Supporting Information

Synthesis of β-Nitro Ketone from Geminal Bromonitroalkane and Silyl Enol Ether by Visible Light Photoredox Catalysis

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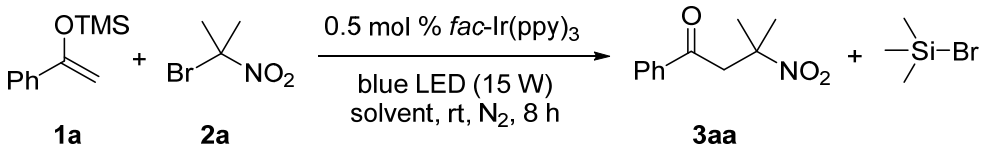
1. General information

All the solvents and reagents were obtained from commercial sources and used without purification unless stated otherwise. THF, Et_2O and 1,4-dioxane were distilled over CaH_2 and $LiAlH_4$ under N_2. Toluene, CH_2Cl_2 and CH_3CN were distilled over CaH_2 under N_2. Acetone, AcOEt, DMSO, DMA, DMF, DME, $CHCl_3$, $C_2H_5NO_2$, CH_3NO_2 and DBU were dried over activated 4A molecular sieves. All glassware was dried overnight at 100 °C prior to use. All visible light induced photocatalytic reactions were performed in a Schlenk tube under N_2 atmosphere. Thin-layer chromatography (TLC) was performed on silica gel plates (0.2–0.25 mm thickness). Visualization of TLC was achieved by the use of UV light (254 nm). Flash column chromatography was performed on a silica gel (Qingdao Haiyang, 200–300 mesh) column. ^1H and ^{13}C NMR spectra were recorded on a JEOL ECZ 400 MHz or 600 MHz spectrometer. The chemical shift (δ) values are given in ppm and are referenced to TMS or residual solvent peaks. Chemical shifts of ^{19}F NMR are referred to $CFCl_3$ (δ = 0). Infrared spectra were obtained on a Nicolet AVATAR 360 FT-IR spectrometer. Melting points were measured on a WRX-4 (Shanghai Yice) micro melting point apparatus. Mass spectra were obtained on an AB Sciex TripleTOF 5600+ mass spectrometer. X-ray diffraction experiment was performed on a Rigaku XtaLAB Synergy diffractometer using Cu Kα radiation.

2. Optimization of reaction conditions

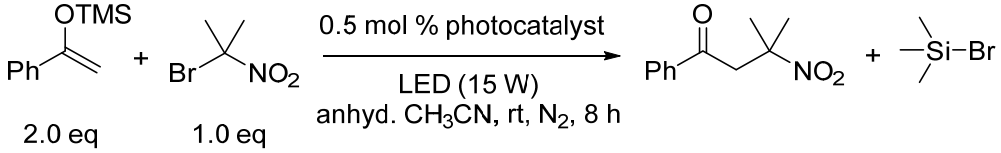
Table S1 Effect of solvent



1a **2a** **3aa**

Entry	**1a** equiv	Solvent	Yield (%)	Entry	**1a** equiv	Solvent	Yield (%)
1		CH_3CN	91	10		1,4-dioxane	0
2		DMSO	85	11	1.5	CH_2Cl_2	36
3		DMF	84	12		$CHCl_3$	36
4		DMA	71	13		toluene	35
5	1.5	acetone	46	14	2.0		98
6		AcOEt	38	15	1.5	CH_3CN	91
7		DME	35	16	1.0		35
8		THF	43	17	0.5		16
9		Et_2O	41				

Table S2 Effect of photocatalyst

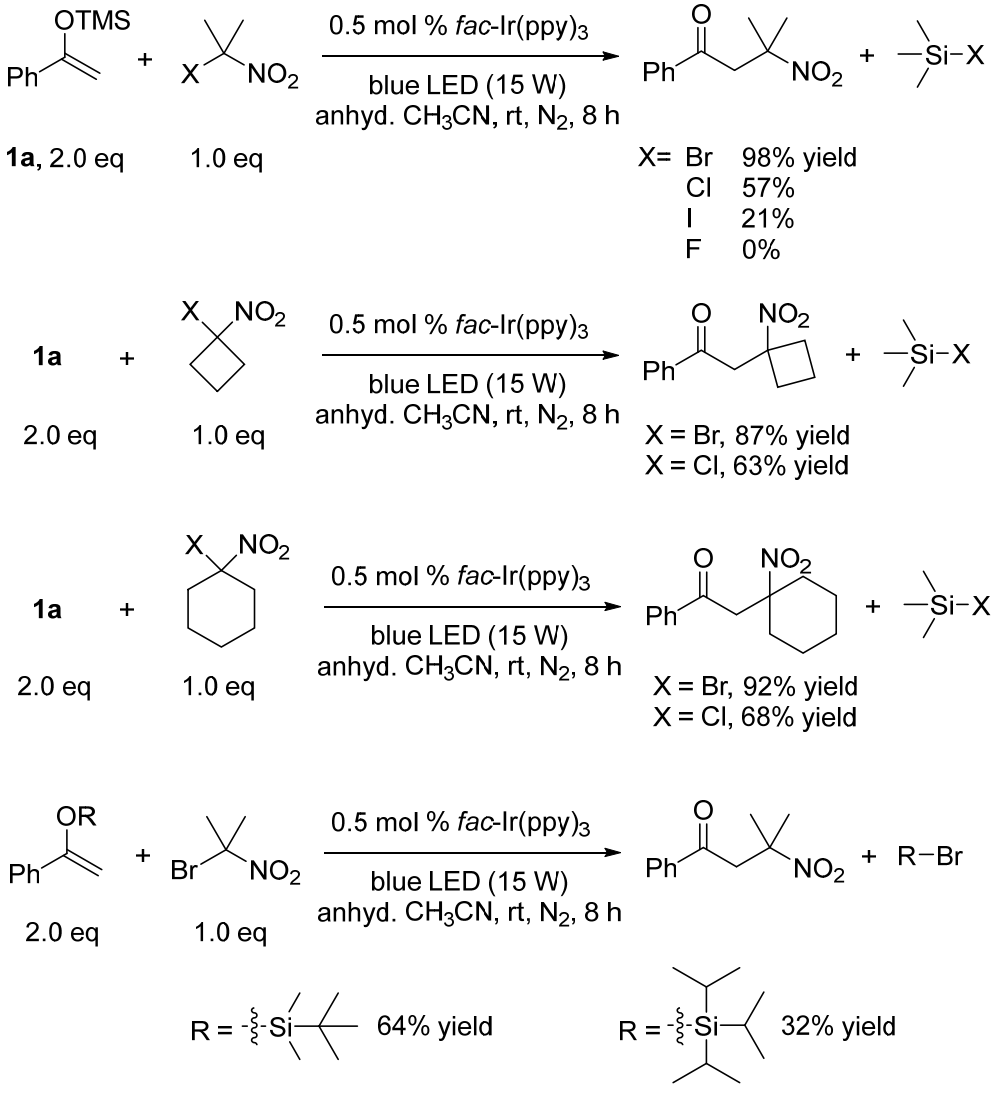


2.0 eq 1.0 eq

Entry	Photocatalyst	Visible light (15 W)	Yield (%)

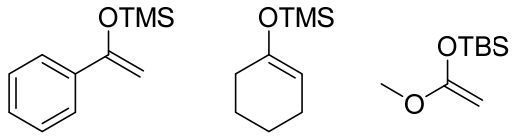
1	*fac*-Ir(ppy)$_3$		98
2	Ir(ppy)$_2$(dtbbpy)PF$_6$		71
3	[Ir(dF(CF$_3$)ppy)$_2$(dtbbpy)](PF$_6$)		trace
4	[Ru(bpy)$_2$]Cl$_2$·6H$_2$O	blue LED belt	32
5	[Ru(bpy)$_2$]Cl$_2$		81
6	[Ru(bpy)$_2$](PF$_6$)$_2$		78
7	NaI / Ph$_3$P (10 mol %)		18
8	Eosin Y, neutral (10 mol %)	green LED belt	trace
9	Eosin Y, disodium salt (10 mol %)		22

Figure S1 Effect of leaving group



3. Preparation of silyl enol ethers

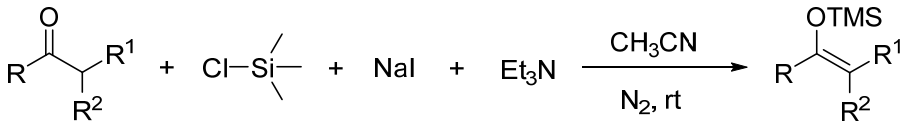
Silyl enol ethers from commercial soures:



1a **1y'** **1o''**

3.1 Preparation of silyl enol ethers

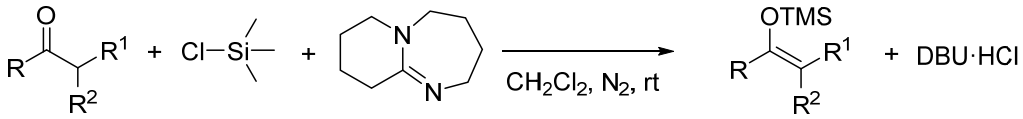
General procedure A[1,2]



1.0 eq 1.25 eq 1.25 eq 1.25 eq

Sodium iodide (1.70 g, 11.3 mmol) in acetonitrile (20 mL) was added at room temperature to a solution of ketone (9.08 mmol), triethylamine (1.90 mL, 11.3 mmol) and chlorotrimethylsilane (1.45 mL, 11.3 mmol) successively introduced to the reaction flask under N_2 atmosphere. This solution was vigorously stirred overnight and the reaction was monitored by TLC. After the reaction was completed, ice-water (50 mL) and cold pentane (50 mL) were successively added. After decantation, the aqueous layer was extracted with pentane (2 × 50 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under vacuum to give the crude trimethylsilyl enol ether. Repeatedly, high vacuum was shortly applied to remove the volatiles. After determining the purity by NMR analysis, the thus obtained silyl enol ether was used for photocatalytic coupling reaction.

General procedure B[3]



1.0 eq 1.2 eq 1.4 eq

A mixture of ketone (5.0 mmol), chlorotrimethylsilane (0.8 mL, 6.0 mmol) and 1,8-diazabicyclo [5.4.0] undec-7-ene (DBU) (1.0 mL, 7.0 mmol) in dichloromethane (5.0 mL) was stirred at room temperature for 12 h. Then the mixture was diluted with pentane (10.0 mL) and washed with $NaHCO_3$ solutions and dried over Na_2SO_4. Solvent was evaporated to furnish the corresponding silyl enol ether.

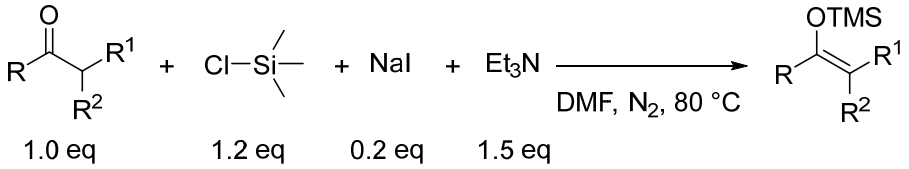
General procedure C[4]

1.0 eq 1.5 eq 2.0 eq

To a solution of LiHMDS (50.0 mL, 1.0 M in THF) was added ketone (25.0 mmol) at 0 °C. After stirring for 30 min at the same temperature, TMSCl (4.8 mL, 37.5 mmol) was added at 0 °C. The mixture was stirred for 45 min at the same temperature before saturated aqueous

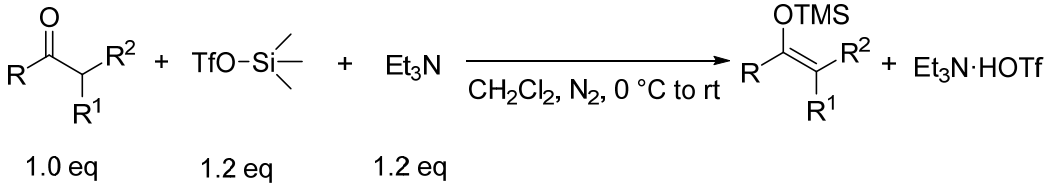
$NaHCO_3$ was added to quench the reaction. The aq. layer was extracted twice with hexanes (150 mL). The combined organic layers were washed with saturated $NaHCO_3$ solution and brine, dried over Na_2SO_4, and concentrated to give a yellow oil.

General procedure D[5]



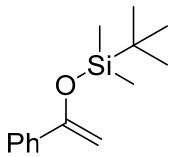
TMSCl (7.5 mL, 60.0 mmol) was added to a stirred solution of ketone (7.0 mL, 50.0 mmol), Et_3N (10.0 mL, 75.0 mmol) and NaI (1.5 g, 10 mmol) in DMF (30 mL). The solution was stirred at 80 °C under N_2 for 12 h. After cooling to room temperature, cold water (50 mL) was added and the solution was extracted with light petroleum (3 × 50 mL, b.p. 30–40 °C). The combined organic layers were washed with saturated $NaHCO_3$ (3 × 50 mL) and brine (3 × 50 mL) and evaporated under reduced pressure.

General procedure E[6]



Ketone (5.0 mmol) was added to a flame-dried round-bottom flask at 0 °C under N_2. Anhydrous dichloromethane (20 mL) was added to the flask, followed by triethylamine (0.85 mL, 6.0 mmol). Then TMSOTf (1.0 mL, 6.0 mmol) was added dropwise via syringe over 10 min. The reaction was stirred overnight at room temperature, which was monitored by TLC. Upon completion, the reaction was quenched with sat. aq. $NaHCO_3$ and diluted with DCM. The phases were separated and the aqueous layer was extracted with DCM (3 × 15 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated in vacuum.

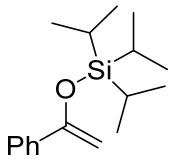
3.2 Physical data



***tert*-Butyldimethyl((1-phenylvinyl)oxy)silane**[7]

Following general procedure A, *t*-butyldimethylchlorosilane (TBSCl) was used instead of chlorotrimethylsilane (TMSCl).

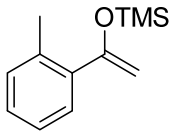
Yellow oil (1.65 g, 94% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.68 (m, 2H), 7.45 – 7.32 (m, 3H), 4.99 (d, *J* = 1.9 Hz, 1H), 4.53 (d, *J* = 1.9 Hz, 1H), 1.27 – 0.83 (m, 9H), 0.32 (d, *J* = 2.5 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 155.98, 137.80, 128.13, 128.02, 125.26, 90.86, 25.84, 18.31, −4.65.



Triisopropyl((1-phenylvinyl)oxy)silane[8]

Following general procedure E, TIPSOTf was used instead of TMSOTf.

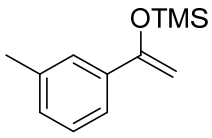
Yellow oil (1.5 g, 90% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.75 (dt, *J* = 7.3, 2.5 Hz, 2H), 7.42 – 7.33 (m, 3H), 4.95 (dd, *J* = 3.6, 1.9 Hz, 1H), 4.56 – 4.44 (m, 1H), 1.39 (dd, *J* = 7.6, 3.5 Hz, 3H), 1.25 – 1.21 (m, 18H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.16, 137.91, 128.06, 128.00, 125.28, 89.89, 18.08, 12.79.



Trimethyl((1-(*o*-tolyl)vinyl)oxy)silane (1b)[9]

Following general procedure A.

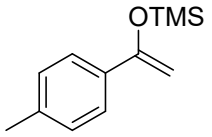
Yellow oil (1.4 g, 75% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 7.4 Hz, 1H), 7.26 – 7.05 (m, 3H), 4.59 (s, 1H), 4.45 (s, 1H), 2.44 (s, 3H), 0.24 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 157.80, 138.96, 135.79, 130.31, 128.67, 127.99, 125.35, 94.83, 20.43, 0.02.



Trimethyl((1-(*m*-tolyl)vinyl)oxy)silane (1c)

Following general procedure A.

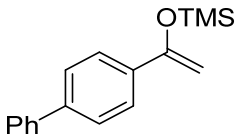
Yellow oil (1.7 g, 92% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 8.3 Hz, 2H), 7.32 (td, *J* = 7.6, 2.9 Hz, 1H), 7.20 (d, *J* = 6.8 Hz, 1H), 5.12 – 4.85 (m, 1H), 4.57 – 4.44 (m, 1H), 2.46 (d, *J* = 2.9 Hz, 3H), 0.39 (d, *J* = 4.0 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 155.79, 137.45, 128.94, 127.94, 125.84, 122.39, 90.88, 21.43, 0.22.



Trimethyl((1-(*p*-tolyl)vinyl)oxy)silane (1d)[10,11]

Following general procedure A.

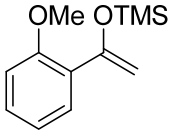
Yellow oil (1.8 g, 96% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 4.95 (d, *J* = 1.7 Hz, 1H), 4.46 (d, *J* = 1.9 Hz, 1H), 2.41 (s, 3H), 0.34 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 155.71, 137.97, 134.76, 128.73, 125.13, 90.31, 21.11, 0.05.



((1-([1,1'-Biphenyl]-4-yl)vinyl)oxy)trimethylsilane (1e)[11]

Following general procedure A.

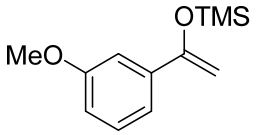
Yellow oil (1.9 g, 78% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.61 (m, 6H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.48 – 7.39 (m, 1H), 5.09 (d, *J* = 1.8 Hz, 1H), 4.59 (d, *J* = 1.8 Hz, 1H), 0.42 (d, *J* = 2.1 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.30, 140.88, 140.60, 136.41, 128.72, 127.28, 126.92, 126.72, 125.59, 91.07, 0.06.



((1-(2-Methoxyphenyl)vinyl)oxy)trimethylsilane (1f)[12]

Following general procedure A.

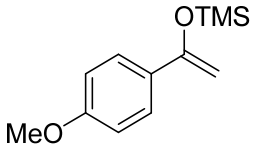
Yellow oil (1.76 g, 87% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.5 Hz, 1H), 7.31 (s, 1H), 7.00 (s, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 5.11 (s, 1H), 4.74 (s, 1H), 3.89 (s, 3H), 0.31 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 157.02, 153.00, 129.05, 128.97, 126.84, 120.06, 110.95, 96.46, 55.16, 0.04.



((1-(3-Methoxyphenyl)vinyl)oxy)trimethylsilane (1g)[10]

Following general procedure A.

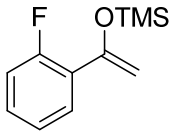
Yellow oil (1.5 g, 73% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 (s, 1H), 7.24 (d, *J* = 1.5 Hz, 1H), 7.20 (s, 1H), 6.87 (d, *J* = 7.6 Hz, 1H), 4.96 (d, *J* = 1.6 Hz, 1H), 4.48 (d, *J* = 1.6 Hz, 1H), 3.84 (s, 3H), 0.32 (d, *J* = 1.4 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.41, 155.36, 138.99, 128.96, 117.72, 113.53, 110.91, 91.32, 55.03, 0.03.



((1-(4-Methoxyphenyl)vinyl)oxy)trimethylsilane (1h)

Following general procedure A.

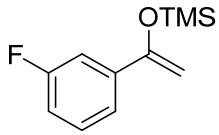
Yellow oil (1.5 g, 76% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.29 (m, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 4.86 (s, 1H), 4.40 (s, 1H), 3.83 (s, 3H), 0.33 (d, *J* = 2.5 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 159.69, 155.38, 130.16, 126.48, 113.33, 89.30, 55.09, 0.00.



((1-(2-Fluorophenyl)vinyl)oxy)trimethylsilane (1i)[13]

Following general procedure A.

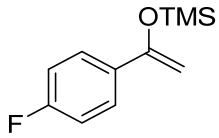
Yellow oil (1.6 g, 84% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.64 – 7.48 (m, 1H), 7.31 – 7.15 (m, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.05 (dd, *J* = 11.7, 8.2 Hz, 1H), 5.04 (s, 1H), 4.71 (s, 1H), 0.27 (s, 9H);^{13}C NMR (151 MHz, Chloroform-*d*) δ 160.93, 159.27, 150.41, 129.40, 128.80, 116.01, 97.22, 97.15, 0.22.



((1-(3-Fluorophenyl)vinyl)oxy)trimethylsilane (1j)[14]

Following general procedure A.

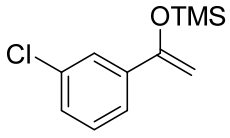
Yellow oil (1.4 g, 76% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.41 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.37 – 7.19 (m, 2H), 7.00 (td, *J* = 8.3, 2.7 Hz, 1H), 4.97 (d, *J* = 1.8 Hz, 1H), 4.51 (t, *J* = 1.8 Hz, 1H), 0.32 (d, *J* = 1.7 Hz, 9H);^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.66, 162.04, 154.47, 129.48, 120.78, 114.83, 112.25, 91.80, 0.13.



((1-(4-Fluorophenyl)vinyl)oxy)trimethylsilane (1k)[9]

Following general procedure A.

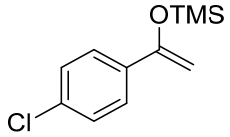
Yellow oil (1.5 g, 82% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 (dd, *J* = 7.7, 5.5 Hz, 2H), 7.05 – 6.99 (m, 2H), 4.86 (s, 1H), 4.43 (s, 1H), 0.30 (s, 9H);^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.04, 161.58, 154.79, 133.72, 133.68, 127.00, 126.92, 114.95, 114.7, 90.54, −0.01.



((1-(3-Chlorophenyl)vinyl)oxy)trimethylsilane (1l)[15]

Following general procedure A.

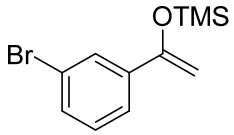
Yellow oil (1.4 g, 70% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (s, 1H), 7.49 (dt, *J* = 6.5, 1.8 Hz, 1H), 7.32 – 7.22 (m, 2H), 4.94 (d, *J* = 1.9 Hz, 1H), 4.48 (d, *J* = 1.9 Hz, 1H), 0.30 (d, *J* = 1.3 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.28, 139.39, 134.09, 129.24, 128.30, 125.32, 123.27, 91.84, −0.05.



((1-(4-Chlorophenyl)vinyl)oxy)trimethylsilane (1m)[9,10]

Following general procedure A.

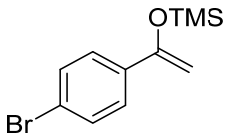
Yellow oil (1.2 g, 75% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (dd, *J* = 8.6, 1.6 Hz, 2H), 7.30 (dt, *J* = 9.4, 2.2 Hz, 2H), 4.91 (t, *J* = 1.7 Hz, 1H), 4.46 (d, *J* = 1.7 Hz, 1H), 0.39 – 0.23 (m, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.62, 136.00, 133.96, 128.19, 126.50, 91.34, 0.00.



((1-(3-Bromophenyl)vinyl)oxy)trimethylsilane (1n)[10]

Following general procedure A.

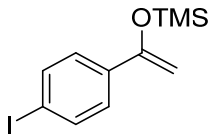
Yellow oil (2.0 g, 81% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 1.8 Hz, 1H), 7.52 (m, *J* = 7.9, 1.8, 1.0 Hz, 1H), 7.41 (m, *J* = 8.0, 2.1, 1.1 Hz, 1H), 7.19 (s, 1H), 4.92 (d, *J* = 2.0 Hz, 1H), 4.47 (d, *J* = 1.9 Hz, 1H), 0.29 (d, *J* = 1.1 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.16, 139.62, 131.02, 129.52, 128.26, 123.72, 122.34, 91.87, -0.28.



((1-(4-Bromophenyl)vinyl)oxy)trimethylsilane (1o)[9]

Following general procedure A.

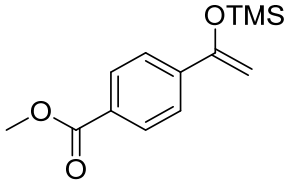
Yellow oil (2.1 g, 84% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.61 – 7.31 (m, 4H), 4.93 (d, *J* = 1.9 Hz, 1H), 4.48 (t, *J* = 1.8 Hz, 1H), 0.30 (d, *J* = 2.9 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 154.66, 136.45, 131.14, 126.79, 122.21, 91.41, 0.00.



((1-(4-Iodophenyl)vinyl)oxy)trimethylsilane (1p)[9]

Following general procedure A.

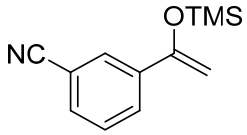
Yellow oil (2.5 g, 86% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 4.93 (d, *J* = 1.5 Hz, 1H), 4.46 (d, *J* = 1.6 Hz, 1H), 0.29 (d, *J* = 1.6 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.71, 137.12, 137.04, 126.98, 93.93, 91.54, 0.03.



Methyl 4-(1-((trimethylsilyl)oxy)vinyl)benzoate (1q)

Following general procedure A.

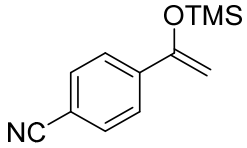
Yellow oil (1.9 g, 84% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 4.99 (s, 1H), 4.50 (s, 1H), 3.86 (s, 3H), 0.25 (d, *J* = 1.7 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.55, 154.60, 141.67, 129.53, 129.29, 124.90, 92.88, 51.78, −0.19.



3-(1-((Trimethylsilyl)oxy)vinyl)benzonitrile (1r)

Following general procedure A.

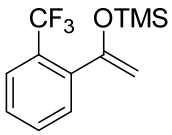
Yellow oil (1.3 g, 65% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 4.91 (s, 1H), 4.46 (s, 1H), 0.24 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 153.19, 138.46, 131.13, 129.01, 128.65, 128.43, 118.47, 112.07, 92.09, −0.36.



4-(1-((Trimethylsilyl)oxy)vinyl)benzonitrile (1s)[13]

Following general procedure A.

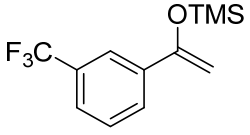
Yellow oil (1.5 g, 78% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.6 Hz, 2H), 7.59 (d, *J* = 8.9 Hz, 2H), 5.01 (d, *J* = 2.2 Hz, 1H), 4.56 (d, *J* = 2.2 Hz, 1H), 0.27 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 153.82, 141.73, 132.40, 131.86, 128.60, 125.59, 93.64, −0.12.



Trimethyl((1-(2-(trifluoromethyl)phenyl)vinyl)oxy)silane (1t)

Following general procedure A.

Dark oil (1.7 g, 72% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 7.9 Hz, 1H), 7.52 (dd, *J* = 16.2, 7.6 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 1H), 4.60 – 4.48 (m, 2H), 0.29 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 156.01, 138.53, 131.59, 130.77, 128.17, 126.41, 125.03, 123.21, 94.44, -0.30.

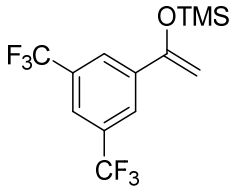


Trimethyl((1-(3-(trifluoromethyl)phenyl)vinyl)oxy)silane (1u)

Following general procedure A.

Yellow oil (1.5 g, 65% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 (s, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 6.7 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 5.00 (s, 1H), 4.54 (s, 1H), 0.30 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 154.26, 138.35,

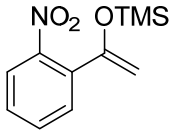
131.02, 130.71, 130.39, 130.07, 128.53, 128.32, 125.51, 124.74, 124.70, 122.80, 121.96, 121.92, 92.05, -0.30.



((1-(3,5-Bis(trifluoromethyl)phenyl)vinyl)oxy)trimethylsilane (1v)

Following general procedure A.

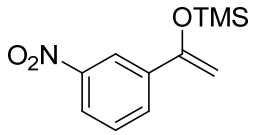
Dark oil (2.3 g, 76% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 (s, 2H), 7.79 (s, 1H), 5.06 (d, *J* = 2.5 Hz, 1H), 4.62 (d, *J* = 2.5 Hz, 1H), 0.31 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.10, 139.80, 131.67 (q, *J* = 33.3 Hz), 127.53, 125.23,124.82, 122.11, 121.72, 121.65, 119.40, 93.21, -0.18.



Trimethyl((1-(2-nitrophenyl)vinyl)oxy)silane (1w)

Following general procedure A.

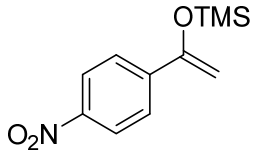
Dark oil (1.2 g, 57% yield); R_f = 0.65 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 – 7.55 (m, 1H), 7.55 – 7.44 (m, 2H), 7.46 – 7.32 (m, 1H), 4.66 (d, *J* = 2.2 Hz, 1H), 4.49 (d, *J* = 2.2 Hz, 1H), 0.21 (d, *J* = 1.1 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ153.70, 133.21, 131.60, 129.98, 128.79, 123.38, 93.85, 7.06, -0.82.



Trimethyl((1-(3-nitrophenyl)vinyl)oxy)silane (1x)[10]

Following general procedure A.

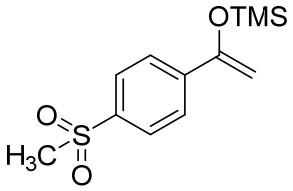
Yellow oil (1.5 g, 72% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 8.13 – 8.08 (m, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 5.02 (d, *J* = 2.4 Hz, 1H), 4.55 (d, *J* = 2.4 Hz, 1H), 0.29 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 153.34, 148.28, 139.29, 129.81, 128.97, 122.72, 120.01, 92.71, −0.11.



Trimethyl((1-(4-nitrophenyl)vinyl)oxy)silane (1y)[16]

Following general procedure A.

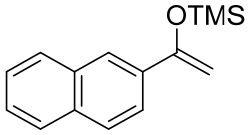
Yellow oil (1.74 g, 81% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 5.07 (d, *J* = 2.3 Hz, 1H), 4.61 (d, *J* = 2.3 Hz, 1H), 0.28 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.57, 147.36, 143.57, 125.73, 123.28, 94.34, -0.81.



Trimethyl((1-(4-(methylsulfonyl)phenyl)vinyl)oxy)silane (1z)[11]

Following general procedure A.

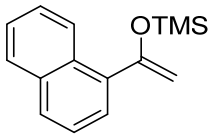
Yellow oil (2.1 g, 87% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.6 Hz, 2H), 7.71 (d, *J* = 8.6 Hz, 2H), 5.00 (d, *J* = 2.3 Hz, 1H), 4.53 (s, 1H), 2.99 (s, 3H), 0.22 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.65, 142.52, 139.57, 127.04, 125.70, 93.74, 44.22, −0.23.



Trimethyl((1-(naphthalen-2-yl)vinyl)oxy)silane (1a′)[9]

Following general procedure A.

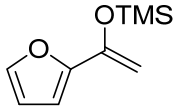
Yellow oil (1.6 g, 71% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.16 (s, 1H), 7.96 – 7.75 (m, 4H), 7.53 (s, 2H), 5.18 – 5.14 (m, 1H), 4.66 – 4.63 (m, 1H), 0.41 (d, *J* = 4.0 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 155.59, 134.76, 133.26, 133.18, 128.48, 127.61, 127.50, 126.09, 126.07, 124.24, 123.33, 91.88, 0.11.



Trimethyl((1-(naphthalen-1-yl)vinyl)oxy)silane (1b′)[9]

Following general procedure A.

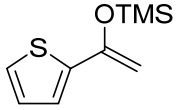
Yellow oil (2.1 g, 98% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.49 (s, 1H), 7.95 – 7.89 (m, 2H), 7.71 – 7.49 (m, 4H), 4.97 – 4.70 (m, 2H), 0.29 (dd, *J* = 8.8, 4.5 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 156.99, 137.30, 133.66, 131.00, 128.63, 128.12, 126.24, 126.13, 125.92, 125.68, 125.00, 96.62, 0.12.



((1-(Furan-2-yl)vinyl)oxy)trimethylsilane (1c′)[10]

Following general procedure A.

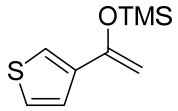
Yellow oil (1.4 g, 84% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 (s, 1H), 6.45 – 6.33 (m, 2H), 4.91 (d, *J* = 1.5 Hz, 1H), 4.39 (d, *J* = 1.6 Hz, 1H), 0.28 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.14, 147.55, 142.29, 111.03, 106.95, 90.27, −0.33.



Trimethyl((1-(thiophen-2-yl)vinyl)oxy)silane (1d′)[10]

Following general procedure A.

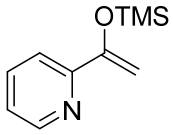
Yellow oil (1.3 g, 73% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.19 (t, *J* = 4.5 Hz, 2H), 6.97 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.84 (d, *J* = 1.9 Hz, 1H), 4.35 (d, *J* = 1.8 Hz, 1H), 0.31 (s, 9H);^{13}C NMR (151 MHz, Chloroform-*d*) δ 150.85, 142.61, 127.18, 124.92, 123.80, 90.15, 0.002.



Trimethyl((1-(thiophen-3-yl)vinyl)oxy)silane (1e′)

Following general procedure A.

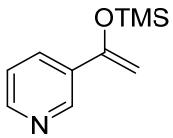
Yellow oil (1.5 g, 82% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.41 – 7.40 (m, 1H), 7.26 – 7.23 (m, 2H), 4.80 (s, 1H), 4.42 (d, *J* = 0.9 Hz, 1H), 0.31 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 152.12, 140.37, 126.30, 125.21, 121.75, 90.76, 0.04.



2-(1-((Trimethylsilyl)oxy)vinyl)pyridine (1f′)[10]

Following general procedure A.

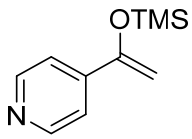
Yellow oil (1.2 g, 71% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 (s, 1H), 7.60 (d, *J* = 11.3 Hz, 2H), 7.09 (t, *J* = 4.4 Hz, 1H), 5.61 (s, 1H), 4.51 (d, *J* = 2.9 Hz, 1H), 0.23 (d, *J* = 3.4 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.79, 136.61,136.33, 126.88, 122.67, 118.86, 93.27, −0.14.



3-(1-((Trimethylsilyl)oxy)vinyl)pyridine (1g′)[17]

Following general procedure A.

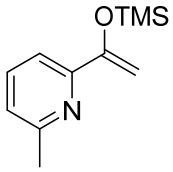
Brown oil (1.2 g, 72% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 1.8 Hz, 1H), 7.63 (t, *J* = 6.2 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.16 – 7.07 (m, 1H), 5.64 (s, 1H), 4.54 (s, 1H), 0.32 – 0.22 (m, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 154.58, 154.27, 148.78, 136.38, 122.71, 118.92, 93.34, -0.08.



4-(1-((Trimethylsilyl)oxy)vinyl)pyridine (1h′)

Following general procedure A.

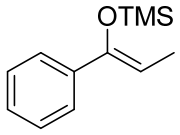
Yellow oil (1.3 g, 76% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.51 – 8.45 (m, 2H), 7.39 – 7.32 (m, 2H), 5.05 – 4.99 (m, 1H), 4.54 – 4.48 (m, 1H), 0.20 (d, *J* = 2.8 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.13, 150.76, 149.67, 144.56, 120.98, 93.79, −0.25.



2-Methyl-6-(1-((trimethylsilyl)oxy)vinyl)pyridine (1i′)

Following general procedure A.

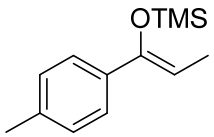
Yellow oil (1.5 g, 79% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.50 (s, 1H), 7.36 (d, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 5.65 (s, 1H), 4.51 (s, 1H), 2.49 (s, 3H), 0.24 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 157.41, 154.50, 153.88, 136.45, 122.35, 115.87, 93.19, 24.46, -0.09.



(Z)-Trimethyl((1-phenylprop-1-en-1-yl)oxy)silane (1j′)[10]

Following general procedure B.

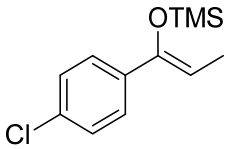
Yellow oil (1.6 g, 87% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.64 – 7.49 (m, 2H), 7.38 – 7.32 (m, 2H), 7.31 – 7.26 (m, 1H), 5.41 (dd, *J* = 6.9, 2.9 Hz, 1H), 1.83 (dd, *J* = 6.3, 2.8 Hz, 3H), 0.24 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 149.90, 139.20, 127.96, 125.16, 105.19, 29.72, 11.61, 0.51.



(Z)-Trimethyl((1-(p-tolyl)prop-1-en-1-yl)oxy)silane (1k′)

Following general procedure B.

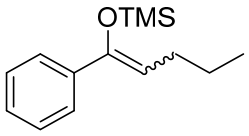
Yellow oil (1.7 g, 86% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.44 – 7.41 (m, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 5.36 (d, *J* = 6.8 Hz, 1H), 2.39 (s, 3H), 1.81 (dd, *J* = 6.9, 2.2 Hz, 3H), 0.22 (d, *J* = 2.3 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.85, 136.91, 136.38, 128.67, 125.08, 104.38, 21.05, 11.58, 0.53.



(Z)-((1-(4-Chlorophenyl)prop-1-en-1-yl)oxy)trimethylsilane (1l′)

Following general procedure B.

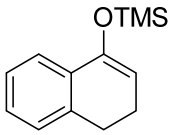
Yellow oil (1.8 g, 83% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 8.8 Hz, 2H), 7.27 (d, *J* = 8.7 Hz, 2H), 5.33 (d, *J* = 6.9 Hz, 1H), 1.75 (d, *J* = 6.9 Hz, 3H), 0.16 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 148.86, 137.70, 132.91, 128.14, 126.37, 105.83, 11.63, 0.48.



(Z)-Trimethyl((1-phenylpent-1-en-1-yl)oxy)silane (1m′)[18,19]

Following general procedure E.

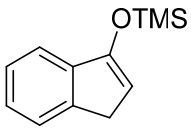
Brown oil (982 mg, 84% yield); R_f = 0.9 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.0 Hz, 2H), 7.34 (d, *J* = 7.8 Hz, 3H), 5.34 (s, 1H), 2.27 (d, *J* = 7.6 Hz, 2H), 1.54 (d, *J* = 7.5 Hz, 2H), 1.05 (s, 3H), 0.24 – 0.18 (m, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.97, 139.29, 127.97, 127.27, 125.30, 111.35, 28.30, 22.93, 14.00, 0.51.



((3,4-Dihydronaphthalen-1-yl)oxy)trimethylsilane (1n′)

Following general procedure A.

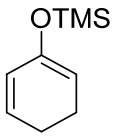
Yellow oil (1.7 g, 85% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (t, *J* = 6.5 Hz, 1H), 7.42 – 7.23 (m, 3H), 5.39 (q, *J* = 5.0 Hz, 1H), 2.98 – 2.89 (m, 2H), 2.55 – 2.44 (m, 2H), 0.51 – 0.42 (m, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.03, 136.85, 133.40, 127.17, 126.83, 126.05, 121.71, 104.98, 28.07, 22.07, 0.07.



((1*H*-Inden-3-yl)oxy)trimethylsilane (1o′)[10]

Following general procedure A.

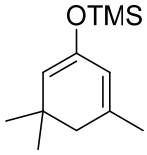
Yellow oil (1.3 g, 69% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.39 (m, 3H), 7.32 (t, *J* = 7.4 Hz, 1H), 5.55 (t, *J* = 2.5 Hz, 1H), 3.38 (d, *J* = 2.4 Hz, 2H), 0.44 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.47, 142.61, 141.73, 125.93, 125.05, 123.66, 118.05, 105.99, 33.84, −0.09.



(Cyclohexa-1,5-dien-1-yloxy)trimethylsilane (1p′)[4]

Following general procedure C.

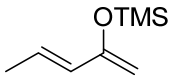
Yellow oil (3.2 g, 78% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.87 – 5.82 (m, 1H), 5.71 – 5.65 (m, 1H), 4.86 (s, 1H), 2.14 (s, 4H), 0.24(s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 128.79, 126.39, 102.32, 35.40, 31.86, 26.88, 22.66, 22.61, 22.55, 21.69, 14.05, 1.87.



Trimethyl((3,3,5-trimethylcyclohexa-1,5-dien-1-yl)oxy)silane (1q′)[20]

Following general procedure C.

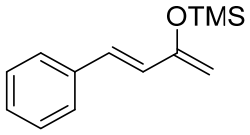
Yellow oil (4.3 g, 82% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.41 (s, 1H), 4.51 (s, 1H), 1.91 (s, 2H), 1.74 (s, 3H), 0.96 (s, 6H), 0.16 (d, *J* = 3.7 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.21, 119.88, 111.60, 43.99, 32.27, 28.88, 23.14, 5.41, 2.43.



(*E*)-Trimethyl(penta-1,3-dien-2-yloxy)silane (1r′)[21]

Following general procedure A.

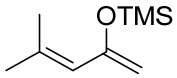
Yellow oil (1.2 g, 84% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.09 – 5.77 (m, 2H), 4.20 (s, 2H), 1.76 (d, *J* = 6.2 Hz, 3H), 0.23 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.88, 129.00, 126.41, 93.63, 17.44, −0.05.



(*E*)-Trimethyl((4-phenylbuta-1,3-dien-2-yl)oxy)silane (1s′)

Following general procedure B.

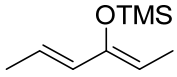
Yellow oil (1.0 g, 87% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.60 – 7.47 (m, 2H), 7.46 – 7.39 (m, 2H), 7.34 (d, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 3.8 Hz, 1H), 6.73 (d, *J* = 15.7 Hz, 1H), 4.60 (d, *J* = 17.6 Hz, 2H), 0.44 (d, *J* = 2.2 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.02, 136.75, 129.20, 128.54, 127.62, 126.74, 126.35, 96.90, 0.04.



Trimethyl((4-methylpenta-1,3-dien-2-yl)oxy)silane (1t′)[21]

Following general procedure B.

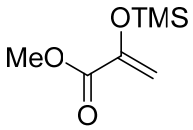
Yellow oil (0.8 g, 89% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.59 (s, 1H), 4.21 (d, *J* = 56.0 Hz, 2H), 1.92 (s, 3H), 1.77 (s, 3H), 0.23 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ155.56, 122.68, 111.54,110.20, 94.56, 27.11, 19.34, 0.27.



(((2*Z*,4*E*)-Hexa-2,4-dien-3-yl)oxy)trimethylsilane (1u′)

Following general procedure A.

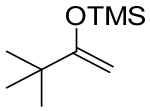
Yellow oil (1.4 g, 88% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.86 (dd, *J* = 15.3, 1.7 Hz, 1H), 5.73 (d, *J* = 6.9 Hz, 1H), 4.72 (q, *J* = 6.9 Hz, 1H), 1.74 (d, *J* = 6.8 Hz, 3H), 1.61 (d, *J* = 7.0 Hz, 3H), 0.20 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 149.36, 129.88, 123.06, 107.10, 17.52, 11.43, 0.36.



Methyl 2-((trimethylsilyl)oxy)acrylate (1v′)[22,23]

Following general procedure D, the solvent changed from DMF to CH_2Cl_2.

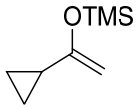
Reddish oil (3.5 g, 80% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.44 (s, 1H), 4.82 (s, 1H), 3.71 (s, 3H), 0.18 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.72, 146.89, 103.84, 51.95, −0.22.



3,3-Dimethylbut-1-en-2-ol (1w′)[9]

Following general procedure A.

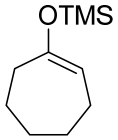
Yellow oil (0.7 g, 80% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.09 (d, *J* = 1.4 Hz, 1H), 3.93 (d, *J* = 1.4 Hz, 1H), 1.06 (s, 9H), 0.22 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.10, 85.73, 36.35, 28.03, 0.09.



1-Cyclopropylethen-1-ol (1x′)[24,25]

Following general procedure E.

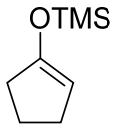
Yellow oil (344 mg, 82% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.11 (d, *J* = 0.8 Hz, 1H), 3.98 (s, 1H), 1.48 – 1.32 (m, 1H), 0.55(m, 4H), 0.17 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 159.03, 87.58, 15.46, 4.37, −0.04.



(Cyclohept-1-en-1-yloxy)trimethylsilane (1z′)[6]

Following general procedure A.

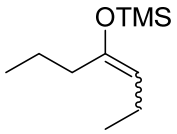
Yellow oil (1.5 g, 91% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.01 (s, 1H), 2.27 – 2.15 (m, 2H), 1.98 (dt, *J* = 9.3, 4.6 Hz, 2H), 1.72 – 1.52 (m, 6H), 0.16 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.02, 108.58, 35.52, 31.59, 27.82, 25.36, 25.23, 0.18.



(Cyclopent-1-en-1-yloxy)trimethylsilane (1a′′)[26,27]

Following general procedure A.

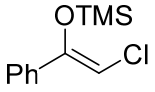
Yellow oil (1.2 g, 85% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.64 – 4.62 (m, 1H), 2.30 – 2.25 (m, 4H), 1.89 – 1.83 (m, 2H), 0.22 (s, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.97, 102.02, 33.47, 28.70, 21.28, -0.06.



(Hept-3-en-4-yloxy)trimethylsilane (1b′′)[28]

Following general procedure A.

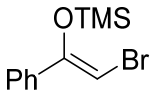
Yellow oil (1.4 g, 84% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.43 (s, 1H), 1.96 (s, 4H), 1.48 (s, 2H), 0.90 (d, *J* = 13.2 Hz, 6H), 0.17 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ149.41, 110.39, 38.67, 20.15, 18.64, 14.45, 13.62, 0.51.



(*Z*)-((2-Chloro-1-phenylvinyl)oxy)trimethylsilane (1c′′)[10]

Following general procedure E.

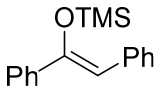
Yellow oil (960 mg, 85% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.47 (m, 2H), 7.35 (dd, *J* = 5.9, 2.2 Hz, 3H), 5.99 (d, *J* = 2.6 Hz, 1H), 0.27 (d, *J* = 3.6 Hz, 9H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.39, 136.34, 128.82, 128.60, 128.45, 128.33, 125.28, 99.92, −0.55.



***(Z)*-((2-Bromo-1-phenylvinyl)oxy)trimethylsilane (1d′′)**[10]

Following general procedure E.

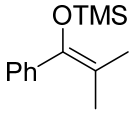
Dark oil (1.2 g, 87% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.45 (m, 2H), 7.38 – 7.32 (m, 3H), 5.97 (s, 1H), 0.26 (d, *J* = 1.2 Hz, 9H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.45, 136.78, 128.67, 128.31, 125.64, 88.28, −0.64.



(*Z*)-((1,2-Diphenylvinyl)oxy)trimethylsilane (1e′′)[29,5]

Following general procedure D.

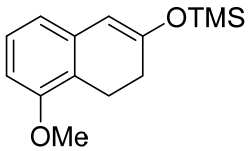
Dark oil (4.69 g, 70% yield); R_f = 0.6 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 – 7.65 (m, 4H), 7.46 – 7.35 (m, 5H), 7.26 (s, 1H), 6.24 (s, 1H), 0.15 (d, *J* = 1.8 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 150.88, 139.66, 136.62, 128.61, 128.11, 128.06, 128.00, 126.14, 126.04, 110.53, 0.65.



Trimethyl((2-methyl-1-phenylprop-1-en-1-yl)oxy)silane (1f′′)[6,28]

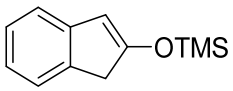
Following general procedure A.

Yellow oil (1.2 g, 65% yield); R_f = 0.75 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.34 – 7.28 (m, 4H), 7.22 (t, *J* = 7.0 Hz, 1H), 1.80 (s, 3H), 1.69 (s, 3H), -0.02 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 143.48, 138.97, 129.07, 127.56, 127.00, 112.71, 18.14, 19.63, -0.20.



((5-Methoxy-3,4-dihydronaphthalen-2-yl)oxy)trimethylsilane (1g′′)[30]

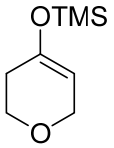
^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.86 – 6.52 (m, 3H), 5.71 (s, 1H),3.83 (s, 3H) 2.58 – 2.50 (m, 2H), 2.38 (t, *J* = 8.5 Hz, 2H), 0.32 (dd, *J* = 2.1, 1.2 Hz, 9H).



((1*H*-Inden-2-yl)oxy)trimethylsilane (1h′′)[10]

Following general procedure C.

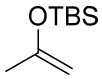
Dark oil (3.8 g, 75% yield); R_f = 0.8 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 (s, 1H), 7.14 – 7.13 (m, 1H), 5.78 (s, 1H), 3.30 (s, 2H), 0.32 (s, 9H).



((3,6-Dihydro-2*H*-pyran-4-yl)oxy)trimethylsilane (1i′′)[10]

Following general procedure A.

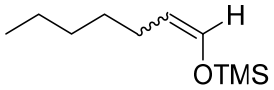
Yellow oil (1.4 g, 89% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.74 (s, 1H), 4.05 (d, *J* = 1.8 Hz, 2H), 3.72 (d, *J* = 5.3 Hz, 2H), 2.04 (s, 2H), 0.13 (d, *J* = 4.8 Hz, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.61, 136.82, 102.02, 64.42, 30.28, 0.06.



***tert*-Butyldimethyl(prop-1-en-2-yloxy)silane (1j′′)**[31,32]

Following general procedure E, TBSOTf was used instead of TMSOTf.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.04 (s, 2H), 1.77 (s, 3H), 0.93 (s, 9H), 0.16 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 156.19, 91.20, 25.63, 22.67, 18.02, −4.68.

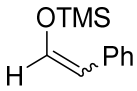


Z:*E* = 75:25

(Hept-1-en-1-yloxy)trimethylsilane (1k′′)[33]

Following general procedure A.

Yellow oil (1.6 g, 95% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.18 (d, *J* = 12.0 Hz, 0.26H), 6.13 (d, *J* = 6.6 Hz, 0.84H), 4.99 (s, 0.32H), 4.48 (d, *J* = 6.1 Hz, 0.88H), 2.06 (d, *J* = 7.3 Hz, 2H), 1.87 (d, *J* = 7.2 Hz, 0.64H), 1.29 (s, 11H), 0.88 (d, *J* = 7.2 Hz, 5H), 0.17 (d, *J* = 2.4 Hz, 11H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.25, 137.56, 112.15, 111.73, 31.51, 31.24, 30.12, 29.39, 27.31, 23.54, 22.60, 22.53, 22.49, 14.04.



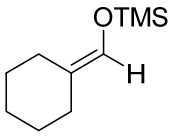
Z:*E* = 2:1

(*E*)-Trimethyl(styryloxy)silane (1l′′)[34]

Following general procedure D, THF was used instead of DMF as the solvent.

Yellow oil (1.7 g, 89% yield); R_f = 0.9 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (s, 2H), 7.56 – 7.11 (m, 11H), 6.26 (ddd, *J* = 12.3, 9.7, 4.8 Hz, 0.6H), 5.58 – 5.49 (m,

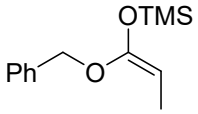
1H), 0.53 – 0.40 (m, 16H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.35, 139.55, 136.21, 136.07, 128.37, 128.10, 127.96, 125.69, 125.60, 125.04, 113.16, 109.47, −0.56.



(1-Cyclohexylideneethoxy)trimethylsilane (1m′′)[35]

Following general procedure A.

Yellow oil (1.5 g, 83% yield); R_f = 0.7 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.97 (s, 1H), 2.16 (t, *J* = 6.0 Hz, 2H), 1.92 (t, *J* = 5.9 Hz, 2H), 1.52 – 1.44 (m, 6H), 0.14 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 130.04, 122.24, 30.51, 28.41, 26.97, 26.90, 25.27, −0.75.



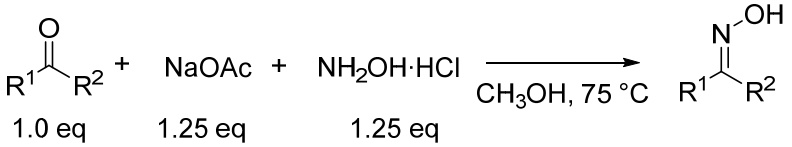
(*E*)-((1-(Benzyloxy)prop-1-en-1-yl)oxy)trimethylsilane (1n′′)[36]

Following general procedure C, the temperature was controlled at −78 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.43 – 7.32 (m, 5H), 4.86 (s, 2H), 3.75 (d, *J* = 6.6 Hz, 1H), 1.53 (dd, *J* = 6.6, 1.0 Hz, 3H), 0.28 – 0.20 (m, 9H).

4. Preparation of *gem*-bromonitroalkanes

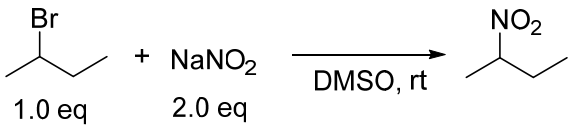
4.1 Preparation of oximes[37,38]



In a round-bottom flask, ketone (50 mmol) was dissolved in CH_3OH (100 mL) under N_2 atmosphere, then sodium acetate (5.12 g, 62.5 mmol) and hydroxylamine hydrochloride (4.35 g, 62.5 mmol) were added. The solution was heated at 75 °C to reflux and stirred overnight. After cooling to room temperature, methanol was evaporated and H_2O (50 mL) was added followed by AcOEt (100 mL). Then the organic layer was washed with saturated brine (50 mL), dried over Na_2SO_4, and concentrated to give a white solid.

4.2 Preparation of nitro compounds

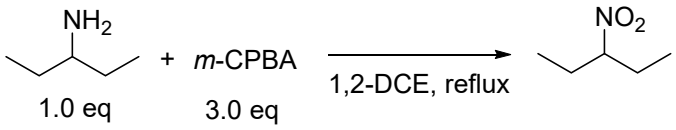
2-Nitrobutane



2-Bromobutane (5.5 mL, 40 mmol) was added to a stirred mixture of $NaNO_2$ (5.5 g, 80 mmol) in DMSO (100 mL). After stirring for 6 h, the reaction mixture was poured into ice-water (60 mL) and layered with hexanes (100 mL). The aq. phase was extracted with hexanes. Then the organic layers were washed with water (2 × 50 mL), dried over anhydrous Na_2SO_4, filtered, concentrated at 30 °C under vacuum (20 Torr) to afford the product as a blue oil (2.5 g, 61%

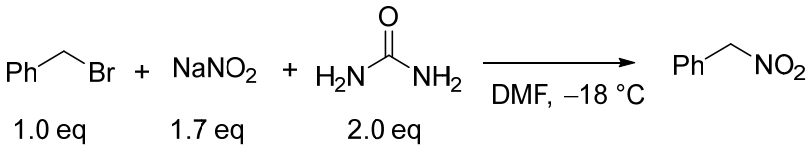
yield).

3-Nitropentane



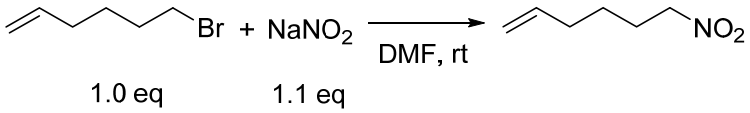
m-Chloroperbenzoic acid (17.2 g, 100.0 mmol) was dissolved in 1,2-dichloroethane (DCE) (20 mL) in a three-necked round-bottom flask equipped with a condenser and a pressure-equalizing dropping funnel. 3-Pentylamine (2.2 mL, 20 mmol) in 1,2-DCE (40 mL) was added dropwise to the refluxing peracid solution. Reflux was continued for 3 h after the addition and then the reaction mixture was cooled, filtered, washed with 1 M NaOH three times, dried over Na_2SO_4, and evaporated at 30 °C under reduced pressure (20 Torr). The crude nitro compound was purified by silica gel chromatography (light petroleum) to afford the product (1.47 g, 63% yield).

Phenyl nitromethane[39]



Benzyl bromide (5.10 g, 30.0 mmol) was added to a stirred mixture of $NaNO_2$ (3.50 g, 50.0 mmol) and urea (3.60 g, 60.0 mmol) in DMF (60 mL) at −18 °C. After stirring at −18 °C for 6 h, the reaction mixture was poured into ice-water (60 mL) and layered with hexanes (100 mL). The aqueous phase was extracted with diethyl ether (3 × 60 mL). Then the extracts were washed with 10% aqueous sodium thiosulfate solution (2 × 20 mL) and water (2 × 50 mL) in sequence. The organic phase was dried over anhydrous Na_2SO_4, filtered, concentrated, and the residue was chromatographed (20:1 hexanes/AcOEt) on silica gel to afford the product (1.85 g, 45% yield).

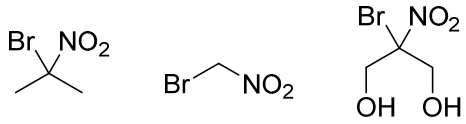
6-Nitro-1-hexene



To a stirred solution of sodium nitrite (1.42 g, 20.56 mmol) in DMF (40 mL) was added 6-bromohex-1-ene (2.50 mL, 18.7 mmol), and the reaction mixture was stirred at room temperature for 2 hours. The pale yellow solution was then partitioned between ice-water (100 mL) and diethyl ether (50 mL), and the organic phase was separated. The aqueous component was extracted with diethyl ether (3 × 50 mL), and the combined organic extracts were subsequently washed with water (2 × 50 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. Purification by flash column chromatography (petroleum) afforded the product as a pale yellow oil (1.0 g, 42% yield).

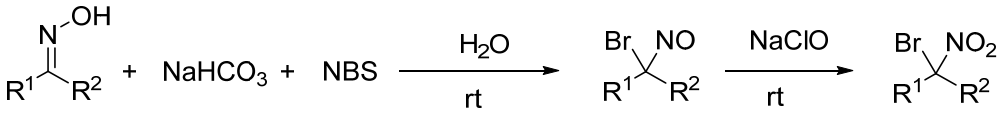
4.3 Preparation of *gem*-bromonitroalkanes

gem-bromonitroalkanes from commercial sources:



2a **2o** Bronopol

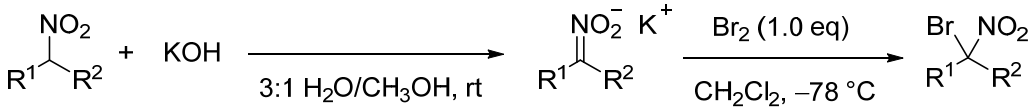
General procedure F



1.0 equiv 2.3 equiv 2.3 equiv

The corresponding oxime (25.0 mmol) was added to a solution of sodium bicarbonate (4.80 g, 57.5 mmol) in 150 mL of water followed by *N*-bromosuccinimide (10.2 g, 57.5 mmol). The reaction mixture was stirred at rt overnight and extracted with AcOEt, and the organic layers were washed with brine and dried over Na_2SO_4. After evaporation of solvents, the residue of bromonitrosoalkane was diluted with benzene (50 mL). To the benzene solution were added tetrabutylammonium hydrogensulfate (4.25 g, 12.5 mmol) and sodium hypochlorite solution (ca. 1.3 M, 60 mL) in portions. Stirring was continued until blue or green color of the reaction mixture faded. After separation and concentration of the organic phase, the crude product was purified by flash column chromatography on silica gel (petroleum ether).

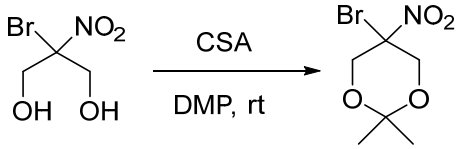
General procedure G[40]



1.0 eq 1.0 eq

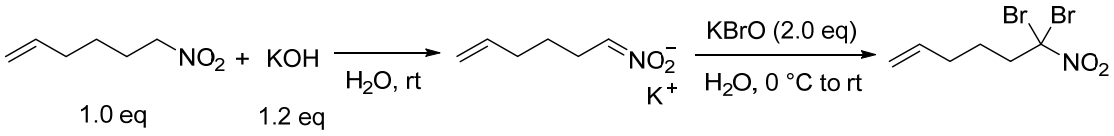
The respective nitro compound (30.0 mmol) was added to a mixture of solid KOH (85%, 2.0 g, 30 mmol), CH_3OH (25 mL) and H_2O (75 mL) at room temperature. The mixture was vigorously stirred until complete dissolution of the starting nitro compound (ca. 30 min), and then cooled to 0 °C. Bromine (1.52 mL, 30 mmol) in CH_2Cl_2 (50 mL, precooled to −78 °C) was added in one pot. The cooling bath was removed, and the mixture was vigorously stirred for 5 min. After separation and concentration of the organic phase, the crude product was chromatographed on silica gel (petroleum ether).

5-Bromo-2,2-dimethyl-5-nitro-1,3-dioxane (2p)[41]



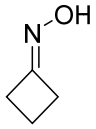
To a solution of 2-bromo-2-nitro-1,3-propanediol (20.0 g, 0.101 mol) in 2,2-dimethoxypropane (80 mL) was added L-camphor-10-sulfonic acid (1.62 g, 8.09 mmol). The mixture was stirred for 3 d at rt under a nitrogen atmosphere. The solvent was evaporated with a rotary evaporator and the residual solid was purified by chromatography on silica gel (petroleum ether) to give a white solid (70% yield).

6,6-Dibromo-6-nitro-1-hexene (2q)



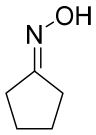
In a round-bottom flask, 6-nitro-1-hexene (1.2 g, 10 mmol) was added to a mixture of solid KOH (85%, 0.79 g, 12 mmol) and H_2O (10 mL) at room temperature. The mixture was stirred at rt for 30 min, then cooled to 0 °C. A solution of KBrO (20 mmol), prepared from bromine (1.0 mL, 20 mmol), solid KOH (85%, 2.63 g, 40.0 mmol) and H_2O (30 mL) at 0 °C, was added dropwise. The mixture was allowed to warm to room temperature and extracted with hexanes. The organic phases were dried over anhydrous Na_2SO_4, filtered and concentrated. The crude product was chromatographed on silica gel (20:1 hexanes/AcOEt) to give 6,6-dibromo-6-nitro-1-hexene as a pale yellow oil (656 mg, 23% yield).

4.4 Physical data



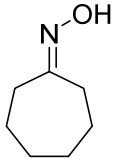
Cyclobutanone oxime[42]

White solid (3.6 g, 85% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 3.18 – 2.71 (m, 4H), 2.14 – 1.93 (m, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 159.72, 31.34, 30.48, 14.40.



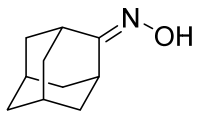
Cyclopentanone oxime[43]

White solid (4.1 g, 83% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.92 (br, J = 354.4 Hz, 1H), 2.40 (d, J = 60.6 Hz, 4H), 1.75 (s, 4H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.31, 31.29, 27.16, 25.13, 24.49.



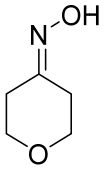
Cycloheptanone oxime[43]

White solid (5.0 g, 79% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.93 (br, 1H), 2.55 (s, 2H), 2.35 (s, 2H), 1.78 – 1.41 (m, 8H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.13, 33.55, 30.32, 30.20, 28.50, 27.40, 24.39.



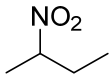
(1*r*,3*r*,5*R*,7*S*)-Adamantan-2-one oxime[44]

White solid (6.7 g, 82% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 3.57 (s, 1H), 2.56 (s, 1H), 2.01 – 1.82 (m, 12H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.97, 38.87, 37.45, 36.47, 36.22, 28.76, 27.83.



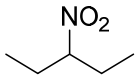
Tetrahydro-4*H*-pyran-4-one oxime[45]

White solid (4.5 g, 79% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 3.78 (d, *J* = 30.4 Hz, 4H), 2.66 (s, 2H), 2.37 (s, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 155.97, 68.15, 66.67, 32.21, 25.95.



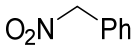
2-Nitrobutane

Blue oil (2.5 g, 61%); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.41 (d, *J* = 6.7 Hz, 1H), 1.95 – 1.64 (m, 2H), 1.47 – 1.34 (m, 3H), 0.90 – 0.81 (m, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 84.62, 28.12, 18.36, 9.67.



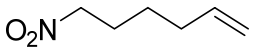
3-Nitropentane[46]

Brown oil (1.5 g, 63%); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.25 (dd, *J* = 7.7, 4.6 Hz, 1H), 1.87 (dd, *J* = 8.3, 6.2 Hz, 2H), 1.71 (d, *J* = 7.4 Hz, 2H), 0.90 – 0.84 (m, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 91.64, 26.55, 9.91.



(Nitromethyl)benzene[47,39]

Yellow oil (1.85 g, 45%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (dd, *J* = 4.5, 1.7 Hz, 5H), 5.43 (s, 2H).



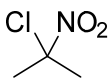
6-Nitrohex-1-ene[48]

Yellow oil (1.0 g, 42%); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.69 (ddd, *J* = 17.0, 8.3, 5.1 Hz, 1H), 4.98 – 4.89 (m, 2H), 4.31 (d, *J* = 2.5 Hz, 2H), 1.98 (dd, *J* = 53.8, 5.4 Hz, 6H), 1.40 (d, *J* = 7.8 Hz, 2H).

2-Fluoro-2-nitropropane (2t)[49,50]

Following general procedure G, Selectfluor was used instead of bromine.

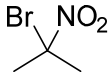
Yellow oil (1.6 g, 82%); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 1.87 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 118.87, 117.30, (*J* = 235.6 Hz)24.87, 24.71 (*J* = 23.9 Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ −111.96.



2-Chloro-2-nitropropane (2r)[51]

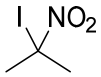
Following general procedure G, *N*-chlorosuccinimide was used instead of bromine.

Yellow oil (0.8 g, 43%); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.09 (d, *J* = 1.3 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 99.99, 30.82.



2-Bromo-2-nitropropane (2a)[52]

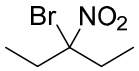
^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.26 (d, *J* = 7.6 Hz, 6H).



2-Iodo-2-nitropropane (2s)[51]

Following general procedure G, iodine was used instead of bromine.

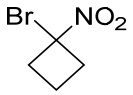
^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.38 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 62.96, 35.55.



3-Bromo-3-nitropentane (2b)[53]

Following general procedure G.

Yellow oil (1.8 g, 75% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.42 (s, 4H), 1.04 – 1.01 (m, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 105.25, 35.51, 9.61.



1-Bromo-1-nitrocyclobutane (2c)[51]

Following general procedure F.

Yellow oil (3.5 g, 72% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 3.29 – 3.17 (m, 2H), 2.92 – 2.77 (m, 2H), 2.30 – 2.12 (m, 1H) 1.97 (dtt, *J* = 11.3, 9.6, 5.0 Hz, 1H) ppm; ^{13}C NMR (101 MHz, Chloroform-*d*) δ = 84.35, 39.58, 13.62.

1-Chloro-1-nitrocyclobutane (2v)

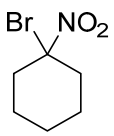
Following general procedure F, NCS was used instead of NBS.

Yellow oil (1.7 g, 75% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.31 – 3.01 (m, 2H), 2.74 (d, *J* = 5.7 Hz, 2H), 2.09 (d, *J* = 51.3 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 96.66, 38.48, 13.16.

1-Bromo-1-nitrocyclopentane (2d)

Following general procedure F.

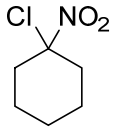
Yellow oil (1.7 g, 68% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.43 (s, 4H), 1.72 (s, 2H), 1.40 (s, 1H), 0.86 (s, 1H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 94.74, 39.26, 23.80, 23.53.



1-Bromo-1-nitrocyclohexane (2e)[51]

Following general procedure F.

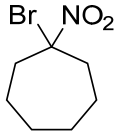
Yellow oil (2.5 g, 71% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.36 (s, 4H), 1.71 – 1.34 (m, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 94.62, 38.97, 23.53, 23.34.



1-Chloro-1-nitrocyclohexane (2u)[59]

Following general procedure F, aqueous NaClO was used instead of NBS.

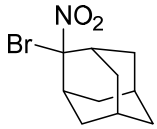
Yellow oil (2.1 g, 68% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.52 – 2.20 (m, 4H), 1.82 – 1.54 (m, 5H), 1.36 (dd, *J* = 9.2, 4.4 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 103.67, 38.16, 23.84, 22.85.



1-Bromo-1-nitrocycloheptane (2f)[51]

Following general procedure F.

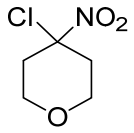
Yellow oil (3.8 g, 70% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.74 (dt, *J* = 14.2, 7.5 Hz, 1H), 2.51 (d, *J* = 7.9 Hz, 1H), 2.39 (s, 2H), 1.59 (d, *J* = 28.5 Hz, 8H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 99.25, 42.98, 27.86, 22.97.



(1*r*,3*r*,5*r*,7*r*)-2-Bromo-2-nitroadamantane (2g)[54,55]

Following general procedure F.

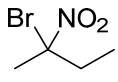
Colorless oil (1.2 g, 43% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.90 (s, 2H), 2.37 (d, *J* = 13.7 Hz, 2H), 1.98 (d, *J* = 14.6 Hz, 2H), 1.95 – 1.75 (m, 8H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 102.45, 38.31, 37.56, 34.95, 34.50, 26.09, 25.59.



4-Chloro-4-nitrotetrahydro-2*H*-pyran (2h)

Following general procedure F, aqueous NaClO was used instead of NBS.

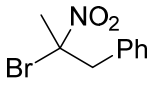
Yellow oil (2.5 g, 71% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ = 4.53 (tt, *J* = 9.9, 4.7 Hz, 2H), 4.01 (dt, *J* = 12.1, 4.0 Hz, 2H), 3.46 (ddd, *J* = 12.1, 10.4, 2.9 Hz, 2H), 2.25 – 2.05 (m, 2H) ppm; ^{13}C NMR (101 MHz, Chloroform-*d*) δ = 80.67, 65.34, 30.48.



2-Bromo-2-nitrobutane (2i)[56]

Following general procedure G.

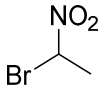
Yellow oil (1.2 g, 75% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 2.41 (dd, *J* = 16.1, 7.4 Hz, 2H), 2.20 (s, 3H), 1.03 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 96.09, 37.39, 29.45, 9.88.



(2-Bromo-2-nitropropyl)benzene (2j)

Following general procedure G.

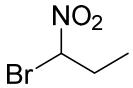
Yellow oil (1.0 g, 75% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.36 – 7.32 (m, 3H), 7.21 (dd, *J* = 6.4, 3.2 Hz, 2H), 3.87 (d, *J* = 14.3 Hz, 1H), 3.65 (d, *J* = 14.3 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 133.12, 130.34, 128.67, 128.20, 93.60, 49.41, 28.98.



1-Bromo-1-nitroethane (2k)[57,51]

Following general procedure G.

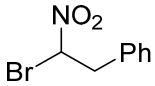
Yellow oil (4.3 g, 94% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.04 (q, *J* = 6.4 Hz, 1H), 2.14 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 74.52, 24.21.



1-Bromo-1-nitropropane (2l)[57,51]

Following general procedure G.

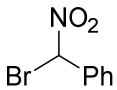
Yellow oil (4.2 g, 86% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.93 – 5.80 (m, 1H), 2.53 – 2.19 (m, 2H), 1.06 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 81.19, 31.03, 10.35.



(2-Bromo-2-nitroethyl)benzene (2m)[58]

Following general procedure G.

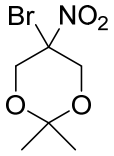
Yellow oil (1.1 g, 75% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.31 (m, 3H), 7.21 (dd, *J* = 7.3, 2.3 Hz, 2H), 6.06 (dd, *J* = 8.3, 6.1 Hz, 1H), 3.76 (dd, *J* = 14.5, 8.2 Hz, 1H), 3.52 (dd, *J* = 14.5, 6.1 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 133.22, 129.14, 129.04, 128.27, 79.12, 43.38.



(Bromo(nitro)methyl)benzene (2n)[59]

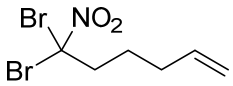
Following general procedure G.

Yellow oil (329 mg, 38% yield); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 – 7.60 (m, 2H), 7.49 – 7.41 (m, 3H), 6.91 (s, 1H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 132.80, 131.39, 129.15, 128.21, 80.37.



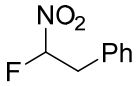
5-Bromo-2,2-dimethyl-5-nitro-1,3-dioxane (2p)[60]

White solid (16.1g, 70% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 4.77 (dd, *J* = 13.3, 1.6 Hz, 2H), 4.26 (d, *J* = 13.4 Hz, 2H), 1.53 (s, 3H), 1.37 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 99.44, 66.14, 27.77, 18.44.



6,6-Dibromo-6-nitrohex-1-ene (2q)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.91 – 5.64 (m, 1H), 5.23 – 4.78 (m, 2H), 2.97 – 2.63 (m, 2H), 2.18 (d, *J* = 9.8 Hz, 2H), 1.77 – 1.57 (m, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 136.63, 116.20, 87.66, 48.30, 32.08, 26.31.



(2-Fluoro-2-nitroethyl)benzene (2w)[49,50]

Following general procedure G, Selectfluor was used instead of bromine.

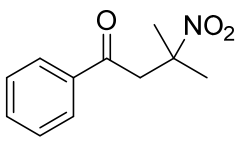
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (dd, *J* = 40.0, 1.3 Hz, 5H), 6.01 (dd, *J* = 6.7, 3.8 Hz, 1H), 3.42 (d, *J* = 16.0 Hz, 2H).

5. Photocatalytic coupling reactions.

5.1 Typical procedure

A dry Schlenk tube charged with a stirring bar was evacuated and backfilled with N_2 (three times). Trimethylsilyl enol ether (**1a**, 457 mg, 2.38 mmol) of acetophenone, 2-bromo-2-nitropropane **2a** (200 mg, 1.19 mmol) and anhydrous acetonitrile (6.0 mL) were added via gastight syringe under N_2 atmosphere followed by *fac*-Ir(ppy)$_3$ (4 mg, 0.5 mol %). The reaction mixture was degassed by freeze-pump-thaw method and then stirred under irradiation with blue LEDs (460 nm, app. 3.0 cm distance from the tube). The mixture was maintained at approximately 25 °C by a desk fan in air-conditioned room. The reaction was monitored by TLC. Upon completion (8 h), the mixture was concentrated in vacuo. The crude product was purified by flash chromatography on silica gel (20:1 to 10:1 hexanes/AcOEt) to give **3aa**.

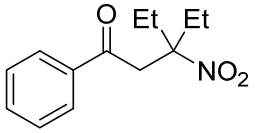
5.2 Physical data



3-Methyl-3-nitro-1-phenylbutan-1-one (3aa)[61]

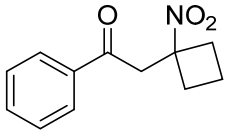
White solid (242 mg, 98% yield); R_f = 0.25 (10:1 hexanes/AcOEt); m.p. 64.0–64.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.90 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz,

2H), 3.68 (s, 2H), 1.77 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.94, 136.42, 133.64, 128.75, 127.93, 84.94, 47.10, 26.61.



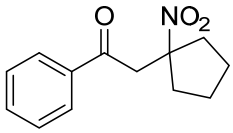
3-Ethyl-3-nitro-1-phenylpentan-1-one (3ab)

Colorless oil (242 mg, 98% yield); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.97 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 15.6 Hz, 2H), 3.68 (s, 2H), 2.22 (dd, *J* = 7.5, 2.5 Hz, 4H), 0.86 (t, *J* = 7.5 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.17, 136.62, 133.60, 128.77, 127.90, 93.17, 40.66, 28.97, 8.37; IR (film) ν_{max} 2930, 1651, 1562, 1460, 1194, 1134, 1076 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{13}H_{17}NO_3Na$ 258.11; Found 258.1106.



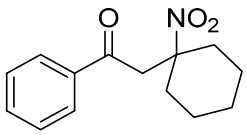
2-(1-Nitrocyclobutyl)-1-phenylethan-1-one (3ac)

White solid (227 mg, 87% yield); R_f = 0.19 (10:1 hexanes/AcOEt); m.p. 112.4–113.9 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 – 7.92 (m, 2H), 7.60 (s, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 3.90 (s, 2H), 3.09 – 3.02 (m, 2H), 2.37 (t, *J* = 4.9 Hz, 2H), 2.14 (s, 1H), 1.97 (s, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.11, 136.07, 133.71, 128.76, 128.01, 84.81, 44.46, 32.70, 14.38; IR (film) ν_{max} 2957, 1678, 1533, 1449, 1400, 1360, 1269, 1225, 1078, 1001. 880, 752.27, 692.47 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{12}H_{13}NO_3Na$ 242.0787; Found 242.0786.



2-(1-Nitrocyclopentyl)-1-phenylethan-1-one (3ad)

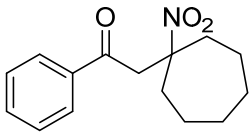
White solid (244 mg, 88% yield); R_f = 0.25 (10:1 hexanes/AcOEt); m.p. 113.5–114.8 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.57 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 3.81 (s, 2H), 2.71 (d, *J* = 12.1 Hz, 2H), 1.95 (s, 4H), 1.77 (s, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.38, 136.24, 133.60, 128.73, 127.99, 94.64, 47.21, 38.87, 24.94; IR (film) ν_{max} 2963, 1686, 1599, 1539, 1447, 1400, 1364, 1221,1180, 1142, 1074, 1001, 754, 691 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^{+}$ Calcd for $C_{13}H_{15}NO_3Na$ 256.0944; Found 256.0948.



2-(1-Nitrocyclohexyl)-1-phenylethan-1-one (3ae)

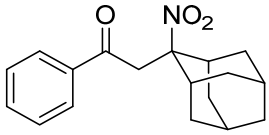
Colorless oil (271 mg, 92% yield); R_f = 0.27 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.86 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.39 (m, 2H), 3.64 (s, 2H), 2.35 (dd, *J* = 13.5, 8.4 Hz, 2H), 2.00 (dd, *J* = 13.5, 8.6 Hz, 2H), 1.50 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.15, 136.49, 133.44, 128.58, 127.82, 88.44, 44.84, 34.53, 24.62,

22.32; IR (film) ν_{max} 2953, 2926, 2855, 1690, 1682, 1537, 1450, 1364, 1215, 1007, 750,688 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{14}H_{17}NO_3Na$ 270.11; Found 270.1096.



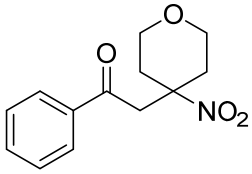
2-(1-Nitrocycloheptyl)-1-phenylethan-1-one (3af)

White solid (255 mg, 82% yield); R_f = 0.27 (10:1 hexanes/AcOEt); m.p. 116.3–118.2 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.51 – 7.43 (m, 2H), 2.66 – 2.55 (m, 2H), 2.05 (dd, *J* = 15.9, 10.0 Hz, 2H), 1.62 (d, *J* = 35.4 Hz, 10H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.16, 136.53, 133.56, 128.72, 127.94, 92.12, 47.29, 38.12, 29.98, 23.45; IR (film) ν_{max} 2924, 1688, 1539, 1180,1142, 1074, 758, 689 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{19}NO_3Na$ 284.1257; Found 284.1264.



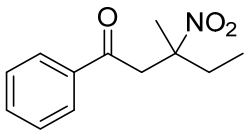
2-((1*R*,3*S*,5*r*,7*r*)-2-Nitroadamantan-2-yl)-1-phenylethan-1-one (3ag)

White solid (335 mg, 94% yield); R_f = 0.3 (10:1 hexanes/AcOEt); m.p. 122.8–124.5 °C; ^1H NMR (600 MHz, Chloroform-*d*) δ 7.82 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 3.60 (s, 2H), 2.75 (s, 2H), 2.11 (s, 2H), 1.95 (s, 3H), 1.86 (d, *J* = 15.5 Hz, 3H), 1.76 (d, *J* = 9.1 Hz, 4H); ^{13}C NMR (151 MHz, Cyclohexane-d_{12}) δ 196.09, 137.17, 133.60, 128.72, 127.92, 95.58, 43.16, 37.91, 34.50, 33.89, 26.38; IR (film) ν_{max} 2918, 1688, 1535, 1449, 1354, 764, 691 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{18}H_{21}NO_3Na$ 322.1413; Found 322.1416.



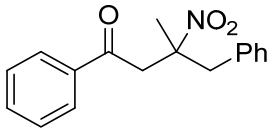
2-(4-Nitrotetrahydro-2*H*-pyran-4-yl)-1-phenylethan-1-one (3ah)

Colorless oil (131 mg, 44% yield); R_f = 0.1 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 6.9 Hz, 2H), 7.89 (d, *J* = 7.1 Hz, 2H), 7.61 – 7.57 (m, 2H), 7.46 (t, *J* = 7.9 Hz, 4H), 3.82 – 3.73 (m, 4H), 3.66 (s, 2H), 2.53 (d, *J* = 14.6 Hz, 2H), 2.11 (s, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.58, 171.40, 136.26, 133.88, 133.71, 130.17, 129.32, 128.83, 128.47, 127.99, 85.40, 63.91, 46.32, 34.44, 29.67; IR (film) ν_{max} 2924, 1535, 1451, 1383, 1180, 1142, 1074, 1042, 1015 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{13}H_{15}NO_4Na$ 272.0893; Found 272.0897.



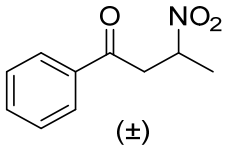
3-Methyl-3-nitro-1-phenylpentan-1-one (3ai)

Colorless oil (218 mg, 90% yield); R_f = 0.4 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.90 (m, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 3.84 (d, *J* = 18.0 Hz, 1H), 3.49 (d, *J* = 18.0 Hz, 1H), 2.10 – 1.99 (m, 2H), 1.74 (s, 3H), 0.93 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.07, 136.40, 133.53, 128.66, 127.84, 88.48, 45.37, 33.70, 22.02, 8.17; IR (film) ν_{max} 2967, 2932, 2878, 1711, 1551, 1458, 1375, 700 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0947.



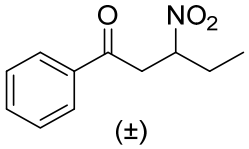
3-Methyl-3-nitro-1,4-diphenylbutan-1-one (3aj)

Colorless oil (307 mg, 91% yield); R_f = 0.3 (8:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.60 (s, 1H), 7.47 (t, *J* = 7.9 Hz, 2H), 7.31 – 7.25 (m, 3H), 7.09 (dd, *J* = 6.8, 2.8 Hz, 2H), 3.71 (d, *J* = 18.1 Hz, 1H), 3.54 – 3.39 (m, 3H), 1.77 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.23, 136.51, 134.57, 133.65, 130.09, 128.75, 128.66, 127.90, 127.69, 88.76, 45.25, 44.68, 23.73; IR (film) ν_{max} 2924, 2853, 1684, 1539, 1450, 1383, 1358, 1142, 1074, 1042, 1013, 756, 727, 689, 557 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{17}H_{17}NO_3Na$ 306.11; Found 306.1099.



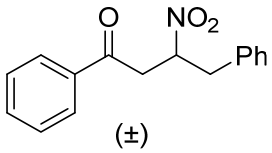
3-Nitro-1-phenylbutan-1-one (3ak)[62]

Colorless oil (214 mg, 93% yield); R_f = 0.17 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 7.1 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.45 (m, 2H), 5.20 – 5.16 (m, 1H), 3.91 (dd, *J* = 18.0, 8.0 Hz, 1H), 3.29 (d, *J* = 5.0 Hz, 1H), 1.68 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.11, 135.76, 133.81, 128.45, 128.03, 78.08, 42.36, 19.60;



3-Nitro-1-phenylpentan-1-one (3al)[62]

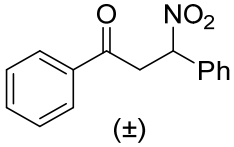
Colorless oil (234 mg, 95% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 5.15 – 5.04 (m, 1H), 3.95 – 3.85 (m, 1H), 3.27 (dd, *J* = 18.2, 4.3 Hz, 1H), 2.07 – 1.99 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.24, 135.80, 133.84, 128.79, 128.07, 83.88, 40.57, 27.21, 10.03.



3-Nitro-1,4-diphenylbutan-1-one (3am)

White solid (295 mg, 92% yield); R_f = 0.37 (8:1 hexanes/AcOEt); m.p. 114.4–115.3 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.2 Hz, 2H), 7.60 (s, 1H), 7.46 (d, *J* = 7.8 Hz,

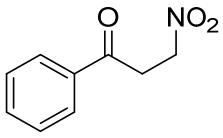
2H), 7.33 (d, J = 7.8 Hz, 3H), 7.23 (s, 2H), 5.42 – 5.33 (m, 1H), 3.84 (dd, J = 18.4, 8.6 Hz, 1H), 3.42 (dd, J = 13.9, 6.6 Hz, 1H), 3.30 – 3.21 (m, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.15, 135.80, 134.91, 133.87, 129.09, 129.02, 128.80, 128.08, 127.74, 83.58, 40.02, 39.80; IR (film) ν_{max} 1680, 1543, 1437, 1383, 1283, 1219, 1074, 928, 750, 700, 546 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{16}H_{15}NO_3Na$ 292.0944; Found 292.0938.



(±)

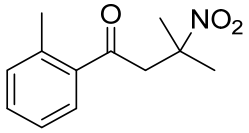
3-Nitro-1,3-diphenylpropan-1-one (3an)

White solid (45 mg, 35% yield); R_f = 0.37 (10:1 hexanes/AcOEt); m.p. 114.4–116.1 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 (dd, J = 8.4, 1.3 Hz, 2H), 7.62 (s, 1H), 7.52 – 7.42 (m, 7H), 6.16 (dd, J = 10.1, 3.6 Hz, 1H), 4.42 (dd, J = 18.3, 10.1 Hz, 1H), 3.51 (dd, J = 18.3, 3.6 Hz, 1H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.84, 135.73, 134.35, 133.94, 130.00, 129.28, 128.85, 128.18, 127.46, 85.48, 42.35; IR (film) ν_{max} 1687, 1552, 1365, 756, 690 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{15}H_{13}NO_3Na$ 278.0895; Found 278.0788.



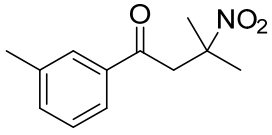
3-Nitro-1-phenylpropan-1-one (3ao)[63]

White solid (164 mg, 77% yield); R_f = 0.25 (10:1 hexanes/AcOEt); m.p. 76.8–78.0 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.95 (m, 2H), 7.65 – 7.60 (m, 1H), 7.53 – 7.48 (m, 2H), 4.83 (t, J = 6.1 Hz, 2H), 3.67 (t, J = 6.1 Hz, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.94, 135.67, 133.95, 128.86, 128.12, 69.26, 34.85.



3-Methyl-3-nitro-1-(*o*-tolyl)butan-1-one (3ba)

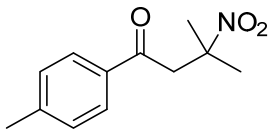
Colorless oil (229 mg, 87% yield); R_f = 0.22 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.63 (dd, J = 7.8, 1.4 Hz, 1H), 7.39 (d, J = 1.3 Hz, 1H), 7.28 – 7.23 (m, 2H), 3.59 (s, 2H), 2.47 (s, 3H), 1.75 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 198.84, 138.50, 137.09, 132.17, 131.78, 128.16, 125.73, 84.98, 49.73, 26.66, 21.22; IR (film) ν_{max} 2932, 1811, 1786, 1746, 1709, 1516, 1368, 1173, 976, 879, 698 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0947.



