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.86 – 7.94 (m, 2H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 28.1, 36.6, 39.1, 41.6, 91.9, 127.0, 128.5, 132.0, 135.9, 185.5, 201.4 ppm;
HRMS (ESI): calcd for $C_{19}H_{23}O_2$ $[M+H]^+$ 283.1698, found 283.1690.



1-(furan-2-yl)-3-phenylpropane-1,3-dione (2r): yellow solid (35.8 mg, 84%). Mp: 67-69 ℃. (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 6.58 (dd, *J* = 3.5, 1.5 Hz, 1H), 6.76 (s, 1H), 7.24 (dd, *J* = 3.5, 0.5 Hz, 1H), 7.42 – 7.50 (m, 2H), 7.53 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.61 (dd, *J* = 1.5, 0.5 Hz, 1H), 7.91 – 7.99 (m, 2H), 16.19 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 92.7, 112.6, 115.7, 127.0, 128.6, 132.3, 134.7, 146.0, 151.1, 177.5, 182.6 ppm;
HRMS (ESI): calcd for $C_{16}H_{15}O_2$ $[M+H]^+$ 215.0708, found 215.0708.

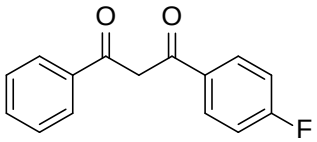


1-(2-ethoxyphenyl)-3-phenylpropane-1,3-dione (2s): Pale yellow solid (51.1 mg, 95%). Mp: 85-86 ℃. (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.55 (t, *J* = 7.0 Hz, 3H), 4.16 (q, *J* = 7.0 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.01 – 7.08 (m, 1H), 7.33 (s, 1H), 7.40 – 7.48 (m, 3H), 7.52 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.93 – 7.99 (m, 2H), 8.00 (dd, *J* = 8.0, 1.5 Hz, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 14.9, 64.3, 98.6, 112.6, 120.7, 124.6, 127.1, 128.6, 130.3, 132.1, 133.1, 136.2, 158.1, 183.5, 186.0 ppm;
HRMS (ESI) calcd for $C_{17}H_{17}O_3$ $[M+H]^+$ 269.1178, found 268.1170.

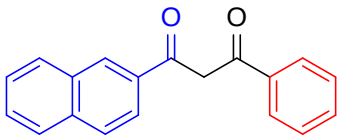


1-(2-ethoxyphenyl)-3-phenylpropane-1,3-dione (2t)[4]: yellow solid (47.6 mg, 99%). Mp: 85-86℃.

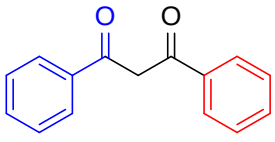
(lit. Mp 80−82 °C). (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 2.42 (s, 3H), 6.82 (s, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.44 – 7.50 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.94 – 8.00 (m, 2H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.6, 92.8, 127.1, 127.2, 128.6, 129.4, 132.3, 132.9, 135.6, 143.2, 185.1, 186.0 ppm;
HRMS (ESI): calcd for $C_{16}H_{15}O_2$ $[M+H]^+$ 239.1072, found 239.1070.



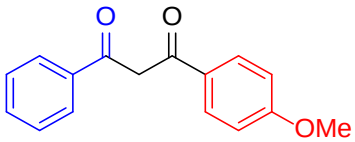
1-(4-fluorophenyl)-3-phenylpropane-1,3-dione (2u): Pale yellow solid. Mp: 81-83℃. From **1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one** (44.8 mg, 0.20 mmol), (45.7 mg, 94%), or from **3-(4-fluorophenyl)-1-phenylprop-2-yn-1-one** (44.3 mg, 0.20 mmol), (42.3 mg, 88%). (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 6.79 (s, 1H), 7.18 – 7.15 (m, 2H), 7.43 – 7.51 (m, 2H), 7.55 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.95 – 8.03 (m, 4H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 92.82, 115.8(d, *J* = 21.8 Hz), 127.1, 128.7, 129.6 (d, *J* = 9.1 Hz), 132.0 (d, *J* = 3.0 Hz), 132.5, 135.3, 165.4 (d, *J* = 252.4 Hz), 185.0, 185.1 ppm;
^{19}F NMR (471 MHz, $CDCl_3$): δ = -106.2 ppm;
HRMS (ESI): calcd for $C_{15}H_{12}FO_2$ $[M+H]^+$ 243.0821, found 243.0816.



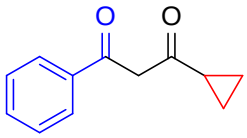
1-(naphthalen-2-yl)-3-phenylpropane-1,3-dione (2v): white solid (52.0 mg, 95%). Mp: 101-103℃. (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 6.97 (s, 1H), 7.45 – 7.60 (m, 5H), 7.83 – 7.91 (m, 2H), 7.92 – 8.04 (m, 4H), 8.51 (s, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$) δ = 93.4, 123.2, 126.8, 127.2, 127.7, 128.1, 128.3, 128.4, 128.7, 129.3, 132.4, 132.7, 132.8, 135.3, 135.6, 185.5, 185.7 ppm;
HRMS (ESI): calcd for $C_{19}H_{15}O_2$ $[M+H]^+$ 275.1072, found 275.1071.



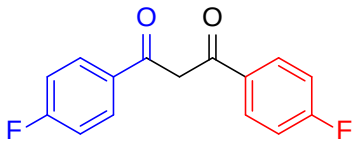
1,3-diphenylpropane-1,3-dione (2w)[4]: White solid (92%, 41.5 mg): Mp: 77-78℃. (Lit. 76−77 °C). (PE/EA = 80/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 6.85 (s, 1H), 7.45 – 7.52 (m, 4H), 7.55 (tt, *J* = 7.5, 1.5 Hz, 2H), 7.93 – 8.00 (m, 4H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 93.2, 127.2, 128.7, 132.4, 135.6, 185.8 ppm;
HRMS (ESI): calcd for $C_{15}H_{13}O_2$ $[M+H]^+$ 225.0916, found 225.0913.



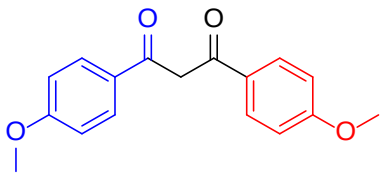
1-(4-Methoxyphenyl)-3-phenylpropane-1,3-dione (2x)[4]: white solid (45.7 mg, 90%). Mp: 130-132℃. (Lit. 127−128 °C). (PE/EA = 40/1)
(enol form) ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.79 (s, 1H), 6.97 (d, *J* = 9.0 Hz, 2H), 7.43 – 7.51 (m, 2H), 7.53 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.90 – 7.98.004 (m, 4H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$) δ = 55.4, 92.4, 114.0, 127.0, 128.2, 128.6, 129.3, 132.1, 135.6, 163.3, 184.0, 186.2 ppm;
HRMS (ESI): calcd for $C_{16}H_{15}O_3$ $[M+H]^+$ 255.1021, found 255.1018.



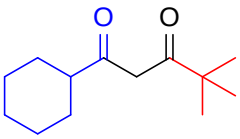
1-cyclopropyl-3-phenylpropane-1,3-dione (2y): White solid (35.9 mg, 94%). Mp: 38-40℃. (PE/EA = 40/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 0.94 – 1.00 (m, 2H), 1.16 – 1.22 (m, 2H), 1.80 (tt, *J* = 8.0, 3.5 Hz, 1H), 6.28 (s, 1H), 7.40 – 7.46 (m, 2H), 7.50 (tt, *J* = 7.5, 1.5 Hz, 1H), 7.83-7.88 (m, 2H), 16.25 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 10.6, 19.3, 54.9, 96.1, 126.7, 128.5, 131.9, 134.5, 178.5, 200.23 ppm;
HRMS (ESI): calcd for $C_{12}H_{13}O_2$ $[M+H]^+$ 189.0916, found 189.0911.



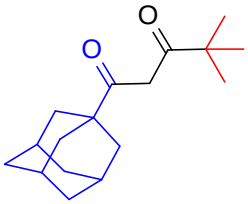
1,3-bis(4-fluorophenyl)propane-1,3-dione (2z): Pale yellow solid (43.2 mg, 83%). Mp: 118-120℃. (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 6.74 (s, 1H), 7.13 – 7.19 (m, 4H), 7.95 – 8.05 (m, 4H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 92.5, 115.8 (d, *J* = 21.8 Hz), 129.6 (d, *J* = 9.1 Hz), 131.71 (d, *J* = 2.8 Hz), 165.5 (d, *J* = 252.5 Hz), 184.5 ppm;
^{19}F NMR (471 MHz, $CDCl_3$): δ = -106.1 ppm;
HRMS (ESI): calcd for $C_{15}H_{11}F_2O_2$ $[M+H]^+$ 261.0727, found 261.0718.



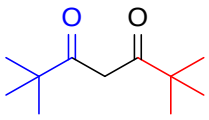
1,3-bis(4-methoxyphenyl)propane-1,3-dione (2A)[5]: White solid (49.3 mg, 87%). Mp: 118-120℃. (PE/EA = 20/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 3.87 (s, 6H), 6.72 (s, 1H), 6.97 (d, *J* = 9.0 Hz, 4H), 7.95 (d, *J* = 9.0 Hz, 4H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 55.4, 91.5, 113.9, 128.2, 129.1, 163.0, 184.6 ppm;
HRMS (ESI): calcd for $C_{17}H_{17}O_4$ $[M+H]^+$ 285.1127, found 285.1128.



1-cyclohexyl-4,4-dimethylpentane-1,3-dione (2B): Light brown oil (36.0 mg, 85%). (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.17 (s, 9H), 1.16 – 1.34 (m, 4H), 1.36 – 1.46 (m 2H), 1.62 – 1.92 (m, 4H), 2.19 (tt, *J* = 11.5, 3.5 Hz, 1H), 5.60 (s, 1H), 15.96 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ =25.8, 27.4, 29.6, 39.2, 45.0, 93.3, 198.5, 201.2 ppm;
HRMS (ESI): calcd for $C_{13}H_{23}O_2$ $[M+H]^+$ 211.1698, found 211.1691.

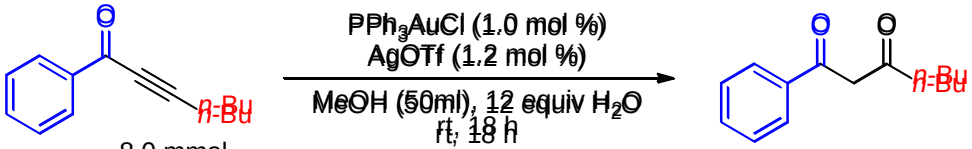


1-{(3r,5r,7r)-Adamantan-1-yl}-4,4-dimethylpentane-1,3-dione (2C): White solid (51.1 mg, 97%). Mp: 86-87℃. (PE/EA = 100/1)
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.17 (s, 9H), 1.67 - 1.77 (m, 6H), 1.83 (s, 6H), 2.04 (s, 3H), 5.68 (s, 1H), 16.25 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.4, 28.1, 36.6, 39.1, 41.2, 90.5, 199.9, 202.7 ppm;
HRMS (ESI): calcd for $C_{17}H_{27}O_2$ $[M+H]^+$ 263.2011, found 263.2006.



2,2,6,6-tetramethylheptane-3,5-dione (2D): colorless oil (19.4 mg, 53%). (PE/EA = 200/1).
(enol form) **^{1}H NMR (500 MHz, $CDCl_3$)**: δ = 1.18 (s, 18H), 5.73 (s, 1H), 16.16 (br, 1H) ppm;
^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.4, 39.4, 90.7, 201.45 ppm;
HRMS (ESI): calcd for $C_{11}H_{21}O_2$ $[M+H]^+$ 185.1542, found 185.1547.

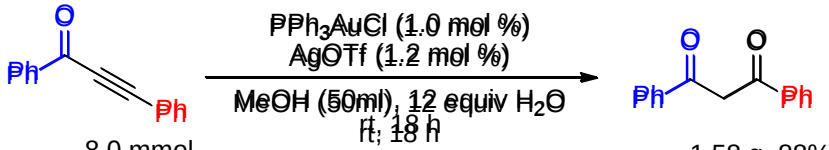
Gram-scale reactions



1a; 8.0 mmol

2a; 1.60 g, 96%

To a 100 mL round bottom flask equipped with a stirring bar was charged with PPh_3AuCl (39.5 mg, 0.08 mmol), AgOTf (26.4 mg, 0.10 mmol), ynone **1a** (1.493 g, 8.0 mmol), methanol (50 mL), and H_2O (1.73 mL, 1.73 g, 96.1 mmol) sequentially without any protection. The reaction was then stirred at room temperature for 18 h (open to the air, monitored by TLC). Upon completion the solvent was removed under reduced pressure and the crude product was purified by column chromatography (eluent: PE /EA=120/1) to afford the 1,3-diketone product **2a** (1.5956 g, 96%).

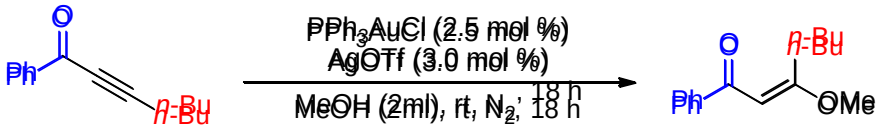


1w; 8.0 mmol

2w; 1.58 g, 88%

To a 100 mL round bottom flask equipped with a stirring bar was charged with PPh_3AuCl (40.0 mg, 0.08 mmol), AgOTf (27.0 mg, 0.10 mmol), ynone **1w** (1.6482 g, 8.0 mmol), methanol (50 mL), and H_2O (1.73 mL, 1.73 g, 96.1 mmol) sequentially without any protection. The reaction was then stirred at room temperature for 18 h (open to the air, monitored by TLC). Upon completion the solvent was removed under reduced pressure and the crude product was purified by column chromatography (eluent: PE /EA=100/1) to afford the 1,3-diketone product **2w** (1.5844 g, 88%).

Synthesis of (E)-3-methoxy-1-phenylhept-2-en-1-one (3a)



1a

3a

To an oven-dried 10 mL Schlenk tube equipped with a stirring bar was charged with PPh_3AuCl (2.5 mg, 0.005 mmol), AgOTf (1.8 mg, 0.007 mmol), ynone **1a** (38.3 mg, 0.21 mmol), and dry methanol (2 mL) sequentially under N_2. The tube was then sealed and the reaction was stirred at room temperature for 18 h. Upon completion the solvent was removed under reduced pressure and the crude product was purified by Pre-TLC (eluent: PE/EA = 80/1) to afford the enolether **3a** (36.7 mg, 82%).

^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.93 (t, *J* = 7.5 Hz, 3H), 1.36 – 1.45 (m, 2H), 1.56 – 1.64 (m, 2H), 2.85 (t, *J* = 7.8 Hz, 2H), 3.76 (s, 3H), 6.11 (s, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 2H) ppm;

^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.9, 22.6, 29.6, 32.7, 55.5, 95.7, 127.6, 128.3, 131.6, 140.6, 178.6, 189.9 ppm;

HRMS (ESI): calcd for $C_{14}H_{19}O_2$ $[M+H]^+$ 219.1385, found 219.1383.

References:

1. K. Okamoto, T. Shimbayashi, E. Tamura, K.Ohe, *Org. Lett.* 2015, **17**, 5843-5845.
2. a) H. Koshimura, J. Saio, T. Okuba, *Bull Chem. Soc. Jpn*. **1973**, *46*, 632; b) Padwa, A. H.; Hornbuckle, S. F. *J. Org. Chem.* **1990**, *55*, 5297-5299.
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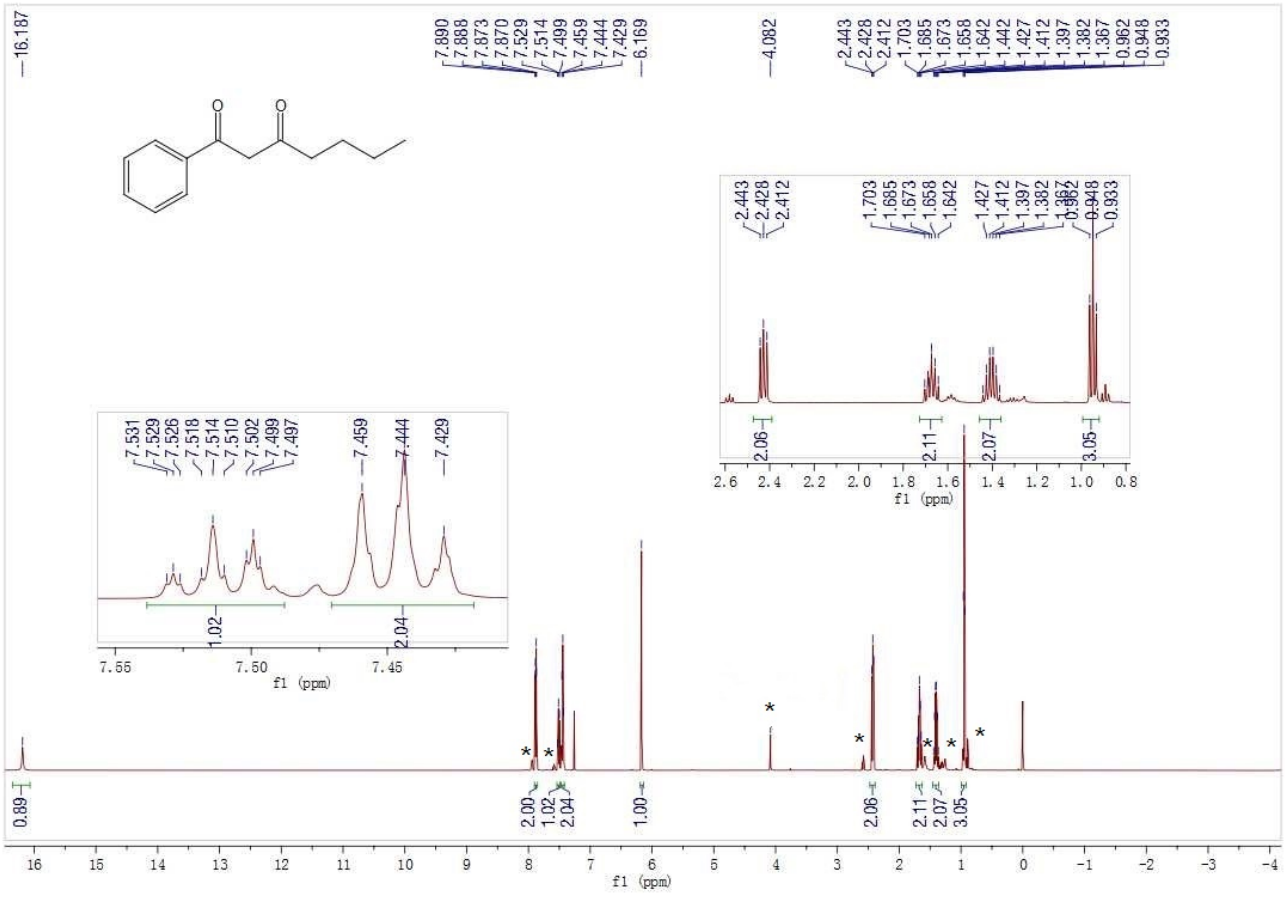
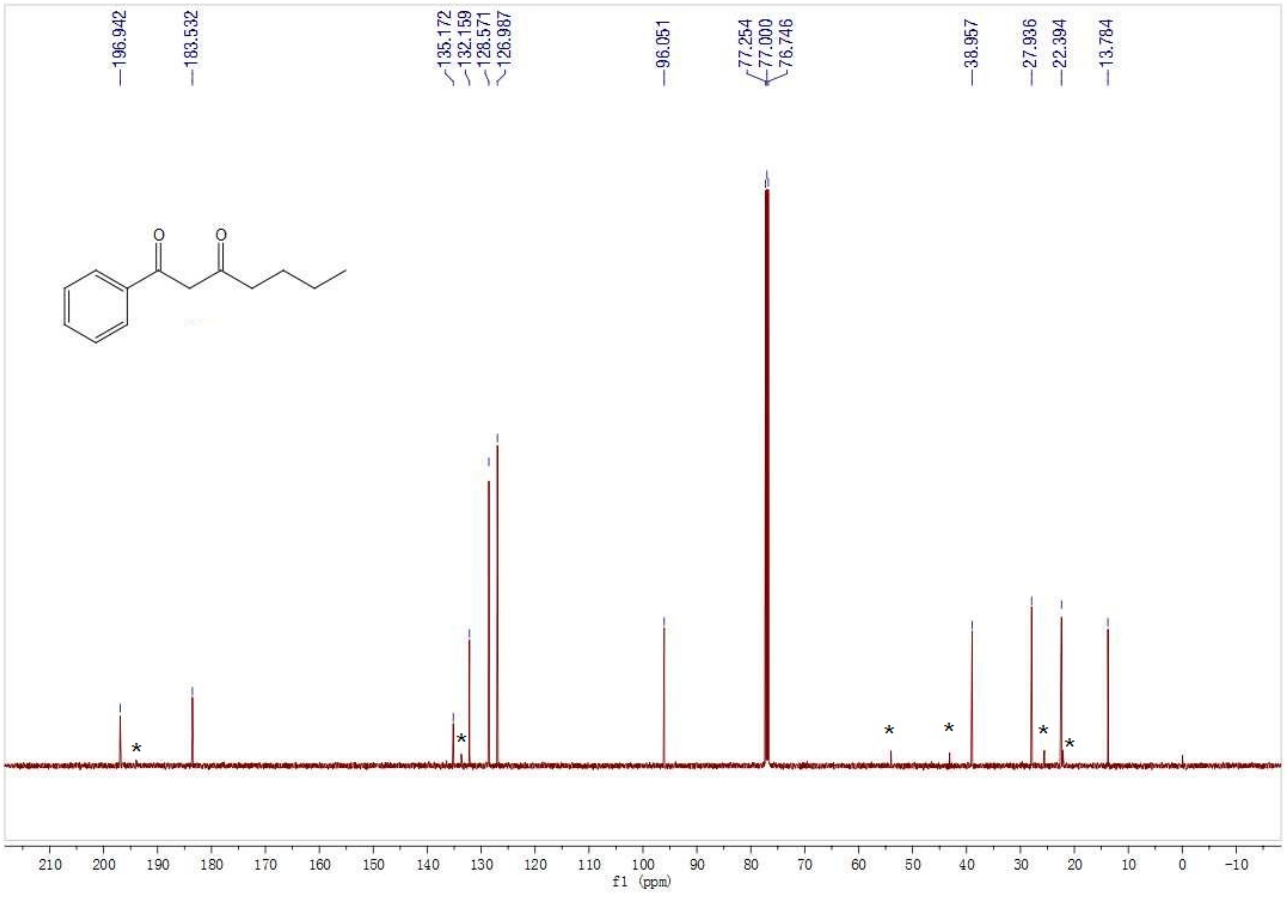
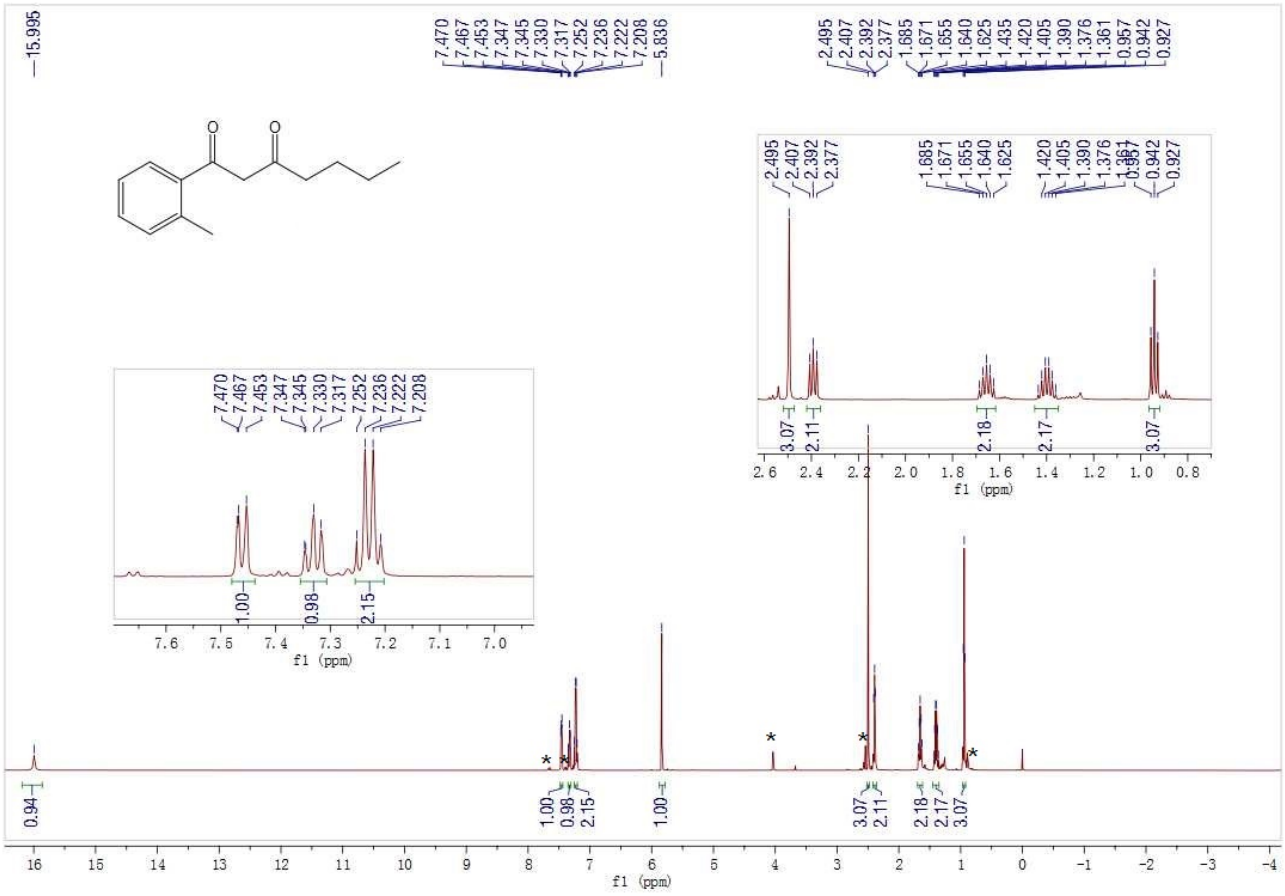
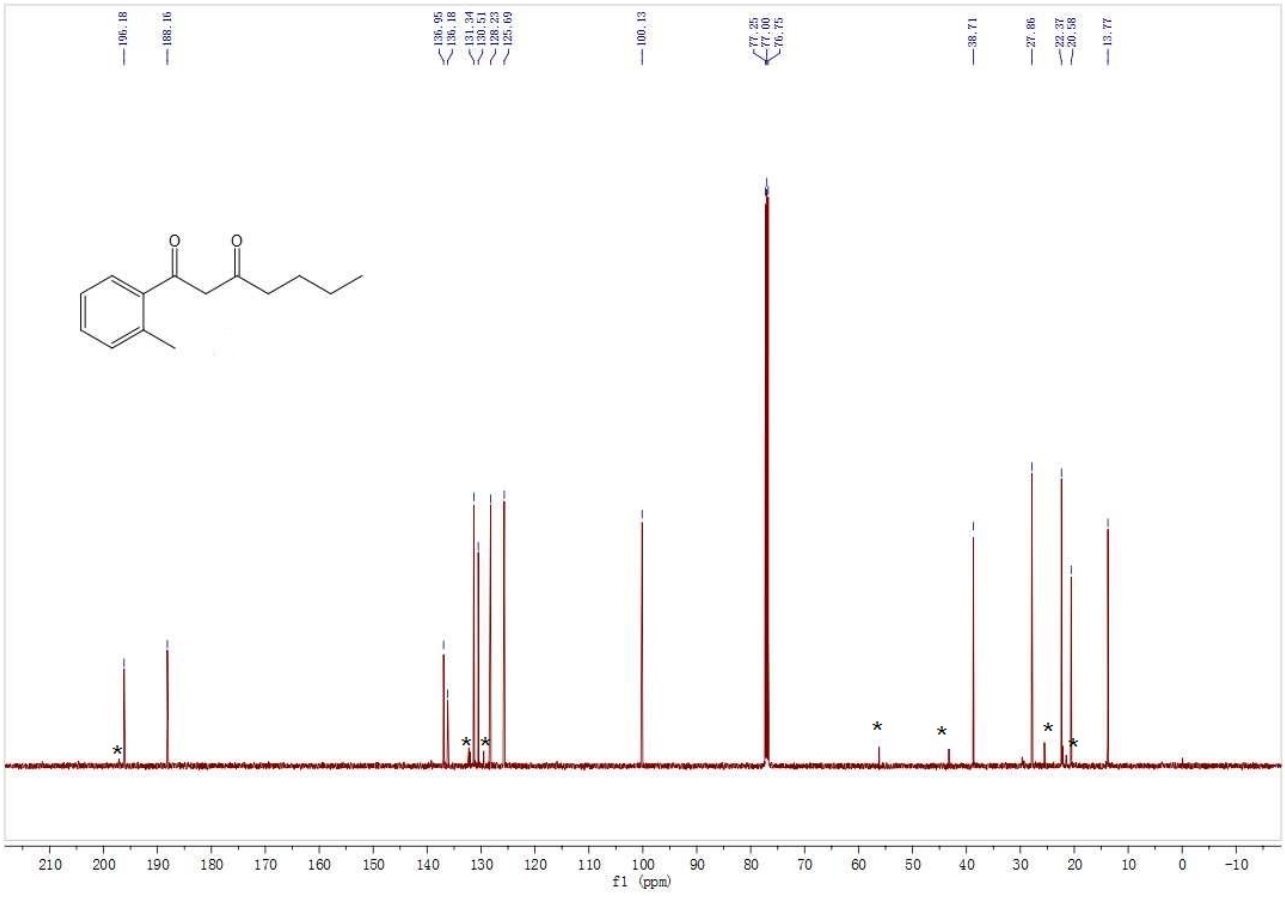
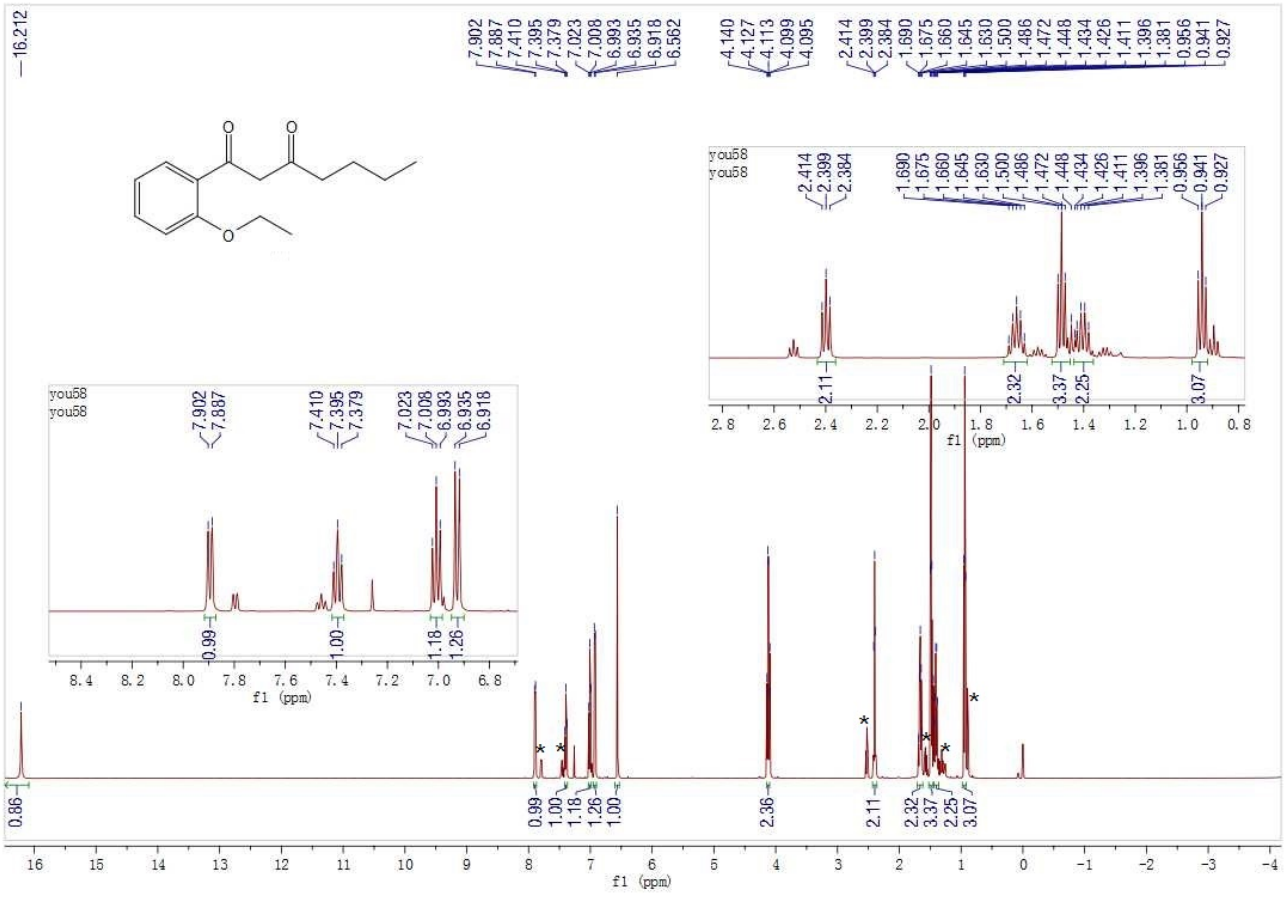
4. E. Hasegawa, K. Ishiyama, T. Horaguchi, T. Shimizu, *J. Org. Chem*. **1991**, *56*, 1631.
5. K. Nomura, K. Asano, T. Kurahashi, S. Matsubara, *Heterocycles* **2008**, *76*, 1381-1399.