3-Methyl-3-nitro-1-(*m*-tolyl)butan-1-one (3ca)

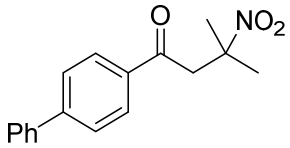
Colorless oil (234 mg, 89% yield); R_f = 0.22 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.74 – 7.68 (m, 2H), 7.38 (d, J = 7.5 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 3.67 (s, 2H), 2.38 (s, 3H), 1.74 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.15, 138.44, 136.27,

134.25, 128.47, 128.32, 125.00, 84.73, 47.02, 26.48, 21.14; IR (film) ν_{max} 2932, 1811, 1786, 1746, 1709, 1516, 1368, 1173, 976, 879, 698 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0947.



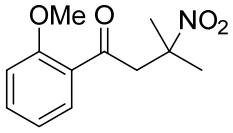
3-Methyl-3-nitro-1-(*p*-tolyl)butan-1-one (3da)

White solid (237 mg, 90% yield); R_f = 0.22 (10:1 hexanes/AcOEt); m.p. 58.2–58.9 °C; ^1H NMR (600 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.28 (s, 2H), 3.65 (s, 2H), 2.42 (s, 3H), 1.76 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.55, 144.57, 134.03, 129.42, 128.07, 85.05, 46.98, 26.60, 21.65; IR (film) ν_{max} 2932, 1811, 1786, 1746, 1709, 1516, 1368, 1173, 976, 879, 698 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0947.



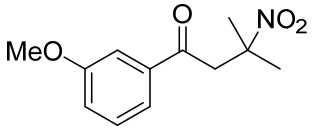
1-([1,1'-Biphenyl]-4-yl)-3-methyl-3-nitrobutan-1-one (3ea)

Colorless oil (320 mg, 95% yield); R_f = 0.19 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 6.9 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 1H), 3.71 (s, 2H), 1.79 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.51, 146.35, 139.64, 135.14, 129.00, 128.56, 128.40, 127.37, 127.27, 85.04, 47.11, 26.63; IR (film) ν_{max} 2932, 1543, 1404, 1370, 1348, 1074, 762, 692 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{17}H_{17}NO_3Na$ 306.1106; Found 306.1106.



1-(2-Methoxyphenyl)-3-methyl-3-nitrobutan-1-one (3fa)

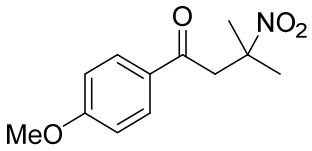
Colorless oil (234 mg, 83% yield); R_f = 0.18 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.50 – 7.44 (m, 1H), 6.98 (dd, *J* = 14.5, 8.1 Hz, 2H), 3.92 (s, 3H), 3.70 (s, 2H), 1.71 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.71, 158.68, 134.16, 130.45, 127.25, 120.77, 111.56, 85.07, 55.49, 52.39, 26.59; IR (film) ν_{max} 1680, 1601, 1543, 1362, 1262, 1231, 1175, 1074, 1017, 835, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{16}NO_4$ 238.1073; Found 238.1078.



1-(3-Methoxyphenyl)-3-methyl-3-nitrobutan-1-one (3ga)

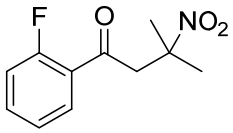
Yellow solid (246 mg, 87% yield); R_f = 0.18 (10:1 hexanes/AcOEt); m.p. 70.3–71.7 °C; ^1H NMR (600 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 7.8 Hz, 1H), 7.45 (s, 1H), 7.41 – 7.35 (m, 1H), 7.16 – 7.11 (m, 1H), 3.85 (s, 3H), 3.66 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-

d) δ 194.79, 159.92, 137.72, 129.71, 120.48, 120.18, 112.12, 84.88, 55.43, 47.21, 26.59; IR (film) ν_{max} 1680, 1601, 1543, 1362, 1262, 1231, 1175, 1074, 1017, 835, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{16}NO_4$ 238.1073; Found 238.1078.



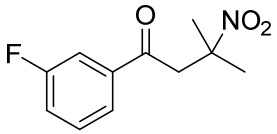
1-(4-Methoxyphenyl)-3-methyl-3-nitrobutan-1-one (3ha)

White solid (240 mg, 85% yield); R_f = 0.18 (10:1 hexanes/AcOEt); m.p. 78.7–79.9 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 – 7.88 (m, 2H), 6.96 – 6.91 (m, 2H), 3.87 (s, 3H), 3.62 (s, 2H), 1.75 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.40, 163.87, 130.24, 129.50, 113.85, 85.02, 55.50, 46.74, 26.60; IR (film) ν_{max} 1680, 1601, 1543, 1362, 1262, 1231, 1175, 1074, 1017, 835, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{12}H_{16}NO_4$ 238.1073; Found 238.1078.



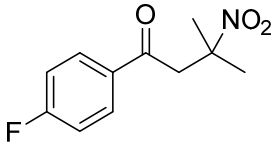
1-(2-Fluorophenyl)-3-methyl-3-nitrobutan-1-one (3ia)

Colorless oil (228 mg, 85% yield); R_f = 0.3 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.84 (t, *J* = 7.7 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.26 – 7.20 (m, 1H), 7.14 (dd, *J* = 11.0, 8.8 Hz, 1H), 3.67 (d, *J* = 3.0 Hz, 2H), 1.74 (d, *J* = 1.4 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.12, 162.76, 135.20, 130.61, 124.87, 124.65, 116.66, 84.64, 51.92, 26.65; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.47; IR (film) ν_{max} 1692, 1587, 1543, 1441, 1360, 1252, 1142, 866, 783 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}NO_3FNa$ 248.0693; Found 248.0696.



1-(3-Fluorophenyl)-3-methyl-3-nitrobutan-1-one (3ja)

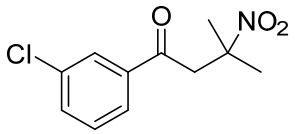
White solid (214 mg, 80% yield); R_f = 0.3 (10:1 hexanes/AcOEt); m.p. 127.1–128.2 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 9.4 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.30 (d, *J* = 2.6 Hz, 1H), 3.65 (s, 2H), 1.77 (d, *J* = 1.1 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.73, 161.61, 138.41, 130.51, 123.66, 120.60, 114.85, 84.79, 47.20, 26.60; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -111.70; IR (film) ν_{max} 1692, 1587, 1543, 1441, 1360, 1252, 1142, 866, 783 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}NO_3FNa$ 248.0693; Found 248.0696.



1-(4-Fluorophenyl)-3-methyl-3-nitrobutan-1-one (3ka)

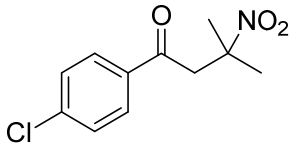
Colorless oil (233 mg, 87% yield); R_f = 0.3 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz,

Chloroform-*d*) δ 7.96 (dd, *J* = 8.8, 5.3 Hz, 2H), 7.21 – 7.10 (m, 2H), 3.64 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.37, 165.20, 132.89, 130.64, 115.98, 84.92, 46.99, 26.62; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -103.93; IR (film) ν_{max} 1692, 1587, 1543, 1441, 1360, 1252, 1142, 866, 783 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{11}H_{12}NO_3FNa$ 248.0693; Found 248.0696.



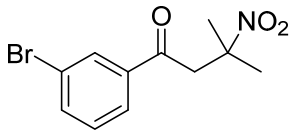
1-(3-Chlorophenyl)-3-methyl-3-nitrobutan-1-one (3la)

Colorless oil (236 mg, 82% yield); R_f = 0.27 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.90 (t, *J* = 1.8 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.43 (t, *J* = 7.9 Hz, 2H), 3.64 (s, 2H), 1.77 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.71, 137.93, 135.17, 133.57, 130.11, 128.12, 126.01, 84.85, 47.15, 26.62; IR (film) ν_{max} 1694, 1587, 1535, 1396, 1350, 1283, 1227, 1136, 1085, 843, 816, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{11}H_{12}NO_3NaCl$ 264.0397; Found 264.0399.



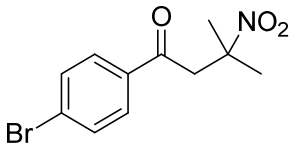
1-(4-Chlorophenyl)-3-methyl-3-nitrobutan-1-one (3ma)

Colorless oil (239 mg, 83% yield); R_f = 0.27 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.89 – 7.84 (m, 2H), 7.48 – 7.43 (m, 2H), 3.63 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.75, 140.21, 134.74, 129.35, 129.10, 84.90, 47.02, 26.62; IR (film) ν_{max} 1694, 1587, 1535, 1396, 1350, 1283, 1227, 1136, 1085, 843, 816, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{11}H_{12}NO_3ClNa$ 264.0397; Found 264.0399.



1-(3-Bromophenyl)-3-methyl-3-nitrobutan-1-one (3na)

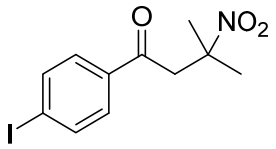
Colorless oil (300 mg, 88% yield); R_f = 0.24 (10:1 hexanes/AcOEt); m.p. 126.3–128.2 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.05 (d, *J* = 1.8 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 3.64 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.63, 138.09, 136.47, 131.03, 130.35, 126.44, 123.09, 84.81, 47.10, 26.61; IR (film) ν_{max} 2957, 1692, 1539, 1395, 1136, 1074, 1010, 810, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M+H]$^+$ Calcd for $C_{11}H_{13}NO_3Br$ 286.0073; Found 286.0070.



1-(4-Bromophenyl)-3-methyl-3-nitrobutan-1-one (3oa)

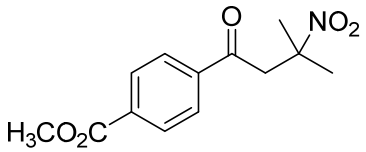
Colorless oil (293 mg, 86% yield); R_f = 0.24 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.76 (m, 2H), 7.66 – 7.58 (m, 2H), 3.63 (s, 2H), 1.76 (s, 6H); ^{13}C NMR

(151 MHz, Chloroform-*d*) δ 193.99, 135.09, 132.05, 129.41, 128.88, 84.83, 46.96, 26.59; IR (film) ν_{max} 2957, 1692, 1539, 1395, 1136, 1074, 1010, 810, 571 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{11}H_{13}NO_3Br$ 286.0073; Found 286.0070.



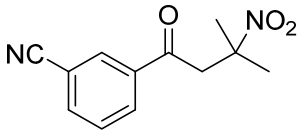
1-(4-Iodophenyl)-3-methyl-3-nitrobutan-1-one (3pa)

Colorless oil (337 mg, 85% yield); R_f = 0.20 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 3.62 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.27, 138.09, 135.62, 129.26, 101.76, 84.83, 46.91, 26.61; IR (film) ν_{max} 1688, 1580, 1539, 1458, 1385, 1356, 1279, 1227, 997, 804 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}NO_3NaI$ 355.9754; Found 355.9751.



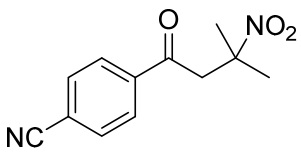
Methyl 4-(3-methyl-3-nitrobutanoyl)benzoate (3qa)

White solid (291 mg, 91% yield); R_f = 0.18 (8:1 hexanes/AcOEt); m.p. 99.0–100.8 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.2 Hz, 2H), 7.98 (d, *J* = 8.2 Hz, 2H), 3.95 (s, 3H), 3.69 (s, 2H), 1.78 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.51, 166.03, 139.50, 134.38, 129.95, 127.87, 84.84, 52.53, 47.37, 26.62; IR (film) ν_{max} 1723, 1696, 1535, 1281, 1182, 1138, 1107, 1074, 1041, 1015, 849, 766, 698 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{13}H_{15}NO_5Na$ 288.0842; Found 288.0845.



3-(3-Methyl-3-nitrobutanoyl)benzonitrile (3ra)

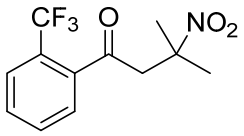
Colorless oil (196 mg, 71% yield); R_f = 0.26 (5:1 hexanes/AcOEt); ^1H NMR (400 MHz, Chloroform-*d*) δ 8.21 (s, 1H), 8.17 – 8.11 (m, 1H), 7.87 (d, *J* = 7.7 Hz, 1H), 7.64 (t, *J* = 7.9 Hz, 1H), 3.66 (s, 2H), 1.78 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.07, 137.09, 136.45, 131.85, 131.63, 129.87, 117.66, 113.38, 84.75, 47.05, 26.66; IR (film) ν_{max} 1692, 1541, 1420, 1361, 1287, 1240, 1142, 1026, 922, 802, 756, 679 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{12}N_2O_3Na$ 255.074; Found 255.0737.



4-(3-Methyl-3-nitrobutanoyl)benzonitrile (3sa)

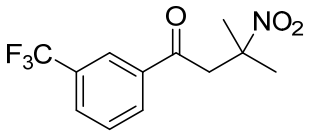
Colorless oil (199 mg, 72% yield); R_f = 0.26 (5:1 hexanes/AcOEt); m.p. 117.3–119.0 °C; ^1H NMR (600 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 3.67 (s, 2H), 1.78 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.74, 139.26, 132.64, 128.38, 117.68, 116.95, 84.80, 47.25, 26.64; IR (film) ν_{max} 1692, 1541, 1420, 1361, 1287, 1240, 1142, 1026,

922, 802, 756, 679 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{12}N_2O_3Na$ 255.074; Found 255.0737.



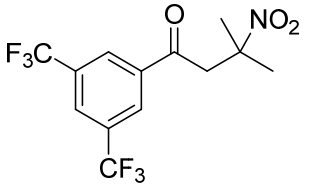
3-Methyl-3-nitro-1-(2-(trifluoromethyl)phenyl)butan-1-one (3ta)

Colorless oil (232 mg, 71% yield); R_f = 0.19 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 7.9 Hz, 1H), 7.64 (s, 1H), 7.58 (s, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 3.52 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.15, 139.36, 132.06, 130.41, 127.00, 126.74, 126.70, 124.46, 84.84, 51.32, 26.30; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.75; IR (film) ν_{max} 1701, 1609, 1545, 1379, 1329, 1179, 1138 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{12}NO_3F_3Na$ 298.0661; Found 298.0666.



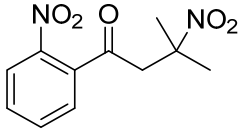
3-Methyl-3-nitro-1-(3-(trifluoromethyl)phenyl)butan-1-one (3ua)

Colorless oil (236 mg, 72% yield); R_f = 0.19 (10:1 hexanes/AcOEt); m.p. 69.4–70.2 °C; ^1H NMR (600 MHz, Chloroform-*d*) δ 8.18 (s, 1H), 8.12 (dt, *J* = 7.8, 1.5 Hz, 1H), 7.87 (mt, *J* = 16.0, 7.7, 2.0, 1.0 Hz, 1H), 7.64 (s, 1H), 3.70 (s, 2H), 1.79 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.68, 136.85, 133.36, 131.08, 130.02, 129.52, 124.77, 84.79, 47.13, 26.64; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.75; IR (film) ν_{max} 1701, 1609, 1545, 1379, 1329, 1179, 1138 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{12}NO_3F_3Na$ 298.0661; Found 298.0666.



1-(3,5-Bis(trifluoromethyl)phenyl)-3-methyl-3-nitrobutan-1-one (3va)

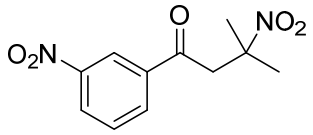
Colorless oil (278 mg, 68% yield); R_f = 0.24 (10:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 8.46 (s, 2H), 8.36 (s, 1H), 3.72 (s, 2H), 1.80 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.41, 137.76, 132.43, 127.95, 126.78, 121.40, 84.70, 47.13, 26.66; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.92; IR (film) ν_{max} 1690, 1287, 1177, 1128 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{13}H_{11}NO_3F_6Na$ 366.0535; Found 366.0531.



3-Methyl-3-nitro-1-(2-nitrophenyl)butan-1-one (3wa)

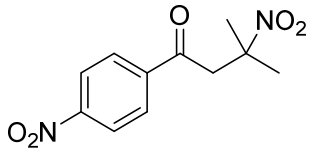
Colorless oil (114 mg, 38% yield); R_f = 0.18 (8:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 1.1 Hz, 1H), 7.64 (s, 1H), 7.47 (dd, *J* = 7.6, 1.4 Hz, 1H), 3.50 (s, 2H), 1.81 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 197.34,

153.25, 137.28, 134.73, 130.79, 127.62, 124.52, 85.12, 53.40, 26.33; IR (film) ν_{max} 1692, 1605, 1533, 1424, 1348, 1285, 1136, 1074, 1013, 982, 930, 795, 714, 561 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}N_2O_5Na$ 275.0638; Found 275.0634.



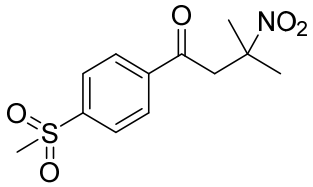
3-Methyl-3-nitro-1-(3-nitrophenyl)butan-1-one (3xa)

White solid (225 mg, 75% yield); R_f = 0.18 (8:1 hexanes/AcOEt); m.p. 193.2–194.9 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.78 – 8.73 (m, 1H), 8.46 (dd, *J* = 8.2, 1.2 Hz, 1H), 8.32 – 8.24 (m, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 3.72 (s, 2H), 1.81 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.92, 148.41, 137.50, 133.50, 130.15, 127.90, 122.84, 84.72, 47.19, 26.69; IR (film) ν_{max} 1692, 1605, 1533, 1424, 1348, 1285, 1136, 1074, 1013, 982, 930, 795, 714, 561 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}N_2O_5Na$ 275.0638; Found 275.0634.



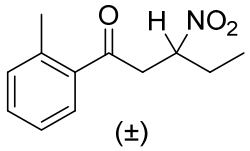
3-Methyl-3-nitro-1-(4-nitrophenyl)butan-1-one (3ya)

White solid (216 mg, 72% yield); R_f = 0.18 (8:1 hexanes/AcOEt); m.p. 193.1–194.9 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 8.32 (s, 1H), 8.11 (s, 1H), 8.09 (s, 1H), 3.70 (s, 2H), 1.80 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.56, 150.64, 140.72, 129.04, 84.82, 47.47, 29.68, 26.67; IR (film) ν_{max} 1692, 1605, 1533, 1424, 1348, 1285, 1136, 1074, 1013, 982, 930, 795, 714, 561 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{12}N_2O_5Na$ 275.0638; Found 275.0634.



3-Methyl-1-(4-(methylsulfonyl)phenyl)-3-nitrobutan-1-one (3za)

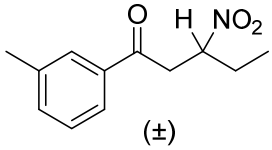
White solid (197 mg, 58% yield); R_f = 0.23 (5:1 hexanes/AcOEt); m.p. 138.2–139.8 °C; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 8.7 Hz, 2H), 8.07 (d, *J* = 8.7 Hz, 2H), 3.69 (s, 2H), 3.09 (s, 3H), 1.79 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.87, 144.70, 140.28, 128.85, 127.97, 84.83, 47.40, 44.30, 26.68; IR (film) ν_{max} 1693, 1661, 1611, 1543, 1316, 1296, 1152, 1086 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{12}H_{15}NO_5NaS$ 308.0563; Found 308.0559.



3-Nitro-1-(*o*-tolyl)pentan-1-one (3bl)

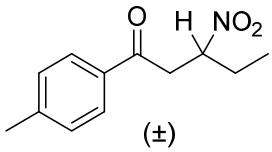
Colorless oil (234 mg, 89% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (m, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 7.3 Hz, 2H), 5.13 –

5.05 (m, 1H), 3.82 (dd, *J* = 18.1, 9.2 Hz, 1H), 3.19 (dd, *J* = 18.1, 4.1 Hz, 1H), 2.49 (s, 3H), 2.07 – 1.95 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 198.60, 138.98, 136.21, 132.25, 132.11, 128.68, 125.82, 84.03, 42.98, 27.12, 21.38, 9.99; IR (film) ν_{max} 2972, 2928, 1692, 1551, 1456, 1379, 980, 759.99 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0949.



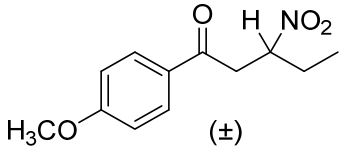
3-Nitro-1-(*m*-tolyl)pentan-1-one (3cl)

Colorless oil (232 mg, 88% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (s, 2H), 7.39 (dd, *J* = 15.8, 7.7 Hz, 2H), 5.14 – 5.03 (m, 1H), 3.87 (dd, *J* = 18.1, 8.7 Hz, 1H), 3.26 (dd, *J* = 18.2, 4.4 Hz, 1H), 2.41 (s, 3H), 2.06 – 1.98 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.41, 138.63, 135.85, 134.55, 128.62, 128.55, 125.26, 83.92, 40.60, 27.17, 21.26, 9.99; IR (film) ν_{max} 2972, 2928, 1692, 1551, 1456, 1379, 980, 759.99 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0949.



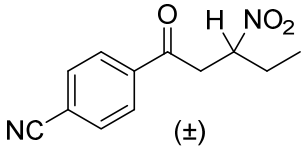
3-Nitro-1-(*p*-tolyl)pentan-1-one (3dl)

Colorless oil (224 mg, 85% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 17.0 Hz, 2H), 5.14 – 5.05 (m, 1H), 3.86 (dd, *J* = 18.0, 8.5 Hz, 1H), 3.25 (dd, *J* = 18.0, 4.5 Hz, 1H), 2.42 (s, 3H), 2.06 – 1.99 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.80, 144.81, 133.44, 129.47, 128.21, 84.02, 40.51, 27.23, 21.68, 10.04; IR (film) ν_{max} 2972, 2928, 1692, 1551, 1456, 1379, 980, 759.99 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_3Na$ 244.0944; Found 244.0949.



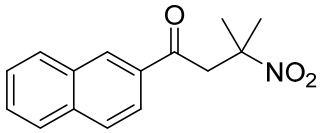
1-(4-Methoxyphenyl)-3-nitropentan-1-one (3hl)

Colorless oil (251 mg, 89% yield); R_f = 0.37 (5:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.90 (m, 2H), 6.97 – 6.92 (m, 2H), 5.09 (d, *J* = 4.5 Hz, 1H), 3.87 (d, *J* = 0.6 Hz, 4H), 3.26 – 3.18 (m, 1H), 2.06 – 1.97 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.63, 164.04, 130.40, 128.93, 113.93, 84.10, 55.51, 40.25, 27.22, 10.04; IR (film) ν_{max} 2974, 2938, 1678, 1601, 1551, 1258, 1175, 1026, 835, 567 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{15}NO_4Na$ 260.0893; Found 260.0897.



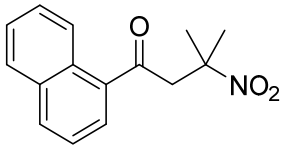
4-(3-Nitropentanoyl)benzonitrile (3sl)

Colorless oil (227 mg, 82% yield); R_f = 0.19 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, *J* = 8.3 Hz, 2H), 7.80 (d, *J* = 8.3 Hz, 2H), 5.10 (dd, *J* = 7.0, 3.6 Hz, 1H), 3.97 – 3.88 (m, 1H), 3.23 (dd, *J* = 18.3, 4.0 Hz, 1H), 2.11 – 1.99 (m, 2H), 1.06 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.13, 138.68, 132.70, 128.53, 117.64, 117.16, 83.49, 40.67, 27.17, 9.99; IR (film) ν_{max} 1692, 1541, 1420, 1361, 1287, 1240, 1142, 1026, 922, 802, 756, 679 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{12}H_{12}N_2O_3Na$ 255.074; Found 255.0737.



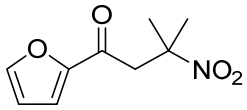
3-Methyl-1-(naphthalen-2-yl)-3-nitrobutan-1-one (3a′a)

White solid (285 mg, 93% yield); R_f = 0.27 (10:1 hexanes/AcOEt); m.p. 119.5–120.5 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 8.02 – 7.95 (m, 2H), 7.90 (dd, *J* = 13.8, 8.5 Hz, 2H), 7.66 – 7.60 (m, 1H), 7.60 – 7.55 (m, 1H), 3.82 (s, 2H), 1.82 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.88, 135.80, 133.84, 132.42, 129.77, 129.60, 128.82, 128.71, 127.84, 127.02, 123.48, 85.14, 47.16, 26.67; IR (film) ν_{max} 2922, 1680, 1539, 1466, 1362, 1126, 858, 818, 748 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{16}NO_3$ 258.1124; Found 258.1129.



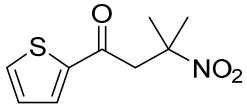
3-Methyl-1-(naphthalen-1-yl)-3-nitrobutan-1-one (3b′a)

White solid (282 mg, 92% yield); R_f = 0.27 (10:1 hexanes/AcOEt); m.p. 119.5–120.5 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.55 (d, *J* = 8.6 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.90 – 7.86 (m, 2H), 7.61 – 7.49 (m, 3H), 3.76 (s, 2H), 1.82 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.13, 135.24, 133.99, 133.23, 129.99, 128.48, 128.26, 127.42, 126.70, 125.57, 124.21, 85.20, 50.26, 26.75; IR (film) ν_{max} 2922, 1680, 1539, 1466, 1362, 1126, 858, 818, 748 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{15}H_{16}NO_3$ 258.1124; Found 258.1129.



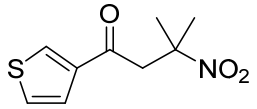
1-(Furan-2-yl)-3-methyl-3-nitrobutan-1-one (3c′a)

Colorless oil (216 mg, 92% yield); R_f = 0.23 (8:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 0.9 Hz, 1H), 7.22 (d, *J* = 3.6 Hz, 1H), 6.56 (dd, *J* = 3.6, 1.7 Hz, 1H), 3.52 (s, 2H), 1.74 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 184.14, 152.35, 146.66, 117.53, 112.60, 85.05, 46.57, 26.51; IR (film) ν_{max} 2365, 2340, 1543, 1464 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{11}NO_4Na$ 220.0586; Found 220.0584.



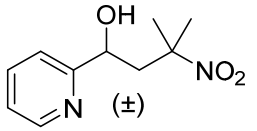
3-Methyl-3-nitro-1-(thiophen-2-yl)butan-1-one (3d′a)

Colorless oil (233 mg, 92% yield); R_f = 0.15 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (dd, *J* = 17.4, 5.0 Hz, 2H), 7.14 (d, *J* = 4.7 Hz, 1H), 3.60 (s, 2H), 1.76 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 187.83, 143.70, 134.44, 132.22, 128.26, 85.18, 47.48, 26.53; IR (film) ν_{max} 1607, 1543, 1462,1413, 1180, 1140, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{11}NO_3SNa$ 236.0351; Found 236.0349.



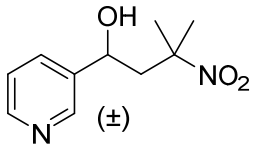
3-Methyl-3-nitro-1-(thiophen-3-yl)butan-1-one (3e′a)

White solid (233 mg, 92% yield); R_f = 0.15 (10:1 hexanes/AcOEt); m.p. 69.6–71.1 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 1.6 Hz, 1H), 7.52 (d, *J* = 5.1 Hz, 1H), 7.33 (d, *J* = 1.4 Hz, 1H), 3.58 (s, 2H), 1.75 (d, *J* = 1.5 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 189.23, 141.73, 132.34, 126.75, 126.70, 85.03, 48.11, 26.54; IR (film) ν_{max} 1607, 1543, 1462,1413, 1180, 1140, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{11}NO_3SNa$ 236.0351; Found 236.0349.



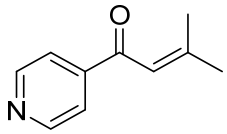
3-Methyl-3-nitro-1-(pyridin-2-yl)butan-1-ol (3f′a)

Colorless oil (195 mg, 78% yield); R_f = 0.86 (AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.52 – 8.48 (m, 1H), 7.73 – 7.66 (m, 1H), 7.30 – 7.19 (m, 2H), 4.82 (dd, *J* = 9.5, 3.1 Hz, 1H), 4.29 (t, *J* = 6.7 Hz, 1H), 2.39 – 2.29 (m, 2H), 1.73 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.00, 148.23, 137.06, 122.70, 120.25, 87.42, 69.60, 48.51, 26.61, 26.34; IR (film) ν_{max} 1593, 1539, 1470, 1142, 1076, 766 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{10}H_{15}N_2O_3$ 211.1077; Found 211.1071.



3-Methyl-3-nitro-1-(pyridin-3-yl)butan-1-ol (3g′a)

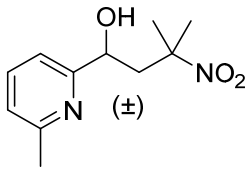
Colorless oil (188 mg, 75% yield); R_f = 0.43 (AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (s, 2H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.26 (s, 1H), 4.87 (dd, *J* = 10.1, 2.7 Hz, 1H), 2.53 (dd, *J* = 15.1, 10.1 Hz, 1H), 2.15 (dd, *J* = 15.1, 2.7 Hz, 1H), 1.71 (d, *J* = 2.3 Hz, 6H); ^{13}C NMR (101 MHz, Benzene-d_6) δ 148.78, 147.08, 140.08, 133.78, 123.75, 86.94, 77.32, 77.00, 76.68, 68.47, 48.49, 27.00, 26.06; IR (film) ν_{max} 1593, 1539, 1470, 1142, 1076, 766 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{10}H_{15}N_2O_3$ 211.1004; Found 211.1071.



3-Methyl-1-(pyridin-4-yl)but-2-en-1-one (3h′a)

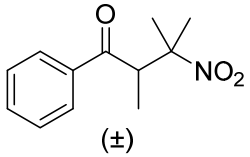
Colorless oil (133 mg, 69% yield); R_f = 0.45 (5:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.77 (d, *J* = 6.1 Hz, 2H), 7.72 – 7.66 (m, 2H), 6.71 (s, 1H), 2.26 (s, 3H), 2.05

(s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 189.79, 160.60, 150.62, 145.46, 121.26, 119.98, 28.26, 21.51; IR (film) ν_{max} 2926, 2384, 1659, 1381, 1132, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{10}H_{12}NO$ 162.0913; Found 162.0914.



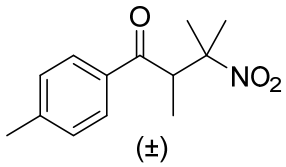
3-Methyl-1-(6-methylpyridin-2-yl)-3-nitrobutan-1-ol (3i′a)

Colorless oil (219 mg, 82% yield); R_f = 0.95 (AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (t, *J* = 7.7 Hz, 1H), 7.06 (t, *J* = 8.3 Hz, 2H), 4.77 (dd, *J* = 10.0, 2.5 Hz, 1H), 4.59 (s, 1H), 2.54 (s, 3H), 2.39 – 2.34 (m, 1H), 2.29 – 2.22 (m, 1H), 1.75 (d, *J* = 3.5 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.86, 157.18, 137.27, 122.14, 117.08, 87.62, 69.12, 48.91, 26.63, 26.46, 24.16; IR (film) ν_{max} 1599, 1539,1460, 1180, 1140, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{11}H_{17}N_2O_3$ 225.1233; Found 225.1231.



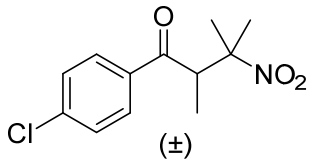
2,3-Dimethyl-3-nitro-1-phenylbutan-1-one (3j′a)[61]

Colorless oil (216 mg, 82% yield); R_f = 0.28 (20:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 7.0 Hz, 2H), 7.62 – 7.56 (m, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 4.41 (q, *J* = 7.2 Hz, 1H), 1.72 (d, *J* = 20.4 Hz, 6H), 1.24 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 200.48, 136.54, 133.52, 128.84, 128.36, 90.67, 46.62, 23.84, 14.20.



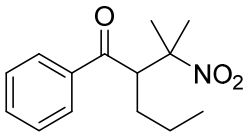
2,3-Dimethyl-3-nitro-1-(*p*-tolyl)butan-1-one (3k′a)

White solid (238 mg, 85% yield); R_f = 0.25 (20:1 hexanes/AcOEt); m.p. 82.1–83.2 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 7.5 Hz, 3H), 4.38 (q, *J* = 7.2 Hz, 1H), 2.42 (s, 3H), 1.70 (d, *J* = 19.7 Hz, 6H), 1.22 (d, *J* = 7.9 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.98, 144.51, 134.05, 129.52, 128.52, 90.72, 46.44, 24.38, 21.60, 14.21.



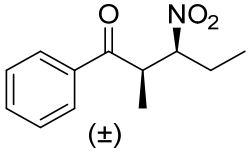
1-(4-Chlorophenyl)-2,3-dimethyl-3-nitrobutan-1-one (3l′a)

White solid (253 mg, 83% yield); R_f = 0.22 (20:1 hexanes/AcOEt); m.p. 122.0–122.8 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.86 (m, 2H), 7.50 – 7.44 (m, 2H), 4.33 (q, *J* = 7.3 Hz, 1H), 1.71 (d, *J* = 6.7 Hz, 6H), 1.24 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.30, 140.11, 134.77, 129.78, 129.17, 90.61, 46.59, 24.27, 14.21.



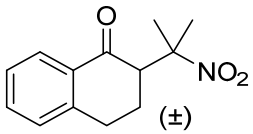
2-(2-Nitropropan-2-yl)-1-phenylpentan-1-one (3m′a)

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 7.0 Hz, 2H), 7.69 – 7.57 (m, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 4.44 (dd, *J* = 11.0, 3.0 Hz, 1H), 1.92 (dddd, *J* = 12.9, 11.0, 9.2, 5.7 Hz, 1H), 1.71 (s, 3H), 1.53 (s, 3H), 1.34 (dt, *J* = 6.7, 3.4 Hz, 1H), 1.25 (s, 2H), 0.84 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 201.07, 138.50, 133.70, 128.91, 128.44, 90.95, 51.35, 31.74, 26.13, 22.10, 21.19, 14.05; IR (film) ν_{max} 2957, 1680, 1537, 1180, 1142, 1076 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{14}H_{19}NO_3Na$ 272.1257; Found 272.1260.



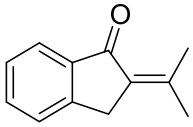
(2*R*,3*S*)-2-Methyl-3-nitro-1-phenylpentan-1-one (3j′l)[64]

Colorless oil (197 mg, 75% yield); R_f = 0.35 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.98 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.48 (m, 2H), 4.99 – 4.94 (m, 1H), 4.18 (dd, *J* = 9.5, 7.3 Hz, 1H), 2.15 (s, 1H), 1.99 – 1.93 (m, 1H), 1.24 (d, *J* = 7.3 Hz, 3H), 1.02 (t, *J* = 7.4 Hz, 3H);^{13}C NMR (151 MHz, Chloroform-*d*) δ 200.31, 135.07, 133.63, 128.84, 128.49, 89.33, 42.41, 23.87, 14.22, 9.33.



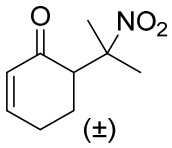
2-(2-Nitropropan-2-yl)-3,4-dihydronaphthalen-1(2H)-one (3n′a)

Colorless oil (172 mg, 62% yield); R_f = 0.15 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 7.9 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 20.0 Hz, 3H), 3.57 (dd, *J* = 13.9, 3.9 Hz, 1H), 3.22 – 3.01 (m, 2H), 2.16 (d, *J* = 9.9 Hz, 1H), 2.00 (s, 1H), 1.73 (s, 3H), 1.65 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.54, 143.07, 133.71, 132.55, 128.56, 127.61, 126.90, 88.69, 77.20, 54.85, 29.50, 25.69, 25.35, 22.37; IR (film) ν_{max} 2924, 2365, 1543, 1181, 1140, 1074, 554 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{13}H_{15}NO_3Na$ 256.0944; Found 256.0937.



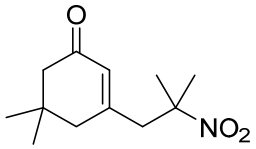
2-(Propan-2-ylidene)-2,3-dihydro-1H-inden-1-one (3o′a)[65]

Colorless oil (168 mg, 82% yield); R_f = 0.33 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.55 (td, *J* = 7.4, 1.3 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 3.65 (s, 2H), 2.44 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.02, 149.64, 147.85, 140.37, 133.67, 130.42, 127.16, 125.90, 123.89, 32.22, 24.53, 20.43.



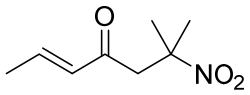
6-(2-Nitropropan-2-yl)cyclohex-2-en-1-one (3p′a)

White solid (112 mg, 51% yield); R_f = 0.3 (10:1 hexanes/AcOEt); m.p. 82.1–83.2 °C; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.97 – 6.93 (m, 1H), 5.99 (dt, *J* = 10.0, 2.0 Hz, 1H), 3.37 (dd, *J* = 14.2, 4.0 Hz, 1H), 2.54 – 2.47 (m, 2H), 2.02 – 1.98 (m, 1H), 1.89 – 1.82 (m, 1H), 1.70 (s, 3H), 1.58 (d, *J* = 8.1 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.66, 149.16, 130.19, 88.68, 29.69, 26.40, 25.09, 24.51, 22.91; IR (film) ν_{max} 3418, 2388, 1615, 1397 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{13}NO_3Na$ 206.0787; Found 206.0788.



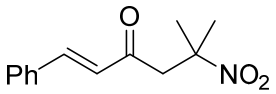
5,5-Dimethyl-3-(2-methyl-2-nitropropyl)cyclohex-2-en-1-one (3q′a)

Colorless oil (156 mg, 58% yield); R_f = 0.2 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.85 (s, 1H), 2.81 (s, 2H), 2.19 (s, 2H), 2.07 (s, 2H), 1.61 (s, 6H), 1.00 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.27, 155.98, 129.52, 86.99, 50.79, 48.33, 44.20, 33.78, 28.10, 26.35; IR (film) ν_{max} 2959, 1670, 1539, 1468, 1371, 1180, 1139, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{20}NO_3$ 226.1437; Found 226.1432.



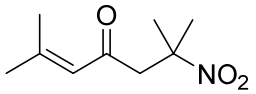
(*E*)-6-Methyl-6-nitrohept-2-en-4-one (3r′a)

Colorless oil (165 mg, 81% yield); R_f = 0.17 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.86 (dd, *J* = 15.7, 6.9 Hz, 1H), 6.09 (dt, *J* = 15.8, 1.6 Hz, 1H), 3.20 (s, 2H), 1.89 (dd, *J* = 6.9, 1.6 Hz, 3H), 1.66 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.71, 143.94, 131.47, 84.90, 48.30, 26.40, 18.22; IR (film) ν_{max} 2918.42, 1543.12, 1132.26, 1076.33, 630.75 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_8H_{13}NO_3Na$ 194.0787; Found 194.0790.



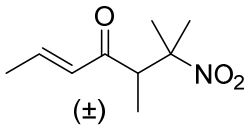
(*E*)-5-Methyl-5-nitro-1-phenylhex-1-en-3-one (3s′a)

Colorless oil (217 mg, 78% yield); R_f = 0.17 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 – 7.54 (m, 3H), 7.42 – 7.40 (m, 2H), 6.73 (s, 1H), 6.70 (s, 1H), 3.35 (s, 2H), 1.73 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 194.70, 134.05, 130.88, 129.03, 128.43, 128.18, 125.64, 85.21, 49.26, 26.50; IR (film) ν_{max} 2922.28, 1541.19, 1076.33, 555.52 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{13}H_{15}NO_3Na$ 256.0944; Found 256.0950.



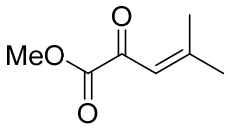
2,6-Dimethyl-6-nitrohept-2-en-4-one (3t′a)[66]

Colorless oil (170 mg, 77% yield); R_f = 0.22 (20:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.00 (d, *J* = 1.3 Hz, 1H), 3.07 (s, 2H), 2.12 (s, 3H), 1.88 (s, 3H), 1.65 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.06, 157.84, 123.17, 52.14, 27.78, 26.42, 20.92.



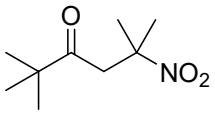
(*E*)-5,6-Dimethyl-6-nitrohept-2-en-4-one (3u′a)

Colorless oil (172 mg, 78% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.94 (dd, *J* = 15.6, 6.9 Hz, 1H), 6.19 (d, *J* = 15.6 Hz, 1H), 3.64 (d, *J* = 7.2 Hz, 1H), 1.92 (d, *J* = 6.9 Hz, 3H), 1.63 (d, *J* = 3.6 Hz, 6H), 1.13 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.03, 144.37, 131.02, 90.29, 49.76, 23.92, 23.61, 18.29, 13.22; IR (film) ν_{max} 1385, 1180, 1142, 1074, 918, 636, 547 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{15}NO_3Na$ 208.0944; Found 208.0950.



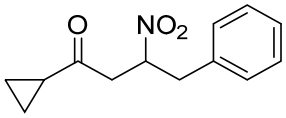
Methyl 4-methyl-2-oxopent-3-enoate (3v′a)

Colorless oil (105 mg, 62% yield); R_f = 0.25 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.87 – 6.34 (m, 1H), 3.86 (s, 3H), 2.26 (s, 3H), 2.03 (d, *J* = 1.3 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.58, 165.03, 162.93, 119.09, 52.82, 21.85.



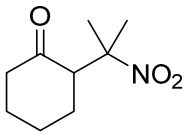
2,2,5-Trimethyl-5-nitrohexan-3-one (3w′a)

Colorless oil (107 mg, 48% yield); R_f = 0.25 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.18 (s, 2H), 1.66 (s, 6H), 1.15 (s, 9H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 211.01, 84.77, 45.50, 44.32, 26.52, 26.22; IR (film) ν_{max} 2922, 1464, 1132, 1076 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_9H_{17}NO_3Na$ 210.1106; Found 210.1102.



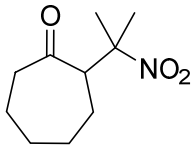
1-Cyclopropyl-3-nitro-4-phenylbutan-1-one (3x′a)

Colorless oil (199 mg, 72% yield); R_f = 0.35 (20:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.34 – 7.31 (m, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.18 – 7.16 (m, 2H), 5.17 (ddd, *J* = 15.4, 7.5, 4.4 Hz, 1H), 3.40 (dd, *J* = 18.2, 8.8 Hz, 1H), 3.31 (s, 1H), 3.14 (s, 1H), 2.88 (d, *J* = 18.2 Hz, 1H), 1.90 (t, *J* = 4.5 Hz, 1H), 1.07 – 1.02 (m, 2H), 0.96 – 0.89 (m, 2H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 205.75, 134.88, 129.08, 128.94, 127.66, 83.31, 44.27, 39.62, 20.75, 11.45, 11.27; IR (film) ν_{max} 2924, 1699, 1551, 1451, 1393, 1180, 1138, 1074, 1018, 918 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{13}H_{15}NO_3Na$ 256.0944; Found 256.0941.



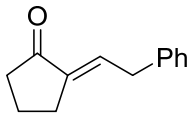
2-(2-Nitropropan-2-yl)cyclohexan-1-one (3y′a)

Colorless oil (130 mg, 59% yield); R_f = 0.17 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.32 (dd, *J* = 13.3, 5.2 Hz, 1H), 2.38 (dd, *J* = 10.6, 5.8 Hz, 2H), 2.16 – 2.08 (m, 1H), 2.00 (s, 2H), 1.73 (m, 2H),1.66 (s, 4H), 1.56 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 208.12, 88.64, 57.23, 42.72, 29.68, 27.58, 25.27, 24.76, 22.73; IR (film) ν_{max} 2924, 1699, 1551, 1451, 1393, 1180, 1138, 1074, 1018, 918 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{13}H_{15}NO_3Na$ 256.0944; Found 256.0941.



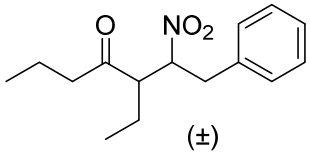
2-(2-Nitropropan-2-yl)cycloheptan-1-one (3z′a)

Colorless oil (171 mg, 72% yield); R_f = 0.18 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 3.46 (dd, *J* = 10.9, 2.5 Hz, 1H), 2.65 – 2.58 (m, 1H), 2.42 (dd, *J* = 11.8, 4.6 Hz, 1H), 1.98 – 1.90 (m, 3H), 1.66 (s, 7H), 1.60 (s, 3H), 1.49 – 1.42 (m, 1H), 1.35 (d, *J* = 11.1 Hz, 1H), 1.28 – 1.22 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-d) δ 211.74, 90.41, 57.14, 43.88, 29.46, 28.71, 27.55, 25.20, 23.53, 22.96; IR (film) ν_{max} 2924, 1699, 1551, 1451, 1393, 1180, 1138, 1074, cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{10}H_{17}NO_3Na$ 222.1106; Found 222.1102.



(*E*)-2-(2-Phenylethylidene)cyclopentan-1-one (3a″m)

Colorless oil (131 mg, 59% yield); R_f = 0.14 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.16 (m, 5H), 6.75 – 6.67 (m, 1H), 3.49 (d, *J* = 7.7 Hz, 2H), 2.73 – 2.65 (m, 2H), 2.36 (t, *J* = 7.8 Hz, 2H), 2.03 – 1.95 (m, 2H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 207.09, 138.51, 137.75, 133.76, 128.67, 128.47, 126.48, 38.60, 35.81, 26.83, 19.76; IR (film) ν_{max} 2963, 1719, 1649, 1175, 1074, 698 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{13}H_{15}O$ 187.1117; Found 187.1110.



(±)

3-Ethyl-2-nitro-1-phenylheptan-4-one (3b″m)

Colorless oil (194 mg, 79% yield); *syn* : *anti* = 40 : 60.

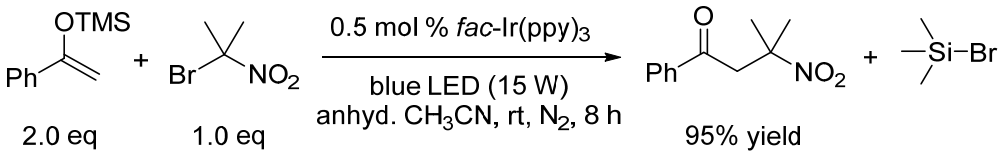
***syn*-isomer:** R_f = 0.42 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.22 (m, 3H), 7.14 – 7.10 (m, 2H), 4.99 (td, *J* = 10.4, 3.4 Hz, 1H), 3.16 (ddd, *J* = 10.0, 6.3, 5.2 Hz, 1H), 3.05 (d, *J* = 10.7 Hz, 1H), 2.99 (d, *J* = 3.3 Hz, 1H), 2.61 – 2.43 (m, 2H), 1.64 (dd, *J* = 7.4, 2.4 Hz, 4H), 0.91 (dt, *J* = 31.0, 7.4 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 209.66, 135.22, 128.77, 128.65, 127.50, 90.49, 55.15, 46.28, 38.40, 22.54, 16.67, 13.60, 10.07; IR (film)

ν_{max} 2967, 2932, 2878, 1711, 1551, 1458, 1375, 700 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{21}NO_3Na$ 286.1413; Found 286.1416.

***anti*-isomer:** R_f = 0.38 (20:1 hexanes/AcOEt); ^1H NMR (600 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 3H), 7.13 – 7.09 (m, 2H), 5.04 – 4.99 (m, 1H), 3.29 (dd, *J* = 14.7, 3.9 Hz, 1H), 3.21 (s, 1H), 3.08 (dd, *J* = 14.7, 8.8 Hz, 1H), 2.55 – 2.40 (m, 2H), 1.86 – 1.75 (m, 2H), 1.60 – 1.54 (m, 2H), 0.90 (dt, *J* = 18.0, 7.5 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 210.15, 134.77, 128.81, 127.60, 77.20, 53.52, 45.11, 36.89, 21.18, 16.55, 13.54, 10.32; IR (film) ν_{max} 2967, 2932, 2878, 1711, 1551, 1458, 1375, 700 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{21}NO_3Na$ 286.1413; Found 286.1416.

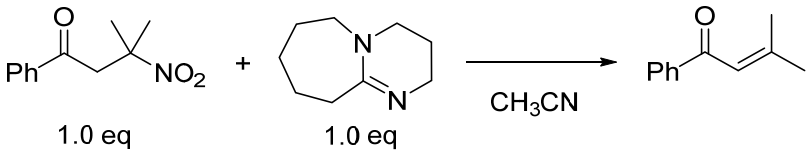
6. Conversions of coupling products

6.1 Gram-scale reaction

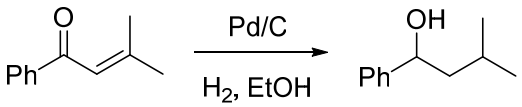


A Schlenk tube equipped with a stirring bar was evacuated and backfilled with N_2 (three times). Geminal bromonitroalkane **2a** (1.00 g, 5.95 mmol), silyl enol ether of acetophenone **1a** (1.23 g, 11.9 mmol) and *fac*-Ir(ppy)$_3$ (20 mg, 0.50 % mmol) were placed. Then, anhydrous acetonitrile (CH_3CN, 20.0 mL) was added via a gastight syringe under N_2 atmosphere. The reaction mixture was degassed by freeze-pump-thaw method and then stirred overnight under irradiation with blue LEDs (460 nm, app. 3.0 cm distance from the tube), maintained at approximately room temperature (25 °C) by a desk fan in the air-conditioned room. Upon completion, the mixture was concentrated under vacuum. The product was purified by flash column chromatography (petroleum ether/ethyl acetate = 50:1–10:1) on silica gel to give the product **3aa** (white solid, 1.17 g, 95% yield).

6.2 Conversions of 3aa and 3al

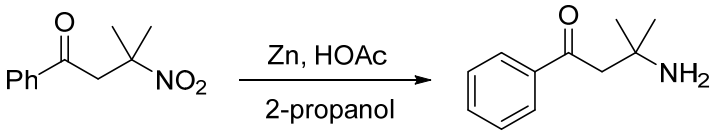


A Schlenk tube equipped with a stirring bar was evacuated and backfilled with N_2 (three times). **3aa** (100 mg, 0.50 mmol) and DBU (75 μL, 0.50 mmol) were added. Then, anhydrous acetonitrile (CH_3CN, 10 mL) was added via a gastight syringe under N_2 atmosphere. The reaction mixture was stirred 5 h, and monitored by TLC. Upon completion, the mixture was concentrated under vacuum. The crude product was purified by flash column chromatography (petroleum ether/ethyl acetate = 10:1) on silica gel to give the product **4a** (colorless oil, 73 mg, 91% yield).

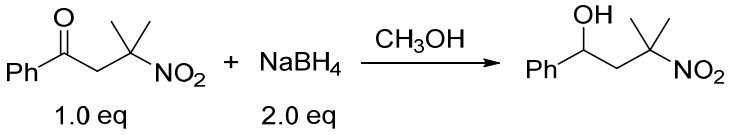


To a Schlenk tube were added **4a** (80 mg, 0.50 mmol), 10% Pd/C (30 mg in wet) and EtOH (15 mL). The mixture was well stirred under hydrogen atmosphere overnight. Pd/C was filtered and

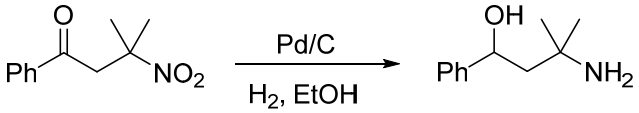
washed with EtOH. The filtrate was concentrated and the residue dried in vacuo. The product was purified by flash column chromatography on silica gel to give 3-methyl-1-phenylbutan-1-ol **4b** as a colorless oil (petroleum ether/ethyl acetate = 2:1).



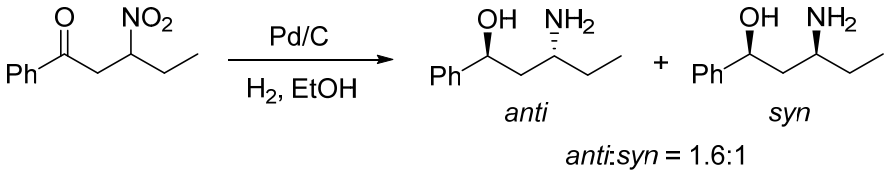
To a solution of **3aa** (100 mg, 0.50 mmol) in 2-propanol (2 mL) was added zinc dust (65 mg, 1.0 mmol) and acetic acid (0.15 mL) at room temperature. The resulting mixture was stirred for 6 h and then quenched with saturated aqueous $NaHCO_3$. The solution was filtrated through Celite to remove zinc dust. The filtrate was extracted with CH_2Cl_2, and the extracts were washed with brine and dried over Na_2SO_4. After evaporation of solvents, the product **4c** was obtained in 82% yield (73 mg).



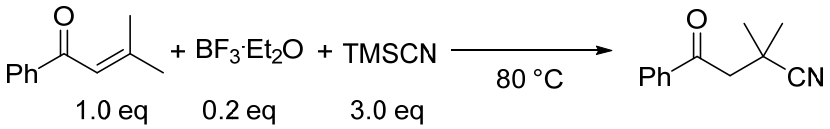
3aa (100 mg, 0.50 mmol) was added to a 100ml flame-dried round-bottomed flask containing methanol (20 mL), followed by $NaBH_4$(38 mg, 1.0 mmol) in portions. After 3 h, the mixture was concentrated under vacuum, diluted by water and extracted with DCM (3 × 10 mL). The organic layers were combined and concentrated under vacuum. The product **4d** was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 10:1–5:1).



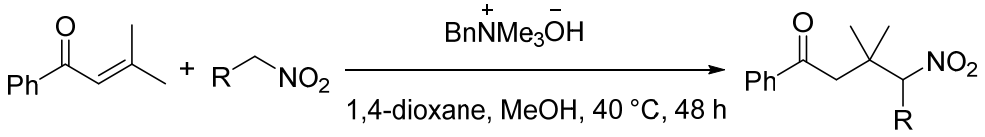
To a transparent Schlenk tube were added **3aa** (100 mg, 0.5 mmol), 10% Pd/C (30 mg in wet), and EtOH (15 mL). The mixture was well stirred under hydrogen atmosphere overnight. Pd/C was filtered and washed with EtOH. The filtrate was concentrated and the residue dried in vacuo. The yield of crude **4e** was 87%. The product was purified by flash column chromatography on silica gel (ethyl acetate/methanol = 1:1).



To a Schlenk tube were added **3al** (100 mg, 0.50 mmol), 10% Pd/C (30 mg in wet) and EtOH (15 mL). The mixture was well stirred under hydrogen atmosphere overnight. Pd/C was filtered and washed with EtOH. The filtrate was concentrated and the residue dried in vacuo. The yield of crude **4f** was 83%. The product was purified by flash column chromatography on silica gel (ethyl acetate/methanol = 1:1).



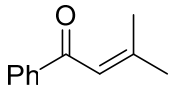
To a solution of **4a** (100 mg, 0.50 mmol) and TMSCN (0.2 mL, 1.5 mmol) was slowly added $BF_3{\cdot}Et_2O$ (15 μL, 0.10 mmol) at room temperature, the mixture was stirred at 80 °C for 12 h. After being cooled to 0 °C, the reaction was carefully quenched with saturated $NaHCO_3$ solution (5 mL) and extracted with ethyl acetate (3 × 10 mL). The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated in vacuo. The product **4g** was purified by flash column chromatography on silica (petroleum ether/ethyl acetate = 50:1–8:1).



1.0 eq 2.0 eq

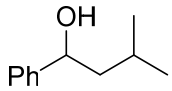
To a solution of nitroalkane (2.00 mmol), **4a** (200 mg, 1.00 mmol) in 1,4-dioxane (1 mL) was added a solution of benzyltrimethylammonium hydroxide (0.15 mL, 40% in MeOH) at ambient temperature. The solution was stirred at 40 °C for 48 h until completion of reaction. The reaction mixture was concentrated in vacuo to give a residue. The crude product was purified by flash column chromatography using 10:1 hexanes/AcOEt to give the product **4h** or **4i** as a colorless oil.

6.2 Physical data



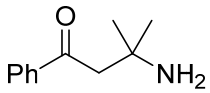
3-Methyl-1-phenylbut-2-en-1-one (4a)[65]

Yellow oil (73 mg, 91% yield); R_f = 0.7 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.83 (m, 2H), 7.53 – 7.39 (m, 3H), 6.79 – 6.67 (m, 1H), 2.20 (d, *J* = 1.3 Hz, 3H), 2.00 (d, *J* = 1.3 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.35, 156.51, 139.18, 132.15, 128.32, 128.07, 121.09, 27.85, 21.04.



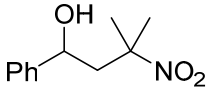
3-Methyl-1-phenylbutan-1-ol (4b)[67]

Colorless oil (66 mg, 80% yield); R_f = 0.1 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.26 (m, 5H), 4.75 (dd, *J* = 8.2, 5.4 Hz, 1H), 1.98(br, 1H),1.71 (d, *J* = 6.3 Hz, 2H), 1.52 (s, 1H), 0.97 (dd, *J* = 6.5, 2.5 Hz, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.21, 128.42, 127.44, 125.84, 72.74, 48.31, 24.75, 23.08, 22.22.



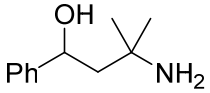
3-Amino-3-methyl-1-phenylbutan-1-one (4c)[68]

Colorless oil (73 mg, 80% yield); R_f = 0.1 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 3.28 (s, 2H), 1.47 (s, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.03, 136.42, 133.97, 128.74, 128.23, 53.78, 45.53, 26.12.



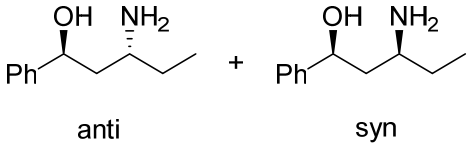
3-Methyl-3-nitro-1-phenylbutan-1-ol (4d)[69]

Colorless oil (108 mg, 93% yield); R_f = 0.3 (5:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.37 – 7.28 (m, 5H), 4.82 (dd, *J* = 10.0, 2.8 Hz, 1H), 2.53 (dd, *J* = 15.1, 10.0 Hz, 1H), 2.16 (dd, *J* = 15.1, 2.8 Hz, 1H), 1.70 (d, *J* = 9.8 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.19, 128.73, 128.03, 125.54, 87.08, 71.10, 48.78, 27.08, 25.92; ; IR (film) ν_{max} 2990, 2930, 1537, 1458, 1384, 1358, 1132, 1063, 756, 700 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{15}NONa$ 232.0944; Found 232.0948.



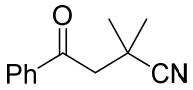
3-Amino-3-methyl-1-phenylbutan-1-ol (4e)[70]

Colorless oil (54 mg, 60% yield); R_f = 0.1 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (dd, *J* = 16.0, 7.1 Hz, 3H), 7.26 (s, 2H), 5.02 (d, *J* = 11.2 Hz, 1H), 2.91 (s, 1H), 1.97 (s, 1H), 1.83 – 1.75 (m, 1H), 1.61 (dd, *J* = 14.6, 2.3 Hz, 1H), 1.39 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.26, 128.29, 127.03, 125.64, 71.75, 51.50, 49.51, 34.10, 29.68, 26.25, 1.31.



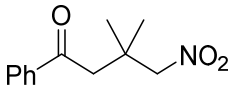
***anti*: (1*S*,3*R*)-3-amino-1-phenylpentan-1-ol; *syn*: (1*S*,3*S*)-3-amino-1-phenylpentan-1-ol (4f)**[70]

Colorless oil (52 mg, 52% yield); R_f = 0.1 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.38 (d, *J* = 8.2 Hz, 3H), 7.33 (td, *J* = 7.6, 3.8 Hz, 3H), 7.26 (s, 1H), 5.11 – 5.05 (m, 1H), 4.92 (dd, *J* = 10.6, 2.2 Hz, 1H), 2.93 (s, 1H), 2.83 (s, 1H), 1.86 – 1.75 (m, 3H), 1.54 – 1.29 (m, 6H), 0.92 (t, *J* = 7.5 Hz, 2H), 0.88 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 145.44, 128.23, 128.15, 126.98, 126.65, 125.63, 125.57, 75.56, 72.22, 50.44, 44.74, 42.49, 33.63, 31.08, 29.68, 10.22, 9.87.



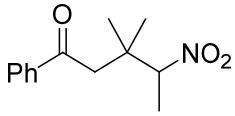
2,2-Dimethyl-4-oxo-4-phenylbutanenitrile (4g)[71,72]

White solid (78 mg, 83% yield); R_f = 0.2 (8:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 (t, *J* = 7.5 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.46 (m, 2H), 3.25 (s, 2H), 1.54 (s, 6H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.16, 136.48, 133.62, 128.75, 124.47, 47.43, 29.59, 26.92.



3,3-Dimethyl-4-nitro-1-phenylbutan-1-one (4h)[73,74]

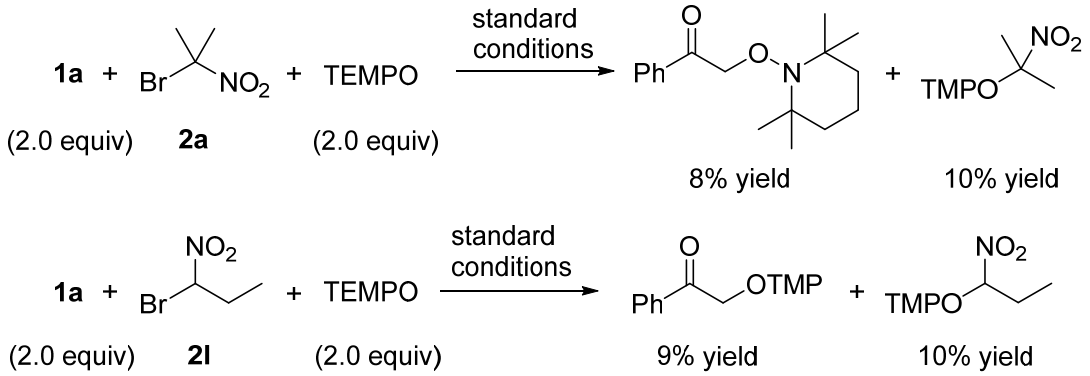
Colorless oil (78 mg, 83% yield); R_f = 0.2 (8:1 hexanes/AcOEt);[1]H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.91 (m, 2H), 7.61 – 7.55 (m, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 4.71 (s, 2H), 3.14 (s, 2H), 1.24 (s, 6H);[13]C NMR (101 MHz, Chloroform-*d*) δ 198.31, 137.46, 133.24, 128.64, 127.85, 83.58, 45.47, 34.48, 26.19.



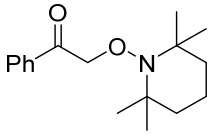
3,3-Dimethyl-4-nitro-1-phenylpentan-1-one (4i)[73,74]

Colorless oil (78 mg, 83% yield); R_f = 0.2 (8:1 hexanes/AcOEt); [1]H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.88 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 5.17 (q, *J* = 6.8 Hz, 1H), 3.20 (d, *J* = 17.1 Hz, 1H), 2.90 (d, *J* = 17.2 Hz, 1H), 1.52 (d, *J* = 6.8 Hz, 3H), 1.18 (d, *J* = 21.8 Hz, 6H); [13]C NMR (101 MHz, Chloroform-*d*) δ 198.32, 137.67, 133.18, 128.62, 127.90, 88.90, 77.20, 45.53, 36.83, 24.27, 23.75, 13.84.

7. Radical-trapping experiments



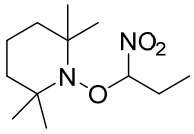
1-Phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethan-1-one[75]



Following the general procedure, obtained in 9% yield (for **2l**) as a colorless liquid after silica gel chromatography.

Colorless oil (59 mg, 9% yield); R_f = 0.65 (20:1 hexanes/AcOEt); [1]H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.89 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 5.10 (s, 2H), 1.45 (dd, *J* = 9.2, 4.0 Hz, 6H), 1.16 (s, 12H); [13]C NMR (101 MHz, Chloroform-*d*) δ 195.55, 135.23, 133.07, 128.41, 127.79, 81.15, 59.96, 39.55, 32.64, 32.15, 20.07, 16.87; IR (film) ν_{max} 2972, 2930, 1703, 1450, 1379, 1362, 1180, 1138, 1097, 1074, 972, 754, 690, 567 cm^{-1}; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{17}H_{26}NO_2$ 276.1958; Found 276.1960.

2,2,6,6-Tetramethyl-1-(1-nitropropoxy)piperidine



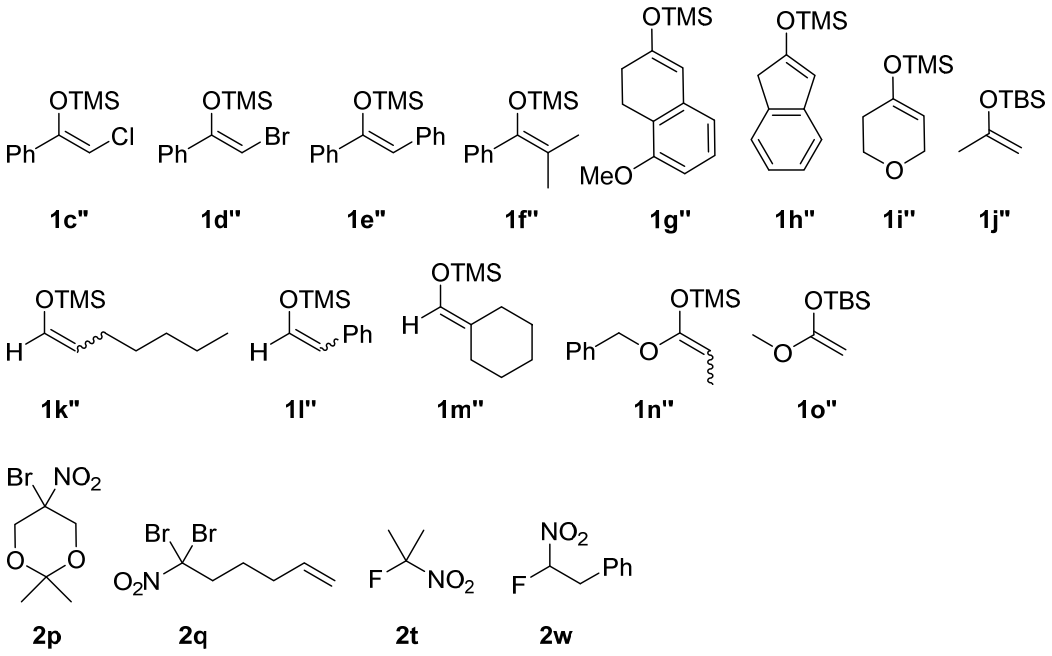
Following the general procedure, obtained in 10% yield as a reddish oil after silica gel

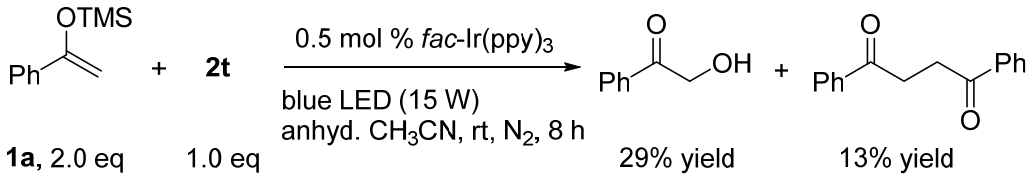
chromatography.

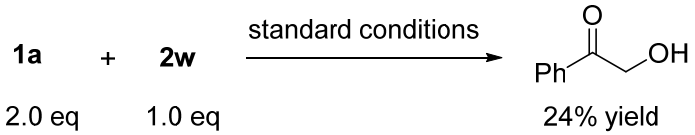
Reddish oil (29 mg, 10% yield); R_f = 0.7 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.61 – 5.52 (m, 1H), 2.27 – 1.93 (m, 2H), 1.52 (d, *J* = 43.1 Hz, 6H), 1.15 (d, *J* = 9.4 Hz, 9H), 0.93 (t, *J* = 7.5 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 94.13, 61.26, 59.55, 40.13, 39.86, 32.88, 31.72, 25.42, 20.05, 19.83, 16.65, 7.97, 0.00; IR (film) ν_{max} 2924, 1180, 1138, 1074 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{24}N_2O_3$ 245.1859; Found 245.1856.

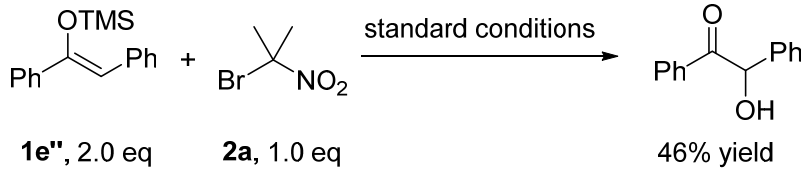
8. Unsuccessful coupling reactions

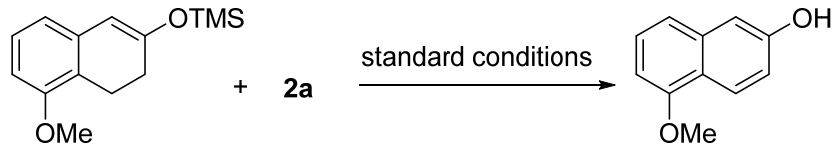
8.1 Unsuccessful coupling reactants

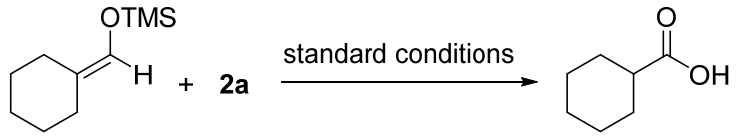


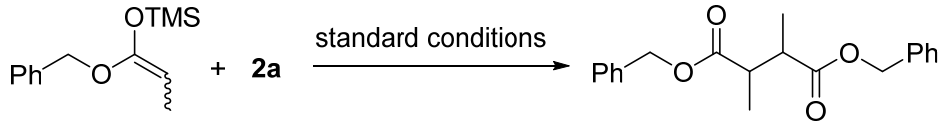




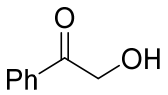






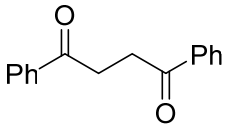


8.2 Physical data



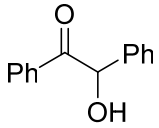
2-Hydroxy-1-phenylethan-1-one[76]

Colorless oil (94 mg, 29% yield); R_f = 0.3 (10:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.56 (d, *J* = 7.4 Hz, 1H), 7.47 (dd, *J* = 8.3, 7.2 Hz, 2H), 5.57 (s, 1H), 3.46 (s, 2H).



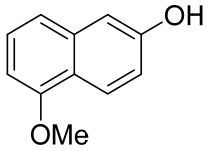
1,4-Diphenylbutane-1,4-dione[77]

White solid (37 mg, 13% yield); R_f = 0.65 (20:1 hexanes/AcOEt); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 8.3, 1.3 Hz, 4H), 7.58 (t, *J* = 7.4 Hz, 2H), 7.50 – 7.46 (m, 4H), 3.47 (s, 4H); ^{13}C NMR (151 MHz, Chloroform-*d*) δ 198.72, 136.79, 133.16, 128.61, 128.13, 32.58.



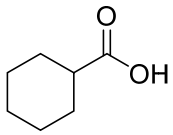
2-Hydroxy-1,2-diphenylethan-1-one[78]

White solid (232 mg, 46% yield); R_f = 0.2 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (dd, *J* = 8.5, 1.3 Hz, 2H), 7.56 – 7.49 (m, 1H), 7.44 – 7.37 (m, 2H), 7.37 – 7.32 (m, 4H), 7.31 – 7.27 (m, 1H), 5.96 (s, 1H), 4.55 (d, *J* = 6.1 Hz, 1H).



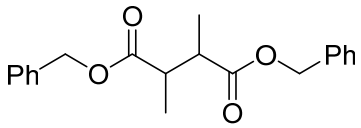
5-Methoxynaphthalen-2-ol[79]

Colorless oil (101 mg, 24% yield); R_f = 0.13 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 9.0 Hz, 1H), 7.38 – 7.30 (m, 1H), 7.27 (s, 1H), 7.14 – 7.02 (m, 2H), 6.67 (d, *J* = 7.5 Hz, 1H), 5.09 (s, 1H), 3.98 (s, 3H).



Cyclohexanecarboxylic acid[80]

Colorless oil (52 mg, 17% yield); R_f = 0.2 (10:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.39 – 2.23 (m, 1H), 1.93 (dd, *J* = 13.3, 2.7 Hz, 2H), 1.84 – 1.56 (m, 4H), 1.53 – 1.39 (m, 2H), 0.92 – 0.81 (m, 2H).



Dibenzyl 2,3-dimethylsuccinate (*dl*:*meso* = 1:1)

Colorless oil (245 mg, 63% yield); R_f = 0.3 (20:1 hexanes/AcOEt); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.29 (m, 10H), 5.08 (d, *J* = 4.7 Hz, 4H), 2.88 (ddd, *J* = 21.9, 4.9, 2.1 Hz, 2H), 1.19 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.84, 174.16, 135.86, 135.76, 128.46, 128.18, 128.11, 128.08, 66.35, 66.32, 42.47, 41.60, 14.63, 13.58; IR (film) ν_{max} 2924, 1685, 1583, 1490, 1452, 1362, 1382, 1200, 1074, 709 cm^{-1}; HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{12}H_{24}N_2O_3$ 327.159; Found 327.1586.

9. References

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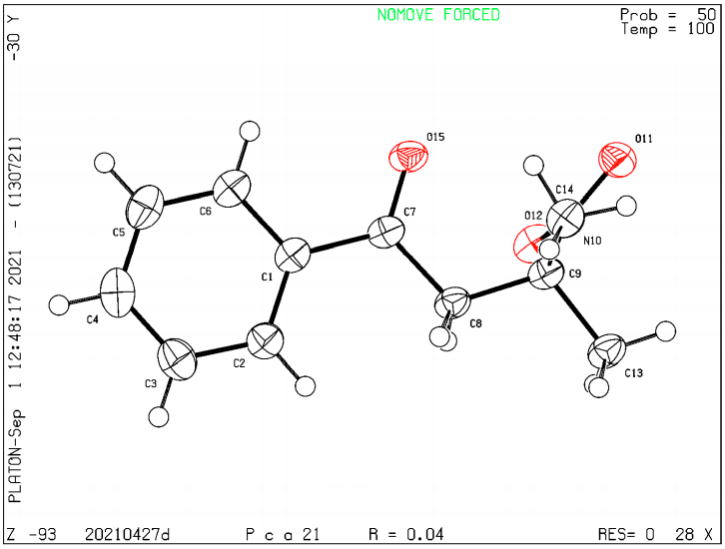
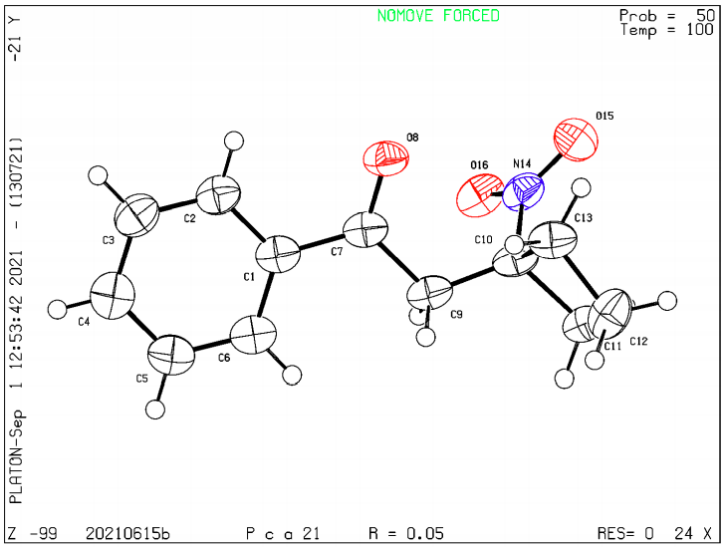
10. Crystal data

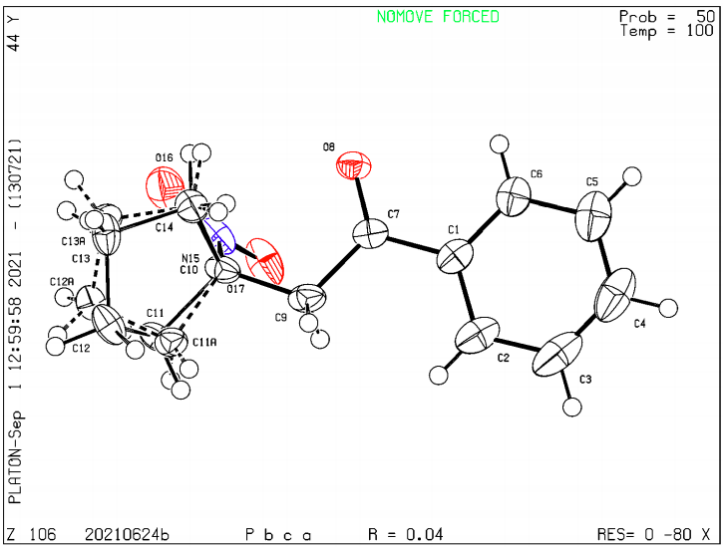
CCDC numbers: 2107700 (**3aa**), 2107697 (**3ac**), 2108083 (**3ad**), 2107698 (**3ag**), 2107699 (**3an**), 2107696 (**3p′a**), 2109233 (**2,2,6,6-tetramethylpiperidine benzoylformate**)



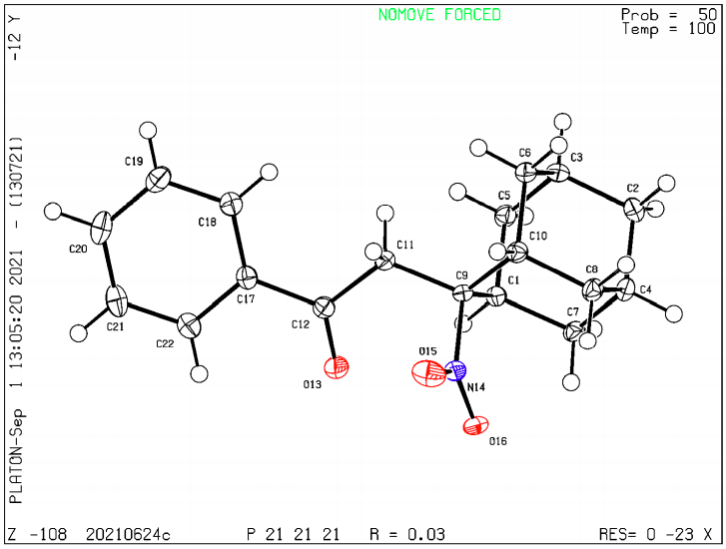
Crystal data and structure refinement for 3aa.	
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	10.2718(2)
b/Å	9.7571(3)
c/Å	10.9209(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1094.53(5)
Z	4
ρ_{calc}g/cm^3	0.261
μ/mm^{-1}	0.207
F(000)	88.0
Crystal size/mm^3	0.5 × 0.2 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.064 to 152.016
Index ranges	$-12 \le h \le 12$, $-12 \le k \le 12$, $-13 \le l \le 12$
Reflections collected	18887
Independent reflections	2179 [R_{int} = 0.0601, R_{sigma} = 0.0273]
Data/restraints/parameters	2179/1/138
Goodness-of-fit on F^2	1.093
Final R indexes [I>=2σ (I)]	R_1 = 0.0356, wR_2 = 0.0975
Final R indexes [all data]	R_1 = 0.0363, wR_2 = 0.0984
Largest diff. peak/hole / e Å^{-3}	0.18/-0.17
Flack parameter	0.17(12)



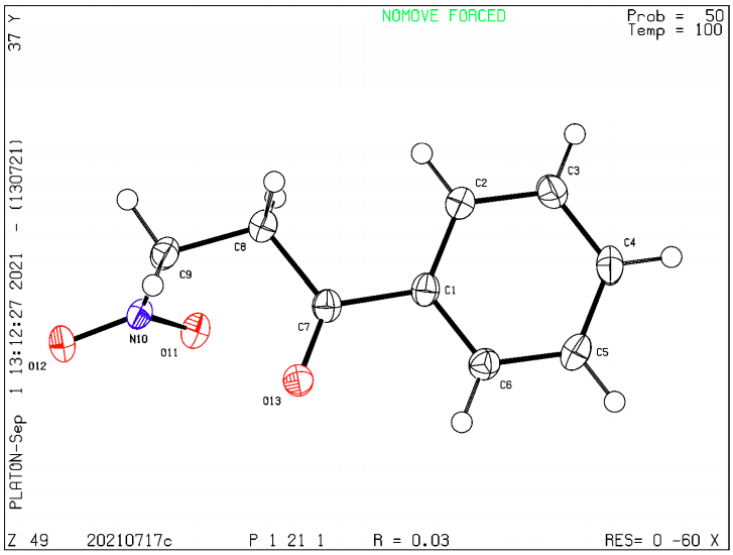
Crystal data and structure refinement for 3ac.	
Temperature/K	100(1)
Crystal system	orthorhombic
Space group	$Pca2_1$
a/Å	10.0228(5)
b/Å	9.8396(5)
c/Å	11.0400(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1088.77(9)
Z	4
ρ_{calc}g/cm^3	1.337
μ/mm^{-1}	0.798
F(000)	464.0
Crystal size/mm^3	0.4 × 0.15 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.988 to 153.54
Index ranges	-12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -13 ≤ l ≤ 13
Reflections collected	18412
Independent reflections	2207 [R_{int} = 0.0938, R_{sigma} = 0.0357]
Data/restraints/parameters	2207/1/146
Goodness-of-fit on F^2	1.127
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.1557
Final R indexes [all data]	R_1 = 0.0580, wR_2 = 0.1625
Largest diff. peak/hole / e Å^{-3}	0.22/-0.31
Flack parameter	-0.1(2)



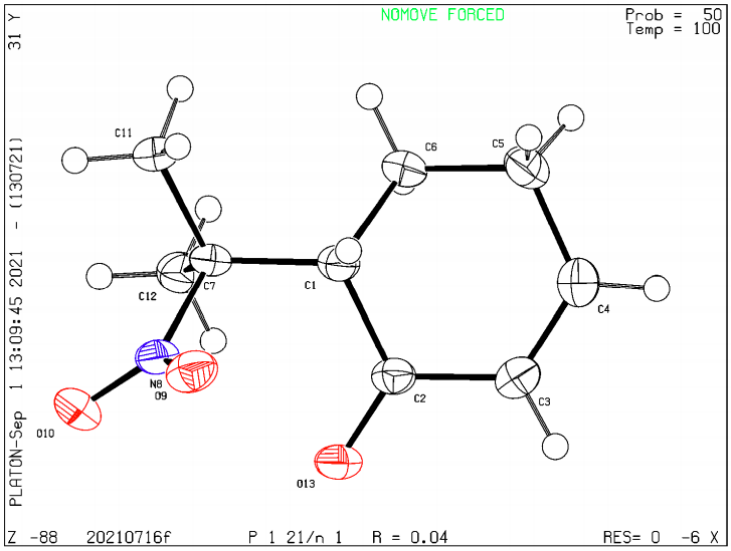
Crystal data and structure refinement for 3ad.	
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	10.15647(11)
b/Å	11.03134(15)
c/Å	20.7789(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2328.05(5)
Z	8
ρ_{calc}g/cm^3	1.331
μ/mm^{-1}	0.778
F(000)	992.0
Crystal size/mm^3	0.4 × 0.2 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.51 to 152.284
Index ranges	-12 ≤ h ≤ 12, -12 ≤ k ≤ 13, -24 ≤ l ≤ 26
Reflections collected	20591
Independent reflections	2397 [R_{int} = 0.0412, R_{sigma} = 0.0181]
Data/restraints/parameters	2397/124/183
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0416, wR_2 = 0.1058
Final R indexes [all data]	R_1 = 0.0450, wR_2 = 0.1084
Largest diff. peak/hole / e Å^{-3}	0.29/-0.24



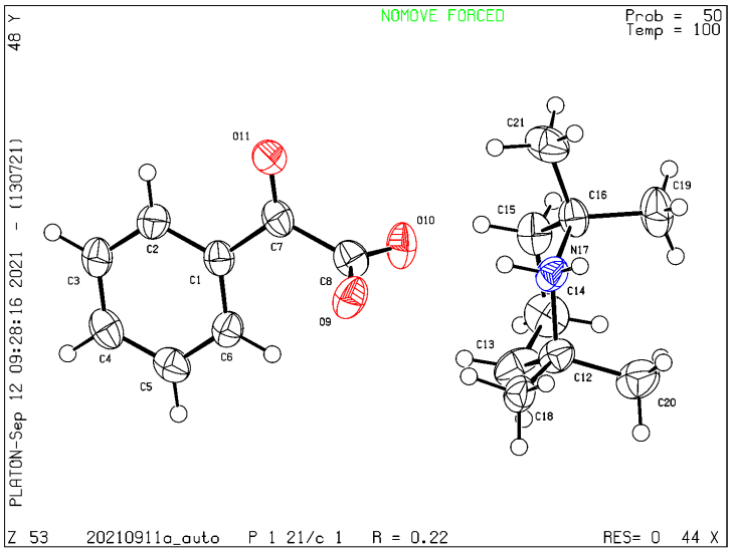
Crystal data and structure refinement for 3ag.	
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.58510(10)
b/Å	10.44770(10)
c/Å	21.3750(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1470.58(3)
Z	4
ρ_{calc}g/cm^3	1.352
μ/mm^{-1}	0.739
F(000)	640.0
Crystal size/mm^3	0.5 × 0.4 × 0.3
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.274 to 152.68
Index ranges	$-5 \le h \le 8$, $-13 \le k \le 13$, $-26 \le l \le 26$
Reflections collected	13735
Independent reflections	2971 [R_{int} = 0.0282, R_{sigma} = 0.0169]
Data/restraints/parameters	2971/0/200
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0275, wR_2 = 0.0739
Final R indexes [all data]	R_1 = 0.0278, wR_2 = 0.0741
Largest diff. peak/hole / e Å^{-3}	0.24/-0.17
Flack parameter	-0.01(6)



Crystal data and structure refinement for 3ao.	
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.61652(15)
b/Å	8.2450(3)
c/Å	9.0227(3)
α/°	90
β/°	92.654(2)
γ/°	90
Volume/Å^3	417.38(2)
Z	2
ρ_{calc}g/cm^3	1.426
μ/mm^{-1}	0.910
F(000)	188.0
Crystal size/mm^3	0.7 × 0.4 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.814 to 151.768
Index ranges	$-6 \le h \le 6$, $-10 \le k \le 10$, $-11 \le l \le 11$
Reflections collected	7648
Independent reflections	1631 [R_{int} = 0.0439, R_{sigma} = 0.0222]
Data/restraints/parameters	1631/1/119
Goodness-of-fit on F^2	1.095
Final R indexes [I>=2σ (I)]	R_1 = 0.0315, wR_2 = 0.0904
Final R indexes [all data]	R_1 = 0.0317, wR_2 = 0.0906
Largest diff. peak/hole / e Å^{-3}	0.24/-0.17
Flack parameter	-0.14(16)

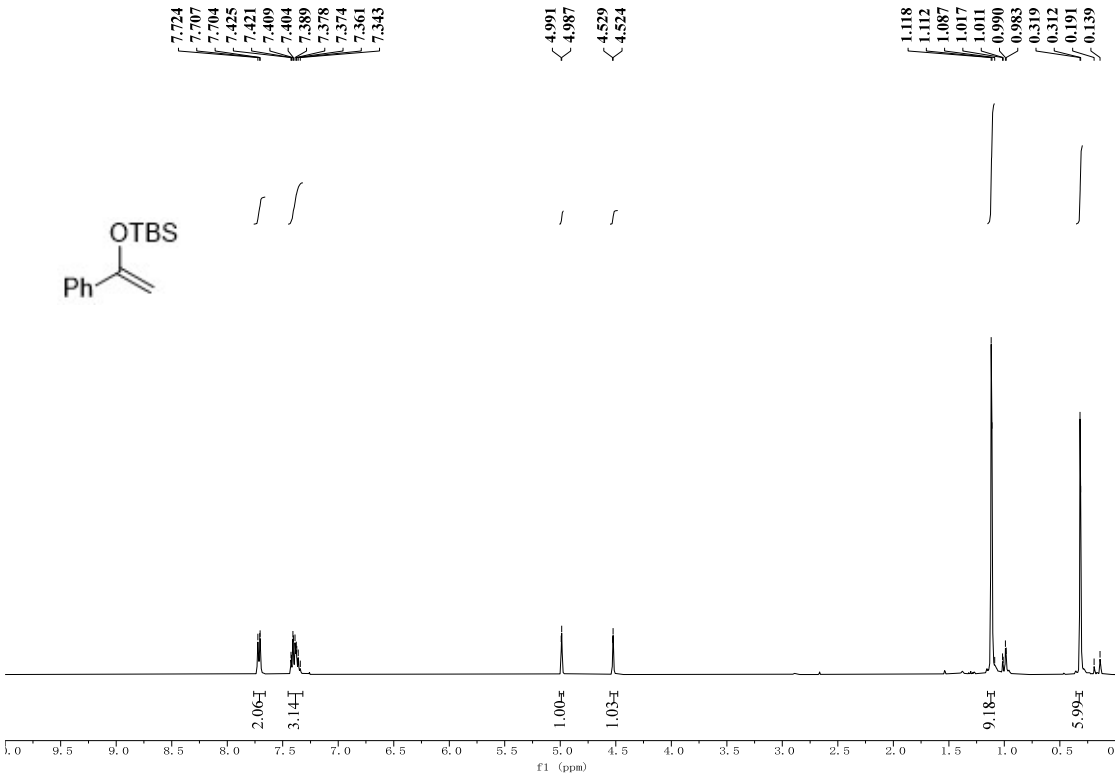


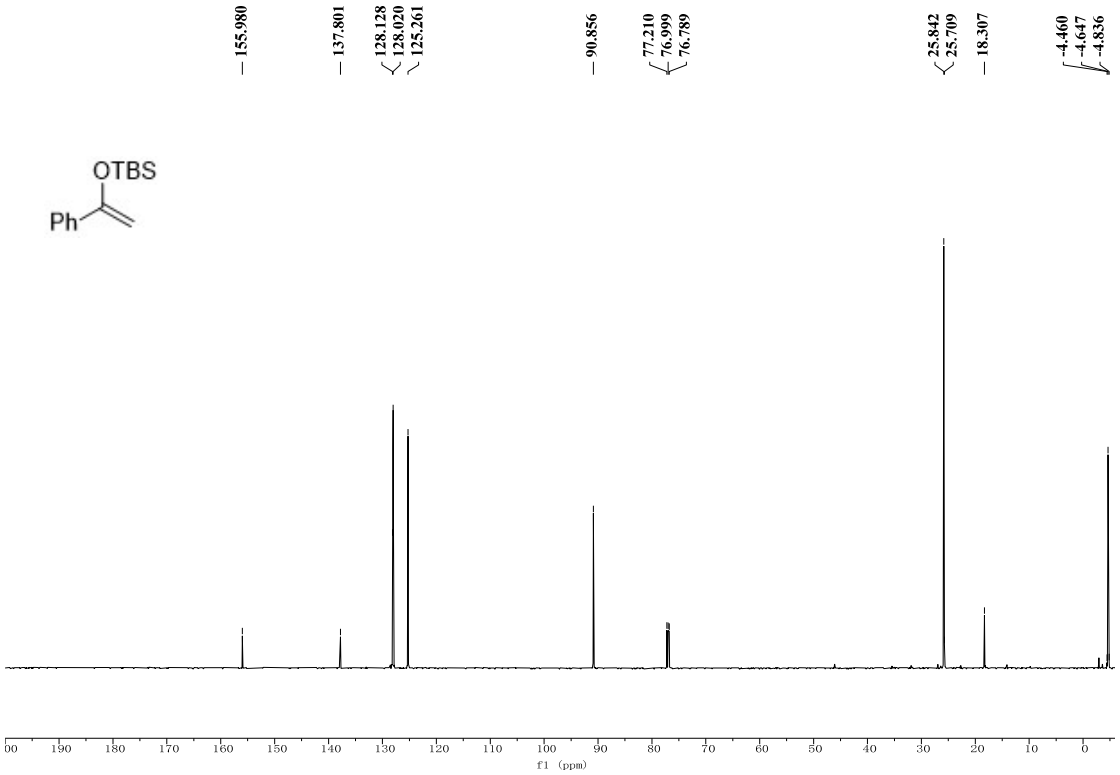
Crystal data and structure refinement for 3p′a.	
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.94438(17)
b/Å	15.3656(5)
c/Å	9.9491(4)
α/°	90
β/°	96.274(3)
γ/°	90
Volume/Å^3	903.30(5)
Z	4
ρ_{calc}g/cm^3	1.347
μ/mm^{-1}	0.843
F(000)	392.0
Crystal size/mm^3	0.4 × 0.3 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.638 to 151.98
Index ranges	$-6 \le h \le 7$, $-19 \le k \le 19$, $-12 \le l \le 12$
Reflections collected	16839
Independent reflections	1860 [R_{int} = 0.0591, R_{sigma} = 0.0262]
Data/restraints/parameters	1860/0/121
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0428, wR_2 = 0.1200
Final R indexes [all data]	R_1 = 0.0459, wR_2 = 0.1233
Largest diff. peak/hole / e Å^{-3}	0.32/-0.20

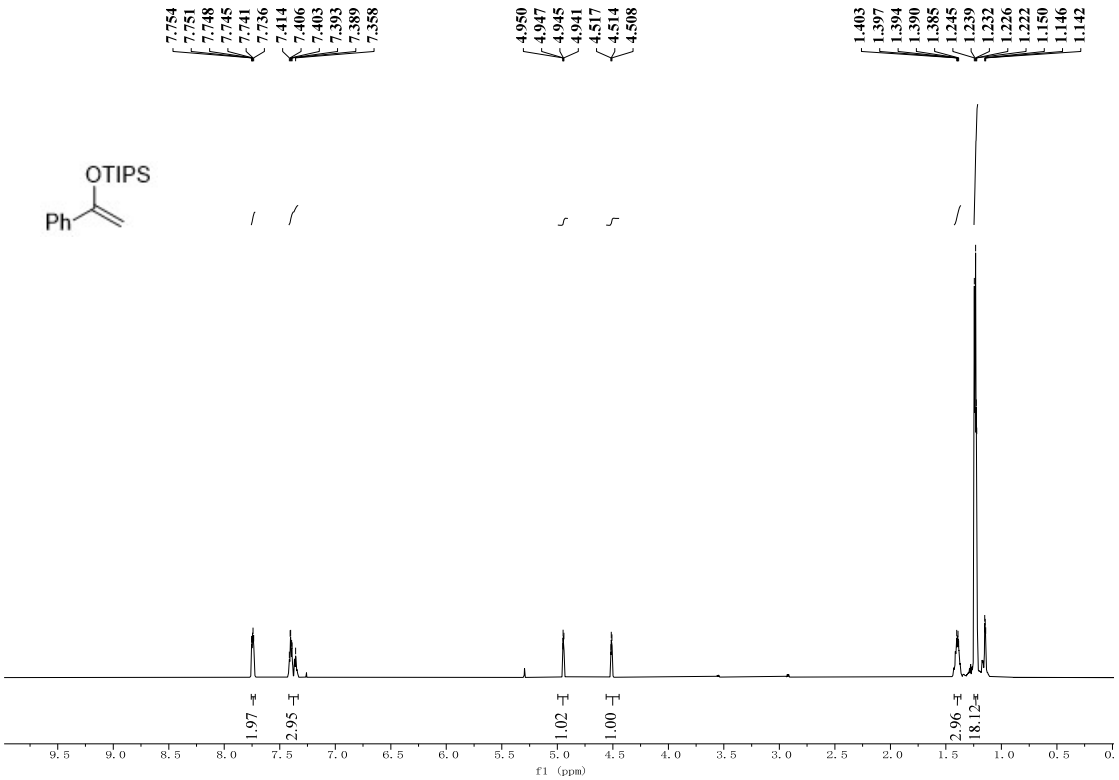


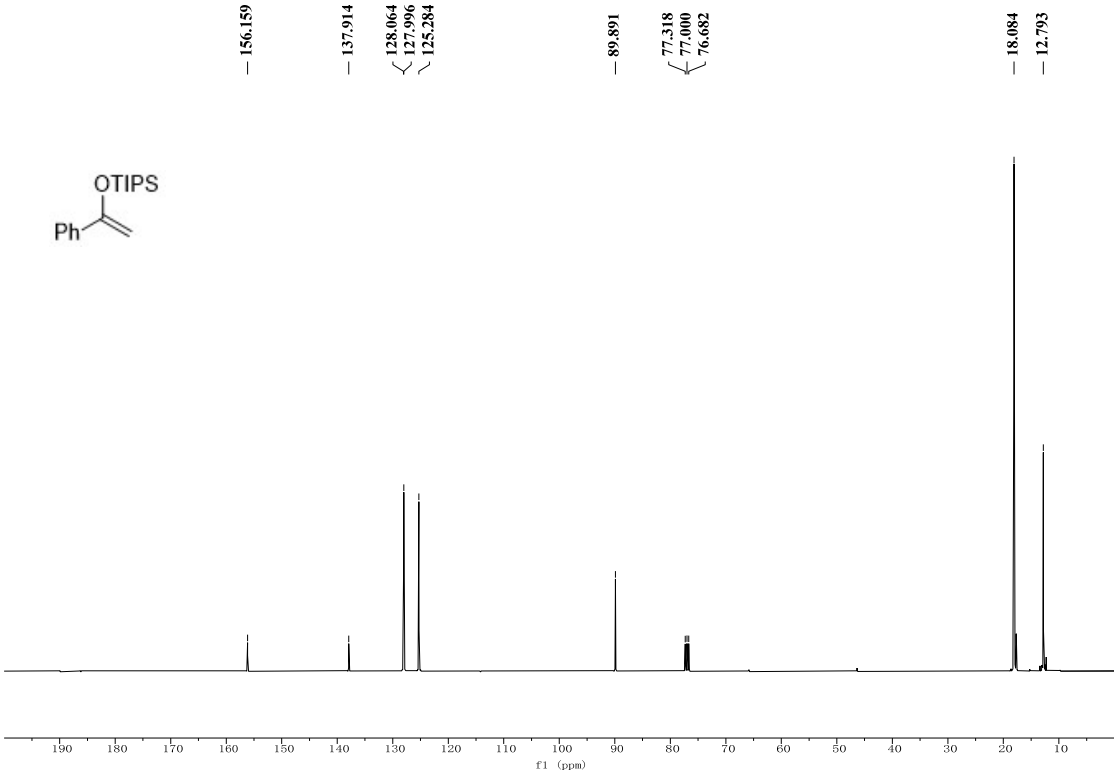
Crystal data and structure refinement for 2,2,6,6-tetramethylpiperidine benzoylformate.	
Temperature/K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.3396(5)
b/Å	10.1521(4)
c/Å	15.1640(8)
α/°	90
β/°	90.266(5)
γ/°	90
Volume/Å^3	1591.73(13)
Z	4
ρ_{calc}g/cm^3	1.222
μ/mm^{-1}	0.651
F(000)	635.0
Crystal size/mm^3	0.6 × 0.3 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.552 to 153.368
Index ranges	$-12 \leq h \leq 13$, $-12 \leq k \leq 12$, $-16 \leq l \leq 19$
Reflections collected	14153
Independent reflections	3188 [R_{int} = 0.0642, R_{sigma} = 0.0369]
Data/restraints/parameters	3188/0/195
Goodness-of-fit on F^2	3.359
Final R indexes [I>=2σ (I)]	R_1 = 0.2227, wR_2 = 0.6254
Final R indexes [all data]	R_1 = 0.2269, wR_2 = 0.6288
Largest diff. peak/hole / e Å^{-3}	1.04/-0.75

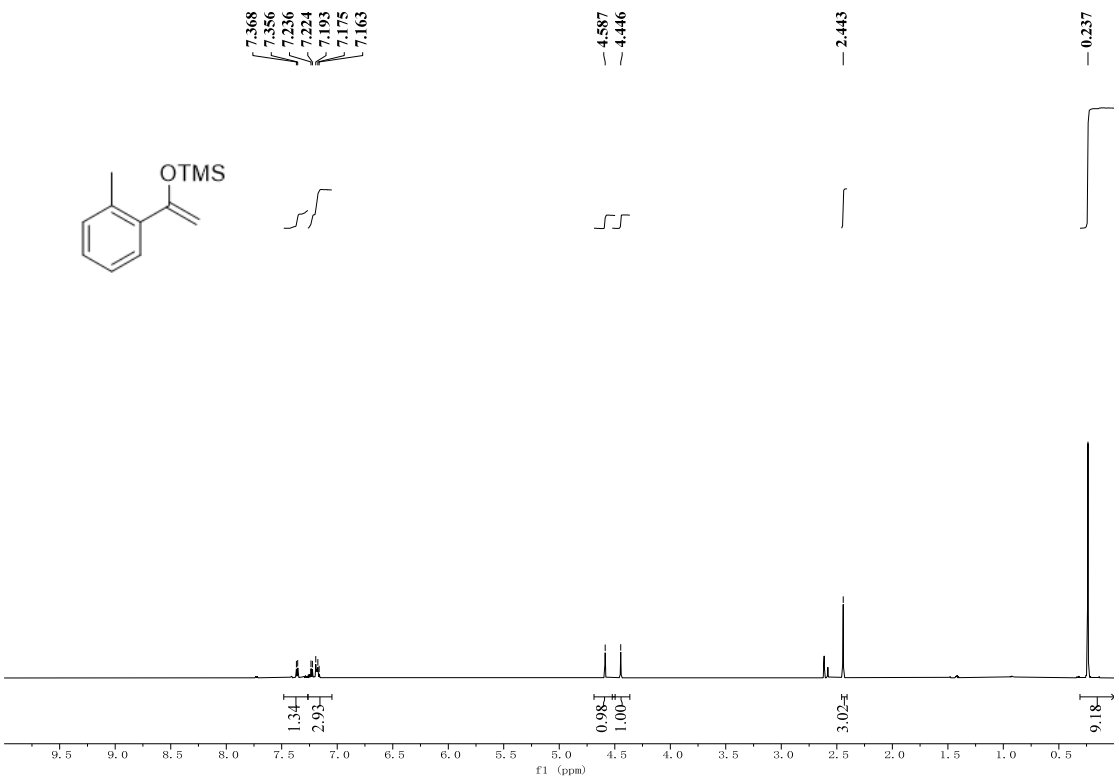
11. NMR spectra

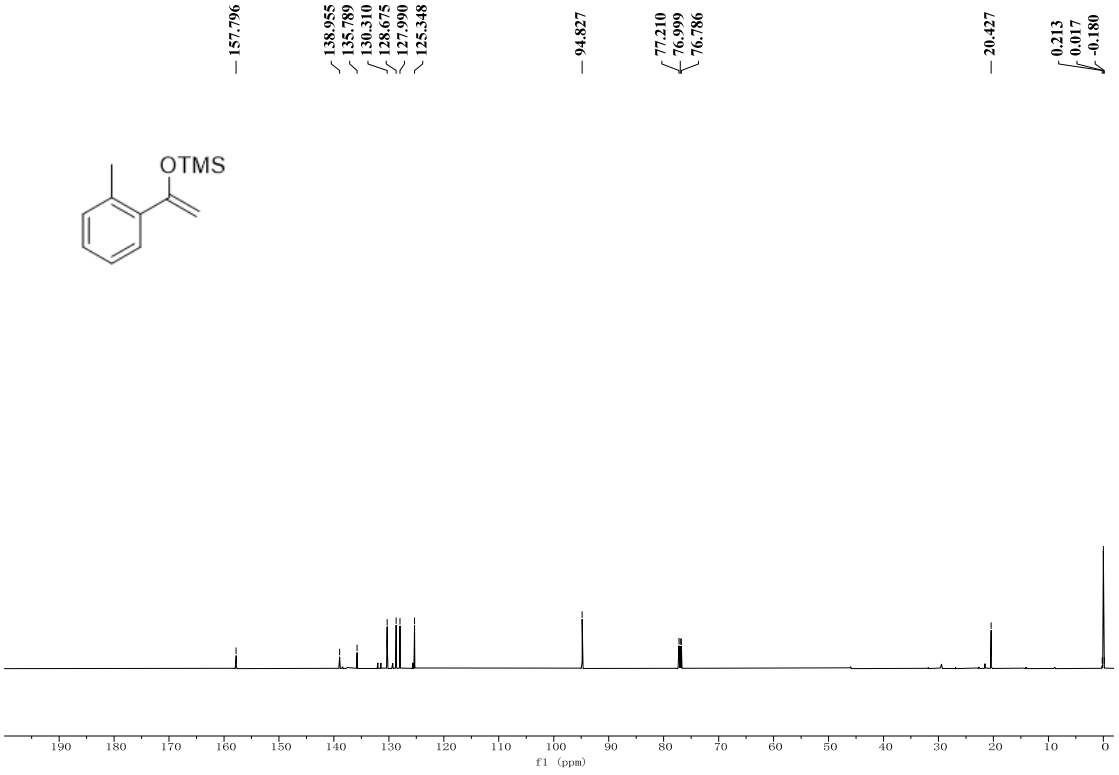


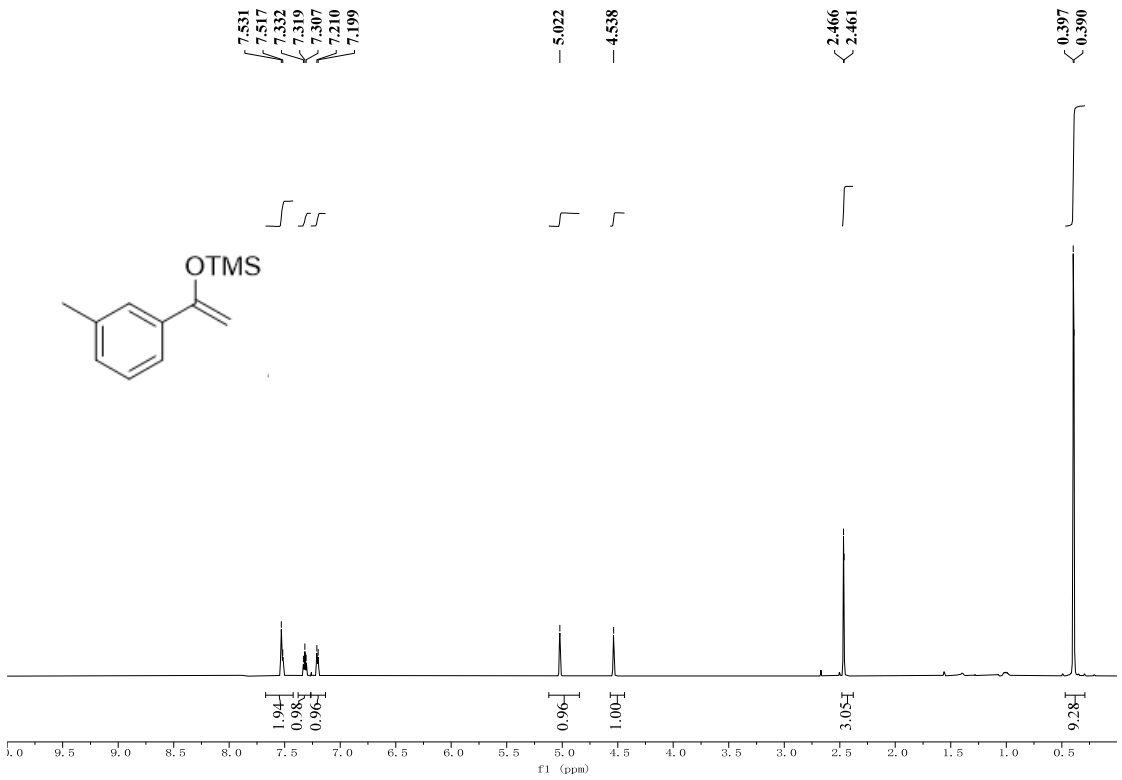


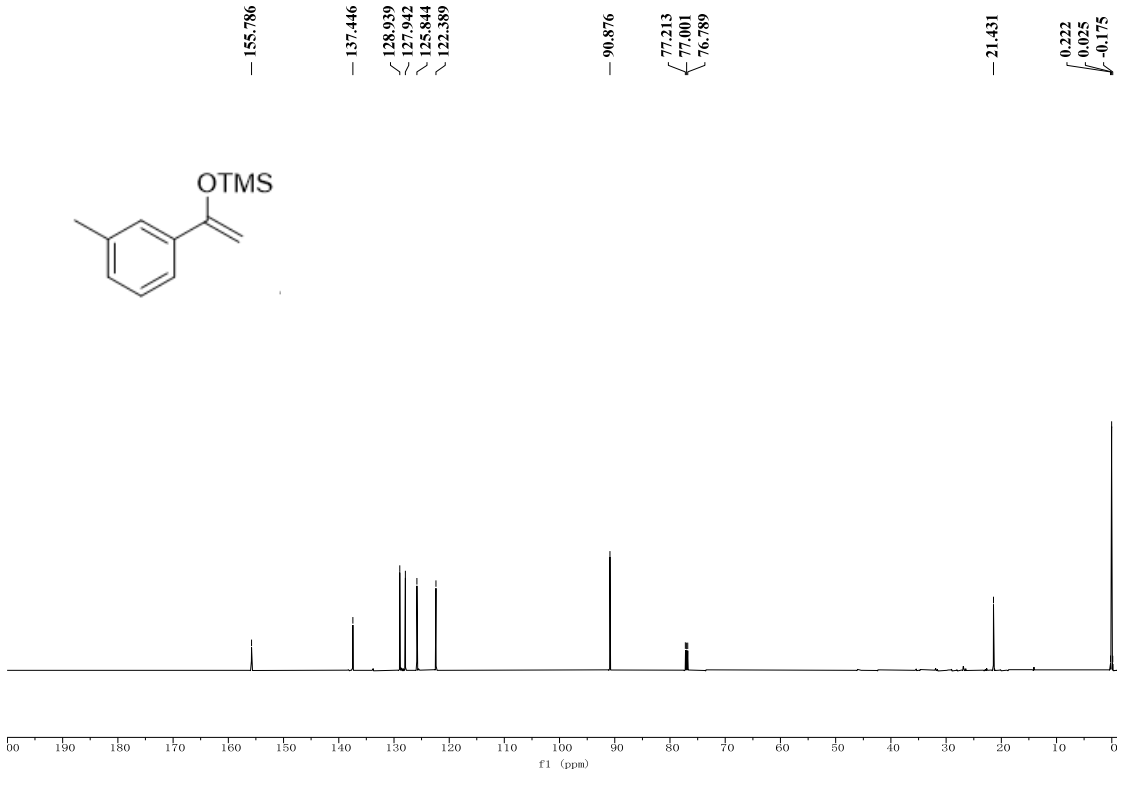

7.754
7.751
7.748
7.745
7.741
7.736
7.414
7.406
7.403
7.393
7.389
7.358
4.950
4.947
4.945
4.941
4.517
4.514
4.508
1.403
1.397
1.394
1.390
1.385
1.245
1.239
1.232
1.226
1.222
1.150
1.146
1.142
OTIPS
Ph
1.97
2.95
1.02
1.00
2.96
18.12
f1 (ppm)

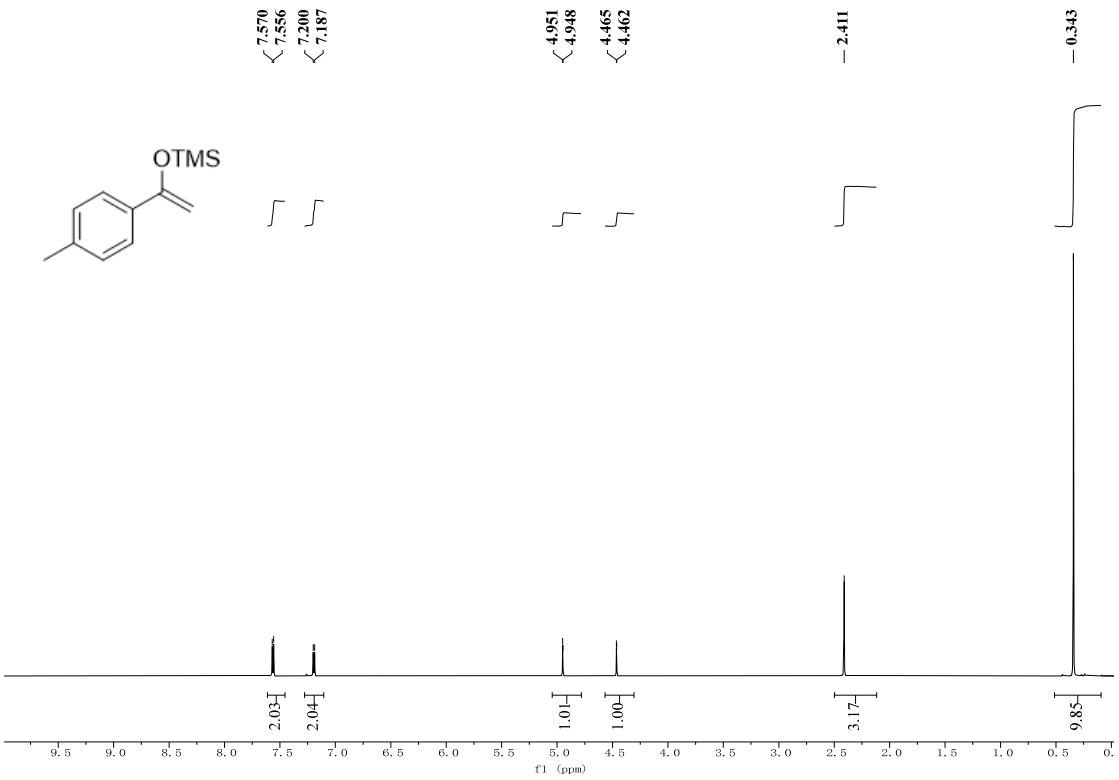

156.159
137.914
128.064
127.996
125.284
89.891
77.318
77.000
76.682
18.084
12.793
OTIPS
Ph
f1 (ppm)

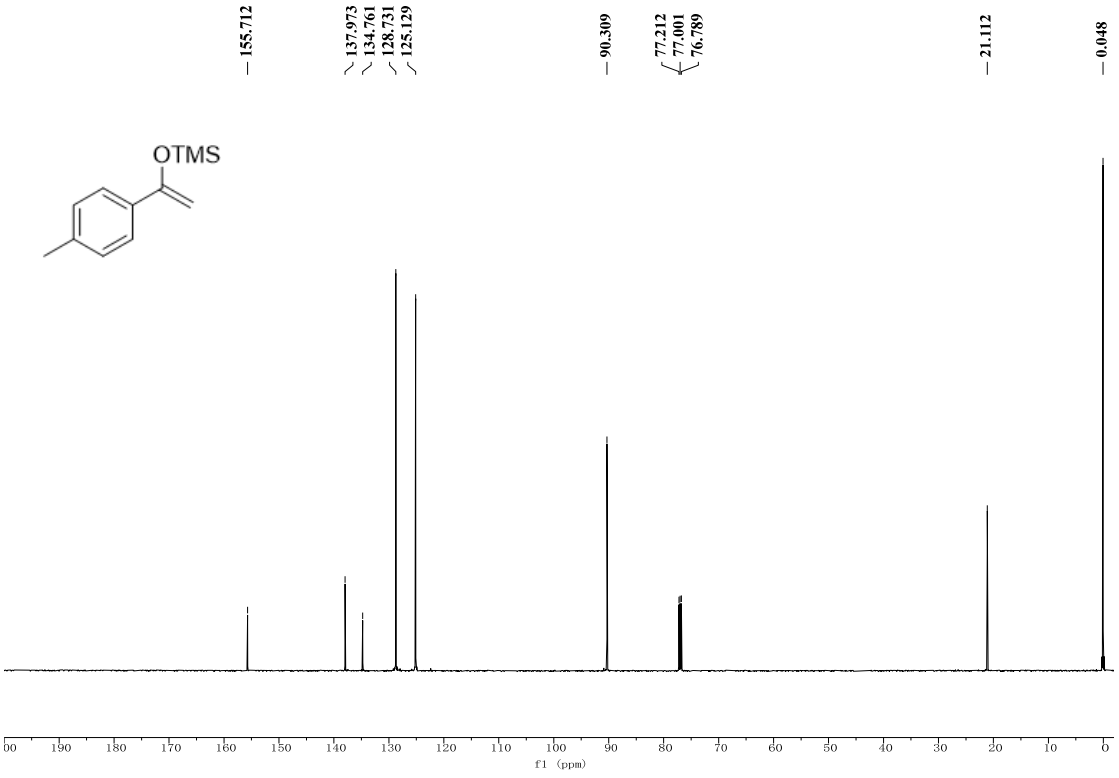

7.368
7.356
7.236
7.224
7.193
7.175
7.163
4.587
4.446
2.443
0.237
OTMS
1.34
2.93
0.98
1.00
3.02
9.18
f1 (ppm)

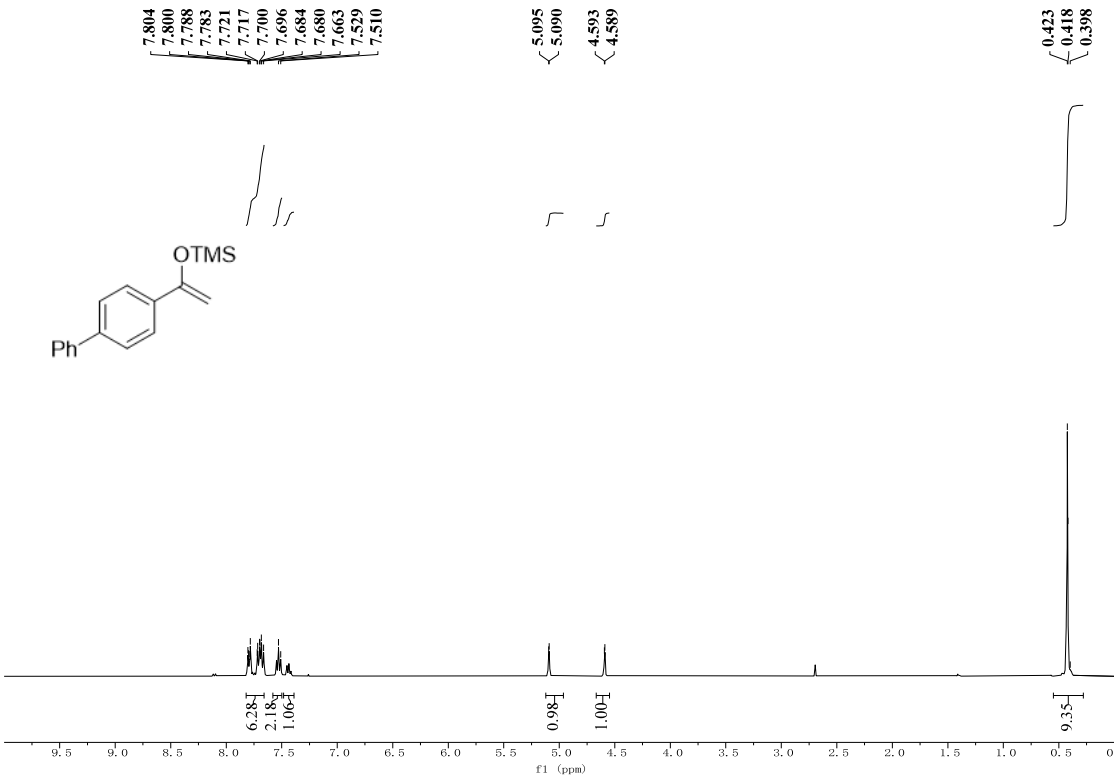

157.796
138.955
135.789
130.310
128.675
127.990
125.348
94.827
77.210
76.999
76.786
20.427
0.213
0.017
-0.180
OTMS
f1 (ppm)

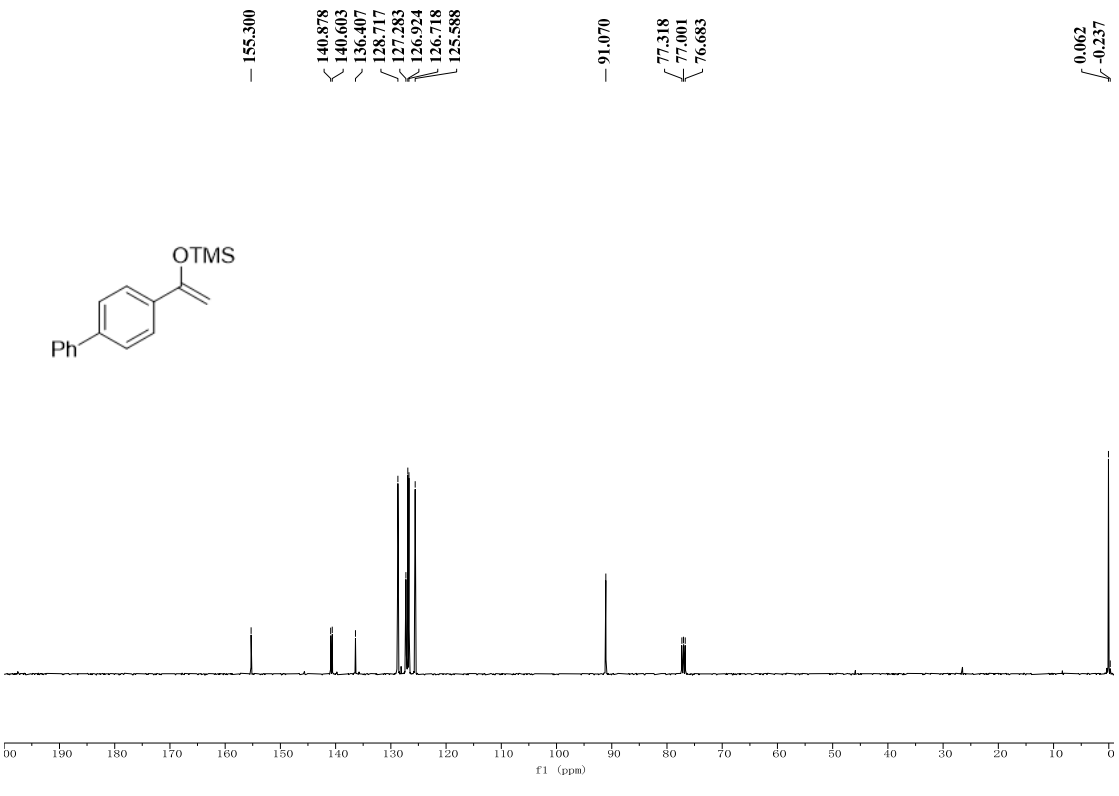

7.531
7.517
7.332
7.319
7.307
7.210
7.199
5.022
4.538
2.466
2.461
0.397
0.390
OTMS
1.94
0.98
0.96
0.96
1.00
3.05
9.28
f1 (ppm)

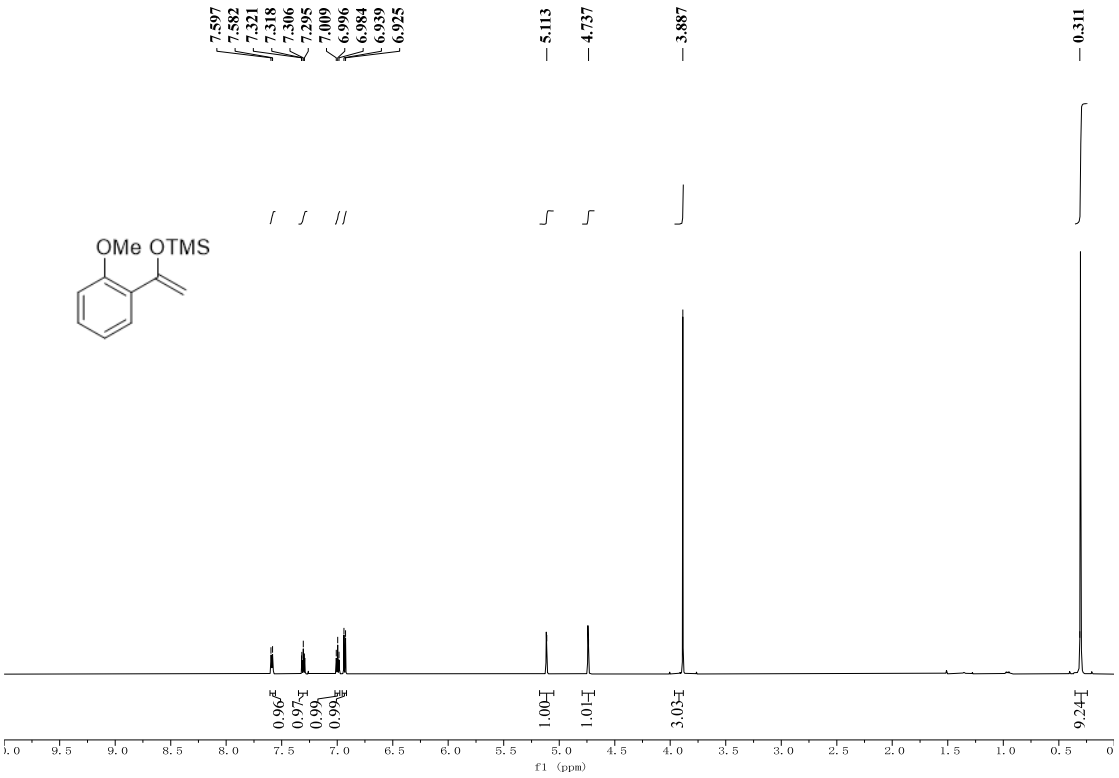

155.786
137.446
128.939
127.942
125.844
122.389
90.876
77.213
77.001
76.789
21.431
0.222
0.025
-0.175
OTMS
f1 (ppm)

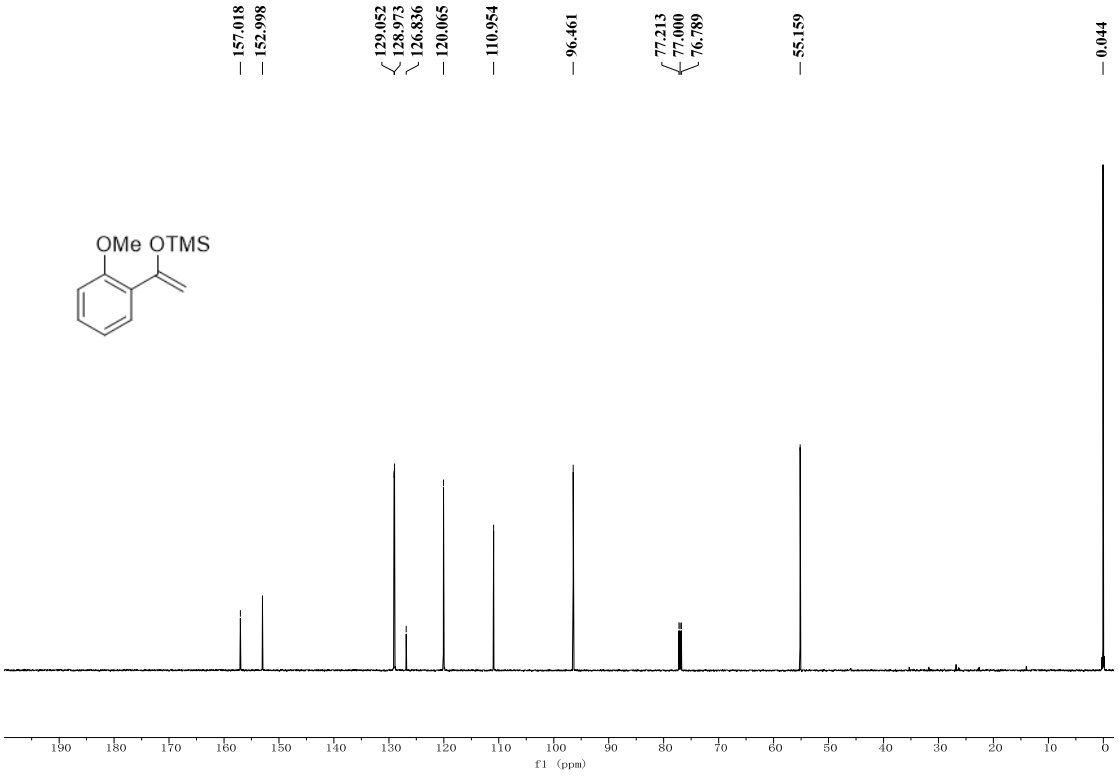

7.570
7.556
7.200
7.187
4.951
4.948
4.465
4.462
2.411
0.343
OTMS
2.03
2.04
1.01
1.00
3.17
9.85
f1 (ppm)

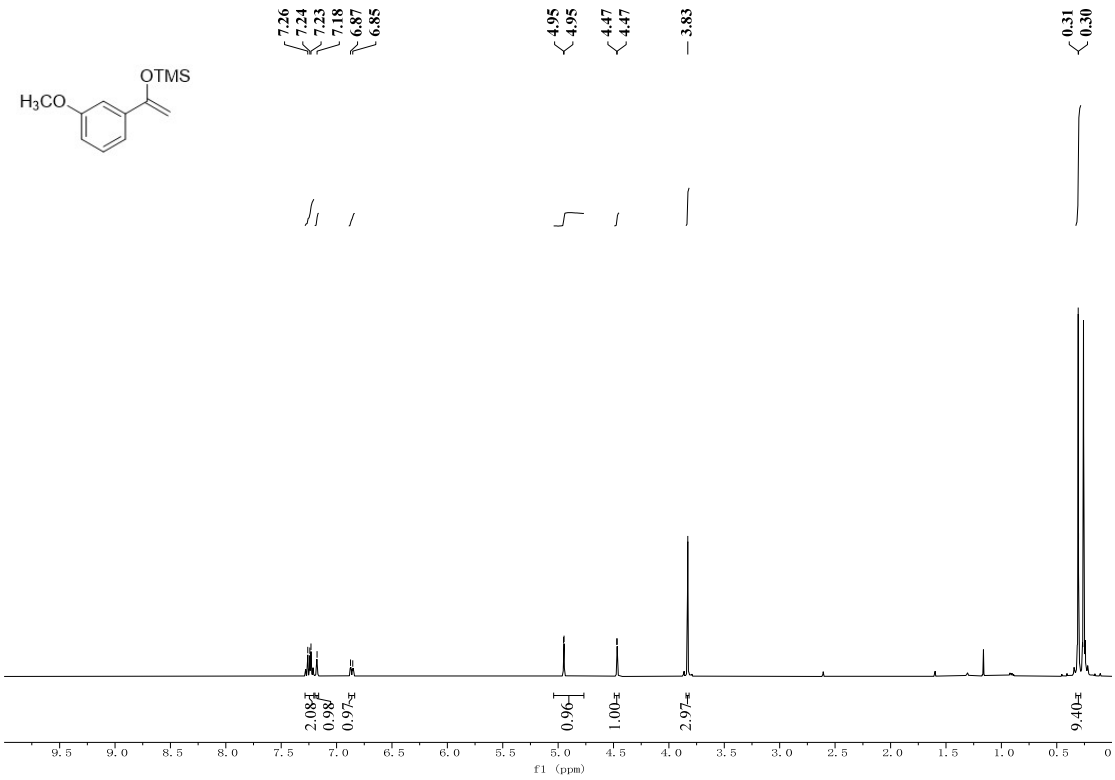

155.712
137.973
134.761
128.731
125.129
90.309
77.212
77.001
76.789
21.112
0.048
OTMS
f1 (ppm)

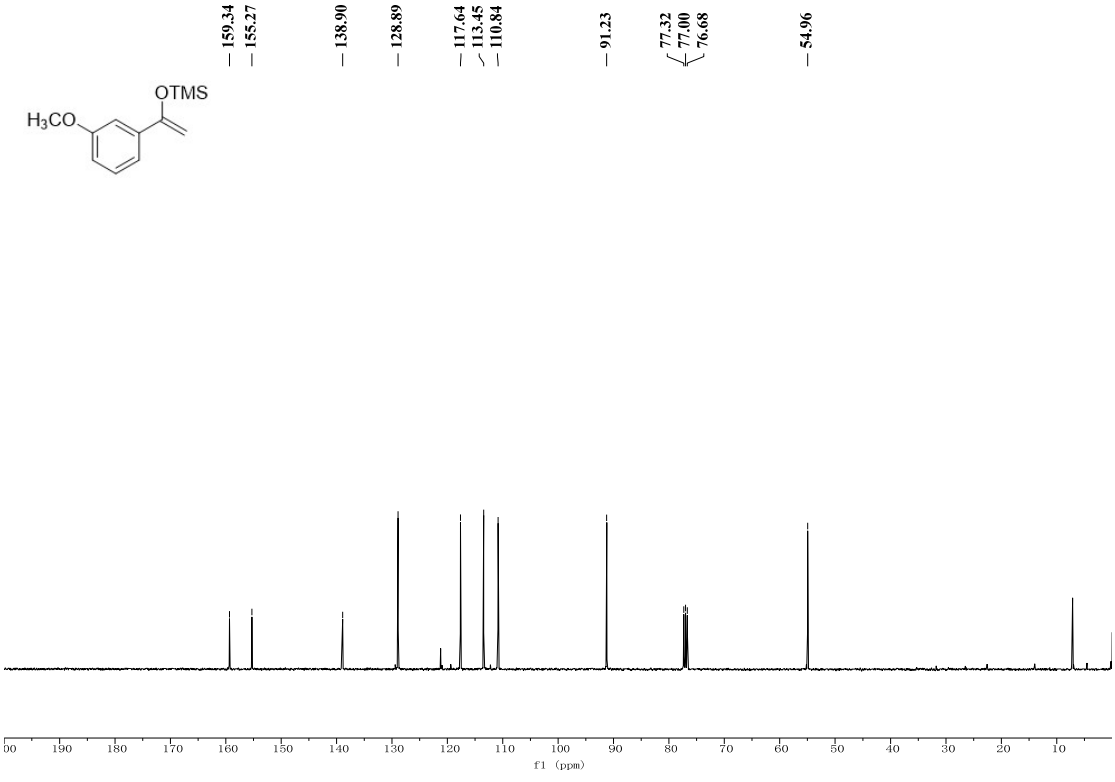

7.804
7.800
7.788
7.783
7.721
7.717
7.700
7.696
7.684
7.680
7.663
7.529
7.510
5.095
5.090
4.593
4.589
0.423
0.418
0.398
OTMS
Ph
6.28
2.18
1.06
0.98
1.00
9.35
f1 (ppm)

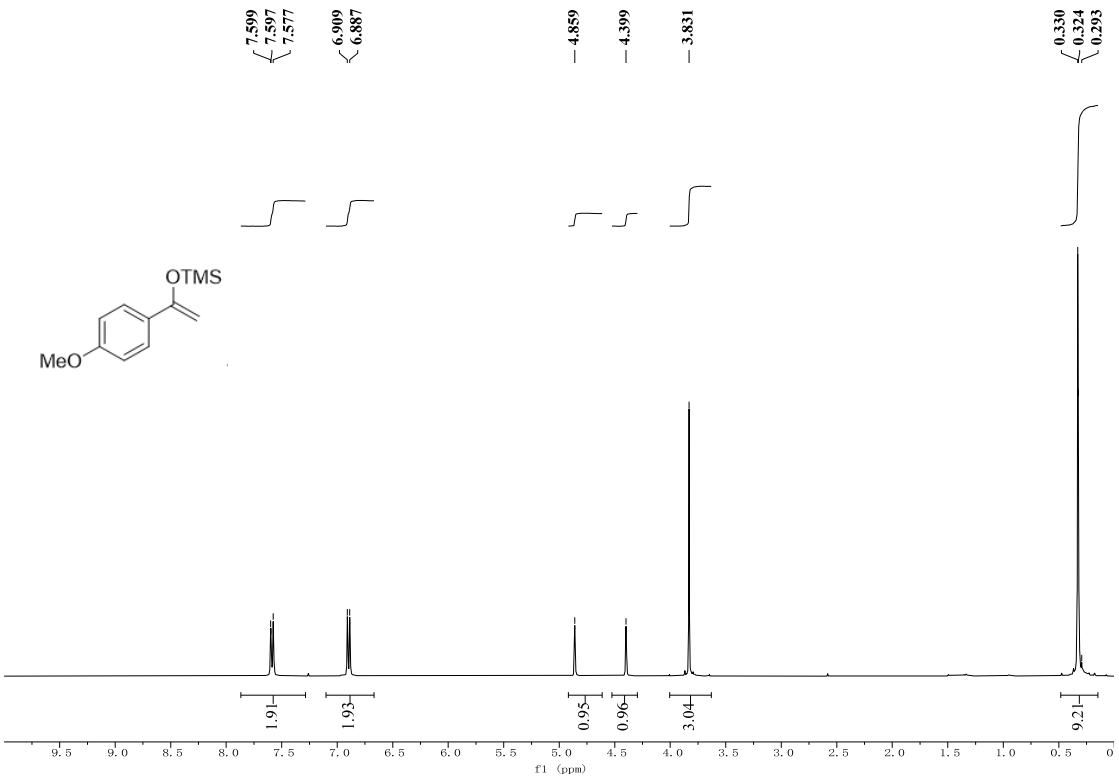

155.300
140.878
140.603
136.407
128.717
127.283
126.924
126.718
125.588
91.070
77.318
77.001
76.683
0.062
-0.237
OTMS
Ph
f1 (ppm)

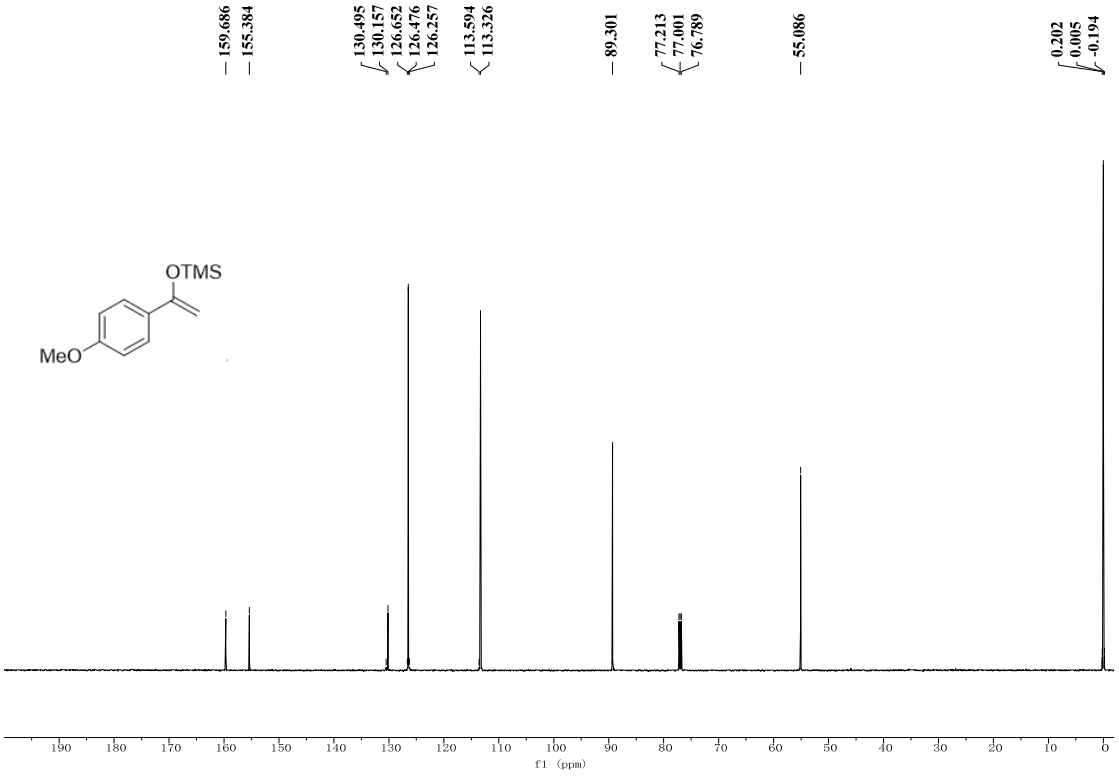

7.597
7.582
7.321
7.318
7.306
7.295
7.009
6.996
6.984
6.939
6.925
5.113
4.737
3.887
0.311
OMe OTMS
0.96
0.97
0.99
0.99
1.00
1.01
3.03
9.24
f1 (ppm)

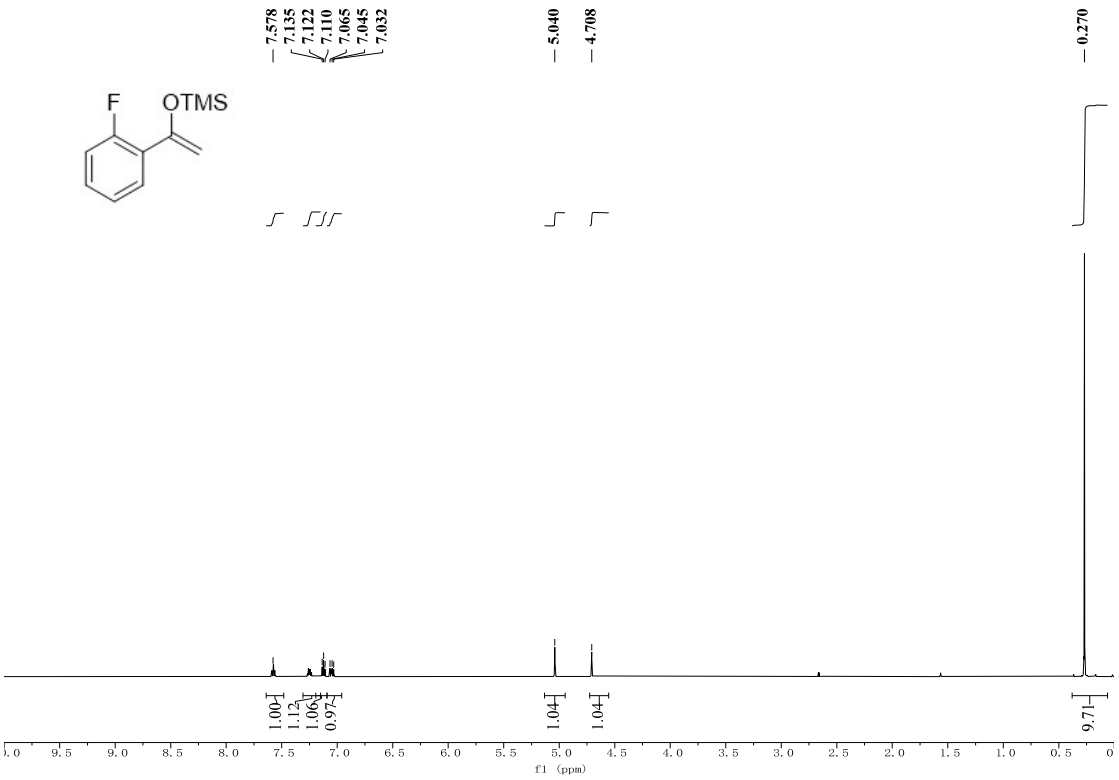

157.018
152.998
129.052
128.973
126.836
120.065
110.954
96.461
77.213
77.000
76.789
55.159
0.044
OMe OTMS
f1 (ppm)

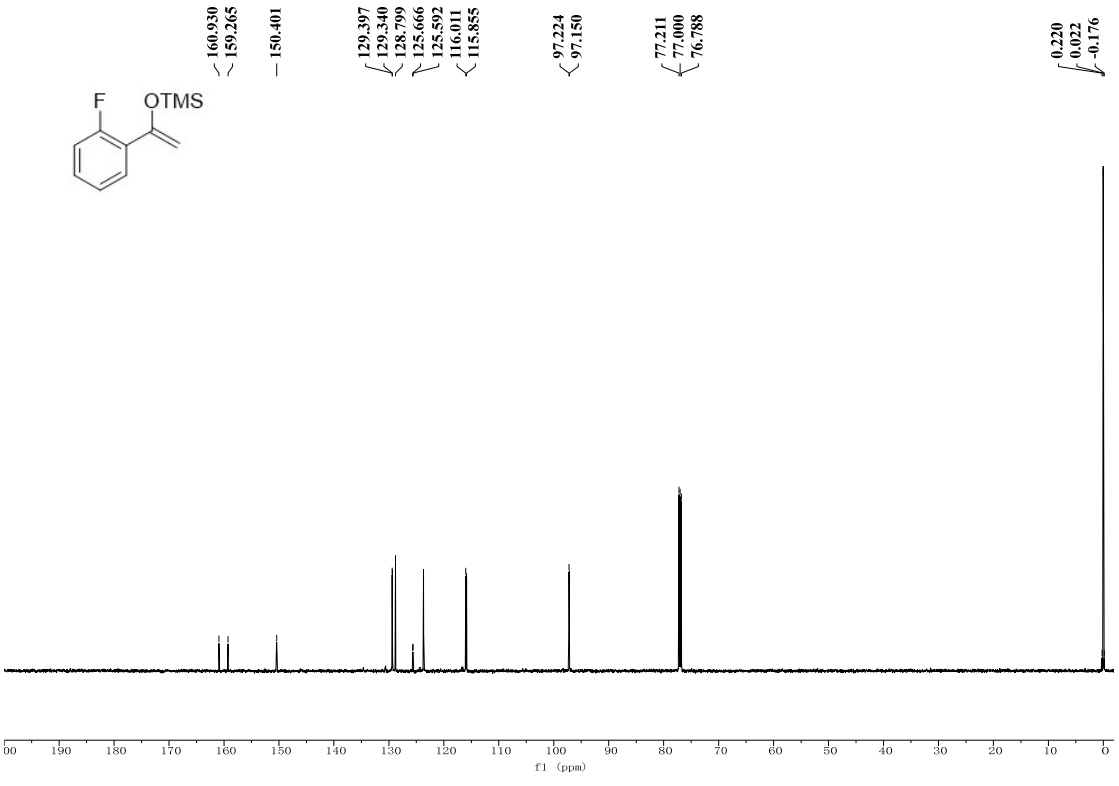

7.26
7.24
7.23
7.18
6.87
6.85
4.95
4.95
4.47
4.47
3.83
0.31
0.30
OTMS
H3CO
2.08
0.98
0.97
0.96
1.00
2.97
9.40
f1 (ppm)

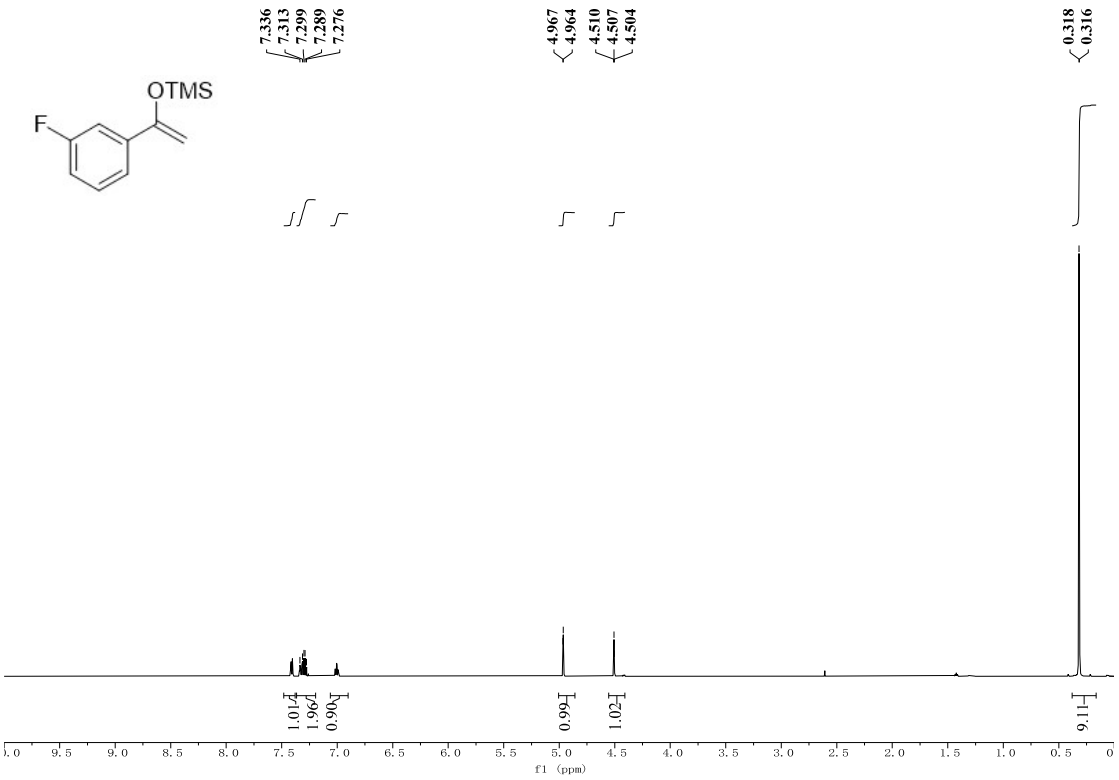

159.34
155.27
138.90
128.89
117.64
113.45
110.84
91.23
77.32
77.00
76.68
54.96
OTMS
H3CO
f1 (ppm)

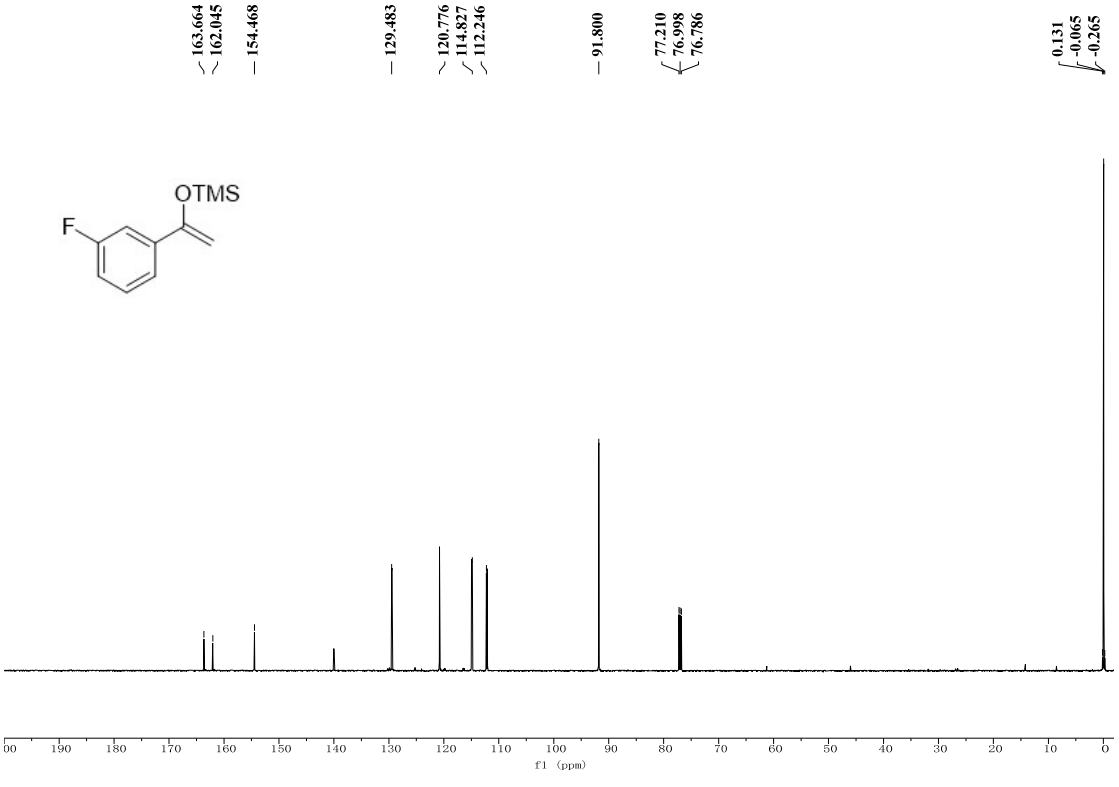

7.599
7.597
7.577
6.909
6.887
4.859
4.399
3.831
0.330
0.324
0.293
OTMS
MeO
1.91
1.93
0.95
0.96
3.04
9.21
f1 (ppm)

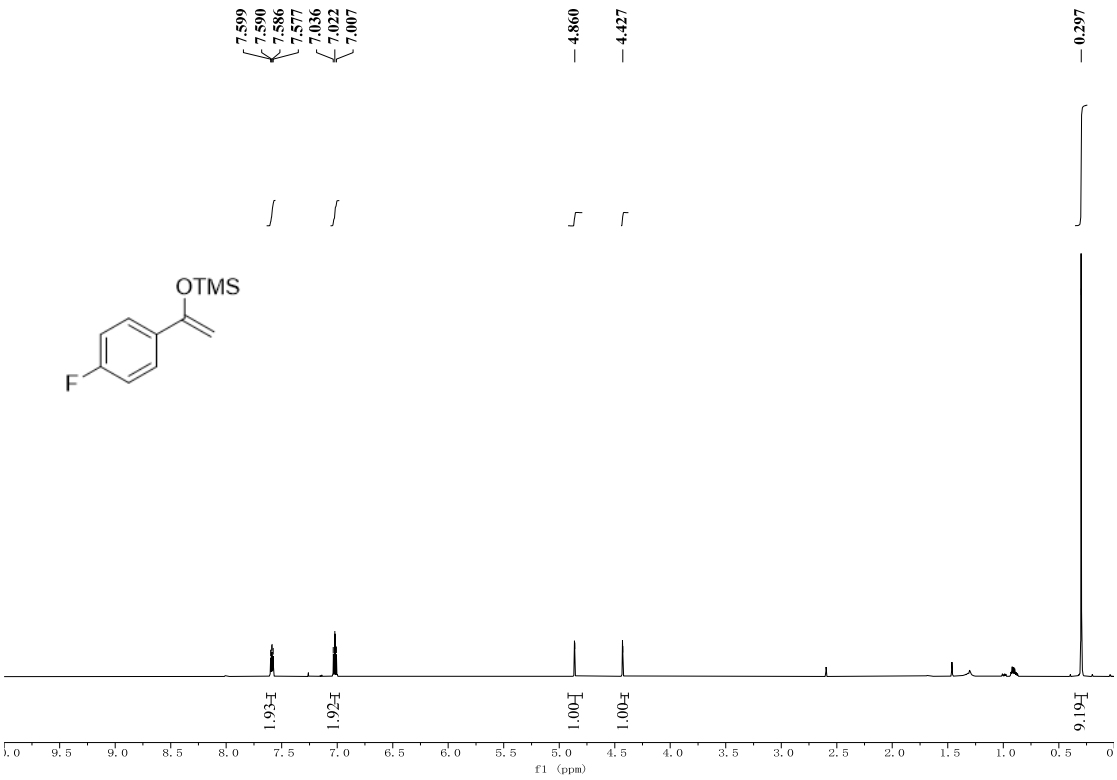

159.686
155.384
130.495
130.157
126.652
126.476
126.257
113.594
113.326
89.301
77.213
77.001
76.789
55.086
0.202
0.005
-0.194
OTMS
MeO
f1 (ppm)

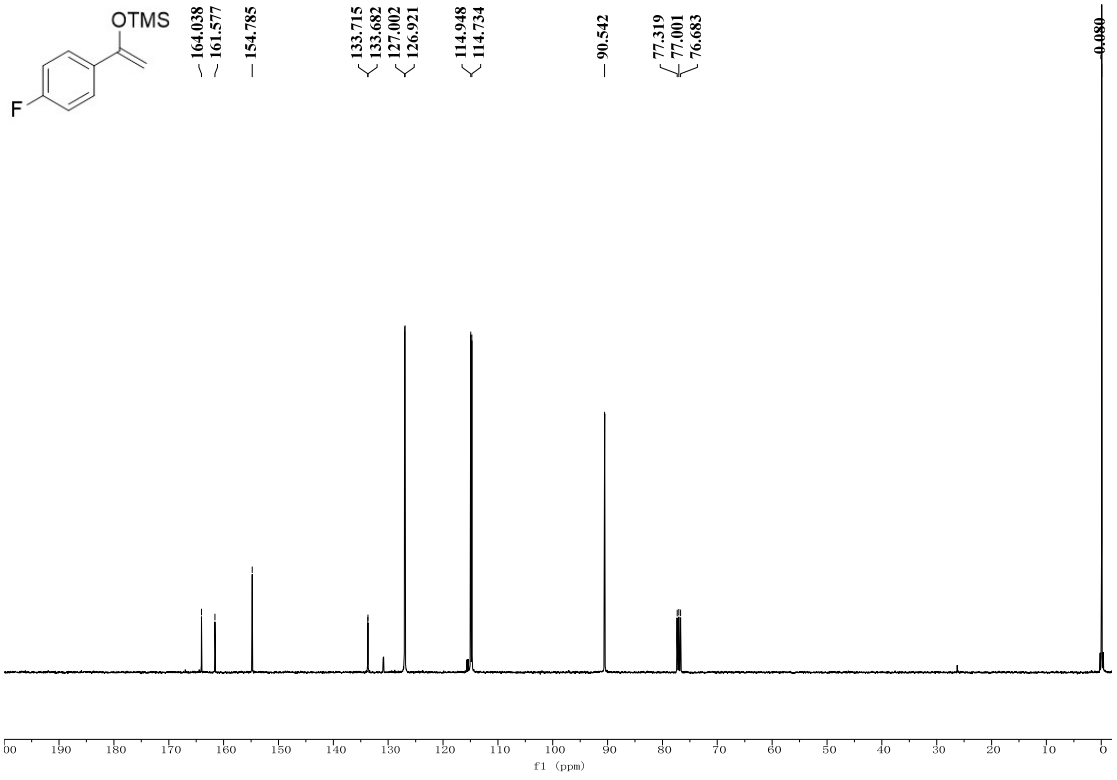

7.578
7.135
7.122
7.110
7.065
7.045
7.032
5.040
4.708
0.270
F
OTMS
1.00
1.12
1.06
0.97
1.04
1.04
9.71
f1 (ppm)

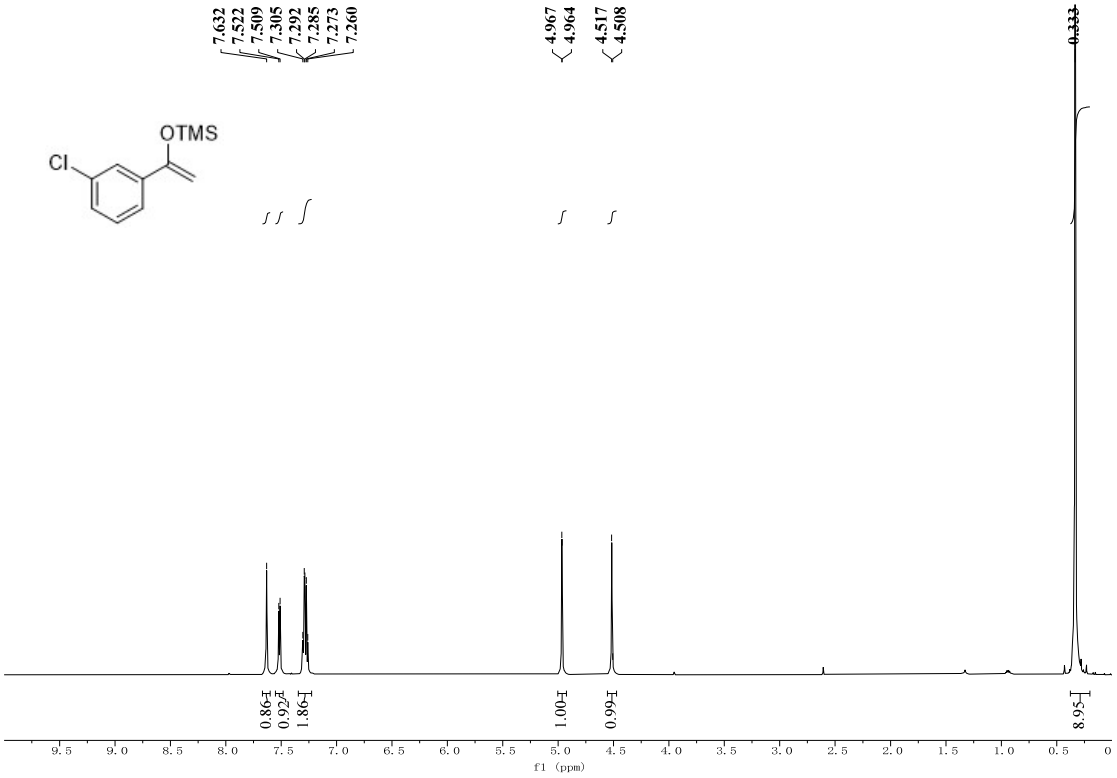

160.930
159.265
150.401
129.397
129.340
128.799
125.666
125.592
116.011
115.855
97.224
97.150
77.211
77.000
76.788
0.220
0.022
-0.176
F
OTMS
f1 (ppm)

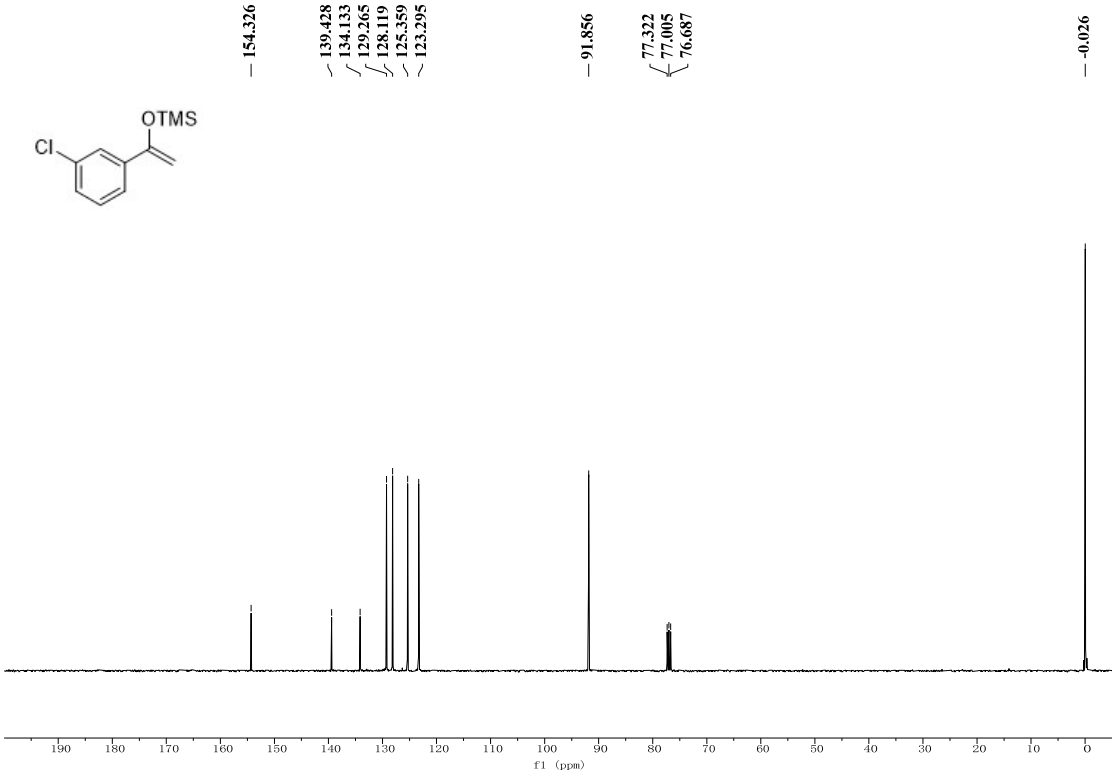

7.336
7.313
7.299
7.289
7.276
4.967
4.964
4.510
4.507
4.504
0.318
0.316
OTMS
F
1.01
1.96
0.90
0.99
1.02
9.11
f1 (ppm)


163.664
162.045
154.468
129.483
120.776
114.827
112.246
91.800
77.210
76.998
76.786
0.131
-0.065
-0.265
OTMS
F
f1 (ppm)


7.599
7.590
7.586
7.577
7.036
7.022
7.007
4.860
4.427
0.297
OTMS
F
1.93
1.92
1.00
1.00
9.19
f1 (ppm)


OTMS
F
164.038
161.577
154.785
133.715
133.682
127.002
126.921
114.948
114.734
90.542
77.319
77.001
76.683
0.080
f1 (ppm)


7.632
7.522
7.509
7.305
7.292
7.285
7.273
7.260
4.967
4.964
4.517
4.508
0.333
OTMS
Cl
0.86
0.92
1.86
1.00
0.99
8.95
f1 (ppm)


154.326
139.428
134.133
129.265
128.119
125.359
123.295
91.856
77.322
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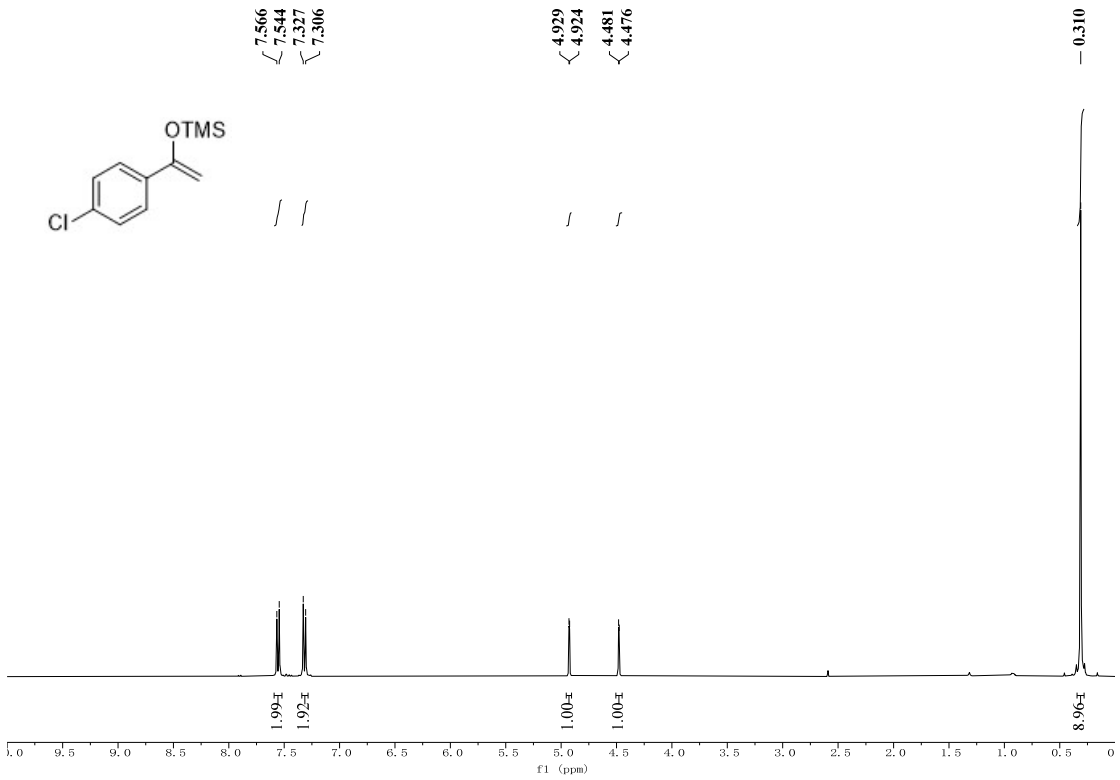
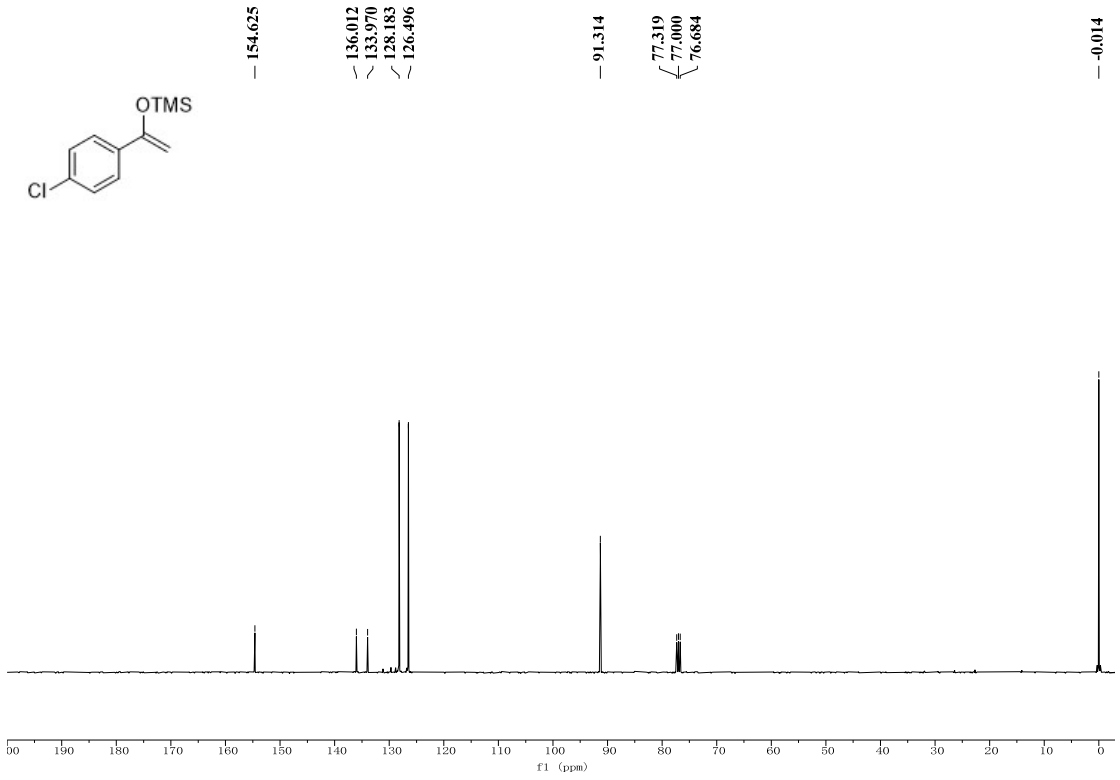
76.687
-0.026
OTMS
Cl
f1 (ppm)


7.566
7.544
7.327
7.306
4.929
4.924
4.481
4.476
0.310
OTMS
Cl
1.99
1.92
1.00
1.00
8.96
f1 (ppm)


154.625
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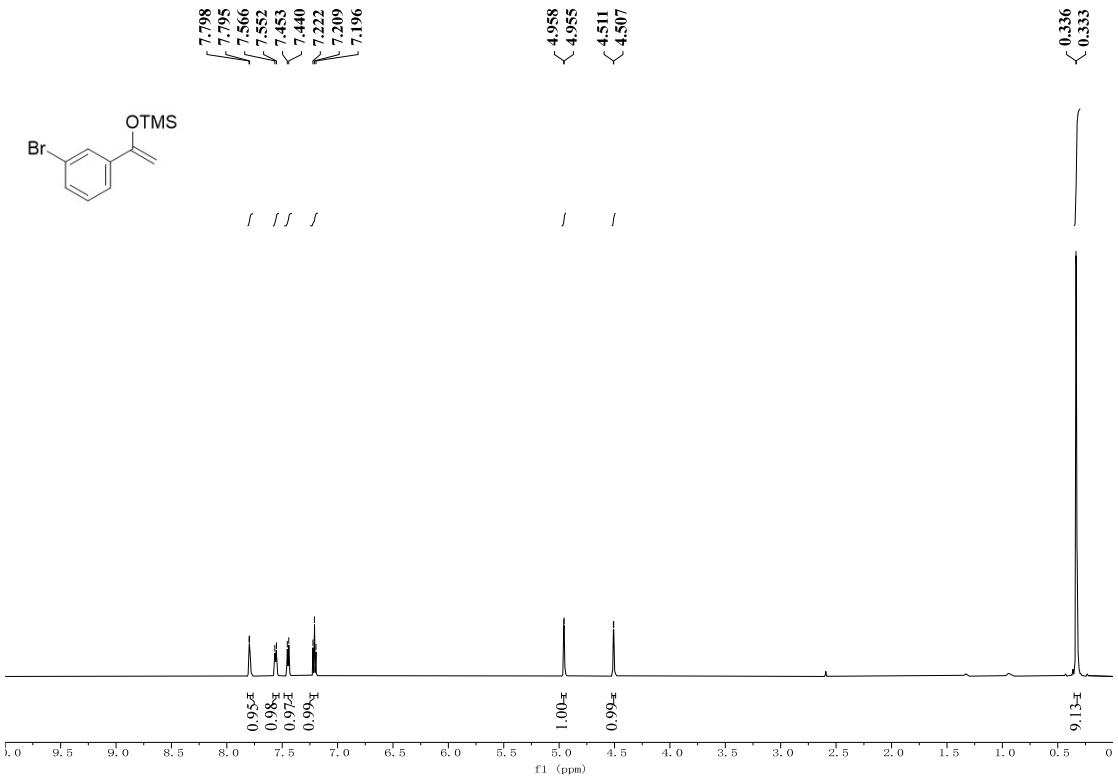
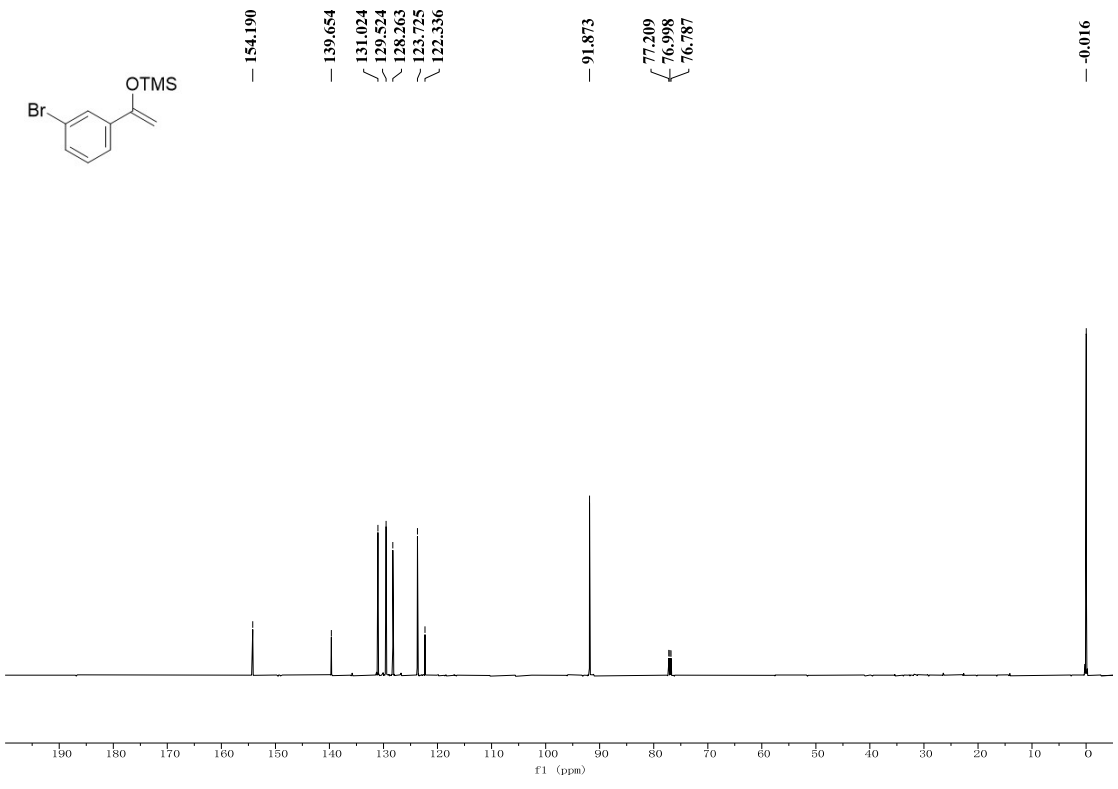
128.183
126.496
91.314
77.319
77.000
76.684
-0.014
OTMS
Cl
f1 (ppm)