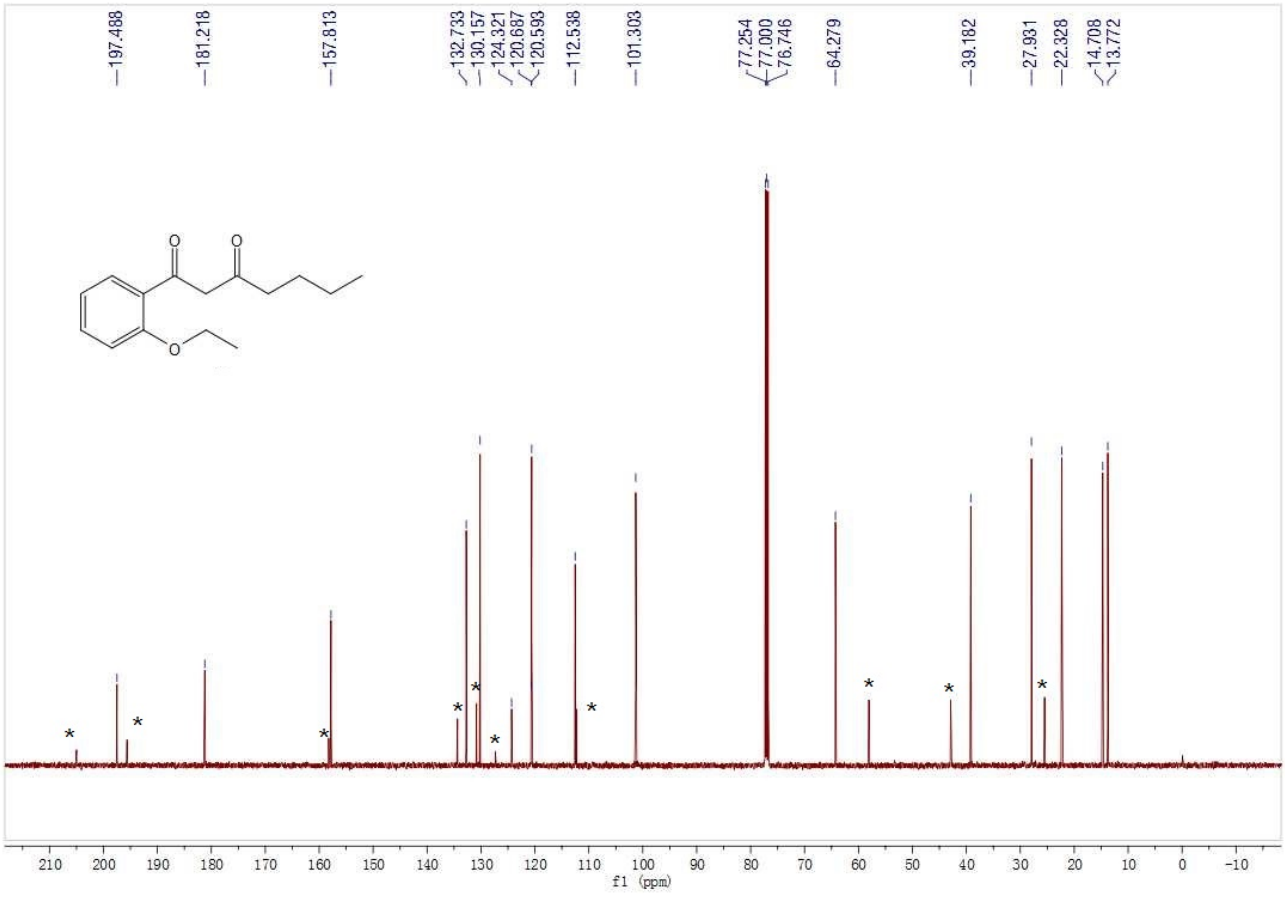

16.187
7.890
7.888
7.873
7.870
7.529
7.514
7.499
7.459
7.444
7.429
6.169
4.082
2.443
2.428
2.412
1.703
1.685
1.673
1.658
1.642
1.442
1.427
1.412
1.397
1.382
1.367
0.962
0.948
0.933
f1 (ppm)

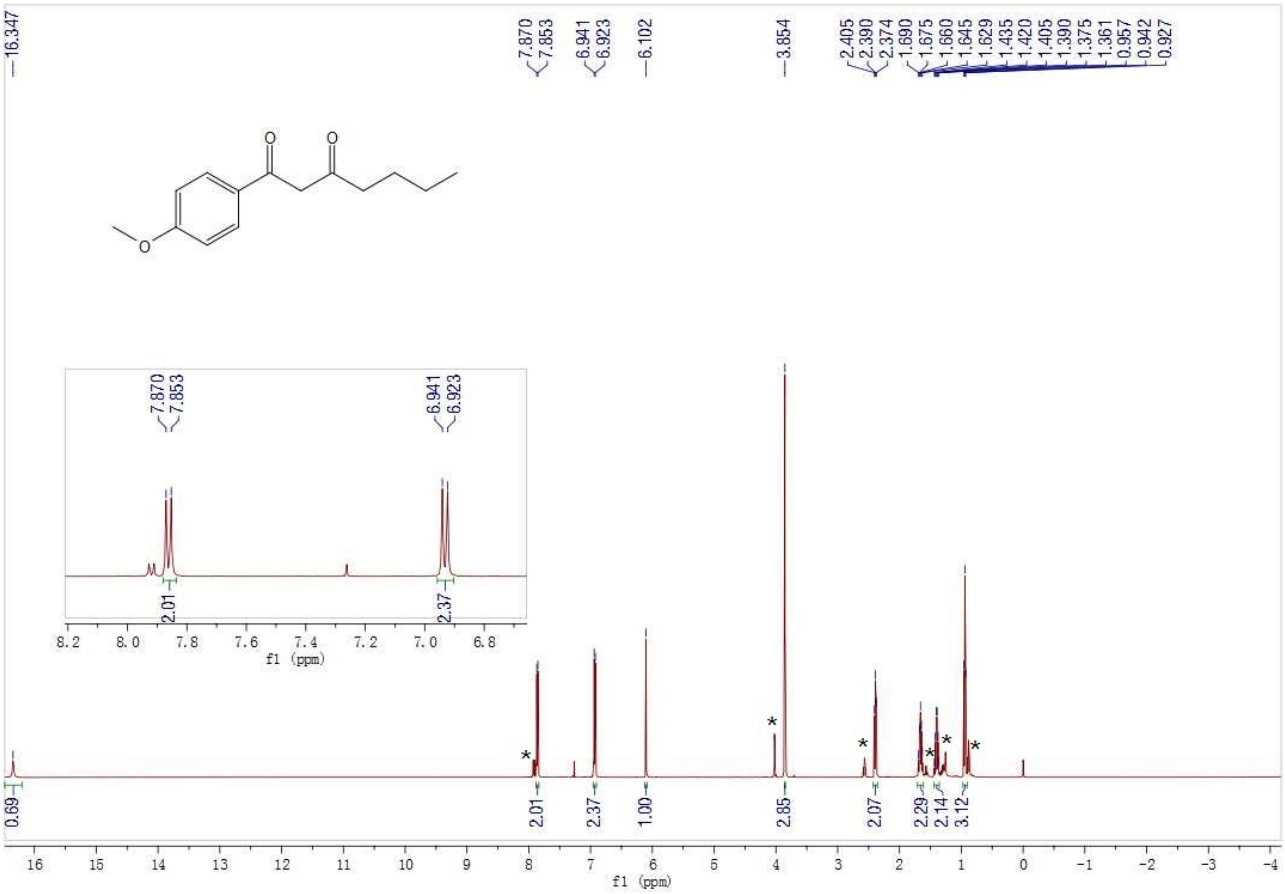

196.942
183.532
135.172
132.159
128.571
126.987
96.051
77.254
77.000
76.746
38.957
27.936
22.394
13.784
f1 (ppm)

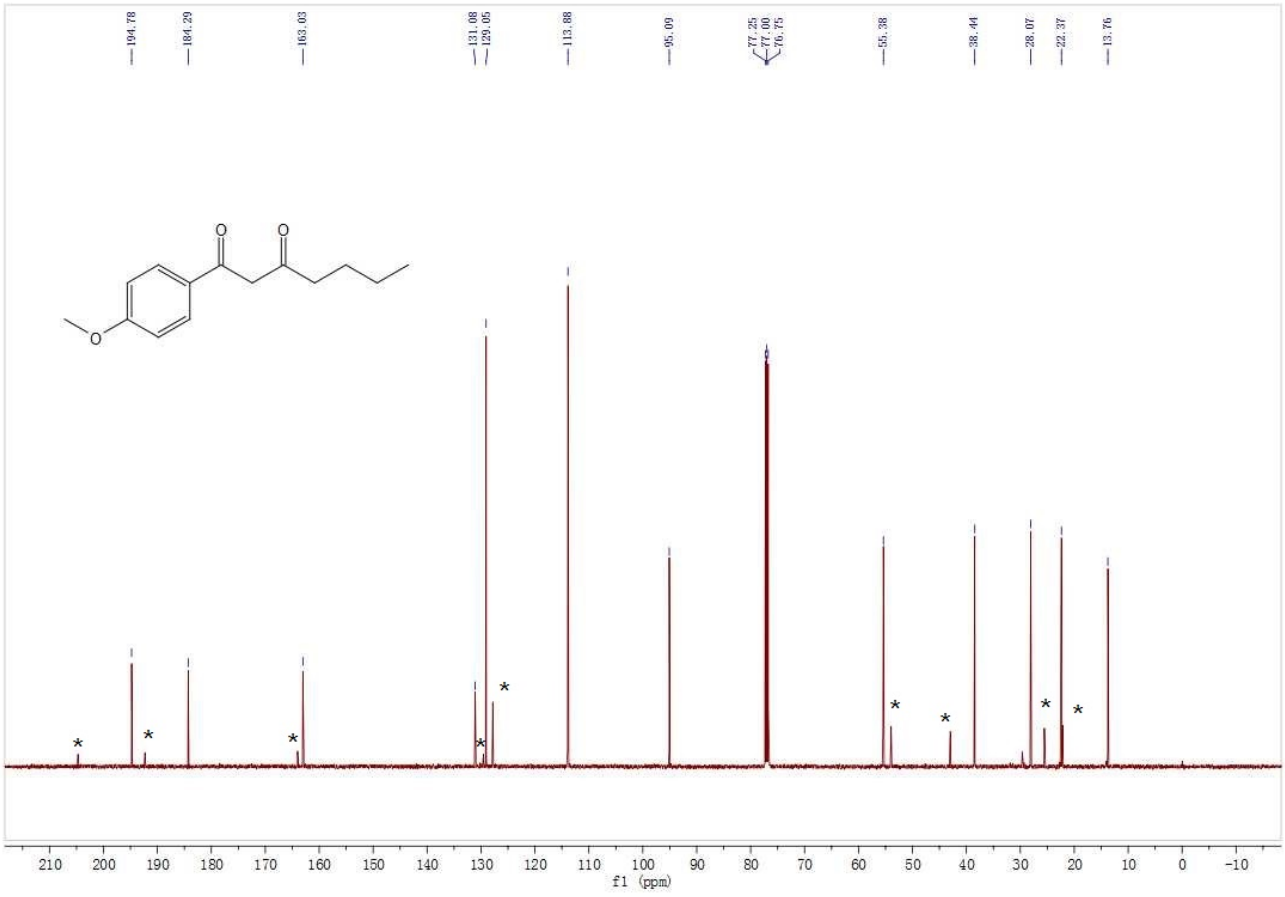

15.995
7.470
7.467
7.453
7.347
7.345
7.330
7.317
7.252
7.236
7.222
7.208
5.836
2.495
2.407
2.392
2.377
1.685
1.671
1.655
1.640
1.625
1.435
1.420
1.405
1.390
1.376
1.361
0.957
0.942
0.927
f1 (ppm)

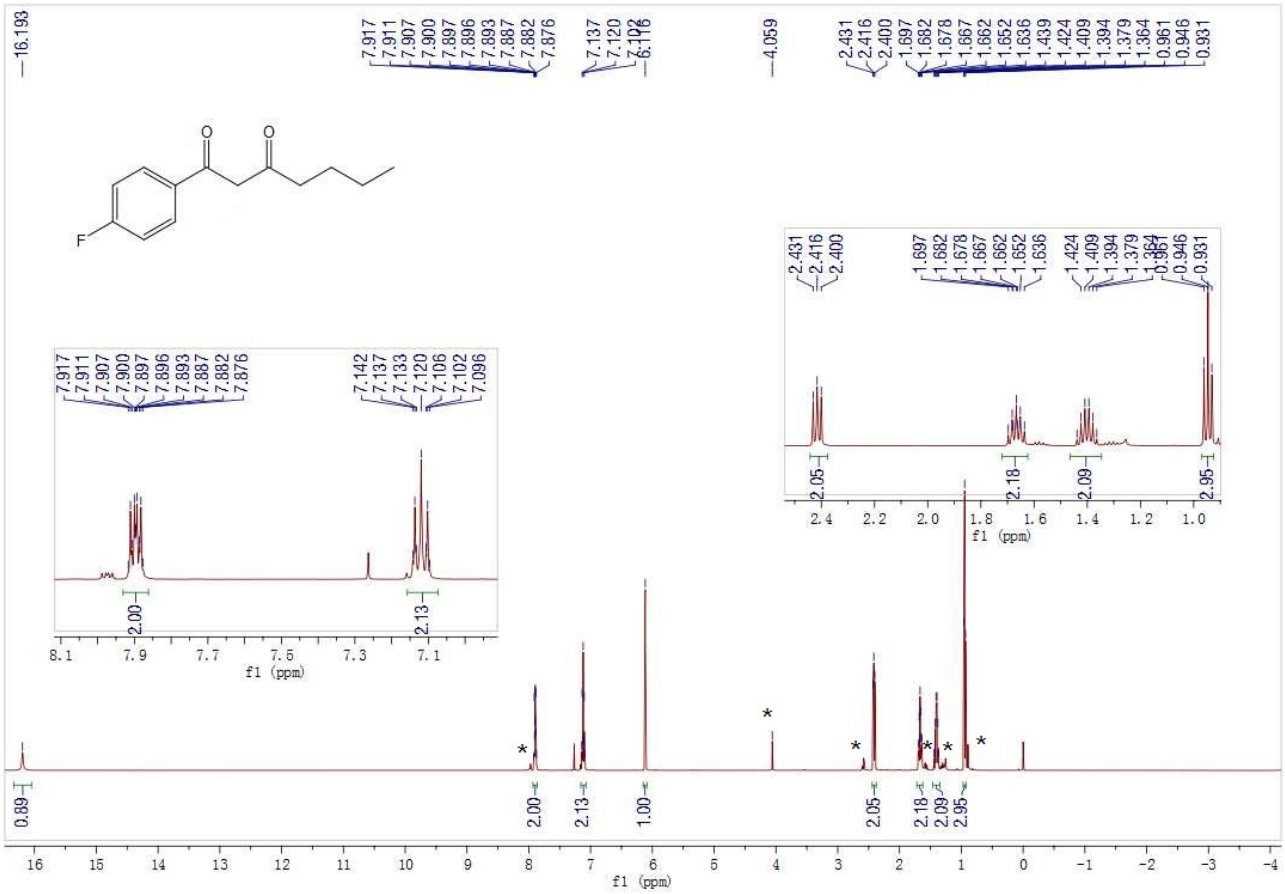

196.18
188.16
136.95
136.18
131.34
130.51
128.23
125.69
100.13
77.25
77.00
76.75
38.71
27.86
22.37
20.58
13.77
f1 (ppm)

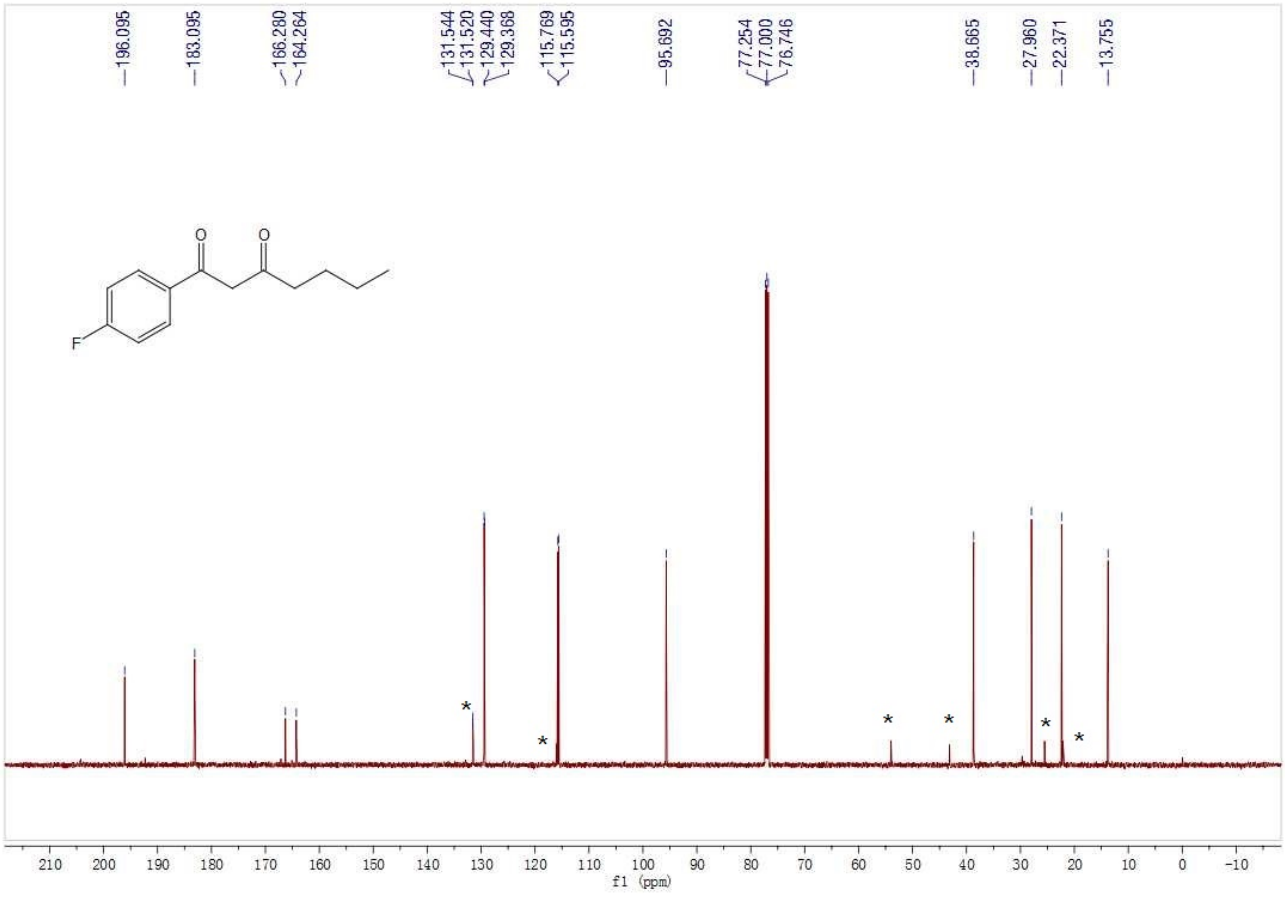

16.212
7.902
7.887
7.410
7.395
7.379
7.023
7.008
6.993
6.935
6.918
6.562
4.140
4.127
4.113
4.099
4.095
2.414
2.399
2.384
1.690
1.675
1.660
1.645
1.630
1.500
1.486
1.472
1.448
1.434
1.426
1.411
1.396
1.381
0.956
0.941
0.927
you58
you58
f1 (ppm)
0.86
0.99
1.00
1.18
1.26
1.00
2.36
2.11
2.32
3.37
2.25
3.07

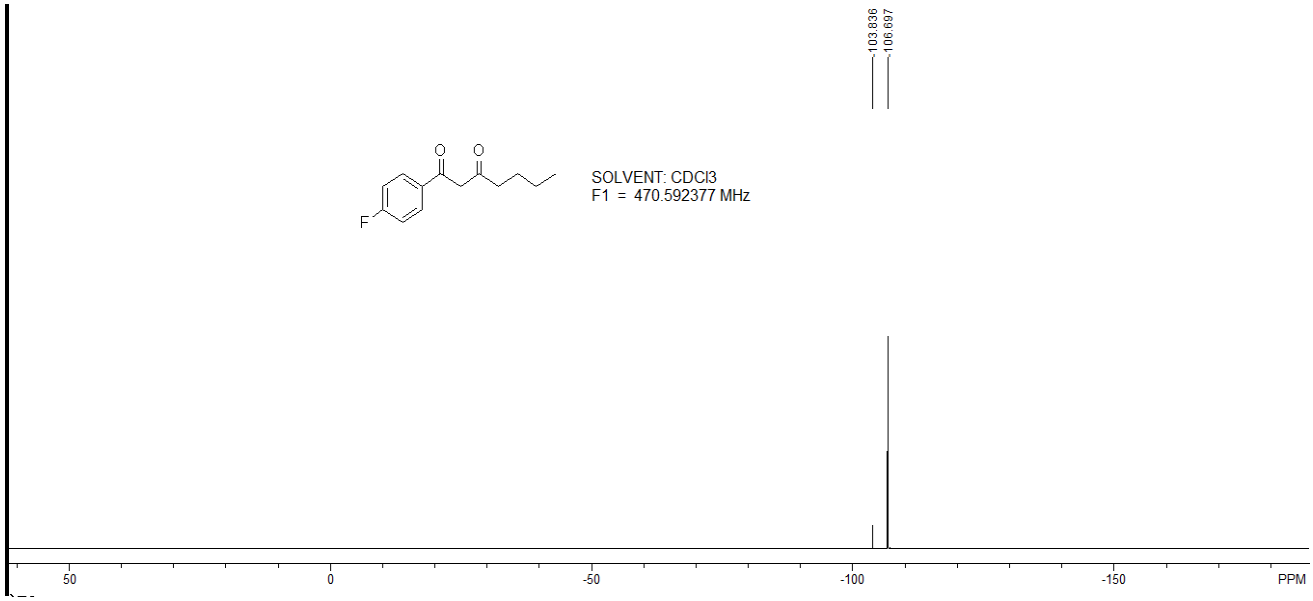

197.488
181.218
157.813
132.733
130.157
124.321
120.687
120.593
112.538
101.303
77.254
77.000
76.746
64.279
39.182
27.931
22.328
14.708
13.772
f1 (ppm)

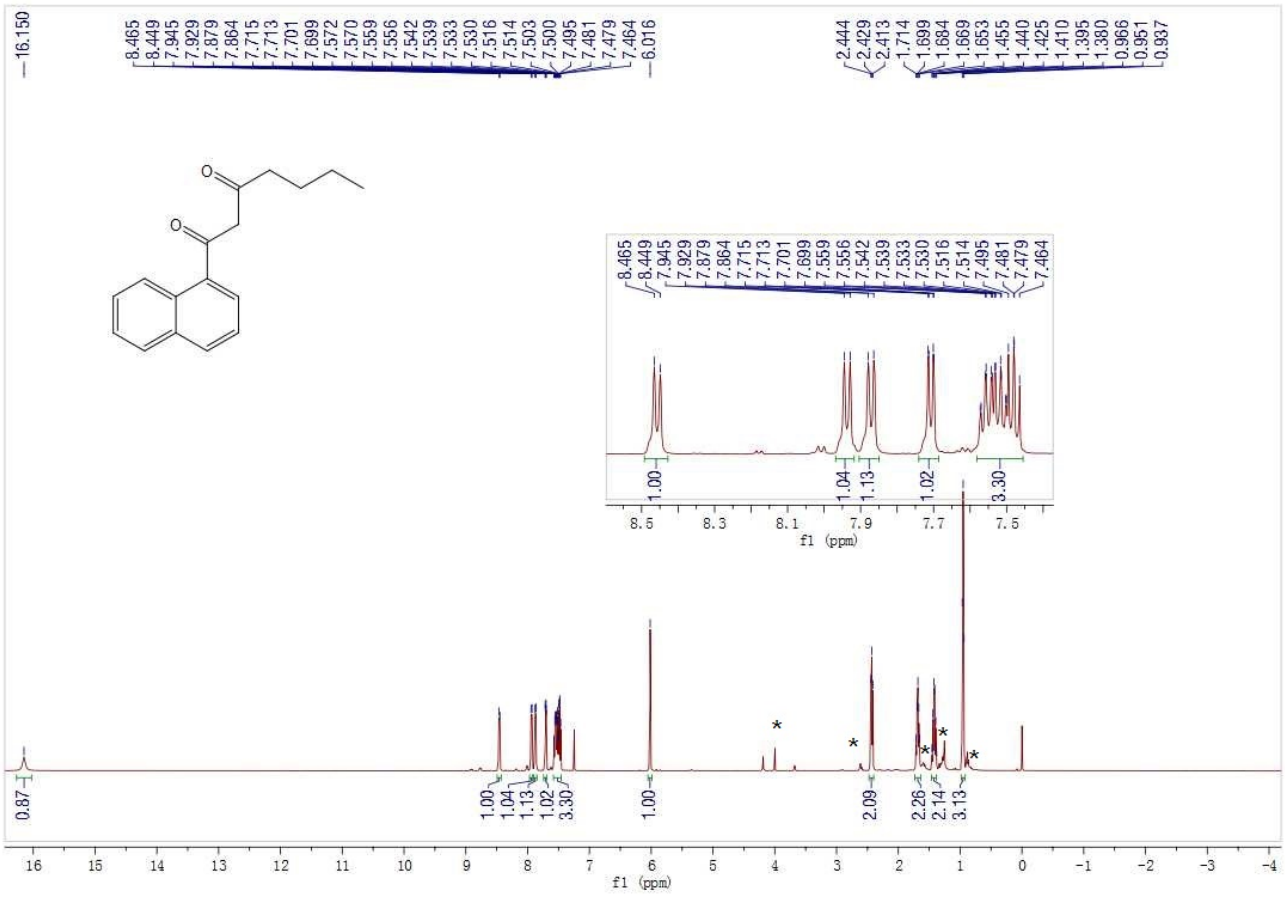

16.347
7.870
7.853
6.941
6.923
6.102
3.854
2.405
2.390
2.374
1.690
1.675
1.660
1.645
1.629
1.435
1.420
1.405
1.390
1.375
1.361
0.957
0.942
0.927
0.69
2.01
2.37
1.00
2.85
2.07
2.29
2.14
3.12
f1 (ppm)

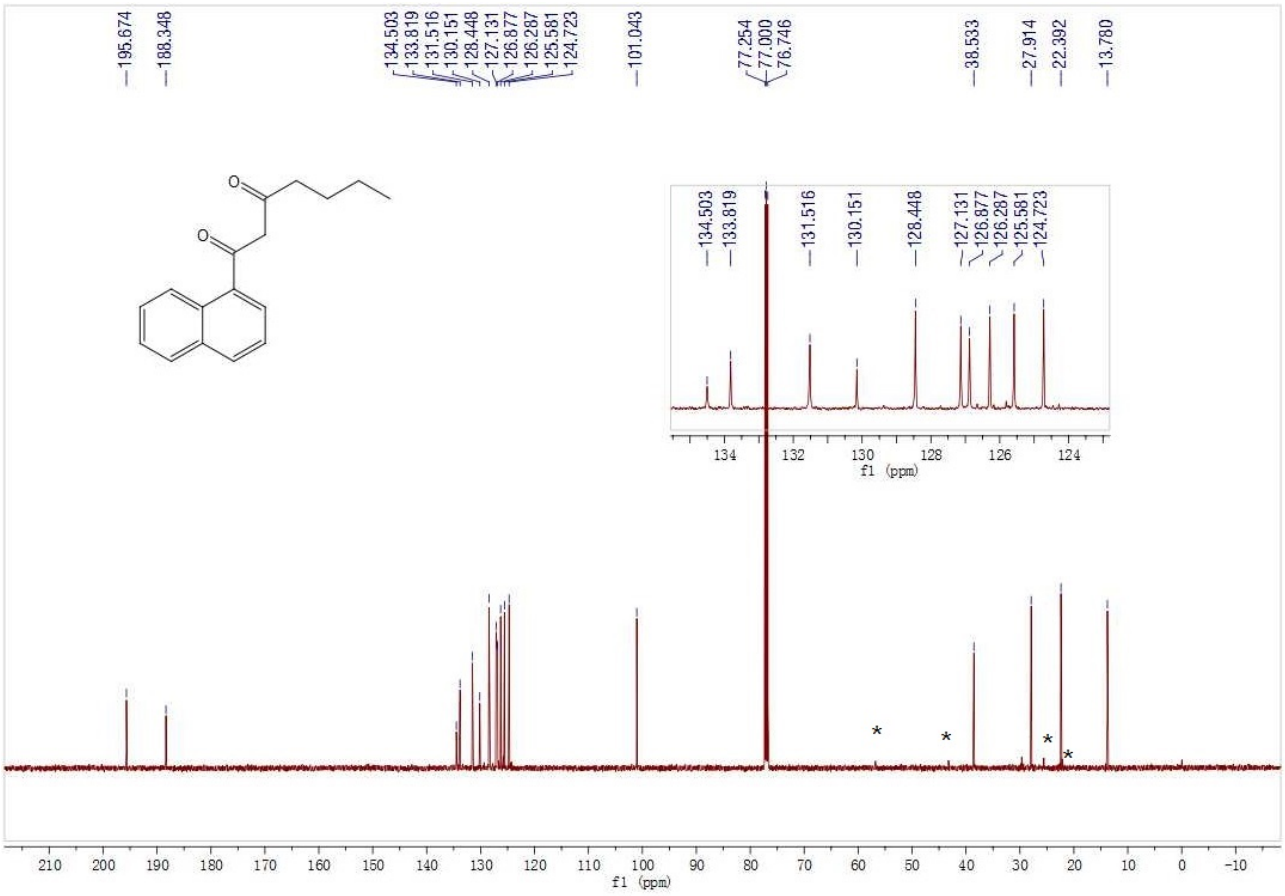

194.78
184.29
163.03
131.08
129.05
113.88
95.09
77.25
77.00
76.75
55.38
38.44
28.07
22.37
13.76
f1 (ppm)

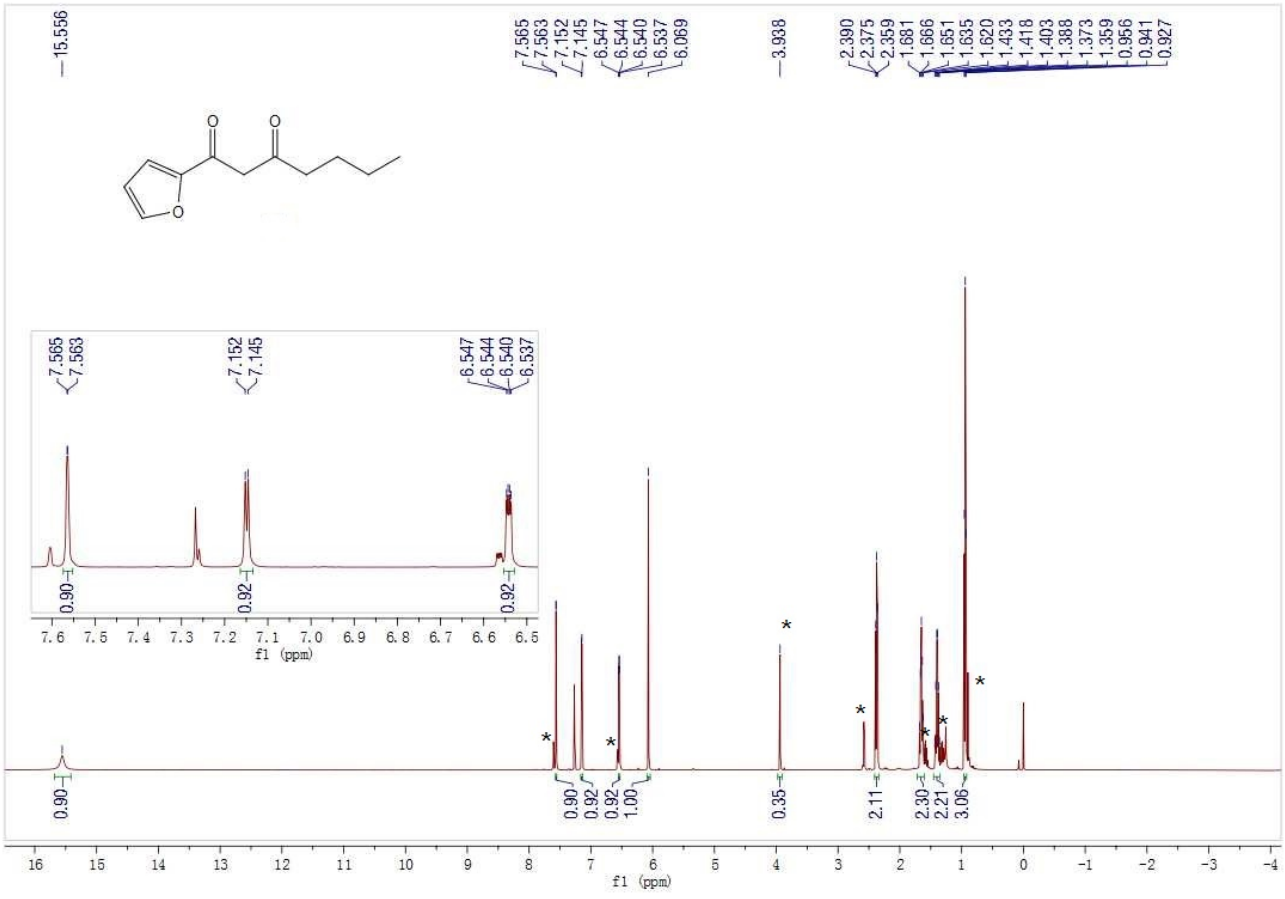

16.193
7.917
7.911
7.907
7.900
7.897
7.896
7.893
7.887
7.882
7.876
7.137
7.120
4.059
2.431
2.416
2.400
1.697
1.682
1.678
1.667
1.662
1.652
1.636
1.439
1.424
1.409
1.394
1.379
0.961
0.946
0.931
O
O
F
2.00
2.13
f1 (ppm)
2.05
2.18
2.09
2.95
f1 (ppm)
0.89
2.00
2.13
1.00
2.05
2.18
2.09
2.95
f1 (ppm)