7.798
7.795
7.566
7.552
7.453
7.440
7.222
7.209
7.196
4.958
4.955
4.511
4.507
0.336
0.333
OTMS
Br
0.95
0.98
0.97
0.99
1.00
0.99
9.13
f1 (ppm)


154.190
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128.263
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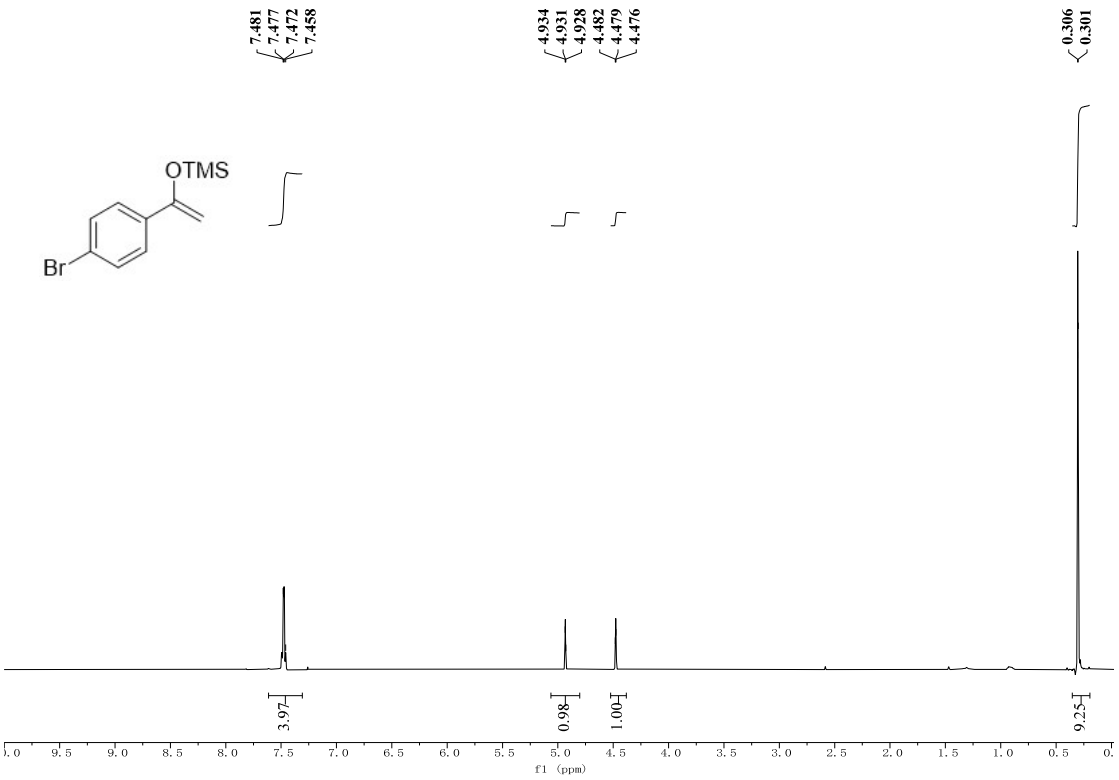
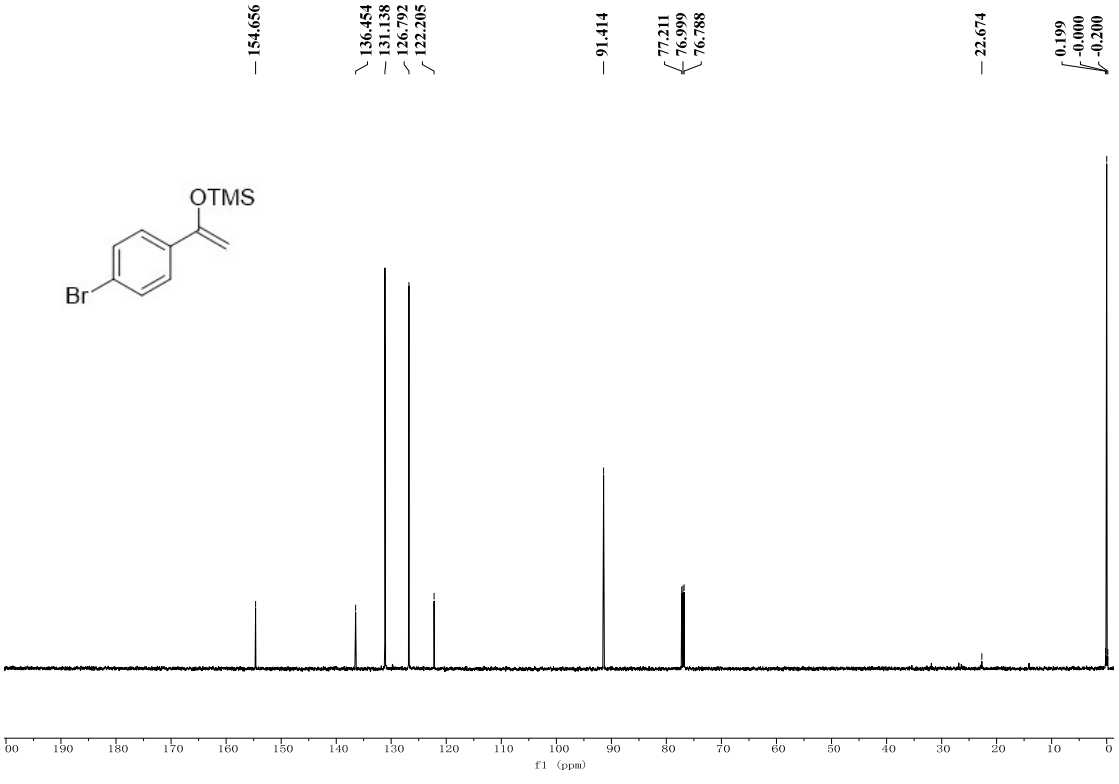
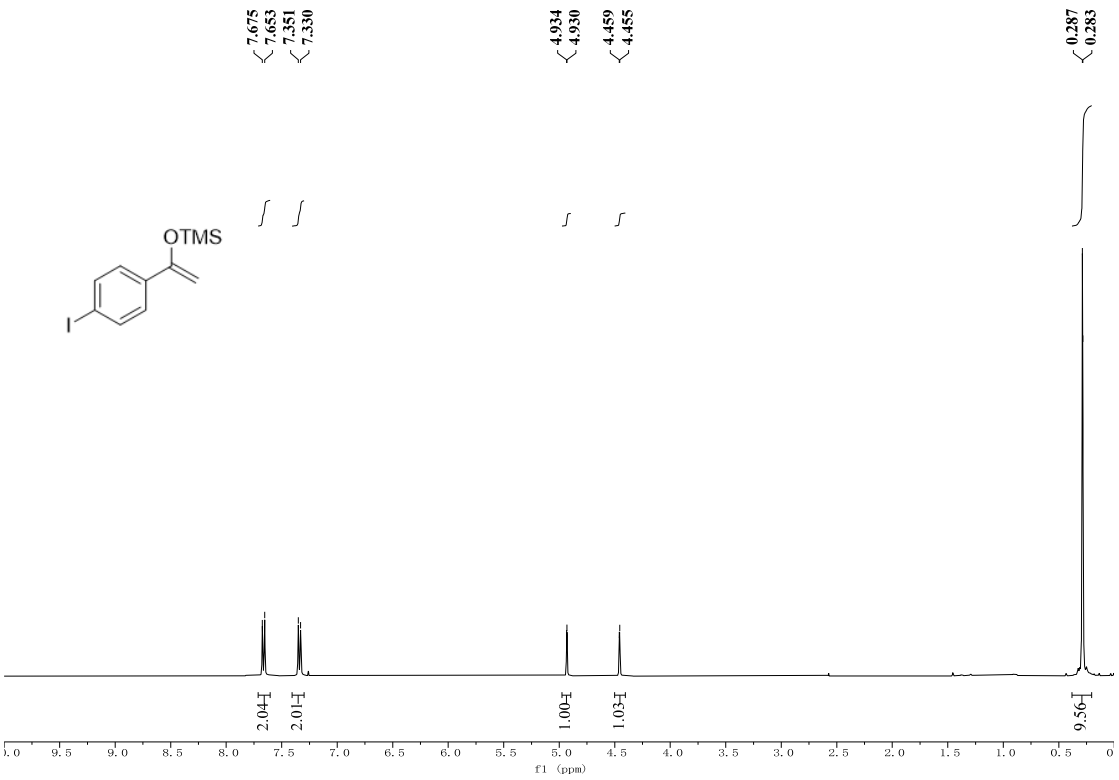
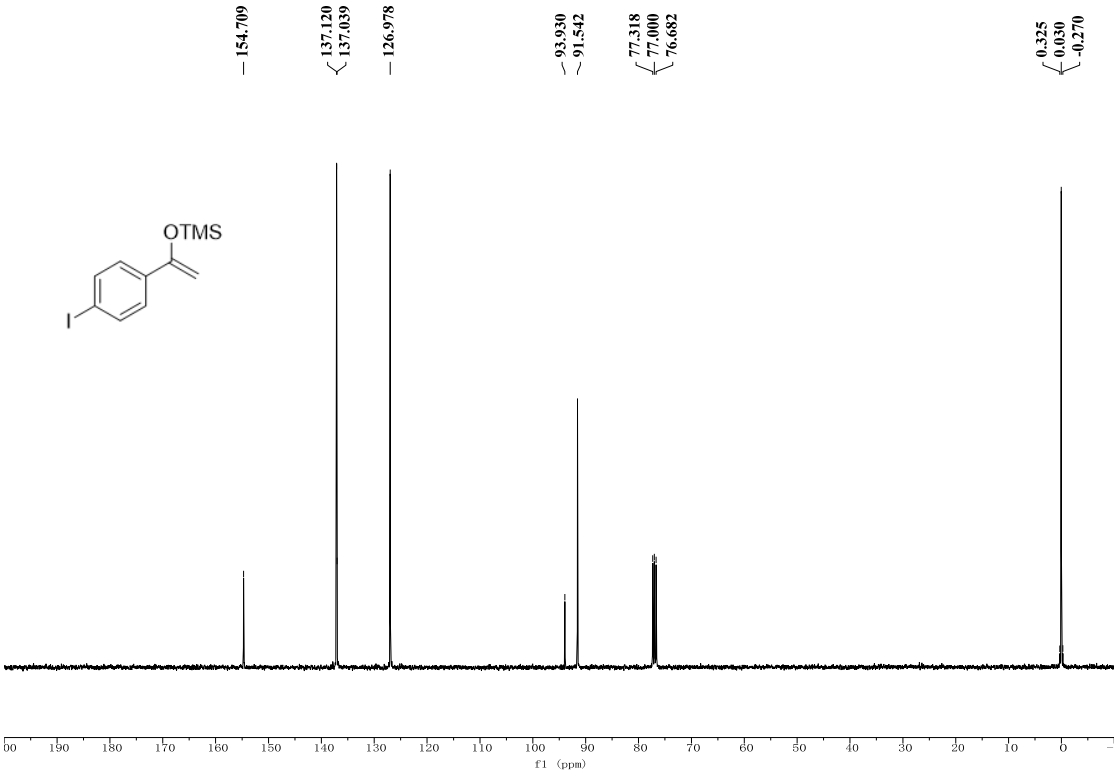
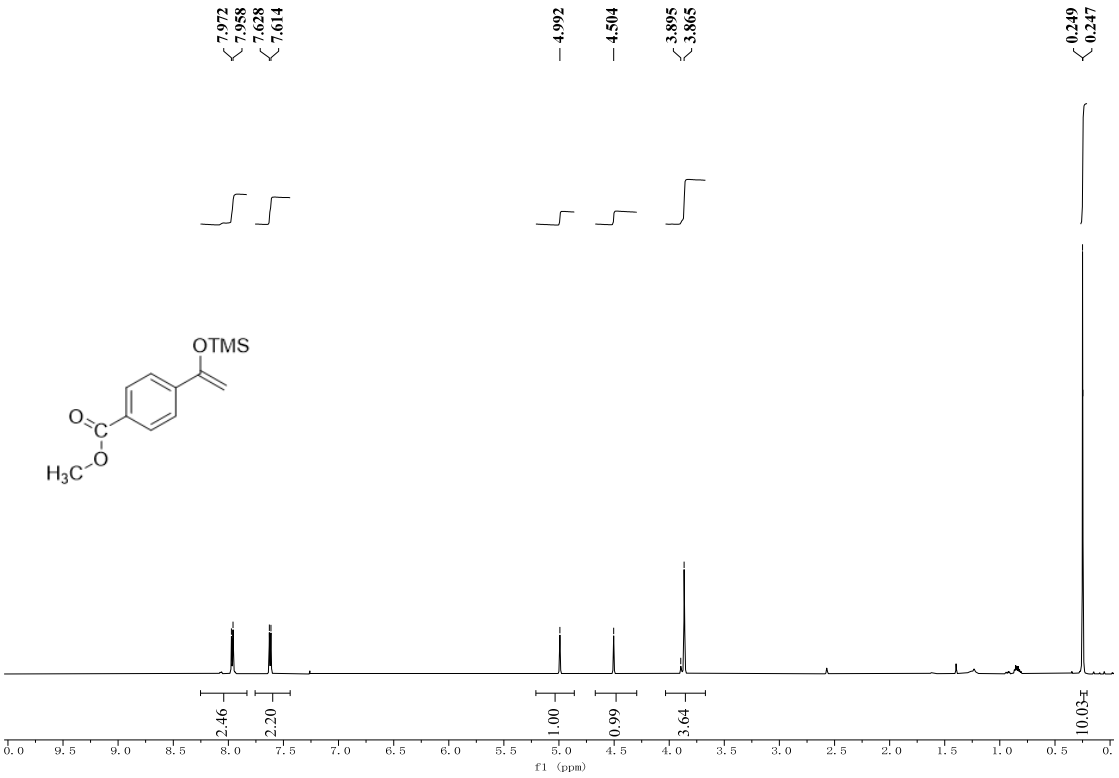
122.336
91.873
77.209
76.998
76.787
-0.016
OTMS
Br
f1 (ppm)

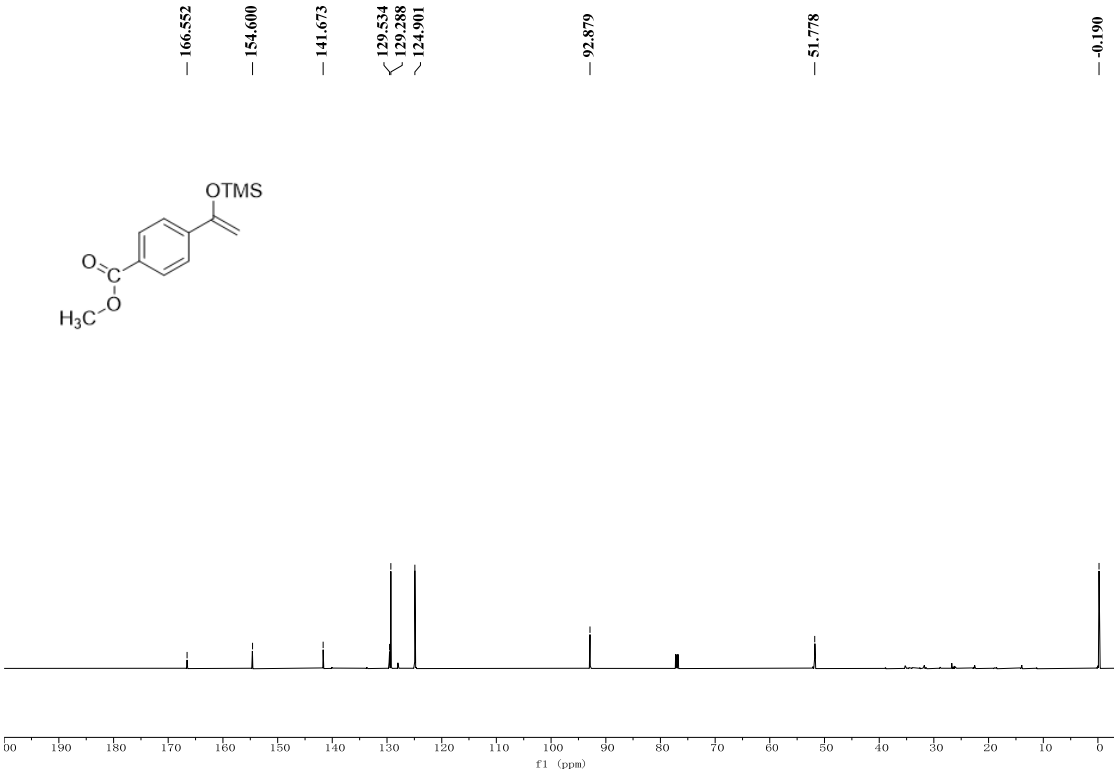

7.481
7.477
7.472
7.458
4.934
4.931
4.928
4.482
4.479
4.476
0.306
0.301
OTMS
Br
3.97
0.98
1.00
9.25
f1 (ppm)

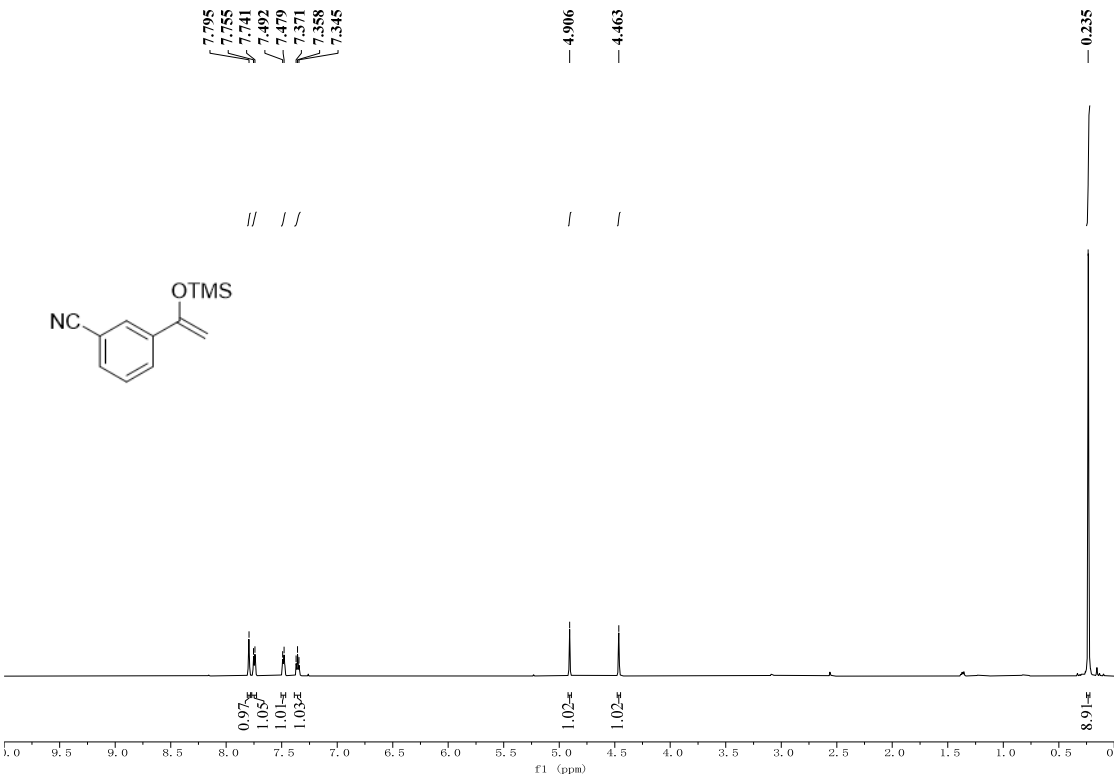

154.656
136.454
131.138
126.792
122.205
91.414
77.211
76.999
76.788
22.674
0.199
-0.000
-0.200
OTMS
Br
f1 (ppm)

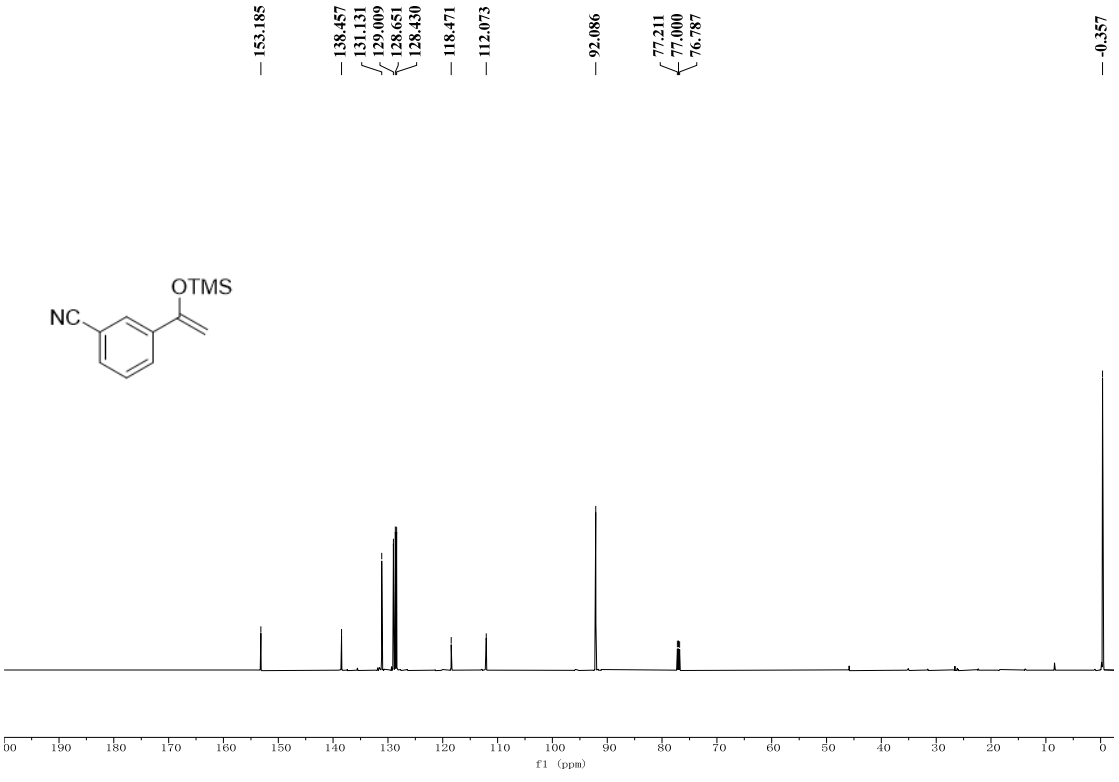

7.675
7.653
7.351
7.330
4.934
4.930
4.459
4.455
0.287
0.283
OTMS
I
2.04
2.01
1.00
1.03
9.56
f1 (ppm)

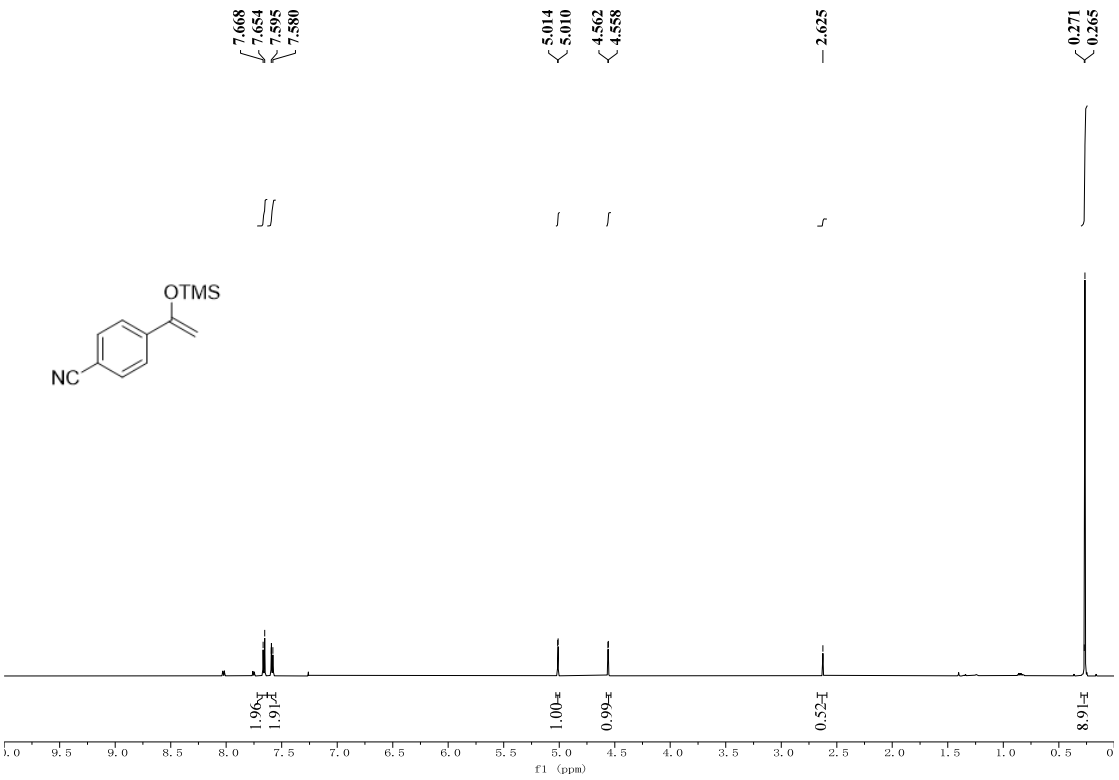

154.709
137.120
137.039
126.978
93.930
91.542
77.318
77.000
76.682
0.325
0.030
-0.270
OTMS
I
f1 (ppm)

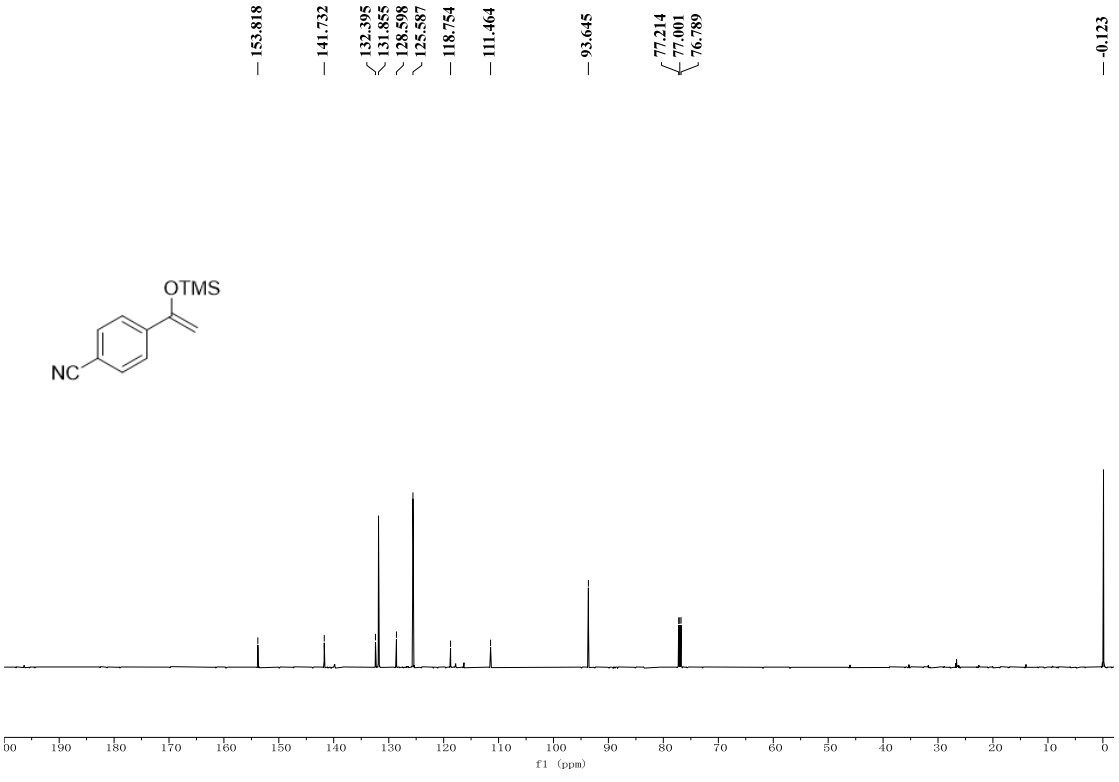

7.972
7.958
7.628
7.614
4.992
4.504
3.895
3.865
0.249
0.247
OTMS
O
C
O
H3C
2.46
2.20
1.00
0.99
3.64
10.03
f1 (ppm)

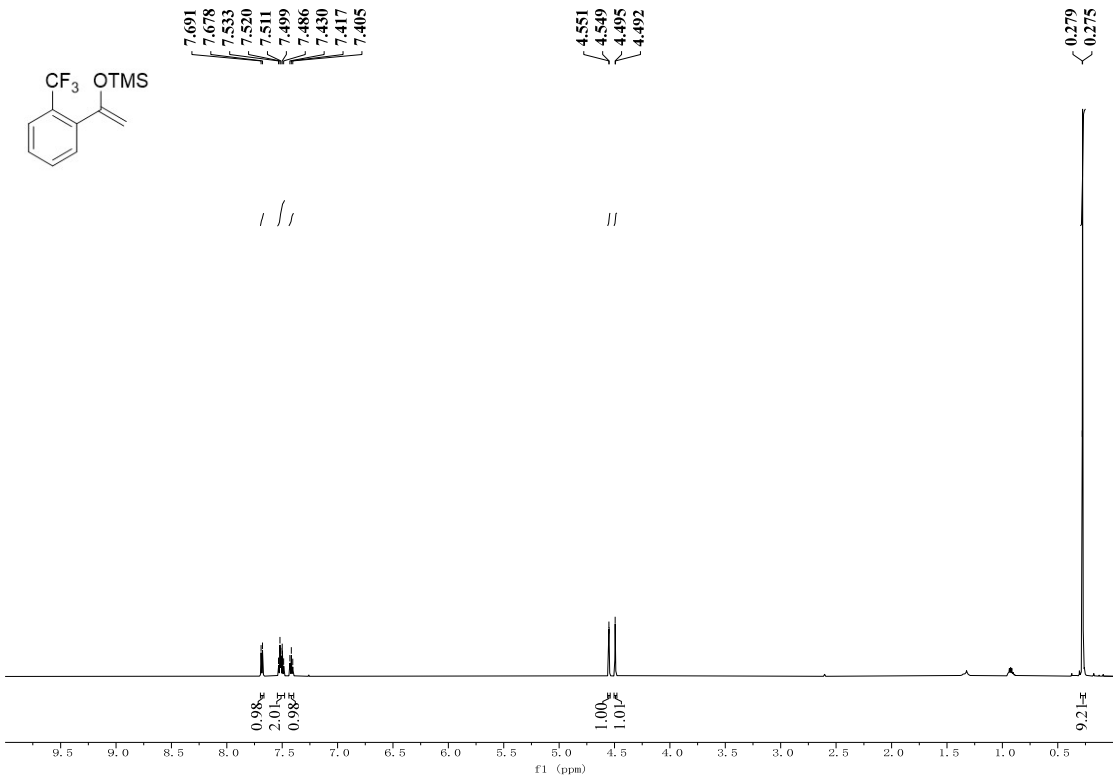

166.552
154.600
141.673
129.534
129.288
124.901
92.879
51.778
-0.190
OTMS
O
C
O
H3C
f1 (ppm)

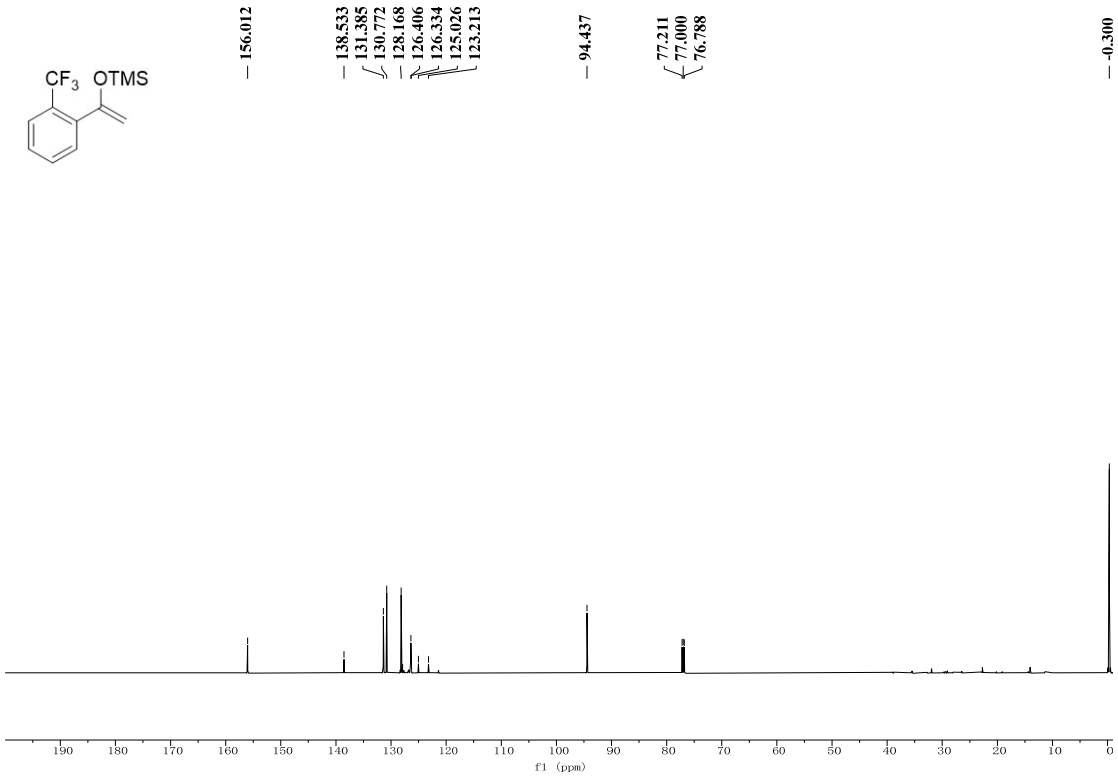

7.795
7.755
7.741
7.492
7.479
7.371
7.358
7.345
4.906
4.463
0.235
OTMS
NC
0.97
1.05
1.01
1.03
1.02
1.02
8.91
f1 (ppm)

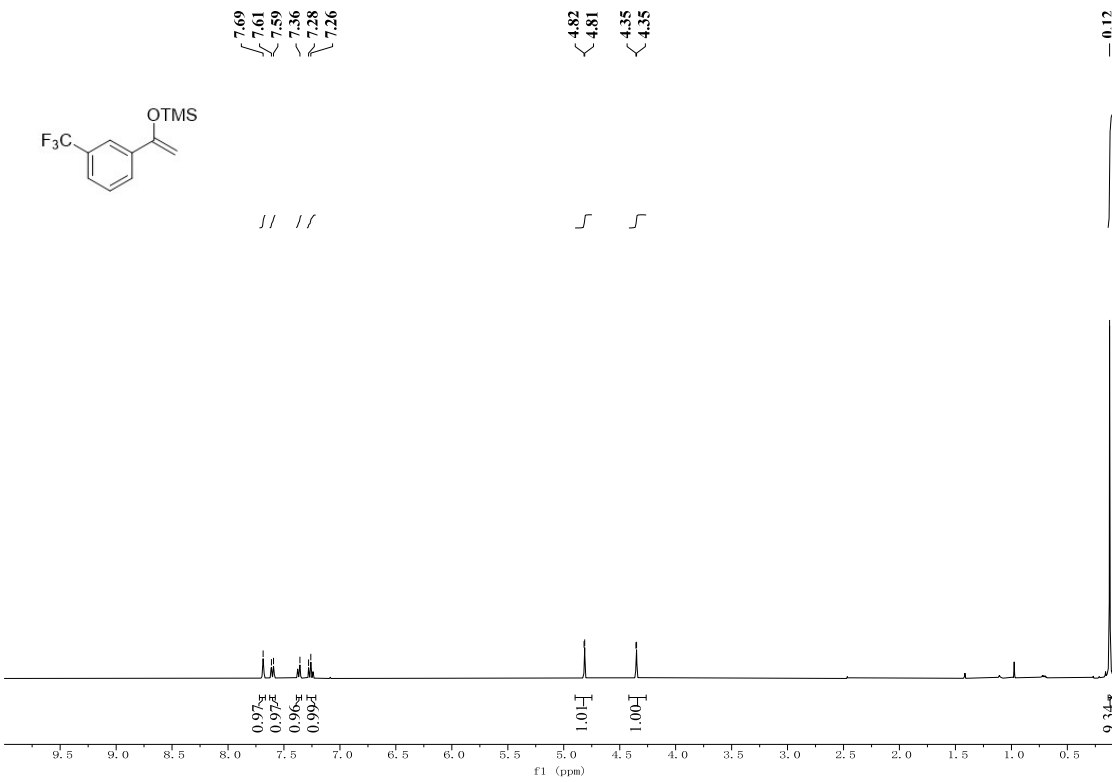

153.185
138.457
131.131
129.009
128.651
128.430
118.471
112.073
92.086
77.211
77.000
76.787
-0.357
OTMS
NC
f1 (ppm)

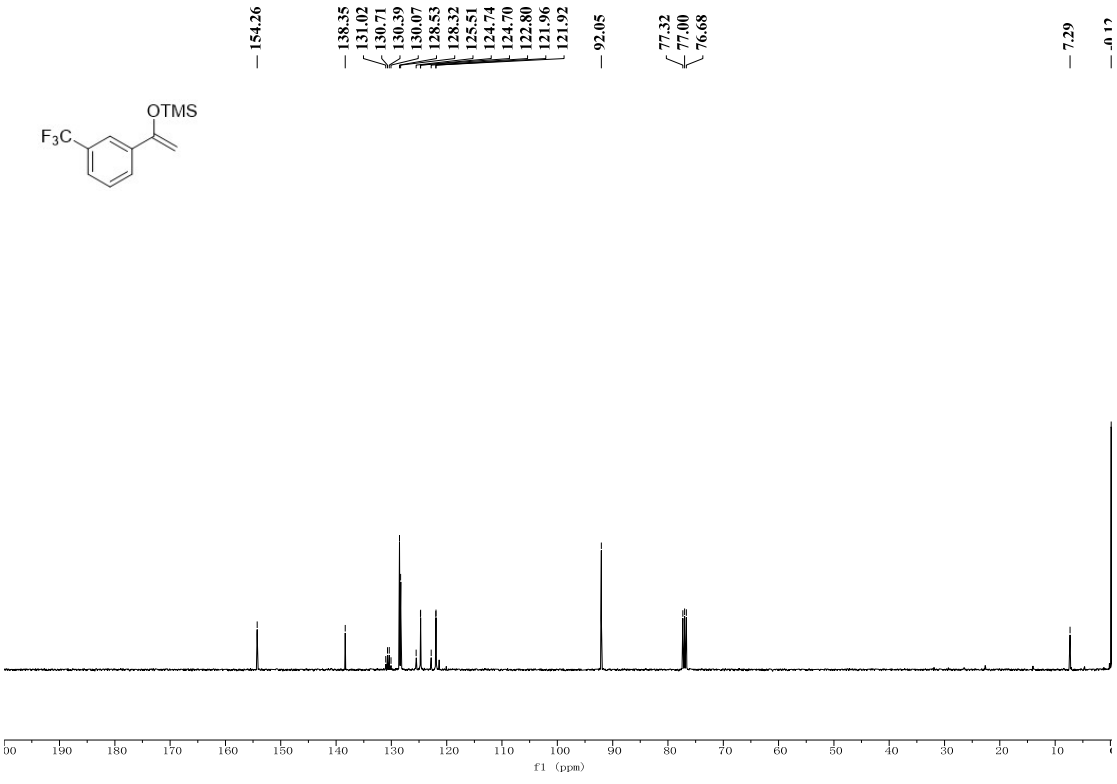

7.668
7.654
7.595
7.580
5.014
5.010
4.562
4.558
2.625
0.271
0.265
OTMS
NC
1.96
1.91
1.00
0.99
0.52
8.91
f1 (ppm)

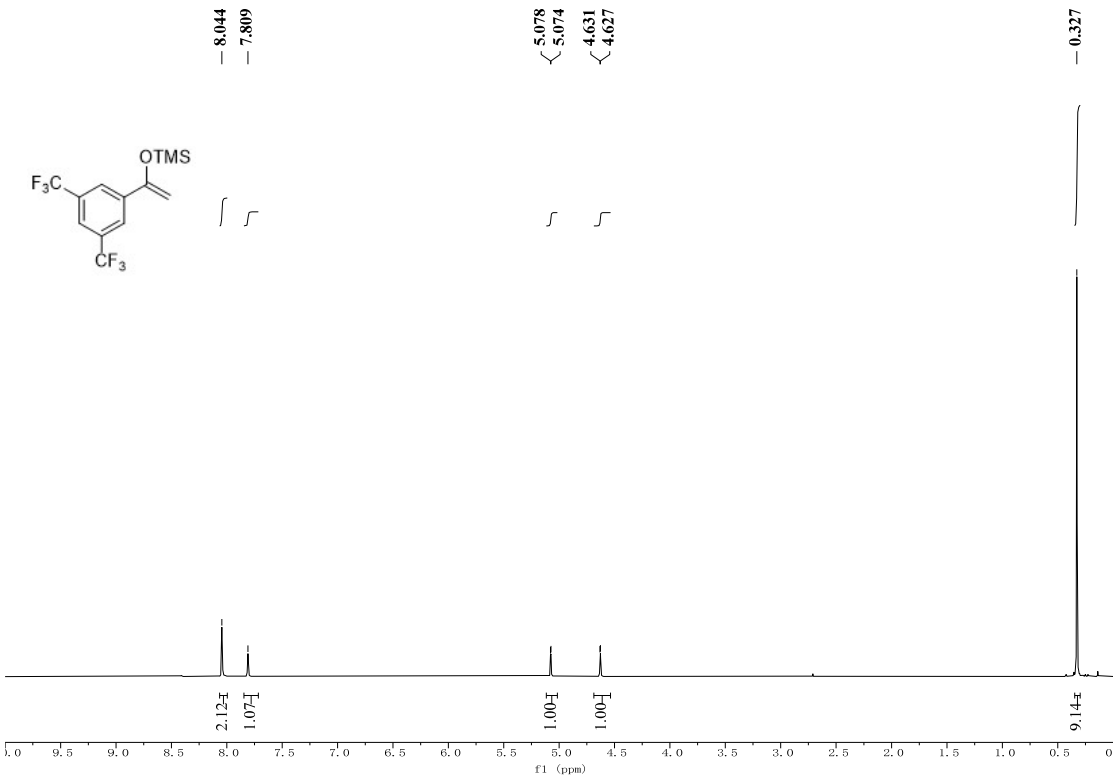

153.818
141.732
132.395
131.855
128.598
125.587
118.754
111.464
93.645
77.214
77.001
76.789
-0.123
OTMS
NC
f1 (ppm)

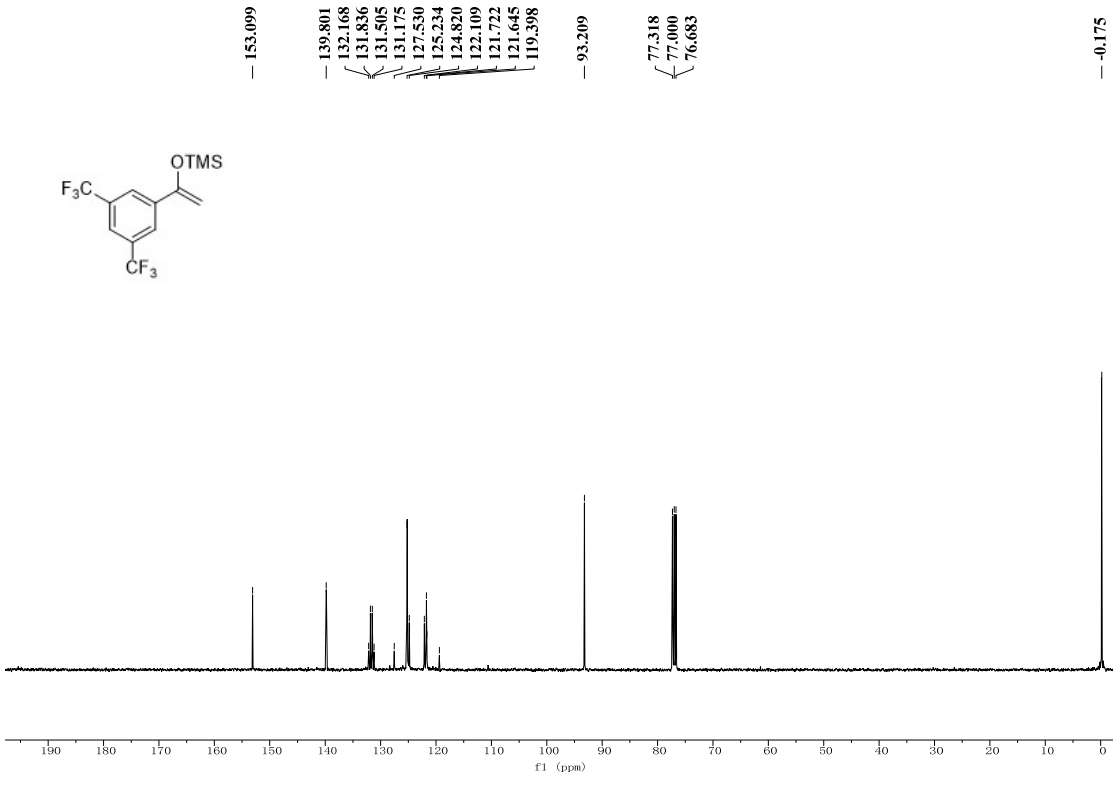

7.691
7.678
7.533
7.520
7.511
7.499
7.486
7.430
7.417
7.405
4.551
4.549
4.495
4.492
0.279
0.275
CF3 OTMS
0.98
2.01
0.98
1.00
1.01
9.21
f1 (ppm)

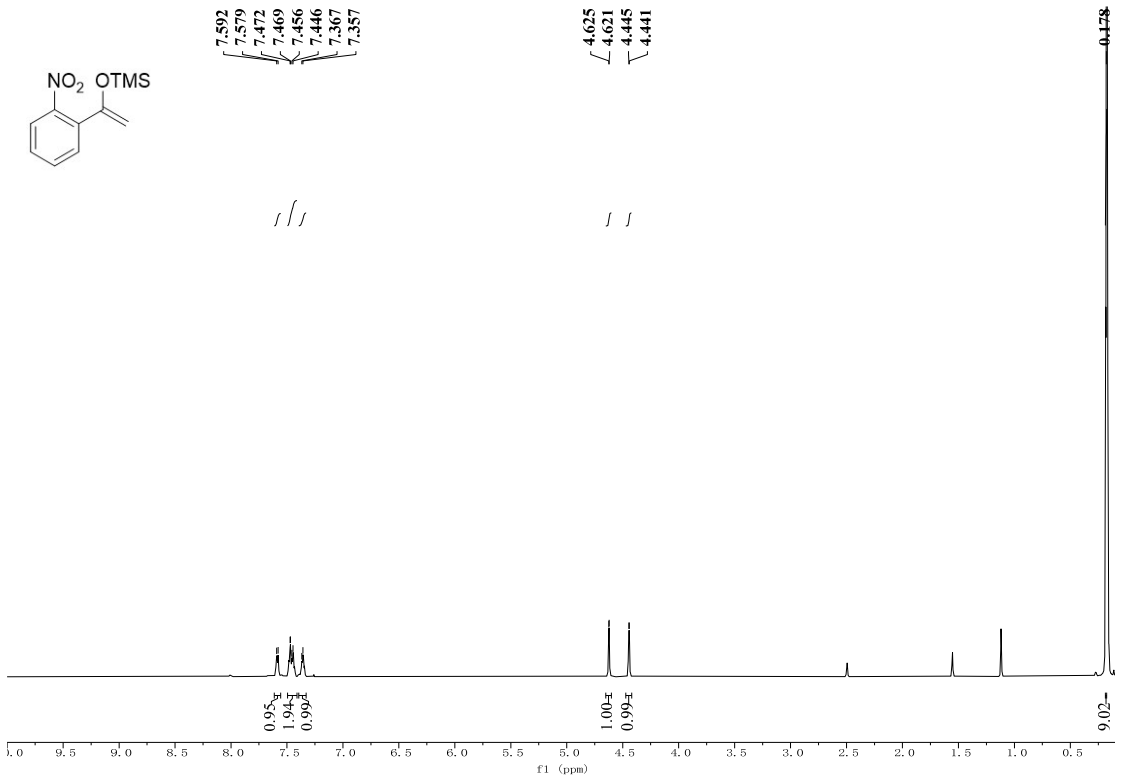

156.012
138.533
131.385
130.772
128.168
126.406
126.334
125.026
123.213
94.437
77.211
77.000
76.788
-0.300
CF3 OTMS
f1 (ppm)

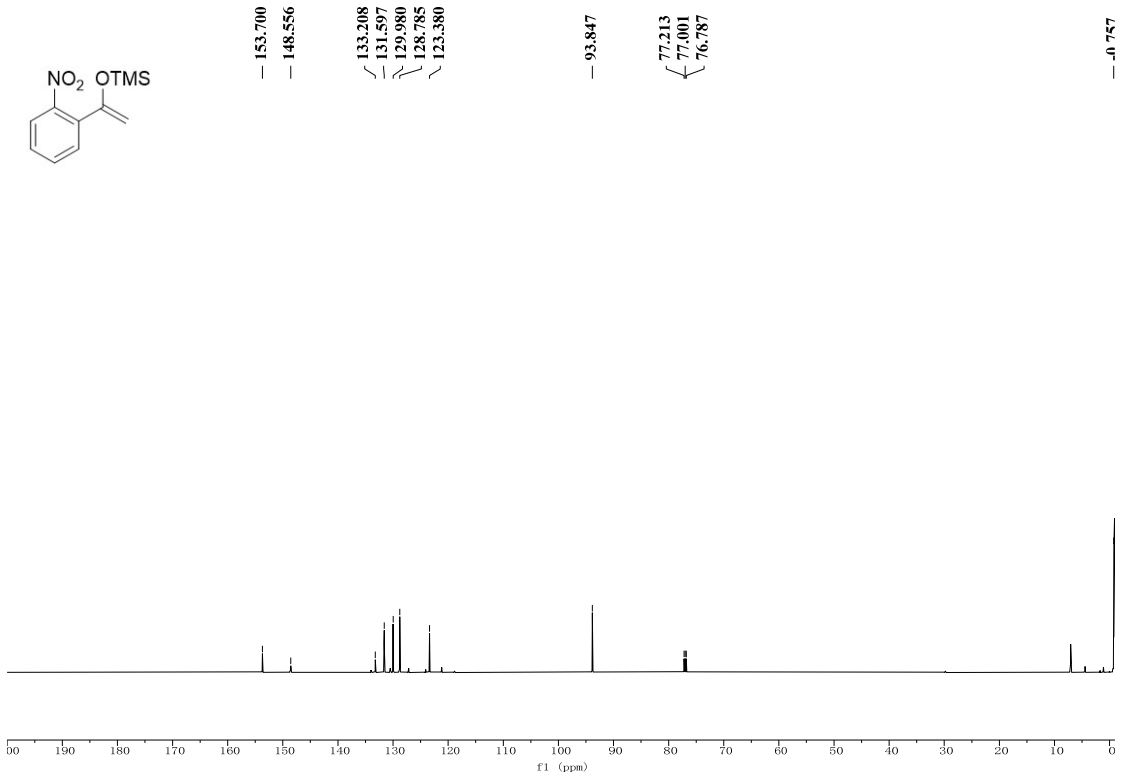

7.69
7.61
7.59
7.36
7.28
7.26
4.82
4.81
4.35
4.35
0.12
OTMS
F3C
0.97
0.97
0.96
0.99
1.01
1.00
9.34
f1 (ppm)

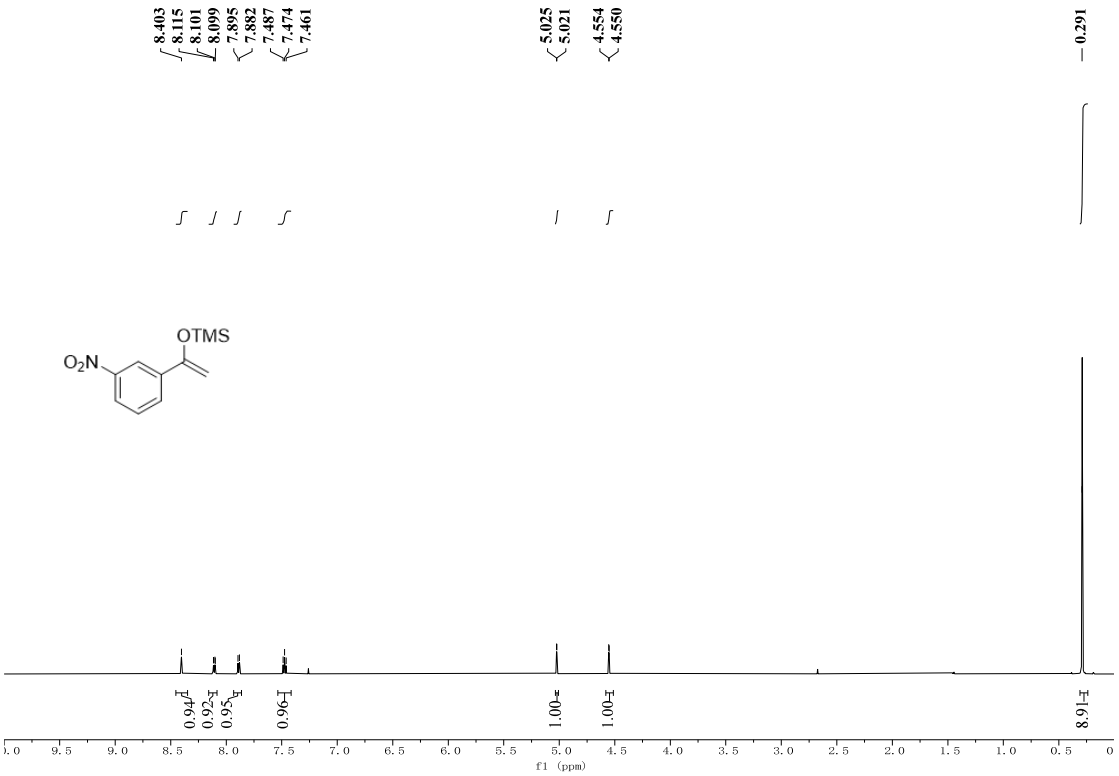

154.26
138.35
131.02
130.71
130.39
130.07
128.53
128.32
125.51
124.74
124.70
122.80
121.96
121.92
92.05
77.32
77.00
76.68
7.29
0.12
OTMS
F3C
f1 (ppm)

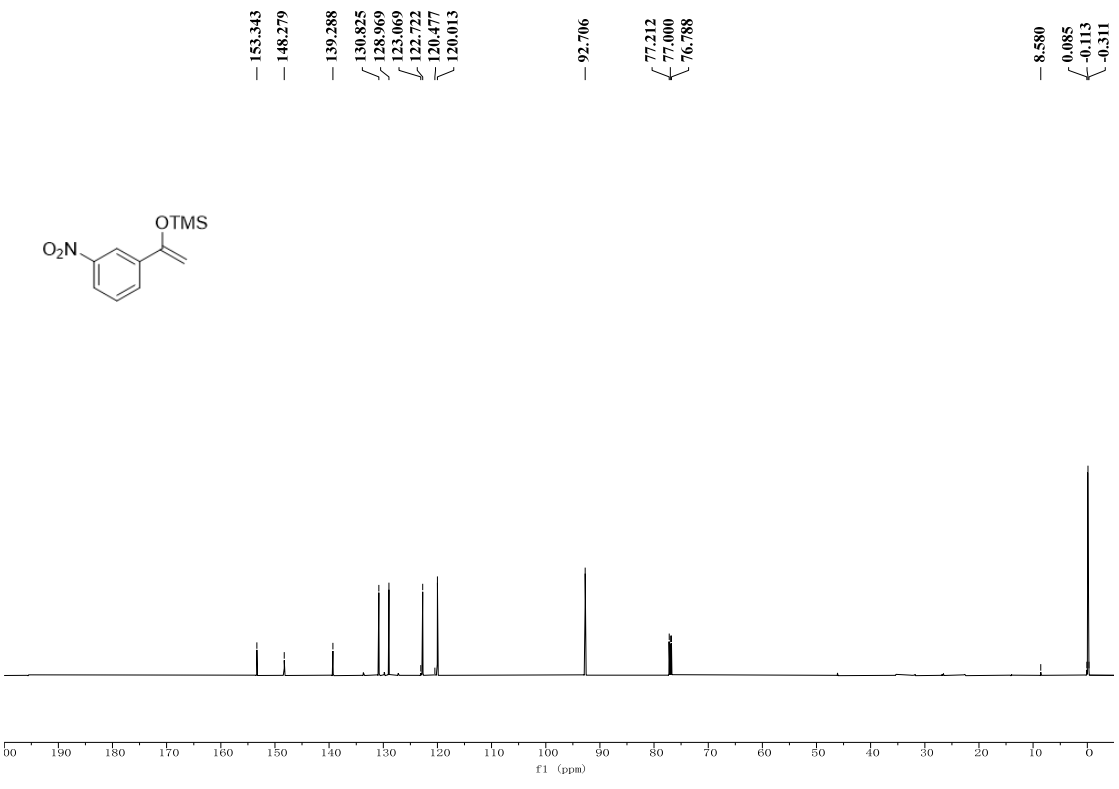

8.044
7.809
5.078
5.074
4.631
4.627
0.327
OTMS
F3C
CF3
2.12
1.07
1.00
1.00
9.14
f1 (ppm)

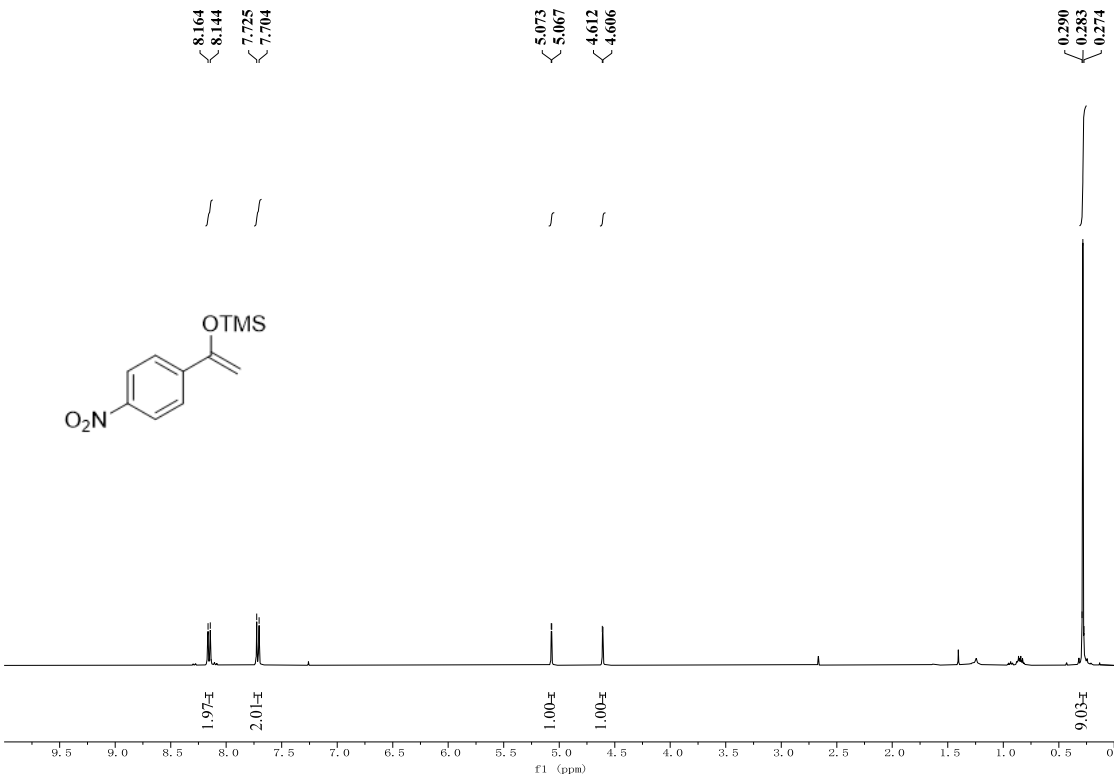

153.099
139.801
132.168
131.836
131.505
131.175
127.530
125.234
124.820
122.109
121.722
121.645
119.398
93.209
77.318
77.000
76.683
-0.175
OTMS
F3C
CF3
f1 (ppm)

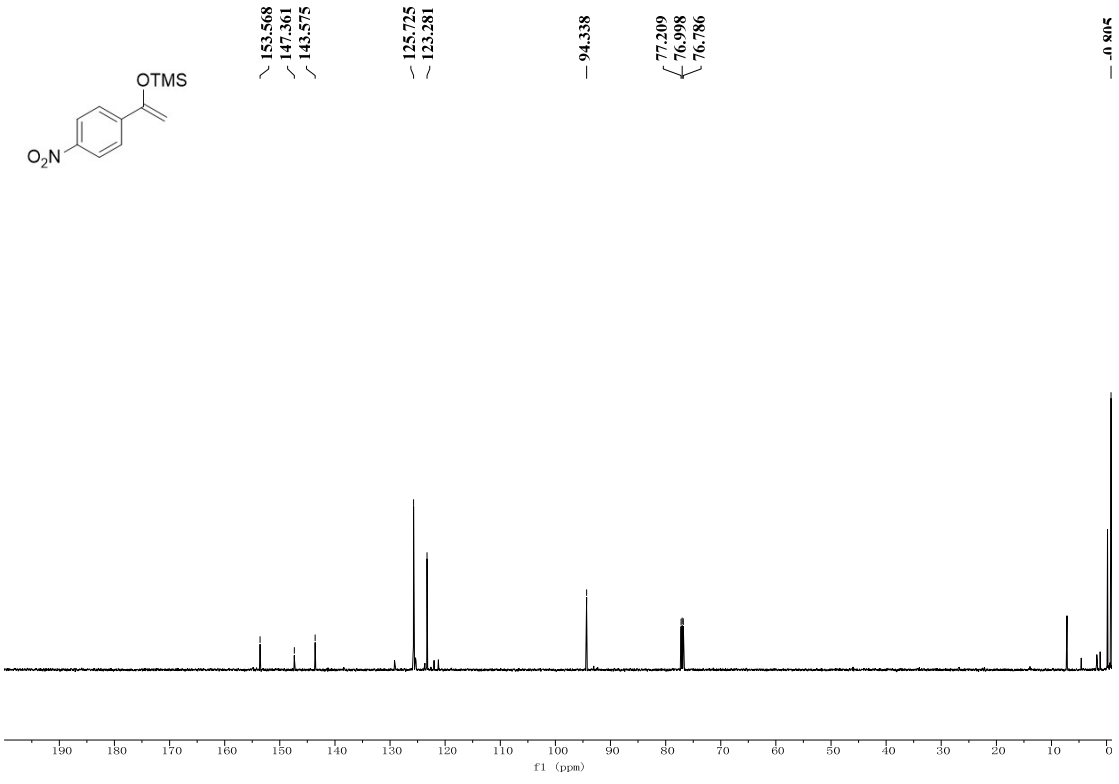

NO2 OTMS
7.592
7.579
7.472
7.469
7.456
7.446
7.367
7.357
4.625
4.621
4.445
4.441
0.178
0.95
1.94
0.99
1.00
0.99
9.02
f1 (ppm)

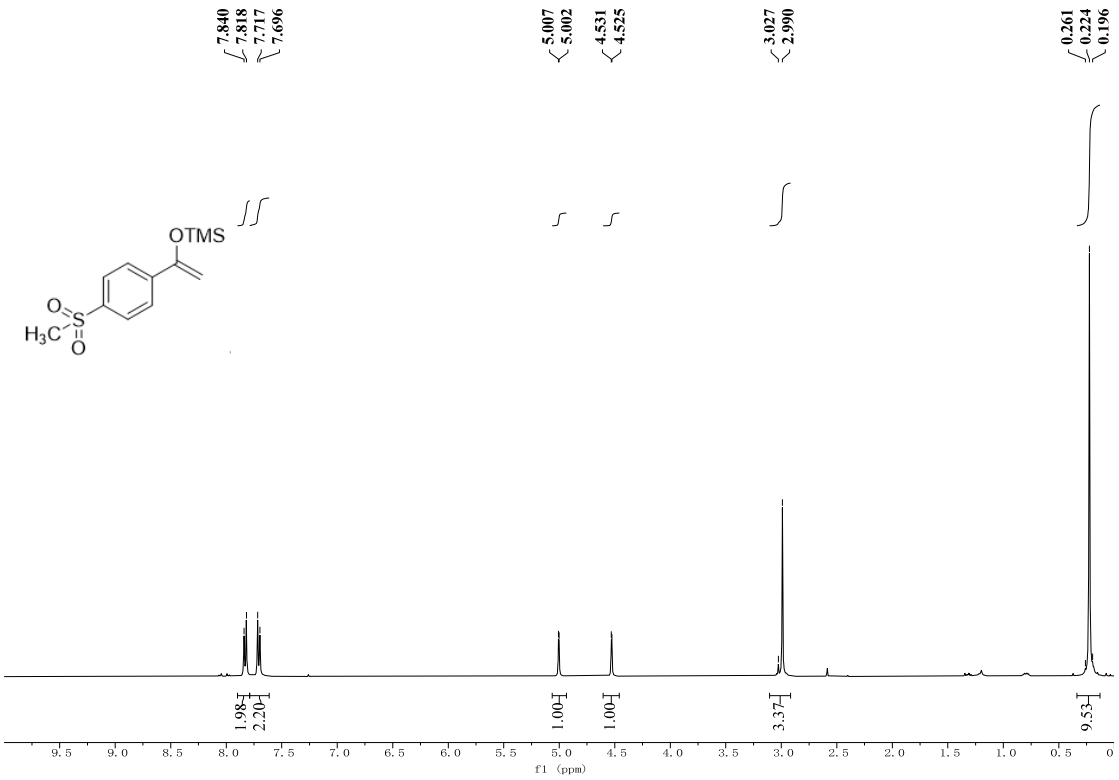

NO2 OTMS
153.700
148.556
133.208
131.597
129.980
128.785
123.380
93.847
77.213
77.001
76.787
-0.757
f1 (ppm)

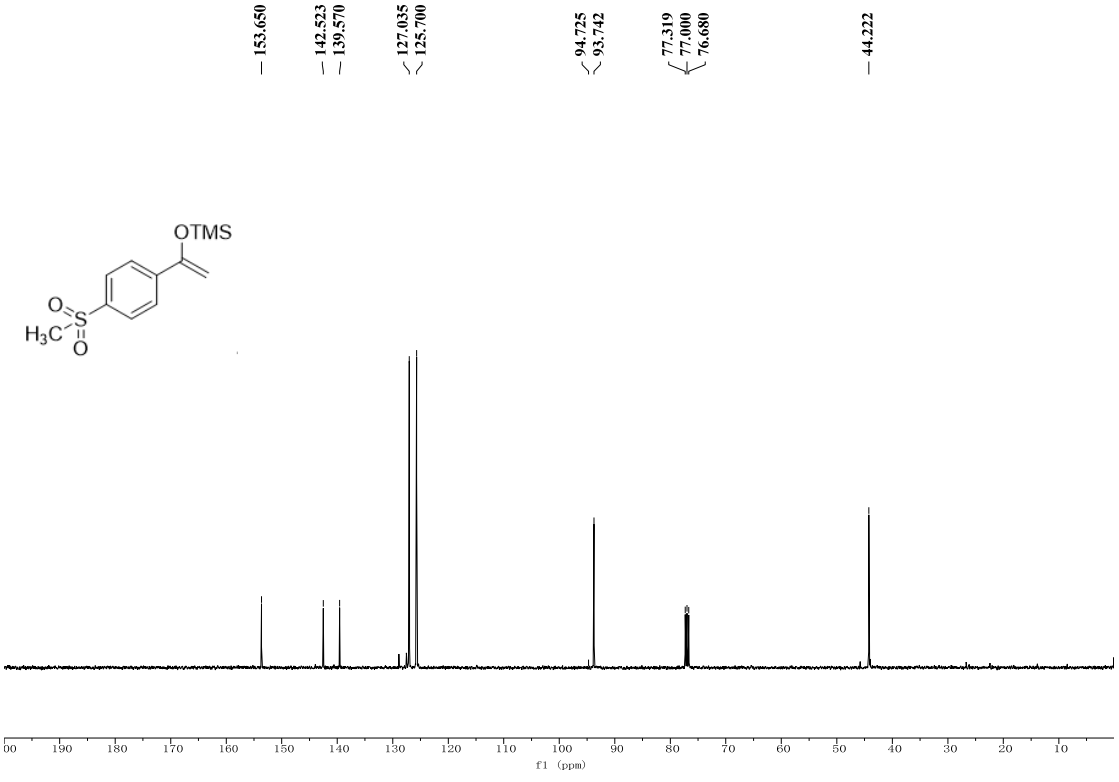

8.403
8.115
8.101
8.099
7.895
7.882
7.487
7.474
7.461
5.025
5.021
4.554
4.550
0.291
OTMS
O2N
0.94
0.92
0.95
0.96
1.00
1.00
8.91
f1 (ppm)

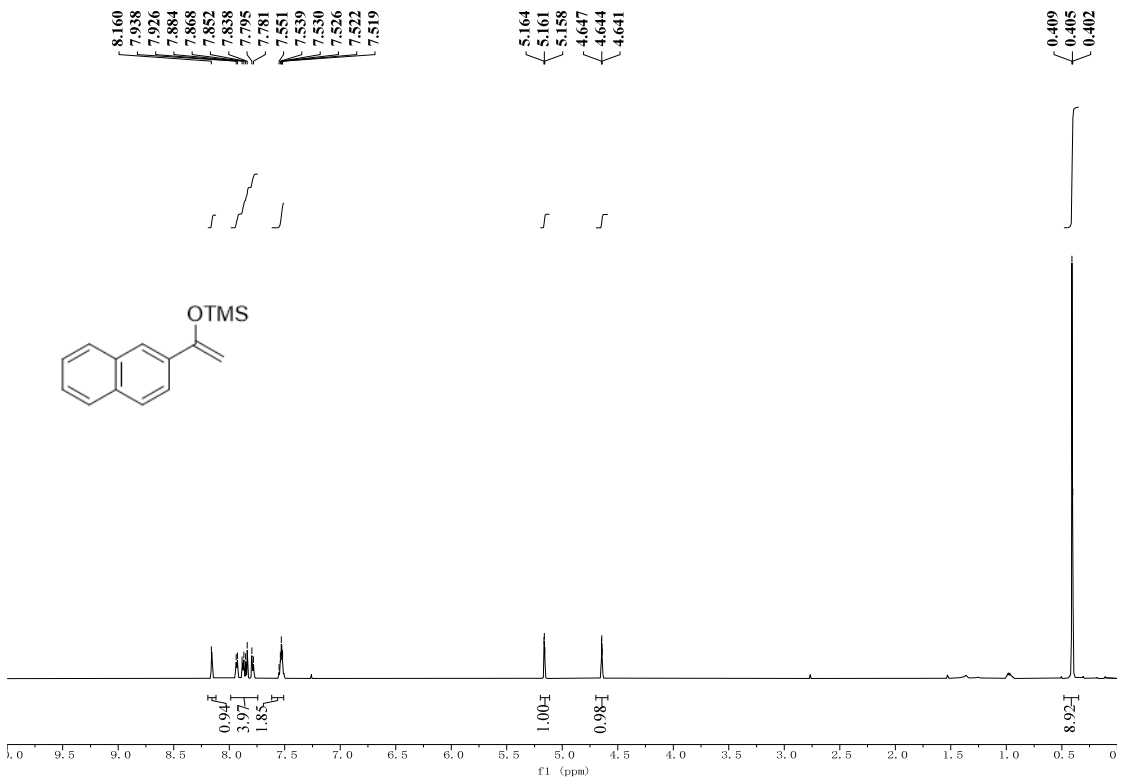

153.343
148.279
139.288
130.825
128.969
123.069
122.722
120.477
120.013
92.706
77.212
77.000
76.788
8.580
0.085
-0.113
-0.311
OTMS
O2N
f1 (ppm)

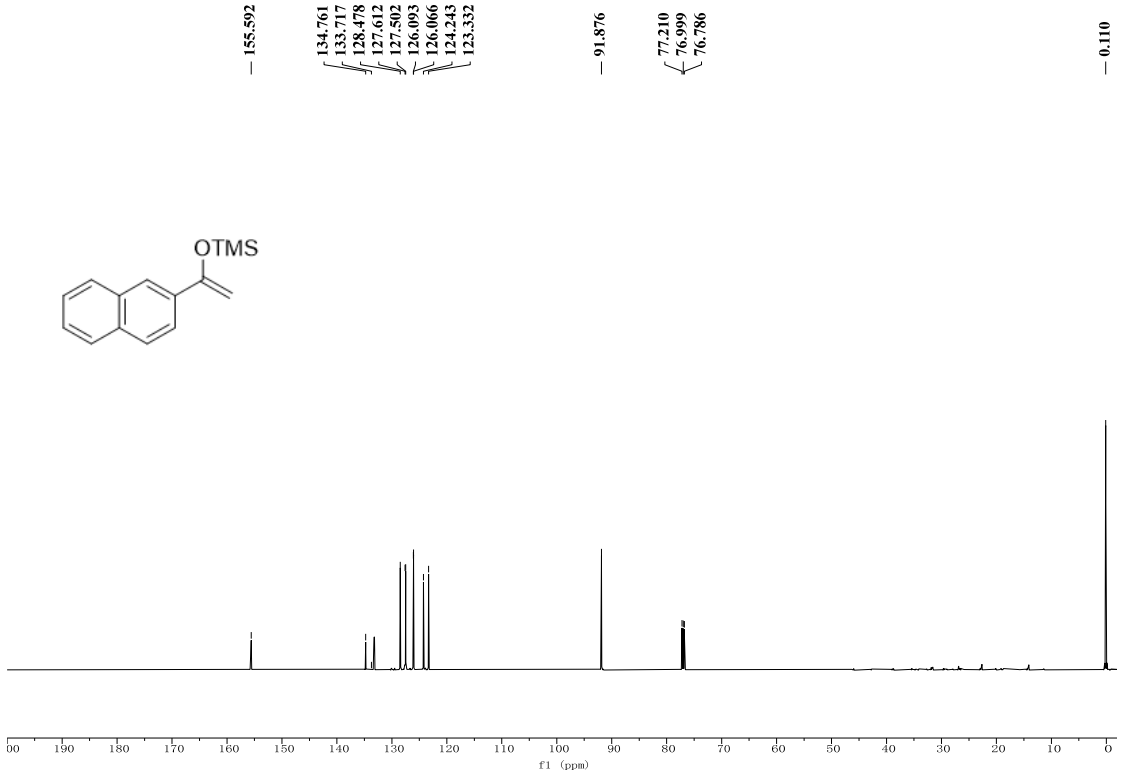

8.164
8.144
7.725
7.704
5.073
5.067
4.612
4.606
0.290
0.283
0.274
OTMS
O2N
1.97
2.01
1.00
1.00
9.03
f1 (ppm)

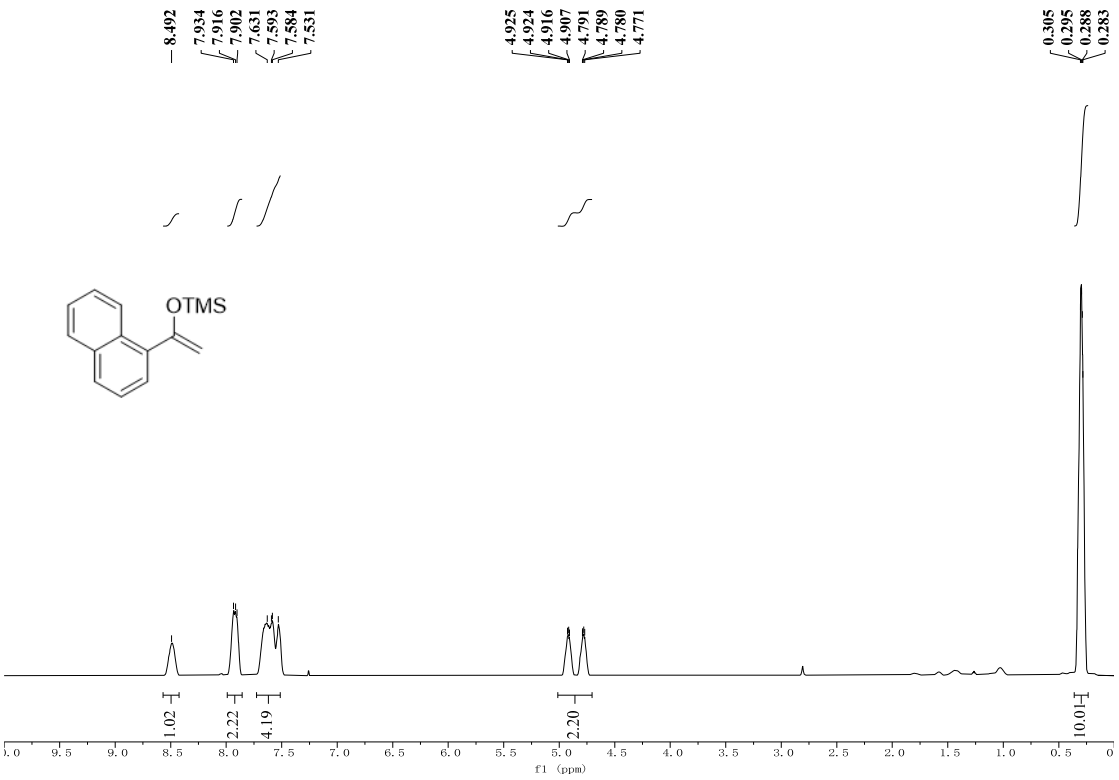

153.568
147.361
143.575
125.725
123.281
94.338
77.209
76.998
76.786
OTMS
O2N
f1 (ppm)

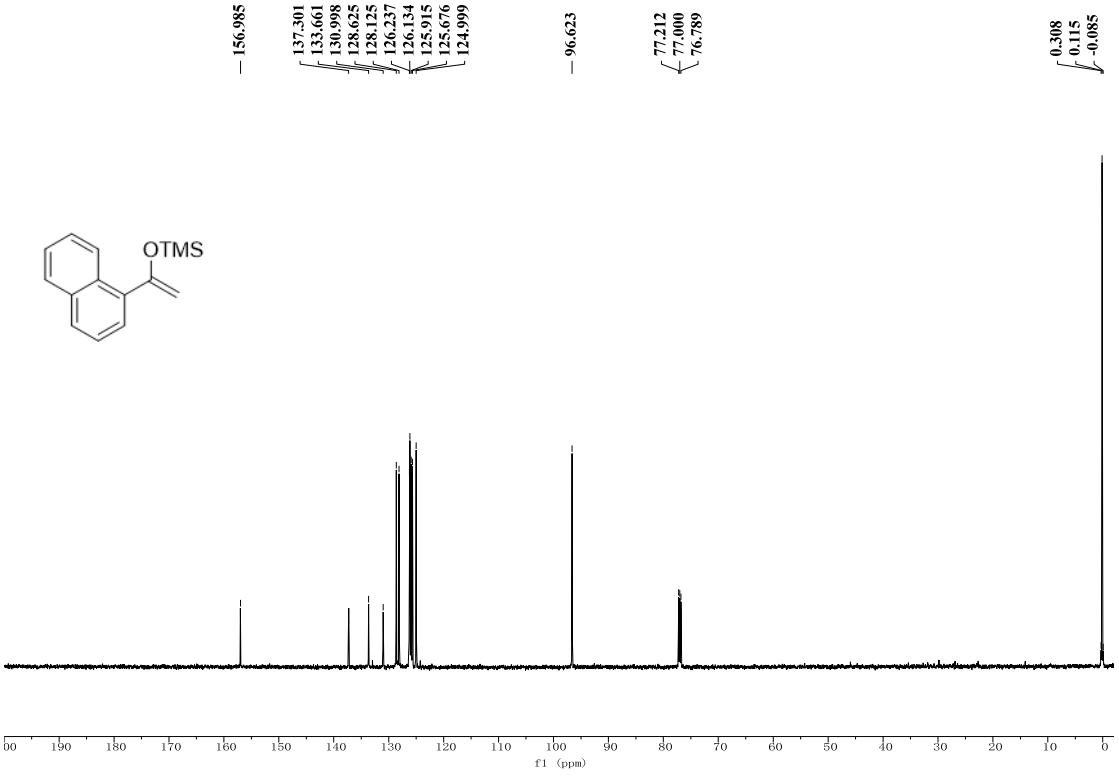

7.840
7.818
7.717
7.696
5.007
5.002
4.531
4.525
3.027
2.990
0.261
0.224
0.196
OTMS
O
S
O
H3C
1.98
2.20
1.00
1.00
3.37
9.53
f1 (ppm)

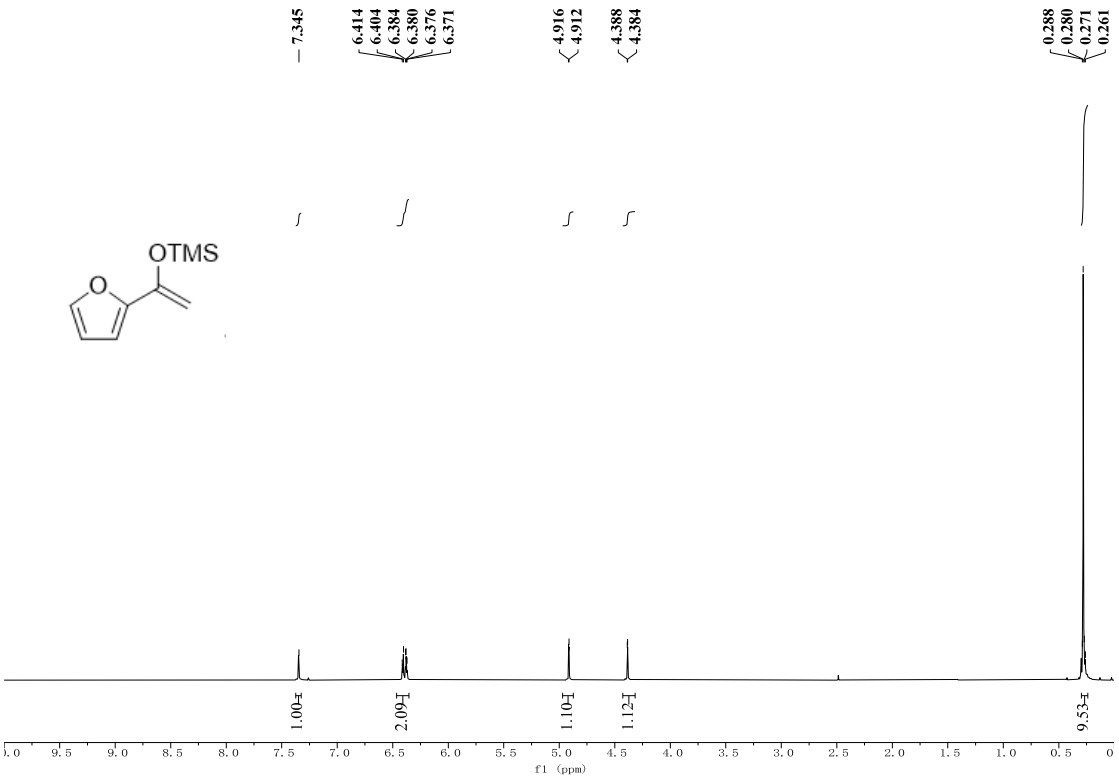

153.650
142.523
139.570
127.035
125.700
94.725
93.742
77.319
77.000
76.680
44.222
OTMS
O
S
O
H3C
f1 (ppm)

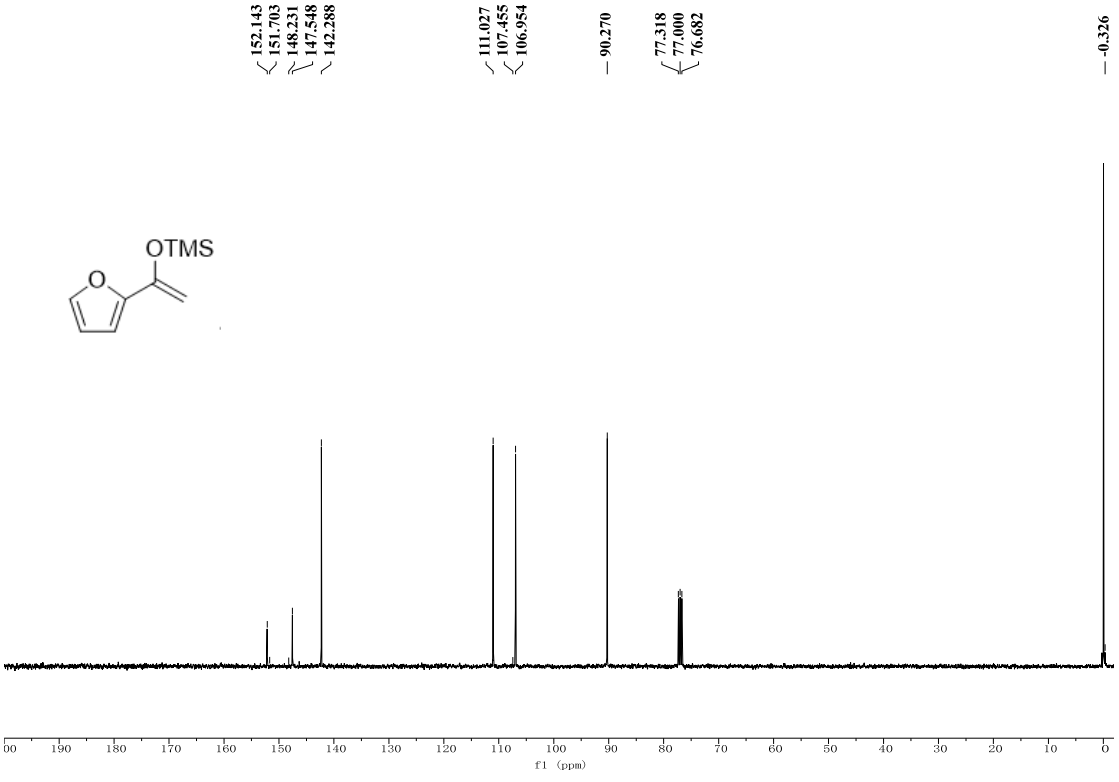

8.160
7.938
7.926
7.884
7.868
7.852
7.838
7.795
7.781
7.551
7.539
7.530
7.526
7.522
7.519
5.164
5.161
5.158
4.647
4.644
4.641
0.409
0.405
0.402
OTMS
0.94
3.97
1.85
1.00
0.98
8.92
f1 (ppm)

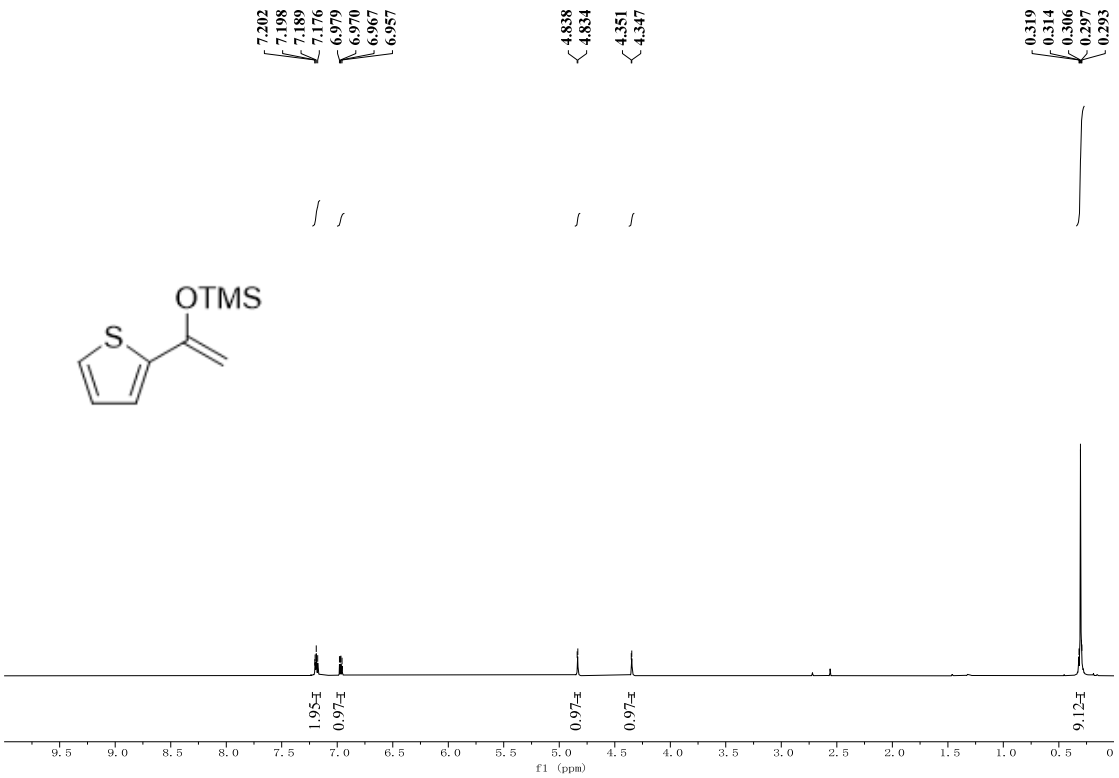

155.592
134.761
133.717
128.478
127.612
127.502
126.093
126.066
124.243
123.332
91.876
77.210
76.999
76.786
0.110
OTMS
f1 (ppm)

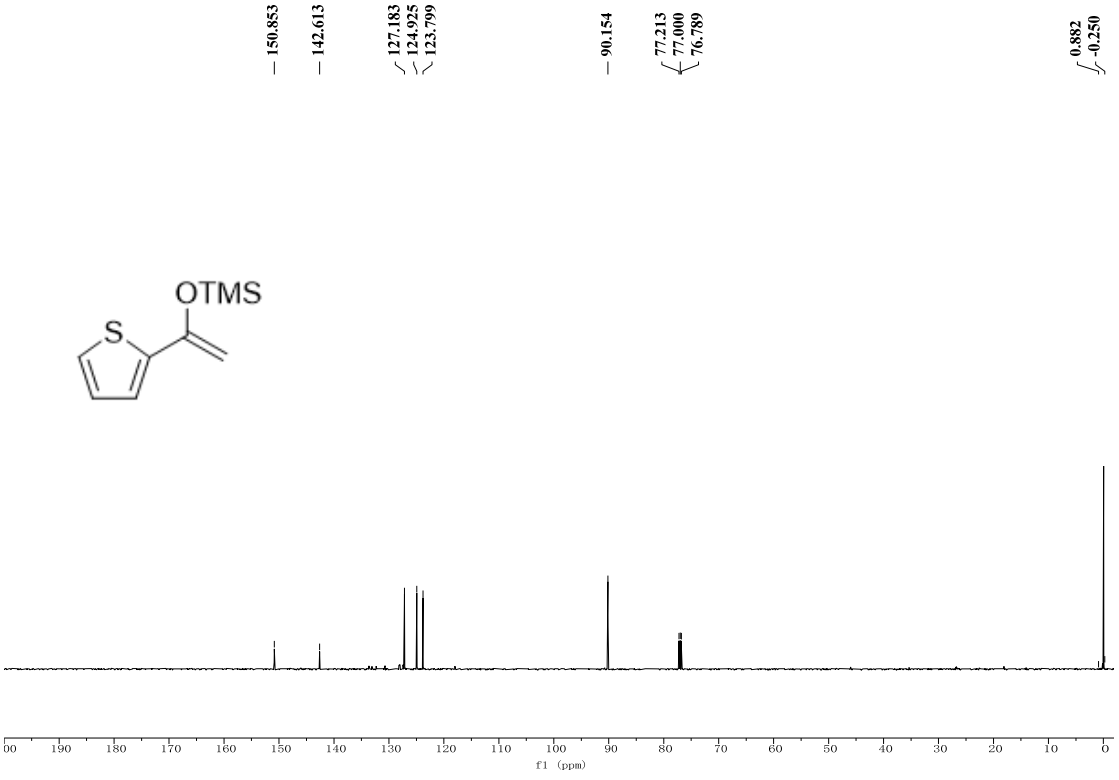

8.492
7.934
7.916
7.902
7.631
7.593
7.584
7.531
4.925
4.924
4.916
4.907
4.791
4.789
4.780
4.771
0.305
0.295
0.288
0.283
OTMS
1.02
2.22
4.19
2.20
10.01
f1 (ppm)

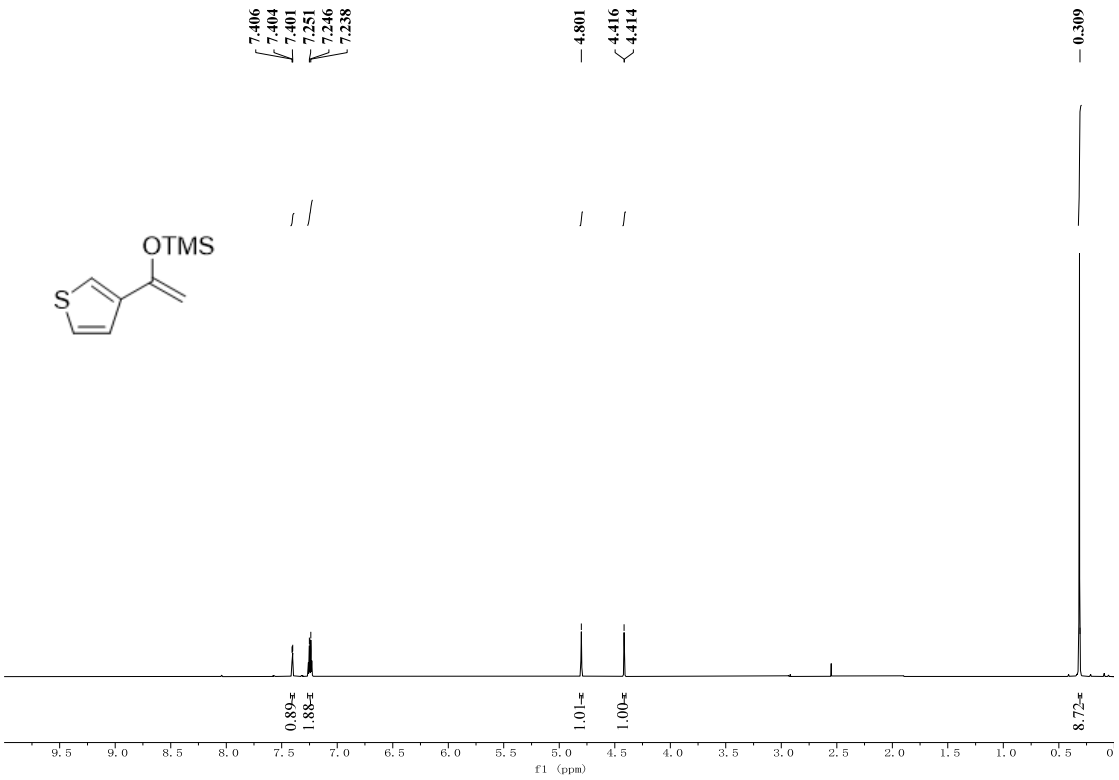

156.985
137.301
133.661
130.998
128.625
128.125
126.237
126.134
125.915
125.676
124.999
96.623
77.212
77.000
76.789
0.308
0.115
-0.085
OTMS
f1 (ppm)

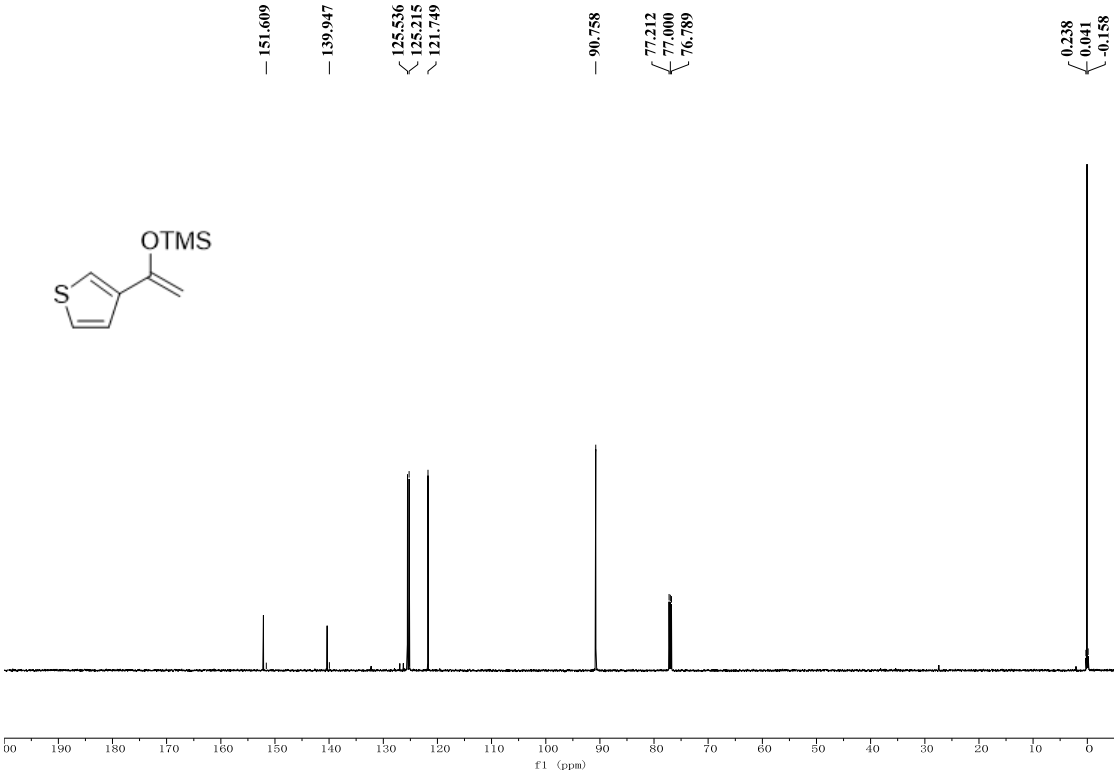

7.345
6.414
6.404
6.384
6.380
6.376
6.371
4.916
4.912
4.388
4.384
0.288
0.280
0.271
0.261
OTMS
O
1.00
2.09
1.10
1.12
9.53
f1 (ppm)

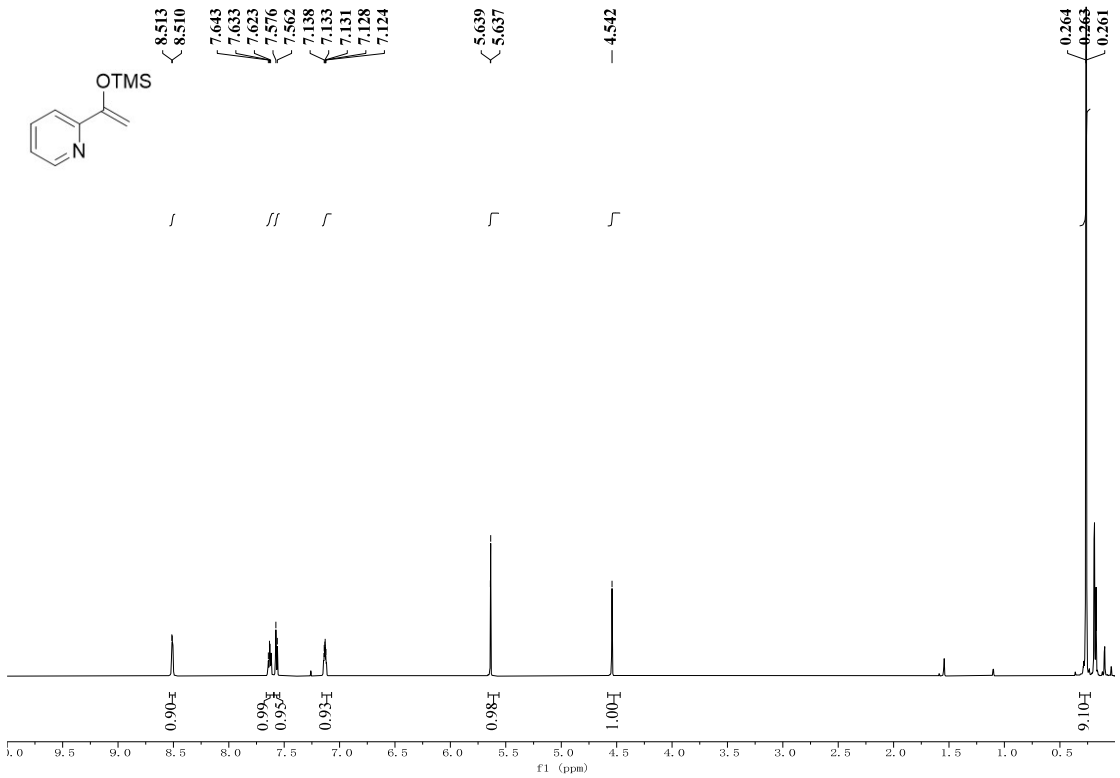

152.143
151.703
148.231
147.548
142.288
111.027
107.455
106.954
90.270
77.318
77.000
76.682
-0.326
OTMS
O
f1 (ppm)

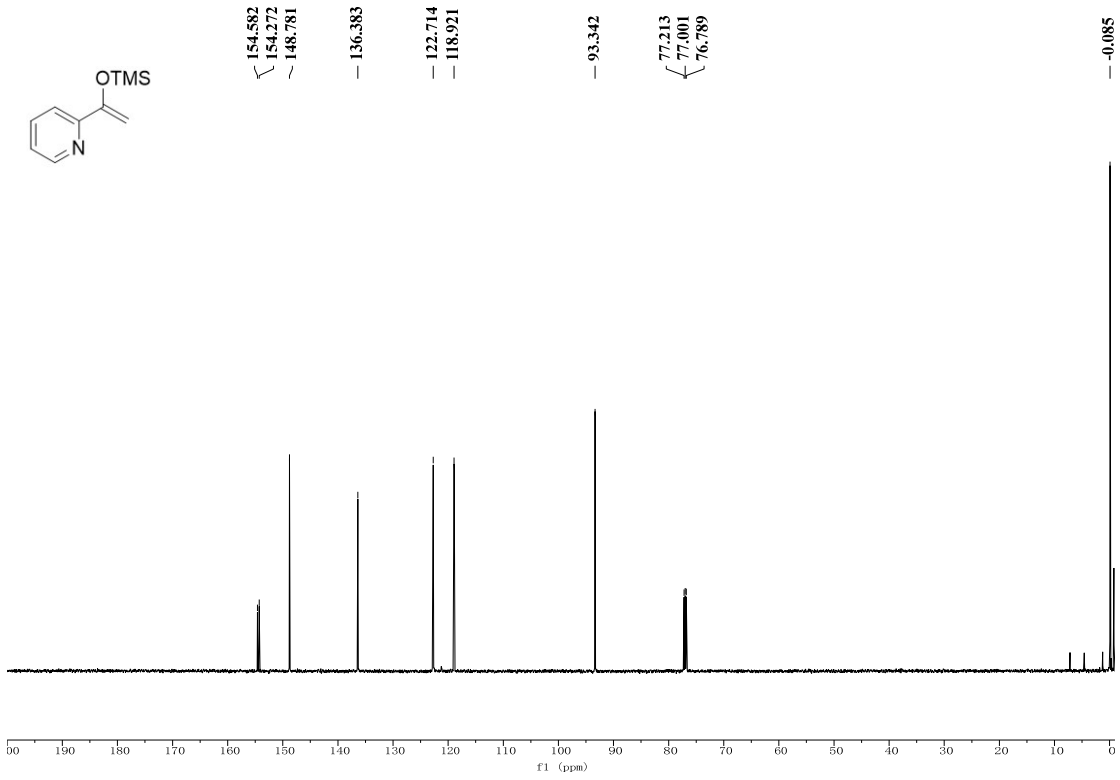

7.202
7.198
7.189
7.176
6.979
6.970
6.967
6.957
4.838
4.834
4.351
4.347
0.319
0.314
0.306
0.297
0.293
OTMS
S
1.95
0.97
0.97
0.97
9.12
f1 (ppm)

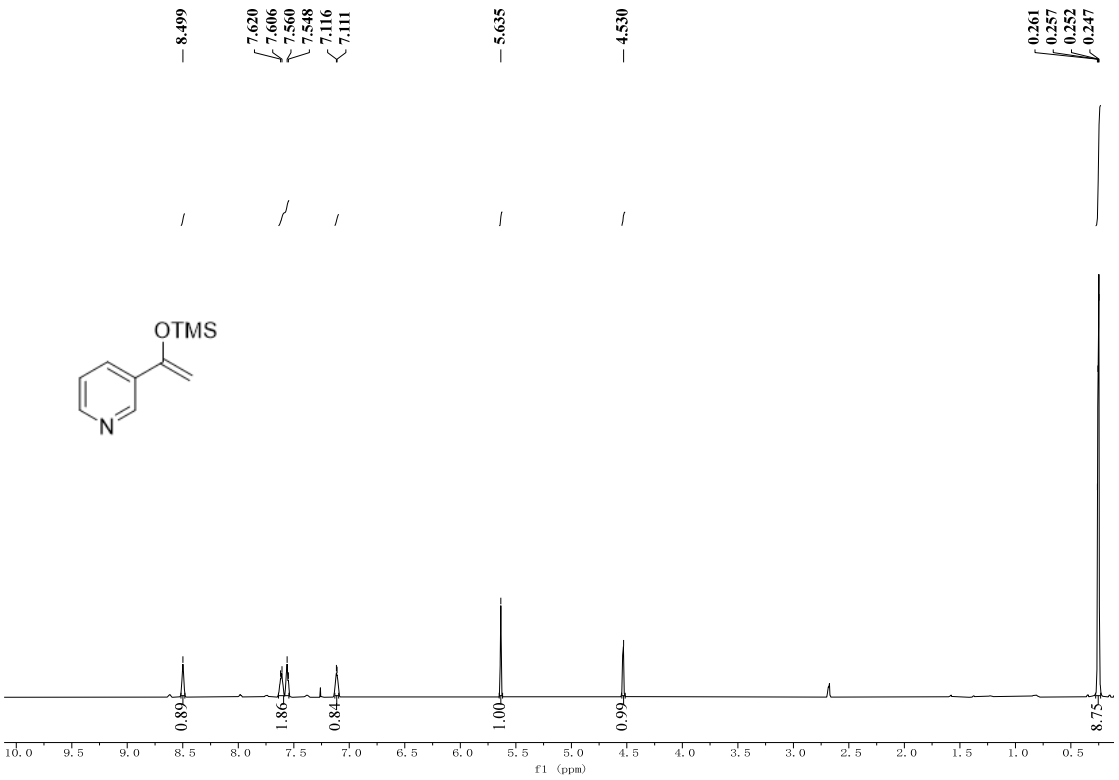

150.853
142.613
127.183
124.925
123.799
90.154
77.213
77.000
76.789
0.882
-0.250
OTMS
S
f1 (ppm)

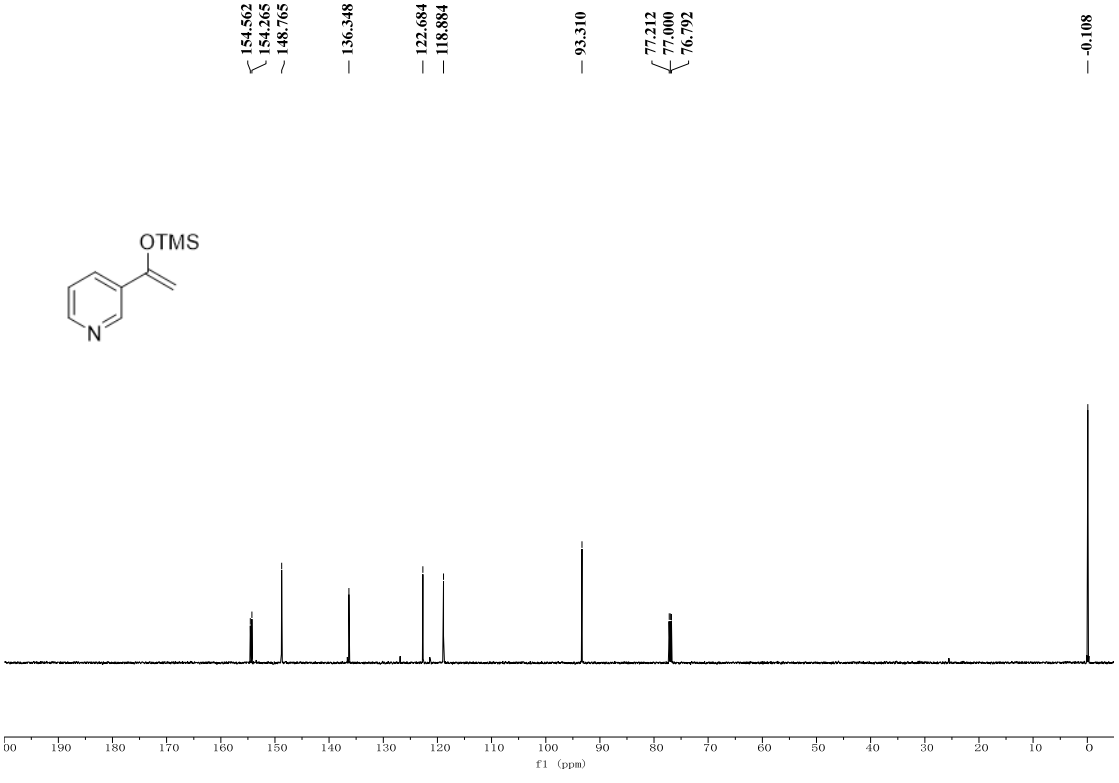

7.406
7.404
7.401
7.251
7.246
7.238
4.801
4.416
4.414
0.309
OTMS
S
0.89
1.88
1.01
1.00
8.72
f1 (ppm)

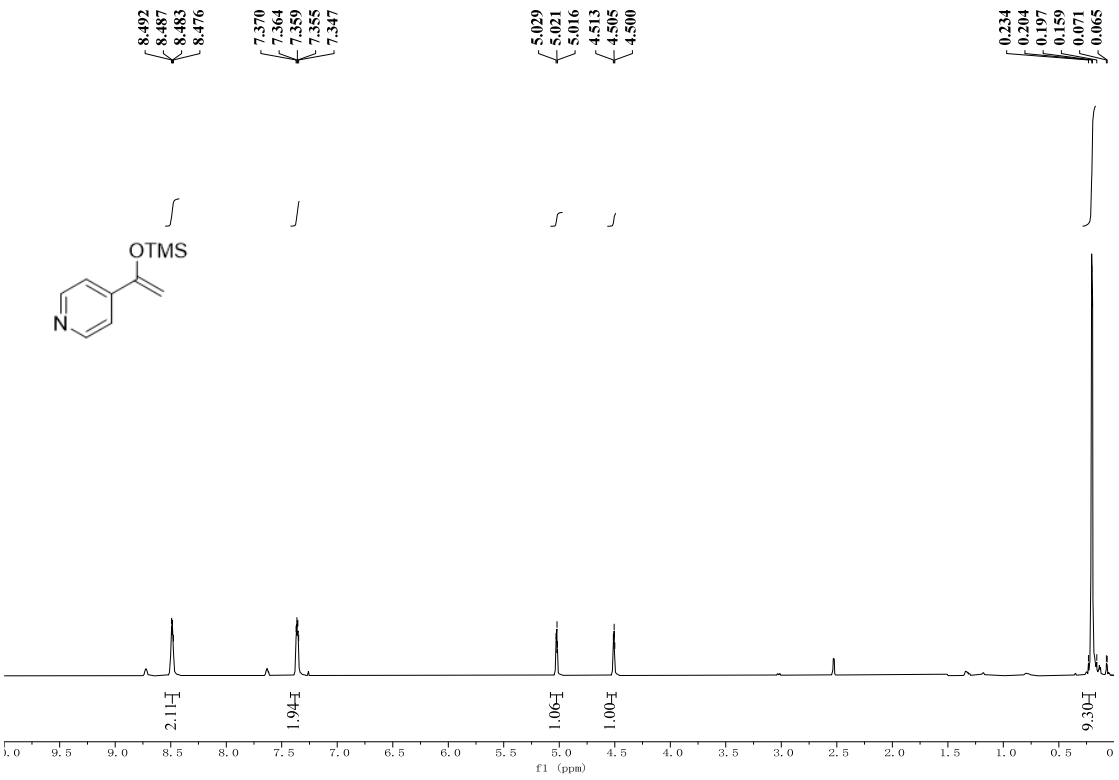

151.609
139.947
125.536
125.215
121.749
90.758
77.212
77.000
76.789
0.238
0.041
-0.158
OTMS
S
f1 (ppm)

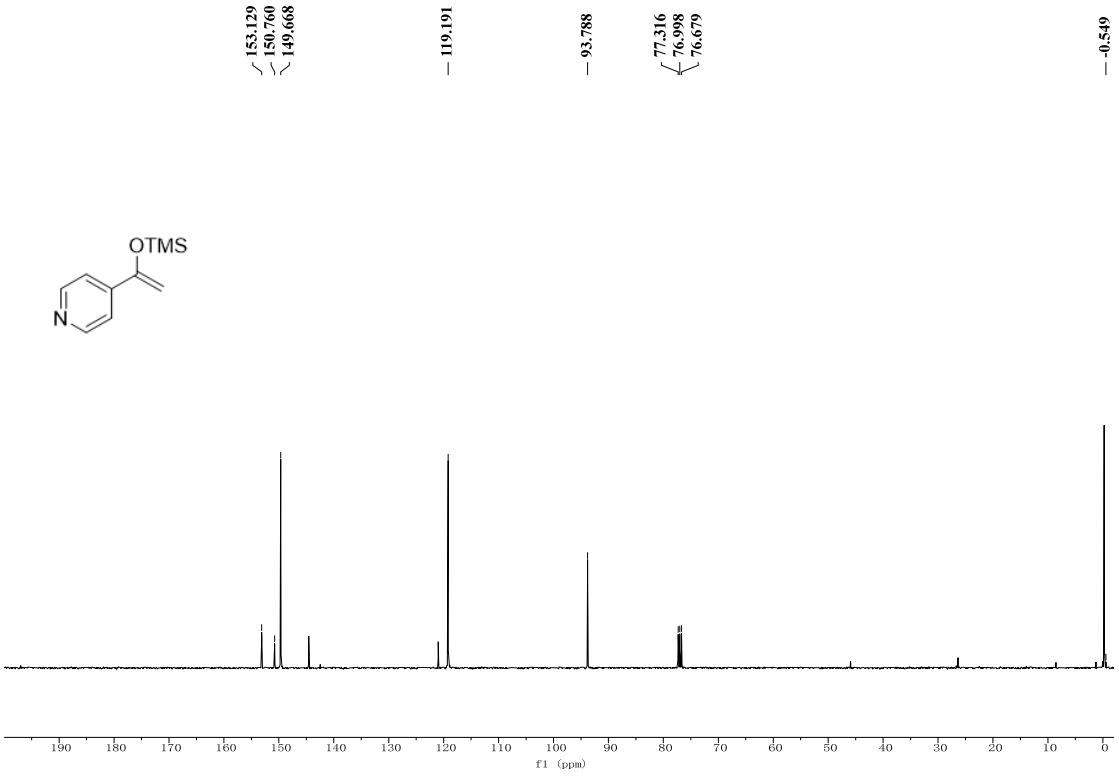

OTMS
N
8.513
8.510
7.643
7.633
7.623
7.576
7.562
7.138
7.133
7.131
7.128
7.124
5.639
5.637
4.542
0.264
0.263
0.261
0.90
0.99
0.95
0.93
0.98
1.00
9.10
f1 (ppm)

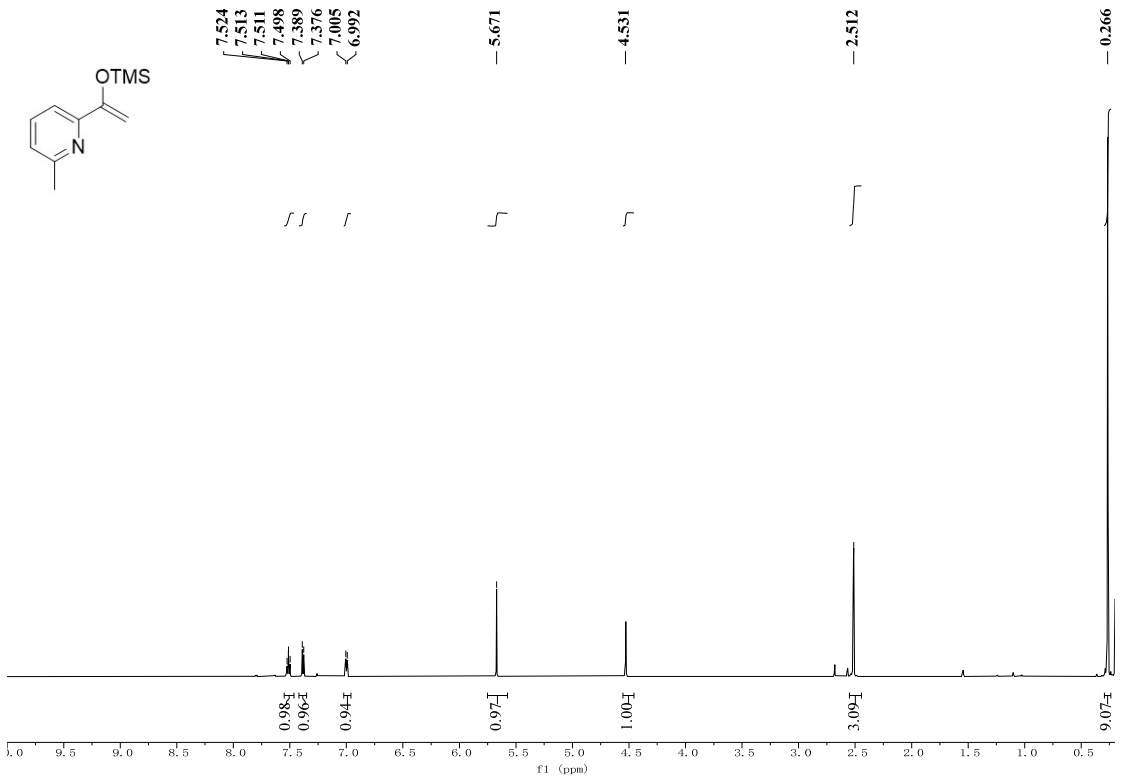

OTMS
N
154.582
154.272
148.781
136.383
122.714
118.921
93.342
77.213
77.001
76.789
-0.085
f1 (ppm)

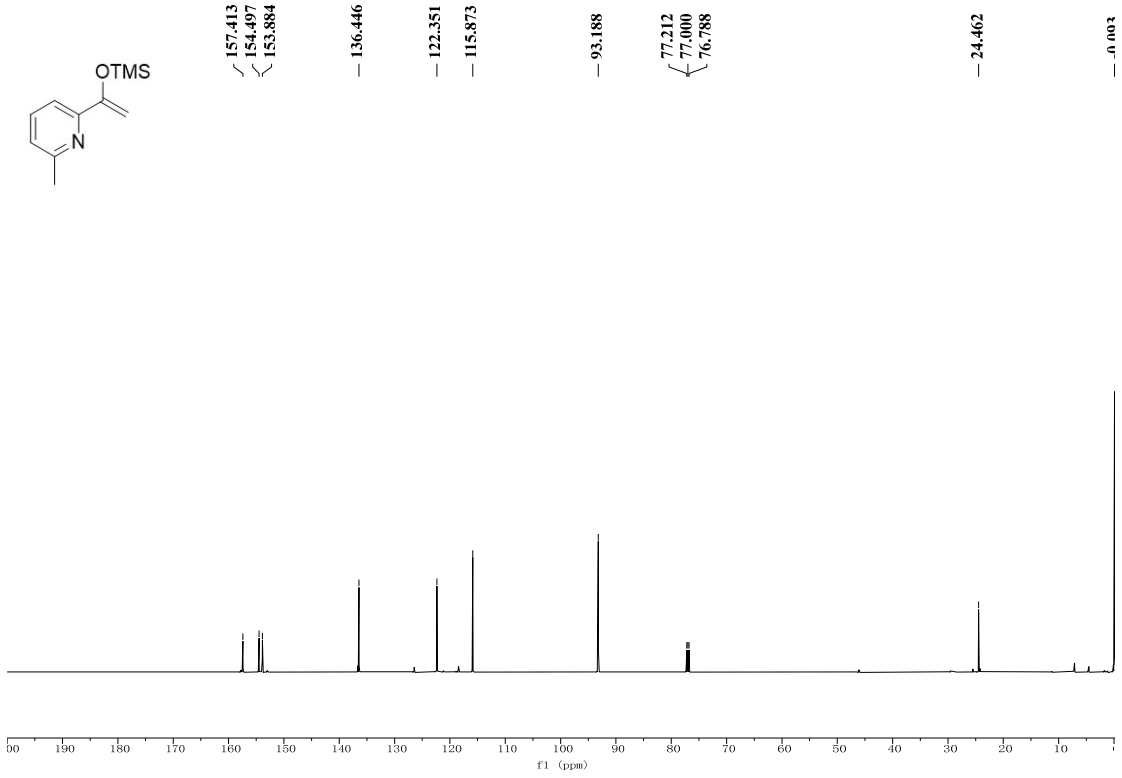

8.499
7.620
7.606
7.560
7.548
7.116
7.111
5.635
4.530
0.261
0.257
0.252
0.247
OTMS
N
0.89
1.86
0.84
1.00
0.99
8.75
f1 (ppm)

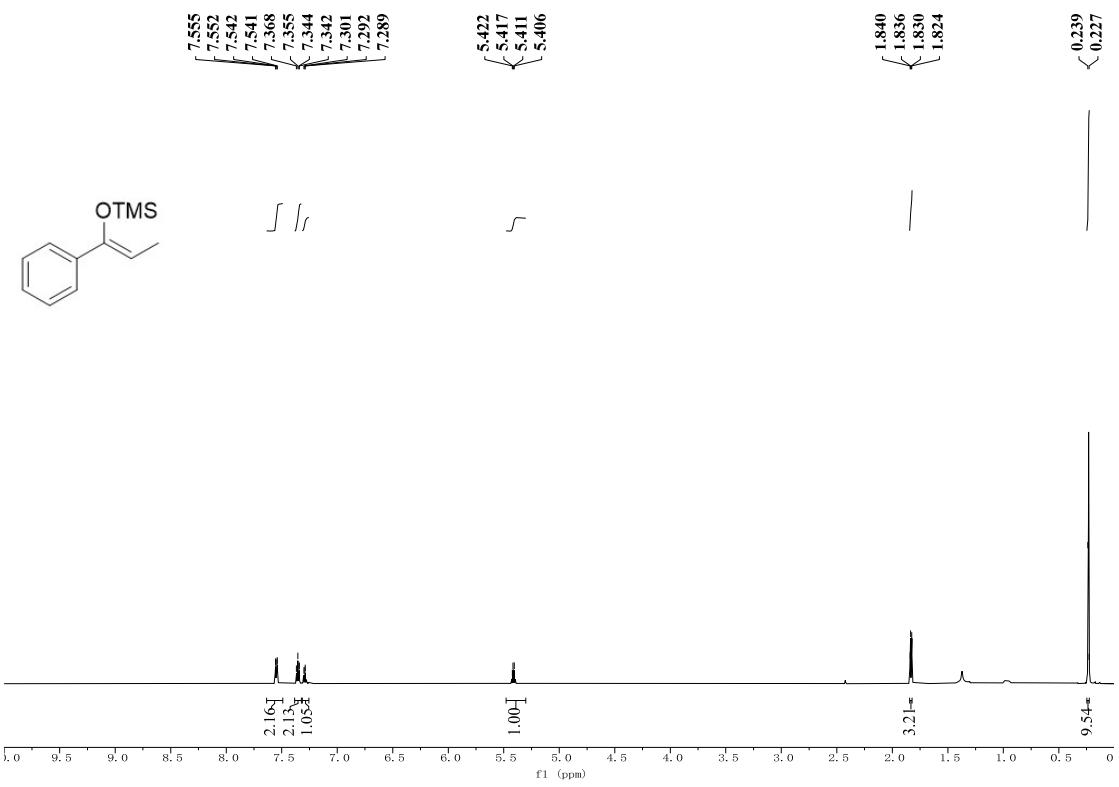

154.562
154.265
148.765
136.348
122.684
118.884
93.310
77.212
77.000
76.792
-0.108
OTMS
N
f1 (ppm)

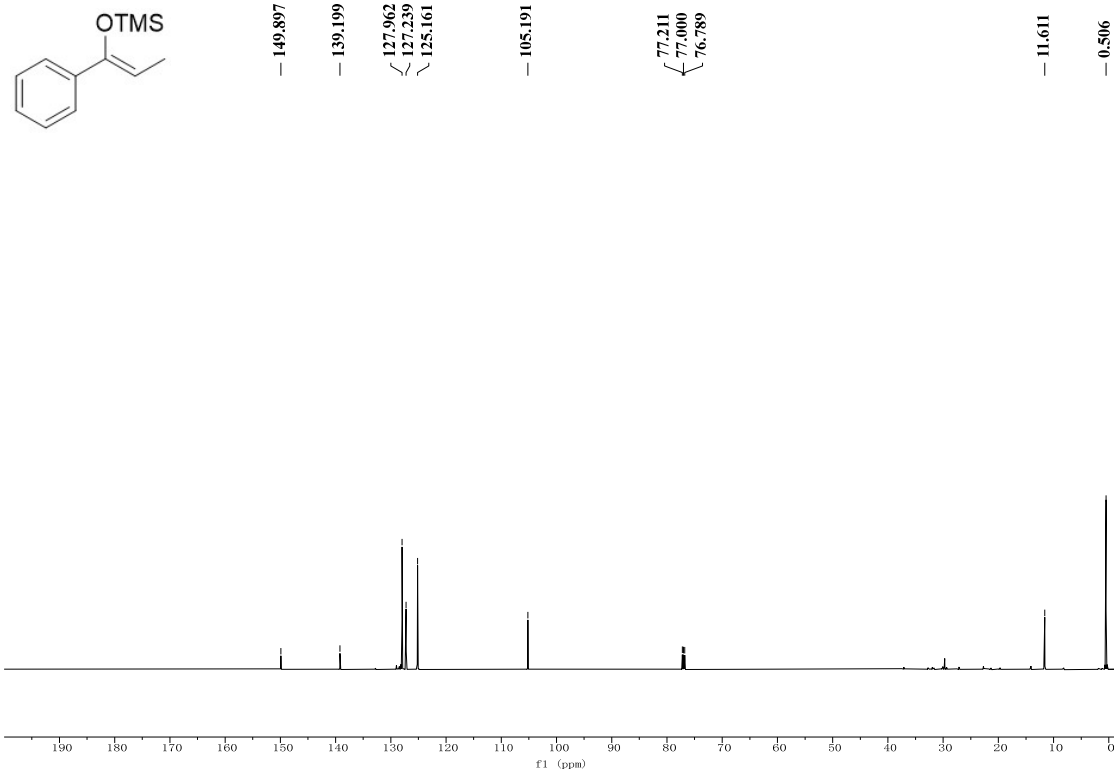

8.492
8.487
8.483
8.476
7.370
7.364
7.359
7.355
7.347
5.029
5.021
5.016
4.513
4.505
4.500
0.234
0.204
0.197
0.159
0.071
0.065
OTMS
N
2.11
1.94
1.06
1.00
9.30
f1 (ppm)

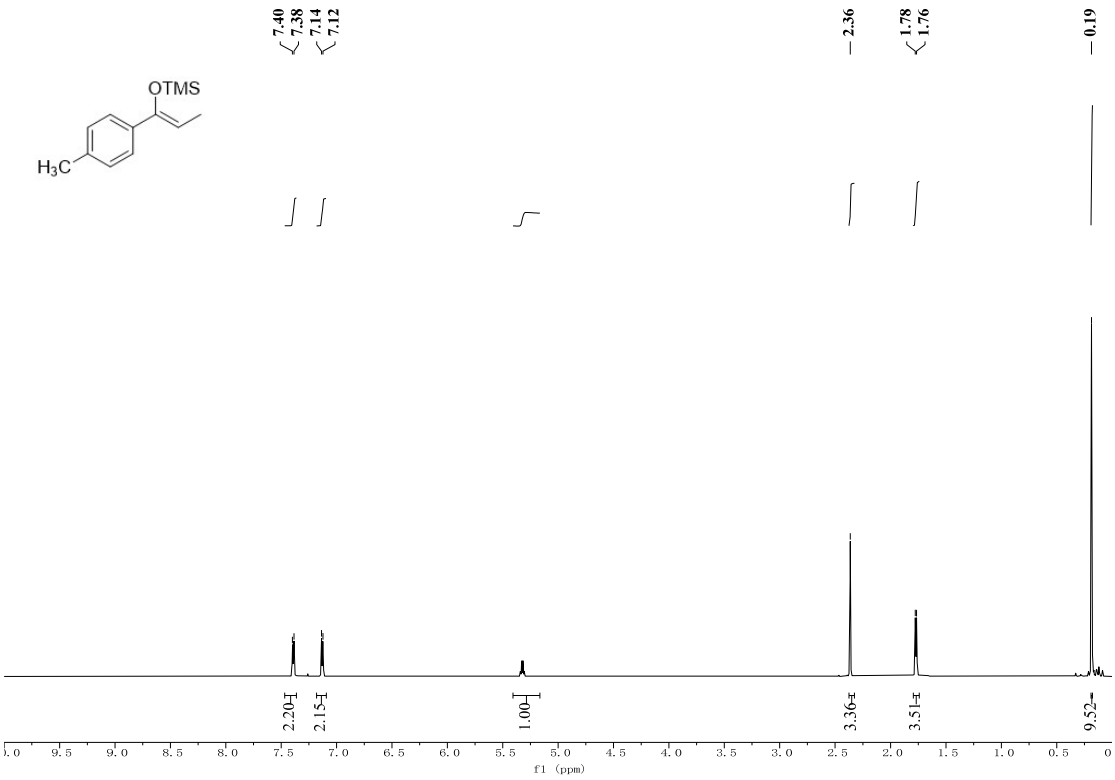

153.129
150.760
149.668
119.191
93.788
77.316
76.998
76.679
-0.549
OTMS
N
f1 (ppm)

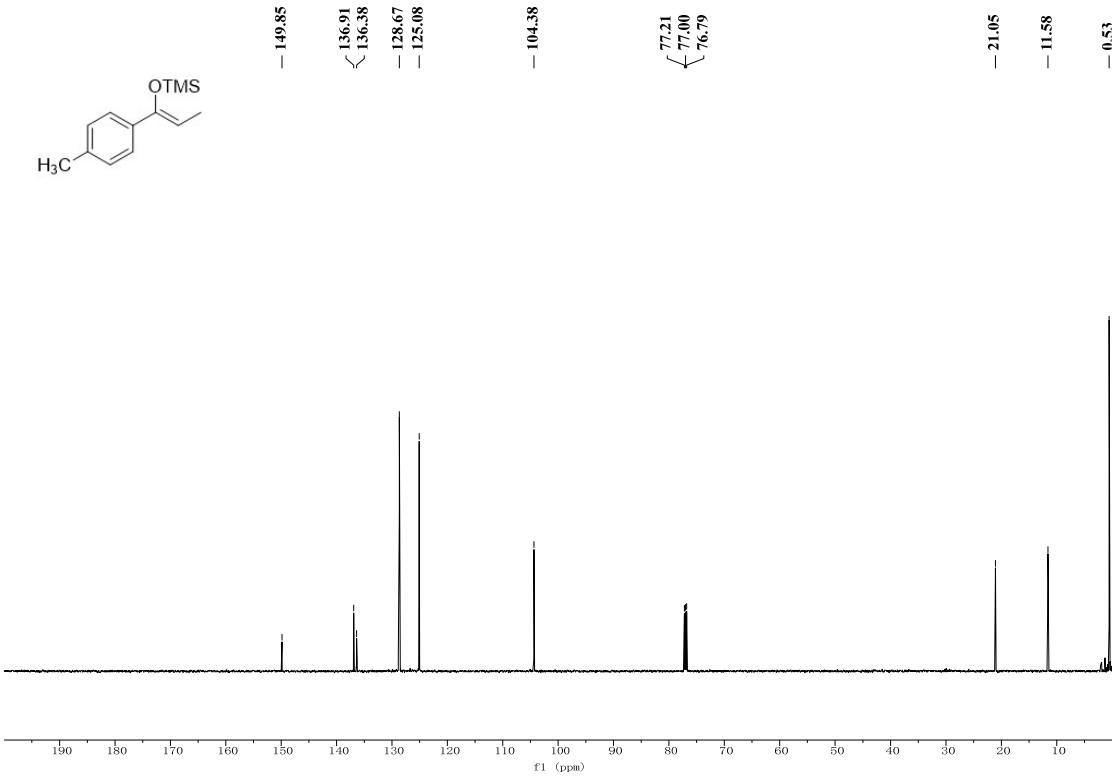

OTMS
N
7.524
7.513
7.511
7.498
7.389
7.376
7.005
6.992
5.671
4.531
2.512
0.266
0.98
0.96
0.94
0.97
1.00
3.09
9.07
f1 (ppm)

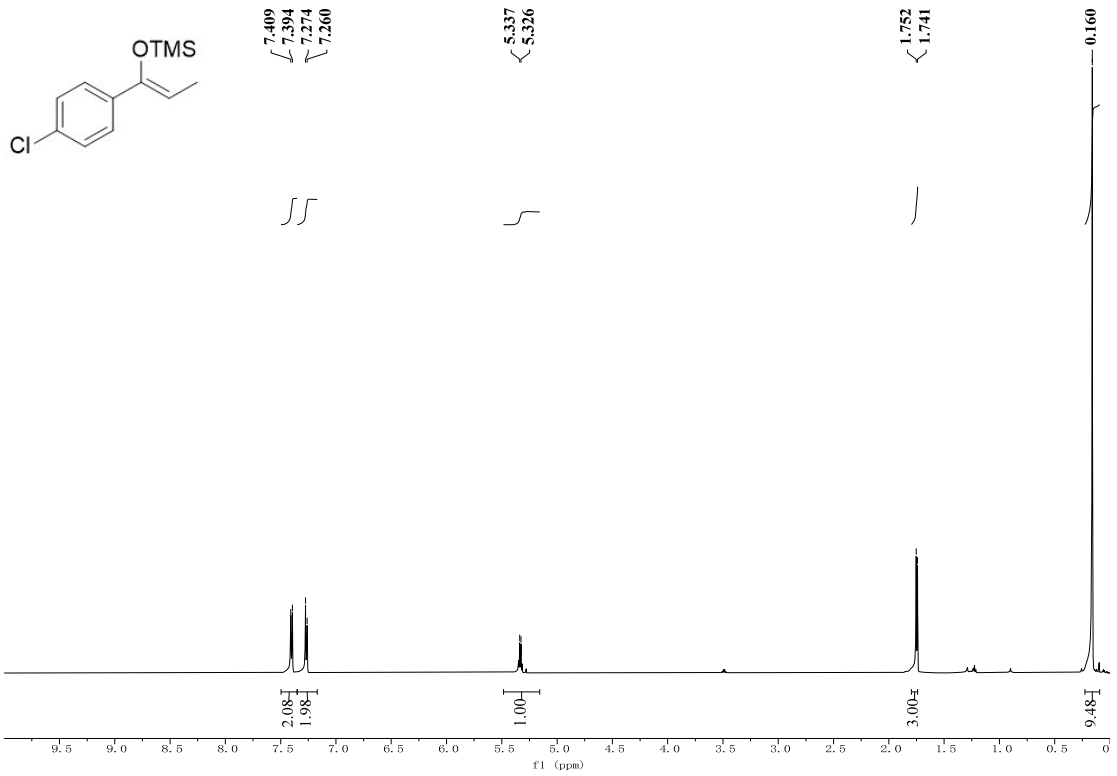

OTMS
N
157.413
154.497
153.884
136.446
122.351
115.873
93.188
77.212
77.000
76.788
24.462
f1 (ppm)

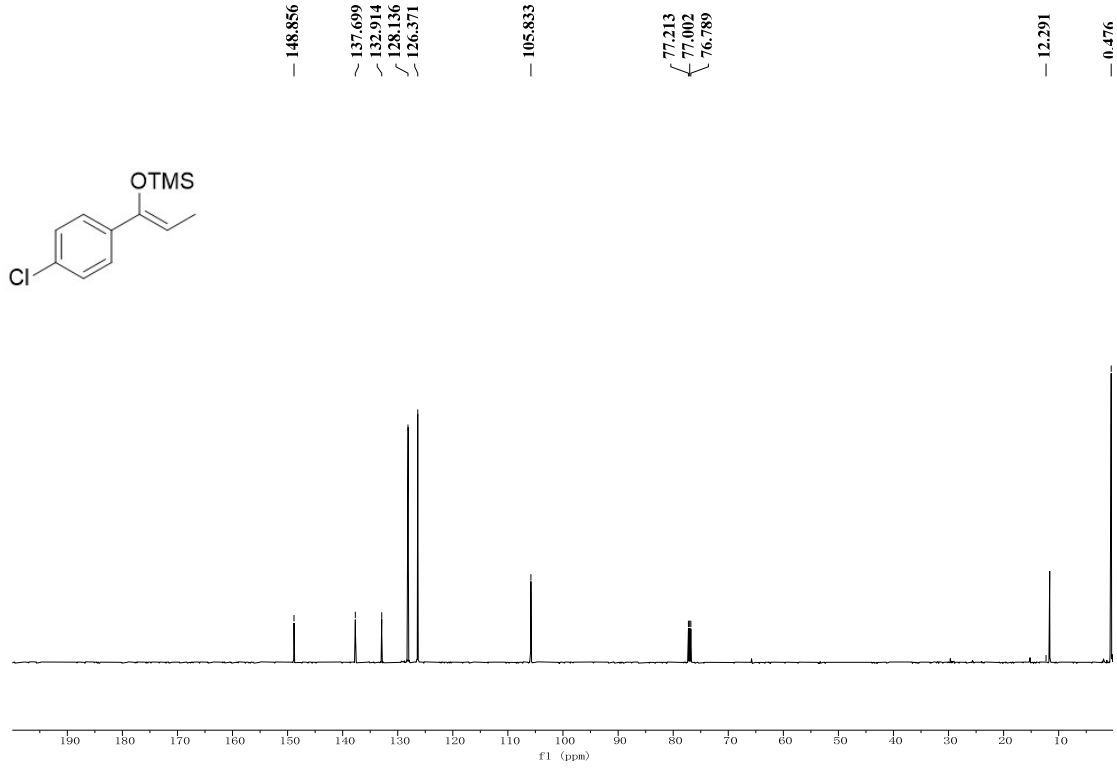

7.555
7.552
7.542
7.541
7.368
7.355
7.344
7.342
7.301
7.292
7.289
5.422
5.417
5.411
5.406
1.840
1.836
1.830
1.824
0.239
0.227
OTMS
2.16
2.13
1.05
1.00
3.21
9.54
f1 (ppm)

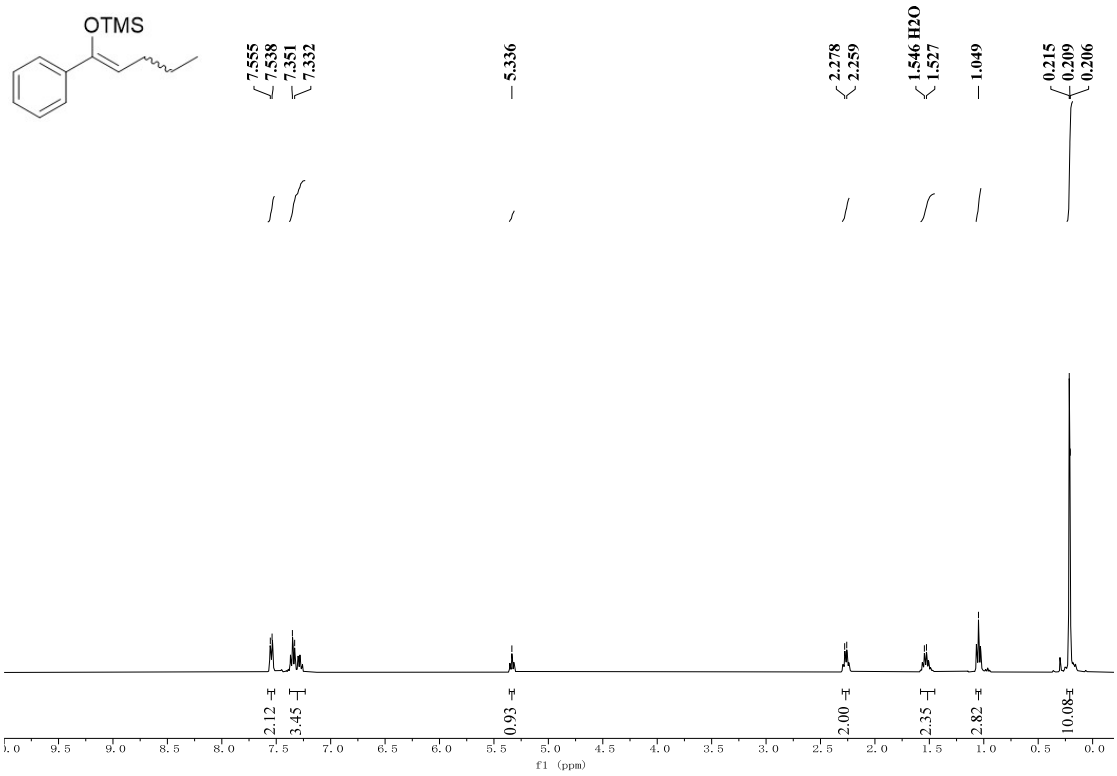

OTMS
149.897
139.199
127.962
127.239
125.161
105.191
77.211
77.000
76.789
11.611
0.506
f1 (ppm)

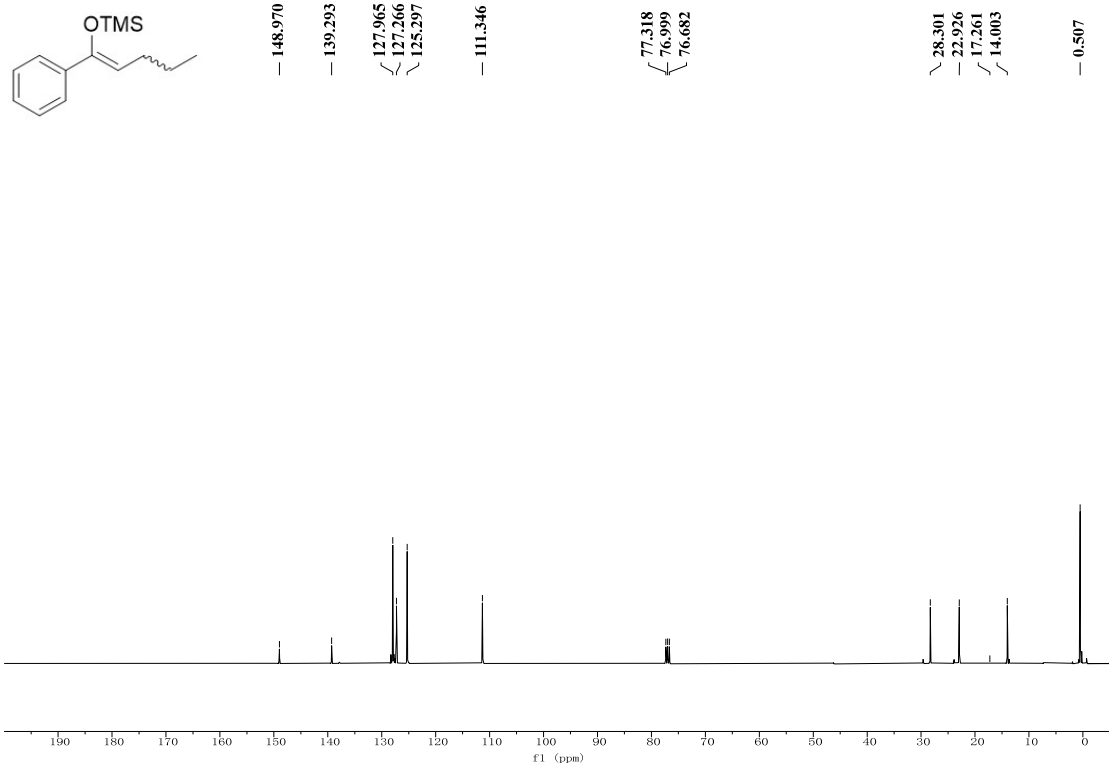

7.40
7.38
7.14
7.12
2.36
1.78
1.76
0.19
OTMS
H3C
2.20
2.15
1.00
3.36
3.51
9.52
f1 (ppm)

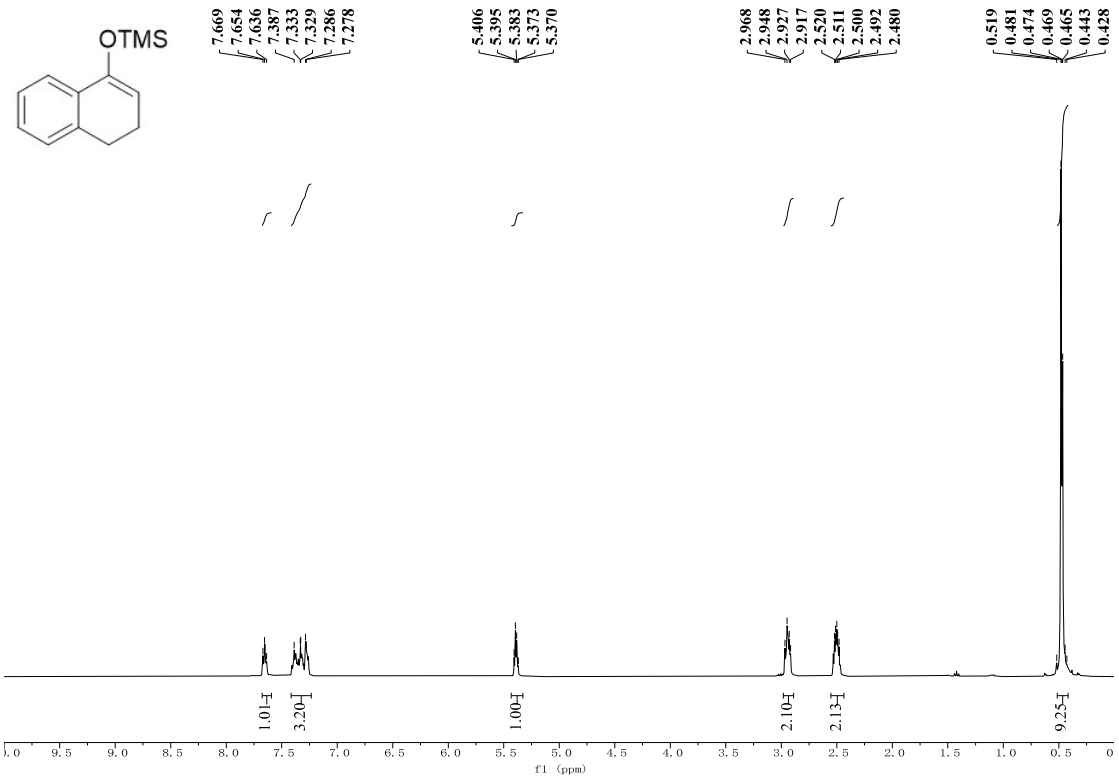

149.85
136.91
136.38
128.67
125.08
104.38
77.21
77.00
76.79
21.05
11.58
0.53
OTMS
H3C
f1 (ppm)

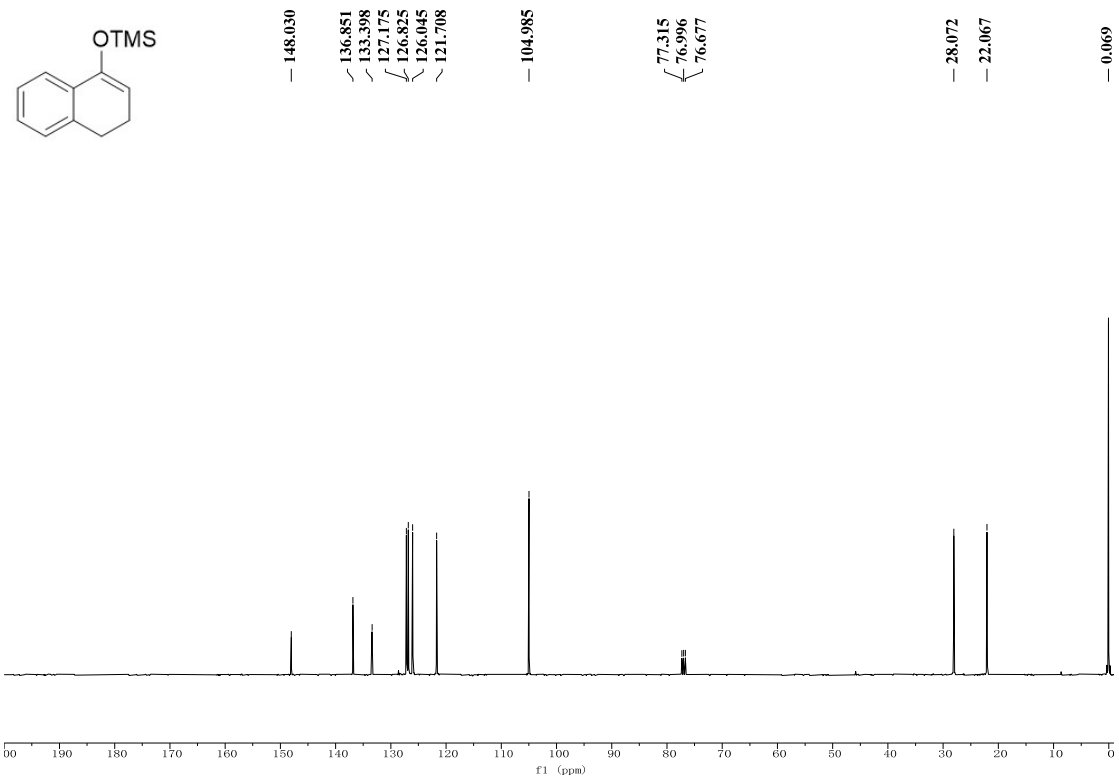

OTMS
Cl
7.409
7.394
7.274
7.260
5.337
5.326
1.752
1.741
0.160
2.08
1.98
1.00
3.00
9.48
f1 (ppm)

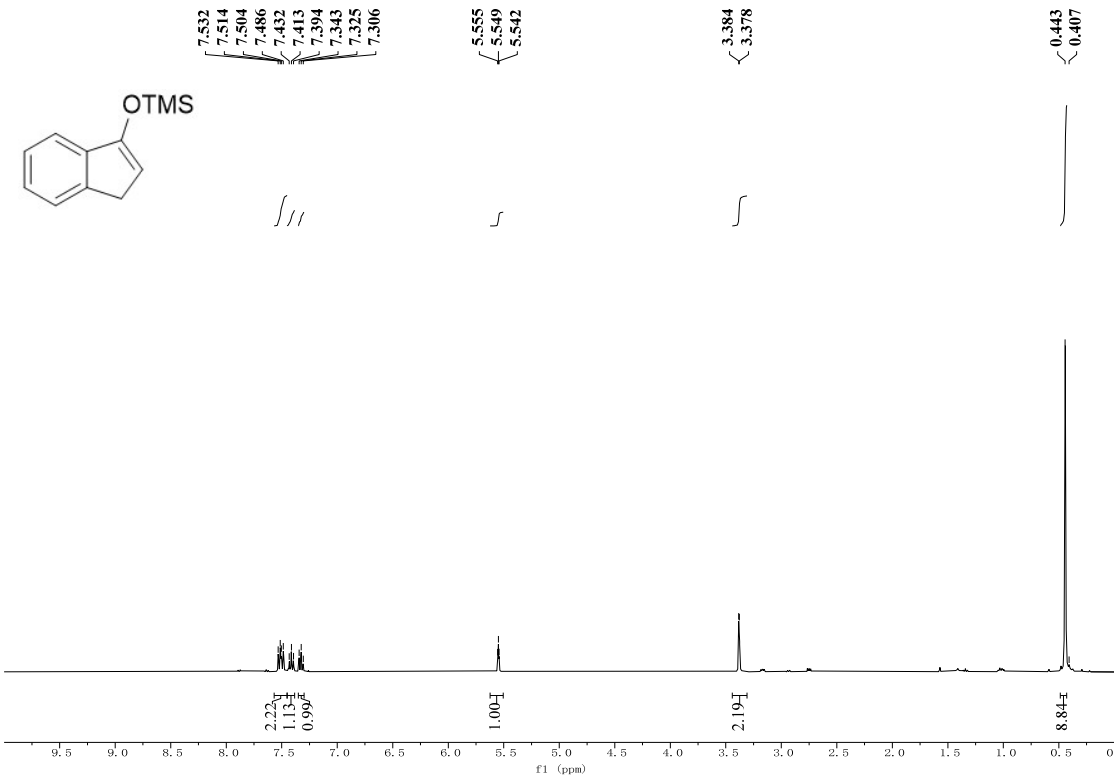

148.856
137.699
132.914
128.136
126.371
105.833
77.213
77.002
76.789
12.291
0.476
OTMS
Cl
f1 (ppm)

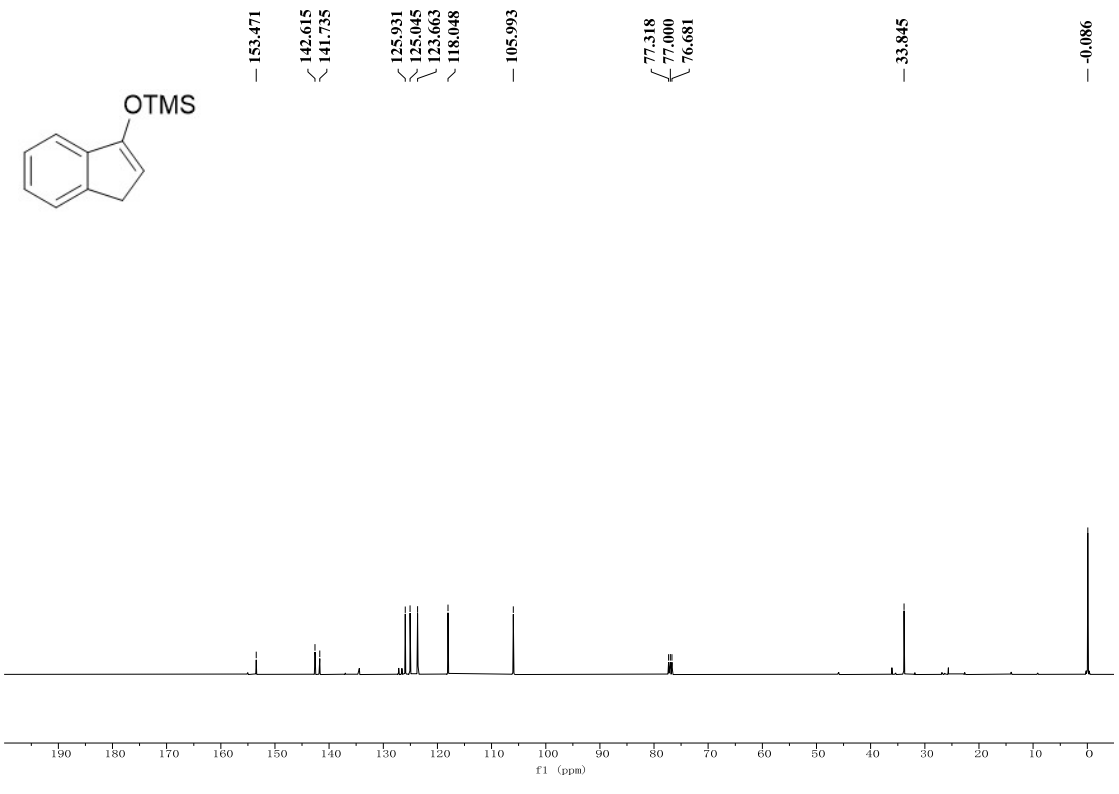

OTMS
7.555
7.538
7.351
7.332
5.336
2.278
2.259
1.546 H2O
1.527
1.049
0.215
0.209
0.206
2.12
3.45
0.93
2.00
2.35
2.82
10.08
f1 (ppm)

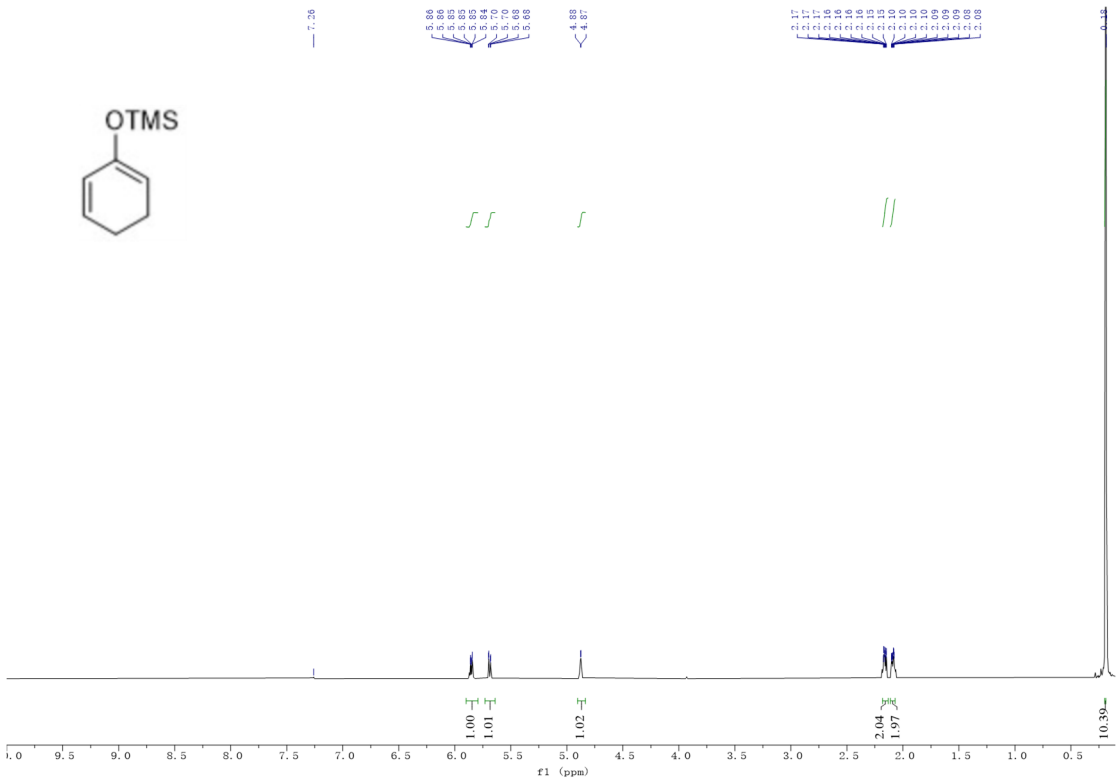

OTMS
148.970
139.293
127.965
127.266
125.297
111.346
77.318
76.999
76.682
28.301
22.926
17.261
14.003
0.507
f1 (ppm)

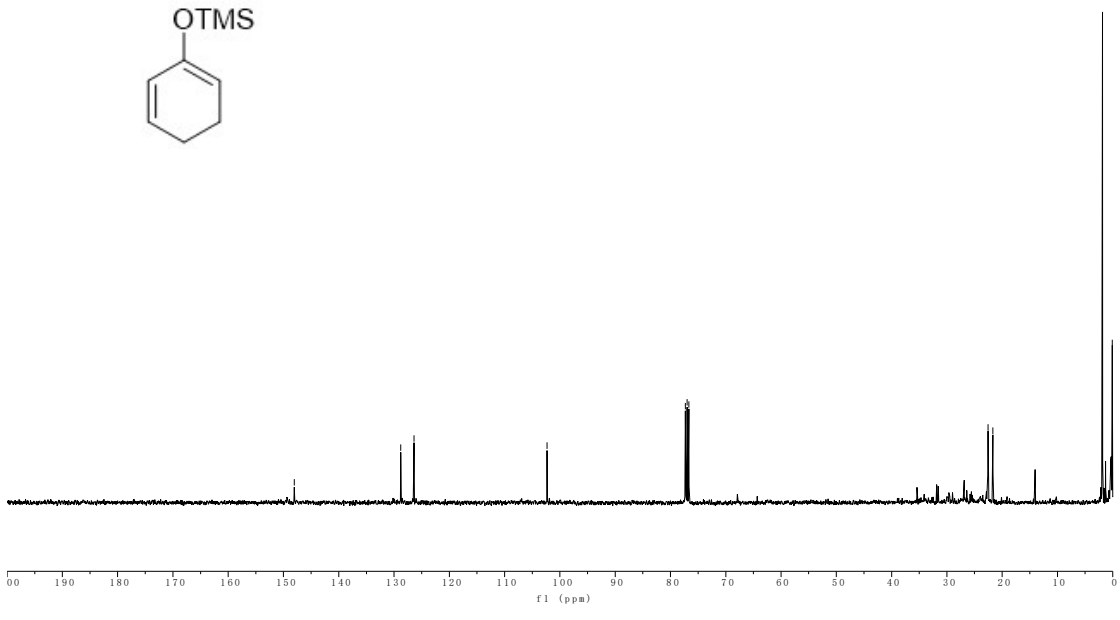

OTMS
7.669
7.654
7.636
7.387
7.333
7.329
7.286
7.278
5.406
5.395
5.383
5.373
5.370
2.968
2.948
2.927
2.917
2.520
2.511
2.500
2.492
2.480
0.519
0.481
0.474
0.469
0.465
0.443
0.428
1.01
3.20
1.00
2.10
2.13
9.25
f1 (ppm)

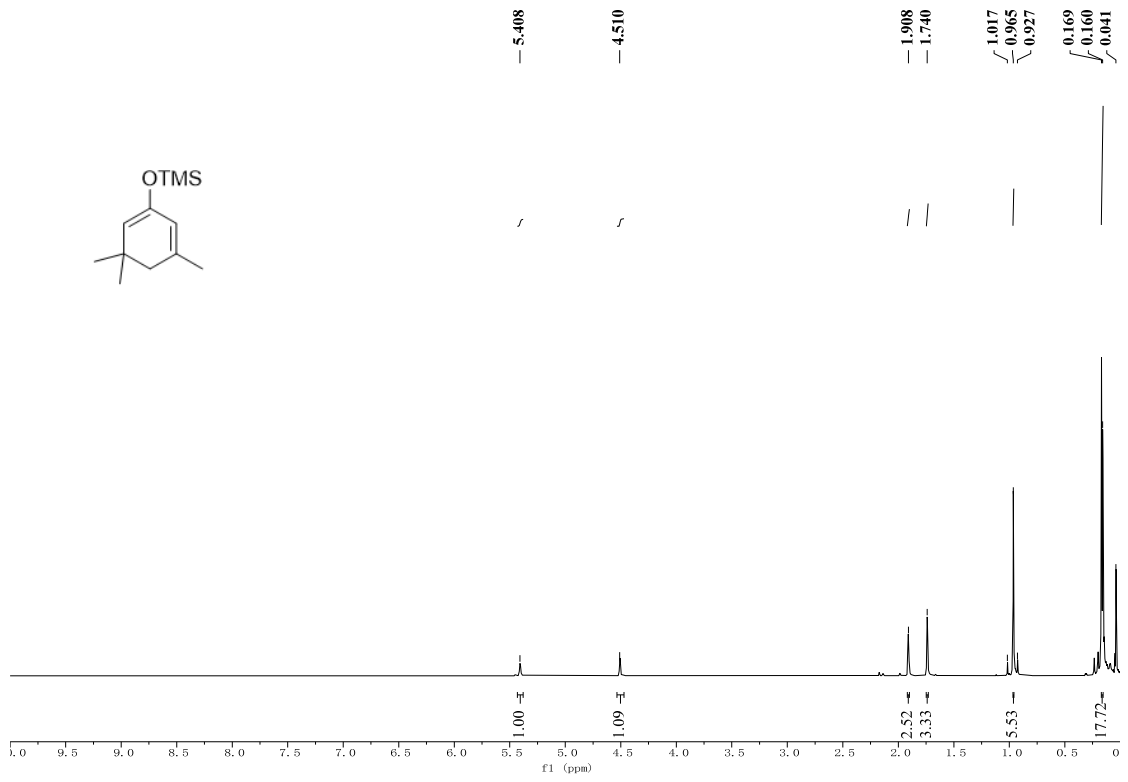

OTMS
148.030
136.851
133.398
127.175
126.825
126.045
121.708
104.985
77.315
76.996
76.677
28.072
22.067
0.069
f1 (ppm)

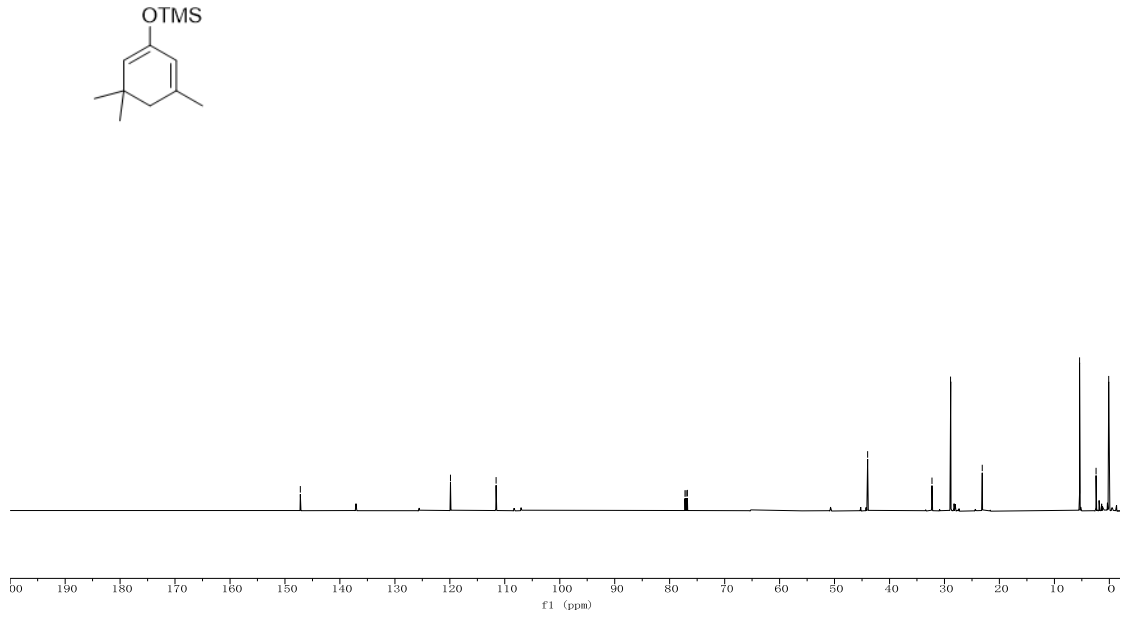

7.532
7.514
7.504
7.486
7.432
7.413
7.394
7.343
7.325
7.306
5.555
5.549
5.542
3.384
3.378
0.443
0.407
OTMS
2.22
1.13
0.99
1.00
2.19
8.84
f1 (ppm)

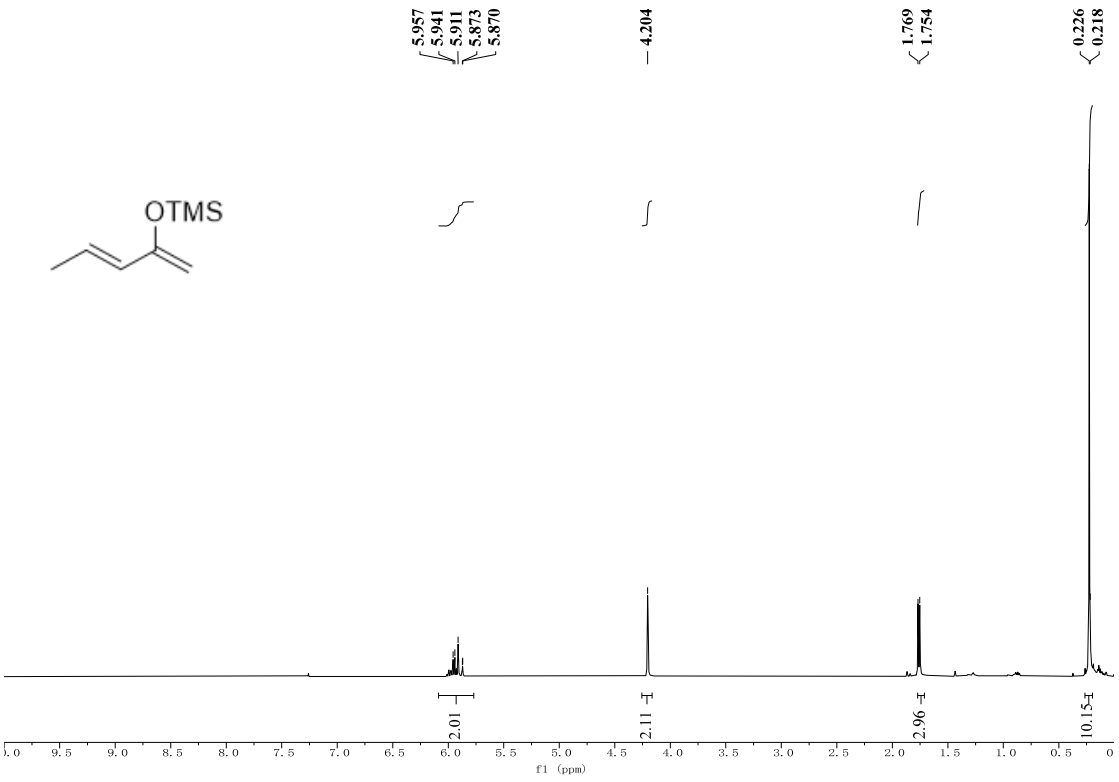

153.471
142.615
141.735
125.931
125.045
123.663
118.048
105.993
77.318
77.000
76.681
33.845
-0.086
OTMS
f1 (ppm)

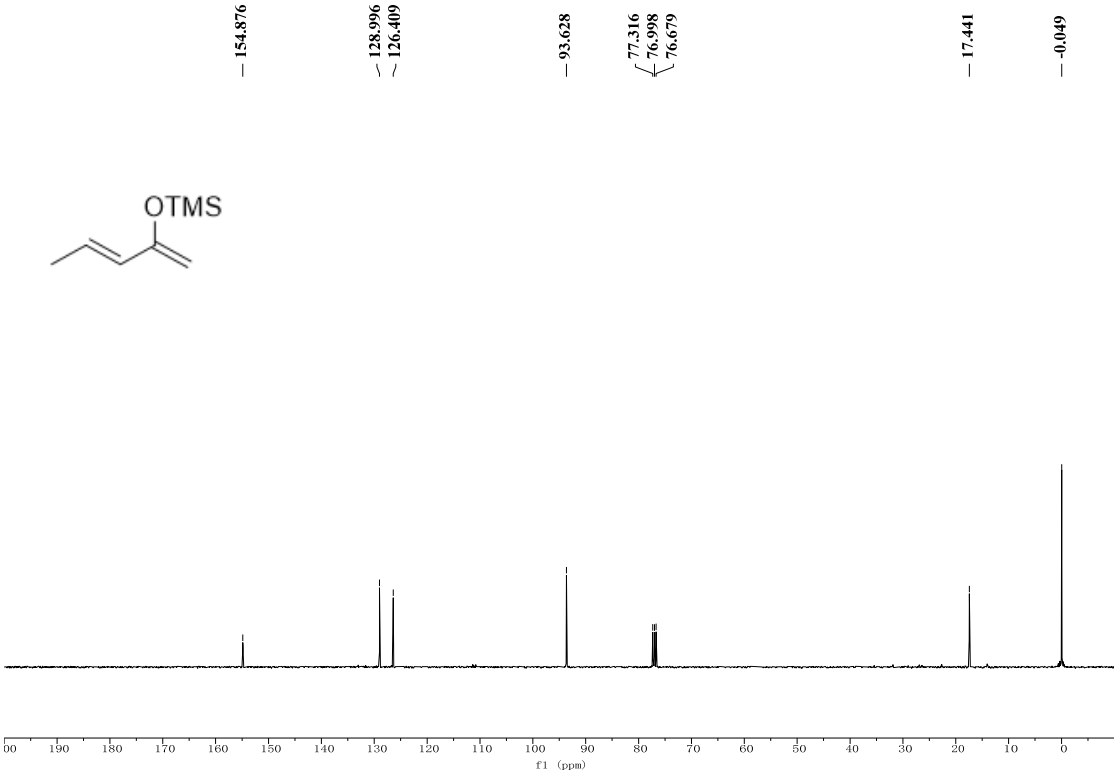

OTMS
7.26
5.86
5.85
5.85
5.85
5.84
5.85
5.70
5.70
5.68
5.68
4.88
4.87
2.17
2.17
2.17
2.16
2.16
2.16
2.15
2.15
2.15
2.10
2.10
2.10
2.09
2.09
2.09
2.08
2.08
0.10
1.00
1.01
1.02
2.04
1.97
10.39
f1 (ppm)