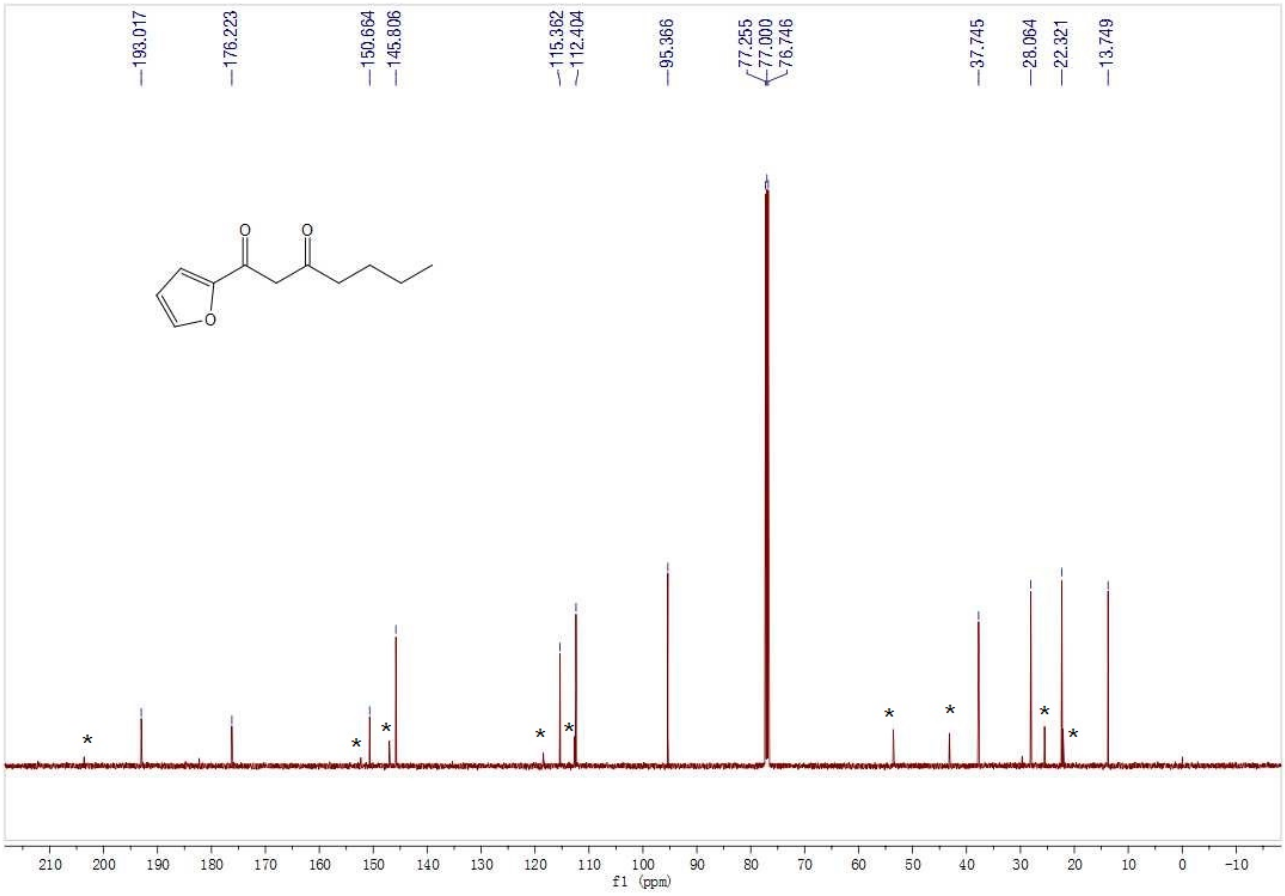

196.095
183.095
166.280
164.264
131.544
131.520
129.440
129.368
115.769
115.595
95.692
77.254
77.000
76.746
38.665
27.960
22.371
13.755
O
O
F
f1 (ppm)

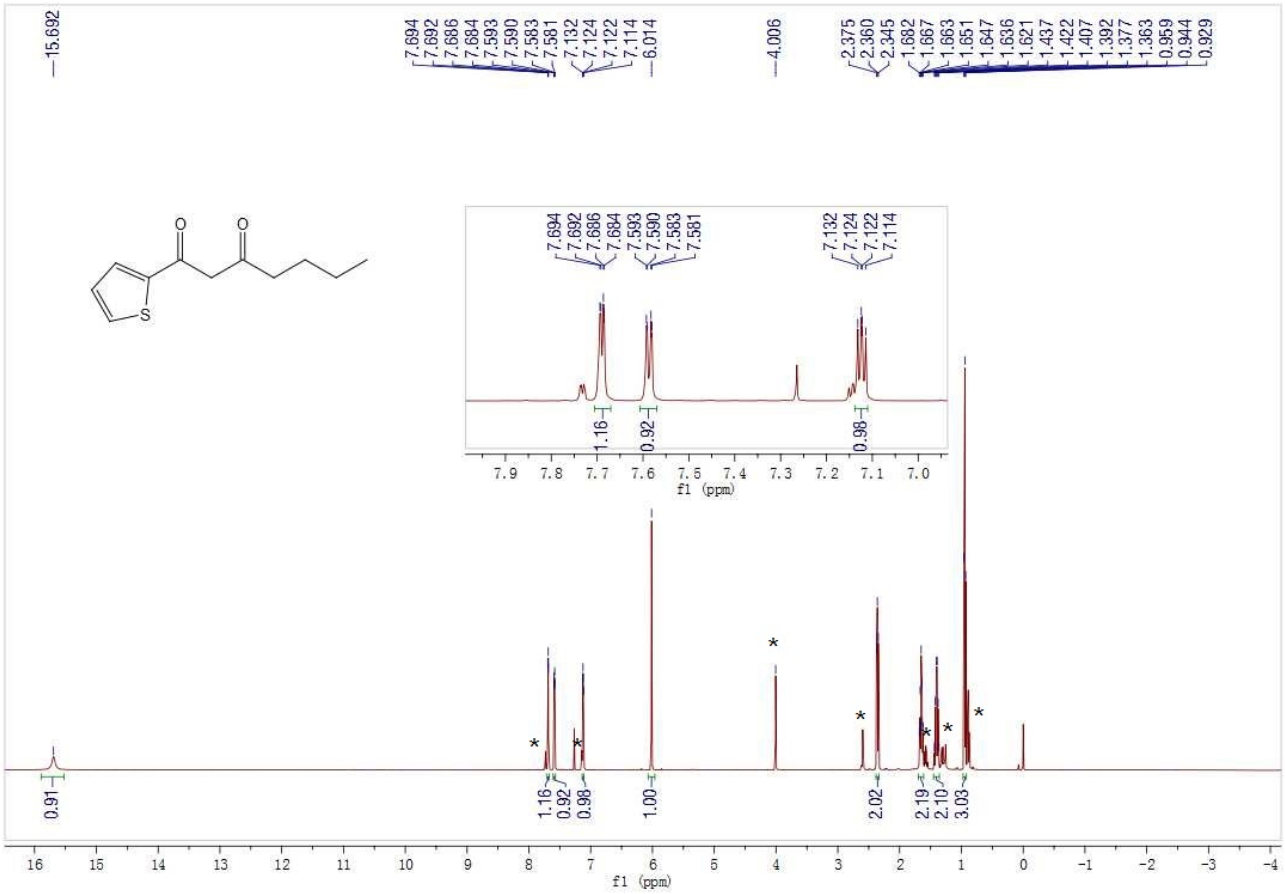

103.836
106.697
SOLVENT: CDCl3
F1 = 470.592377 MHz
50
0
-50
-100
-150
PPM

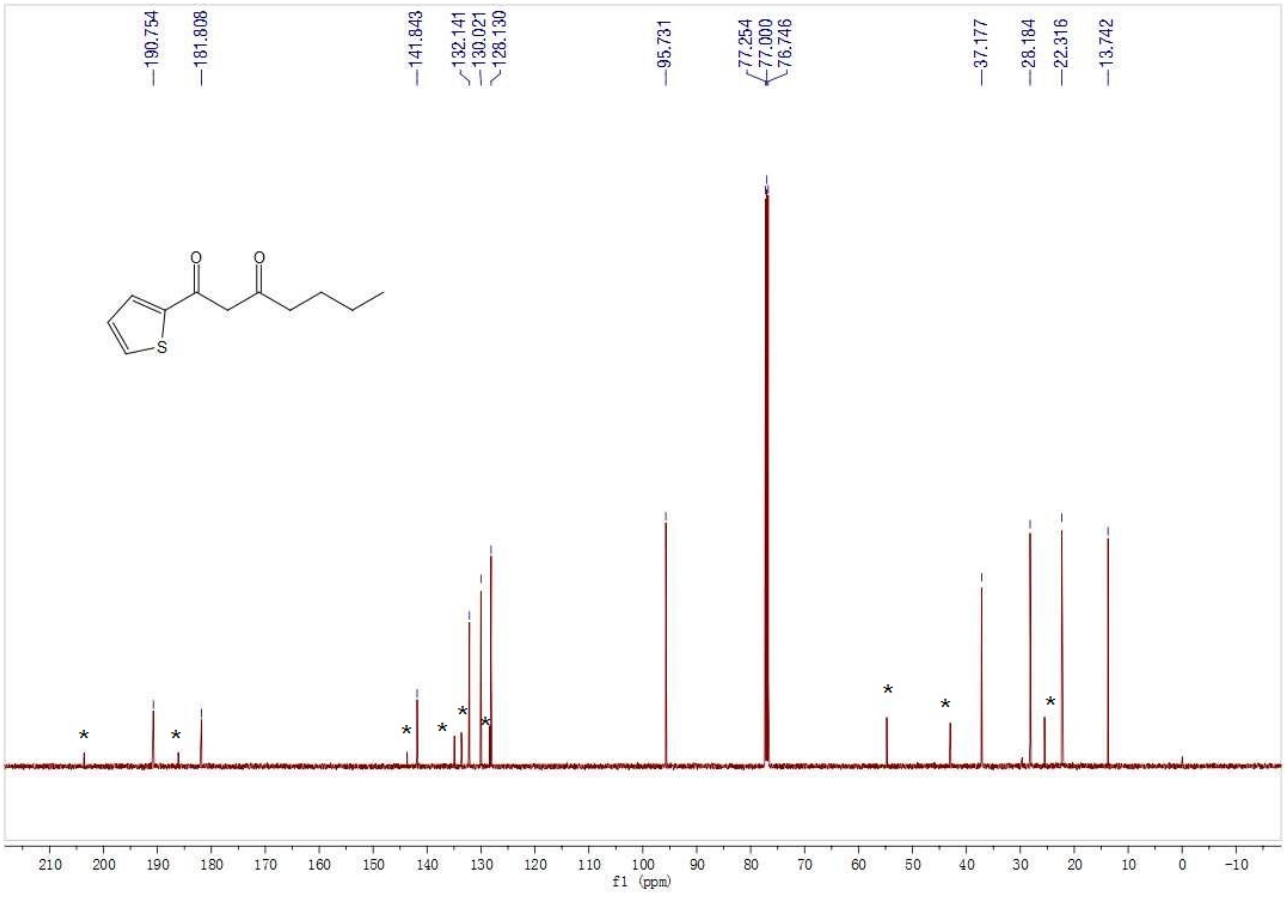

16.150
8.465
8.449
7.945
7.929
7.879
7.864
7.715
7.713
7.701
7.699
7.572
7.570
7.559
7.556
7.542
7.539
7.533
7.530
7.516
7.514
7.503
7.500
7.495
7.481
7.479
7.464
6.016
2.444
2.429
2.413
1.714
1.699
1.684
1.669
1.653
1.455
1.440
1.425
1.410
1.395
1.380
0.966
0.951
0.937
1.00
1.04
1.13
1.02
3.30
8.5
8.3
8.1
7.9
7.7
7.5
f1 (ppm)
0.87
1.00
1.04
1.13
1.02
3.30
1.00
2.09
2.26
2.14
3.13
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
−4
f1 (ppm)

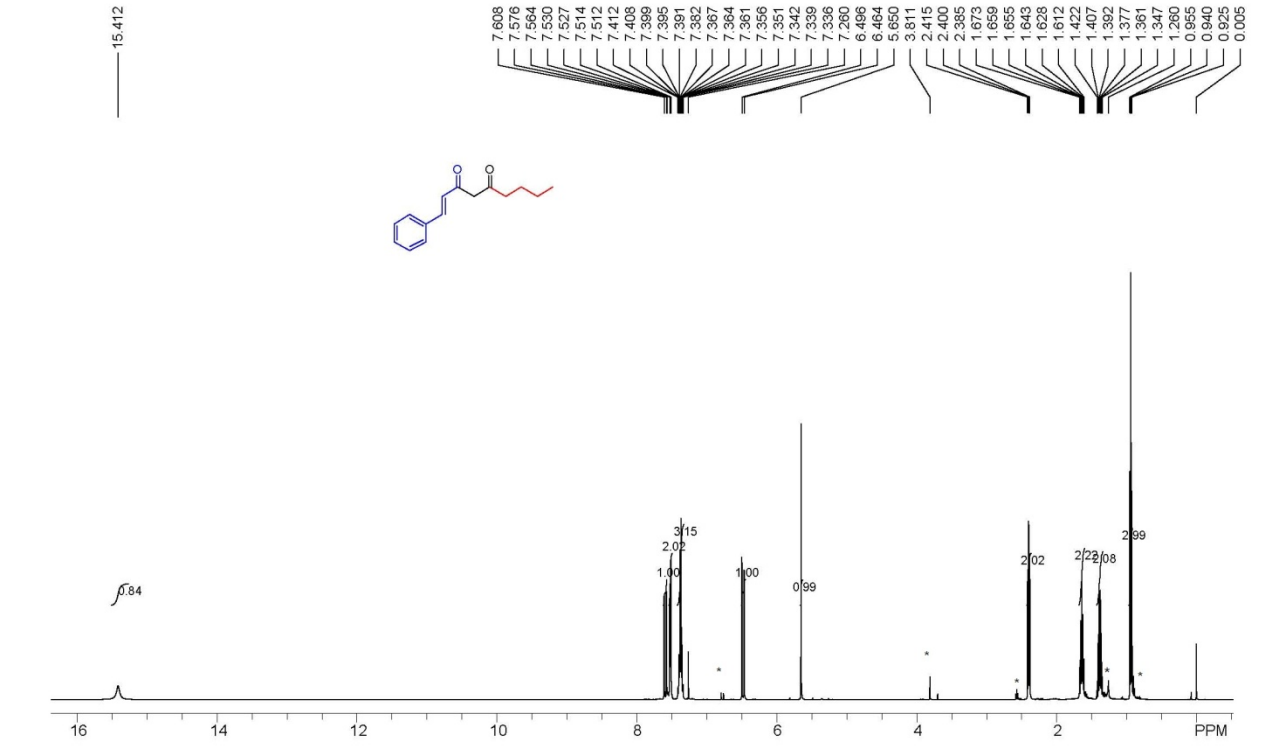

195.674
188.348
134.503
133.819
131.516
130.151
128.448
127.131
126.877
126.287
125.581
124.723
101.043
77.254
77.000
76.746
38.533
27.914
22.392
13.780
f1 (ppm)

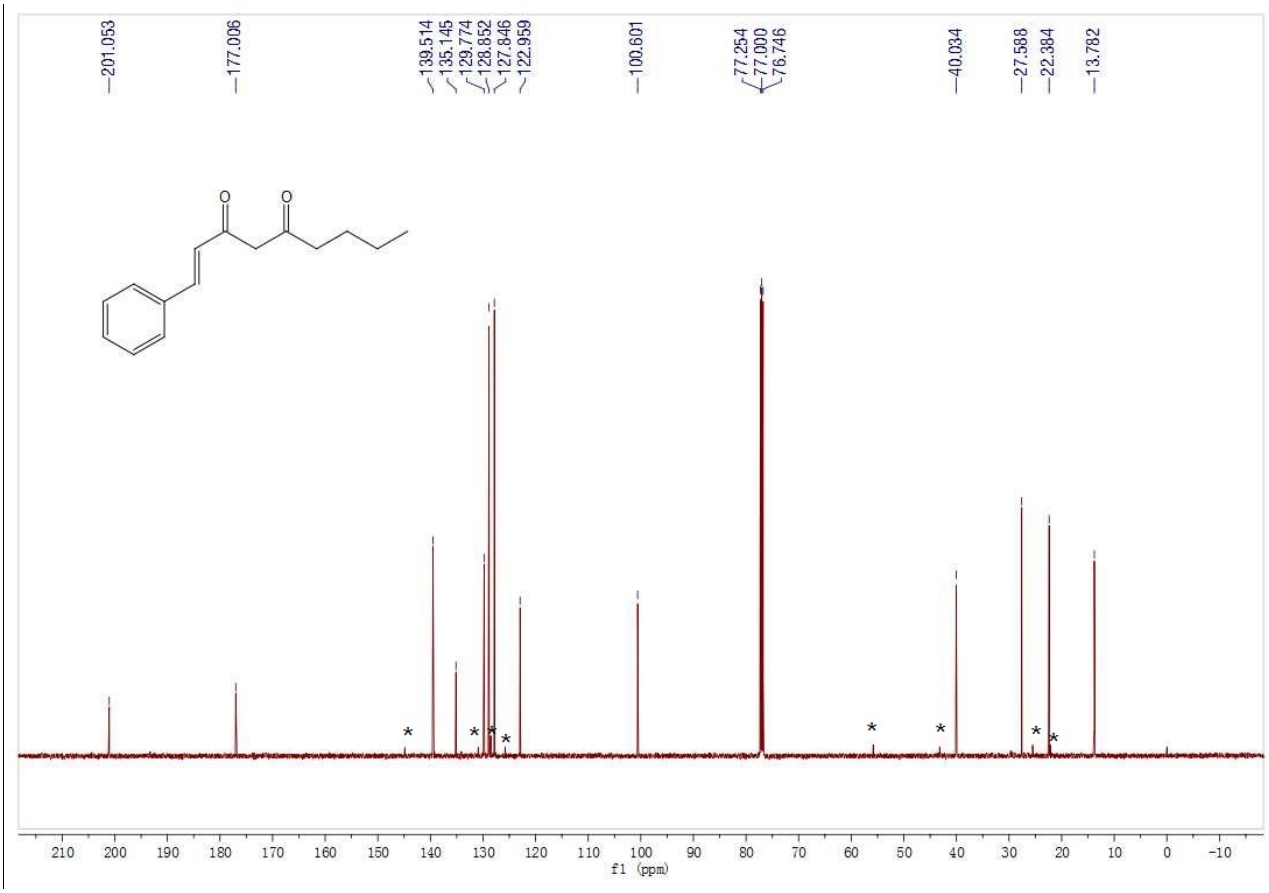

15.556
7.565
7.563
7.152
7.145
6.547
6.544
6.540
6.537
6.069
3.938
2.390
2.375
2.359
1.681
1.666
1.651
1.635
1.620
1.433
1.418
1.403
1.388
1.373
1.359
0.956
0.941
0.927
0.90
0.92
0.92
1.00
0.35
2.11
2.30
2.21
3.06
f1 (ppm)

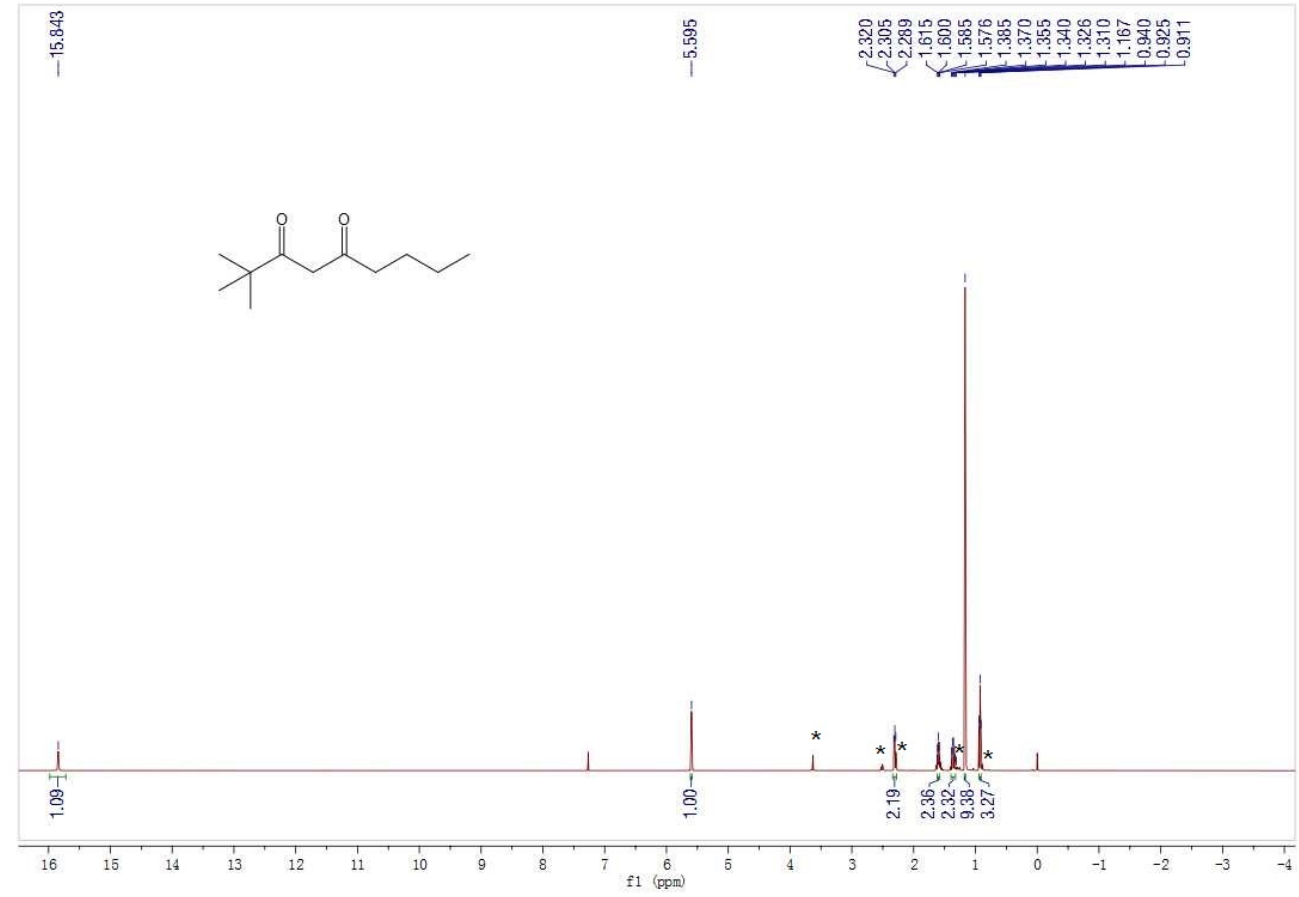

193.017
176.223
150.664
145.806
115.382
112.404
95.366
77.255
77.000
76.746
37.745
28.064
22.321
13.749
O
O
O
f1 (ppm)

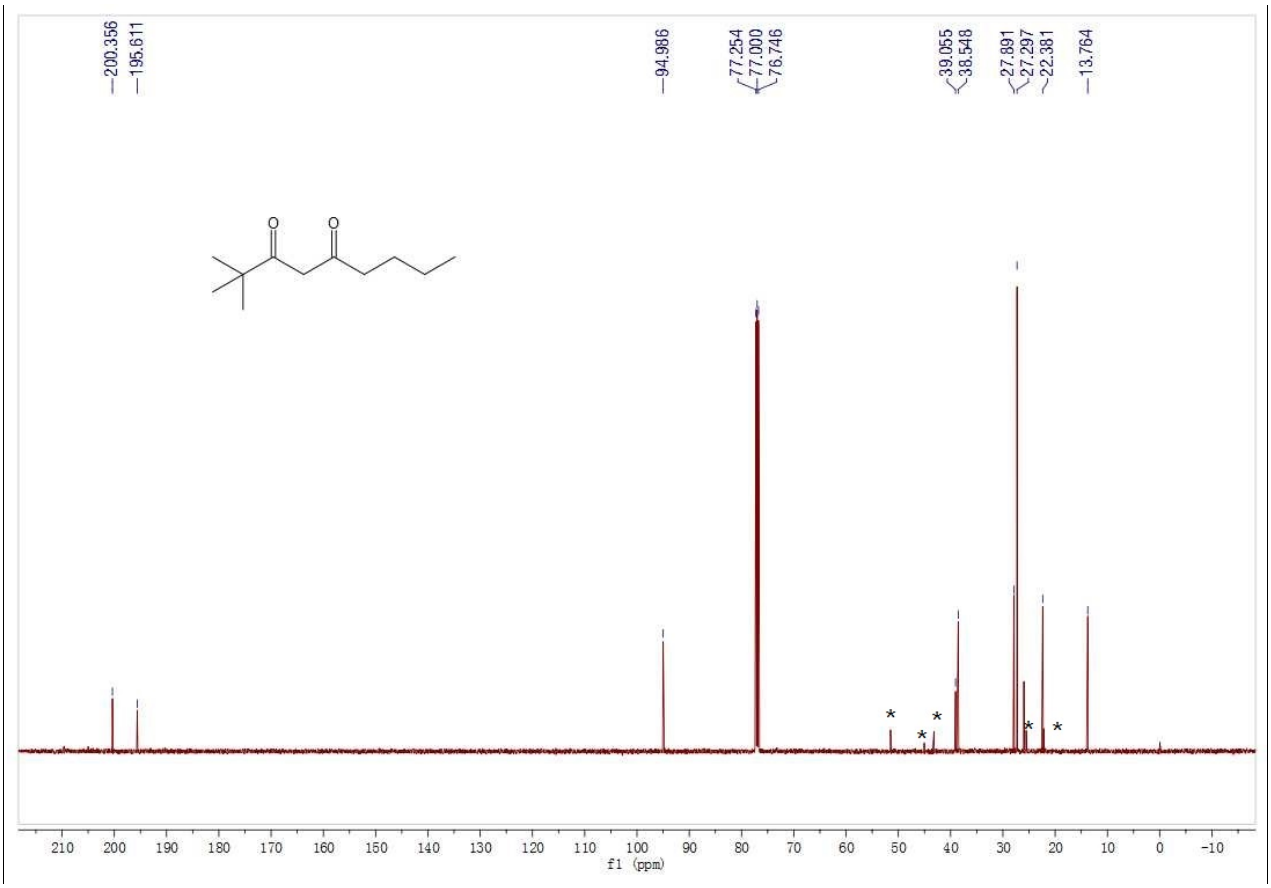

15.692
7.694
7.692
7.686
7.684
7.593
7.590
7.583
7.581
7.132
7.124
7.122
7.114
6.014
4.006
2.375
2.360
2.345
1.682
1.667
1.663
1.651
1.647
1.636
1.621
1.437
1.422
1.407
1.392
1.377
1.363
0.959
0.944
0.929
O
O
S
1.16
0.92
0.98
f1 (ppm)
0.91
1.16
0.92
0.98
1.00
2.02
2.19
2.10
3.03
f1 (ppm)


190.754
181.808
141.843
132.141
130.021
128.130
95.731
77.254
77.000
76.746
37.177
28.184
22.316
13.742
O
O
S
f1 (ppm)


15.412
7.608
7.576
7.564
7.530
7.527
7.514
7.512
7.412
7.408
7.399
7.395
7.391
7.382
7.367
7.364
7.361
7.356
7.351
7.342
7.339
7.336
7.260
6.496
6.464
5.650
3.811
2.415
2.400
2.385
1.673
1.659
1.655
1.643
1.628
1.612
1.422
1.407
1.392
1.377
1.361
1.347
1.260
0.955
0.940
0.925
0.005
O
O
0.84
3.15
2.02
1.00
1.00
0.99
2.02
2.22
2.08
2.99
PPM


201.053
177.006
139.514
135.145
129.774
128.852
127.846
122.959
100.601
77.254
77.000
76.746
40.034
27.588
22.384
13.782
O
O
f1 (ppm)


15.843
5.595
2.320
2.305
2.289
1.615
1.600
1.585
1.576
1.385
1.370
1.355
1.340
1.326
1.310
1.167
0.940
0.925
0.911
O
O
1.09
1.00
2.19
2.36
2.32
9.38
3.27
f1 (ppm)


200.356
195.611
94.986
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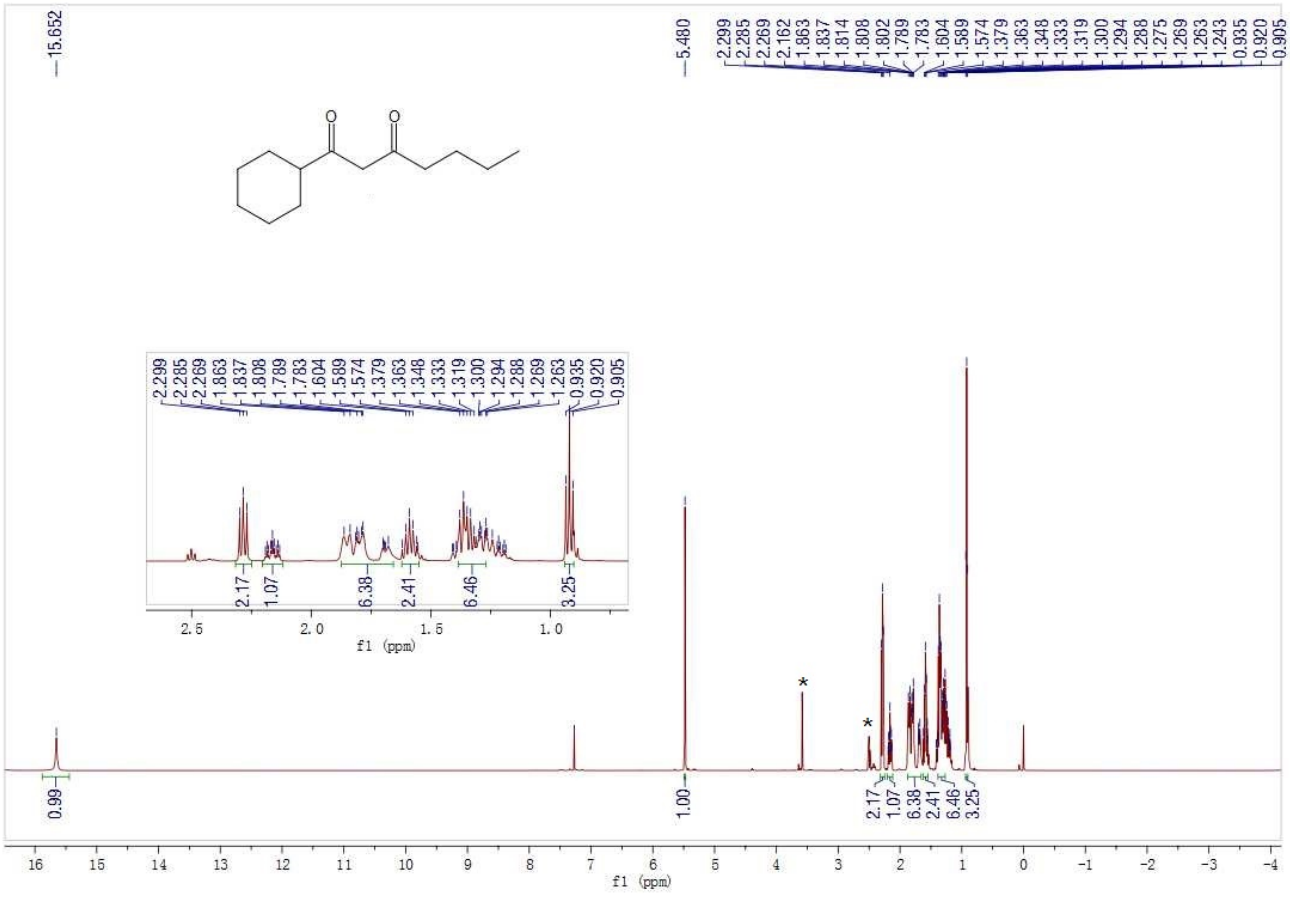
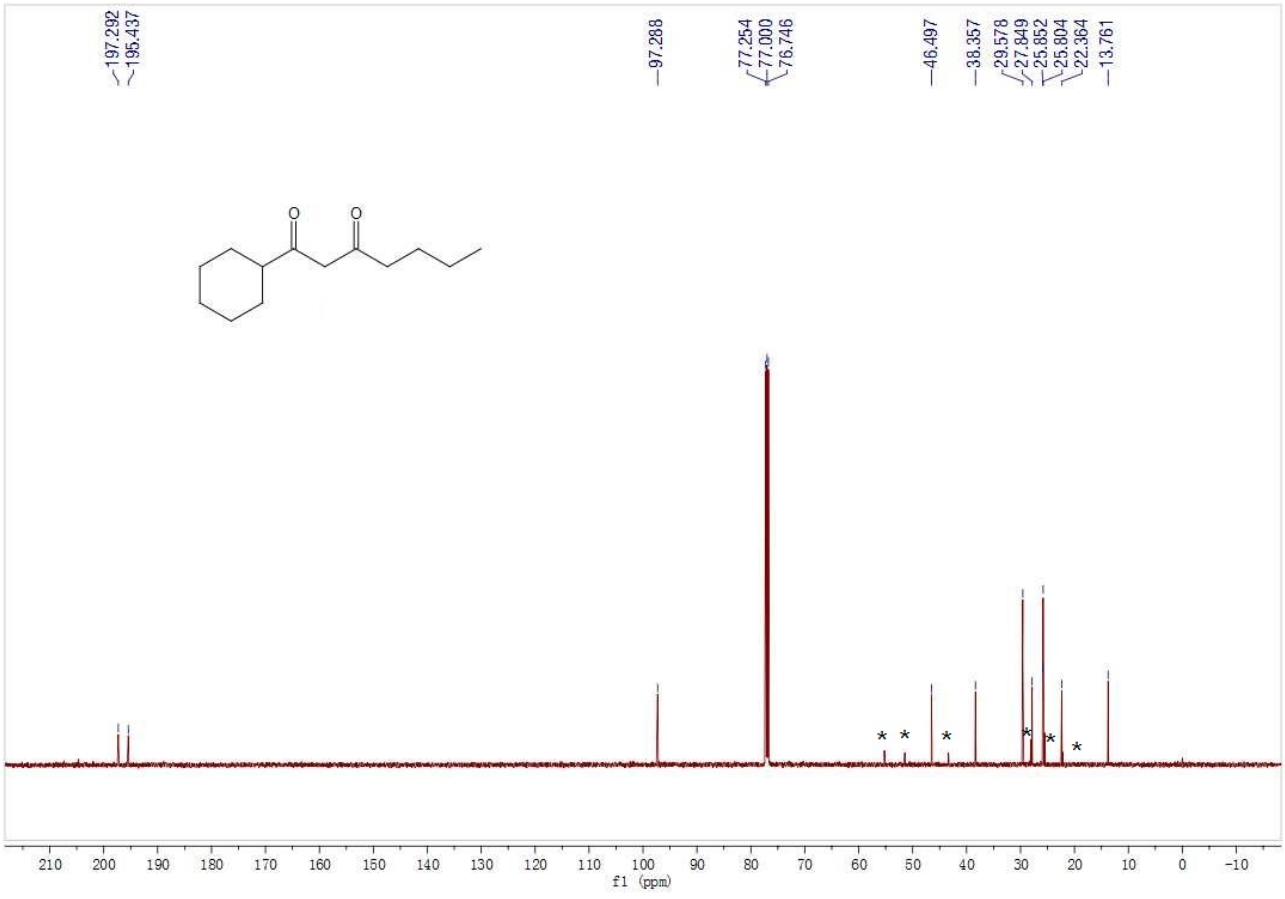
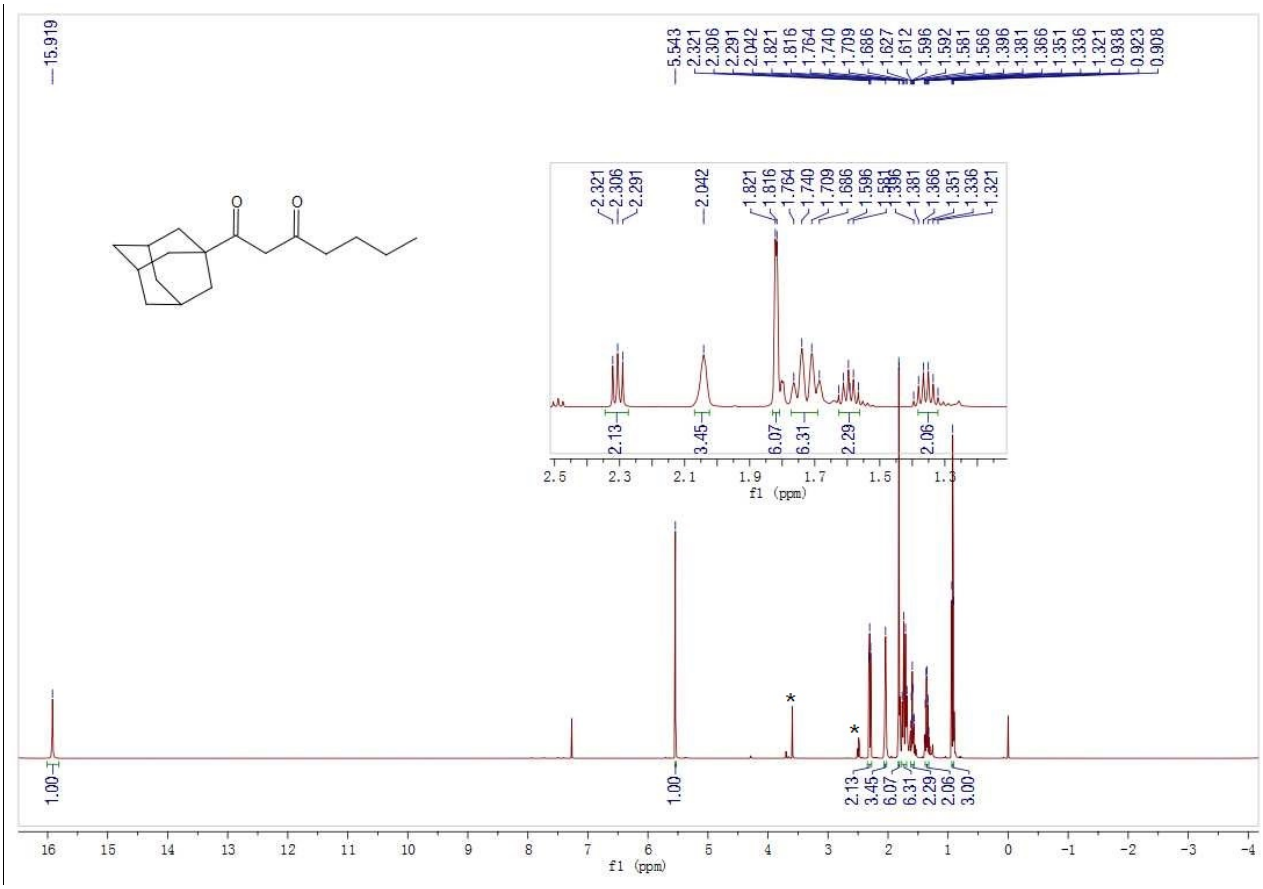
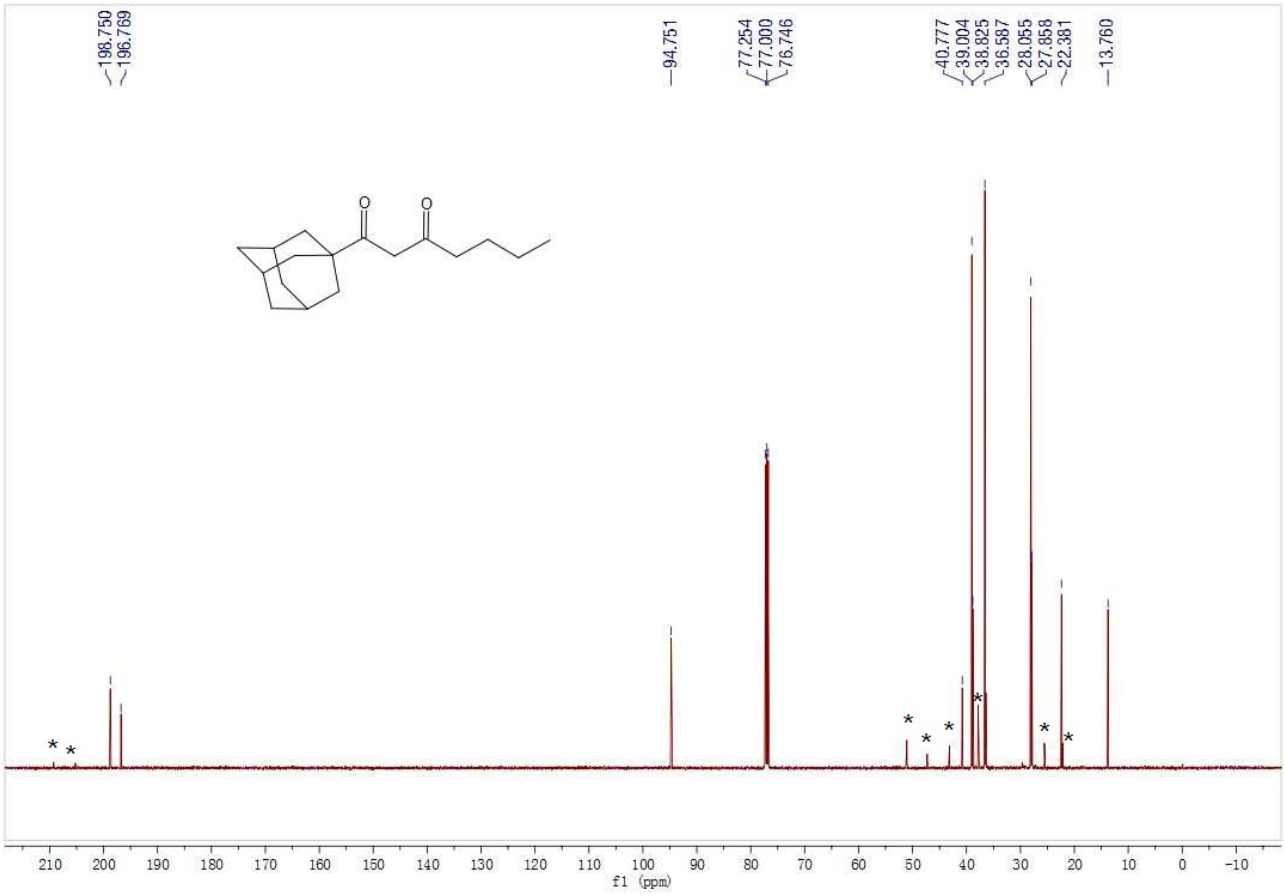
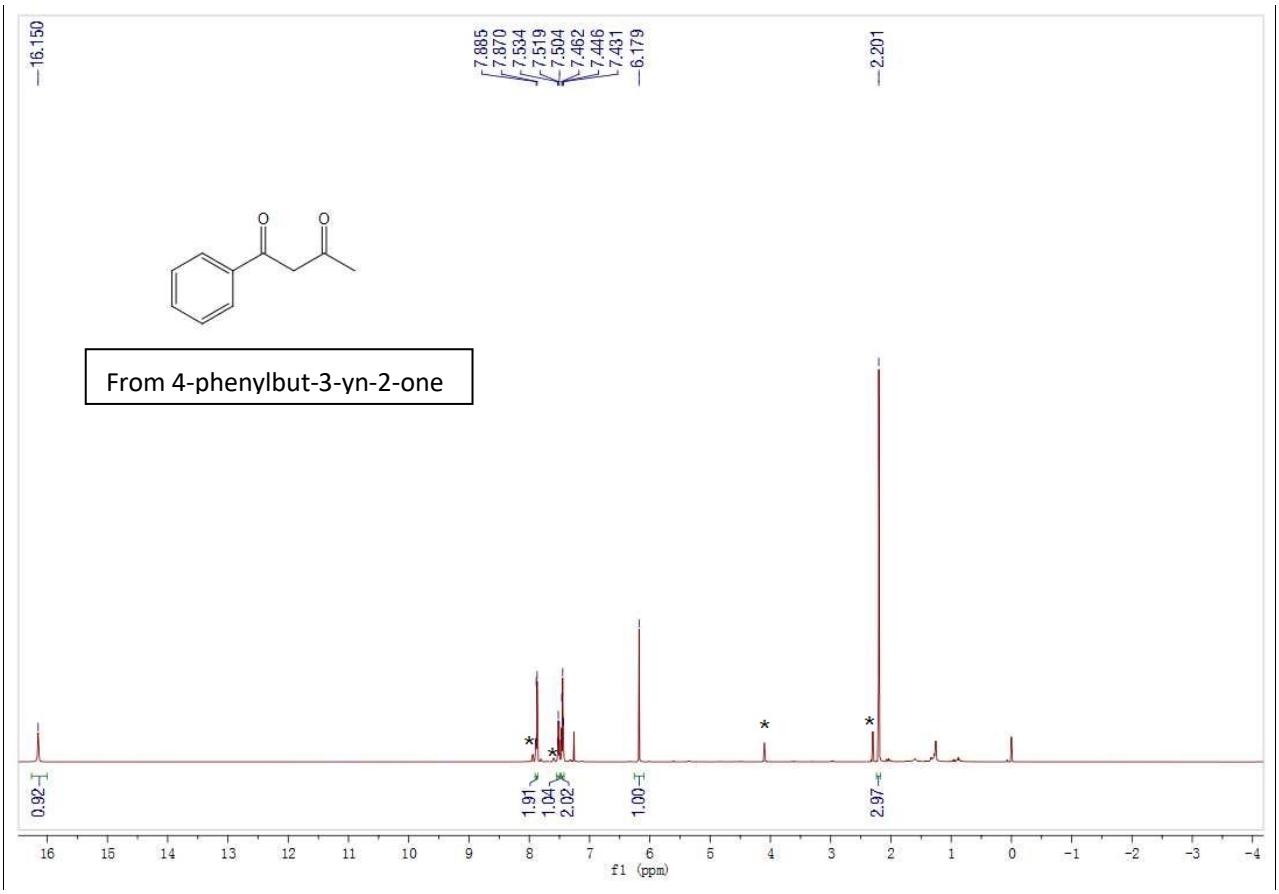
77.000
76.746
39.055
38.548
27.891
27.297
22.381
13.764
f1 (ppm)

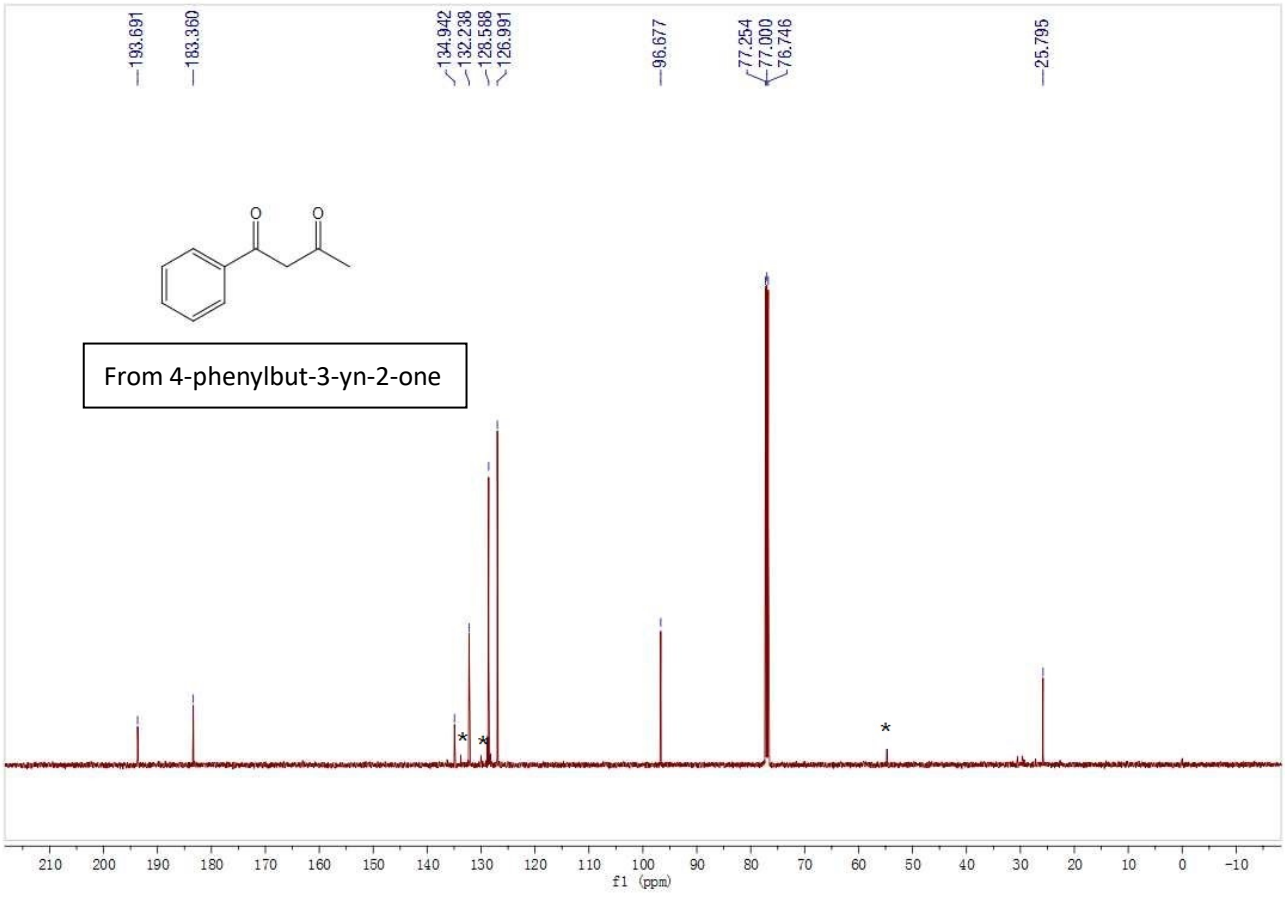

15.652
5.480
2.17
1.07
6.38
2.41
6.46
3.25
0.99
1.00
f1 (ppm)

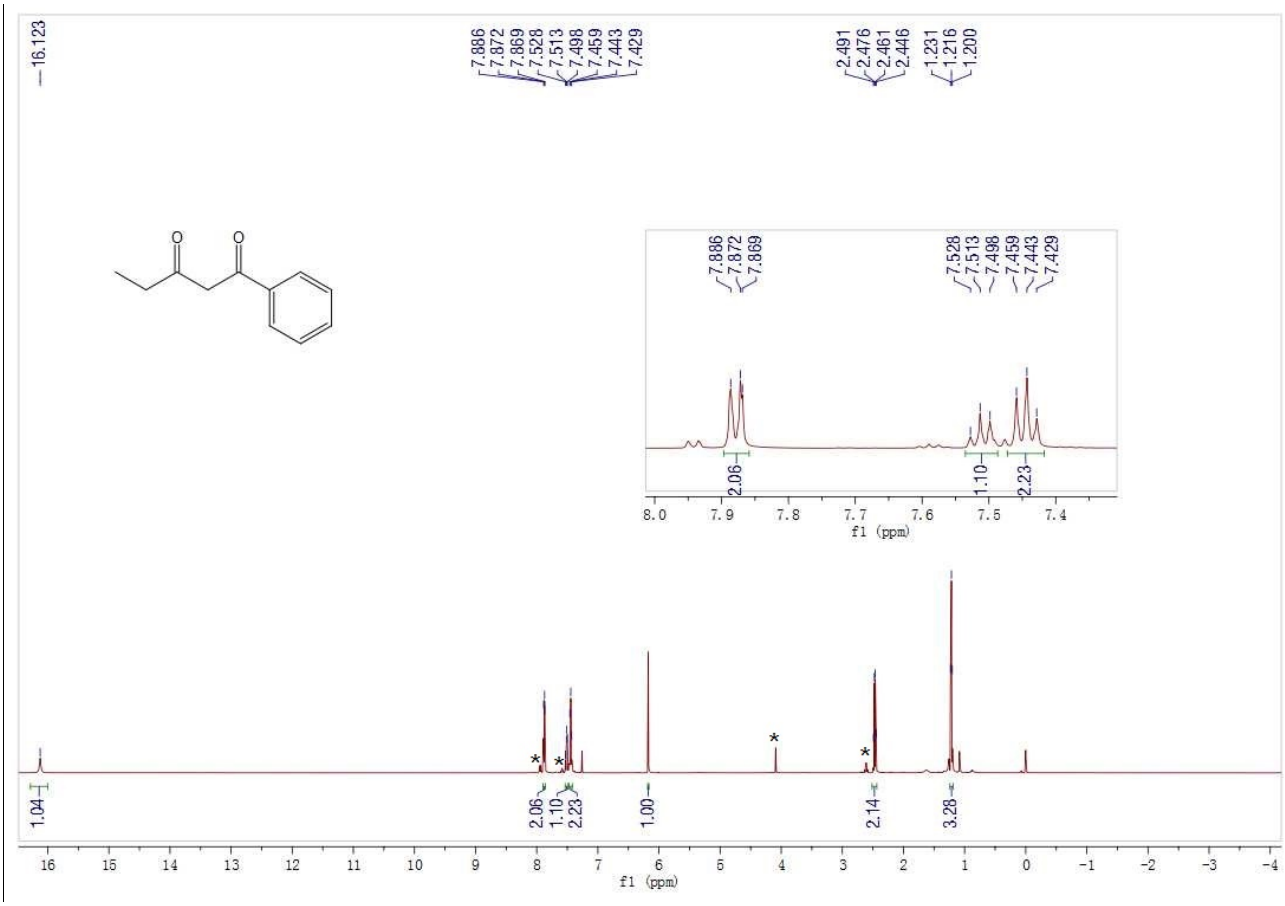

197.292
195.437
97.288
77.254
77.000
76.746
46.497
38.357
29.578
27.849
25.852
25.804
22.364
13.761
f1 (ppm)


15.919
5.543
2.321
2.306
2.291
2.042
1.821
1.816
1.764
1.740
1.709
1.686
1.627
1.612
1.596
1.592
1.581
1.566
1.396
1.381
1.366
1.351
1.336
1.321
0.938
0.923
0.908
2.13
3.45
6.07
6.31
2.29
2.06
3.00
f1 (ppm)


198.750
196.769
94.751
77.254
77.000
76.746
40.777
39.004
38.825
36.587
28.055
27.858
22.381
13.760
f1 (ppm)


16.150
7.885
7.870
7.534
7.519
7.504
7.462
7.446
7.431
6.179
2.201
From 4-phenylbut-3-yn-2-one
0.92
1.91
1.04
2.02
1.00
2.97
f1 (ppm)


193.691
183.360
134.942
132.238
128.588
126.991
96.677
77.254
77.000
76.746
25.795
From 4-phenylbut-3-yn-2-one
f1 (ppm)


16.123
7.886
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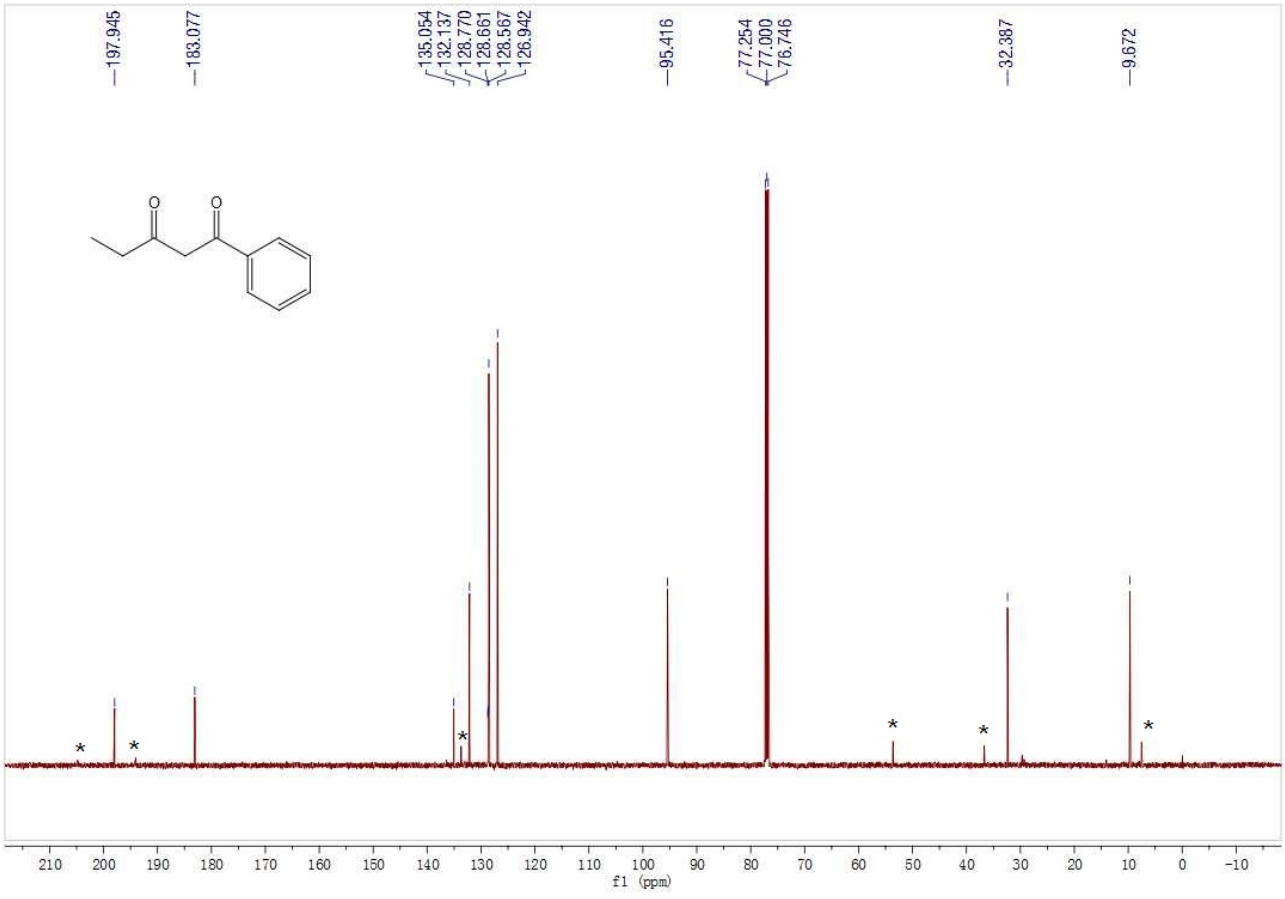
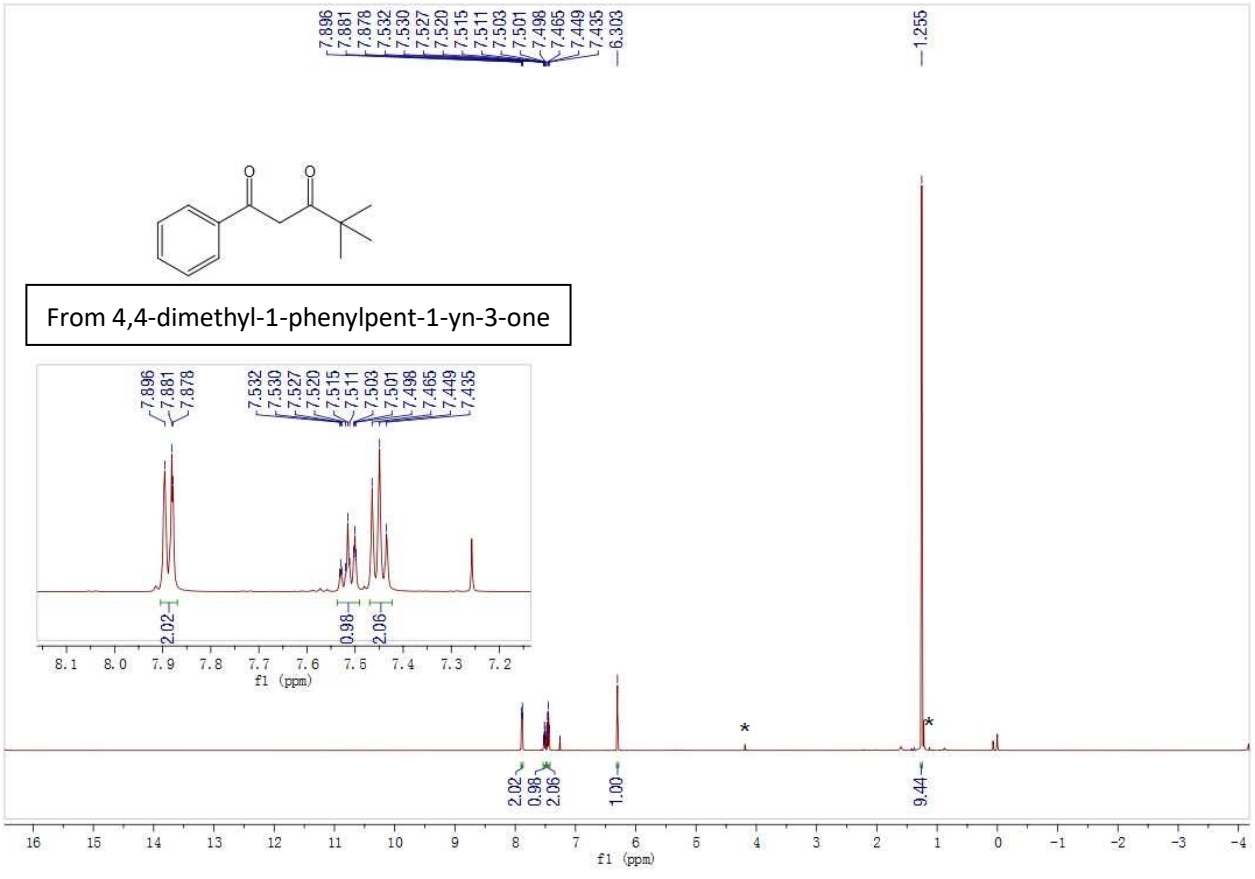
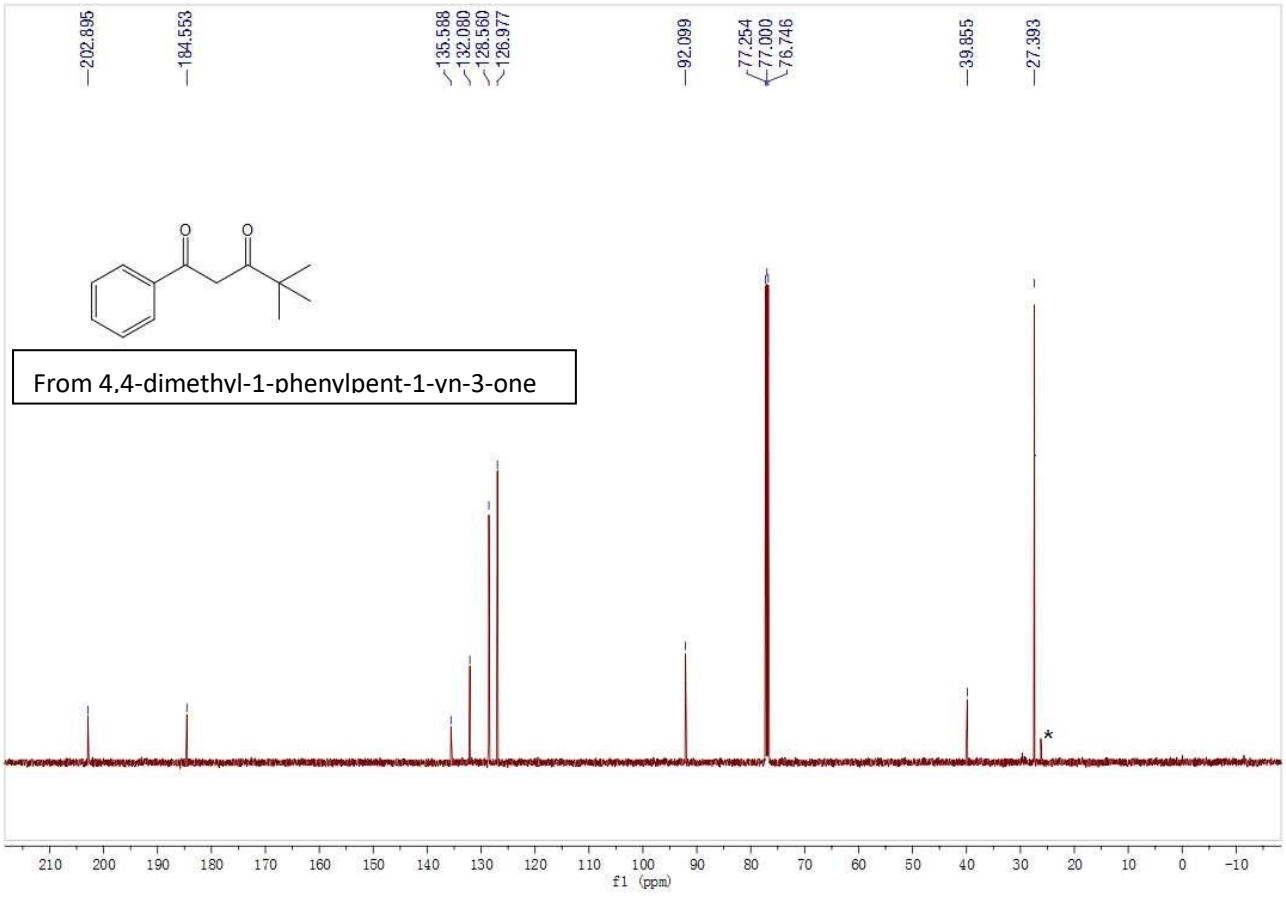
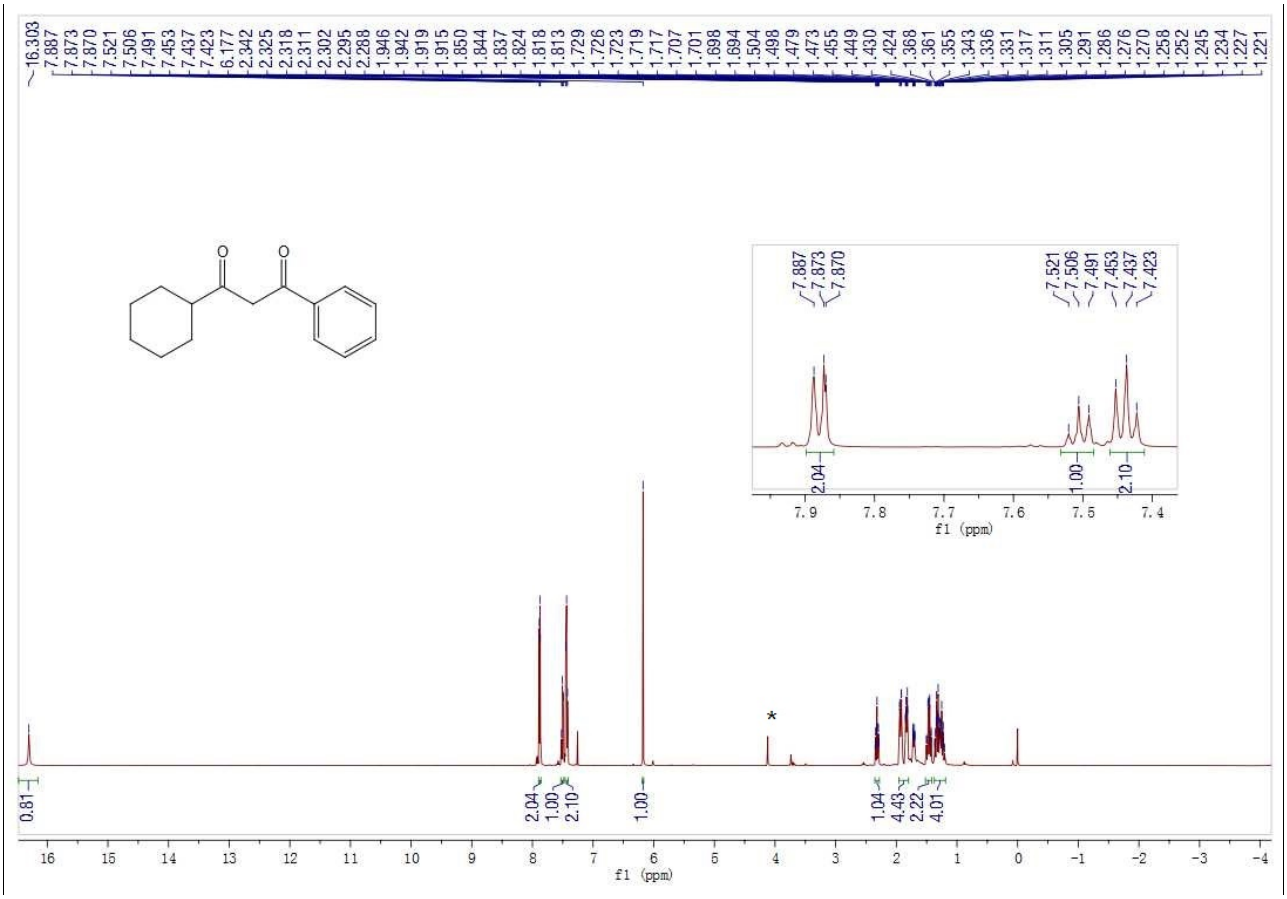
7.869
7.528
7.513
7.498
7.459
7.443
7.429
2.491
2.476
2.461
2.446
1.231
1.216
1.200
2.06
1.10
2.23
1.00
2.14
3.28
f1 (ppm)