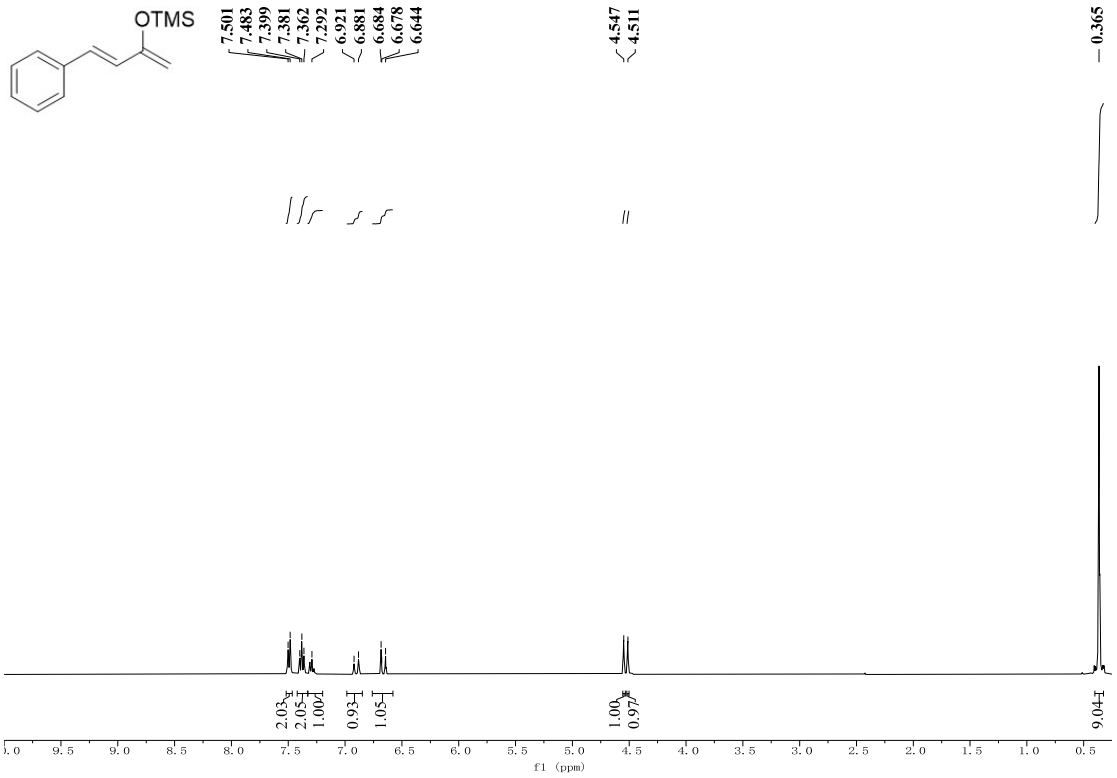

OTMS
148.044
128.789
126.389
102.315
77.319
77.000
76.682
22.554
21.692
1.866
0.087
f1 (ppm)

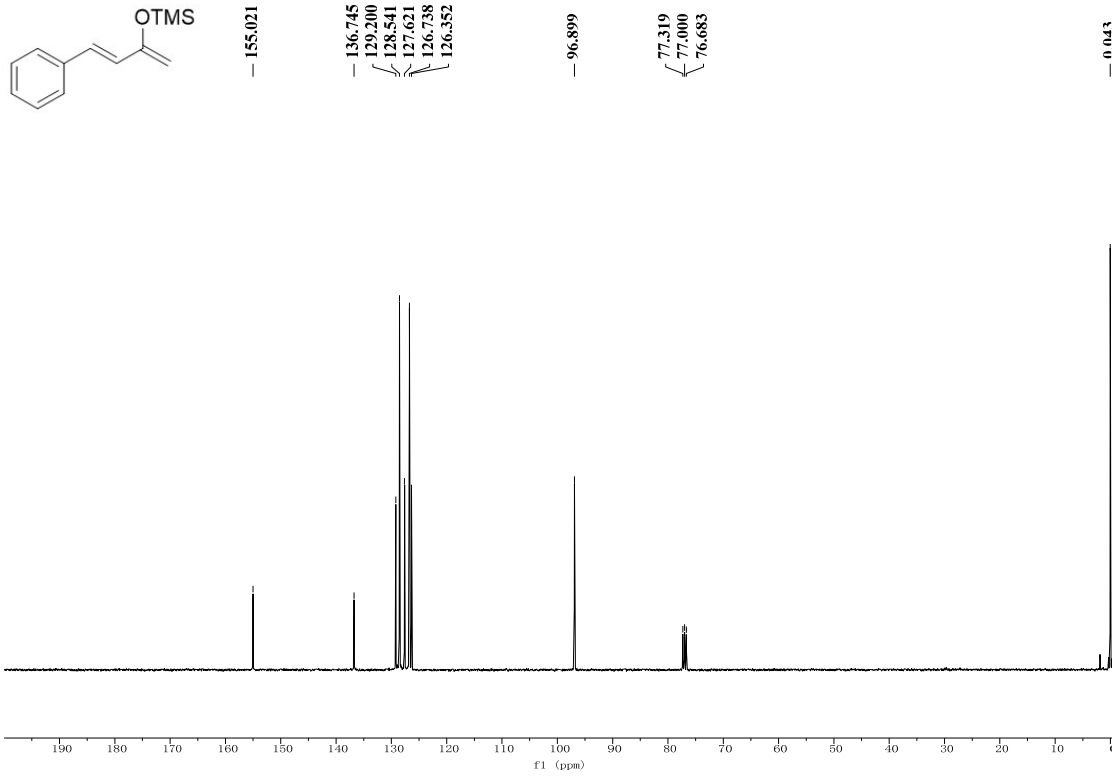

OTMS
5.408
4.510
1.908
1.740
1.017
0.965
0.927
0.169
0.160
0.041
1.00
1.09
2.52
3.33
5.53
17.72
f1 (ppm)

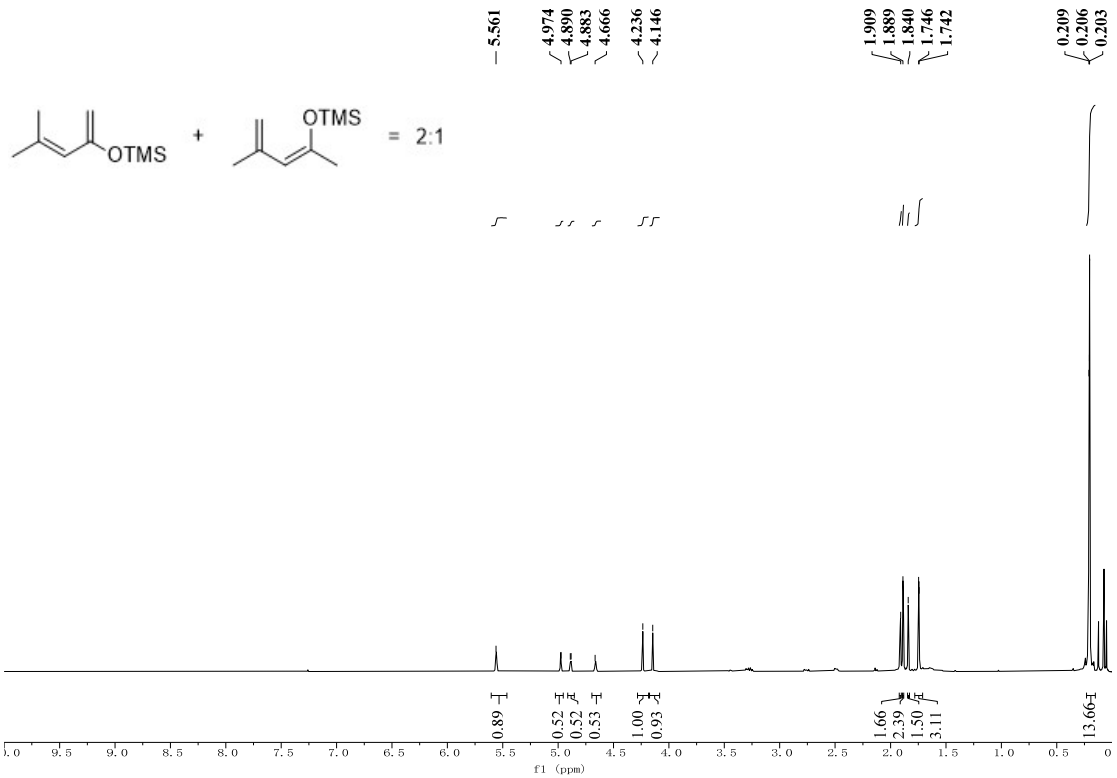

OTMS
147.209
119.877
111.596
77.212
77.001
76.789
43.988
32.270
28.883
23.137
5.411
2.431
0.122
f1 (ppm)

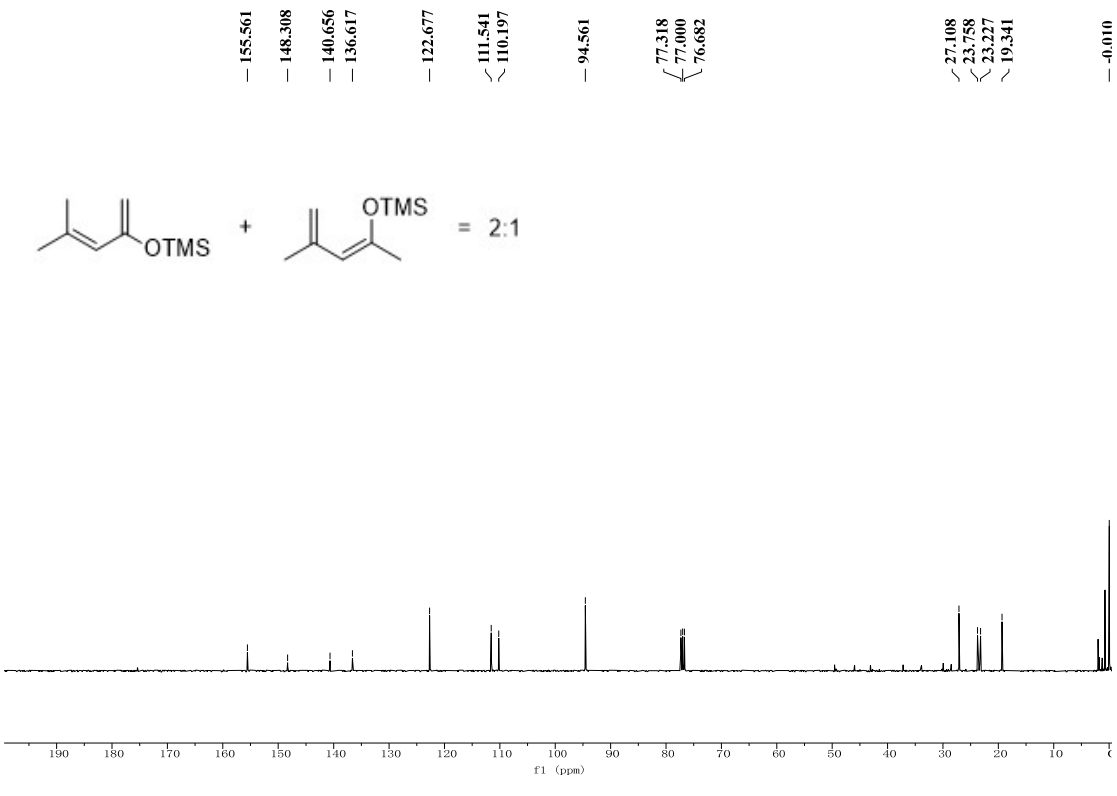

5.957
5.941
5.911
5.873
5.870
4.204
1.769
1.754
0.226
0.218
OTMS
2.01
2.11
2.96
10.15
f1 (ppm)

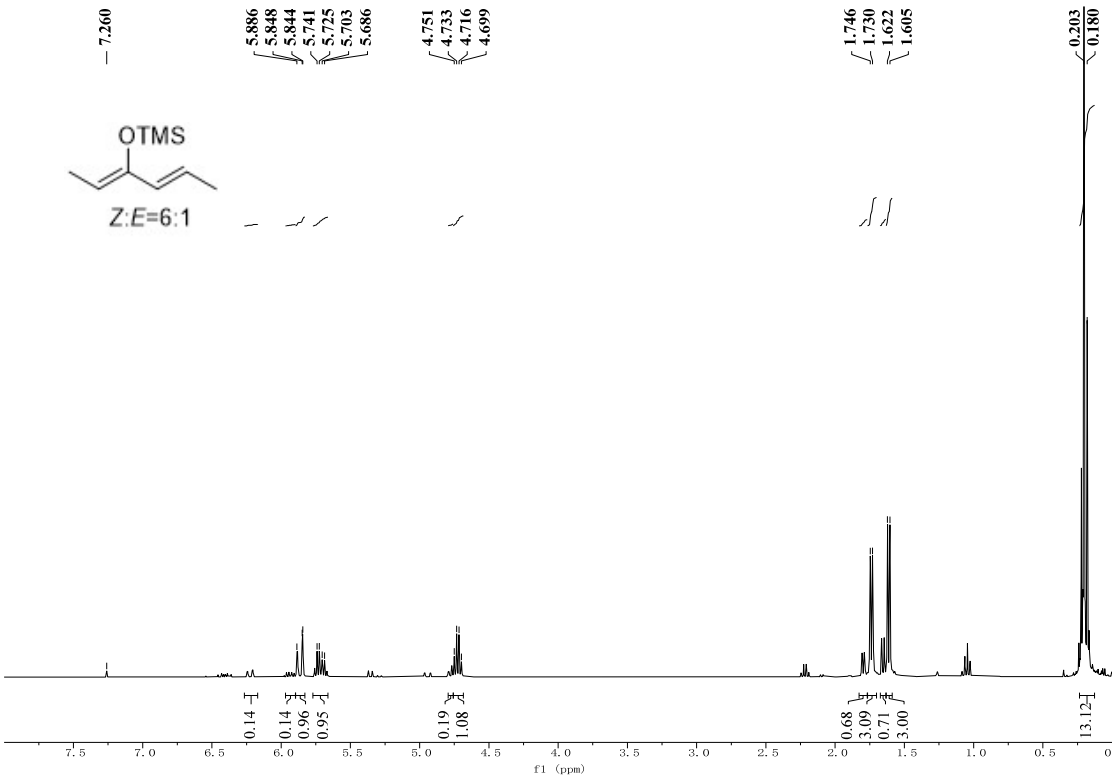

154.876
128.996
126.409
93.628
77.316
76.998
76.679
17.441
-0.049
OTMS
f1 (ppm)

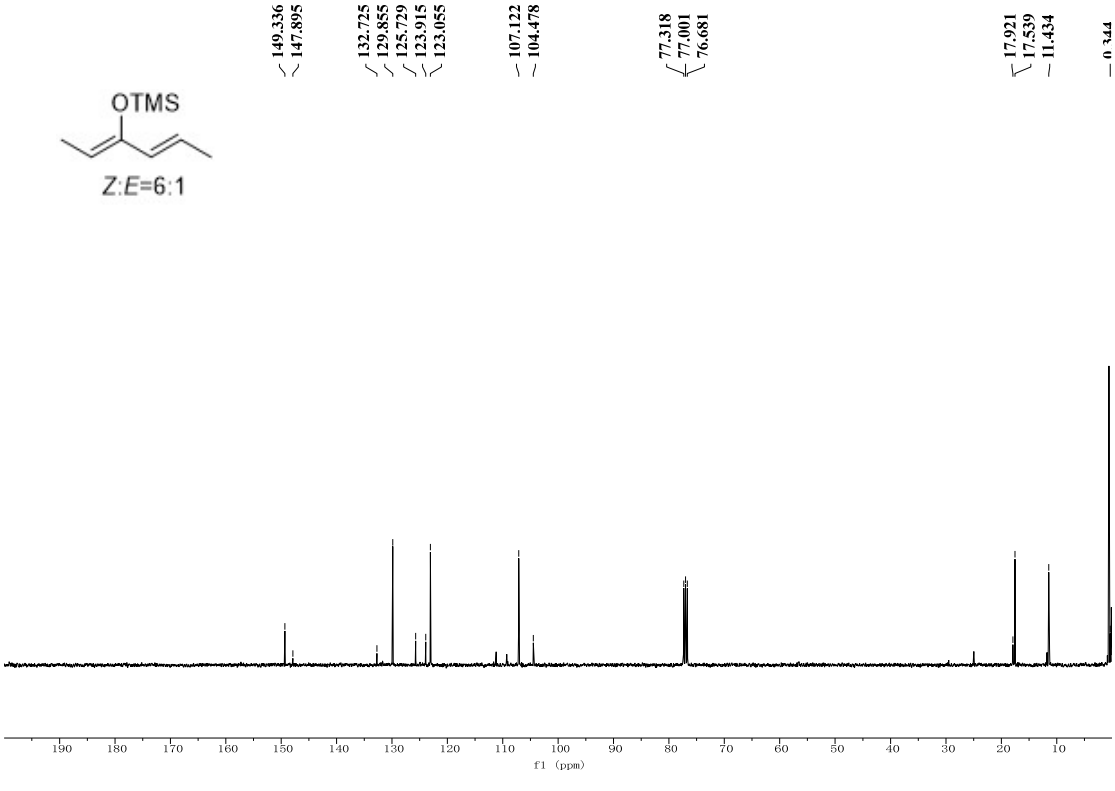

OTMS
7.501
7.483
7.399
7.381
7.362
7.292
6.921
6.881
6.684
6.678
6.644
4.547
4.511
0.365
2.03
2.05
1.00
0.93
1.05
1.00
0.97
9.04
f1 (ppm)

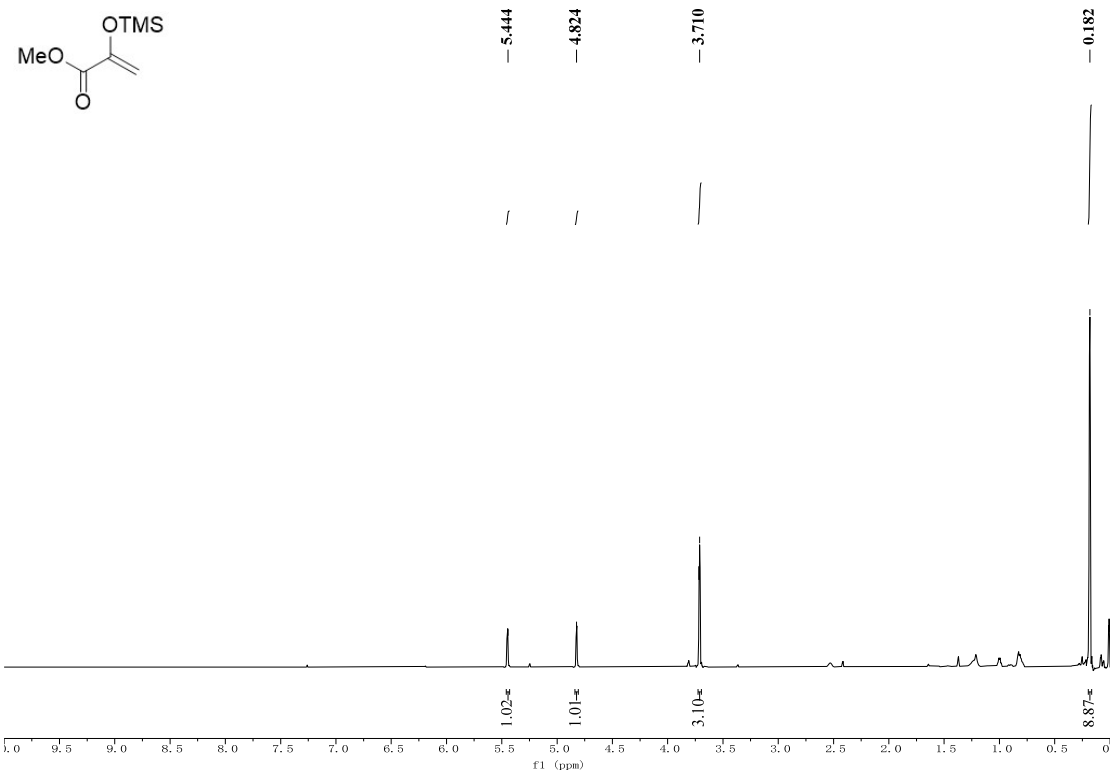

OTMS
155.021
136.745
129.200
128.541
127.621
126.738
126.352
96.899
77.319
77.000
76.683
0.043
f1 (ppm)

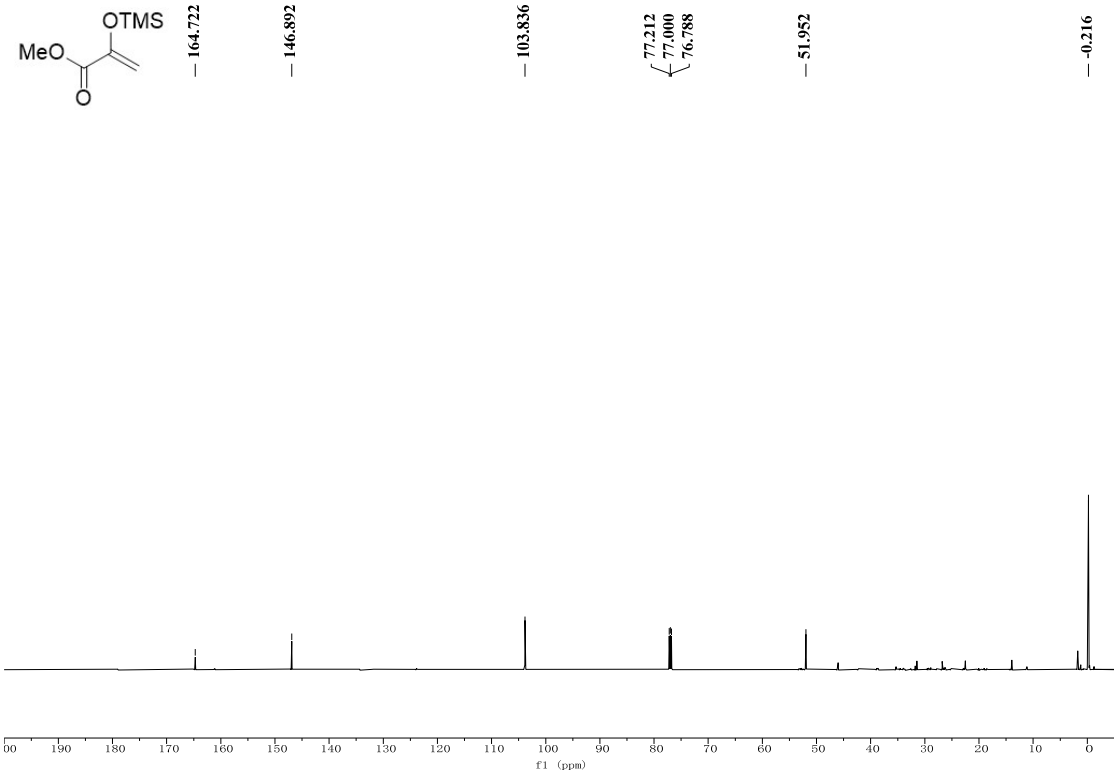

5.561
4.974
4.890
4.883
4.666
4.236
4.146
1.909
1.889
1.840
1.746
1.742
0.209
0.206
0.203
OTMS
+
OTMS
= 2:1
0.89
0.52
0.52
0.53
1.00
0.93
1.66
2.39
1.50
3.11
13.66
f1 (ppm)

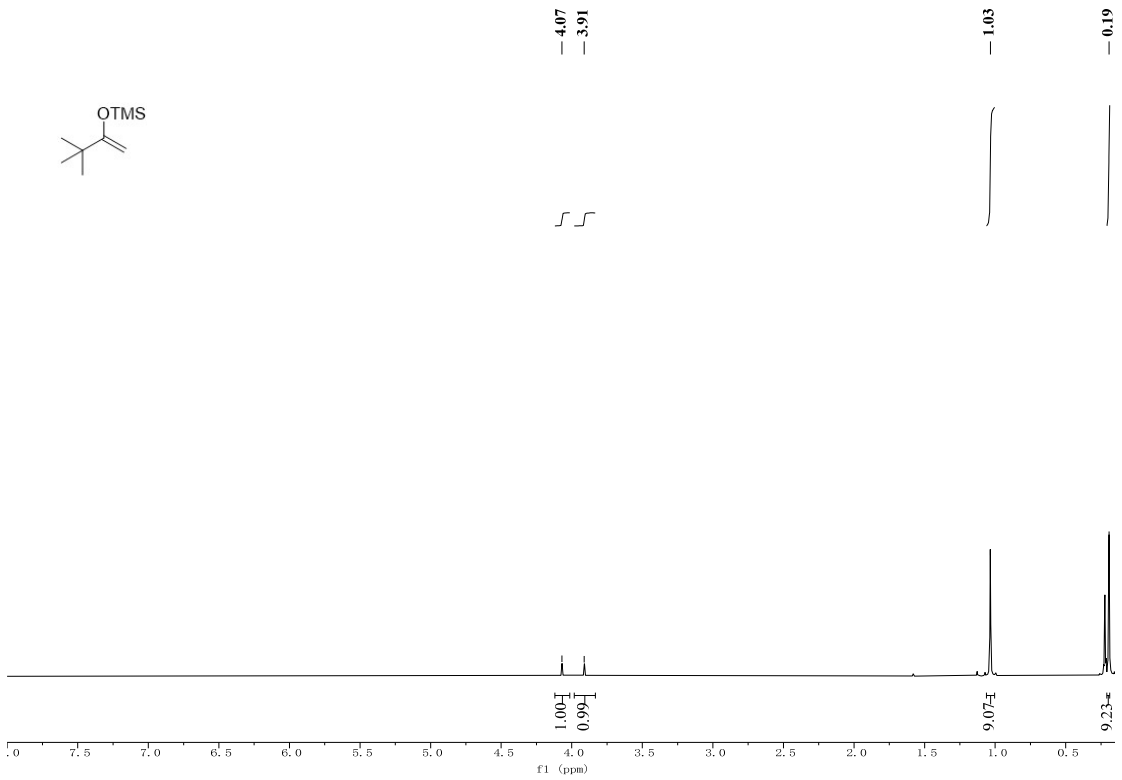

155.561
148.308
140.656
136.617
122.677
111.541
110.197
94.561
77.318
77.000
76.682
27.108
23.758
23.227
19.341
-0.010
OTMS
+
OTMS
= 2:1
f1 (ppm)

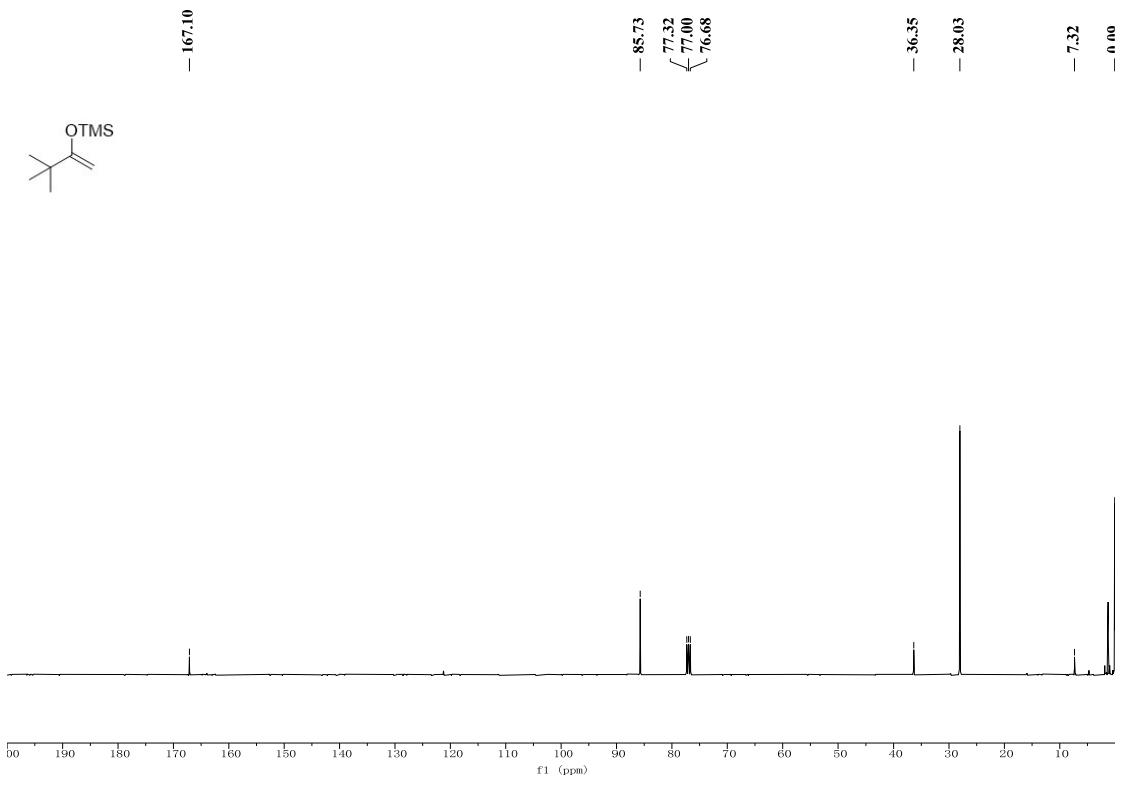

7.260
5.886
5.848
5.844
5.741
5.725
5.703
5.686
4.751
4.733
4.716
4.699
1.746
1.730
1.622
1.605
0.203
0.180
OTMS
Z:E=6:1
0.14
0.14
0.96
0.95
0.19
1.08
0.68
3.09
0.71
3.00
13.12
f1 (ppm)

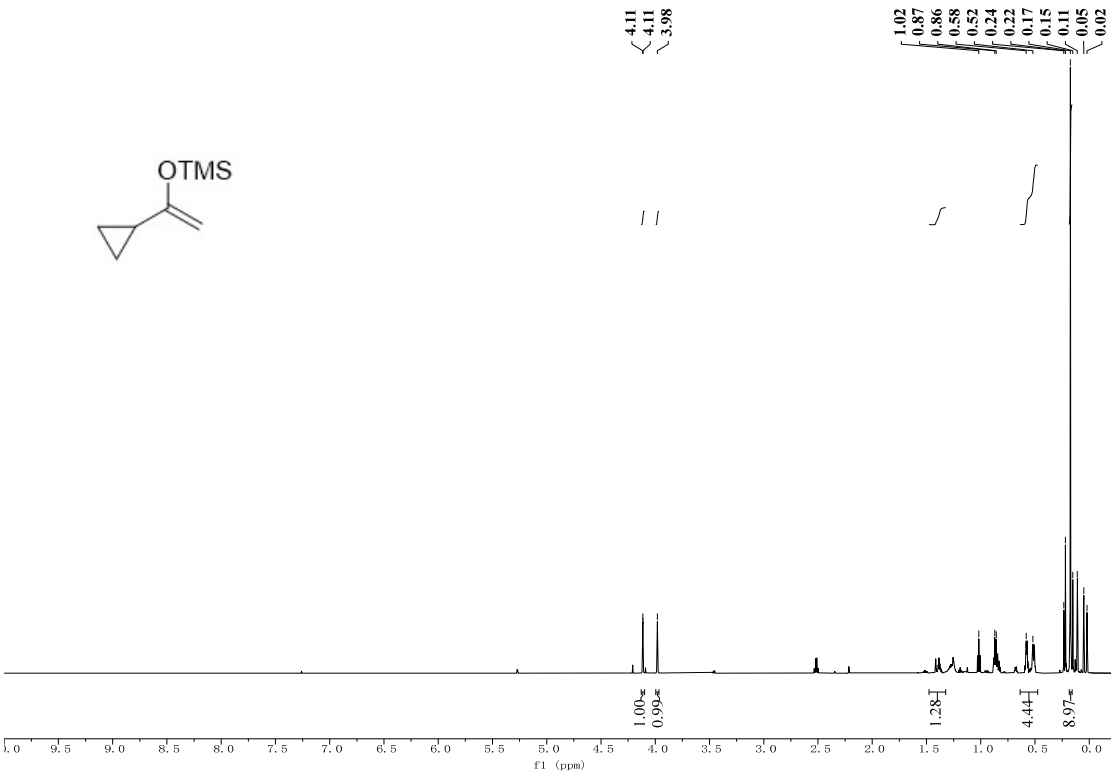

149.336
147.895
132.725
129.855
125.729
123.915
123.055
107.122
104.478
77.318
77.001
76.681
17.921
17.539
11.434
0.344
OTMS
Z:E=6:1
f1 (ppm)

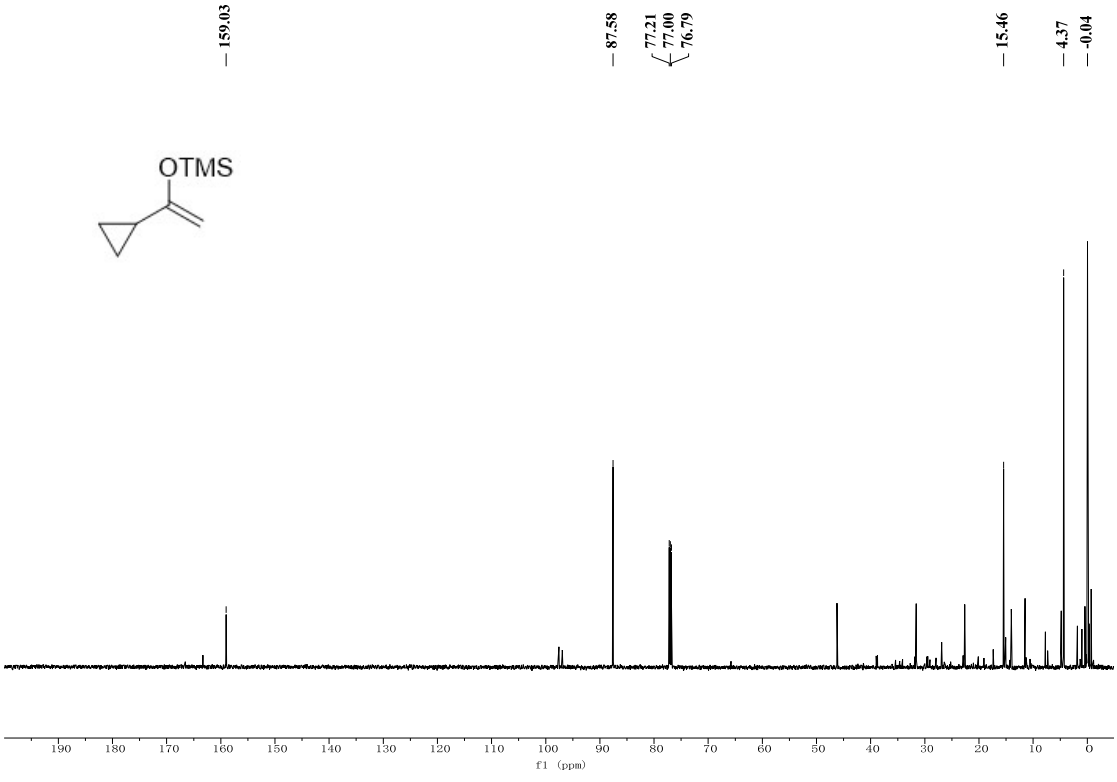

OTMS
MeO
O
5.444
4.824
3.710
0.182
1.02
1.01
3.10
8.87
f1 (ppm)

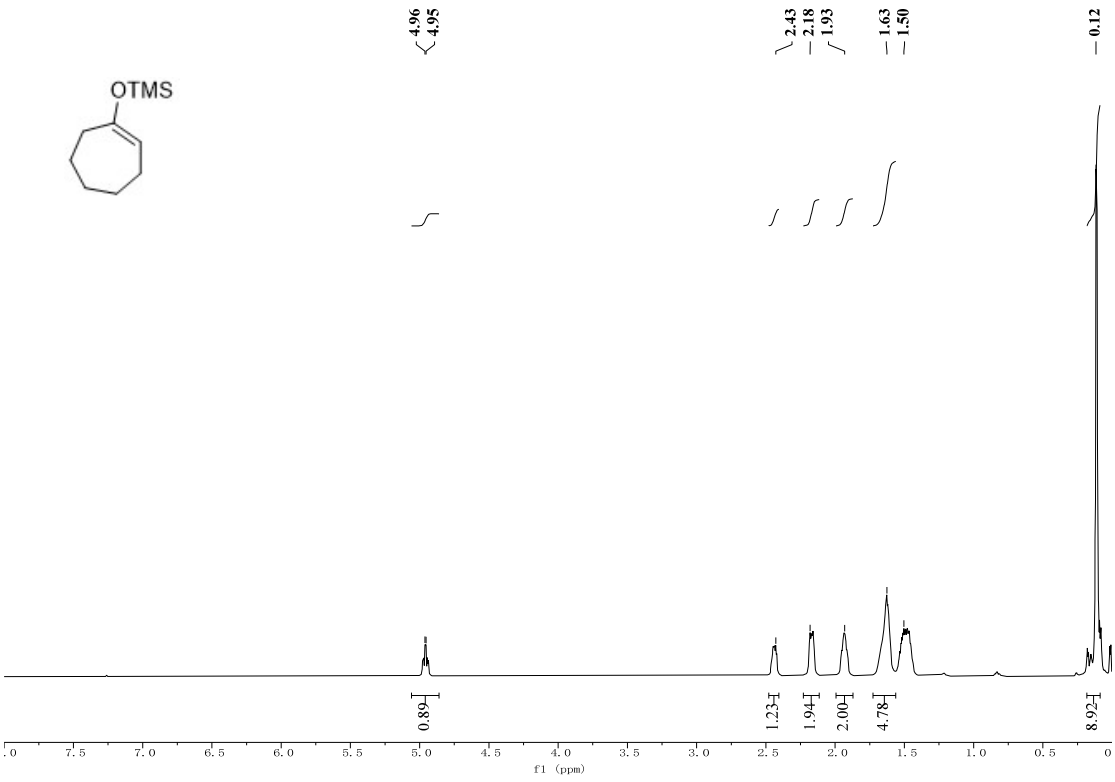

OTMS
MeO
O
164.722
146.892
103.836
77.212
77.000
76.788
51.952
-0.216
f1 (ppm)

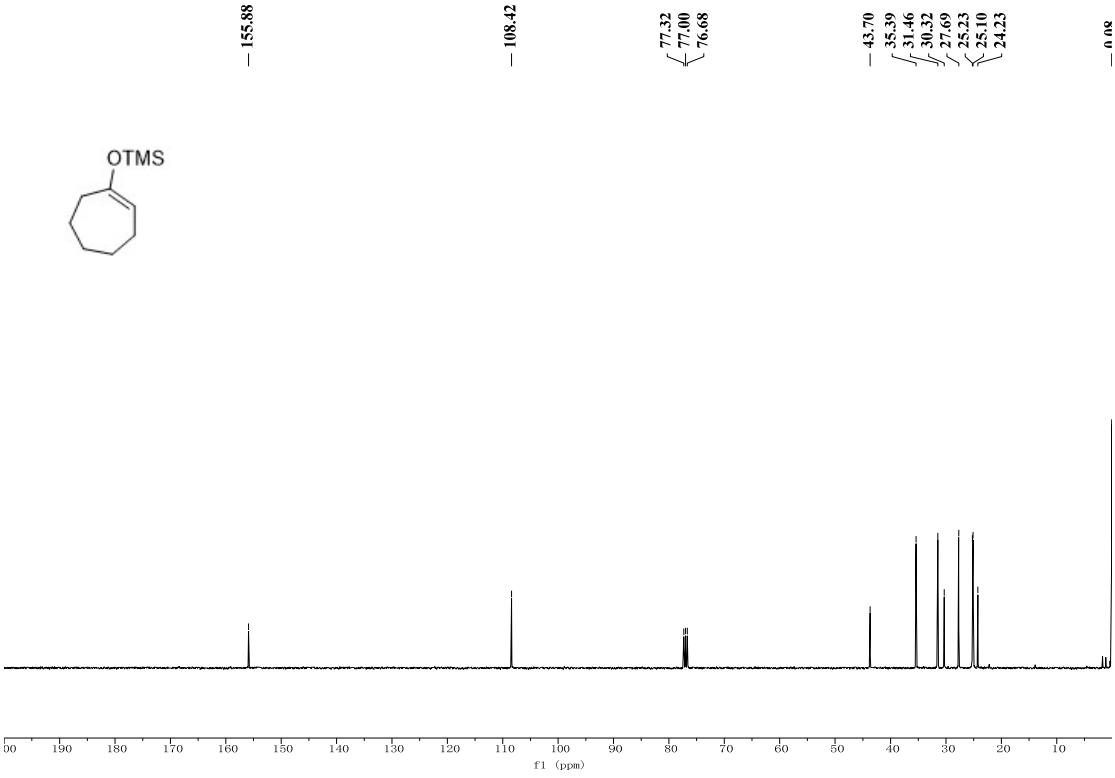

OTMS
4.07
3.91
1.03
0.19
1.00
0.99
9.07
9.23
f1 (ppm)

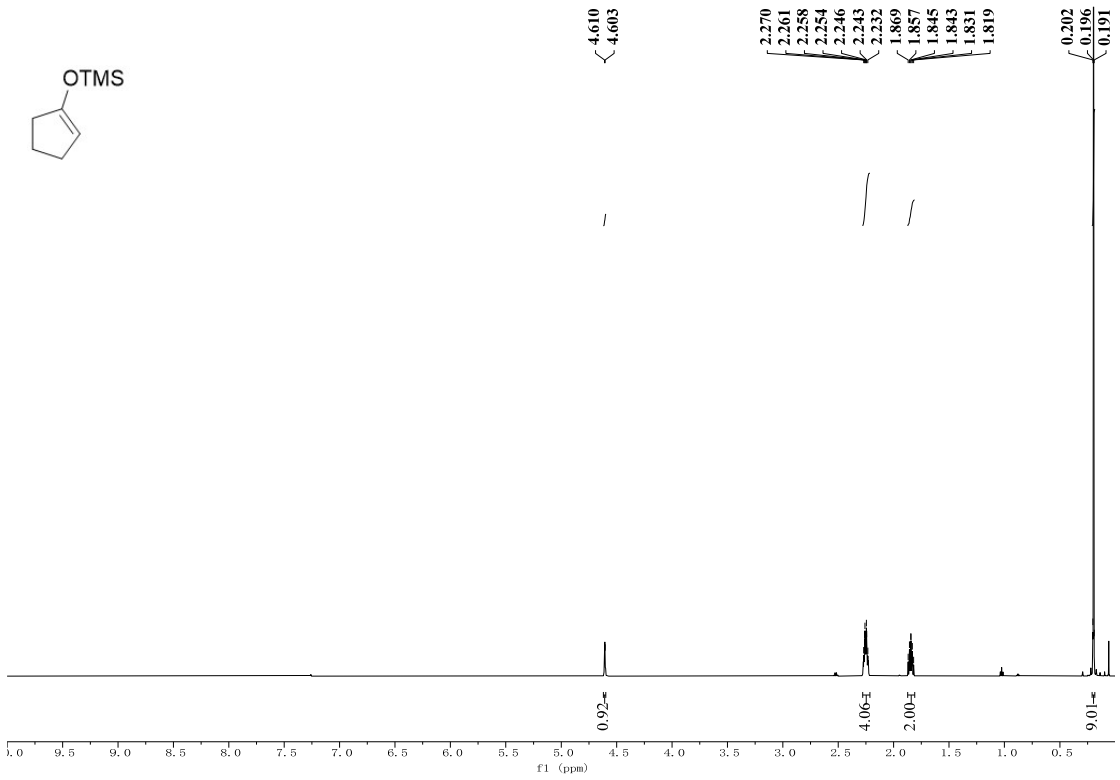

OTMS
167.10
85.73
77.32
77.00
76.68
36.35
28.03
7.32
0.00
f1 (ppm)

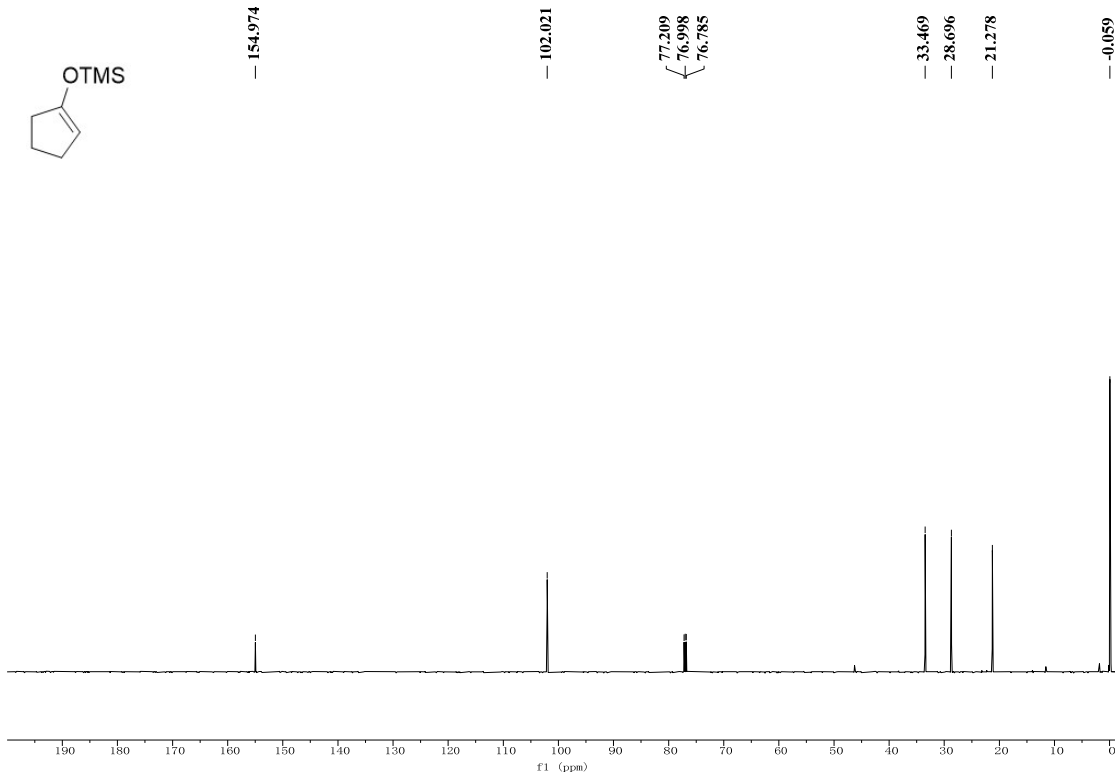

OTMS
4.11
4.11
3.98
1.02
0.87
0.86
0.58
0.52
0.24
0.22
0.17
0.15
0.11
0.05
0.02
1.00
0.99
1.28
4.44
8.97
f1 (ppm)

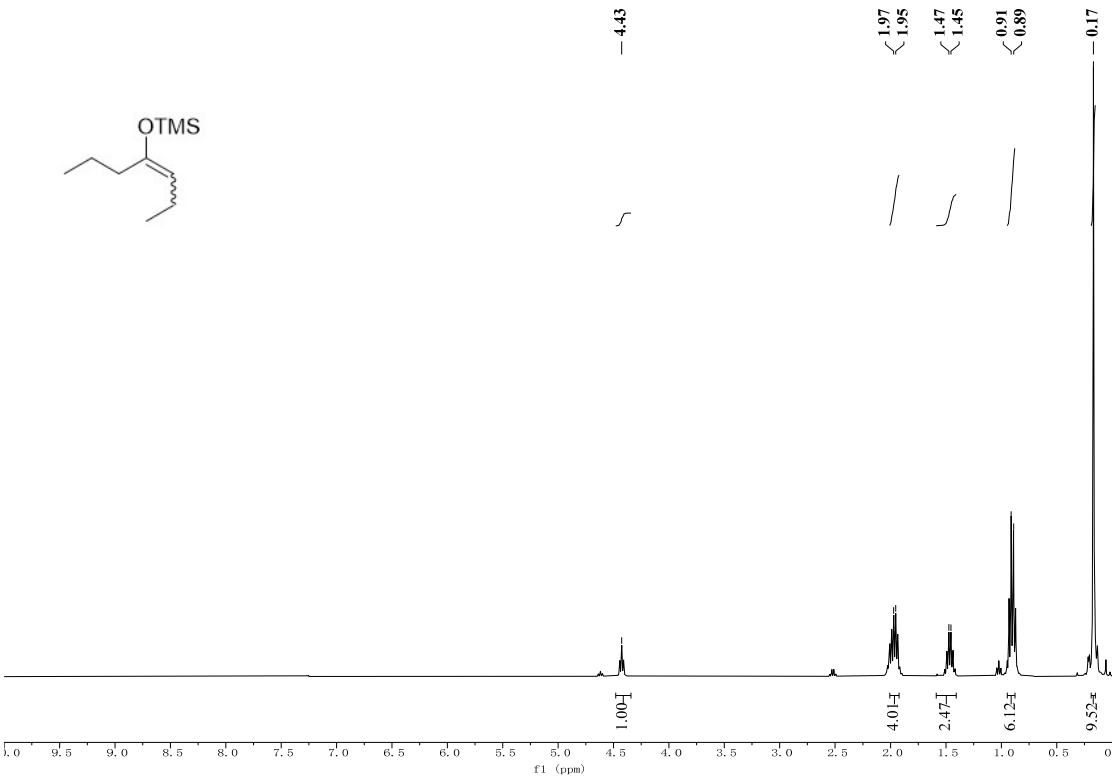

OTMS
159.03
87.58
77.21
77.00
76.79
15.46
4.37
-0.04
f1 (ppm)

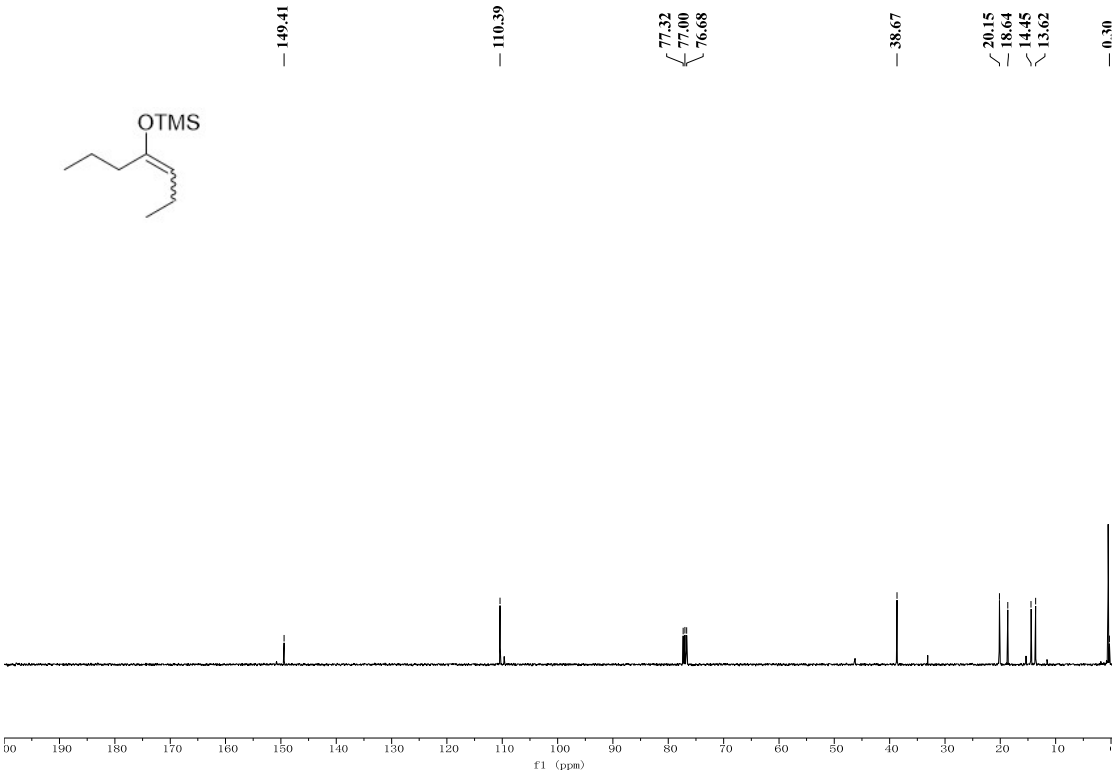

OTMS
4.96
4.95
2.43
2.18
1.93
1.63
1.50
0.12
0.89
1.23
1.94
2.00
4.78
8.92
f1 (ppm)

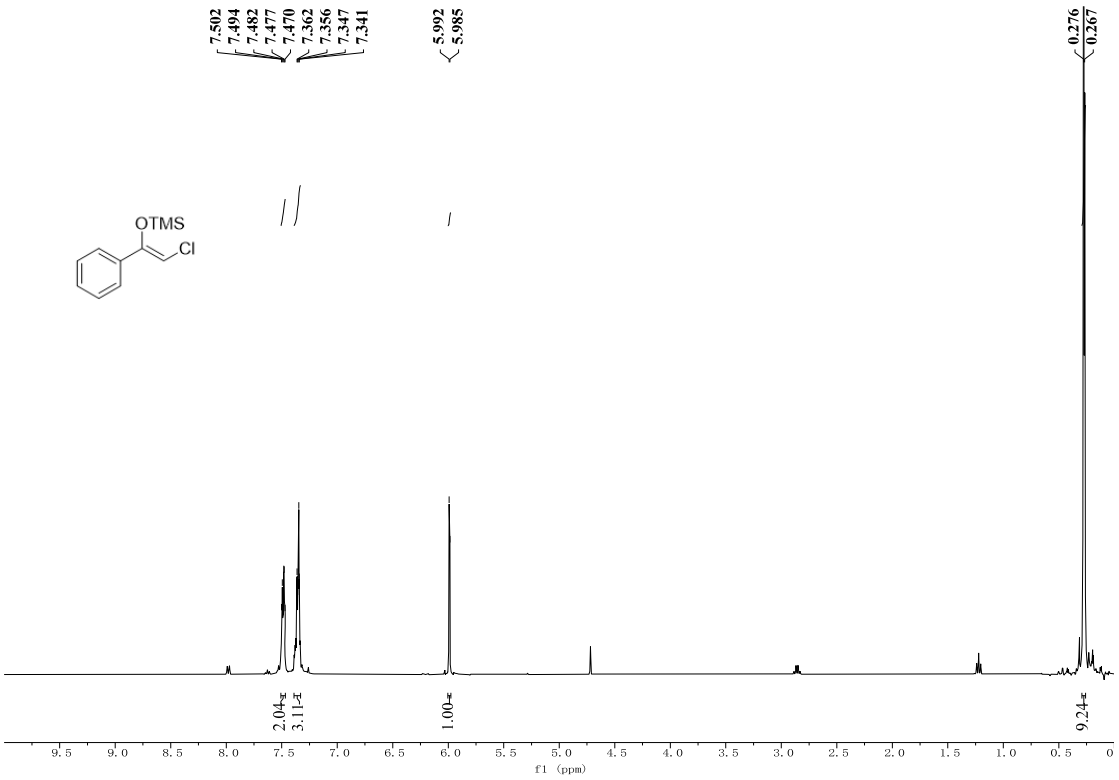

OTMS
155.88
108.42
77.32
77.00
76.68
43.70
35.39
31.46
30.32
27.69
25.23
25.10
24.23
0.08
f1 (ppm)

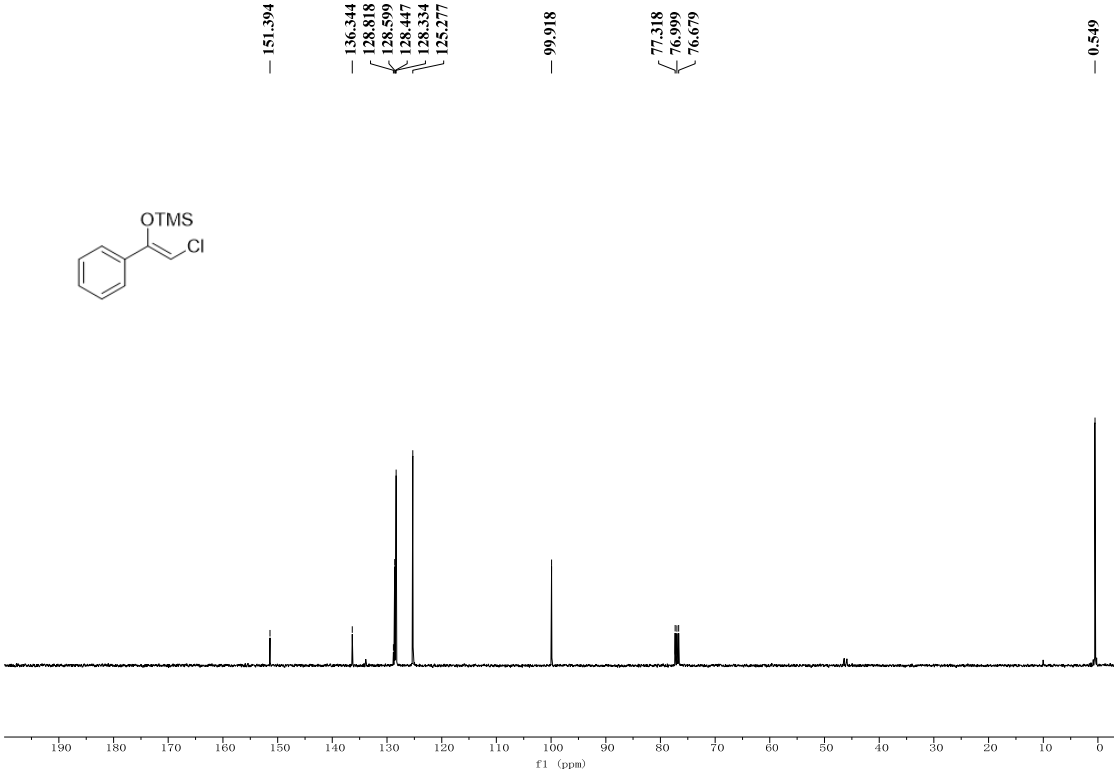

OTMS
4.610
4.603
2.270
2.261
2.258
2.254
2.246
2.243
2.232
1.869
1.857
1.845
1.843
1.831
1.819
0.202
0.196
0.191
0.92
4.06
2.00
9.01
f1 (ppm)

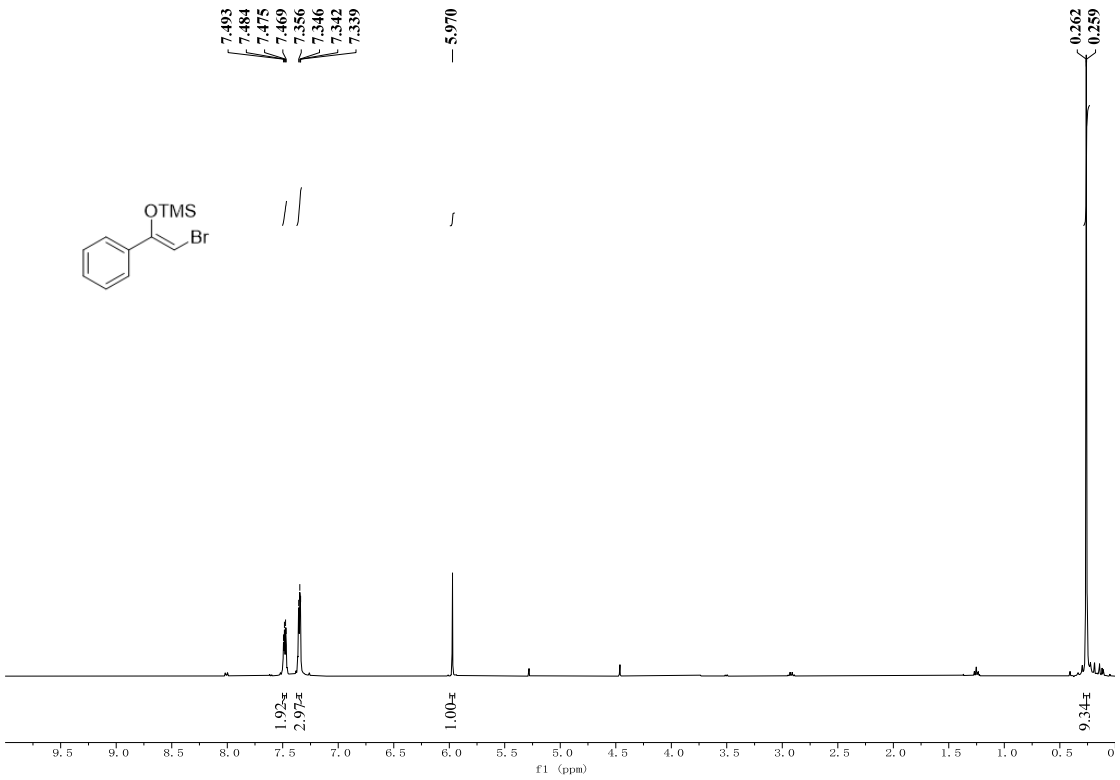

OTMS
154.974
102.021
77.209
76.998
76.785
33.469
28.696
21.278
-0.059
f1 (ppm)

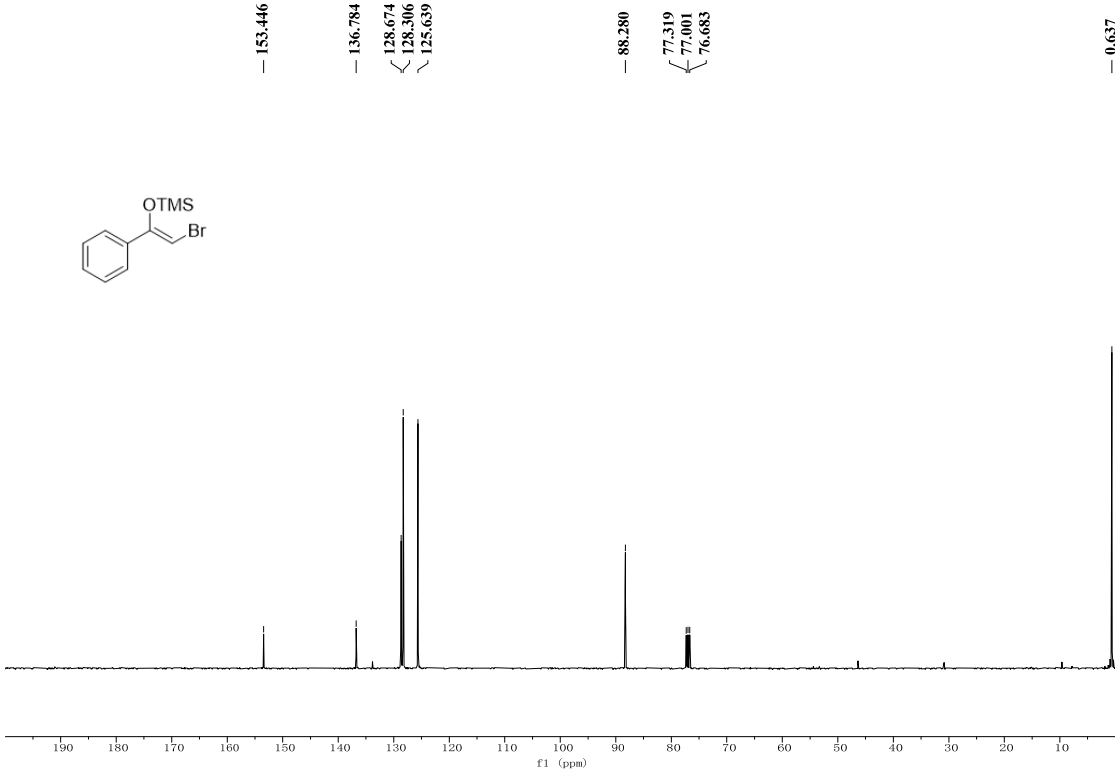

OTMS
4.43
1.97
1.95
1.47
1.45
0.91
0.89
0.17
1.00
4.01
2.47
6.12
9.52
f1 (ppm)

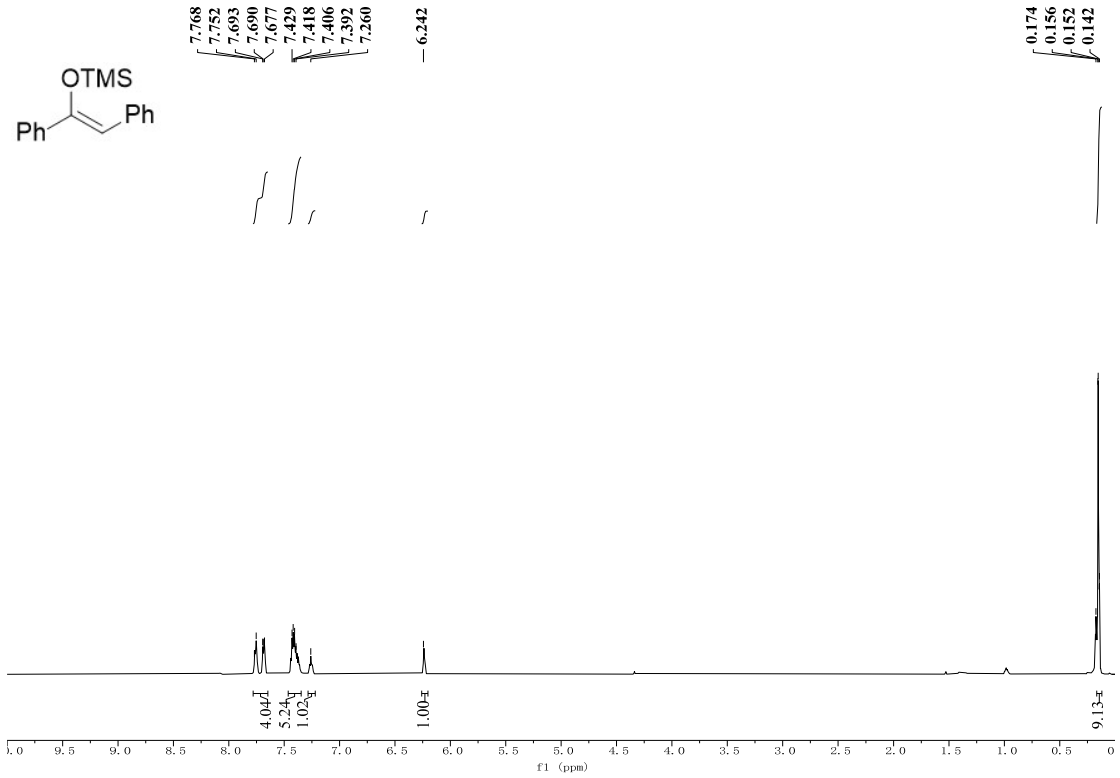

OTMS
149.41
110.39
77.32
77.00
76.68
38.67
20.15
18.64
14.45
13.62
0.30
f1 (ppm)

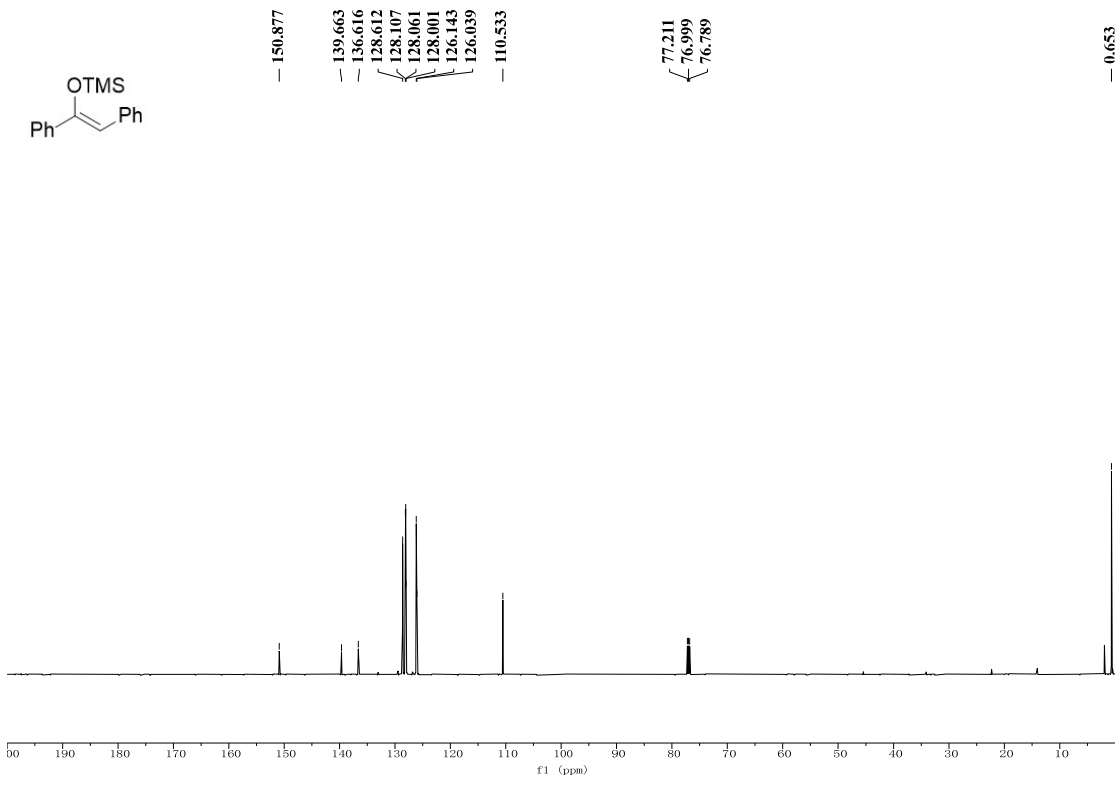

7.502
7.494
7.482
7.477
7.470
7.362
7.356
7.347
7.341
5.992
5.985
0.276
0.267
OTMS
Cl
2.04
3.11
1.00
9.24
f1 (ppm)

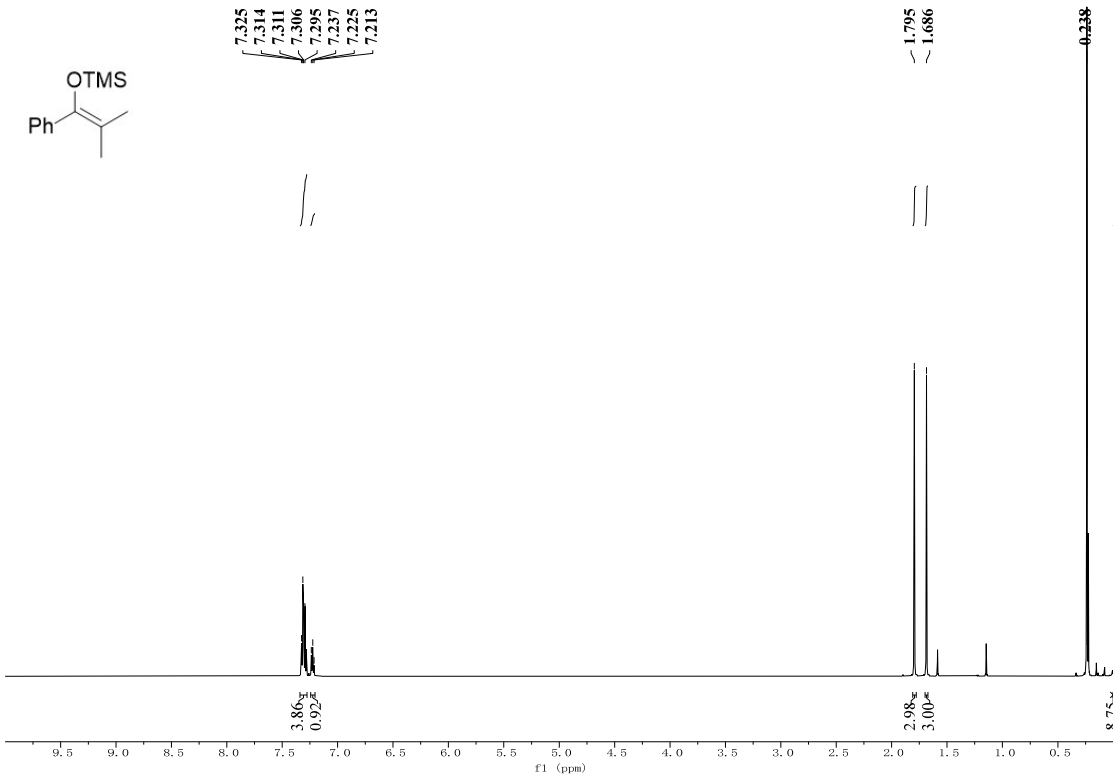

151.394
136.344
128.818
128.599
128.447
128.334
125.277
99.918
77.318
76.999
76.679
0.549
OTMS
Cl
f1 (ppm)

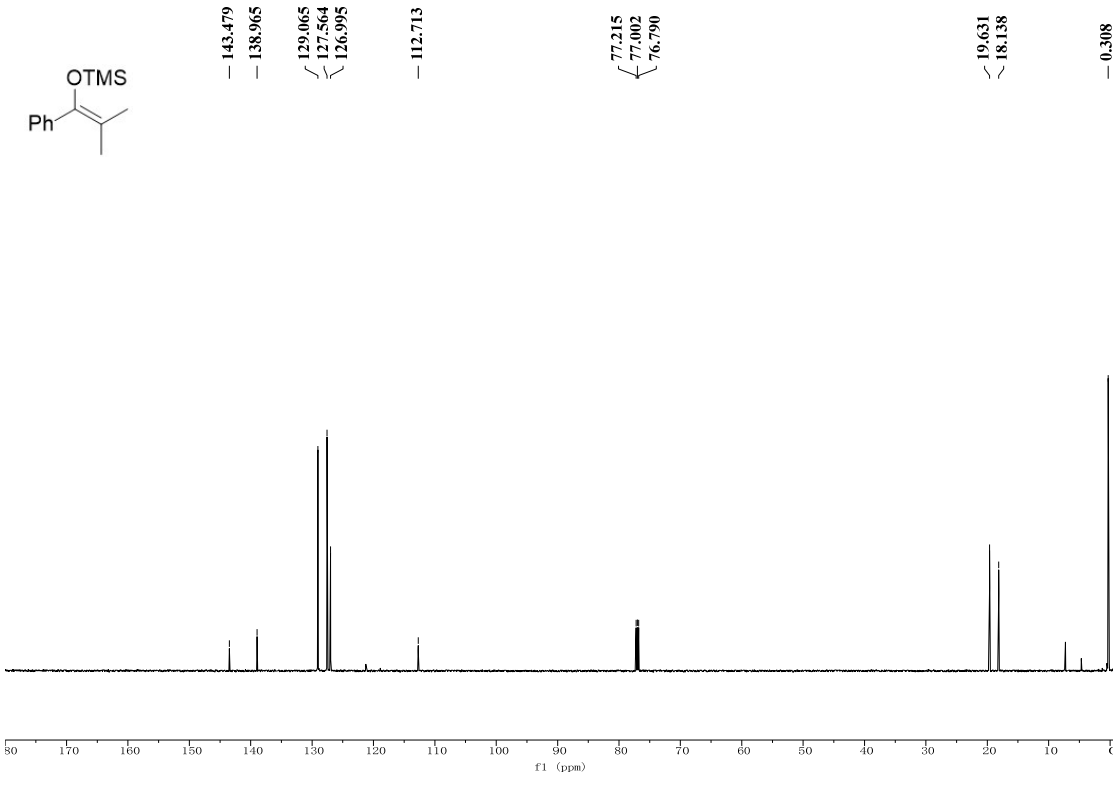

7.493
7.484
7.475
7.469
7.356
7.346
7.342
7.339
5.970
0.262
0.259
OTMS
Br
1.92
2.97
1.00
9.34
f1 (ppm)

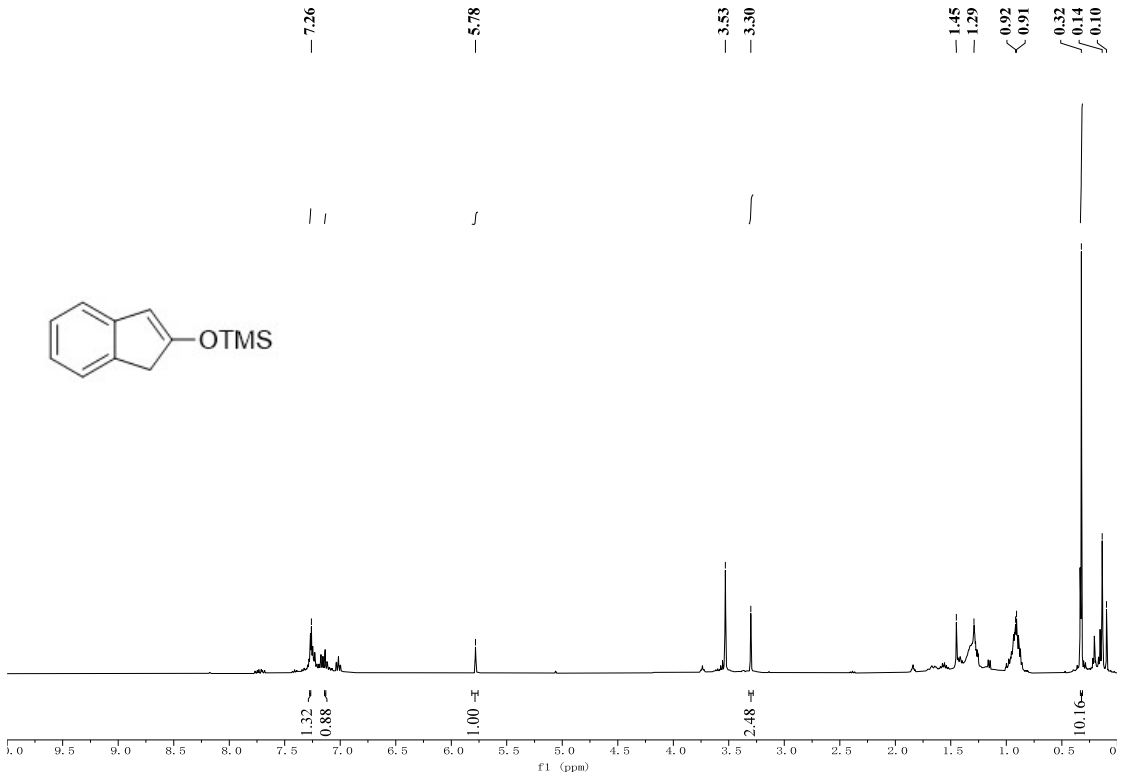

153.446
136.784
128.674
128.306
125.639
88.280
77.319
77.001
76.683
0.637
OTMS
Br
f1 (ppm)

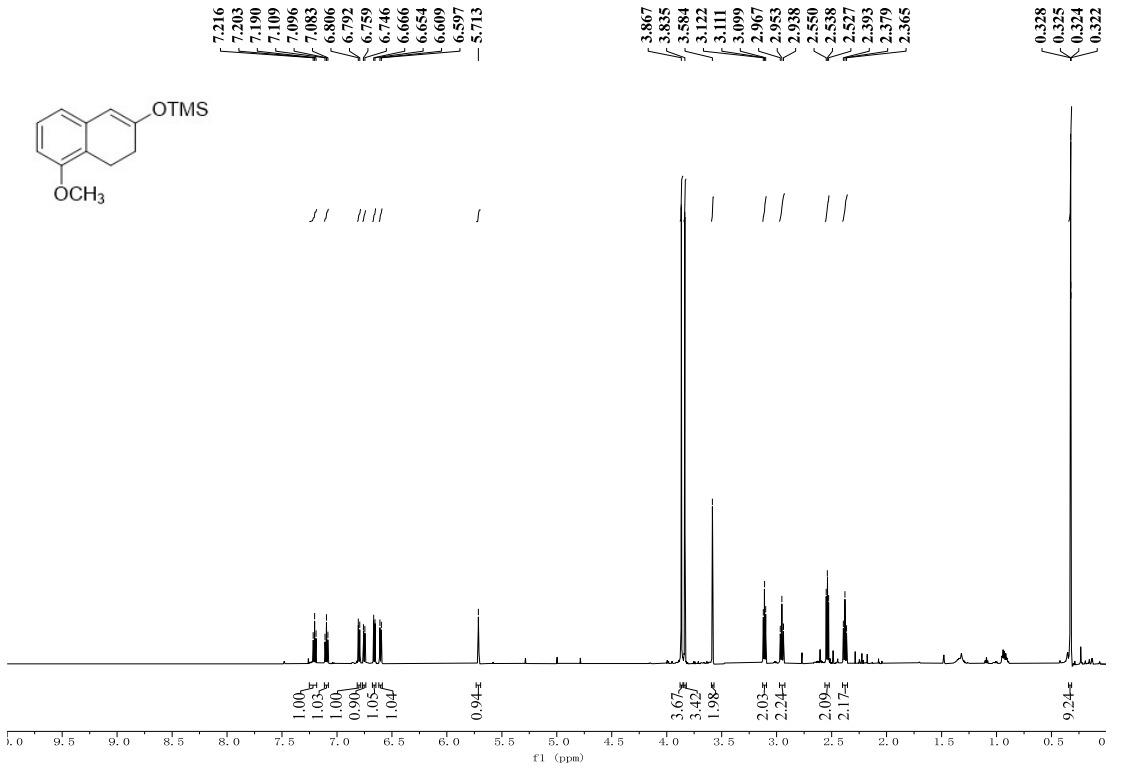

7.768
7.752
7.693
7.690
7.677
7.429
7.418
7.406
7.392
7.260
6.242
0.174
0.156
0.152
0.142
OTMS
Ph
Ph
4.04
5.24
1.02
1.00
9.13
f1 (ppm)

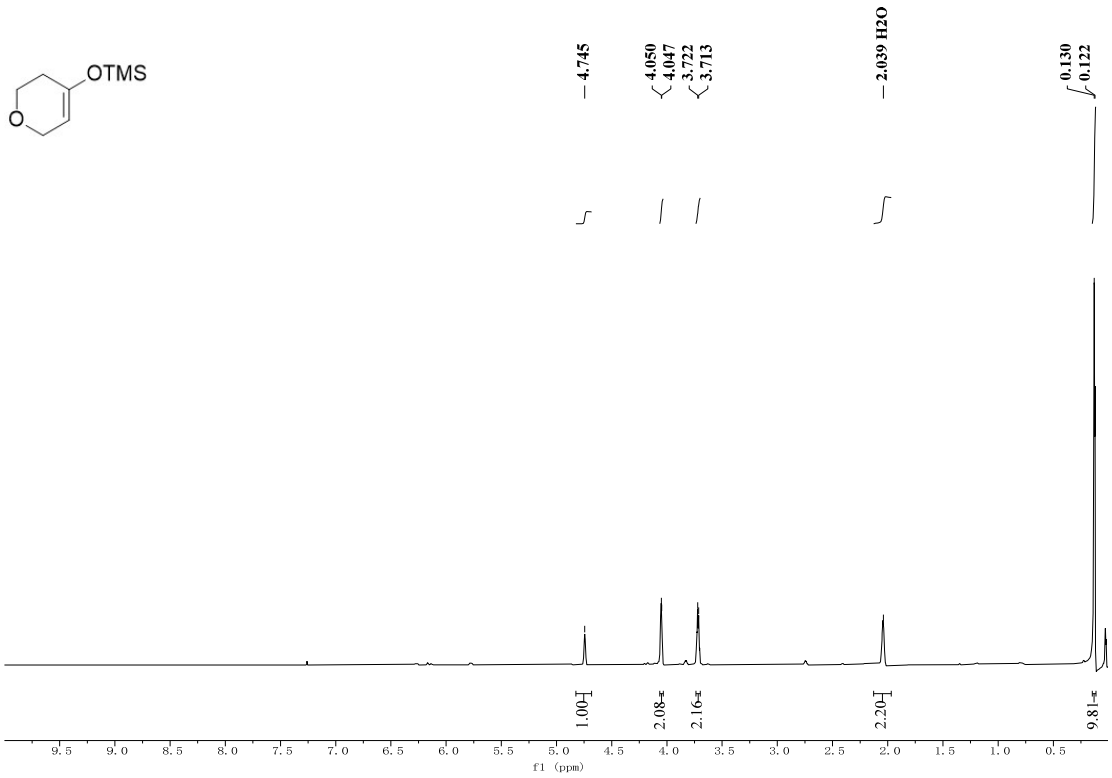

150.877
139.663
136.616
128.612
128.107
128.061
128.001
126.143
126.039
110.533
77.211
76.999
76.789
0.653
OTMS
Ph
Ph
f1 (ppm)

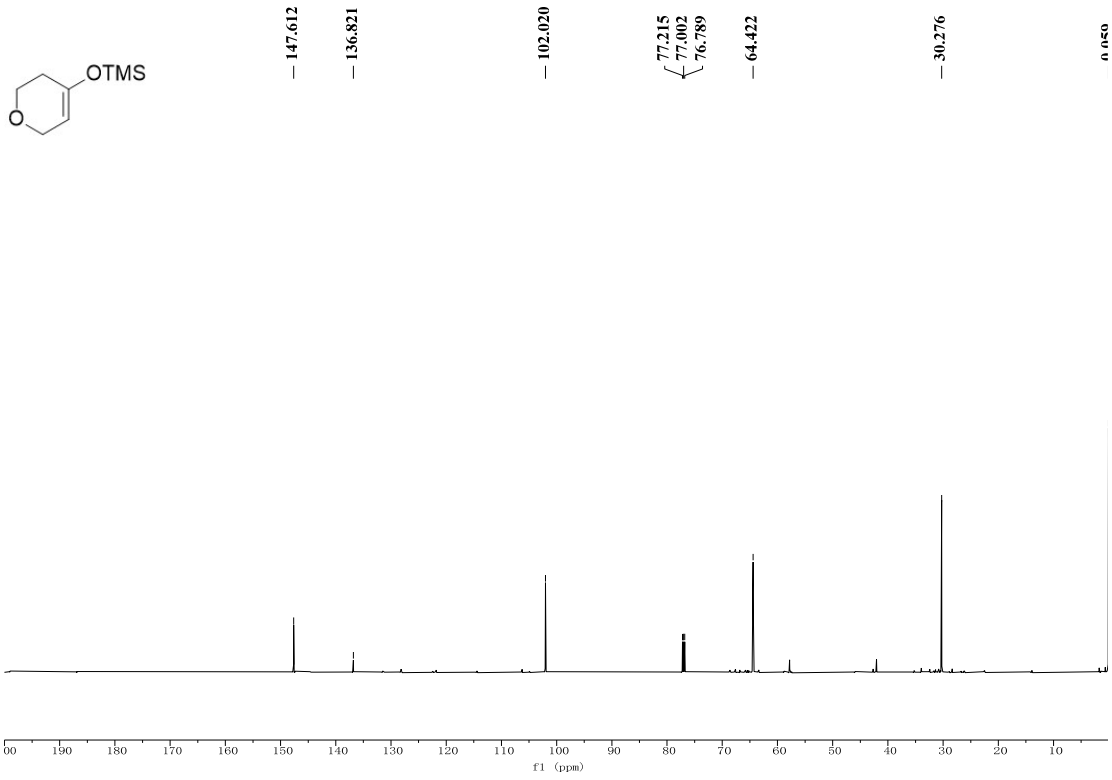

OTMS
Ph
7.325
7.314
7.311
7.306
7.295
7.237
7.225
7.213
1.795
1.686
0.238
3.86
0.92
2.98
3.00
f1 (ppm)