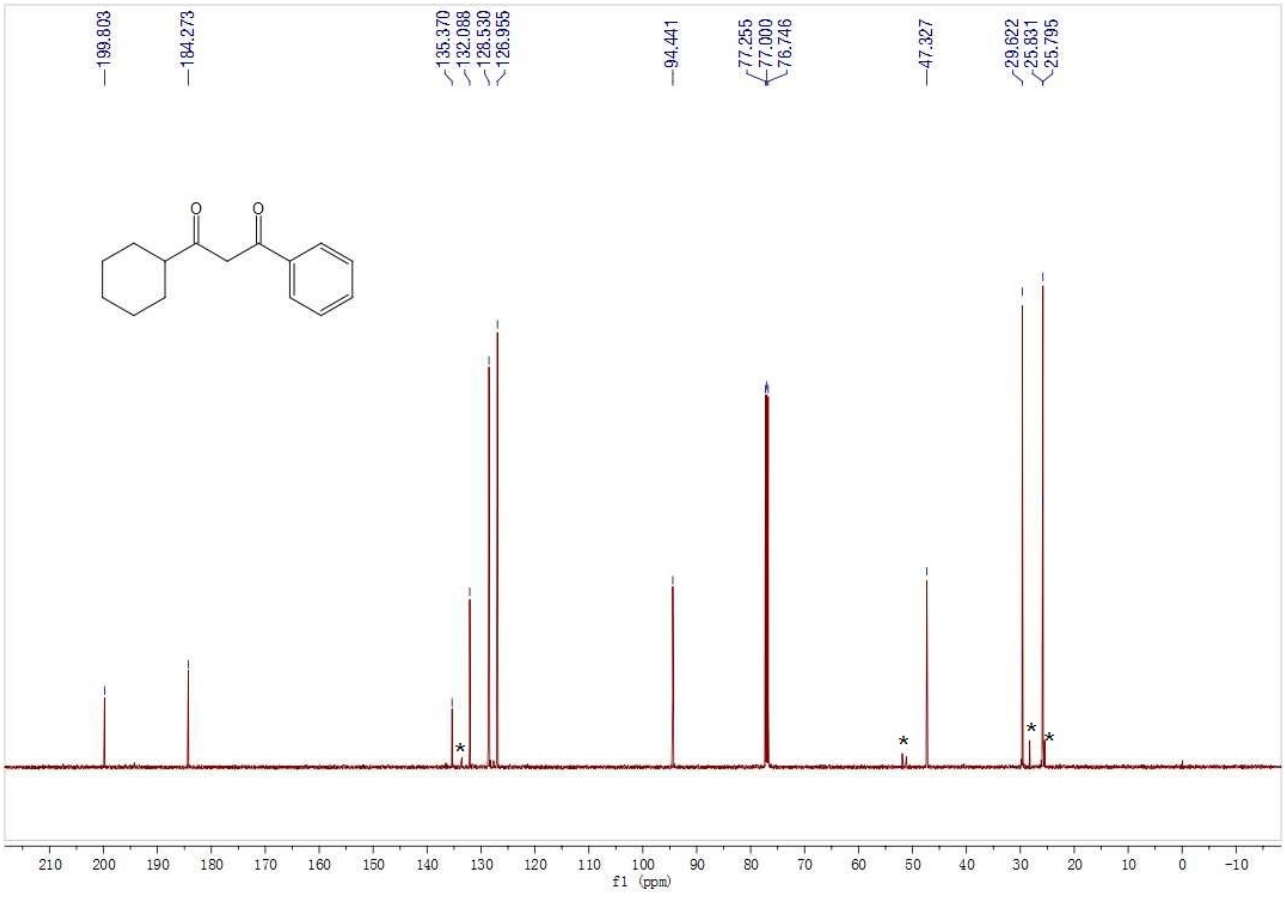


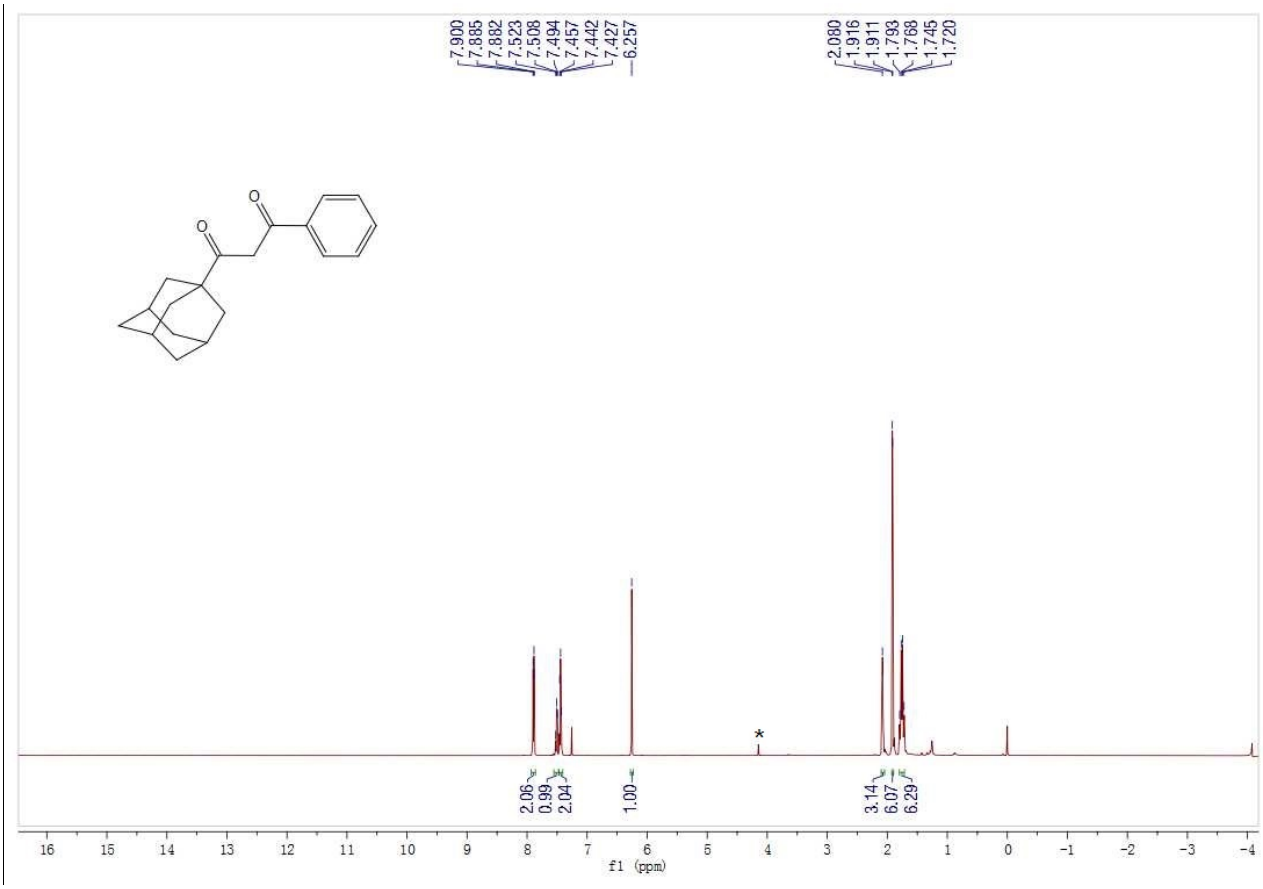


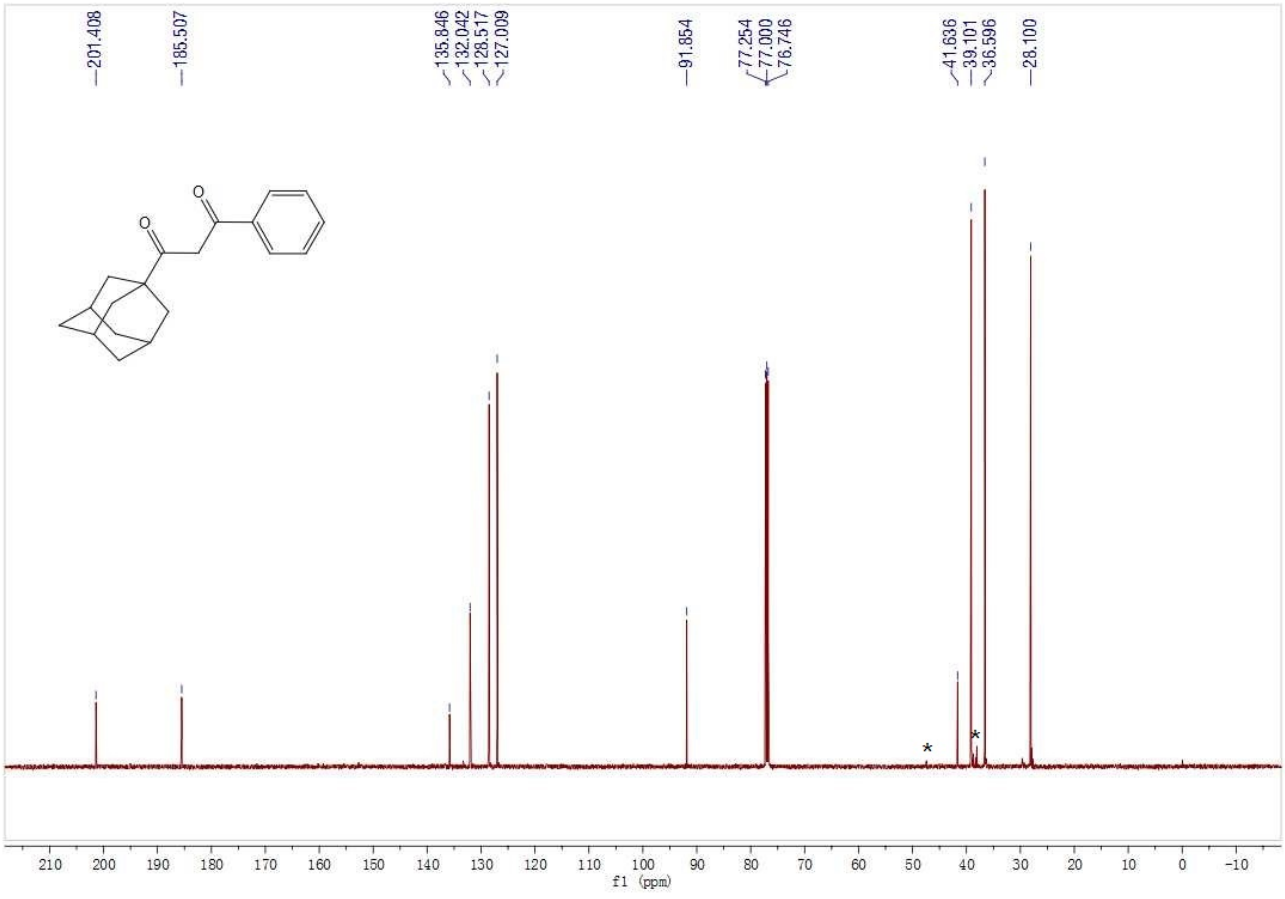
From 4,4-dimethyl-1-phenylpent-1-yn-3-one

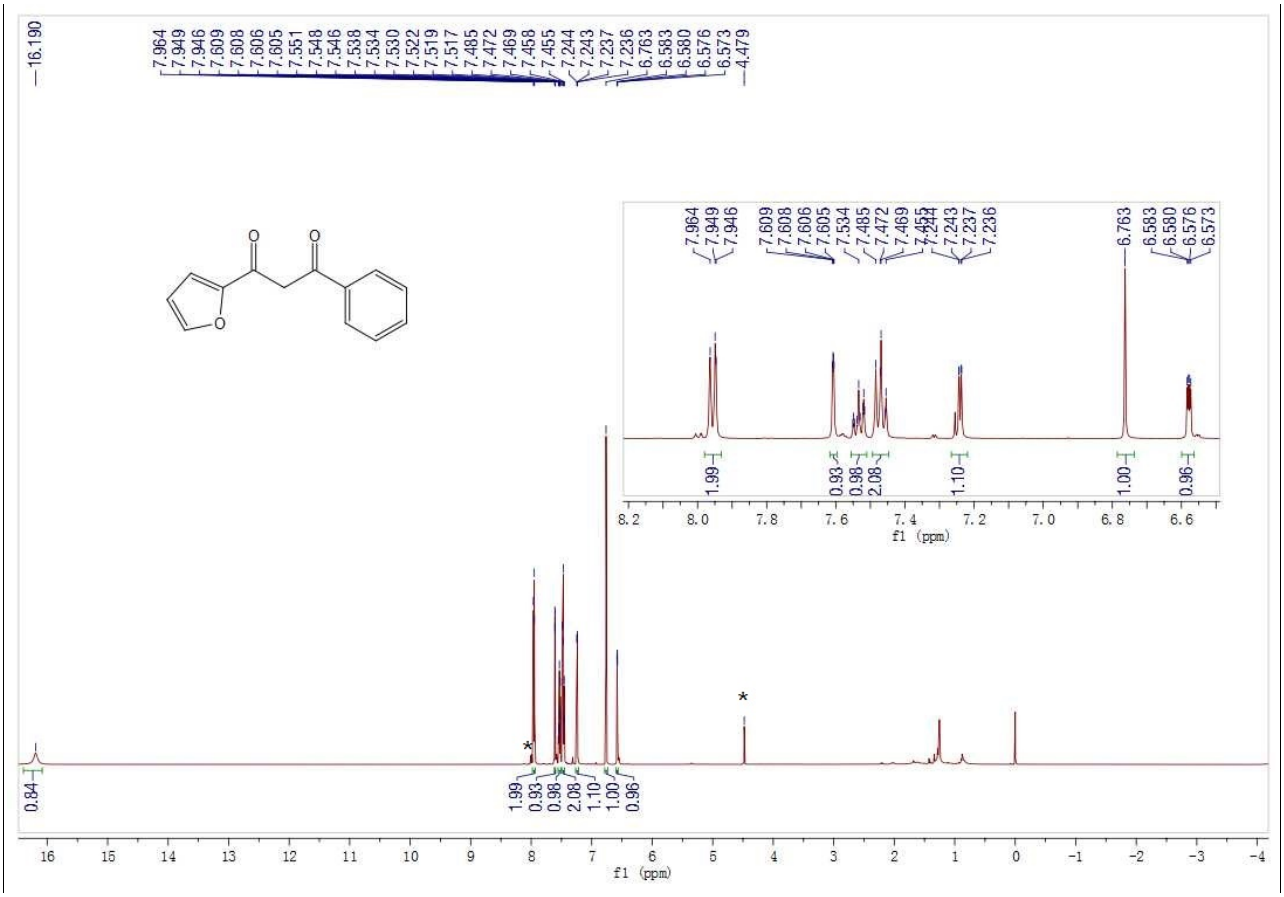

202.895
184.553
135.588
132.080
128.560
126.977
92.099
77.254
77.000
76.746
39.855
27.393
From 4,4-dimethyl-1-phenylpent-1-yn-3-one
f1 (ppm)

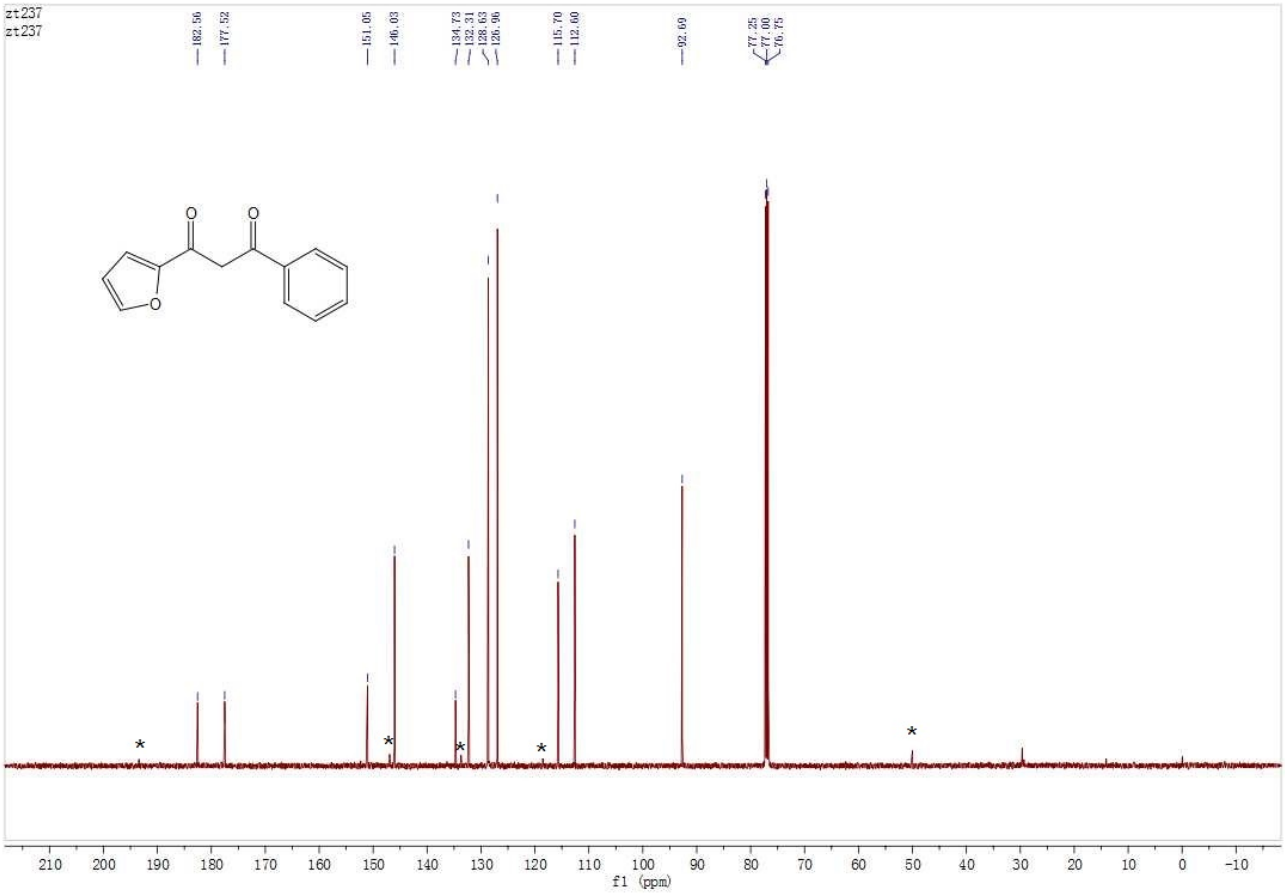

16.303
7.887
7.873
7.870
7.521
7.506
7.491
7.453
7.437
7.423
6.177
2.342
2.325
2.318
2.311
2.302
2.295
2.288
1.946
1.942
1.919
1.915
1.850
1.844
1.837
1.824
1.818
1.813
1.729
1.726
1.723
1.719
1.717
1.707
1.701
1.698
1.694
1.504
1.498
1.479
1.473
1.455
1.449
1.430
1.424
1.368
1.361
1.355
1.343
1.336
1.331
1.317
1.311
1.305
1.291
1.286
1.276
1.270
1.258
1.252
1.245
1.234
1.227
1.221
0.81
2.04
1.00
2.10
1.00
1.04
4.43
2.22
4.01
f1 (ppm)

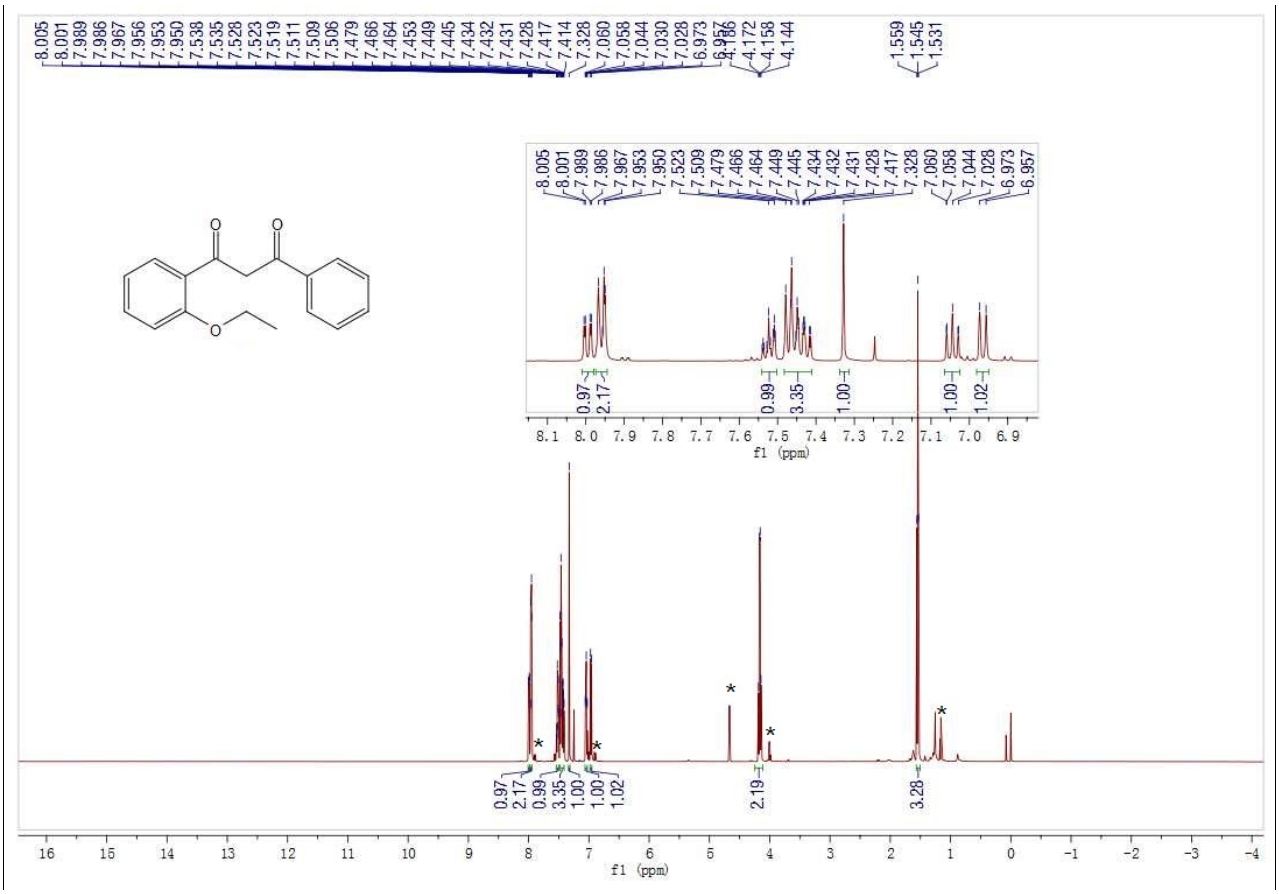

199.803
184.273
135.370
132.088
128.530
126.955
94.441
77.255
77.000
76.746
47.327
29.622
25.831
25.795
f1 (ppm)

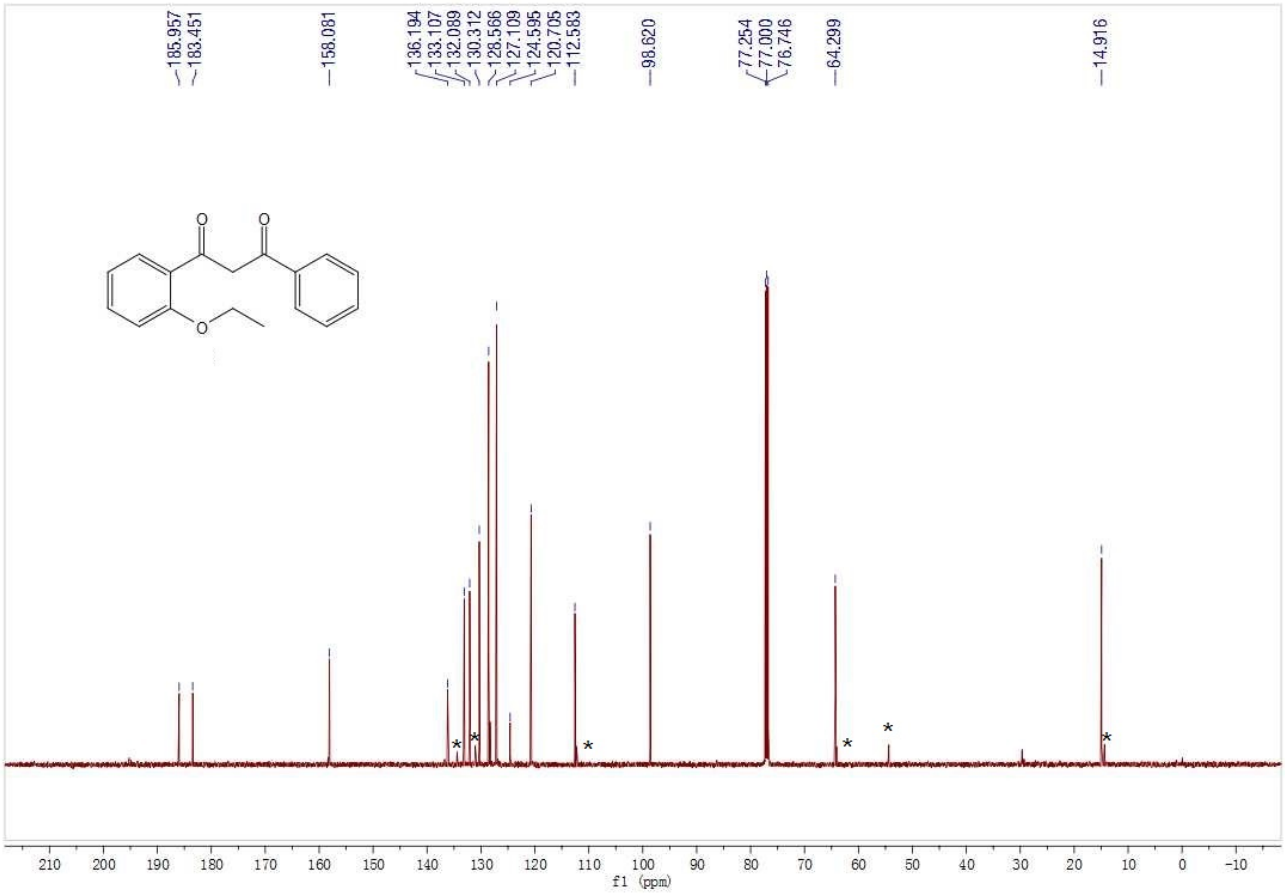

7.900
7.885
7.882
7.523
7.508
7.494
7.457
7.442
7.427
6.257
2.080
1.916
1.911
1.793
1.768
1.745
1.720
2.06
0.99
2.04
1.00
3.14
6.07
6.29
f1 (ppm)

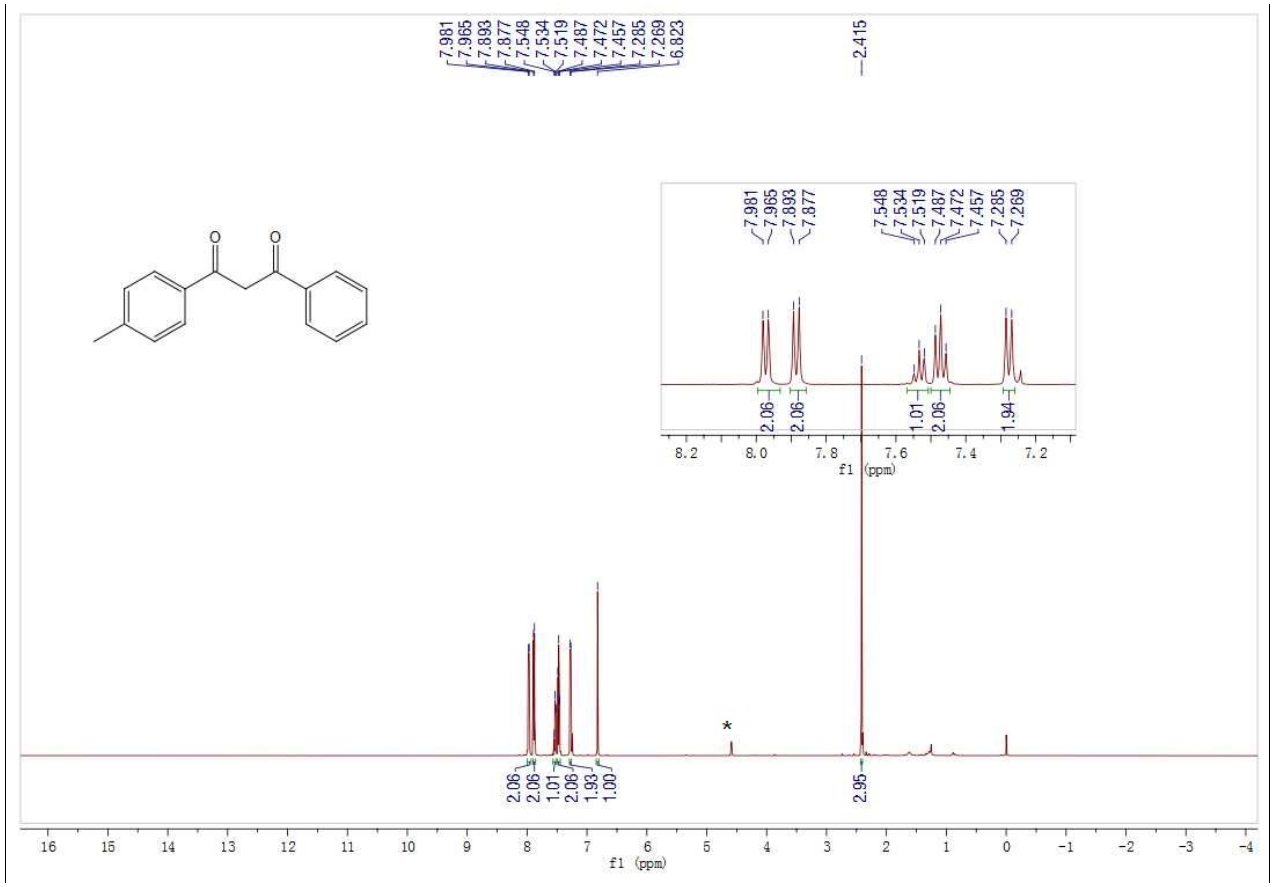

201.408
185.507
135.846
132.042
128.517
127.009
91.854
77.254
77.000
76.746
41.636
39.101
36.596
28.100
f1 (ppm)

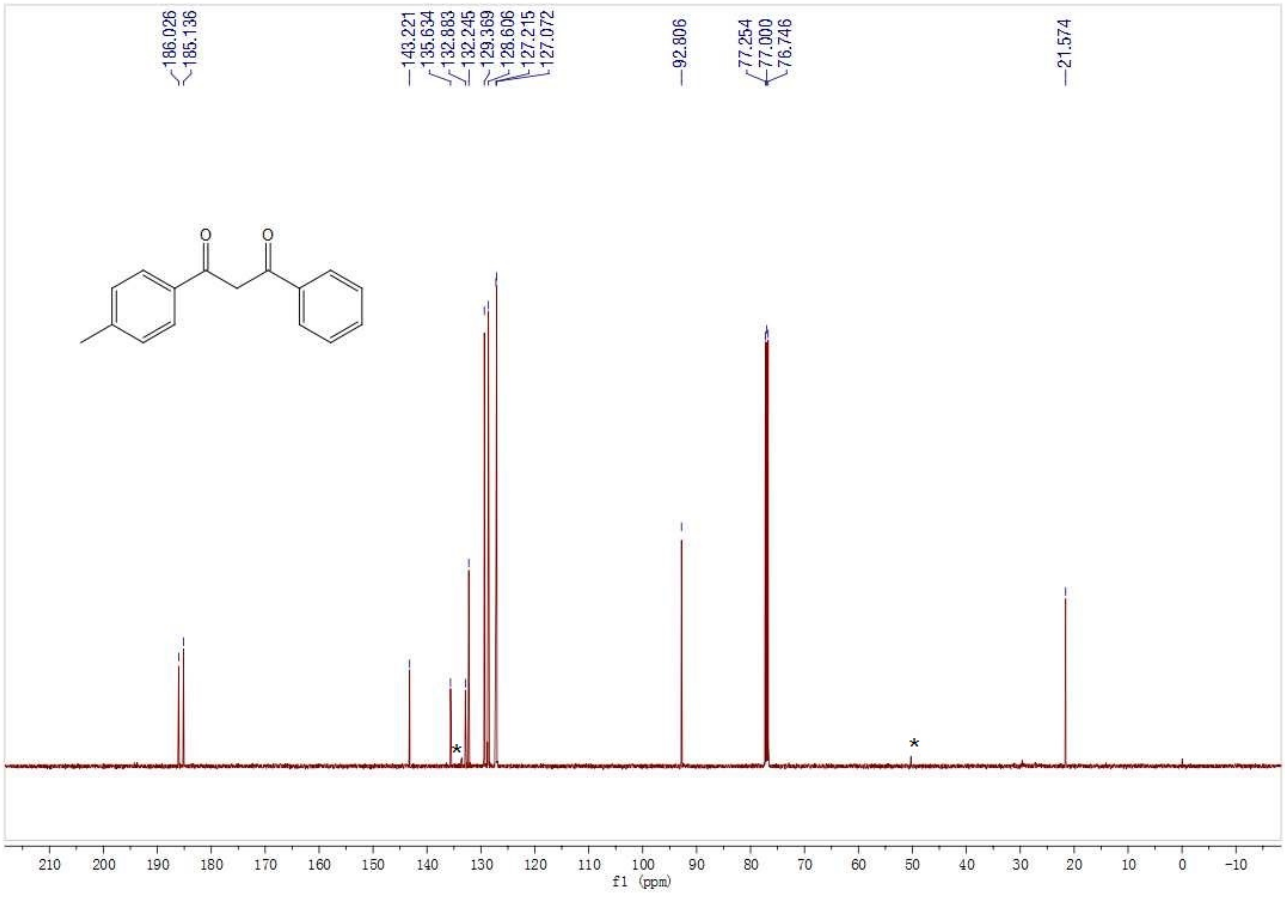

16.190
7.964
7.949
7.946
7.609
7.608
7.606
7.605
7.551
7.548
7.546
7.538
7.534
7.530
7.522
7.519
7.517
7.485
7.472
7.469
7.458
7.455
7.244
7.243
7.237
7.236
6.783
6.763
6.583
6.580
6.576
6.573
4.479
0.84
1.99
0.93
0.98
2.08
1.10
1.00
0.96
f1 (ppm)

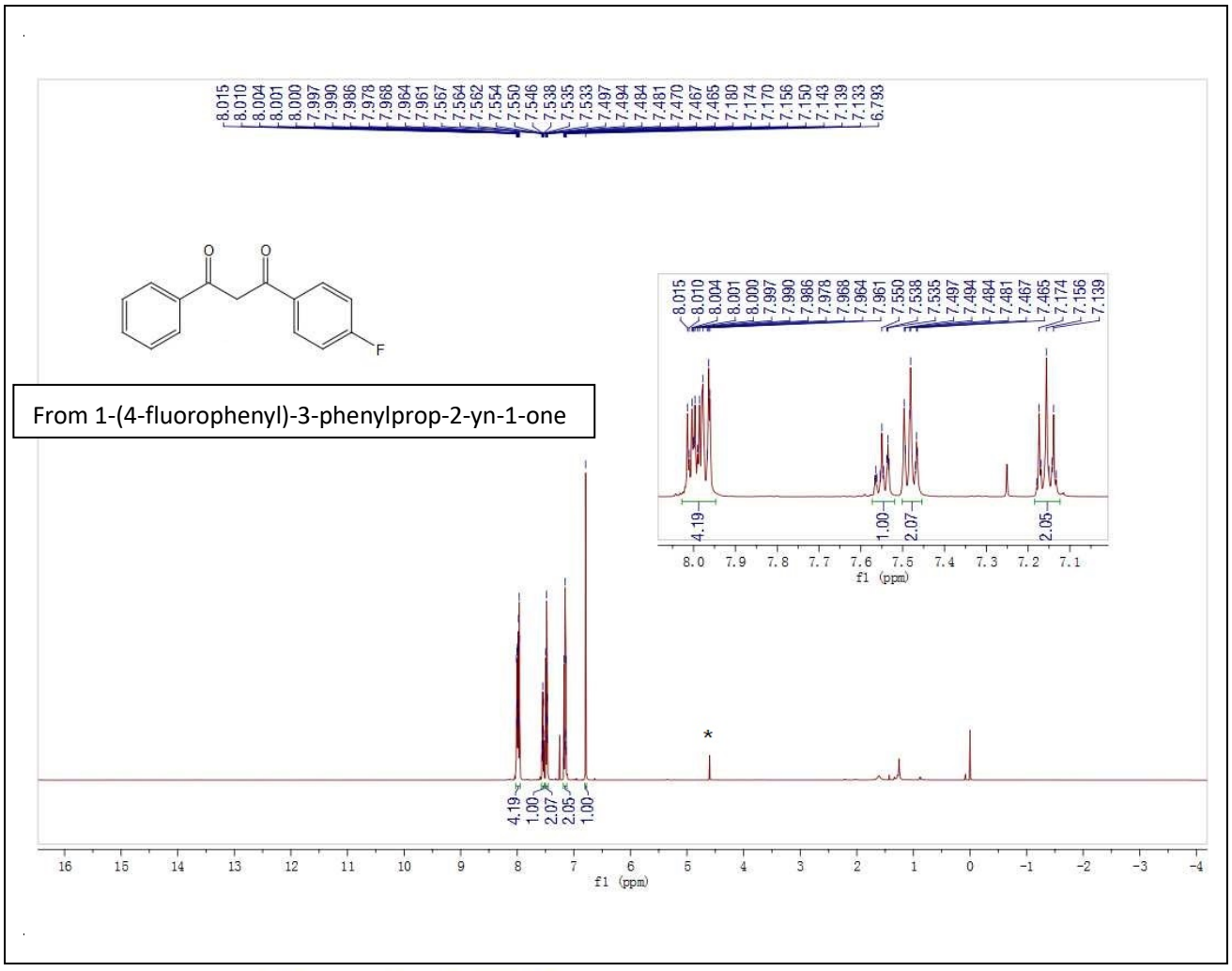

zt237
zt237
182.56
177.52
151.05
146.03
134.73
132.31
128.63
126.96
115.70
112.60
92.69
77.25
77.00
76.75
f1 (ppm)

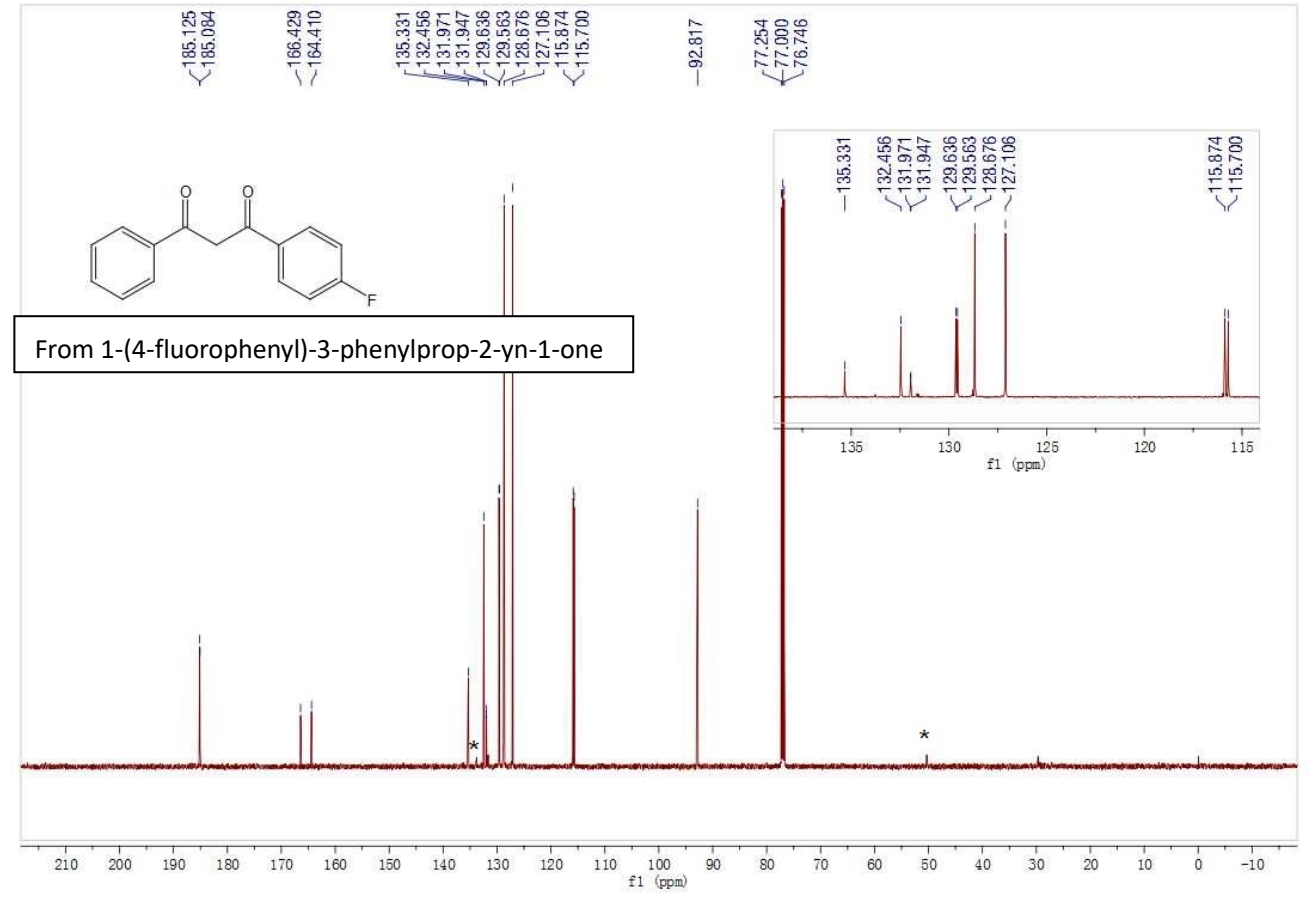

8.005
8.001
7.989
7.986
7.967
7.956
7.953
7.950
7.538
7.535
7.528
7.523
7.519
7.511
7.509
7.506
7.479
7.466
7.464
7.453
7.449
7.445
7.434
7.432
7.431
7.428
7.417
7.414
7.328
7.060
7.058
7.044
7.030
7.028
6.973
4.172
4.158
4.144
1.559
1.545
1.531
0.97
2.17
0.99
3.35
1.00
1.00
1.02
2.19
3.28
f1 (ppm)

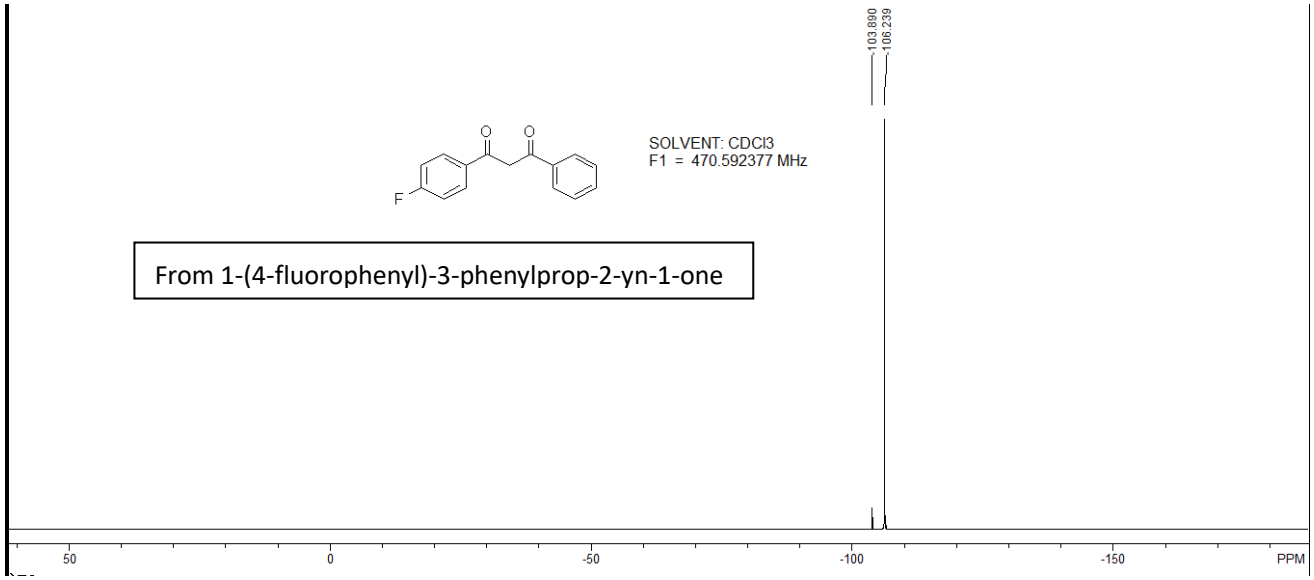

185.957
183.451
158.081
136.194
133.107
132.089
130.312
128.566
127.109
124.595
120.705
112.583
98.620
77.254
77.000
76.746
64.299
14.916
f1 (ppm)

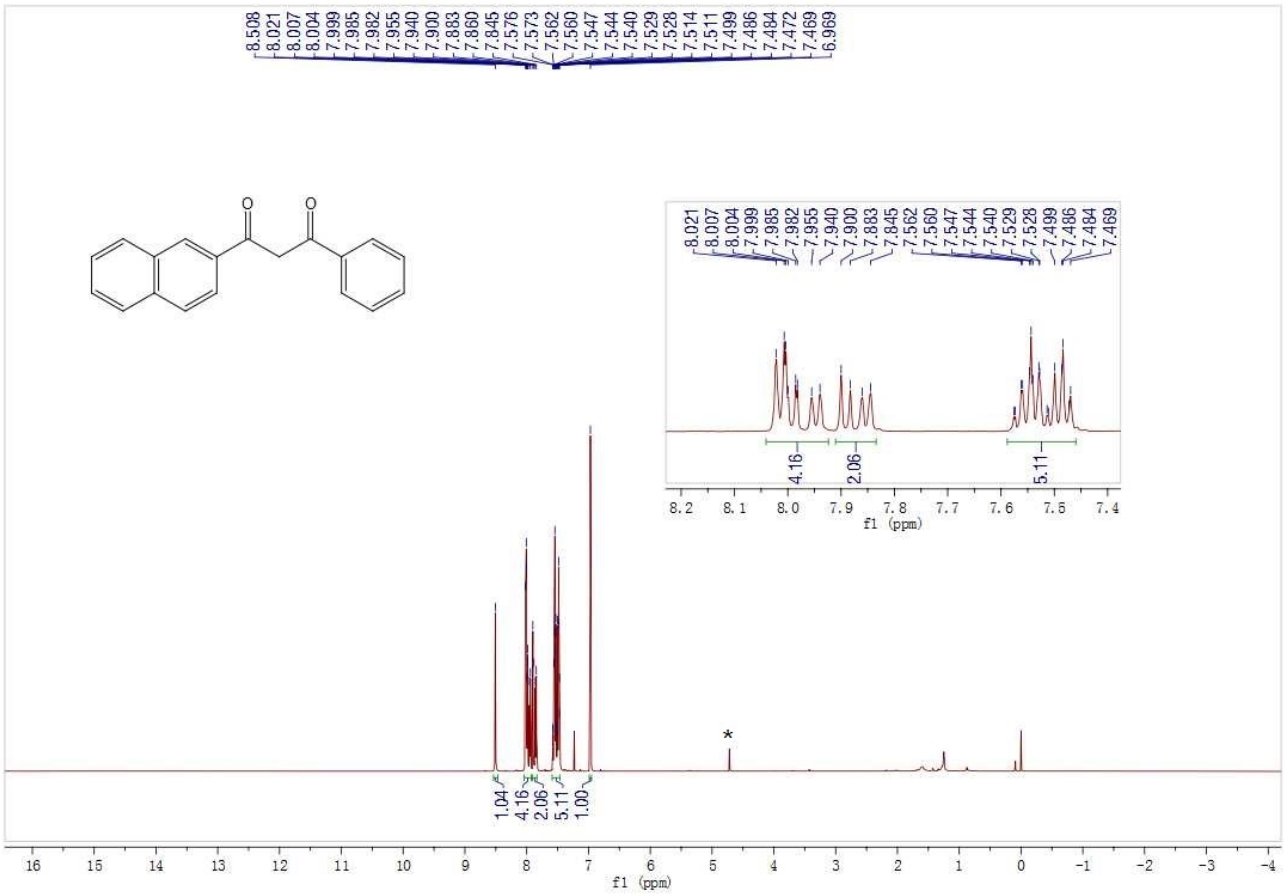

7.981
7.965
7.893
7.877
7.548
7.534
7.519
7.487
7.472
7.457
7.285
7.269
6.823
2.415
2.06
2.06
1.01
2.06
1.93
1.00
2.95
f1 (ppm)

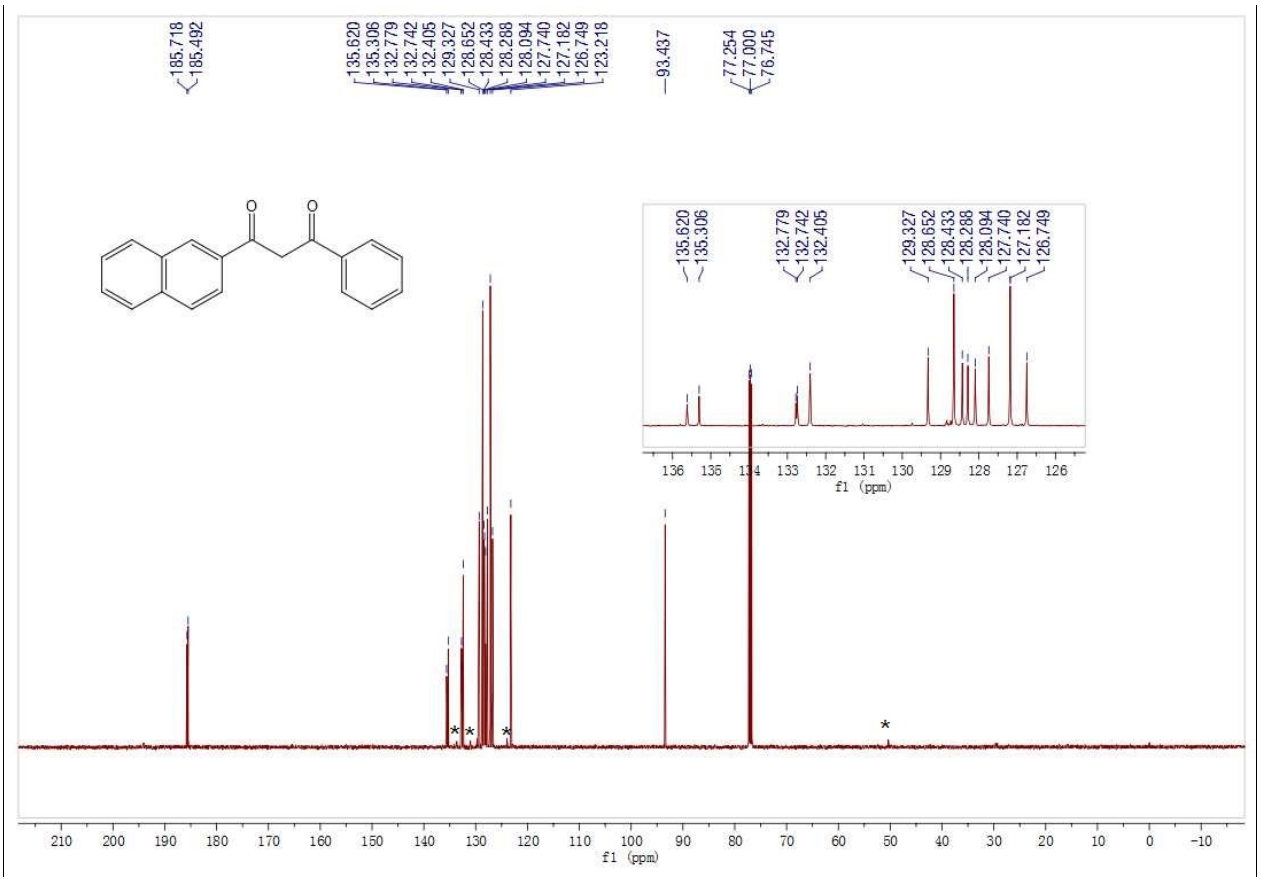

186.026
185.136
143.221
135.634
132.883
132.245
129.369
128.606
127.215
127.072
92.806
77.254
77.000
76.746
21.574
O
O
*
*
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

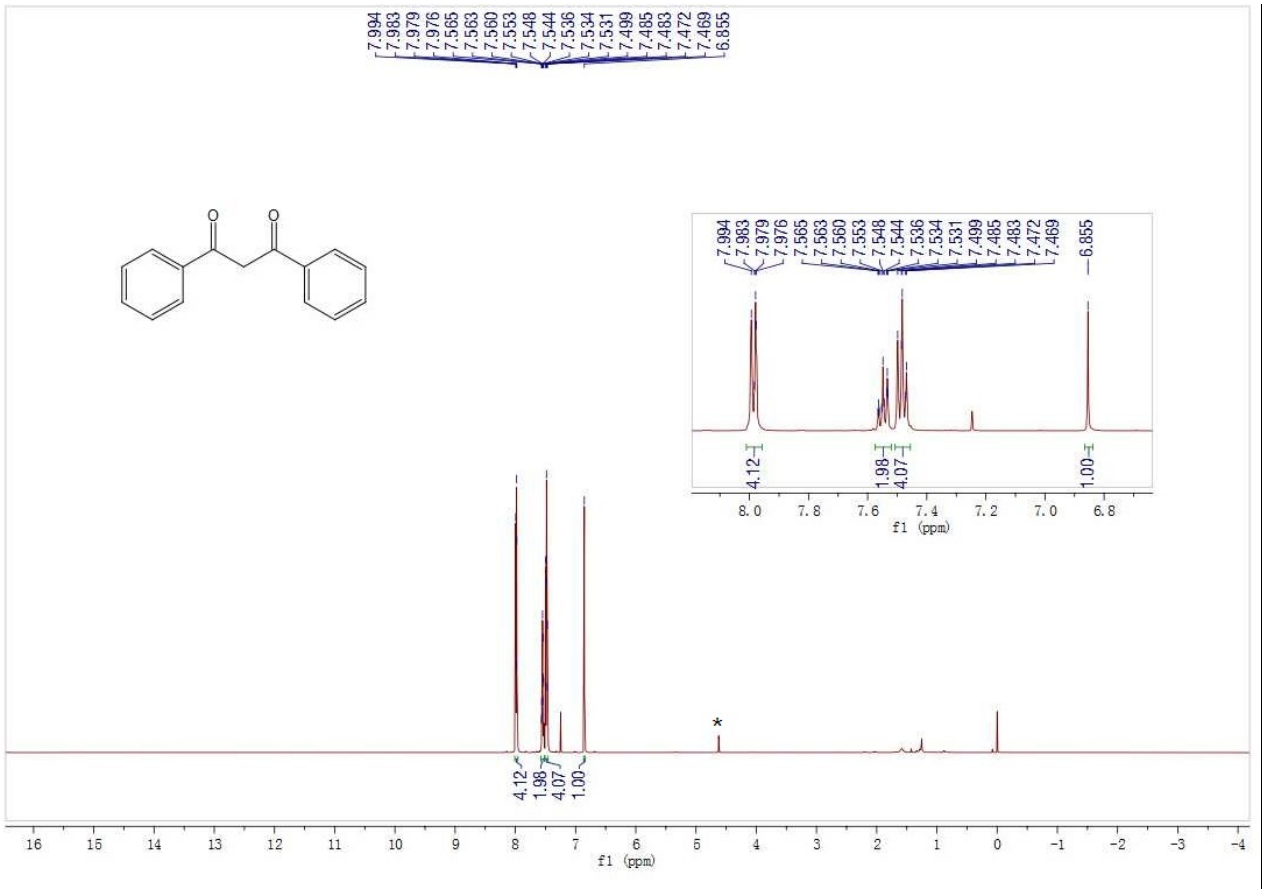

From 1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one
f1 (ppm)

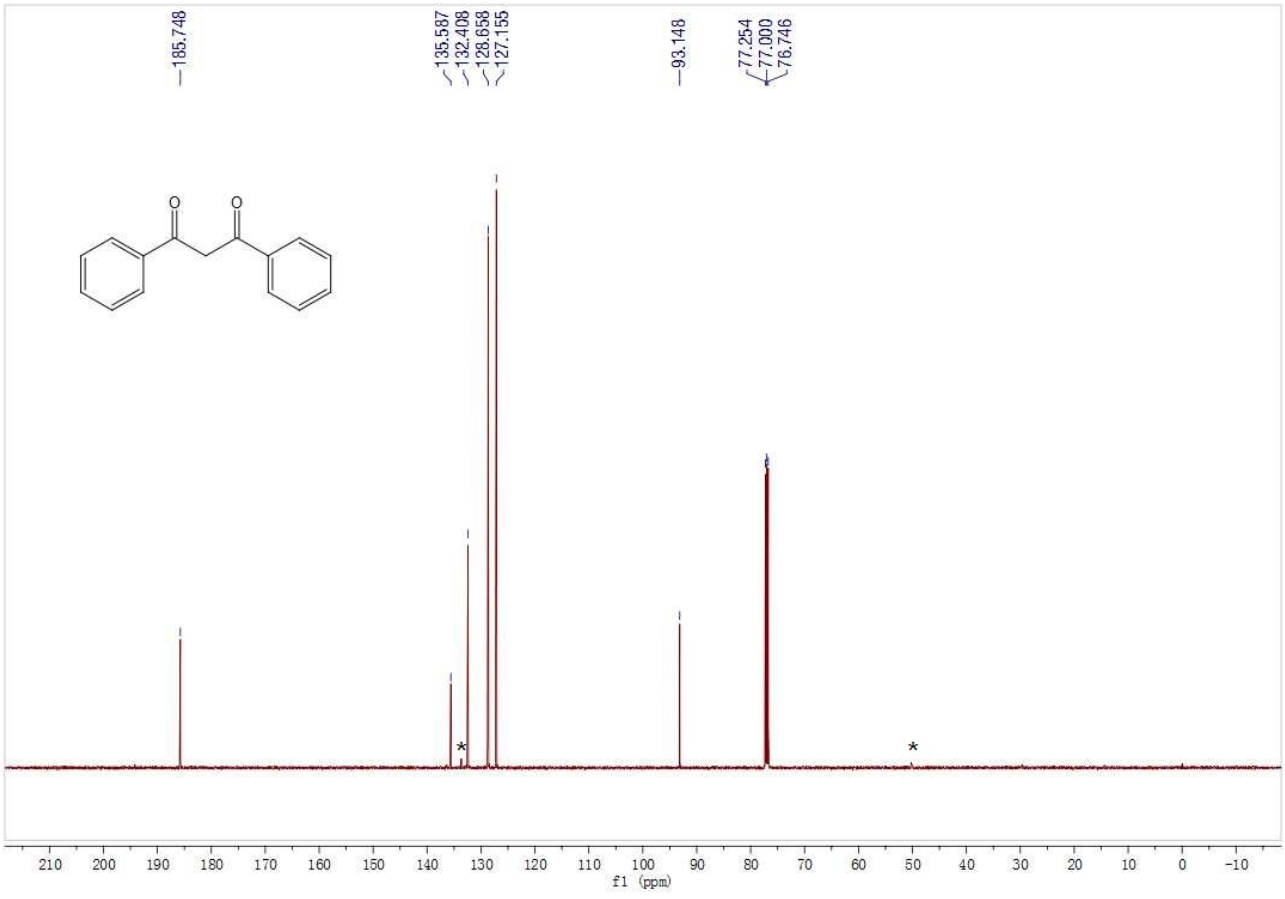

From 1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one
f1 (ppm)


103.890
106.239
SOLVENT: CDCl3
F1 = 470.592377 MHz
F
From 1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one
50
0
-50
-100
-150
PPM


8.508
8.021
8.007
8.004
7.999
7.985
7.982
7.955
7.940
7.900
7.883
7.860
7.845
7.576
7.573
7.562
7.560
7.547
7.544
7.540
7.529
7.528
7.514
7.511
7.499
7.486
7.484
7.472
7.469
6.969
4.16
2.06
5.11
f1 (ppm)
1.04
4.16
2.06
5.11
1.00
*
f1 (ppm)


185.718
185.492
135.620
135.306
132.779
132.742
132.405
129.327
128.652
128.433
128.288
128.094
127.740
127.182
126.749
123.218
93.437
77.254
77.000
76.745
f1 (ppm)


7.994
7.983
7.979
7.976
7.565
7.563
7.560
7.553
7.548
7.544
7.536
7.534
7.531
7.499
7.485
7.483
7.472
7.469
6.855
4.12
1.98
4.07
1.00
f1 (ppm)