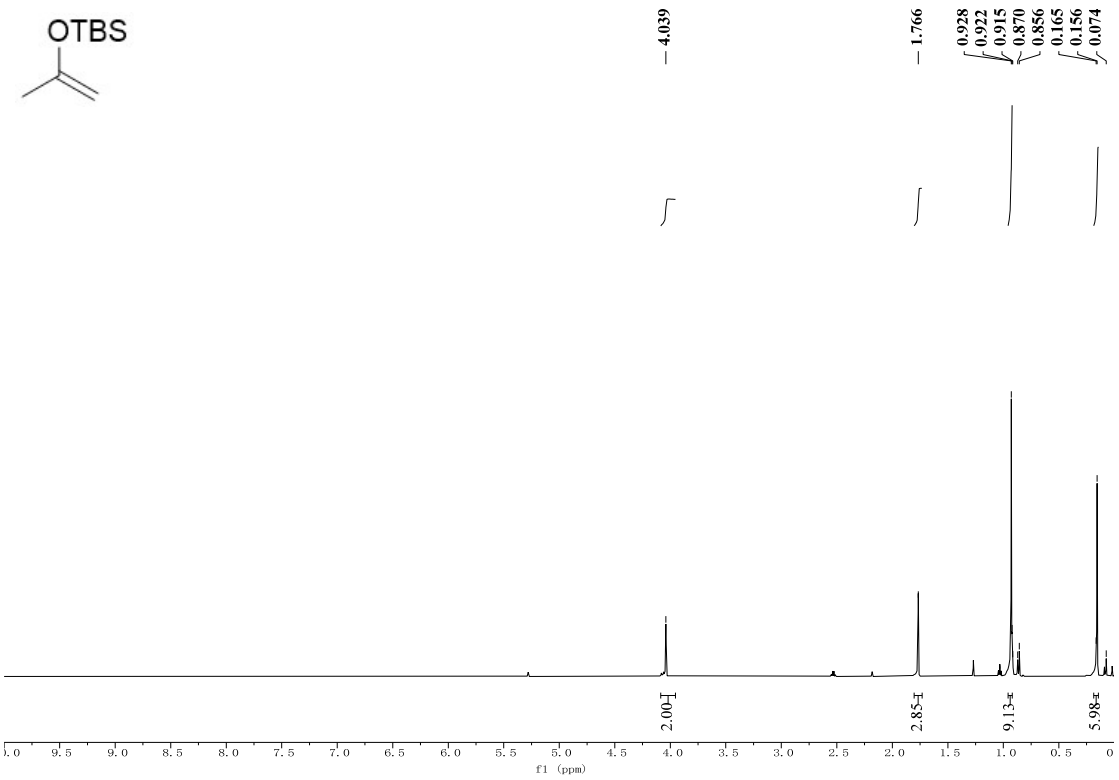

OTMS
Ph
143.479
138.965
129.065
127.564
126.995
112.713
77.215
77.002
76.790
19.631
18.138
0.308
f1 (ppm)

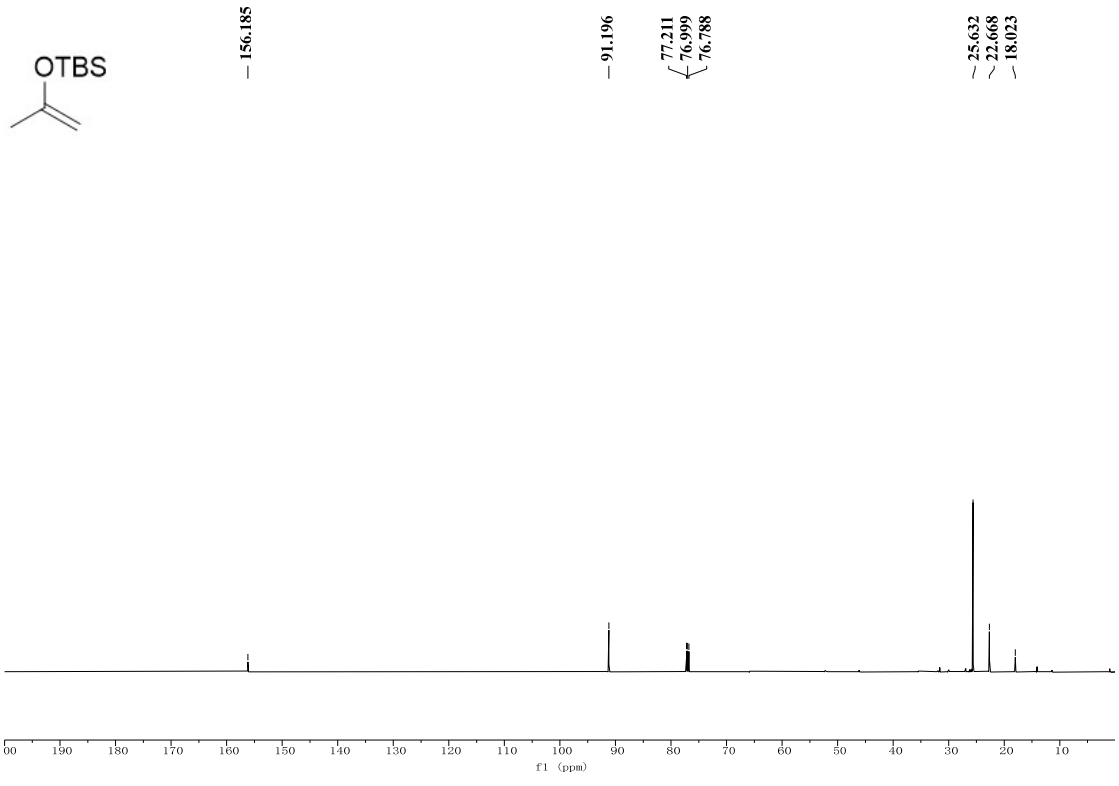

7.26
5.78
3.53
3.30
1.45
1.29
0.92
0.91
0.32
0.14
0.10
OTMS
1.32
0.88
1.00
2.48
10.16
f1 (ppm)

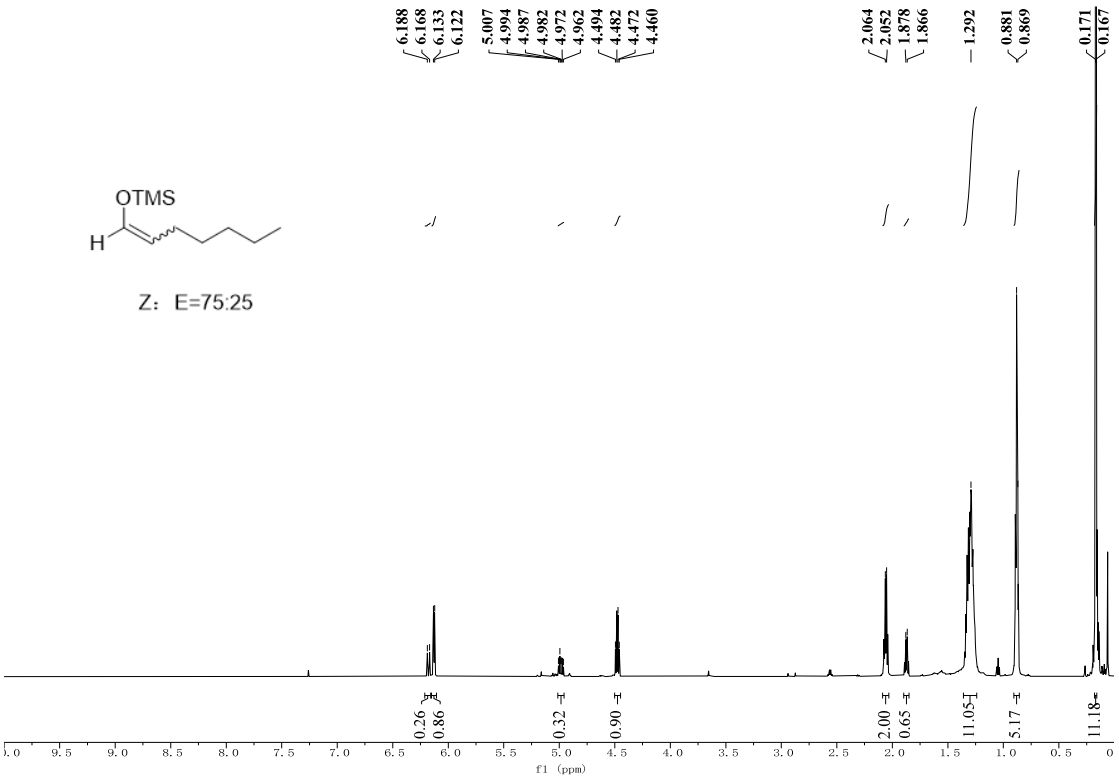

7.216
7.203
7.190
7.109
7.096
7.083
6.806
6.792
6.759
6.746
6.666
6.654
6.609
6.597
5.713
3.867
3.835
3.584
3.122
3.111
3.099
2.967
2.953
2.938
2.550
2.538
2.527
2.393
2.379
2.365
0.328
0.325
0.324
0.322
OTMS
OCH3
1.00
1.03
1.00
0.90
1.05
1.04
0.94
3.67
3.42
1.98
2.03
2.24
2.09
2.17
9.24
f1 (ppm)

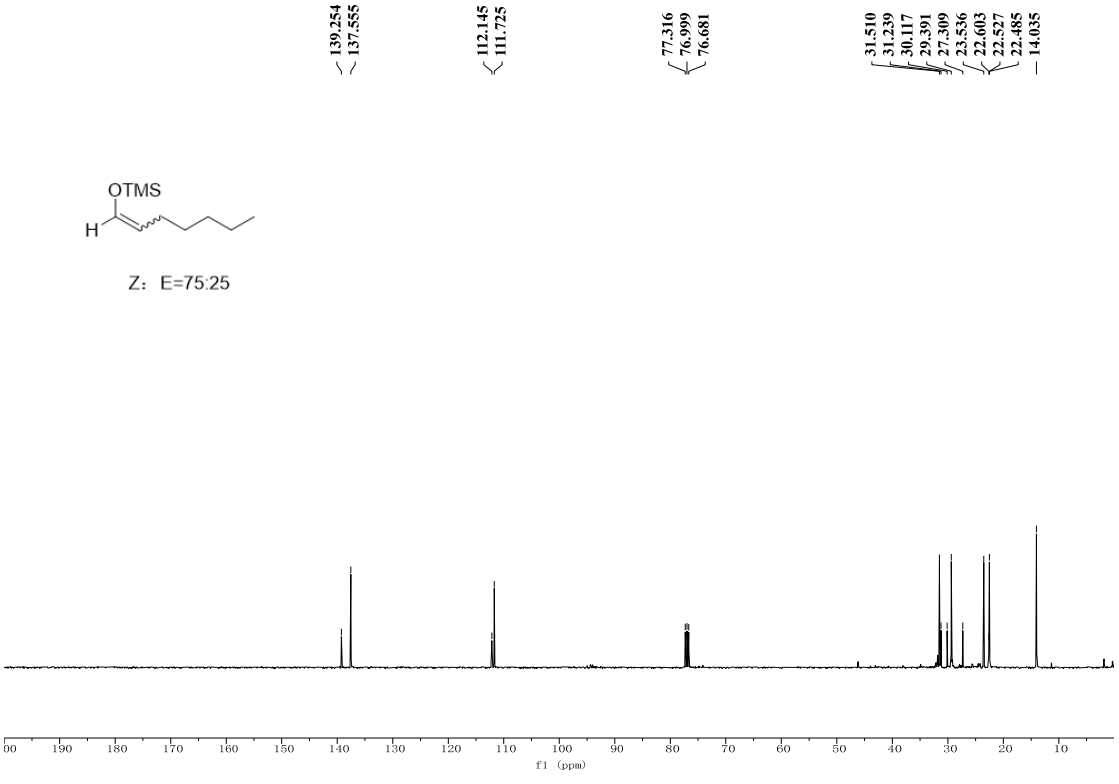

OTMS
O
4.745
4.050
4.047
3.722
3.713
2.039 H2O
0.130
0.122
1.00
2.08
2.16
2.20
9.81
f1 (ppm)

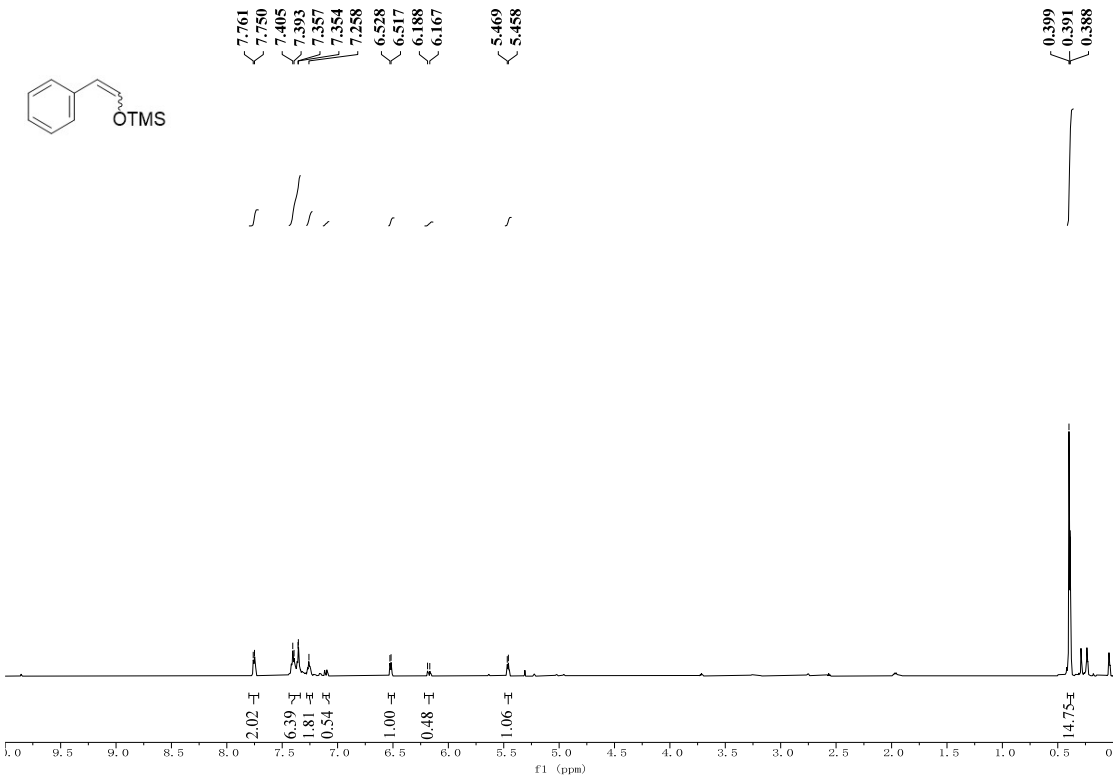

OTMS
O
147.612
136.821
102.020
77.215
77.002
76.789
64.422
30.276
f1 (ppm)

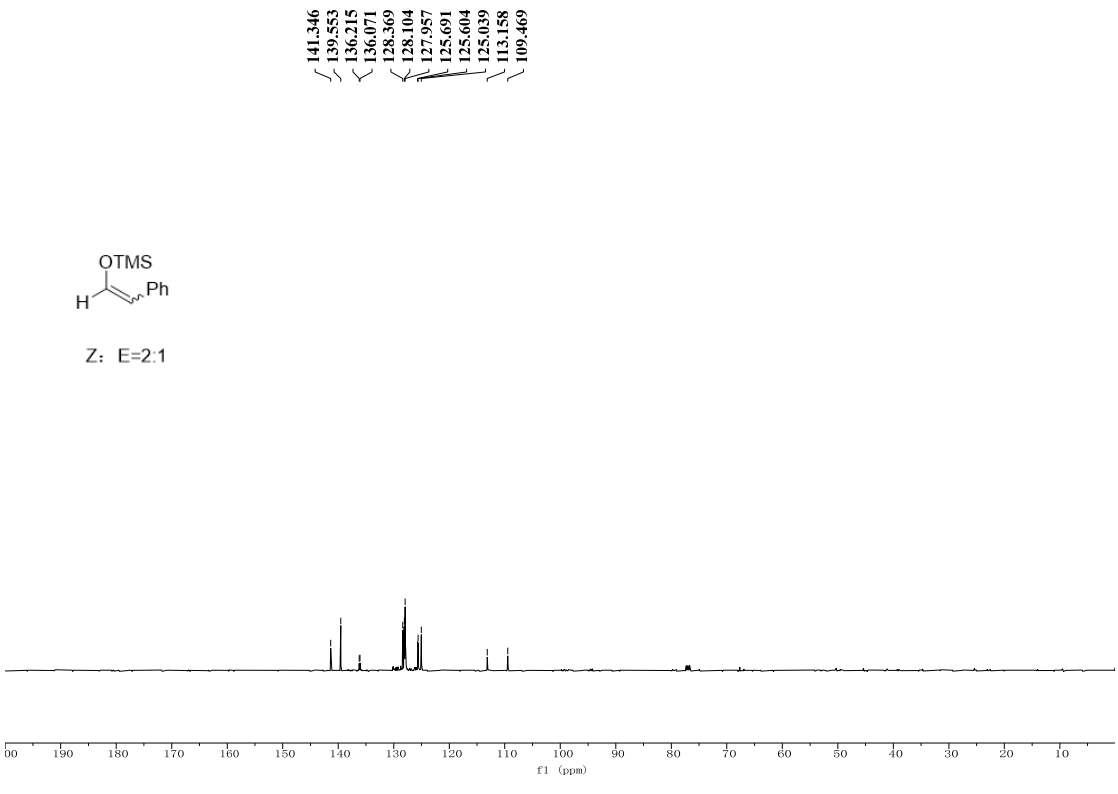

OTBS
4.039
1.766
0.928
0.922
0.915
0.870
0.856
0.165
0.156
0.074
2.00
2.85
9.13
5.98
f1 (ppm)

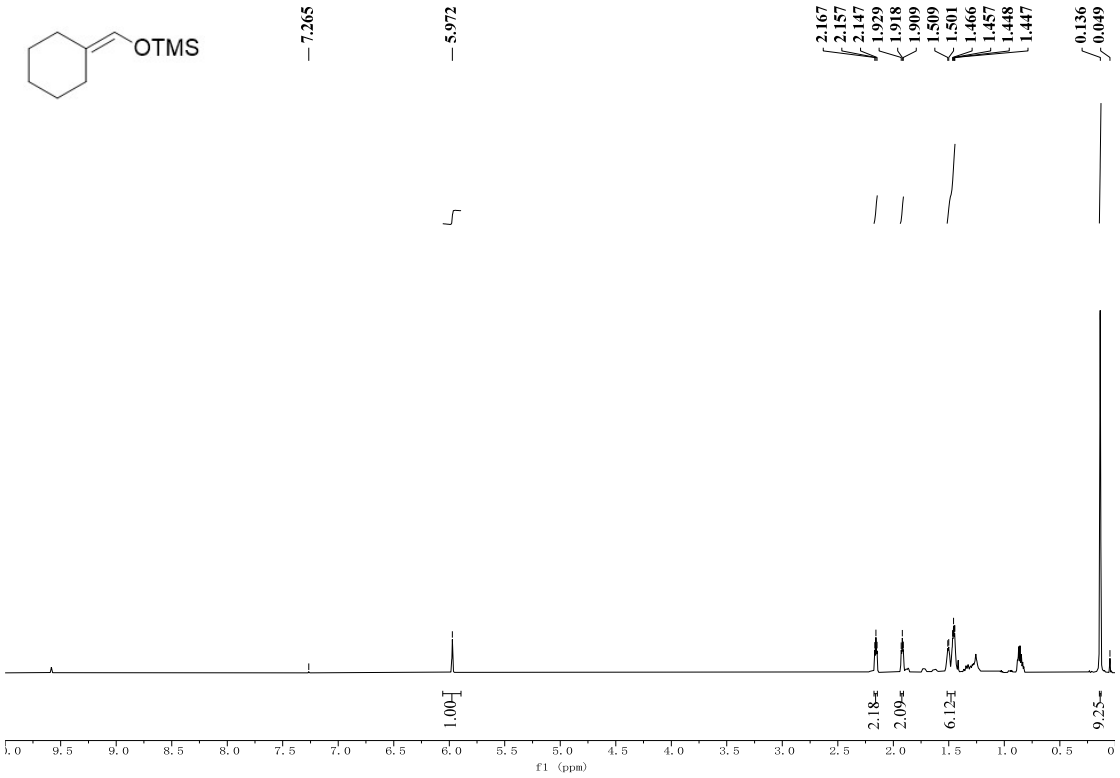

OTBS
156.185
91.196
77.211
76.999
76.788
25.632
22.668
18.023
f1 (ppm)

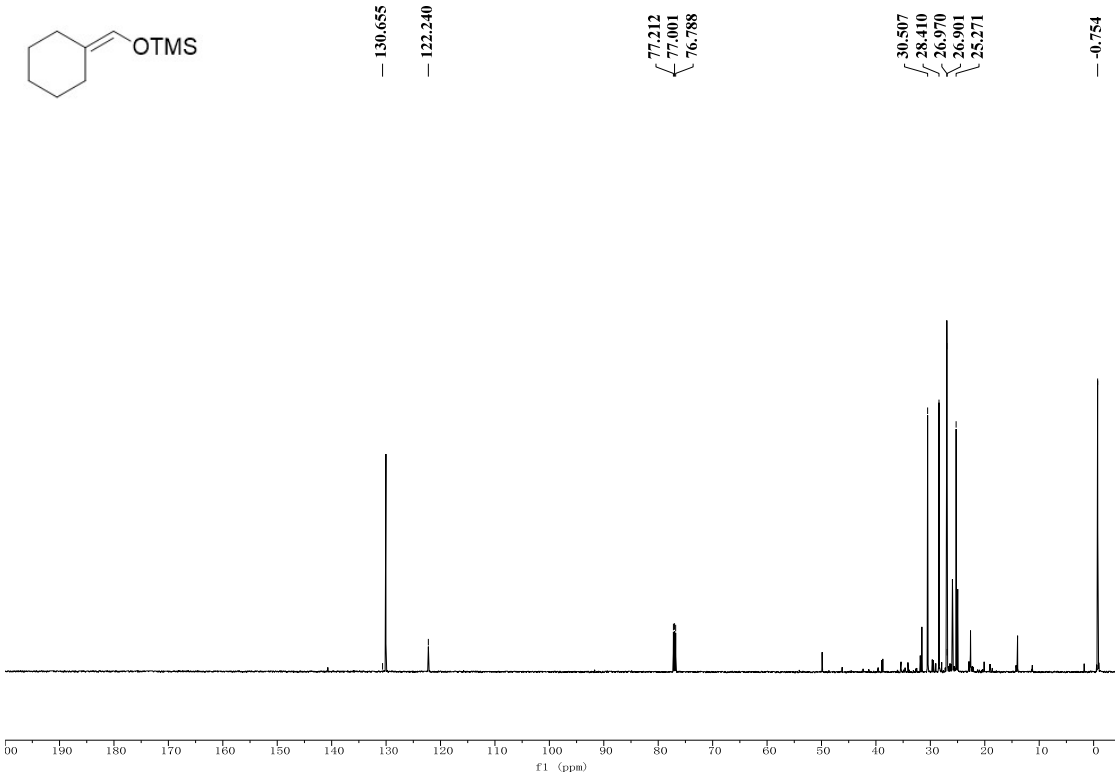

6.188
6.168
6.133
6.122
5.007
4.994
4.987
4.982
4.972
4.962
4.494
4.482
4.472
4.460
2.064
2.052
1.878
1.866
1.292
0.881
0.869
0.171
0.167
OTMS
H
Z：E=75:25
0.26
0.86
0.32
0.90
2.00
0.65
11.05
5.17
11.18
f1 (ppm)

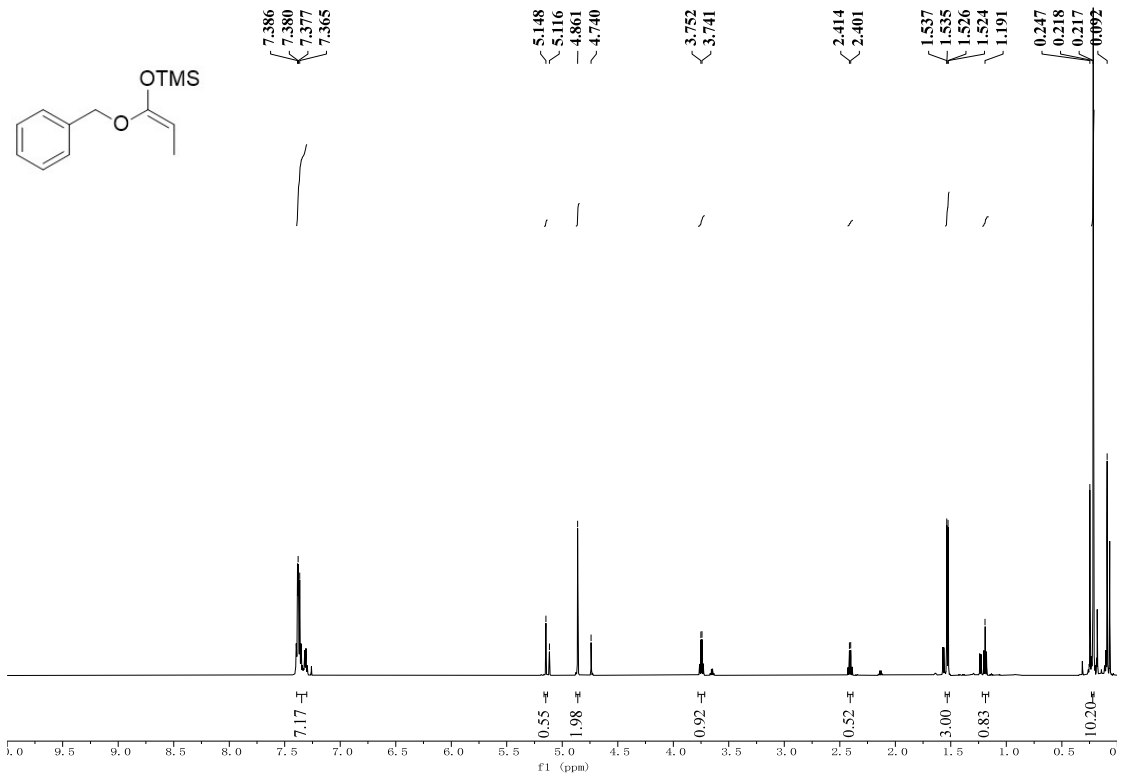

139.254
137.555
112.145
111.725
77.316
76.999
76.681
31.510
31.239
30.117
29.391
27.309
23.536
22.603
22.527
22.485
14.035
OTMS
H
Z：E=75:25
f1 (ppm)

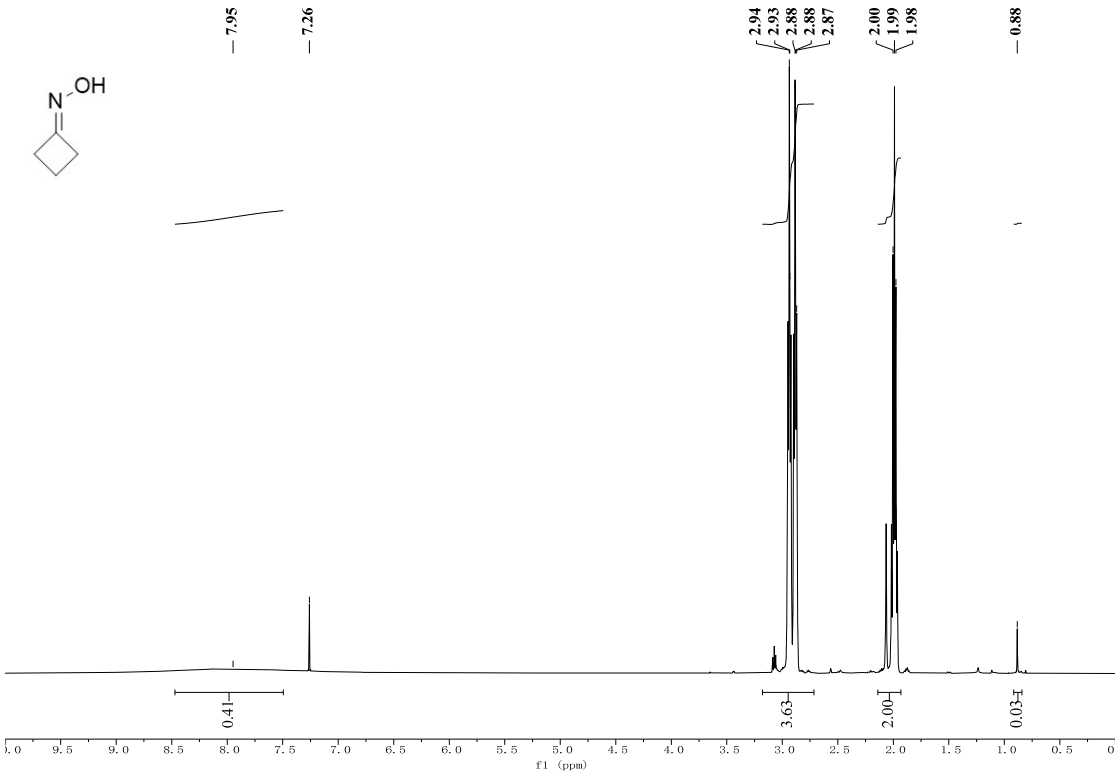

7.761
7.750
7.405
7.393
7.357
7.354
7.258
6.528
6.517
6.188
6.167
5.469
5.458
0.399
0.391
0.388
OTMS
2.02
6.39
1.81
0.54
1.00
0.48
1.06
14.75
f1 (ppm)

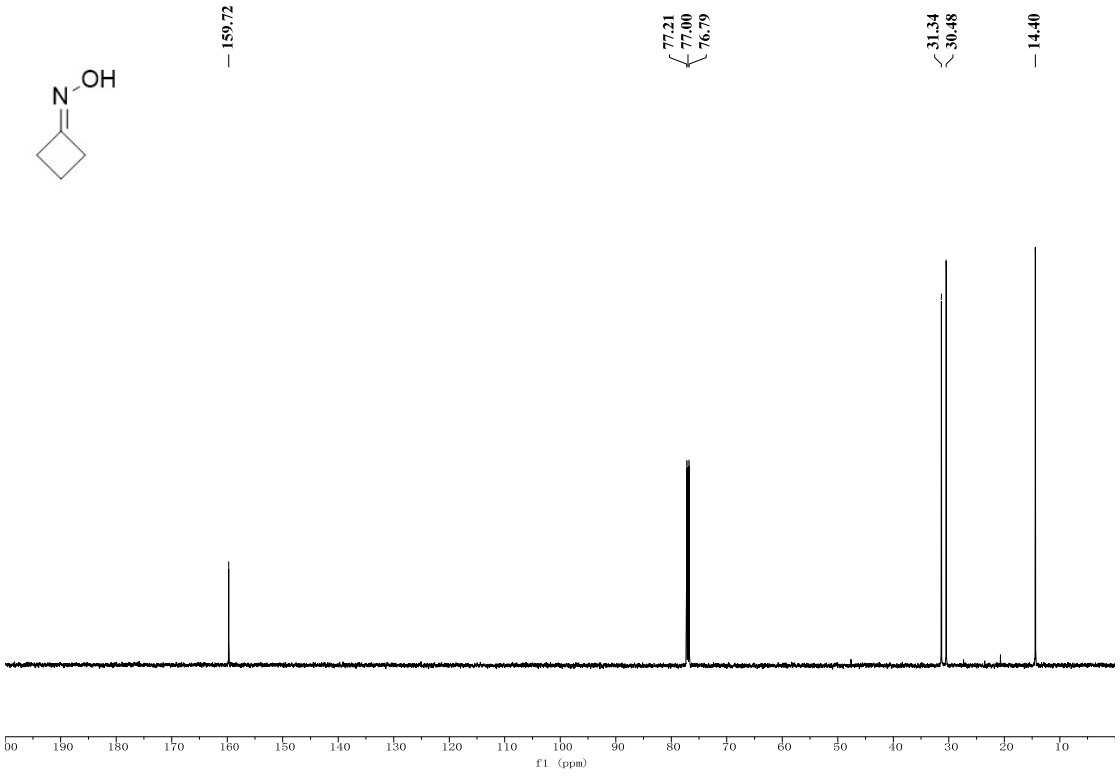

141.346
139.553
136.215
136.071
128.369
128.104
127.957
125.691
125.604
125.039
113.158
109.469
OTMS
H
Ph
Z：E=2:1
f1 (ppm)

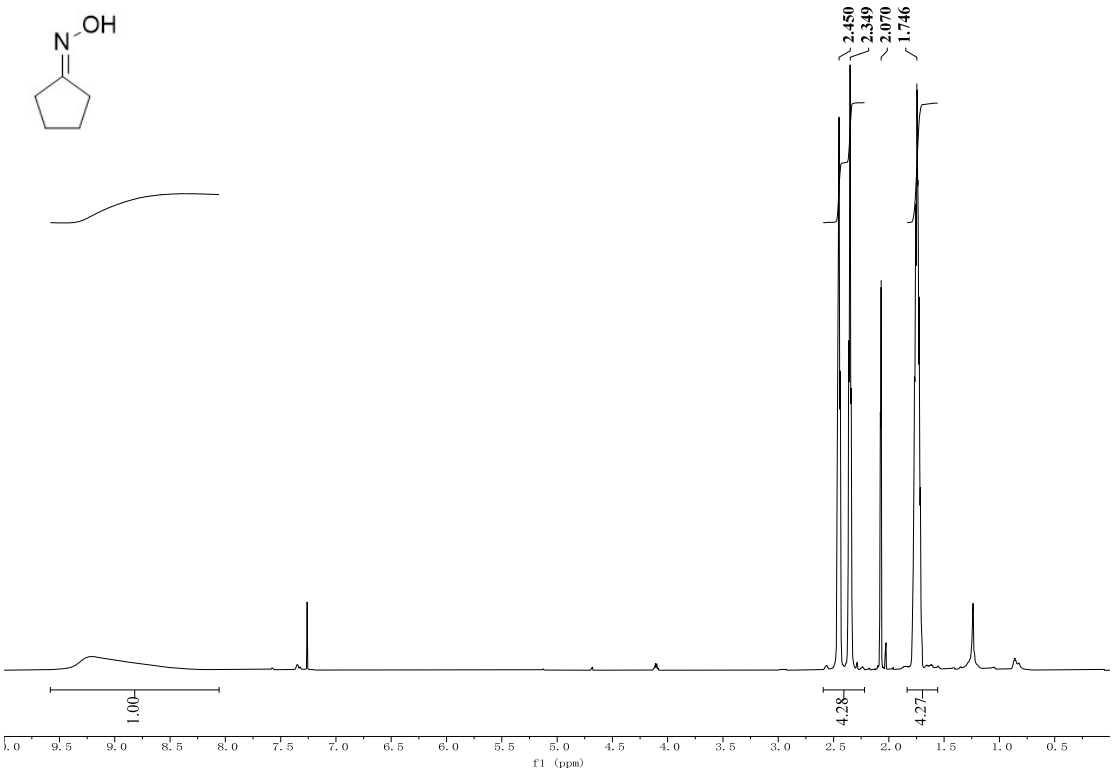

OTMS
7.265
5.972
2.167
2.157
2.147
1.929
1.918
1.909
1.509
1.501
1.466
1.457
1.448
1.447
0.136
0.049
1.00
2.18
2.09
6.12
9.25
f1 (ppm)

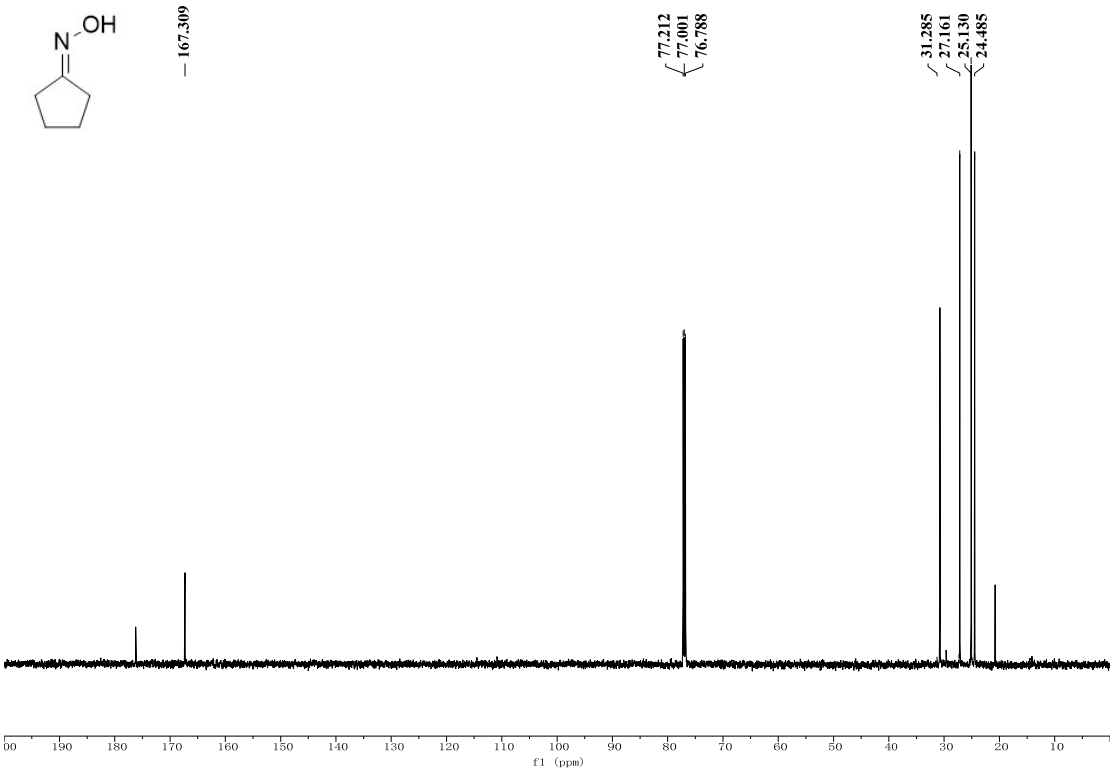

OTMS
130.655
122.240
77.212
77.001
76.788
30.507
28.410
26.970
26.901
25.271
-0.754
f1 (ppm)

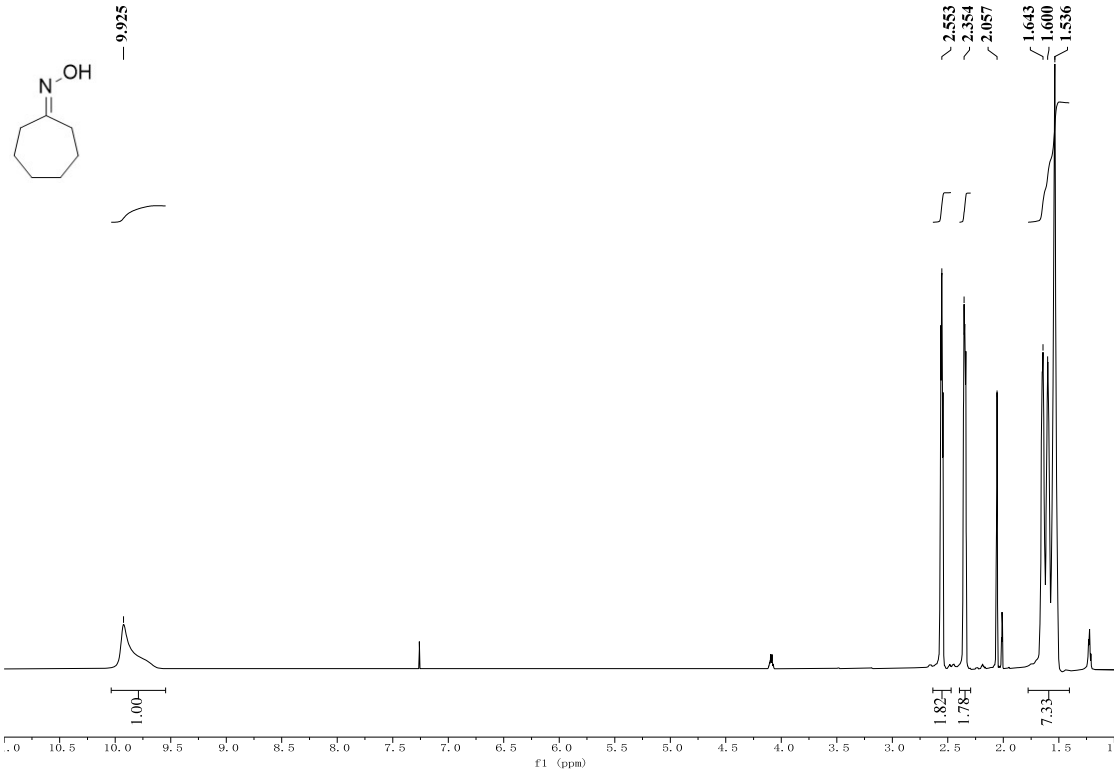

OTMS
O
7.386
7.380
7.377
7.365
5.148
5.116
4.861
4.740
3.752
3.741
2.414
2.401
1.537
1.535
1.526
1.524
1.191
0.247
0.218
0.217
0.092
7.17
0.55
1.98
0.92
0.52
3.00
0.83
10.20
f1 (ppm)

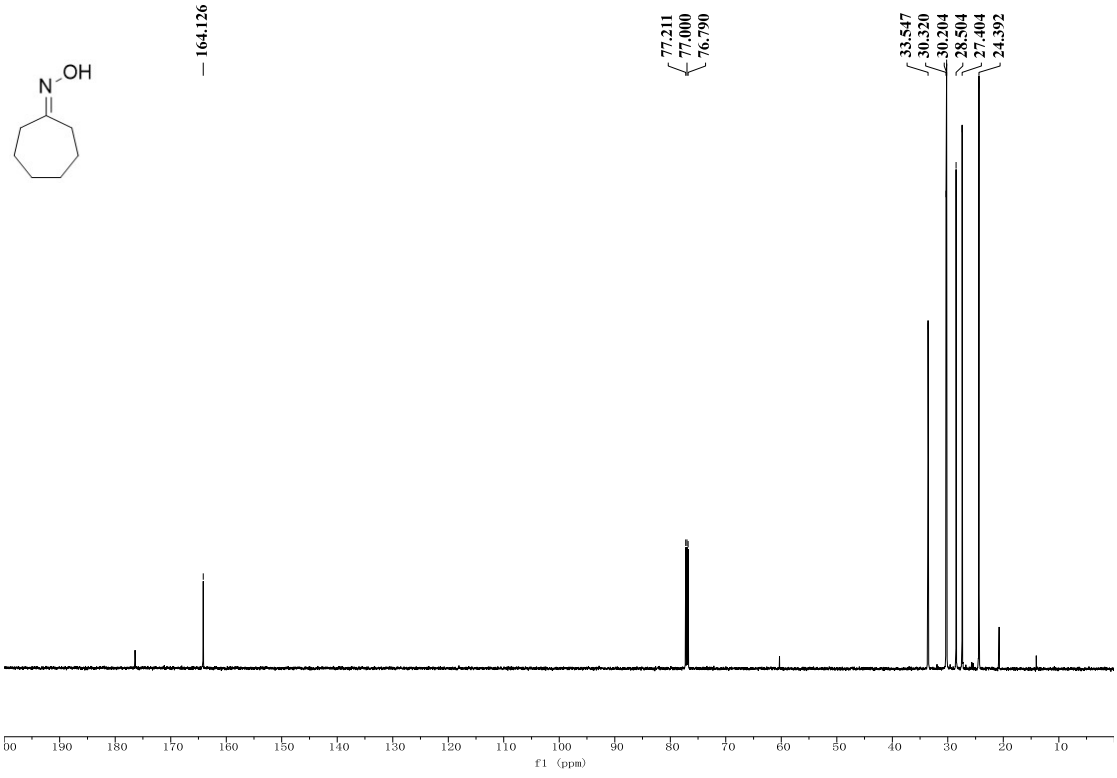

7.95
7.26
2.94
2.93
2.88
2.88
2.87
2.00
1.99
1.98
0.88
0.41
3.63
2.00
0.03
f1 (ppm)

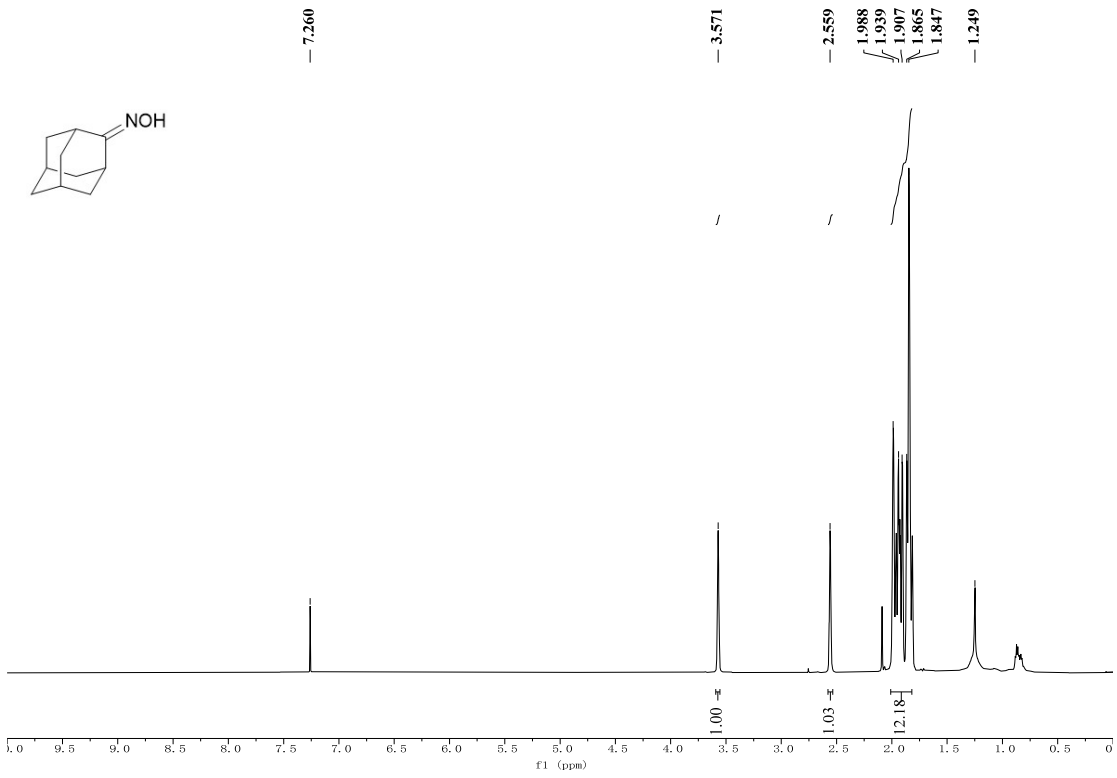

159.72
77.21
77.00
76.79
31.34
30.48
14.40
f1 (ppm)

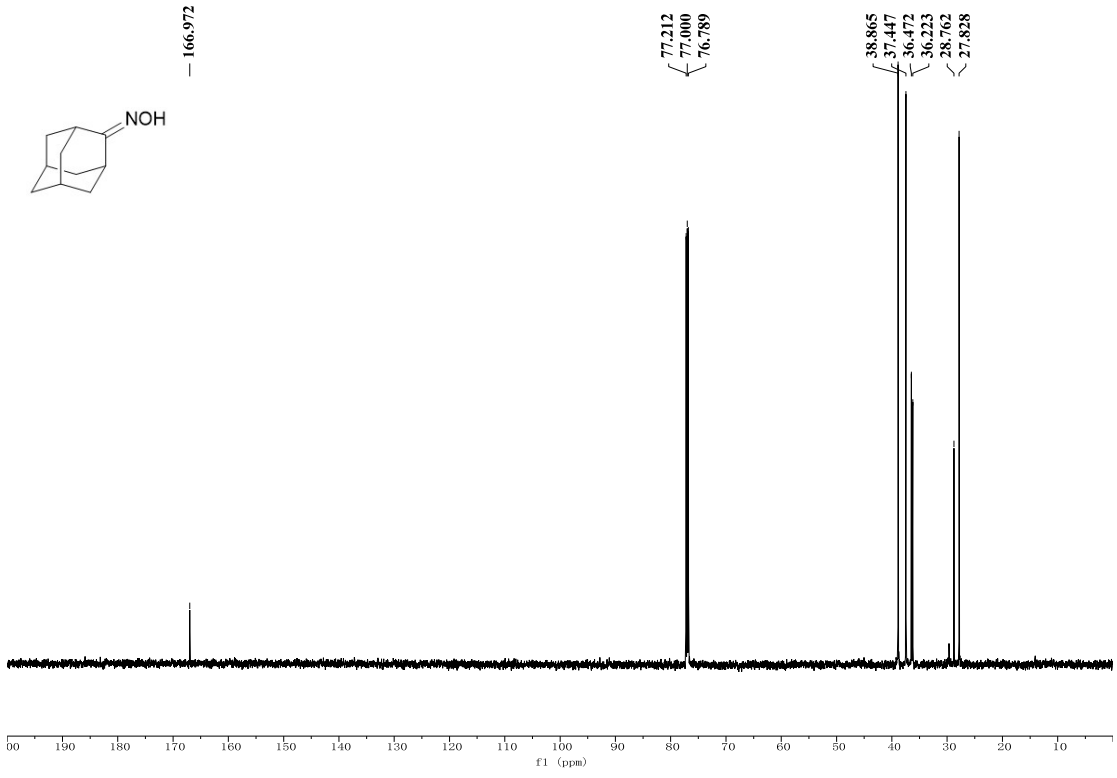

N
OH
2.450
2.349
2.070
1.746
1.00
4.28
4.27
f1 (ppm)

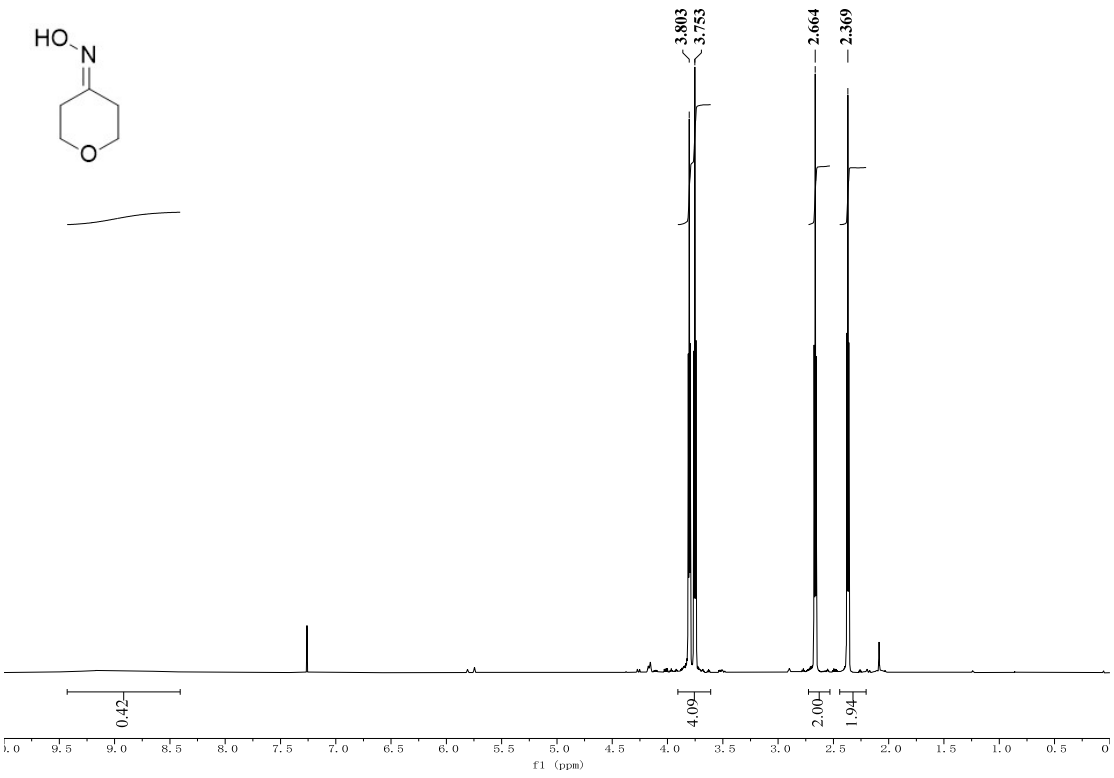

N
OH
167.309
77.212
77.001
76.788
31.285
27.161
25.130
24.485
f1 (ppm)

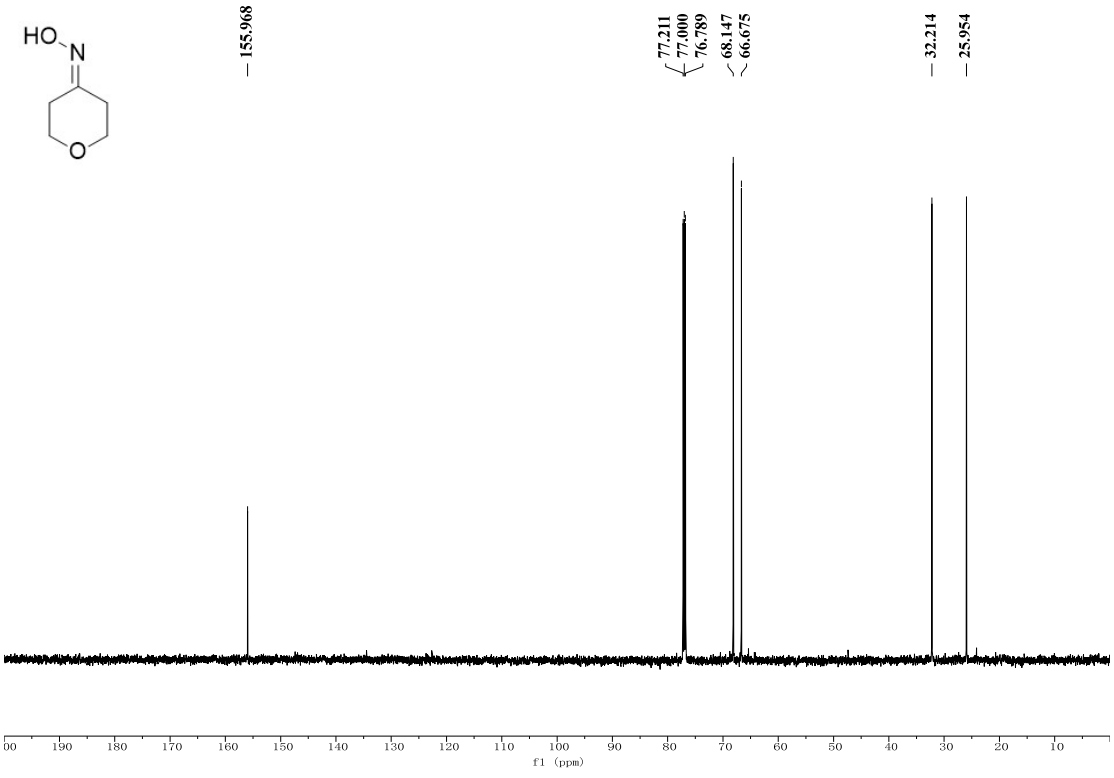

9.925
2.553
2.354
2.057
1.643
1.600
1.536
1.00
1.82
1.78
7.33
f1 (ppm)

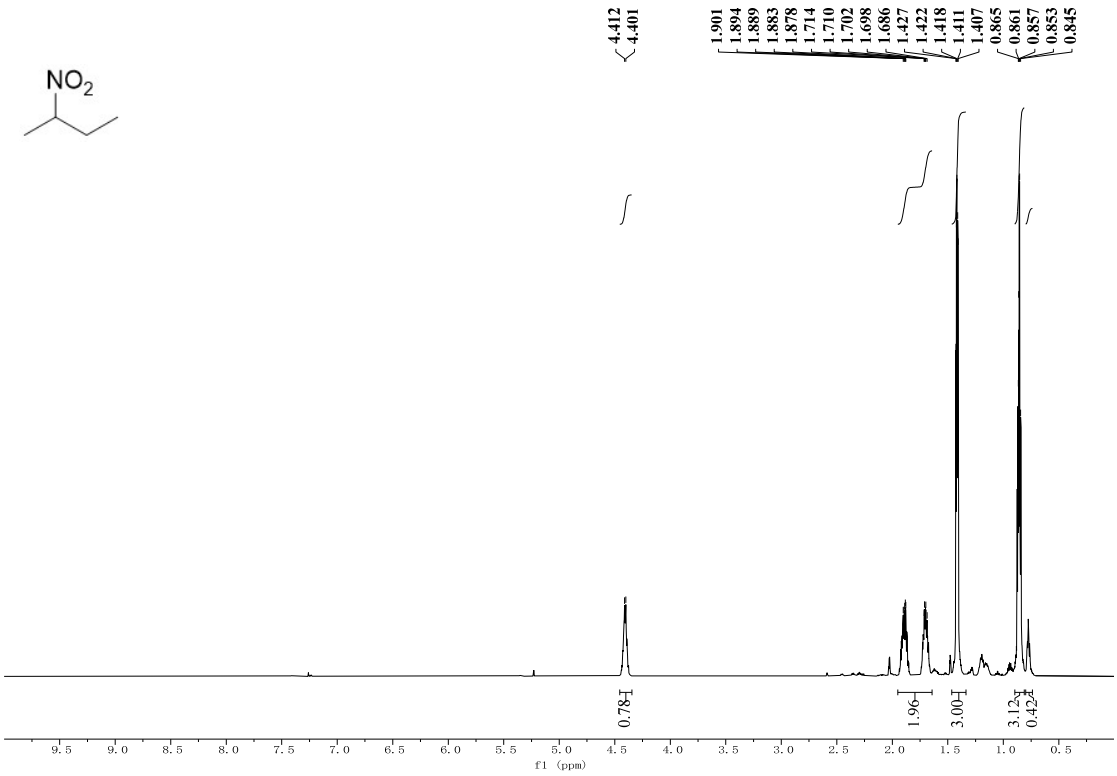

164.126
77.211
77.000
76.790
33.547
30.320
30.204
28.504
27.404
24.392
f1 (ppm)

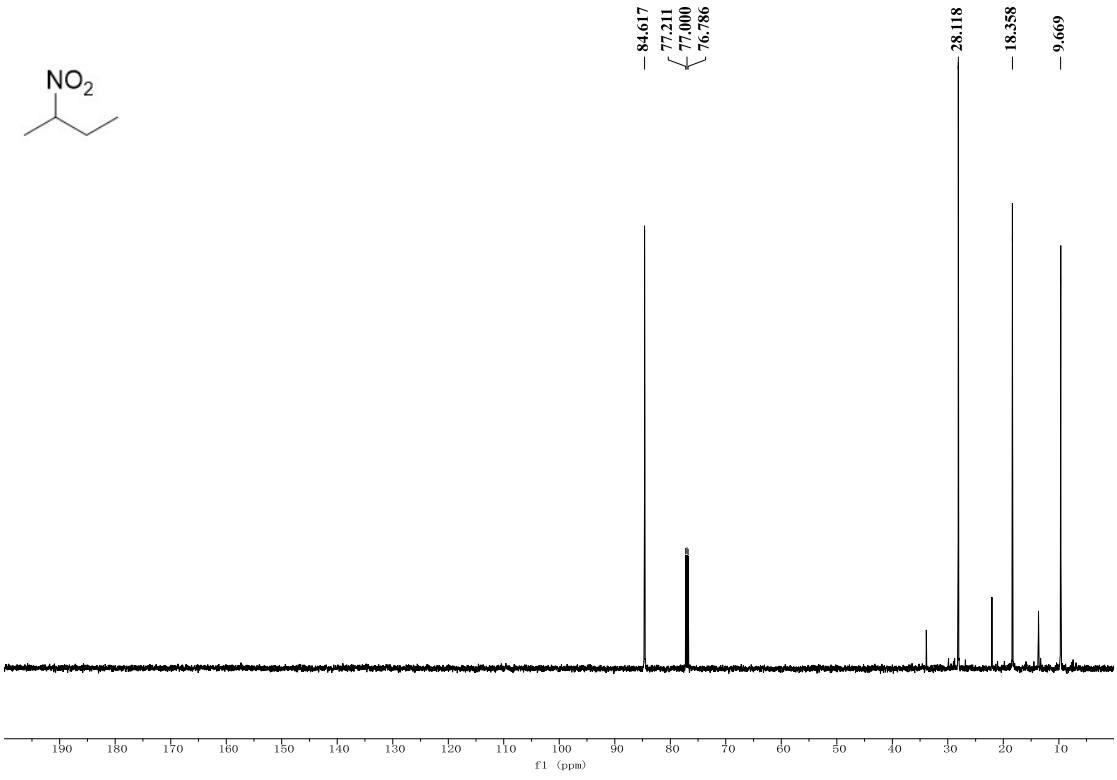

7.260
3.571
2.559
1.988
1.939
1.907
1.865
1.847
1.249
NOH
1.00
1.03
12.18
f1 (ppm)

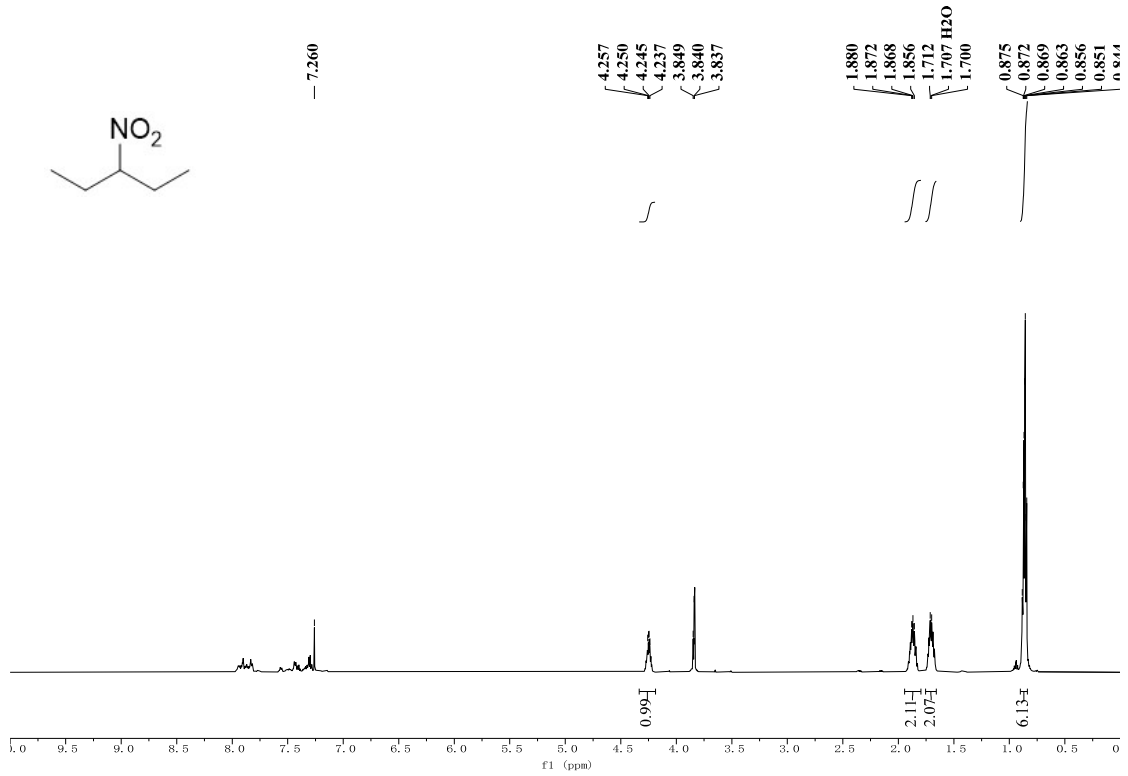

166.972
77.212
77.000
76.789
38.865
37.447
36.472
36.223
28.762
27.828
NOH
f1 (ppm)

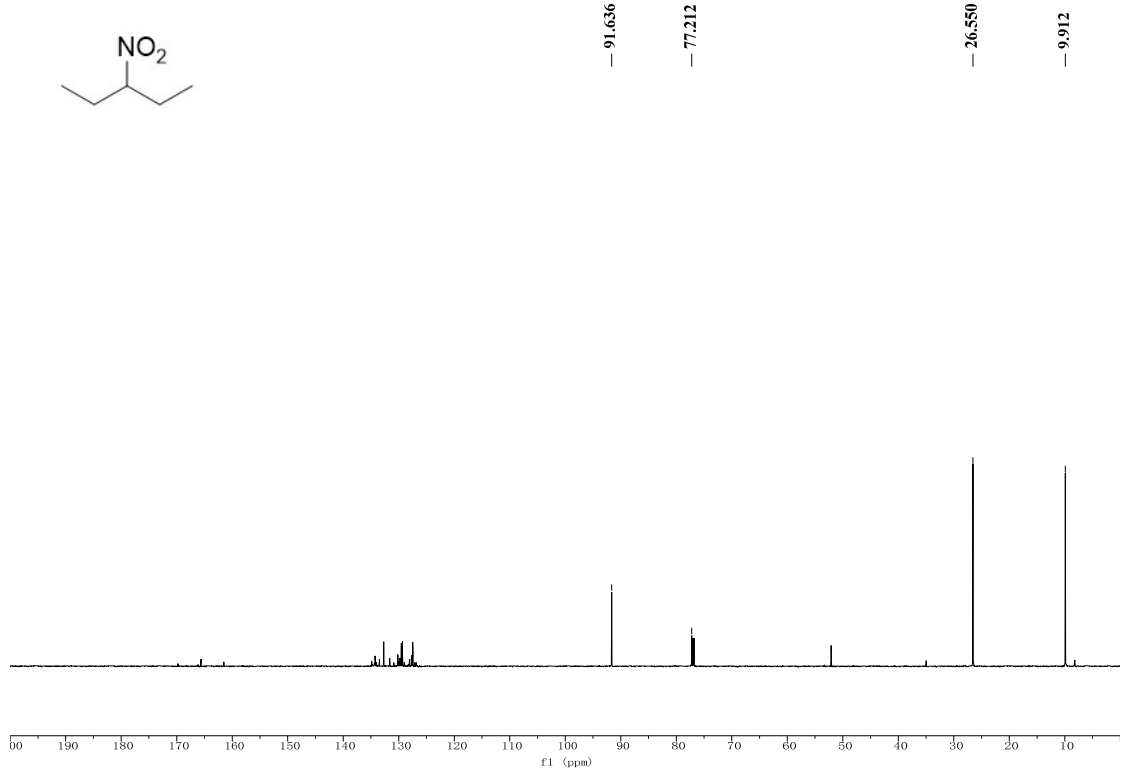

HO
N
O
3.803
3.753
2.664
2.369
0.42
4.09
2.00
1.94
f1 (ppm)

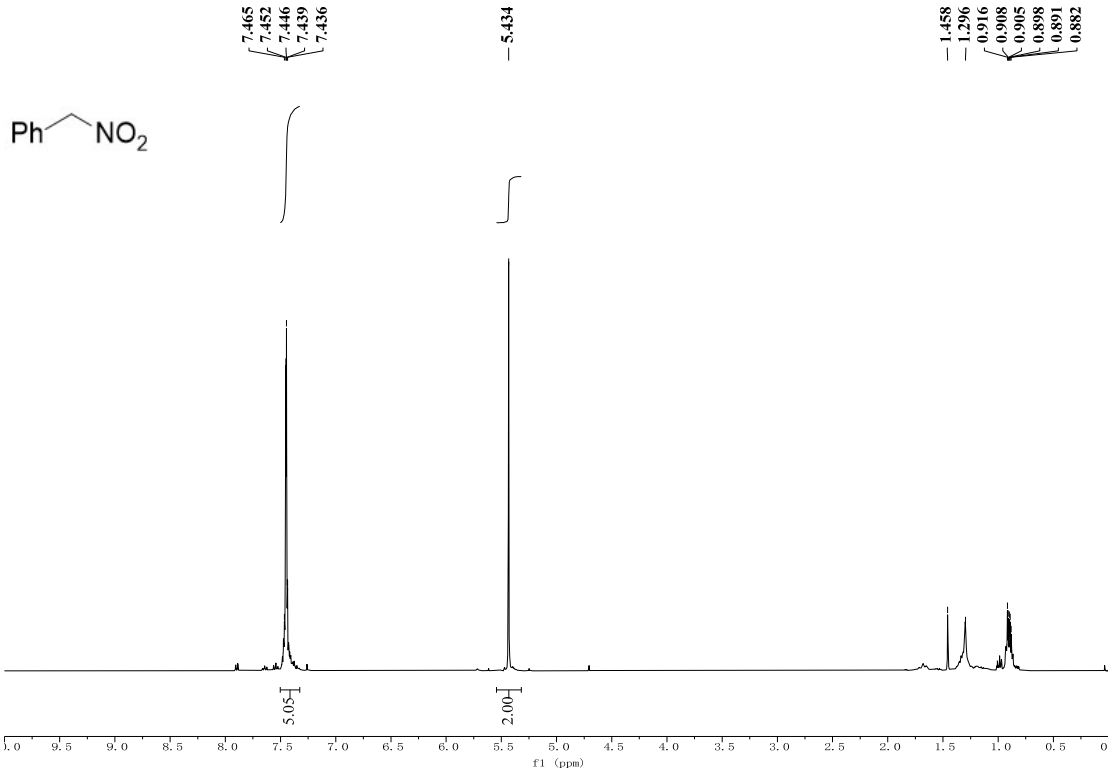

HO
N
O
155.968
77.211
77.000
76.789
68.147
66.675
32.214
25.954
f1 (ppm)

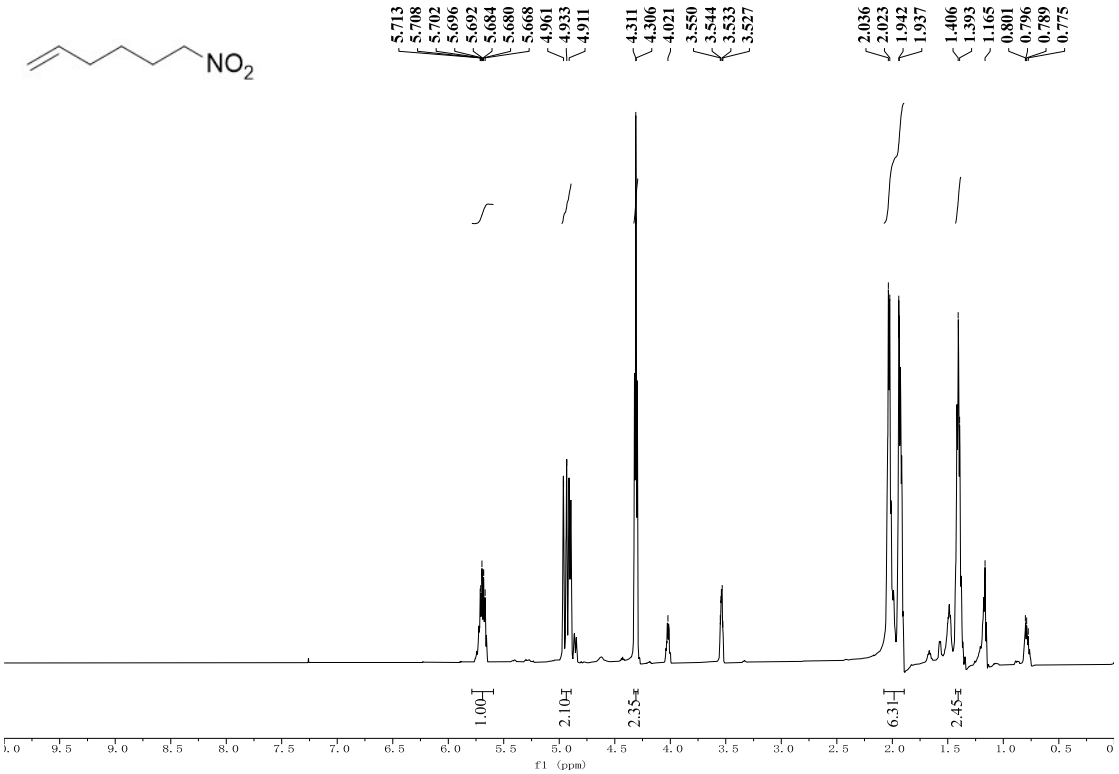

NO2
4.412
4.401
1.901
1.894
1.889
1.883
1.878
1.714
1.710
1.702
1.698
1.686
1.427
1.422
1.418
1.411
1.407
0.865
0.861
0.857
0.853
0.845
0.78
1.96
3.00
3.12
0.42
f1 (ppm)

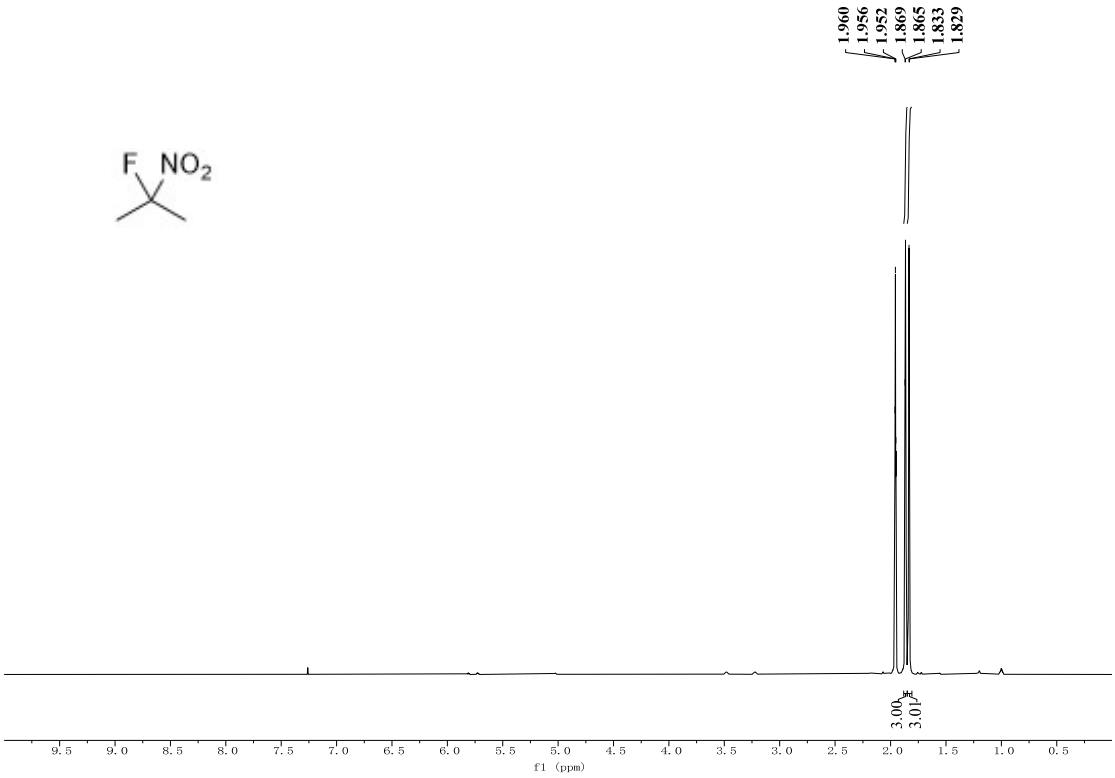

NO2
84.617
77.211
77.000
76.786
28.118
18.358
9.669
f1 (ppm)

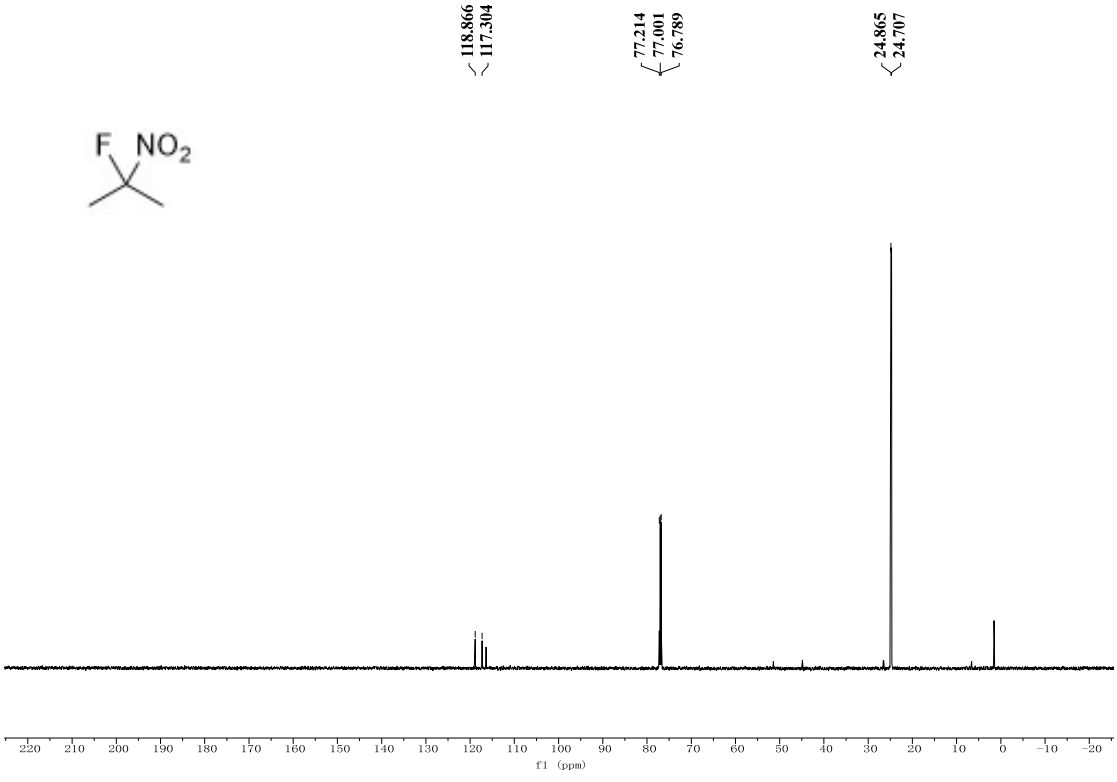

NO2
7.260
4.257
4.250
4.245
4.237
3.849
3.840
3.837
1.880
1.872
1.868
1.856
1.712
1.707 H2O
1.700
0.875
0.872
0.869
0.863
0.856
0.851
0.99
2.11
2.07
6.13
f1 (ppm)

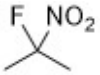

NO2
91.636
77.212
26.550
9.912
f1 (ppm)


7.465
7.452
7.446
7.439
7.436
5.434
1.458
1.296
0.916
0.908
0.905
0.898
0.891
0.882
Ph
NO2
5.05
2.00
f1 (ppm)

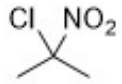

5.713
5.708
5.702
5.696
5.692
5.684
5.680
5.668
4.961
4.933
4.911
4.311
4.306
4.021
3.550
3.544
3.533
3.527
2.036
2.023
1.942
1.937
1.406
1.393
1.165
0.801
0.796
0.789
0.775
NO2
1.00
2.10
2.35
6.31
2.45
f1 (ppm)


1.960
1.956
1.952
1.869
1.865
1.833
1.829
F
NO2
3.00
3.01
f1 (ppm)

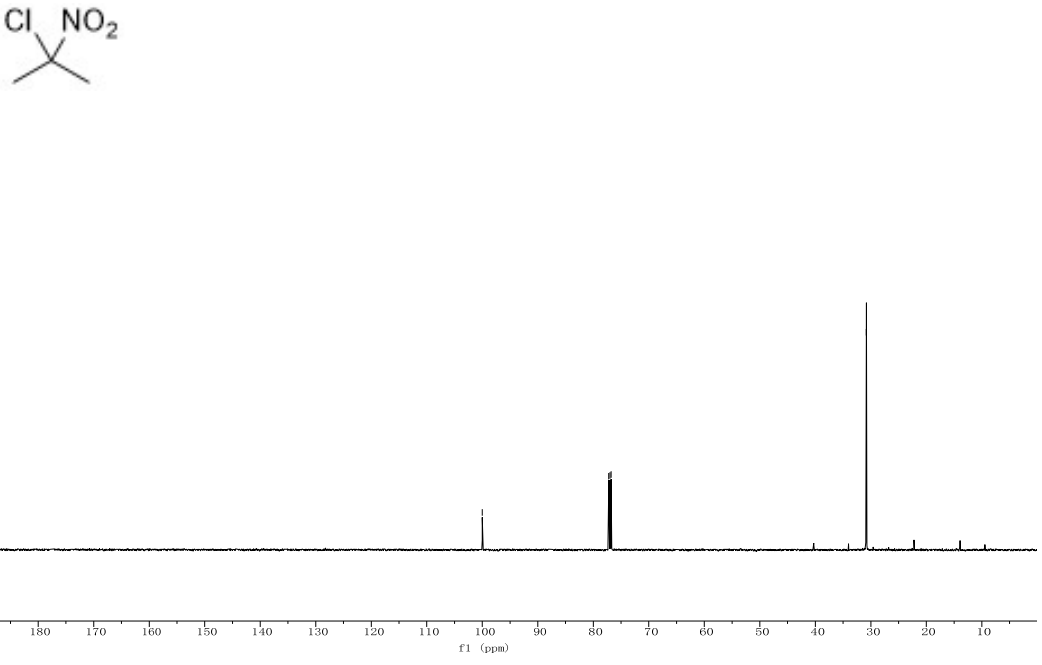

118.866
117.304
77.214
77.001
76.789
24.865
24.707
F
NO2
f1 (ppm)


F
NO2

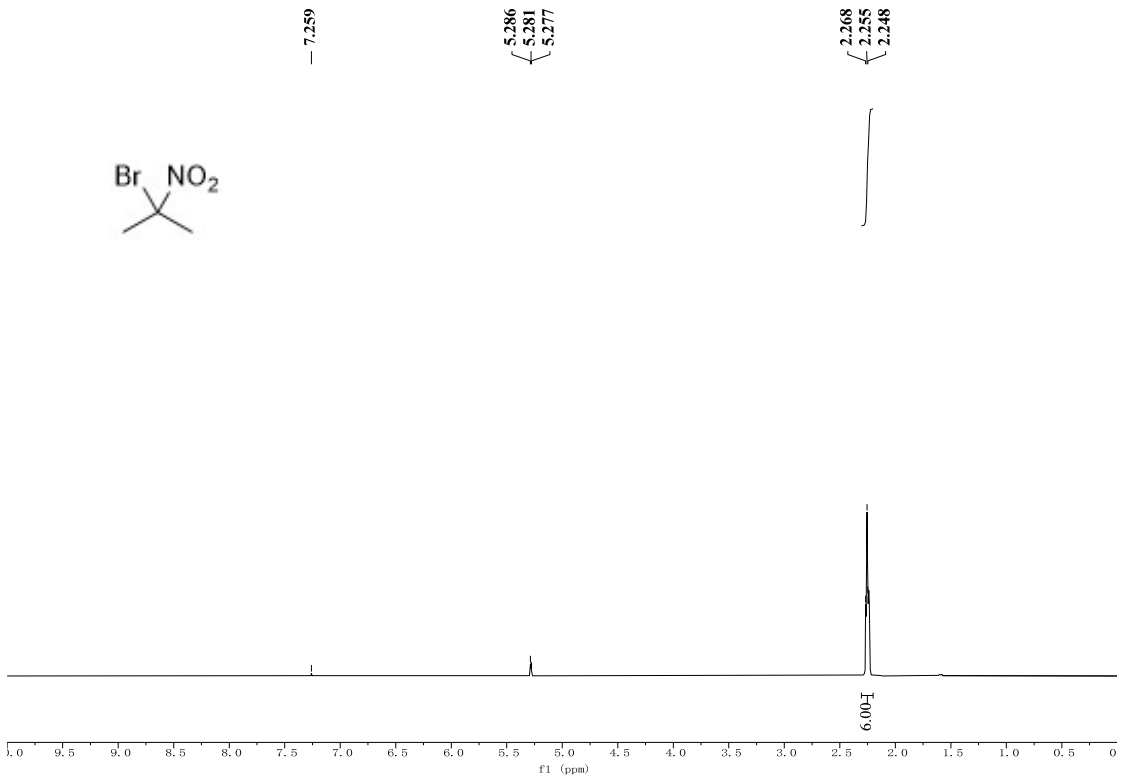
-111.958
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