185.748
135.587
132.408
128.658
127.155
93.148
77.254
77.000
76.746
O
O
*
*
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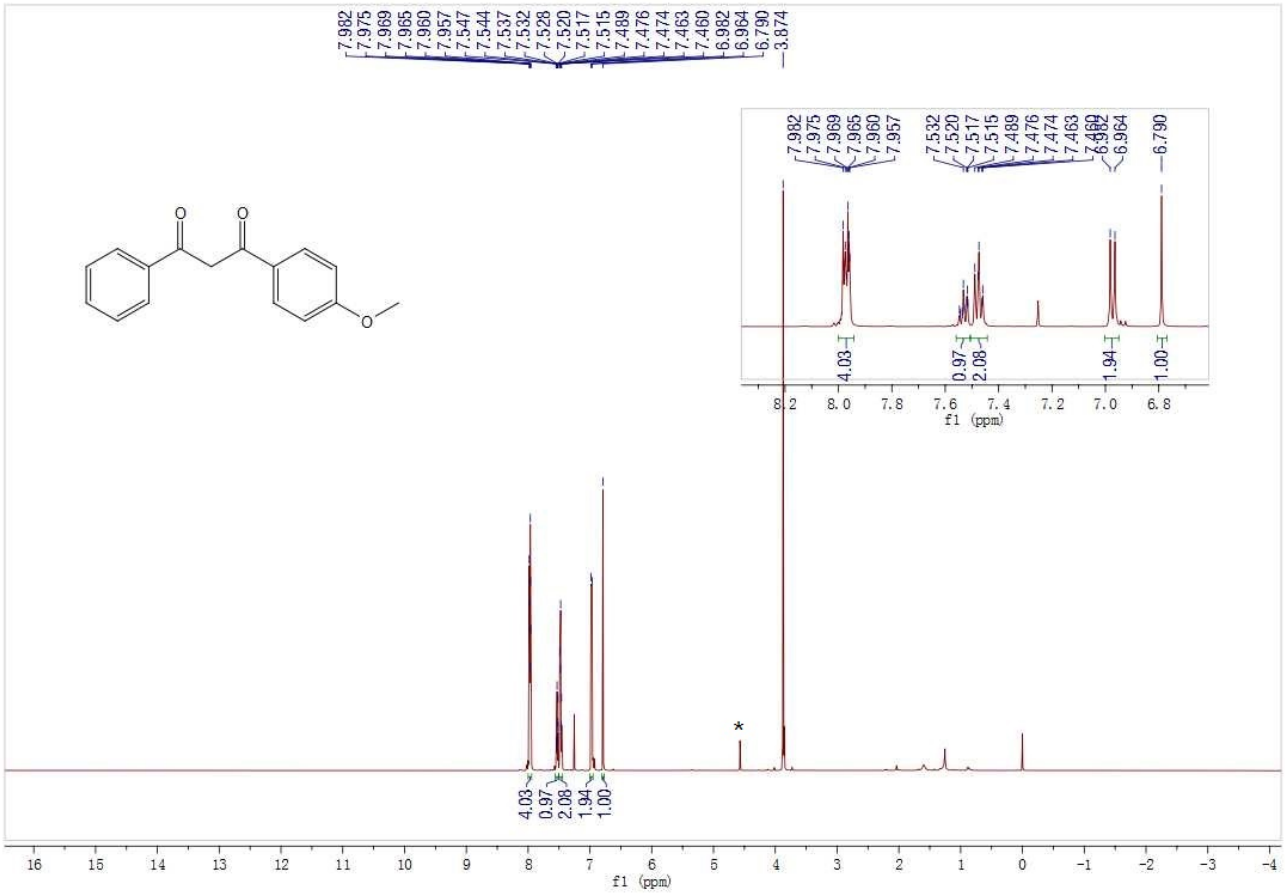
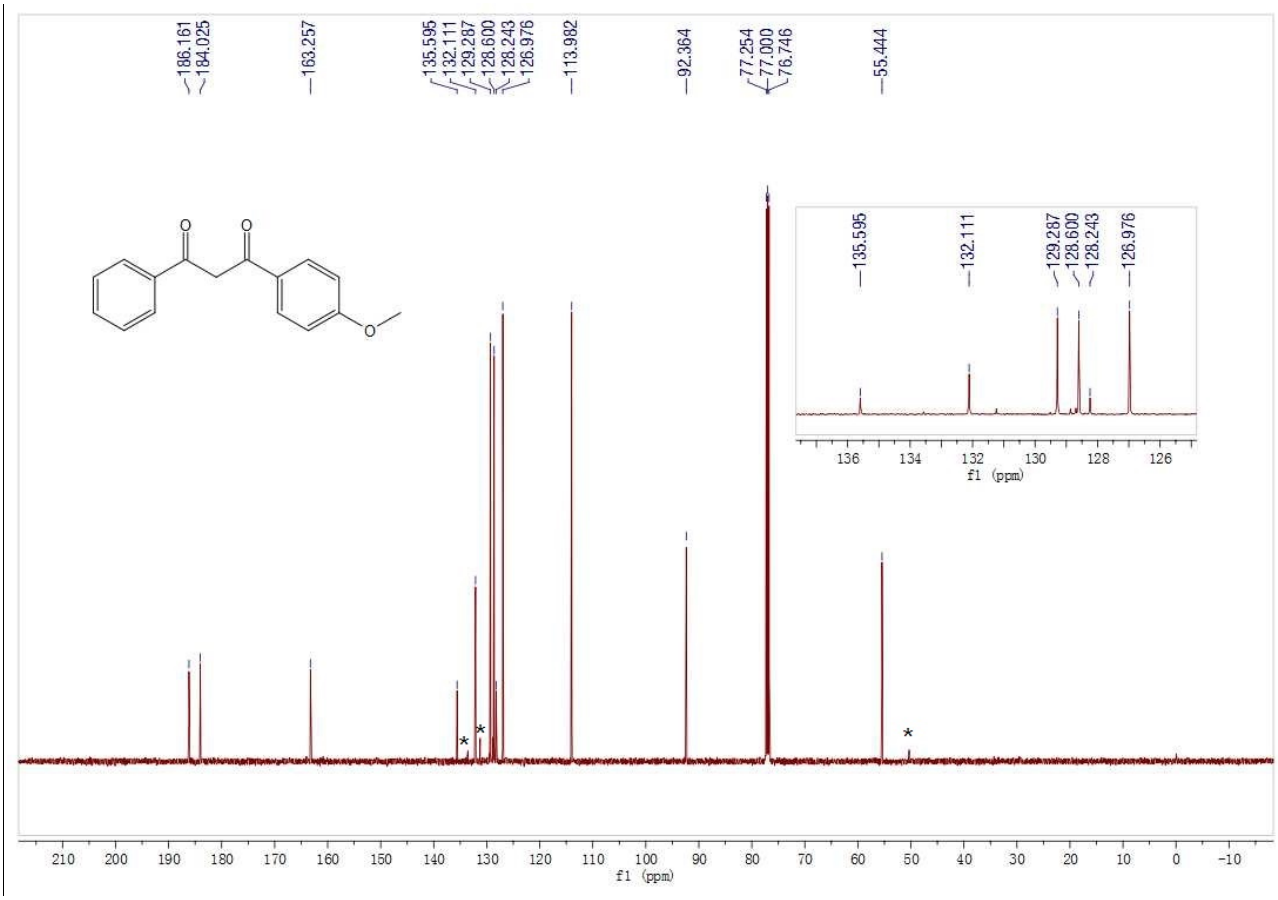
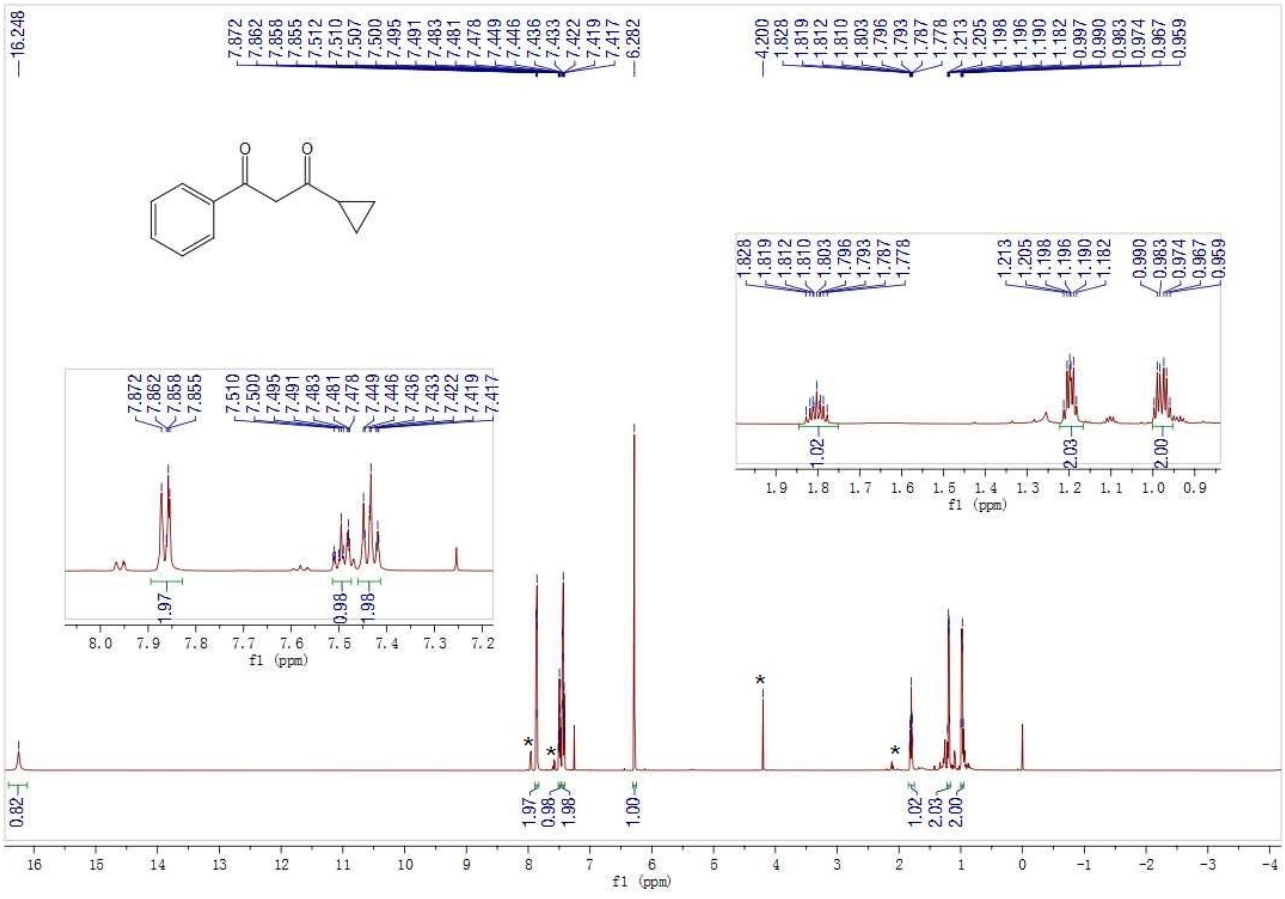
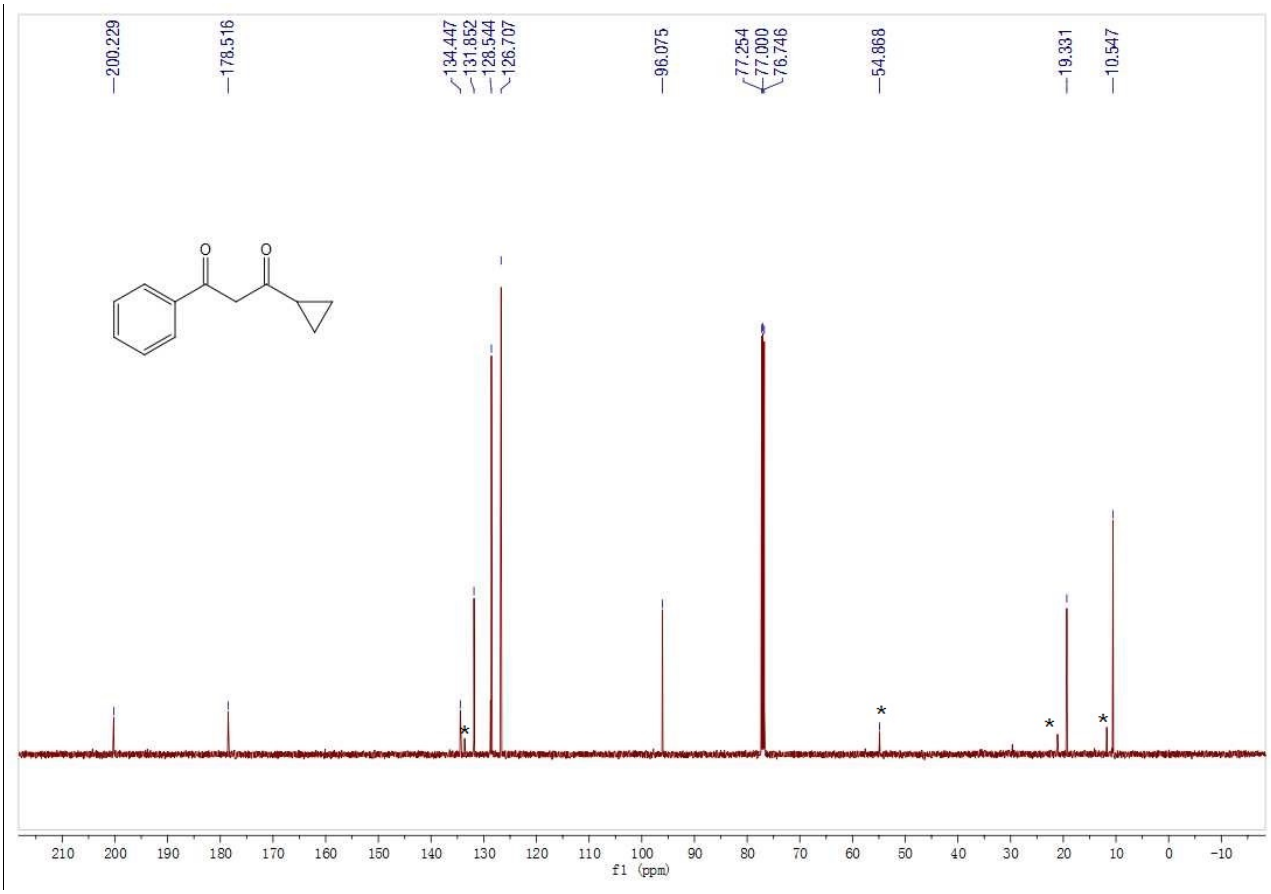
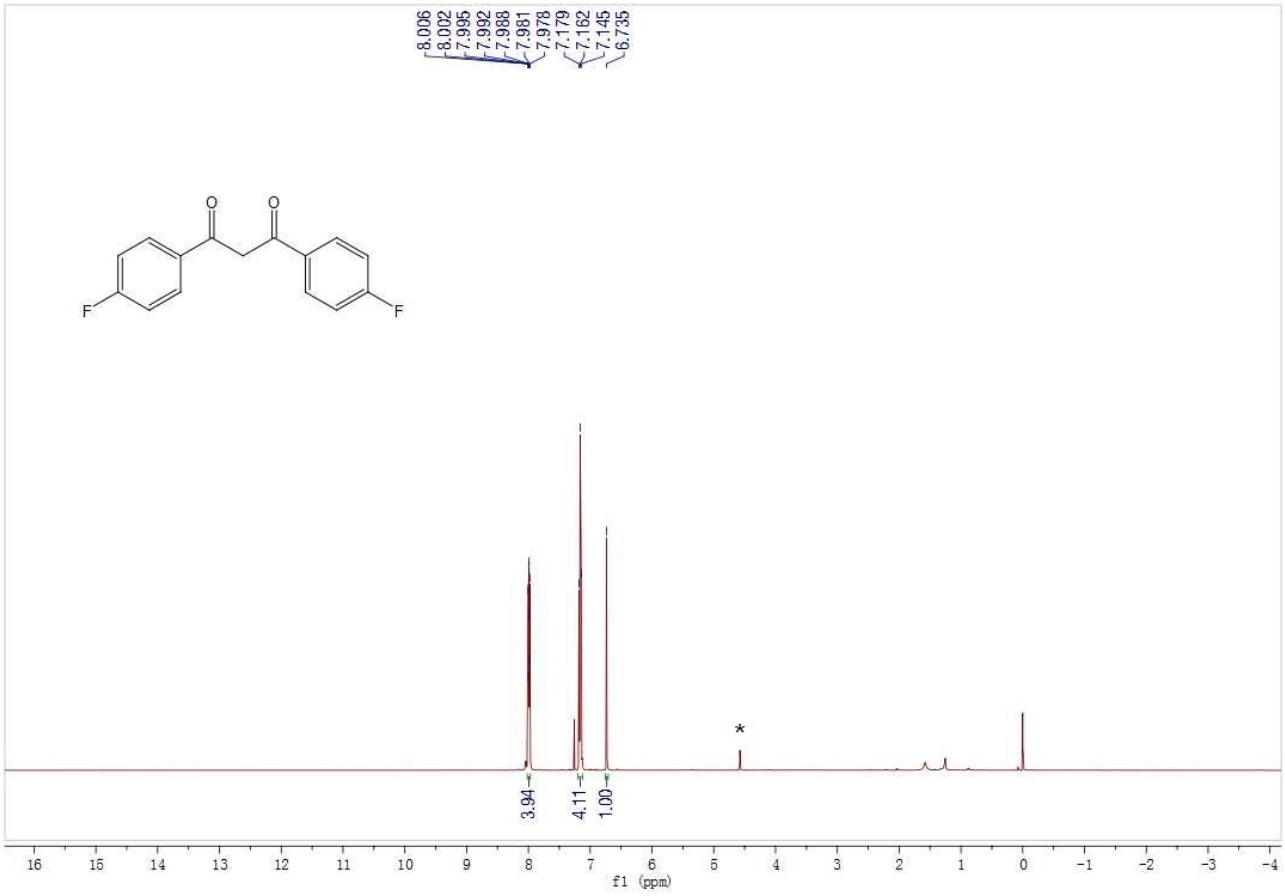
f1 (ppm)

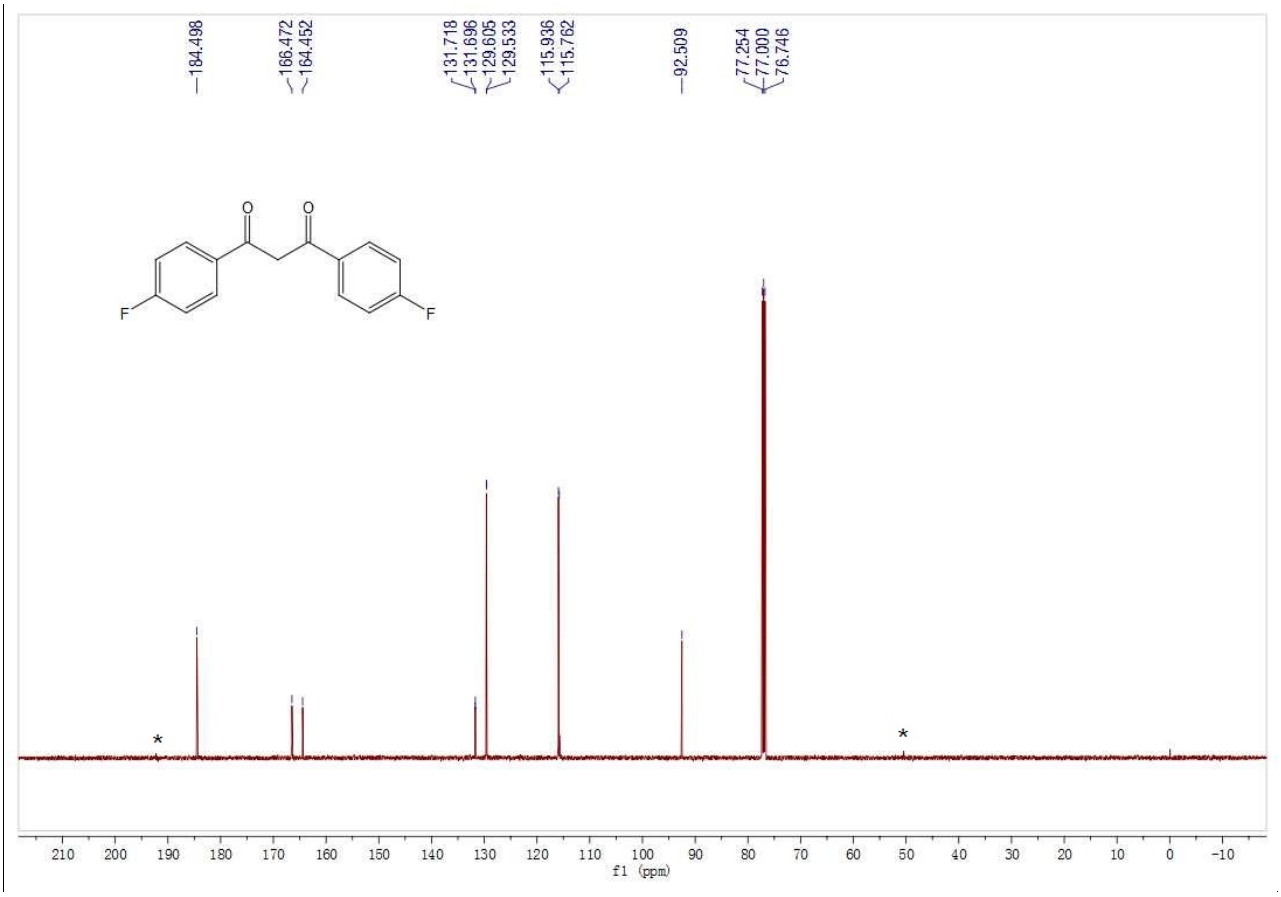

7.982
7.975
7.969
7.965
7.960
7.957
7.547
7.544
7.537
7.532
7.528
7.520
7.517
7.515
7.489
7.476
7.474
7.463
7.460
6.982
6.964
6.790
3.874
4.03
0.97
2.08
1.94
1.00
f1 (ppm)

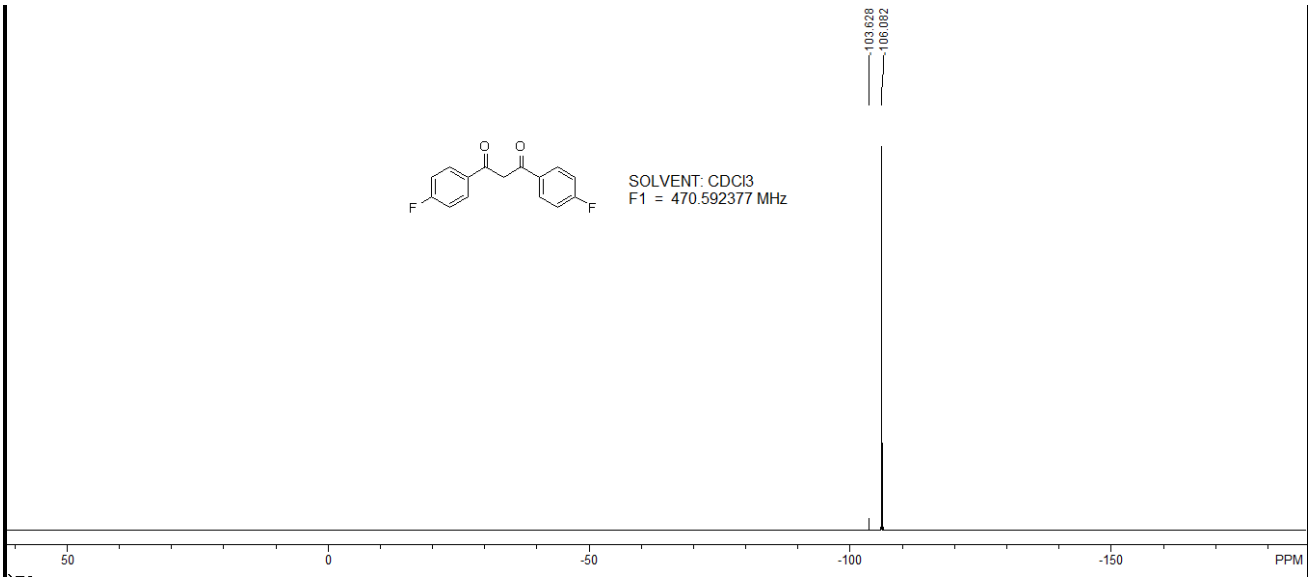

186.161
184.025
163.257
135.595
132.111
129.287
128.600
128.243
126.976
113.982
92.364
77.254
77.000
76.746
55.444
f1 (ppm)

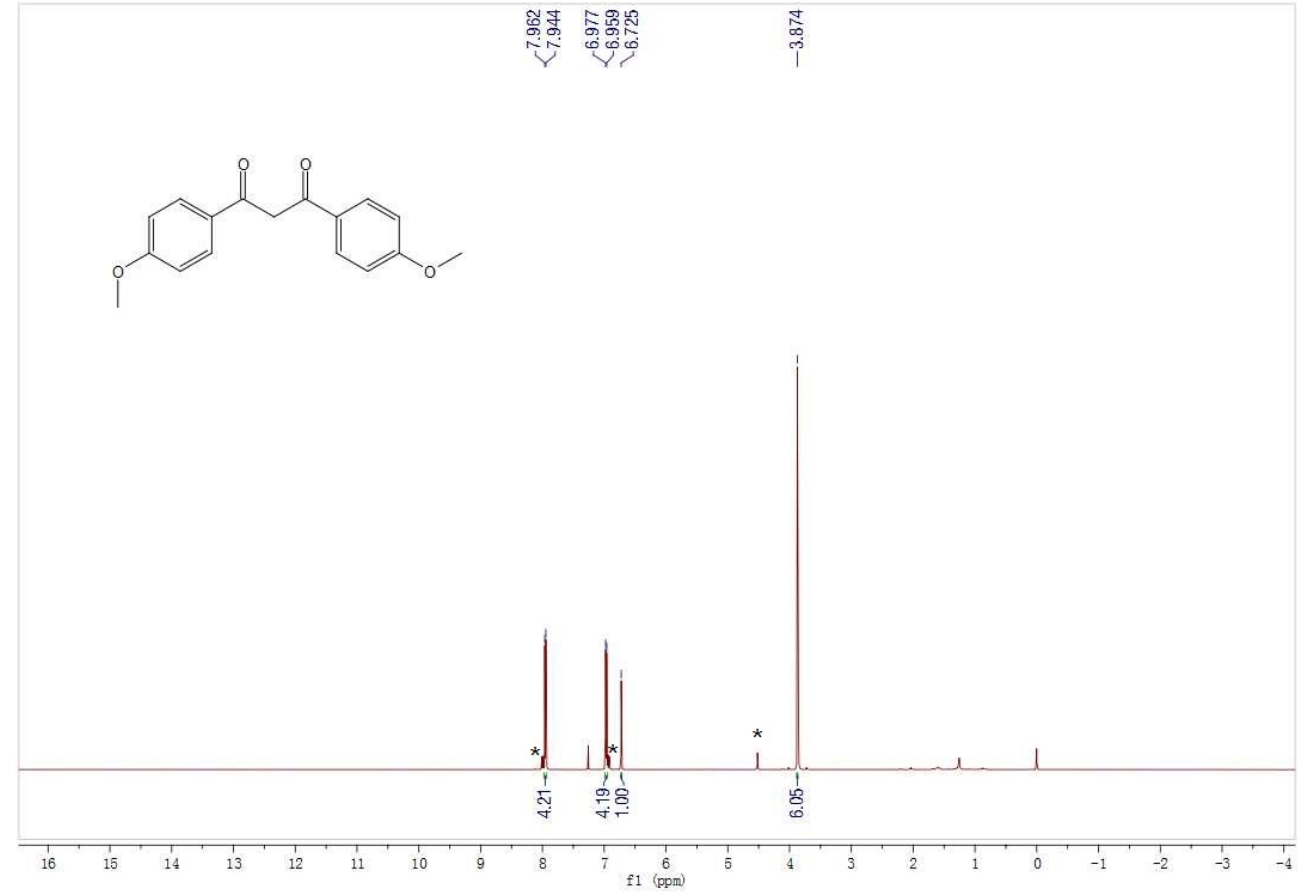


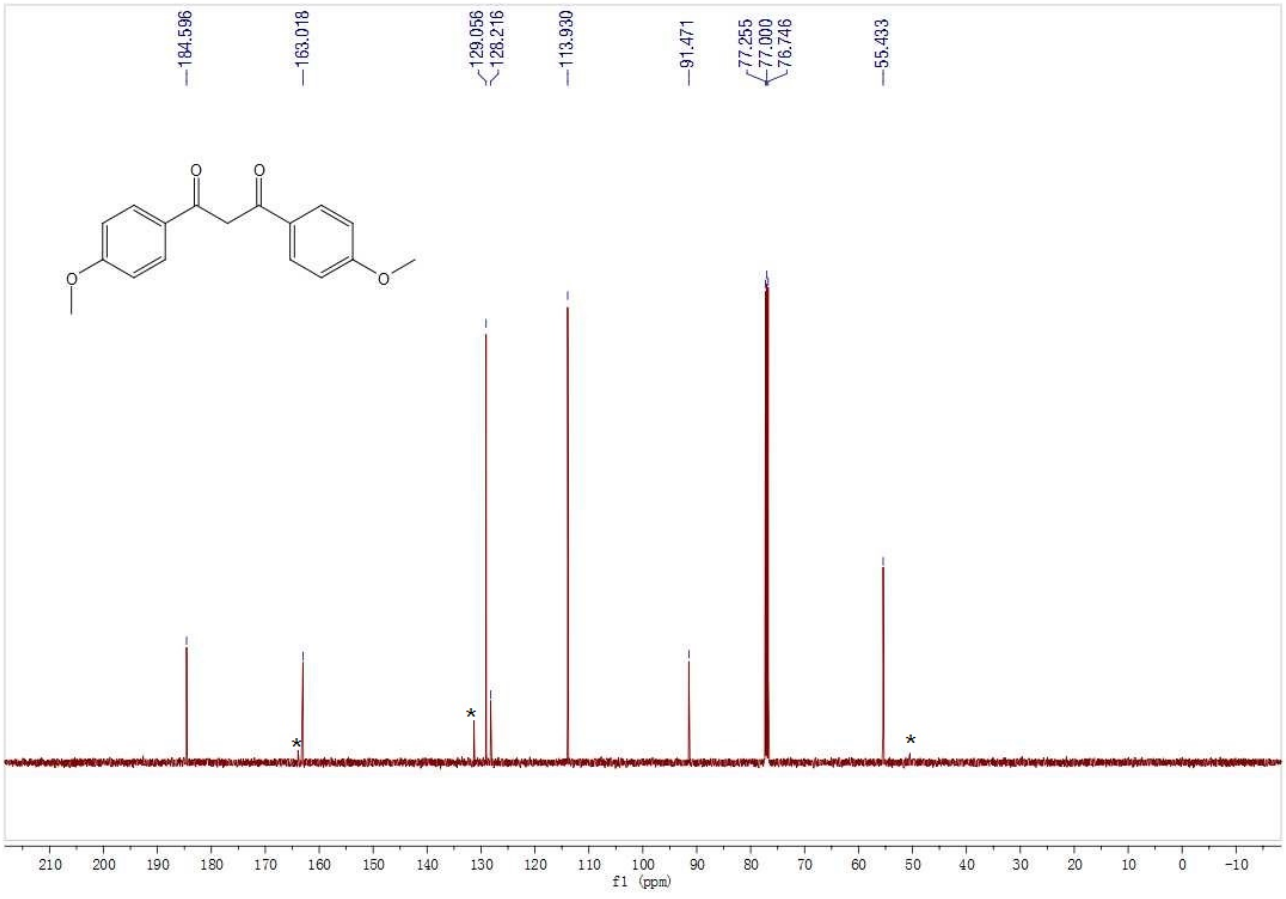


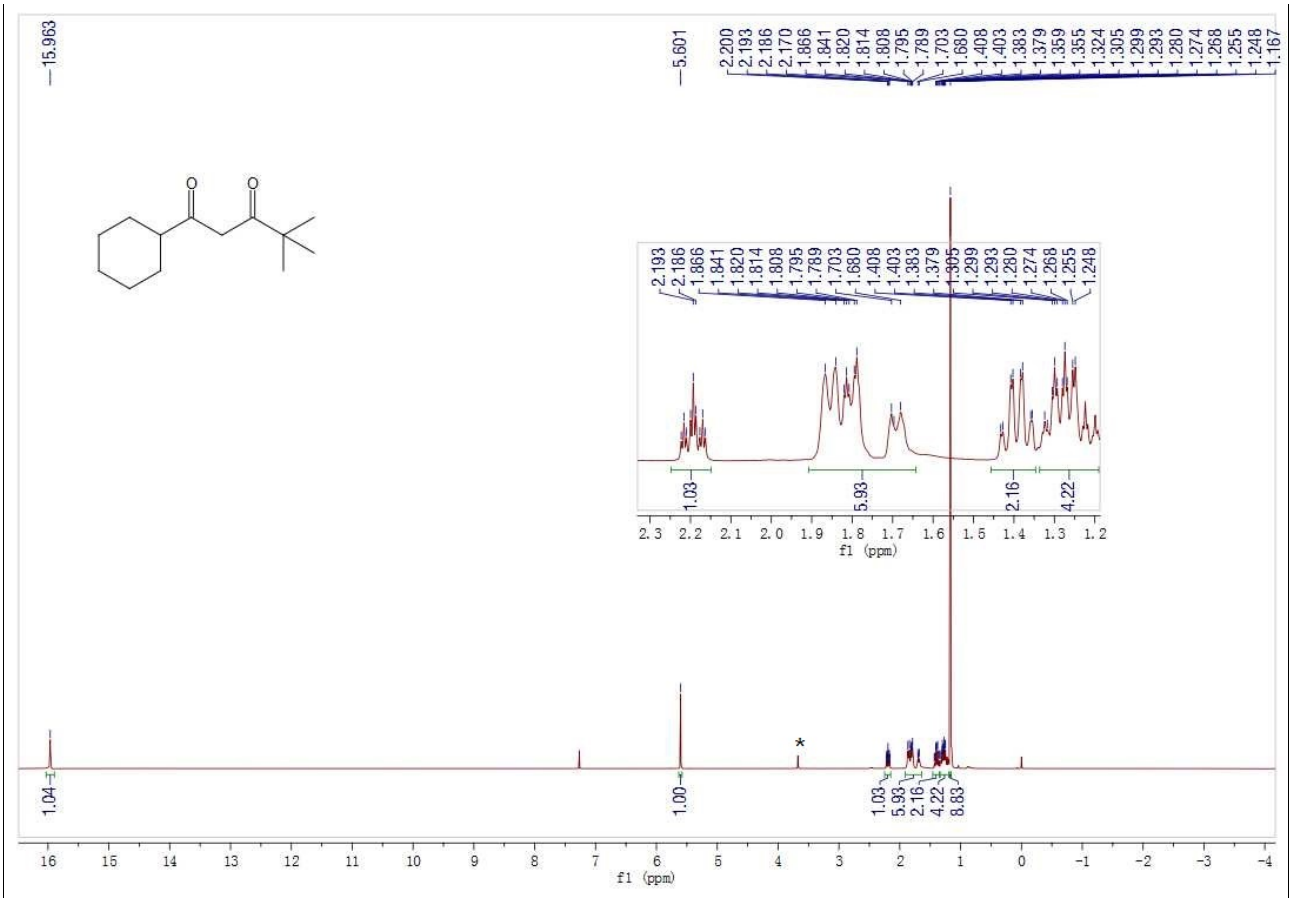

8.006
8.002
7.995
7.992
7.988
7.981
7.978
7.179
7.162
7.145
6.735
O
O
F
F
3.94
4.11
1.00
*
f1 (ppm)

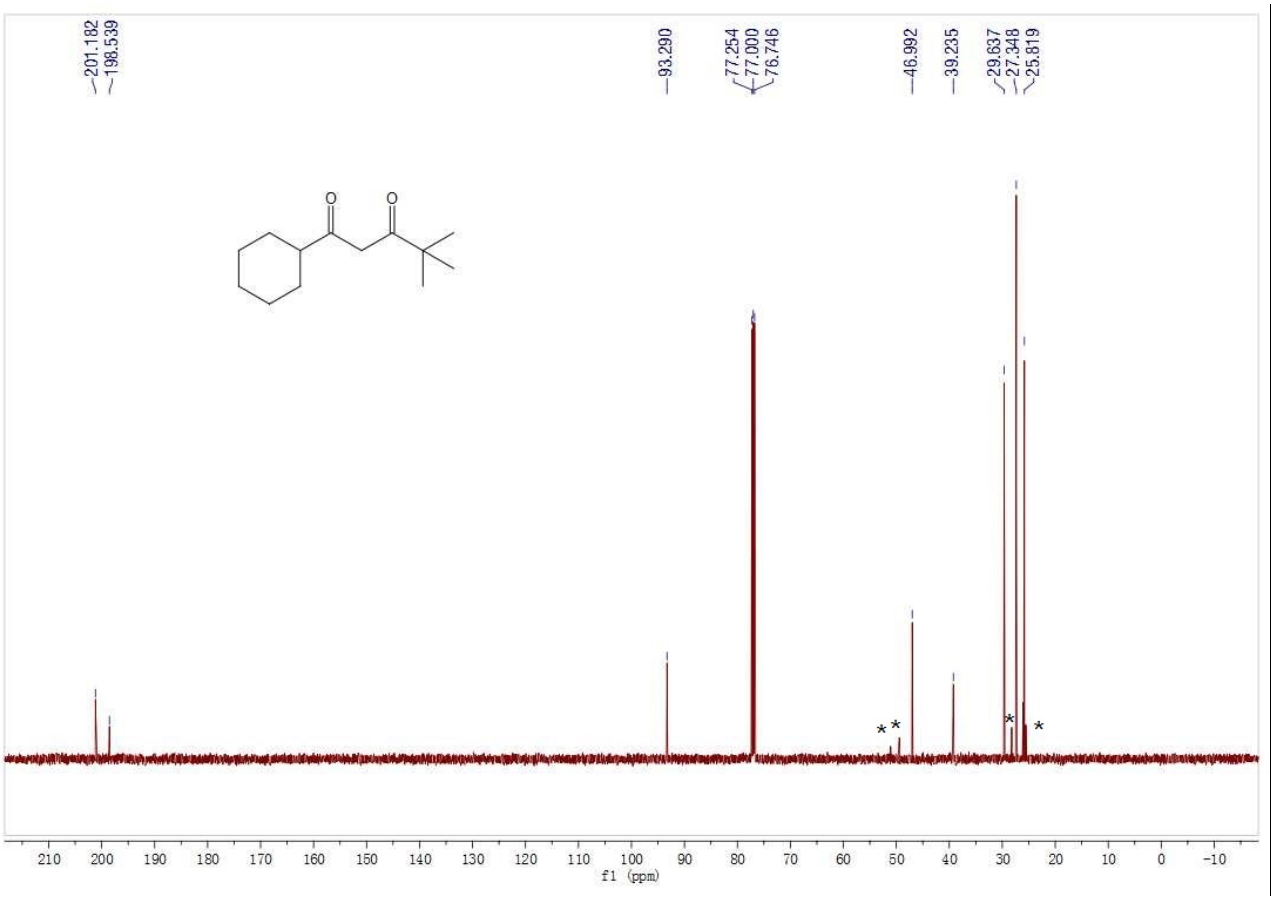

184.498
166.472
164.452
131.718
131.696
129.605
129.533
115.936
115.762
92.509
77.254
77.000
76.746
O
O
F
F
*
*
f1 (ppm)

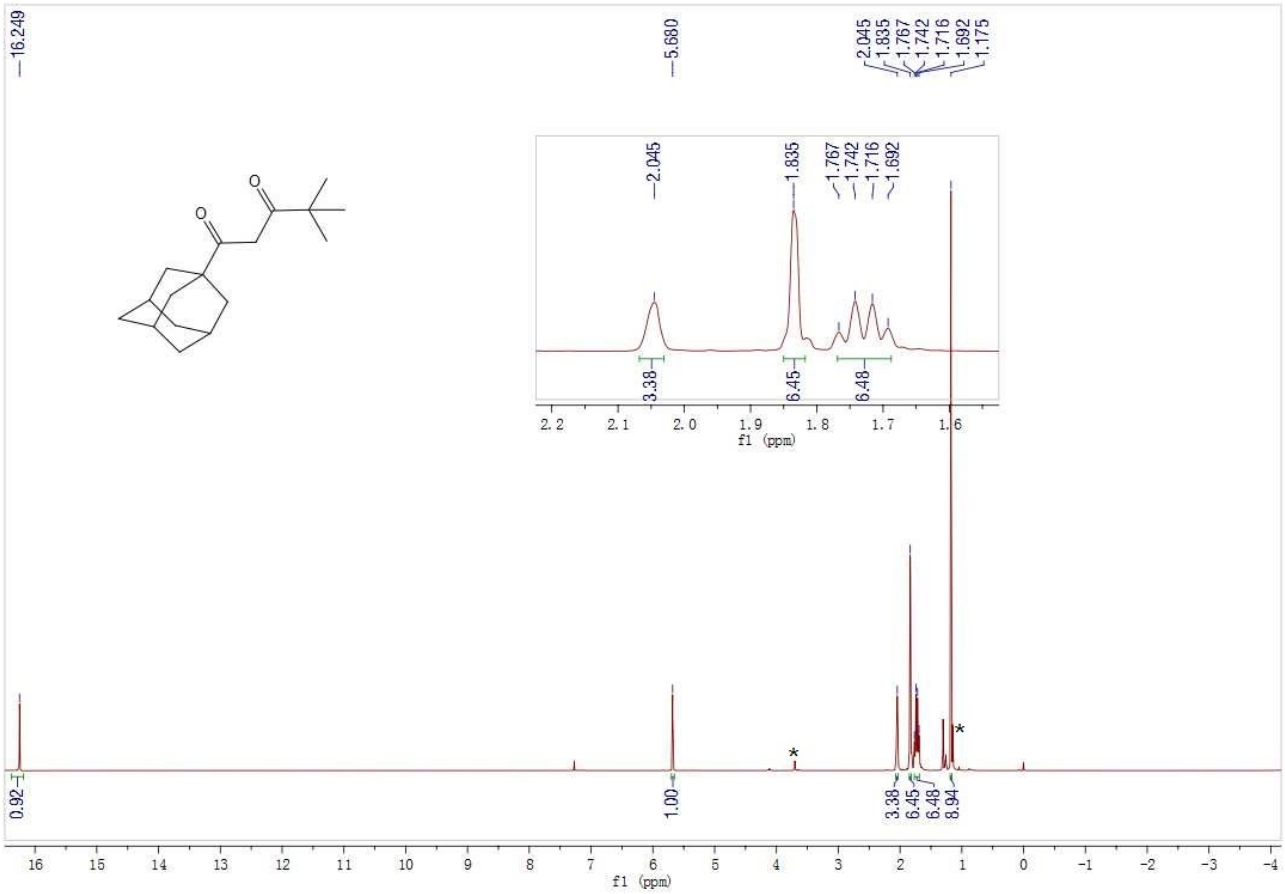

103.628
106.082
SOLVENT: CDCl3
F1 = 470.592377 MHz
50
0
-50
-100
-150
PPM

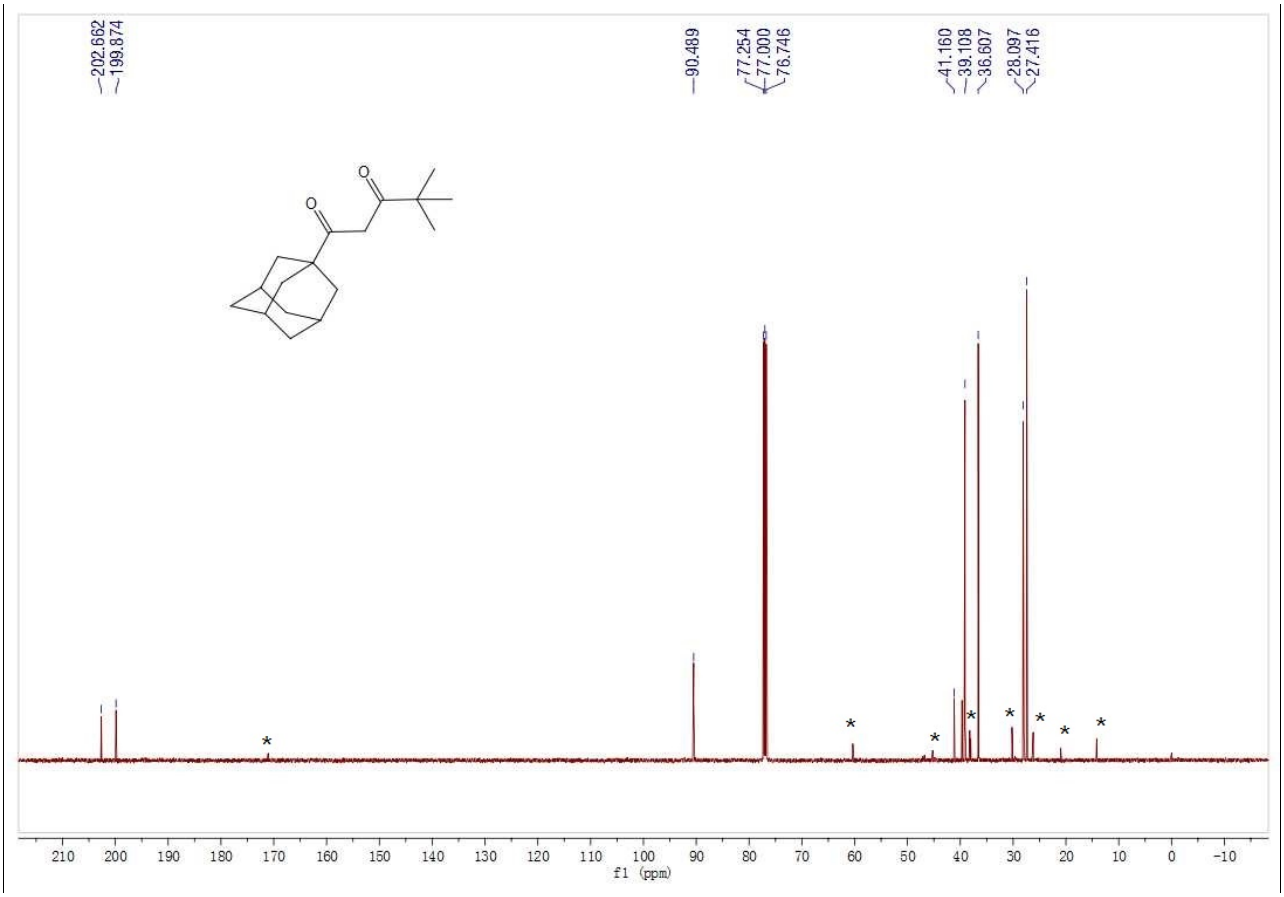

7.962
7.944
6.977
6.959
6.725
3.874
4.21
4.19
1.00
6.05
f1 (ppm)

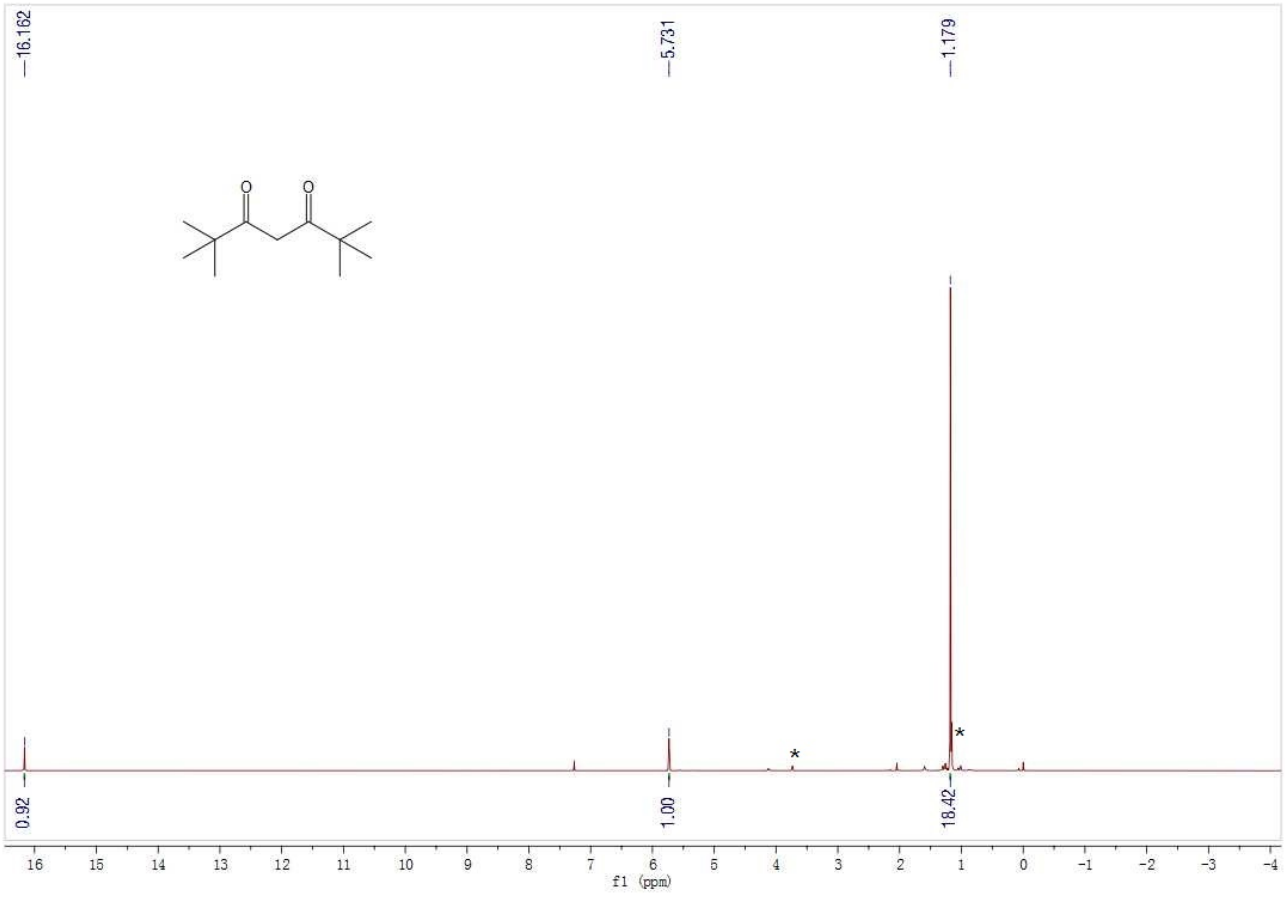

184.596
163.018
129.056
128.216
113.930
91.471
77.255
77.000
76.746
55.433
O
O
O
O
*
*
*
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

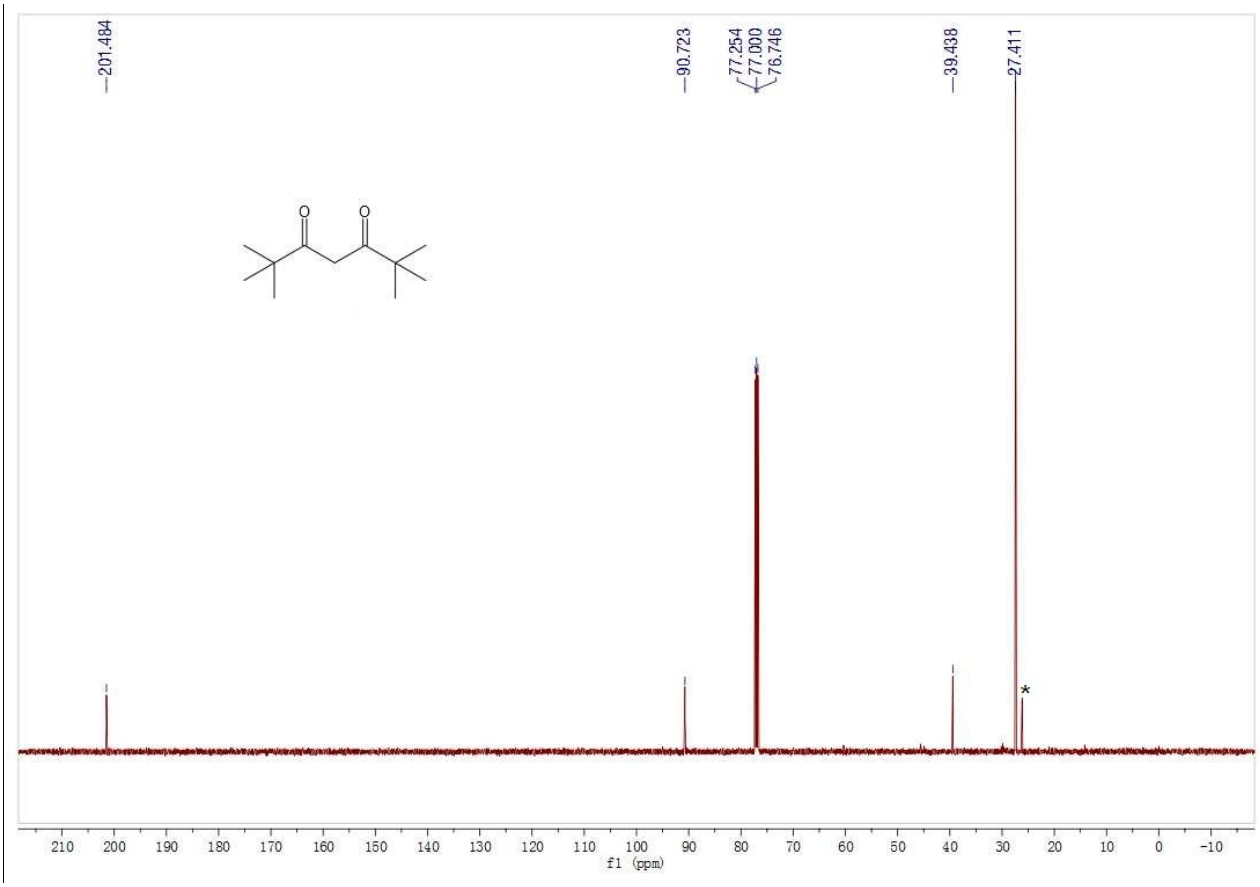

15.963
5.601
2.200
2.193
2.186
2.170
1.866
1.841
1.820
1.814
1.808
1.795
1.789
1.703
1.680
1.408
1.403
1.383
1.379
1.305
1.299
1.293
1.280
1.274
1.268
1.255
1.248
1.167
O
O
1.03
5.93
2.16
4.22
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2
f1 (ppm)
*
1.04
1.00
1.03
5.93
2.16
4.22
8.83
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

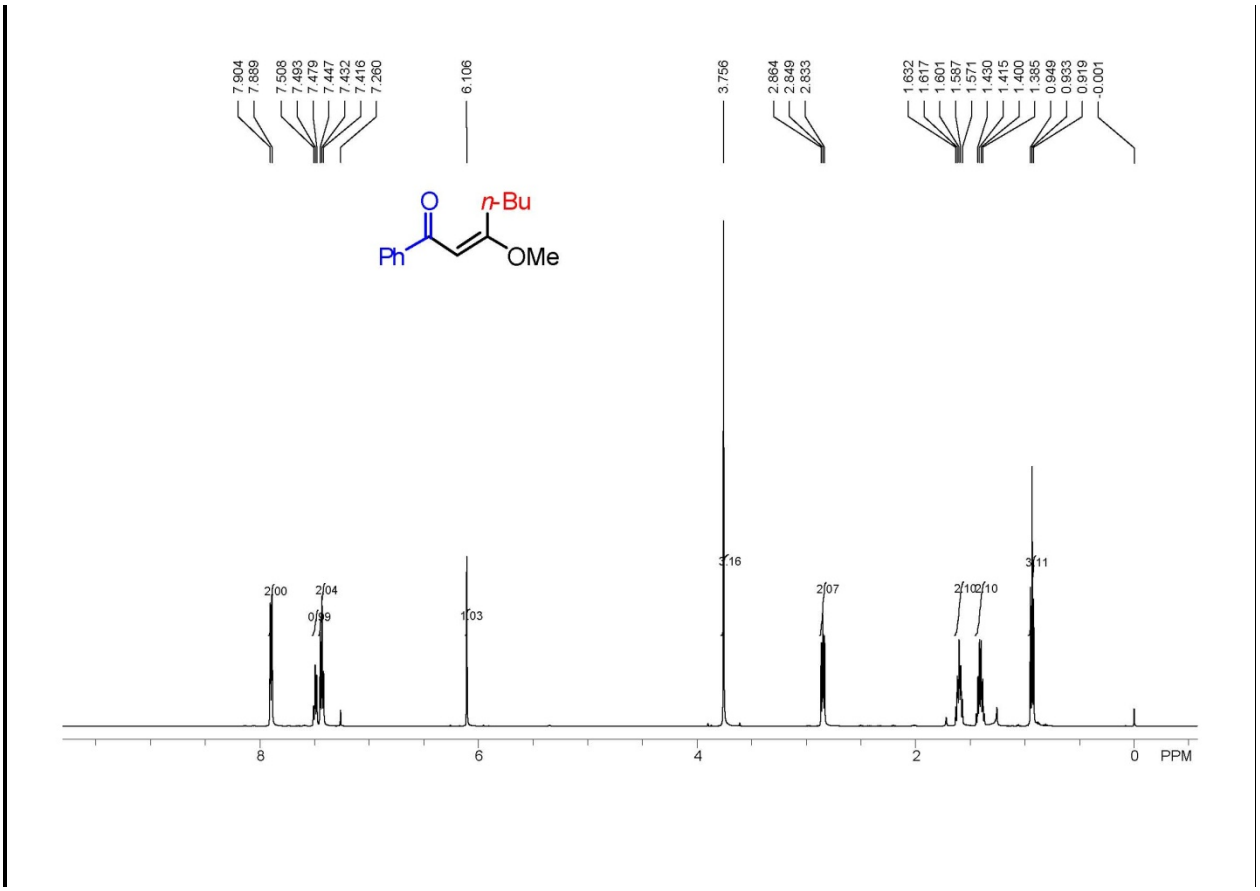

201.182
198.539
93.290
77.254
77.000
76.746
46.992
39.235
29.637
27.348
25.819
O
O
f1 (ppm)

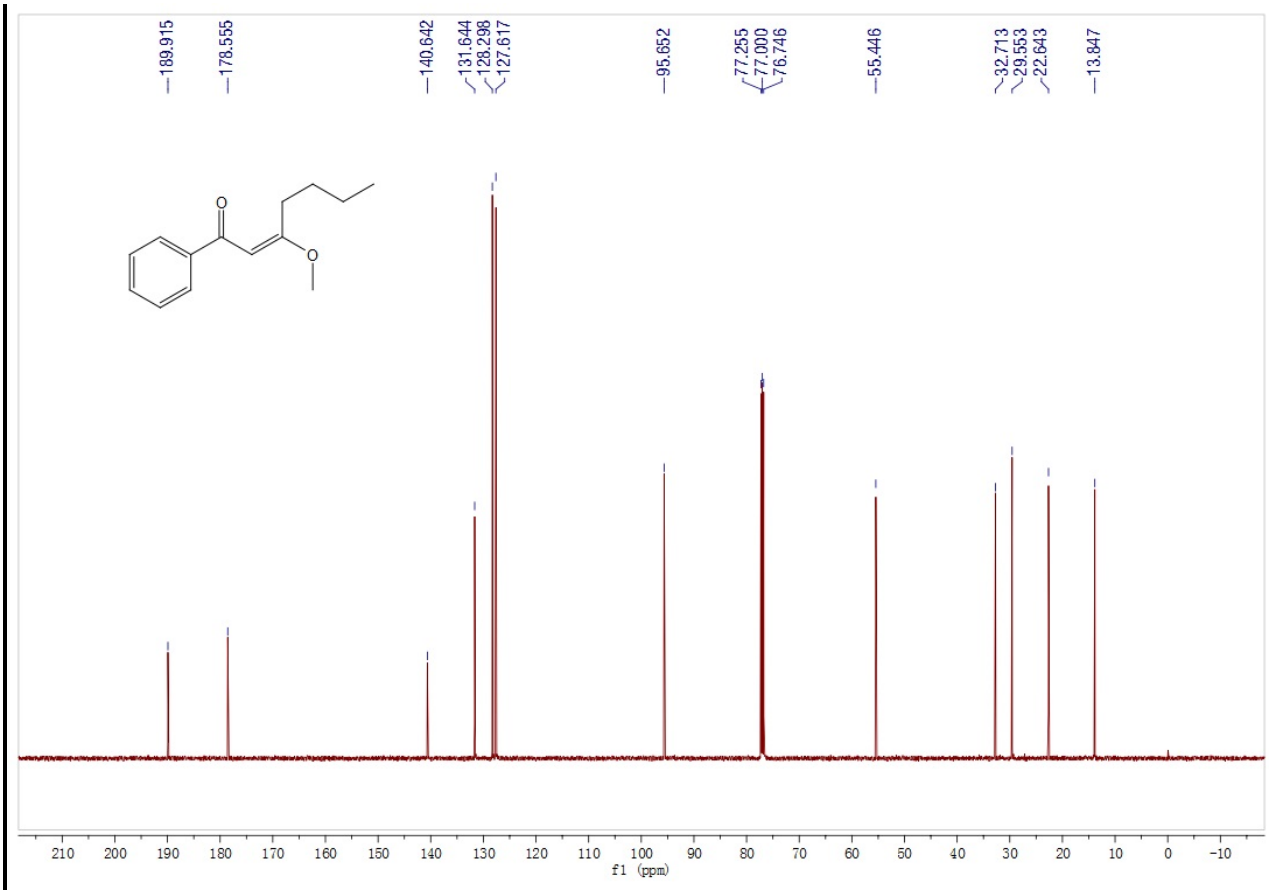

16.249
5.680
2.045
1.835
1.767
1.742
1.716
1.692
1.175
O
O
3.38
6.45
6.48
0.92
1.00
3.38
6.45
6.48
8.94
f1 (ppm)

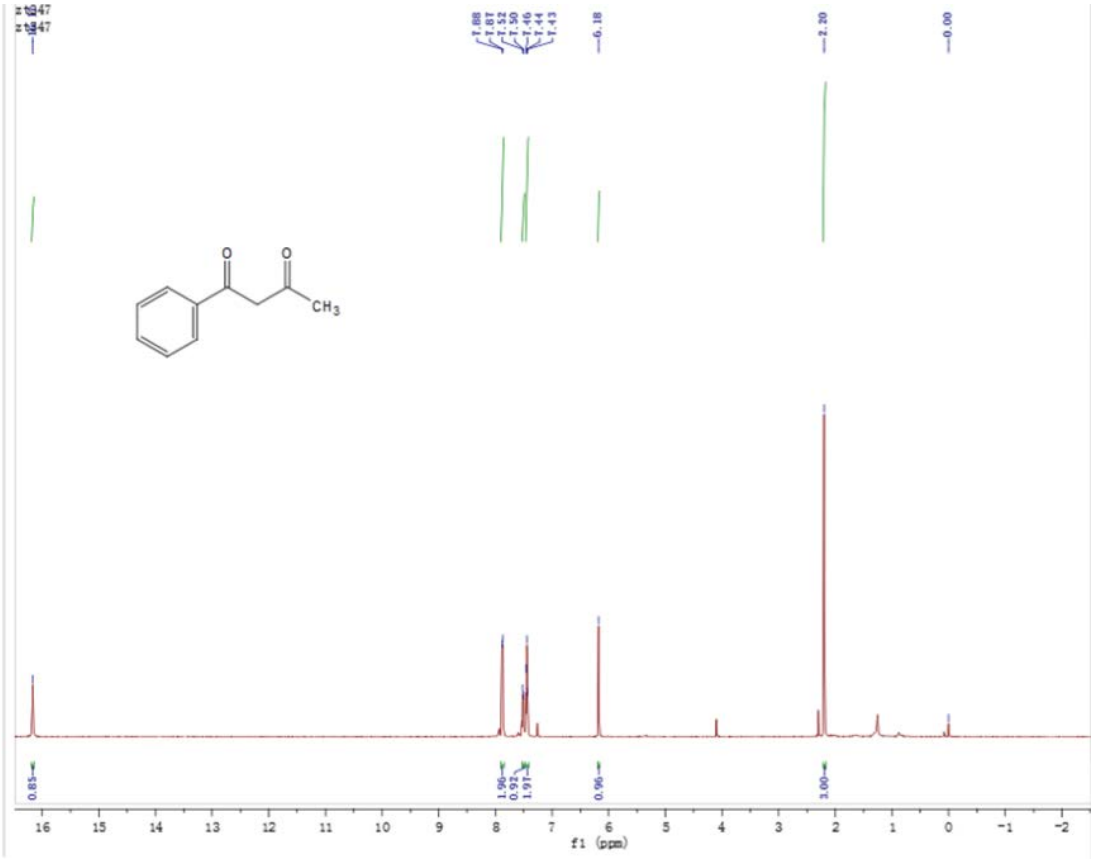

202.662
199.874
90.489
77.254
77.000
76.746
41.160
39.108
36.607
28.097
27.416
O
O
f1 (ppm)


16.162
5.731
1.179
O
O
0.92
1.00
18.42
f1 (ppm)

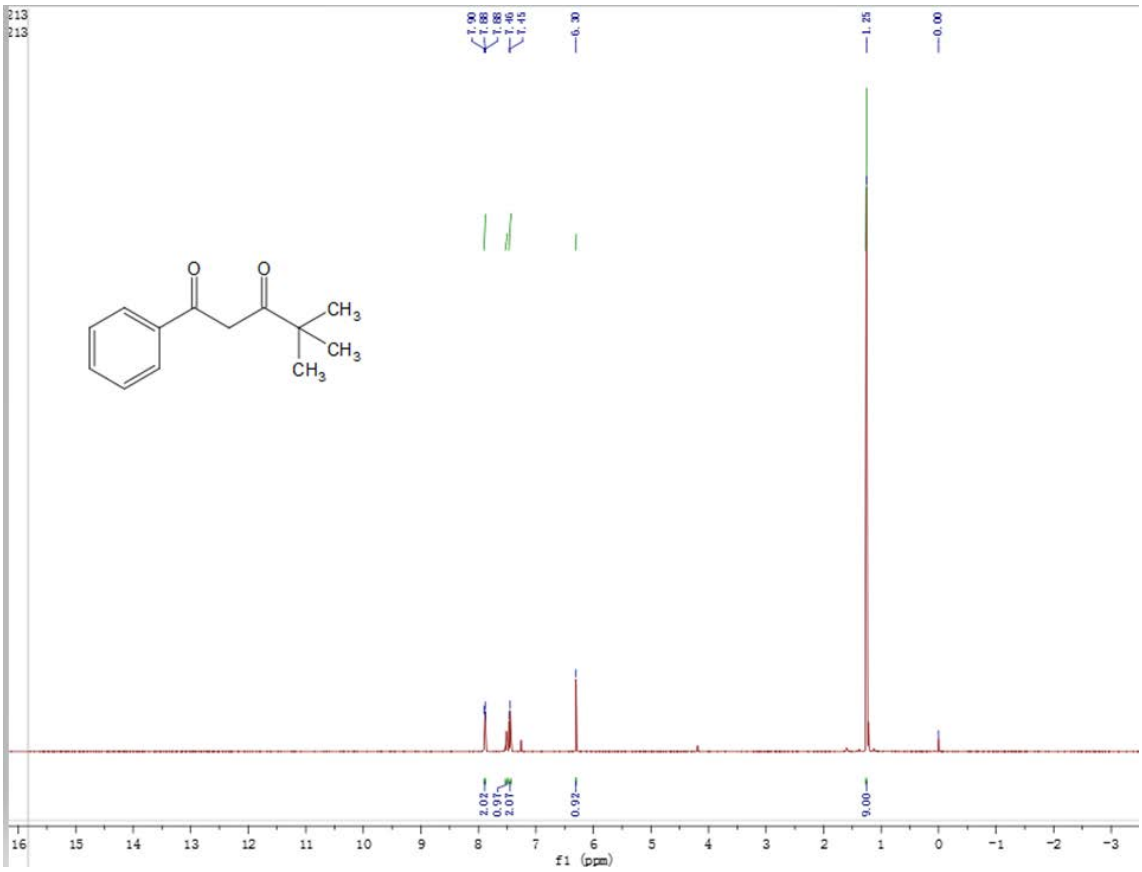

201.484
90.723
77.254
77.000
76.746
39.438
27.411
O
O
*
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.904
7.889
7.508
7.493
7.479
7.447
7.432
7.416
7.260
6.106
3.756
2.864
2.849
2.833
1.632
1.617
1.601
1.587
1.571
1.430
1.415
1.400
1.385
0.949
0.933
0.919
-0.001
O
n-Bu
Ph
OMe
2.00
2.04
0.99
1.03
3.16
2.07
2.10
2.02
3.11
8
6
4
2
0
PPM

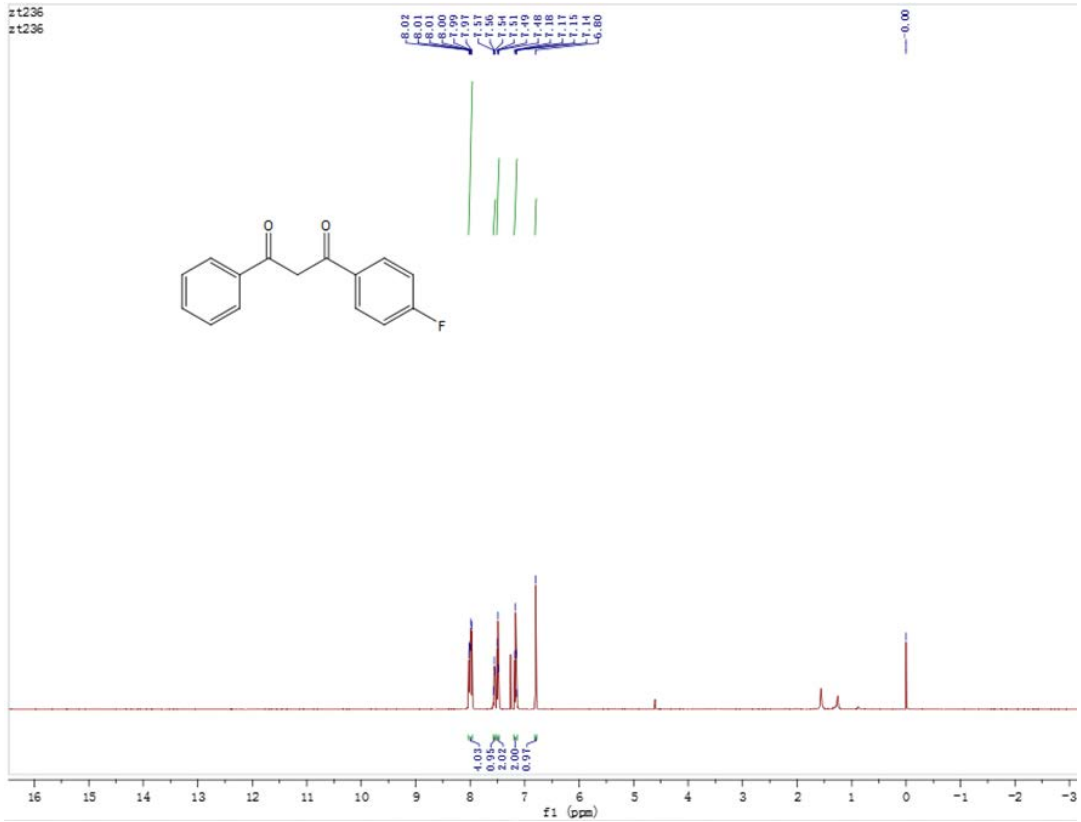




^{1}H NMR for **2m** prepared from 1-phenylbut-2-yn-1-one (Table 3)



^{1}H NMR for **2o** prepared from 4,4-dimethyl-1-phenylpent-2-yn-1-one (Table 3)



^{1}H NMR for **2u** prepared from 3-(4-fluorophenyl)-1-phenylprop-2-yn-1-one (Table 3)