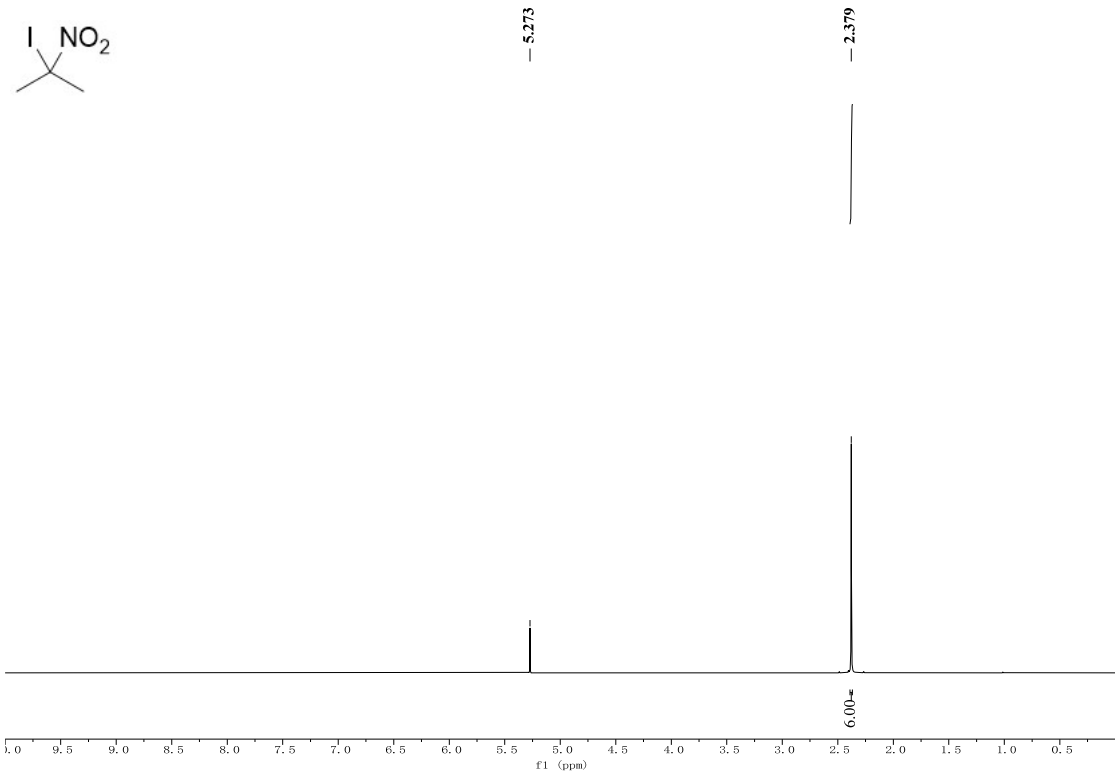

Cl
NO2

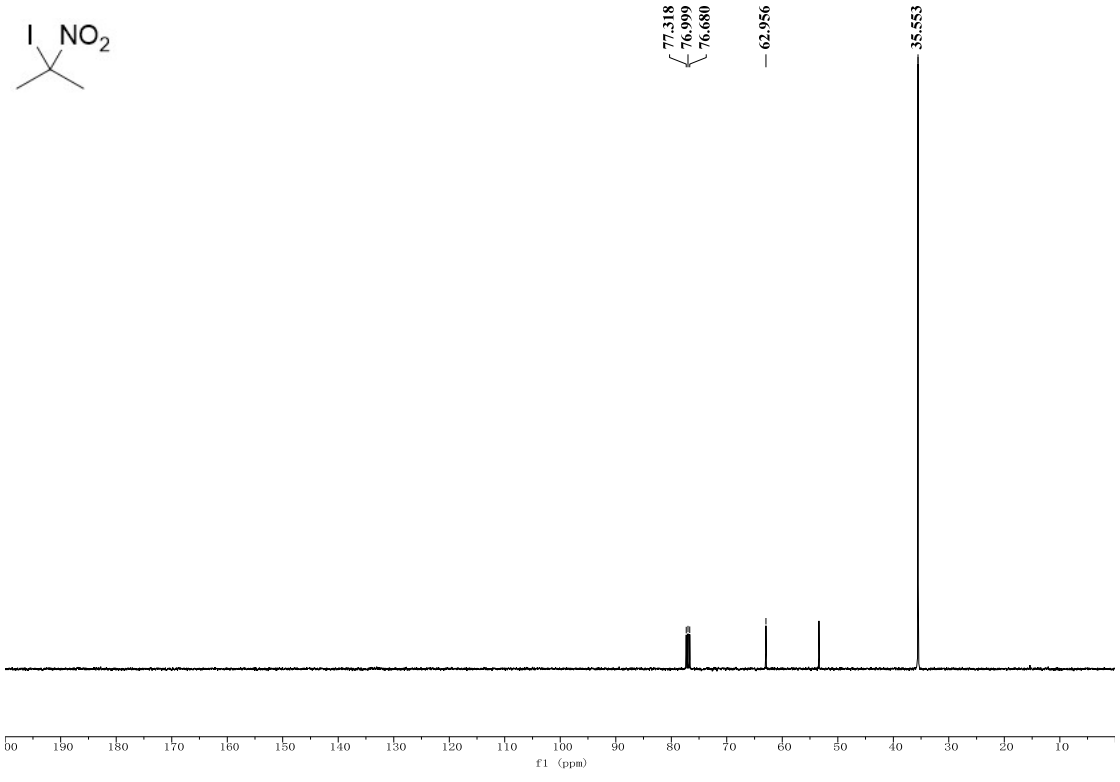
2.096
2.094
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

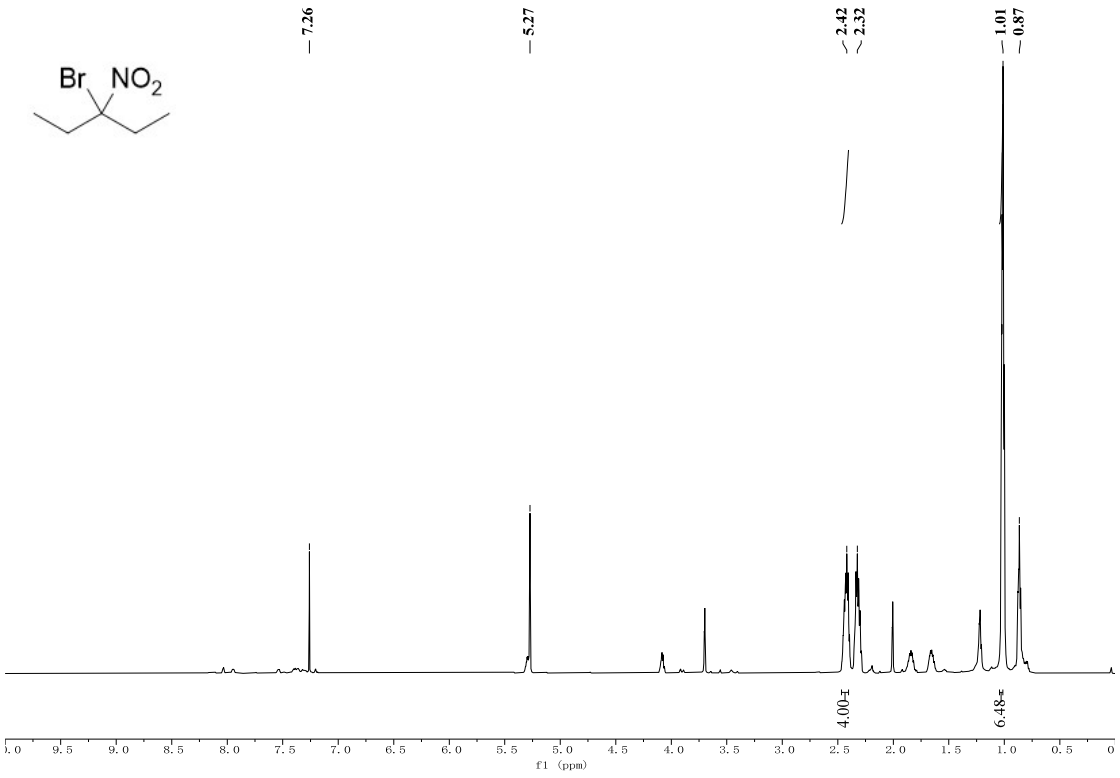

99.991
77.214
77.002
76.790
30.819
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

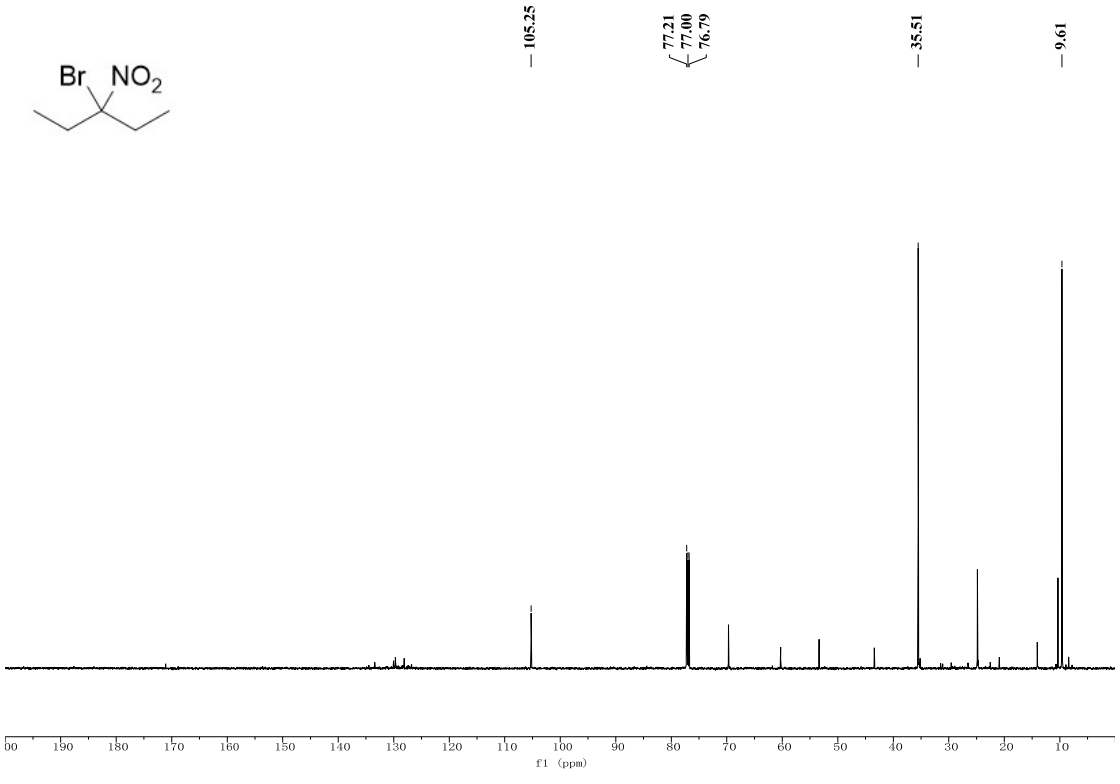
Cl
NO2

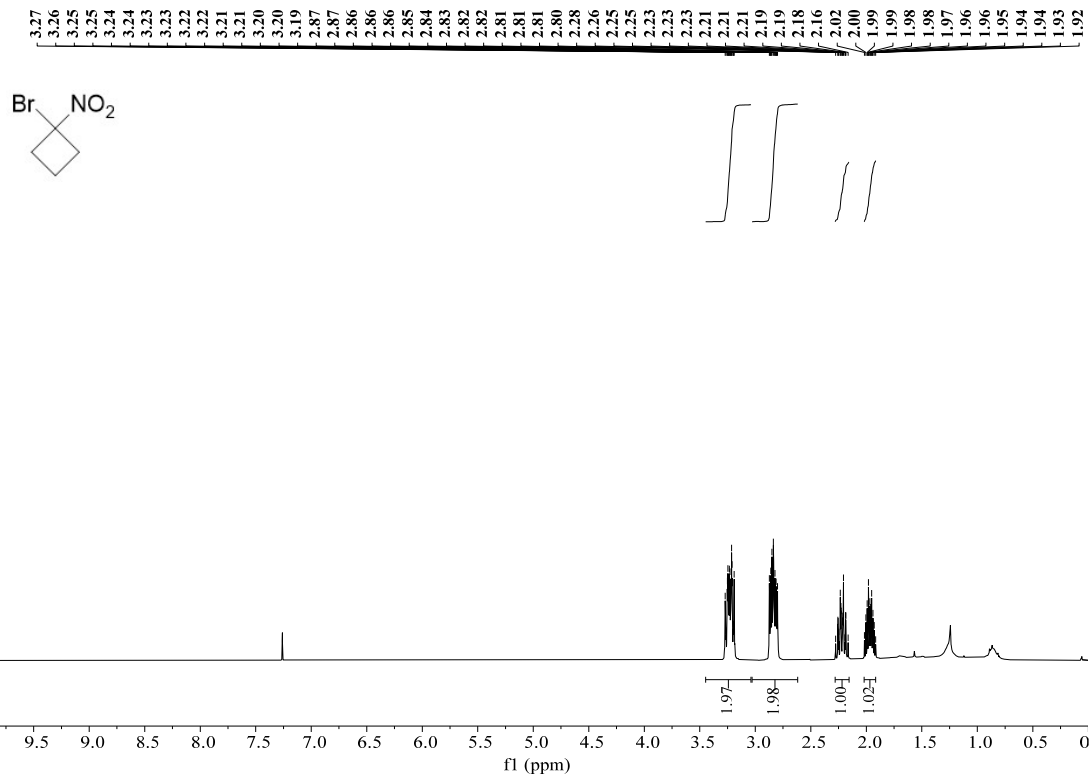

7.259
5.286
5.281
5.277
2.268
2.255
2.248
Br
NO2
6.00
f1 (ppm)

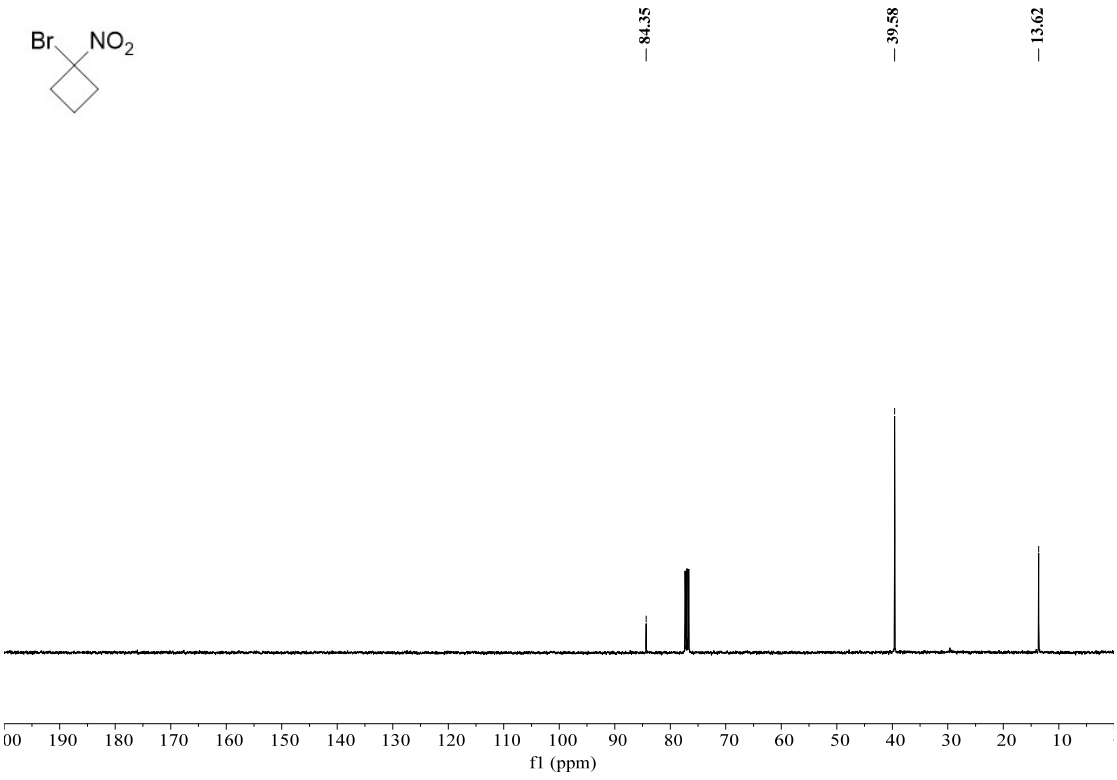

I
NO2
5.273
2.379
6.00
f1 (ppm)

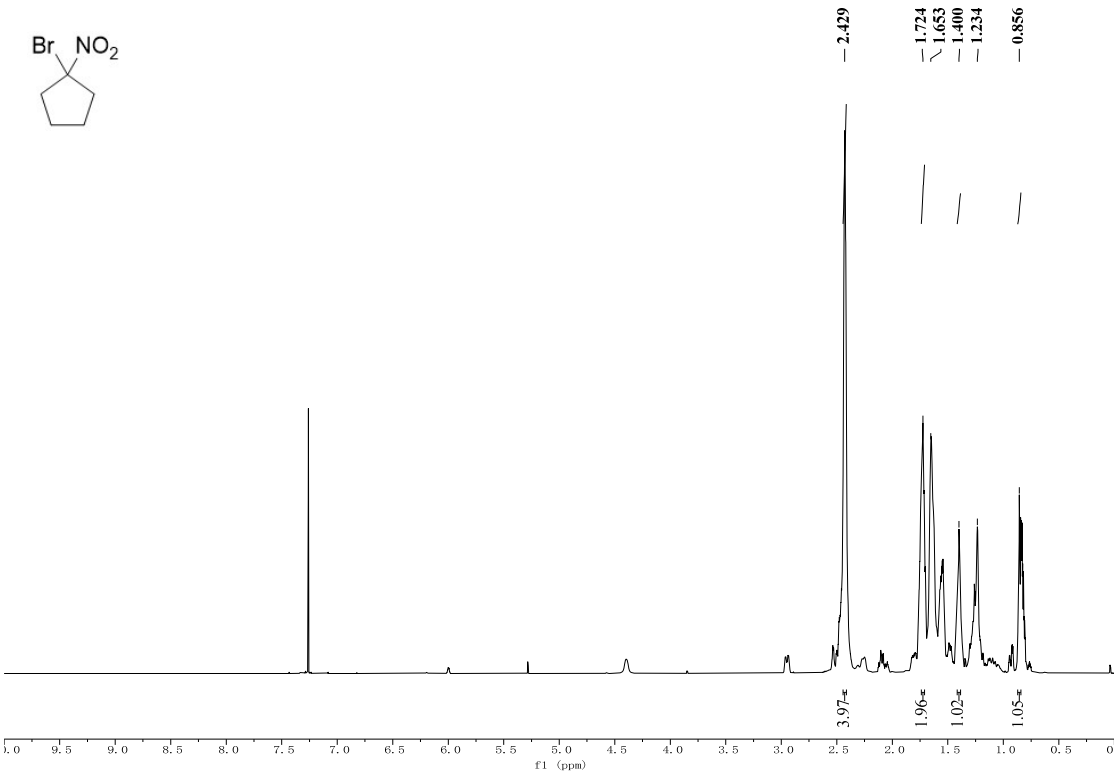

I
NO2
77.318
76.999
76.680
62.956
35.553
f1 (ppm)

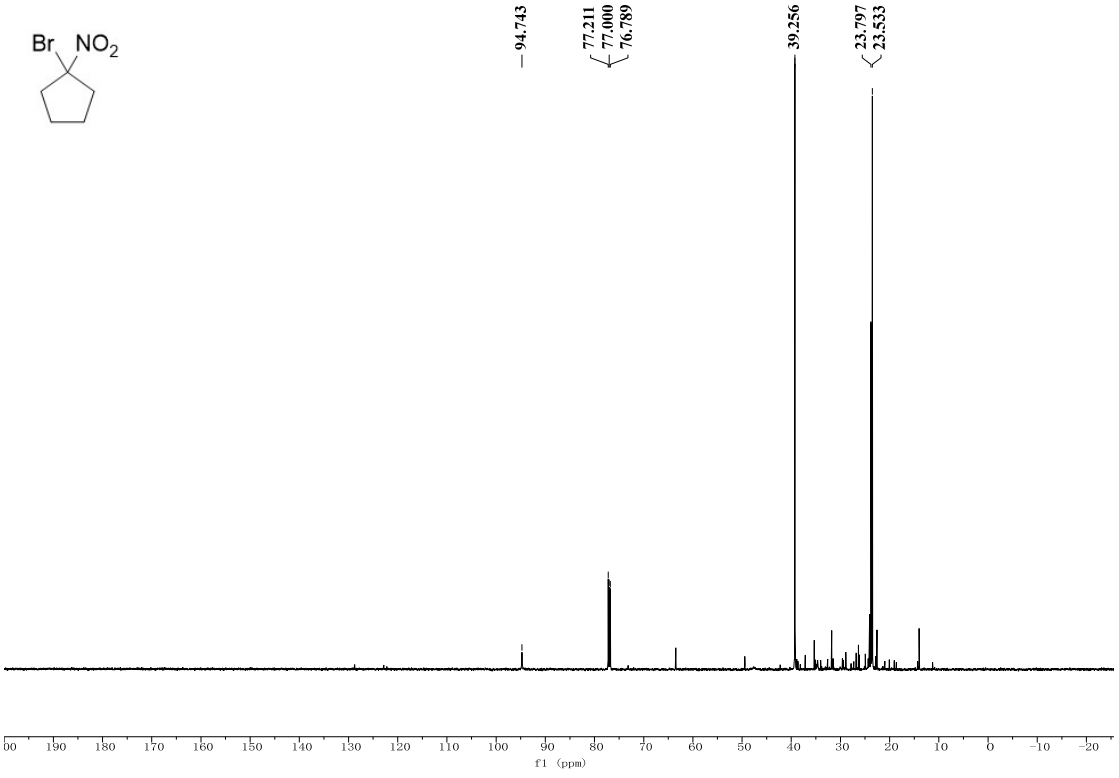

Br NO2
7.26
5.27
2.42
2.32
1.01
0.87
4.00
6.48
f1 (ppm)

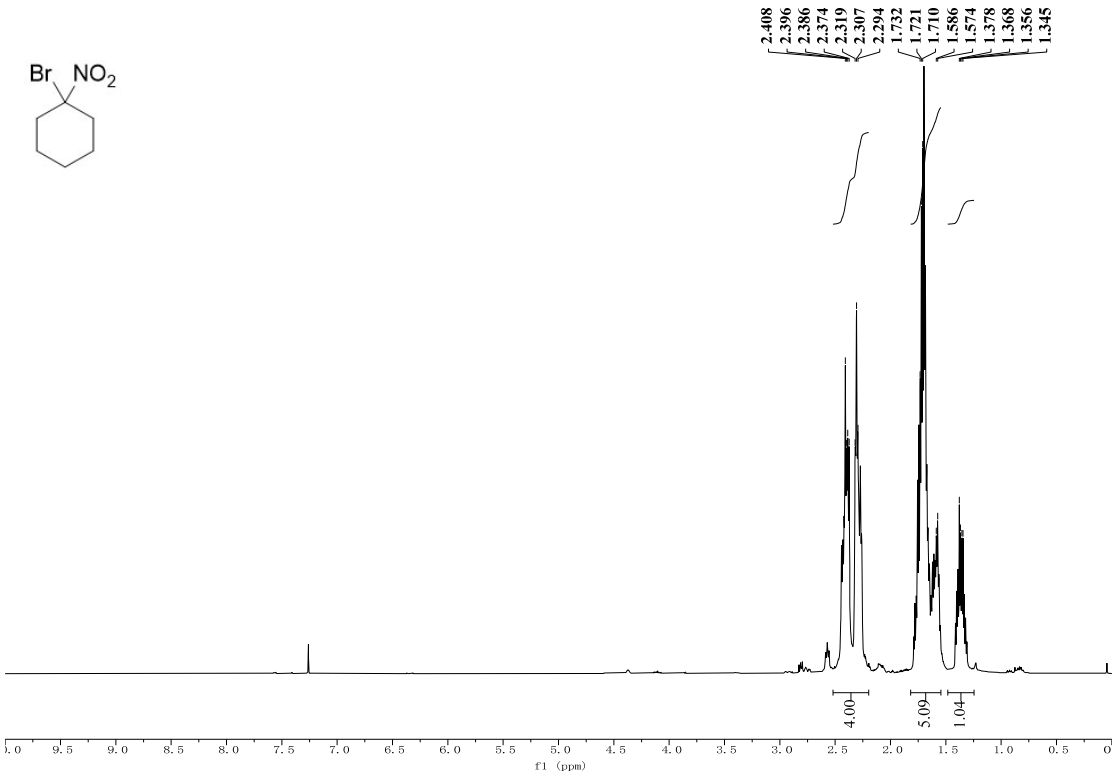

Br NO2
105.25
77.21
77.00
76.79
35.51
9.61
f1 (ppm)

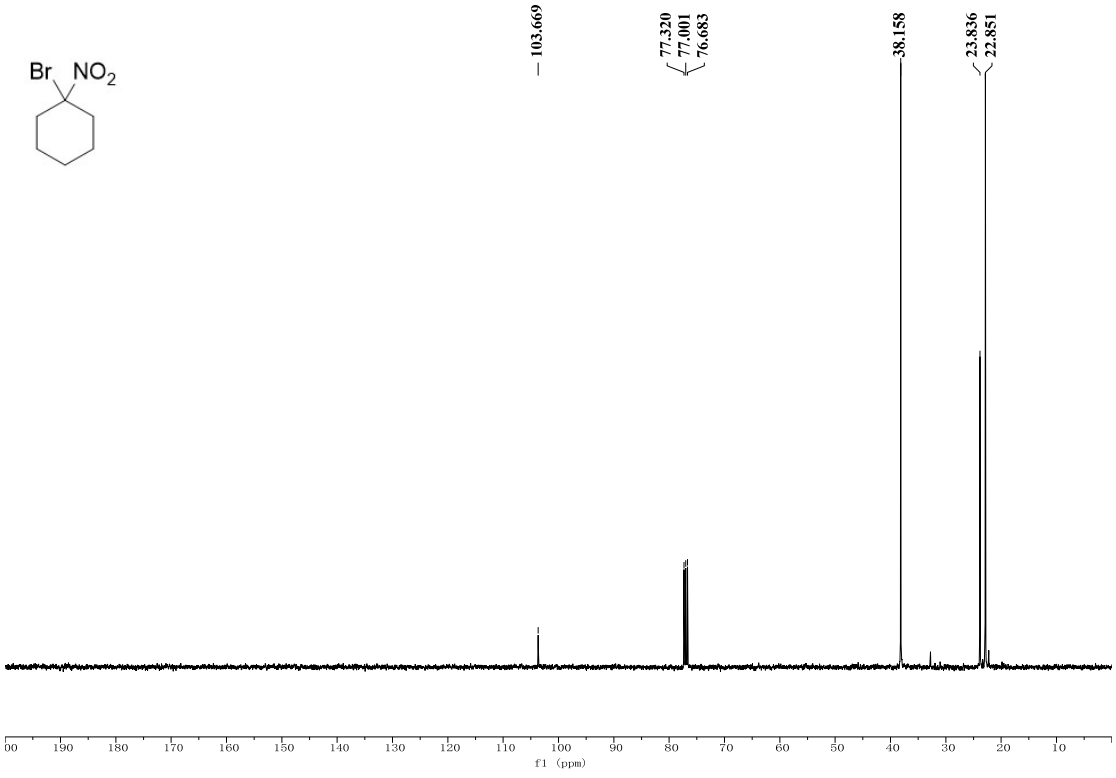

3.27 3.26 3.25 3.25 3.24 3.24 3.23 3.23 3.22 3.22 3.21 3.21 3.20 3.20 3.19 2.87 2.87 2.86 2.86 2.86 2.85 2.84 2.83 2.82 2.82 2.81 2.81 2.81 2.80 2.28 2.26 2.25 2.25 2.23 2.23 2.21 2.21 2.19 2.19 2.18 2.16 2.02 2.00 1.99 1.99 1.98 1.98 1.97 1.96 1.96 1.95 1.94 1.94 1.93 1.92
Br
NO2
1.97
1.98
1.00
1.02
f1 (ppm)

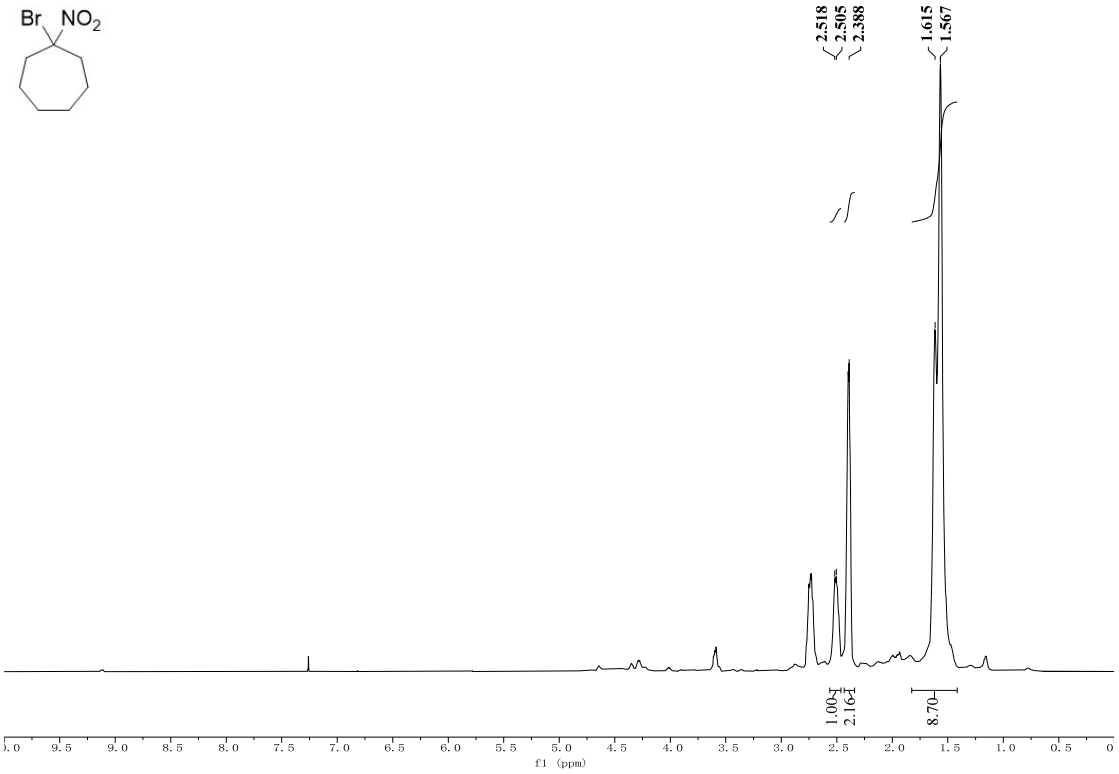

Br
NO2
84.35
39.58
13.62
f1 (ppm)

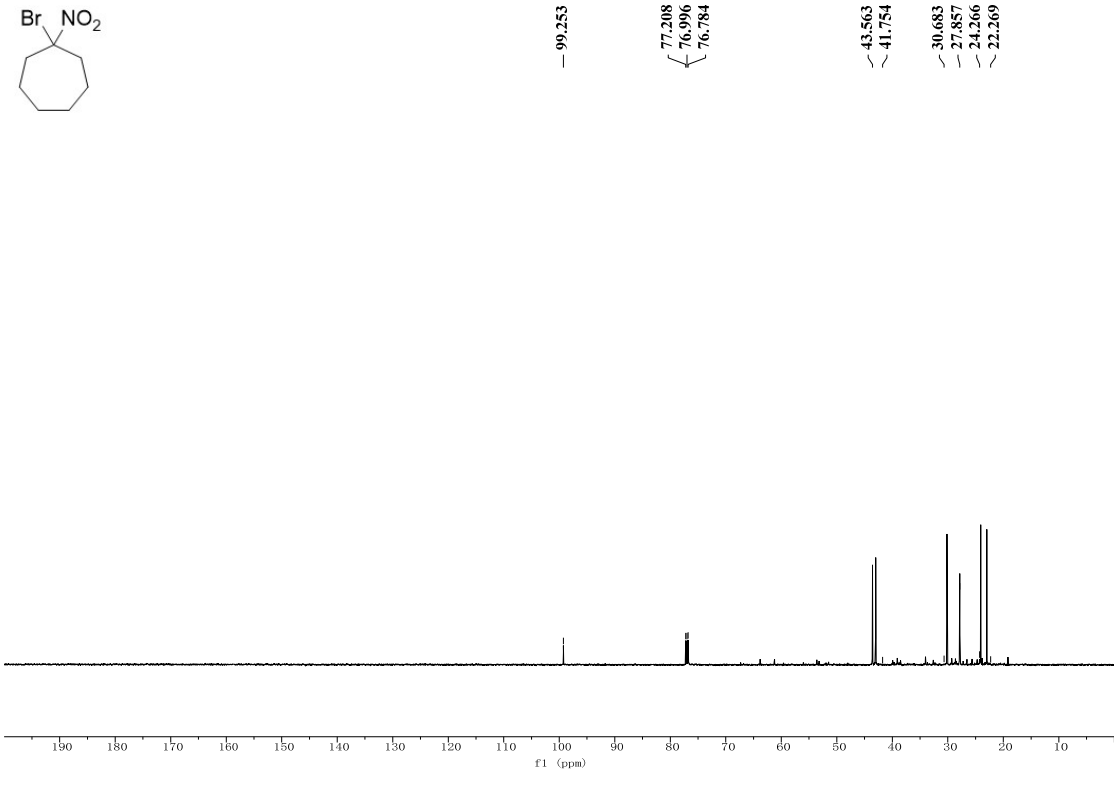

Br
NO2
2.429
1.724
1.653
1.400
1.234
0.856
3.97
1.96
1.02
1.05
f1 (ppm)

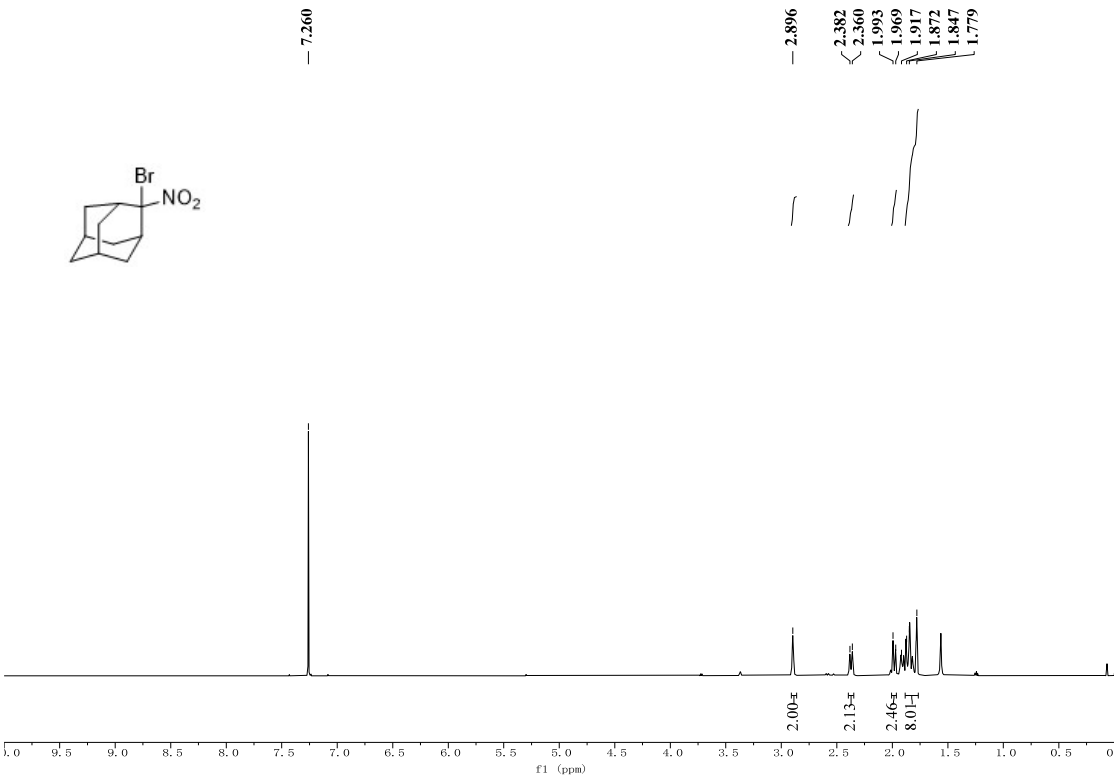

Br
NO2
94.743
77.211
77.000
76.789
39.256
23.797
23.533
f1 (ppm)

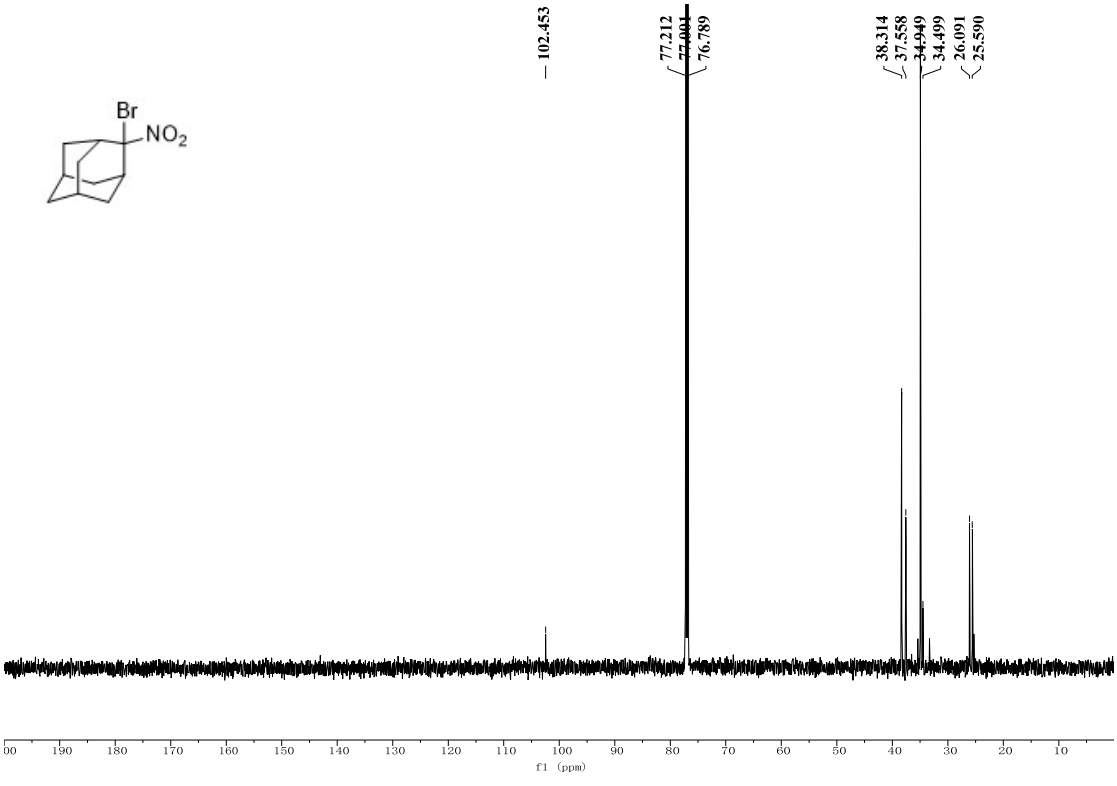

Br NO2
2.408
2.396
2.386
2.374
2.319
2.307
2.294
1.732
1.721
1.710
1.586
1.574
1.378
1.368
1.356
1.345
4.00
5.09
1.04
f1 (ppm)

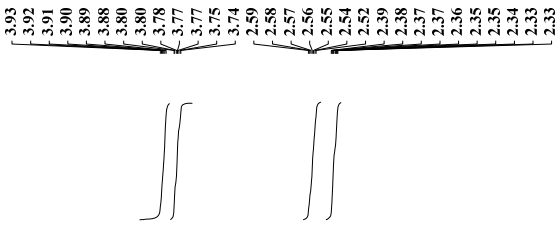

Br NO2
103.669
77.320
77.001
76.683
38.158
23.836
22.851
f1 (ppm)


Br
NO2
2.518
2.505
2.388
1.615
1.567
1.00
2.16
8.70
f1 (ppm)


Br
NO2
99.253
77.208
76.996
76.784
43.563
41.754
30.683
27.857
24.266
22.269
f1 (ppm)


7.260
2.896
2.382
2.360
1.993
1.969
1.917
1.872
1.847
1.779
Br
NO2
2.00
2.13
2.46
8.01
f1 (ppm)


102.453
77.212
77.004
76.789
38.314
37.558
34.949
34.499
26.091
25.590
Br
NO2
f1 (ppm)


3.93
3.92
3.91
3.90
3.89
3.88
3.80
3.80
3.78
3.77
3.77
3.75
3.74
2.59
2.58
2.57
2.56
2.55
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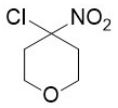
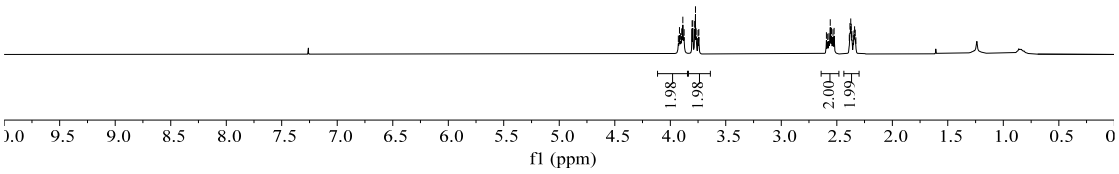
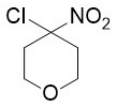
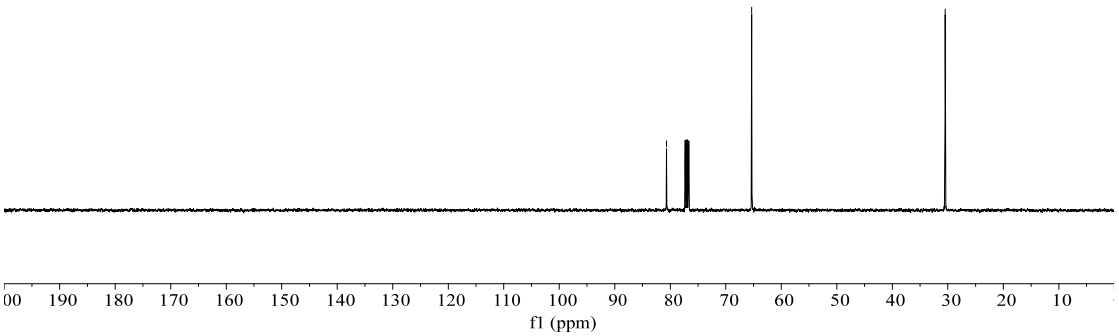
2.36
2.35
2.35
2.34
2.33
2.33

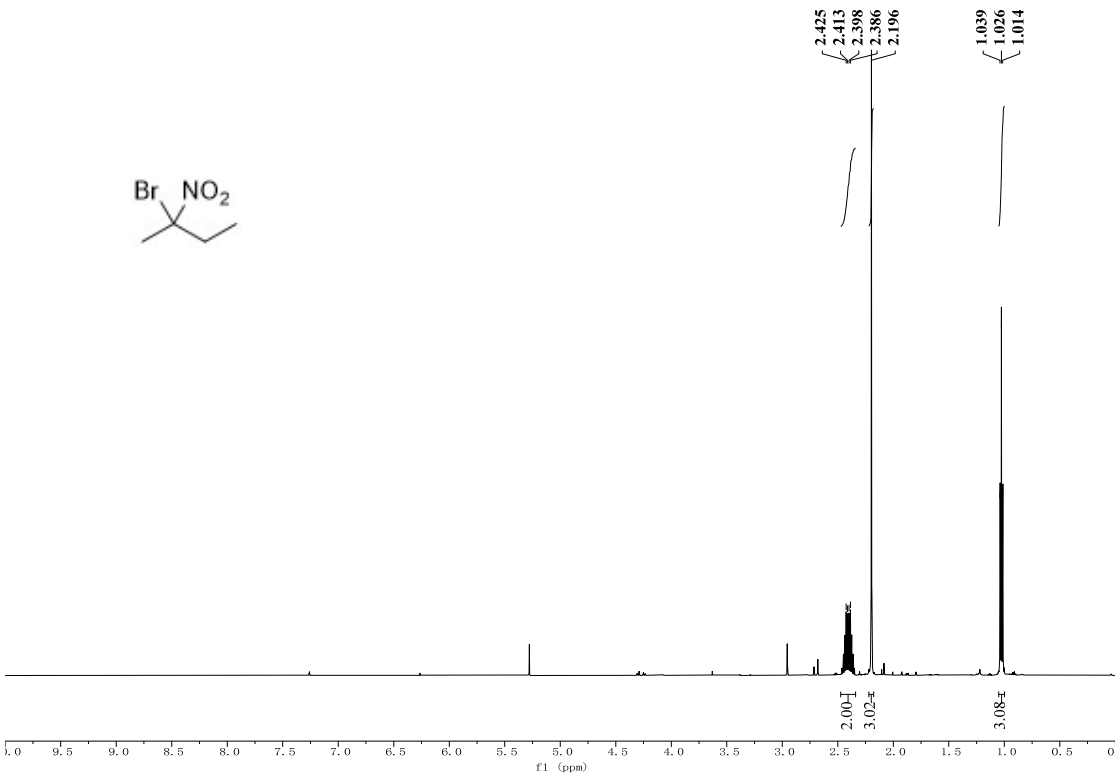

Cl
NO2
O

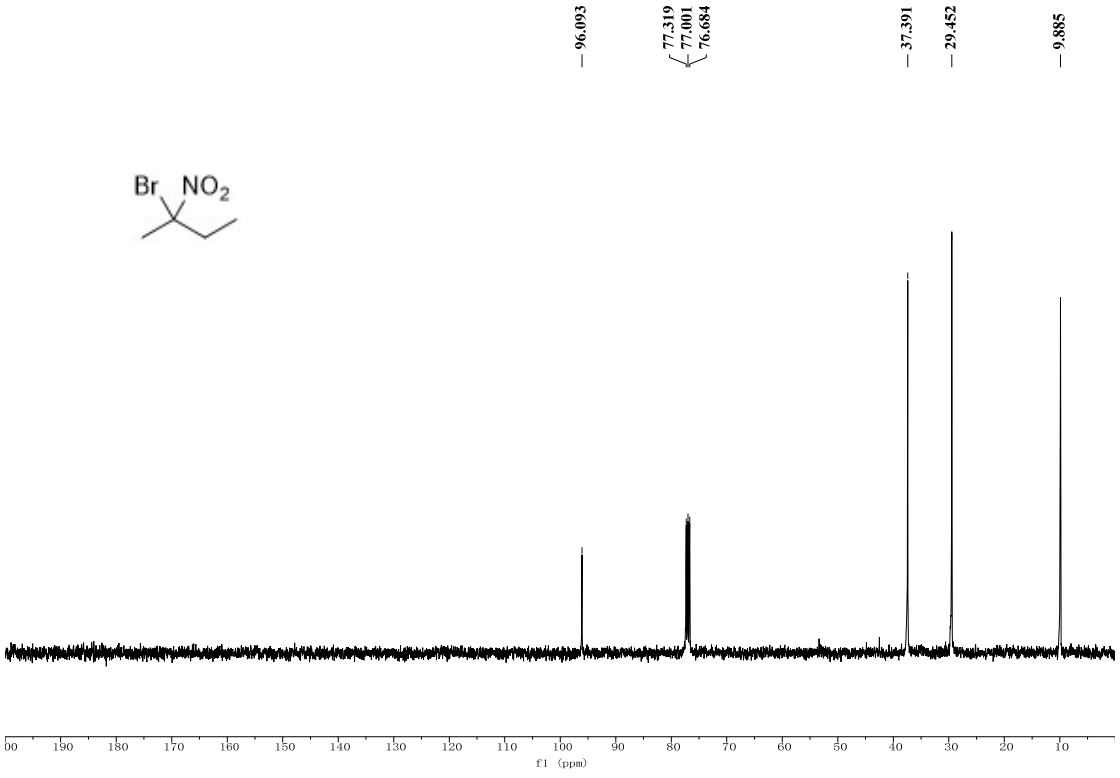

1.98
1.98
2.00
1.99
f1 (ppm)

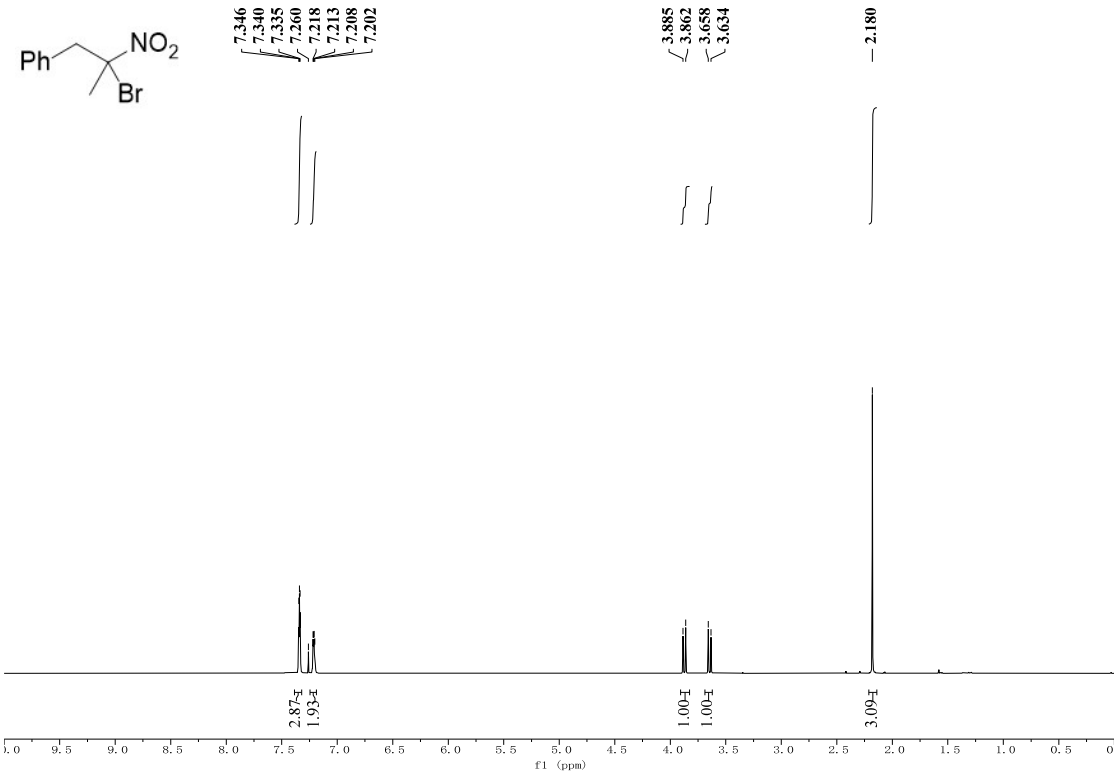

80.67
65.34
30.48


Cl
NO2
O


f1 (ppm)


Br
NO2
2.425
2.413
2.398
2.386
2.196
1.039
1.026
1.014
2.00
3.02
3.08
f1 (ppm)


Br
NO2
96.093
77.319
77.001
76.684
37.391
29.452
9.885
f1 (ppm)


Ph
NO2
Br
7.346
7.340
7.335
7.260
7.218
7.213
7.208
7.202
3.885
3.862
3.658
3.634
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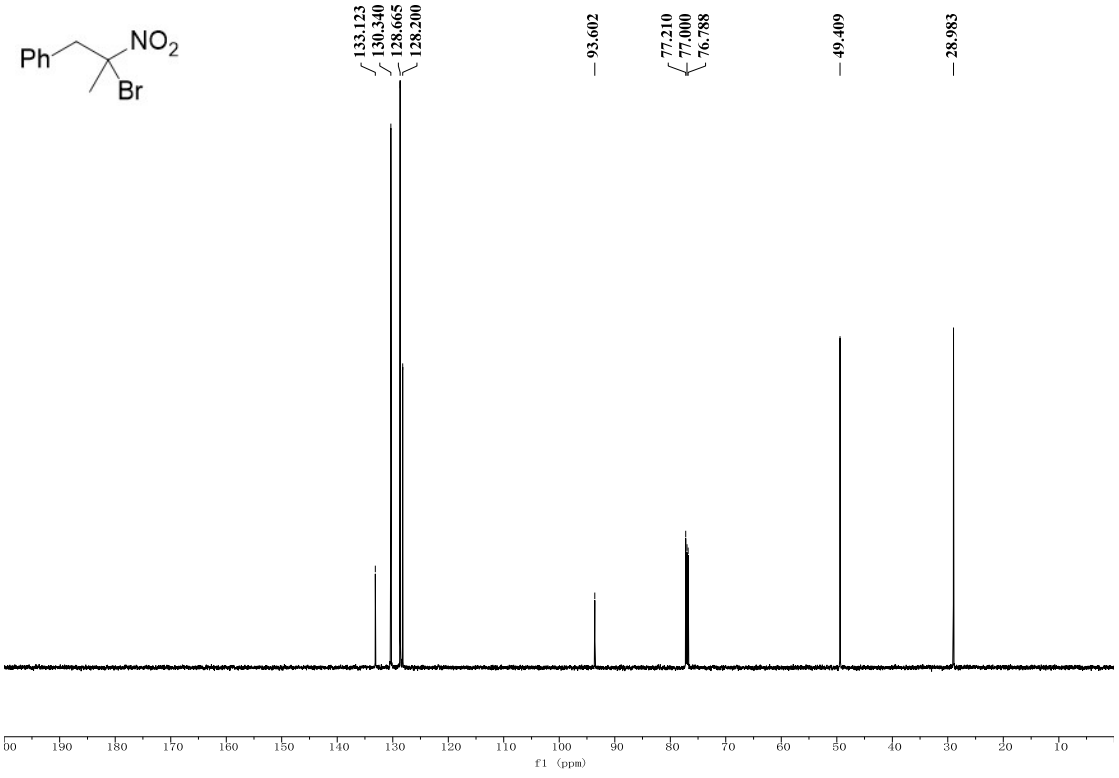
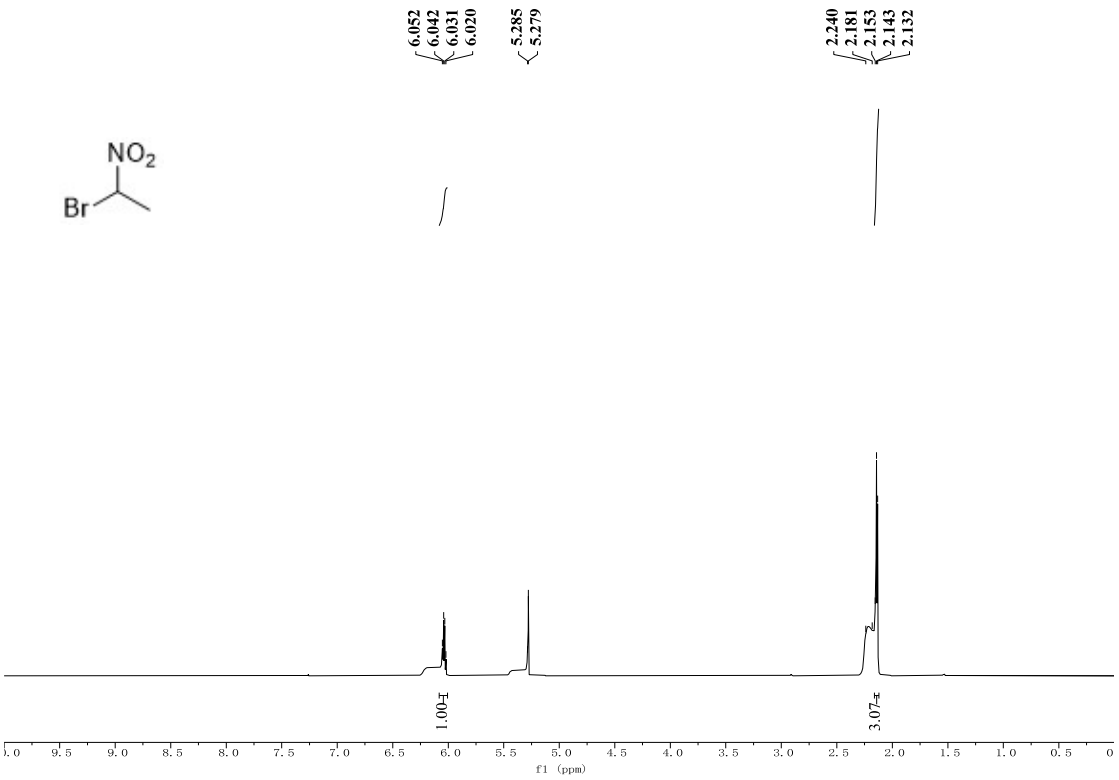
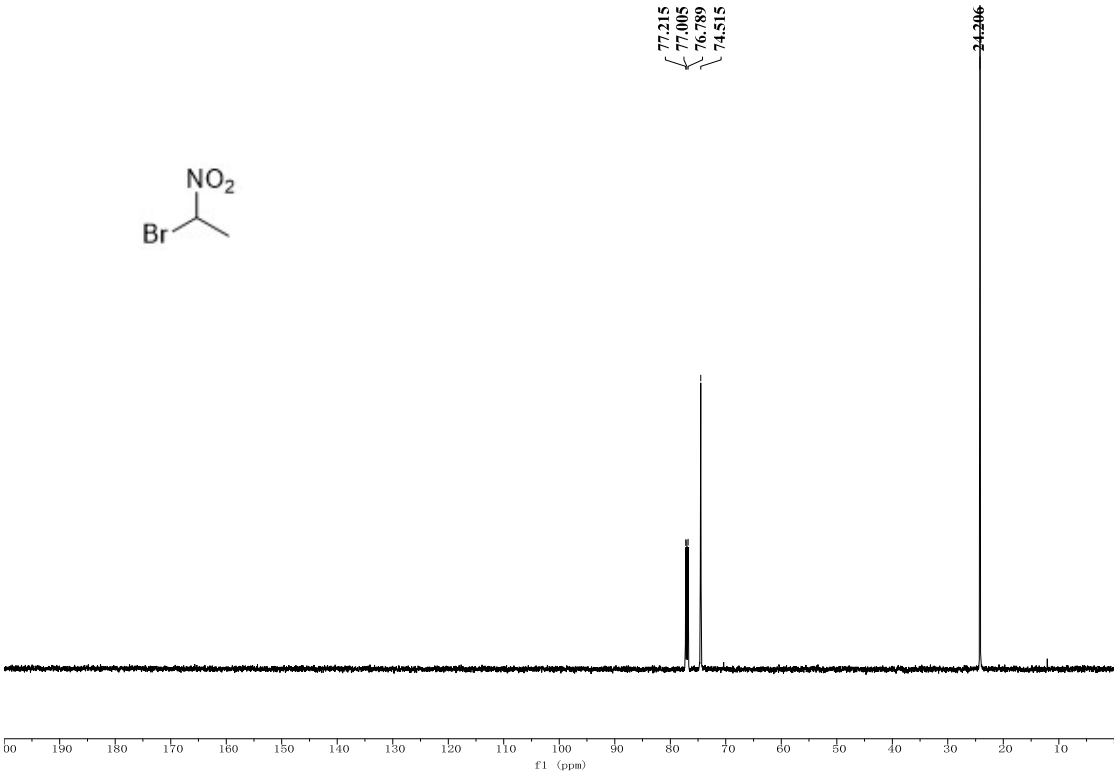
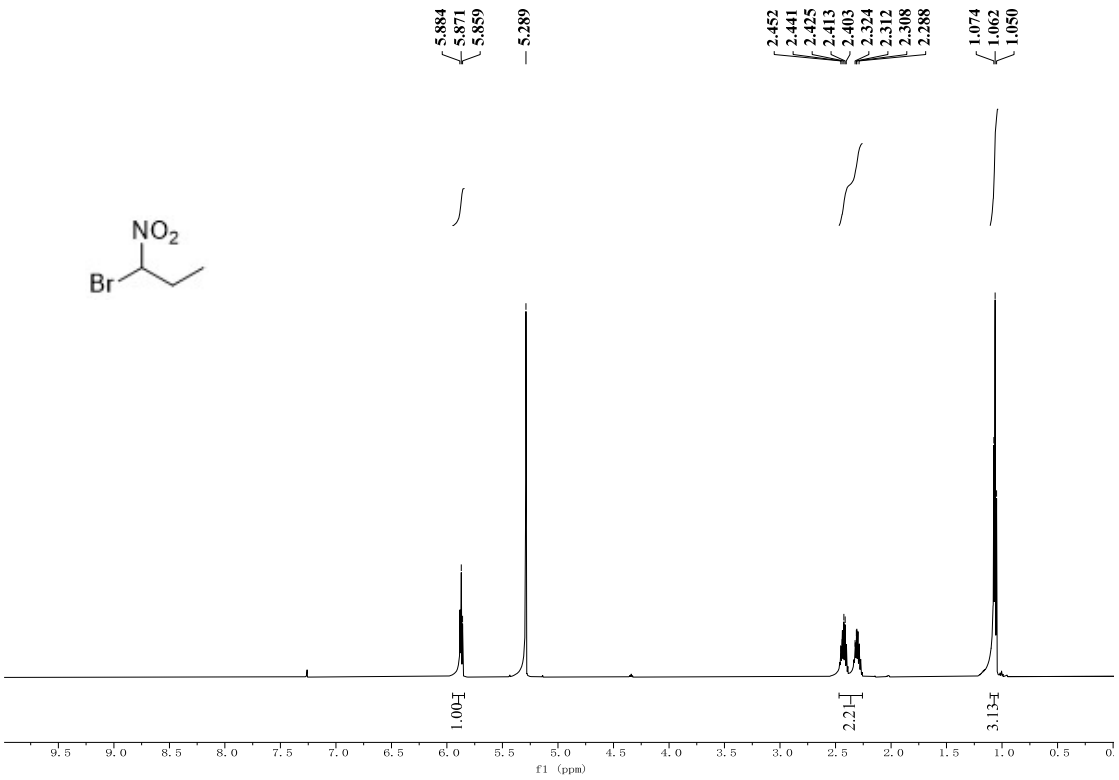
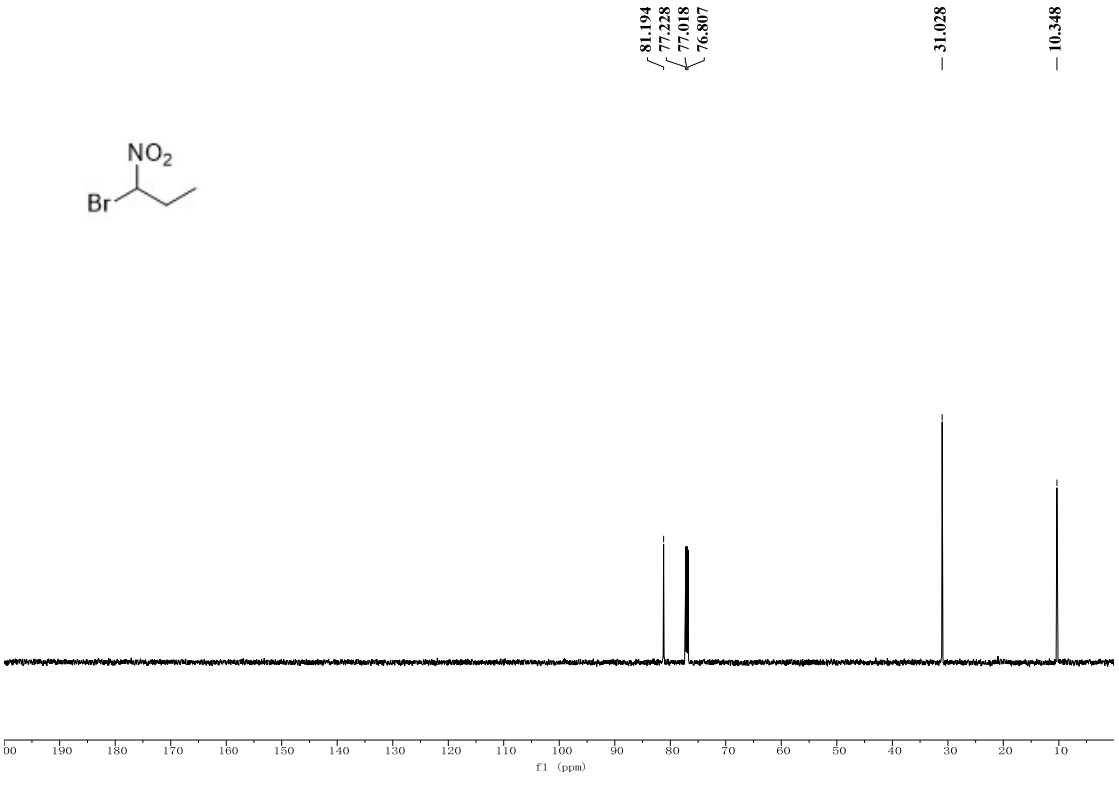
2.87
1.93
1.00
1.00
3.09
f1 (ppm)

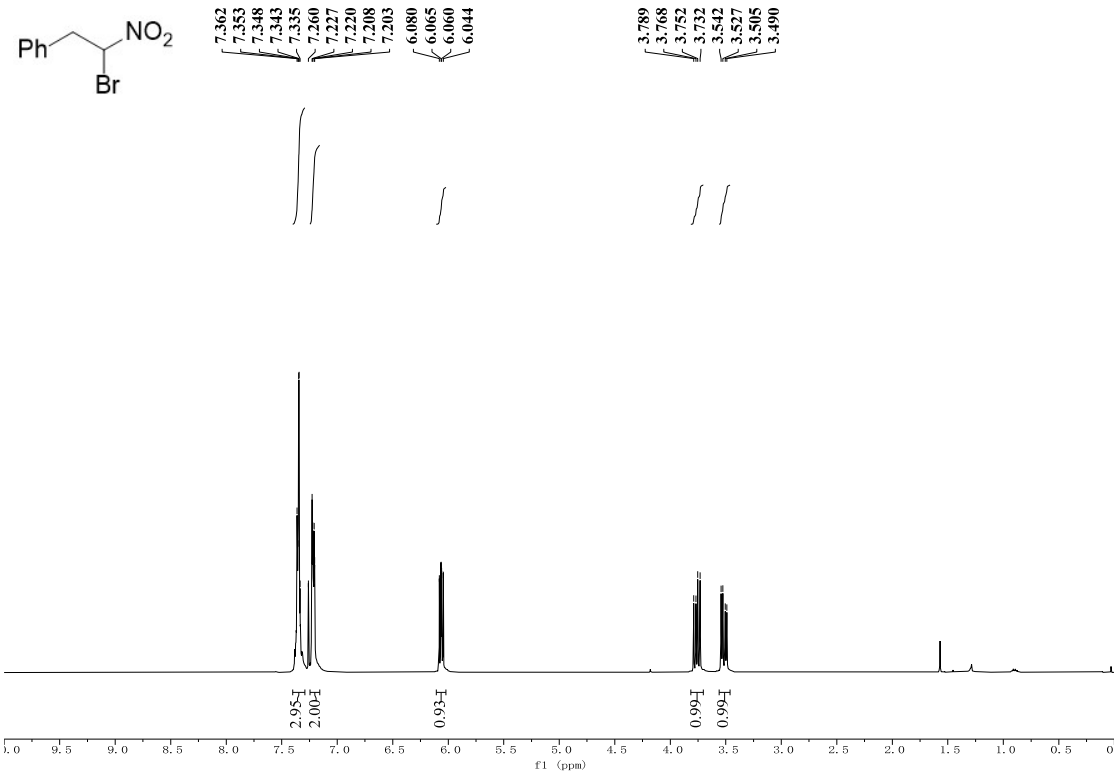

Ph
NO2
Br
133.123
130.340
128.665
128.200
93.602
77.210
77.000
76.788
49.409
28.983
f1 (ppm)

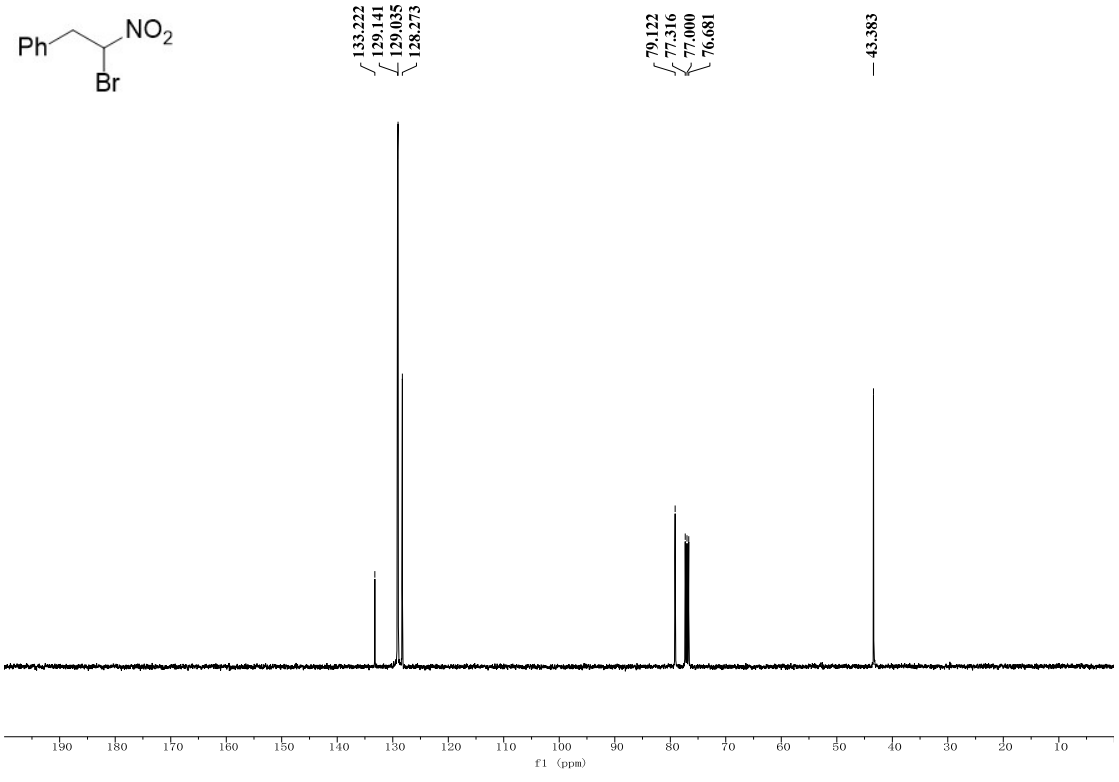

6.052
6.042
6.031
6.020
5.285
5.279
2.240
2.181
2.153
2.143
2.132
NO2
Br
1.00
3.07
f1 (ppm)

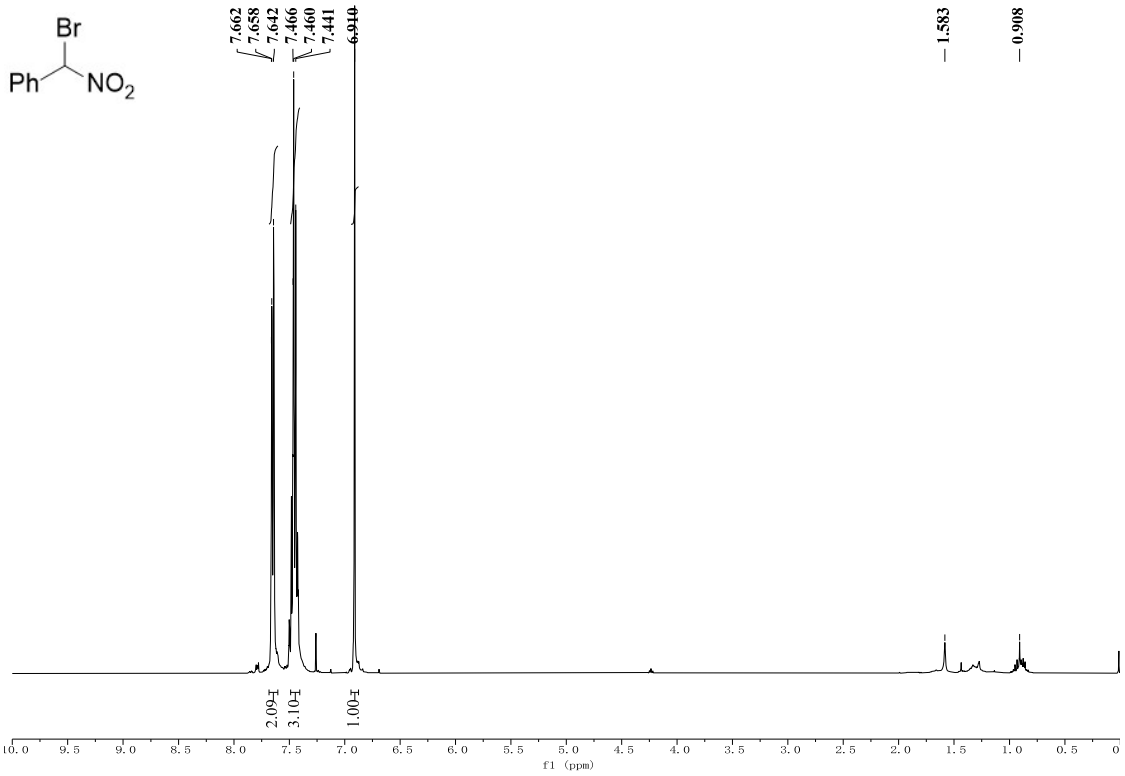

77.215
77.005
76.789
74.515
24.206
NO2
Br
f1 (ppm)

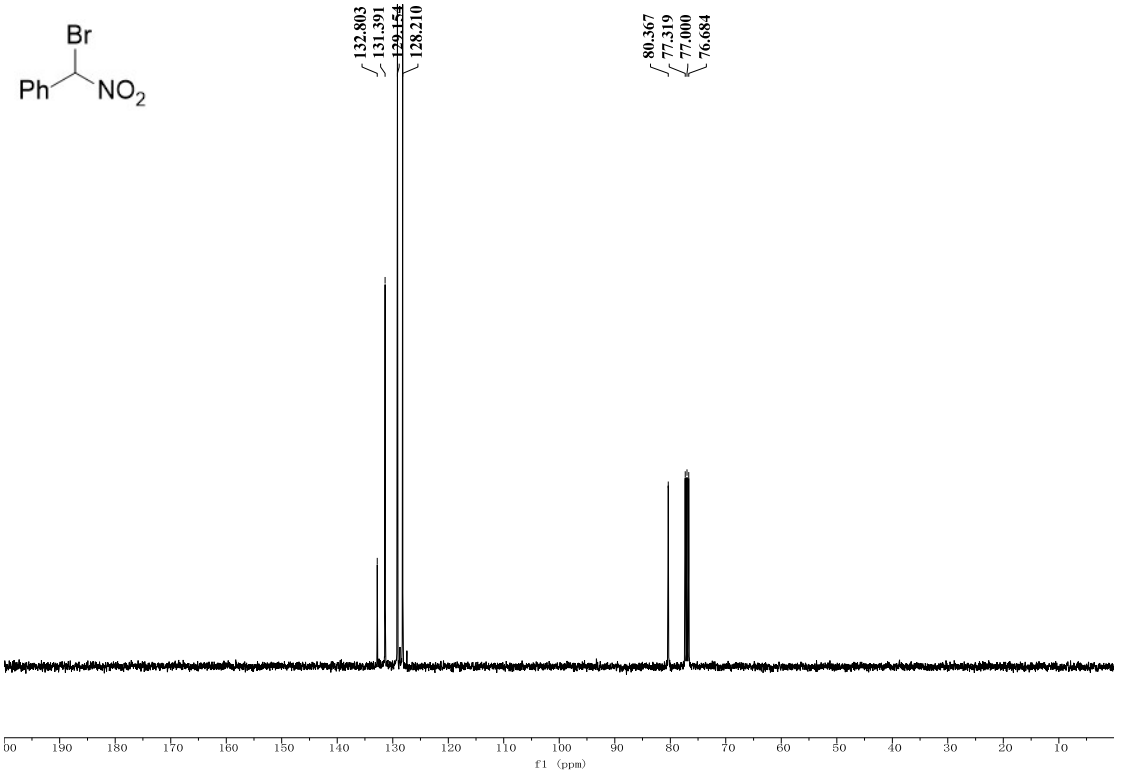

5.884
5.871
5.859
5.289
2.452
2.441
2.425
2.413
2.403
2.324
2.312
2.308
2.288
1.074
1.062
1.050
NO2
Br
1.00
2.21
3.13
f1 (ppm)

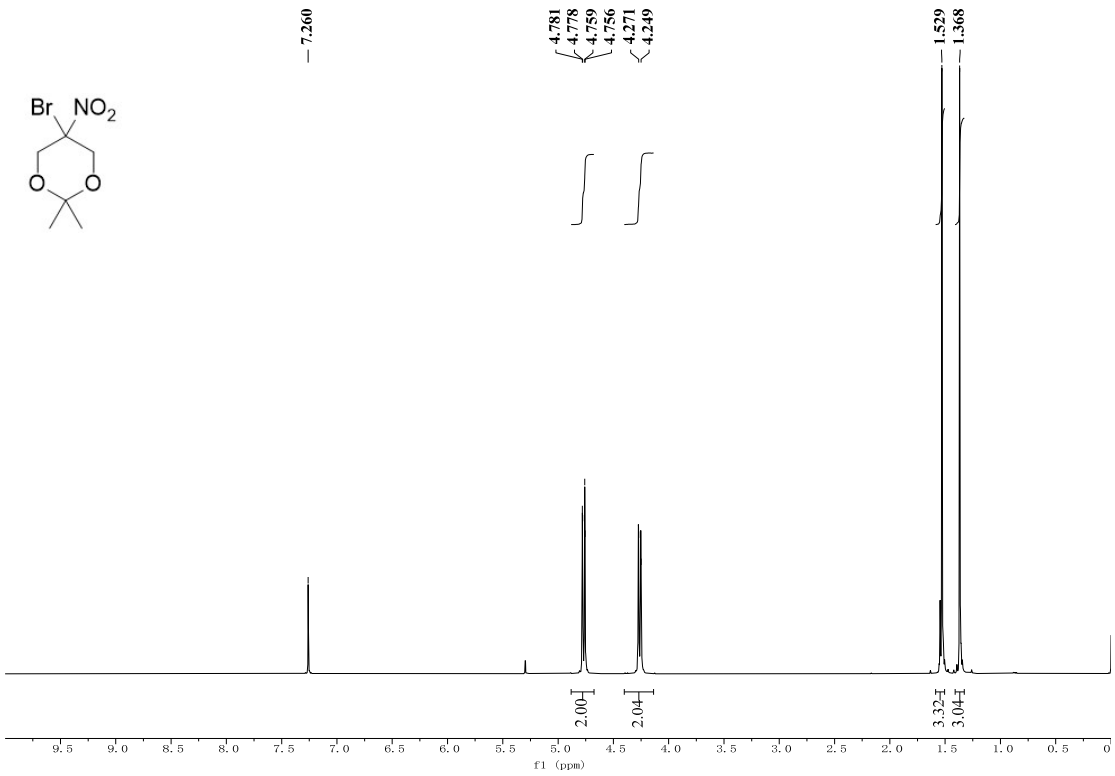

81.194
77.228
77.018
76.807
31.028
10.348
NO2
Br
f1 (ppm)

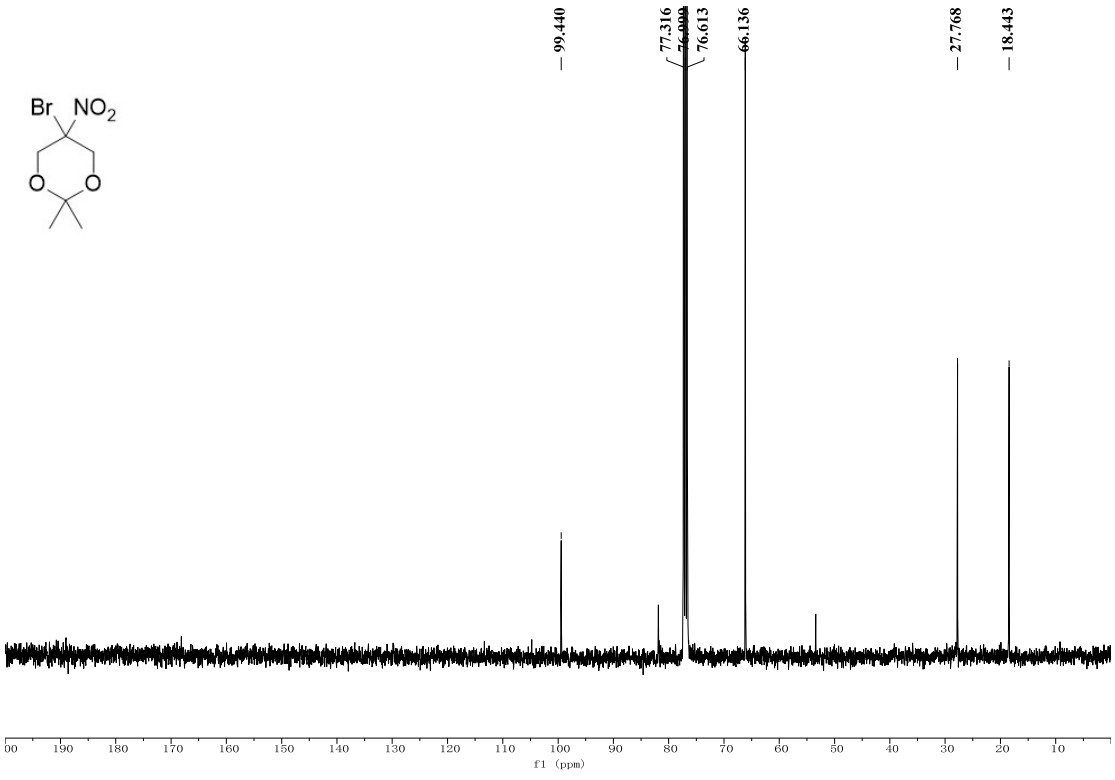

Ph
NO2
Br
7.362
7.353
7.348
7.343
7.335
7.260
7.227
7.220
7.208
7.203
6.080
6.065
6.060
6.044
3.789
3.768
3.752
3.732
3.542
3.527
3.505
3.490
2.95
2.00
0.93
0.99
0.99
f1 (ppm)

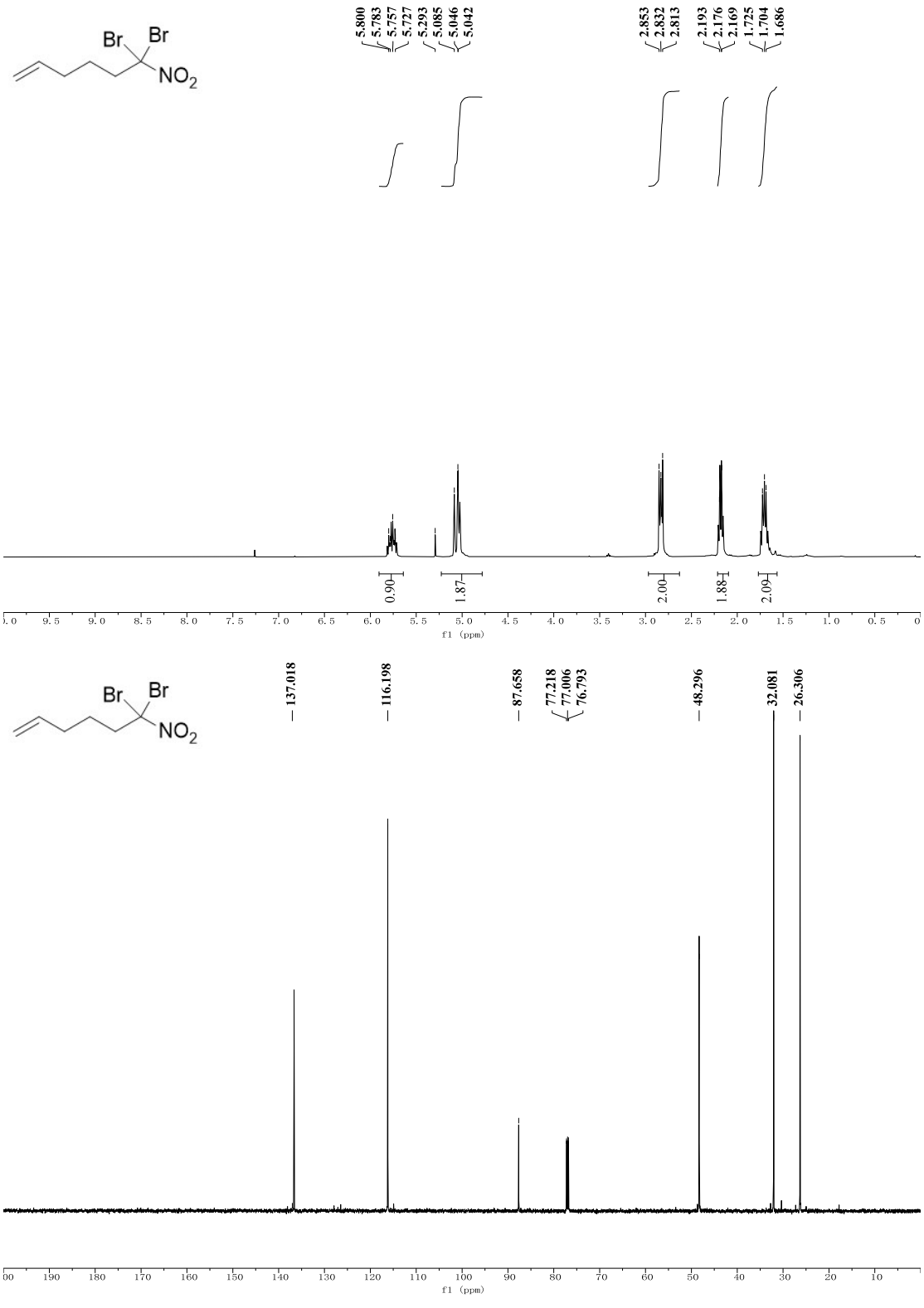

Ph
NO2
Br
133.222
129.141
129.035
128.273
79.122
77.316
77.000
76.681
43.383
f1 (ppm)

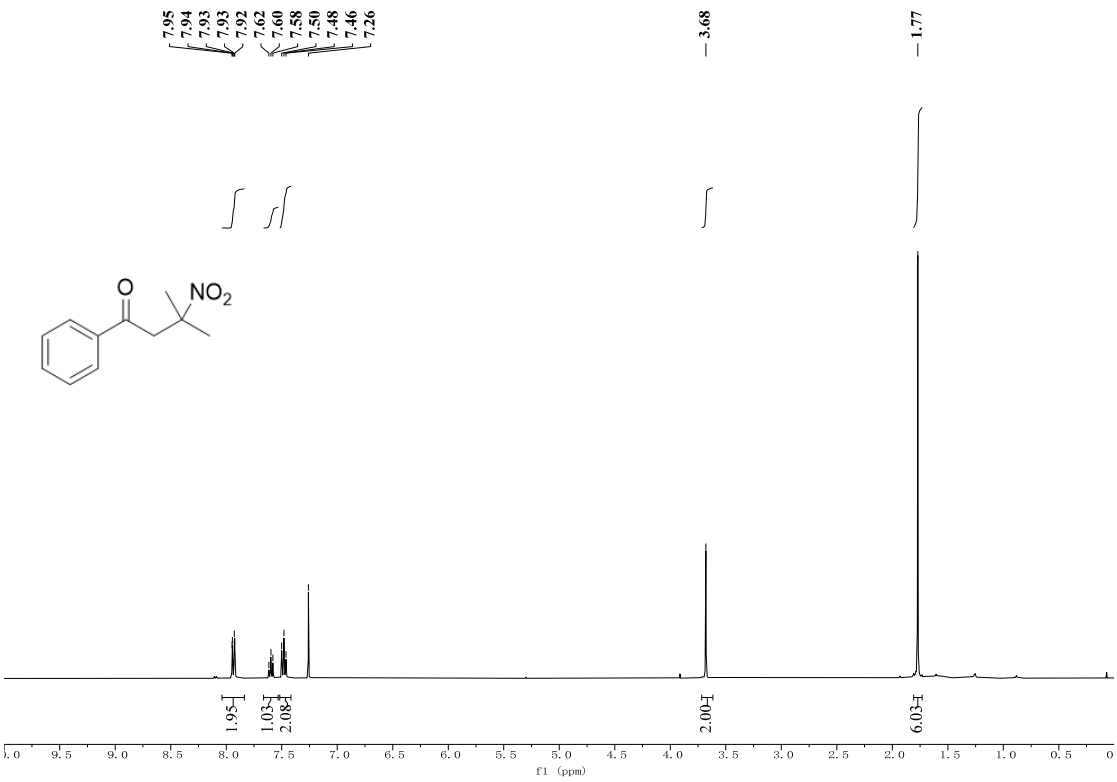

Br
Ph
NO2
7.662
7.658
7.642
7.466
7.460
7.441
6.910
1.583
0.908
2.09
3.10
1.00
f1 (ppm)

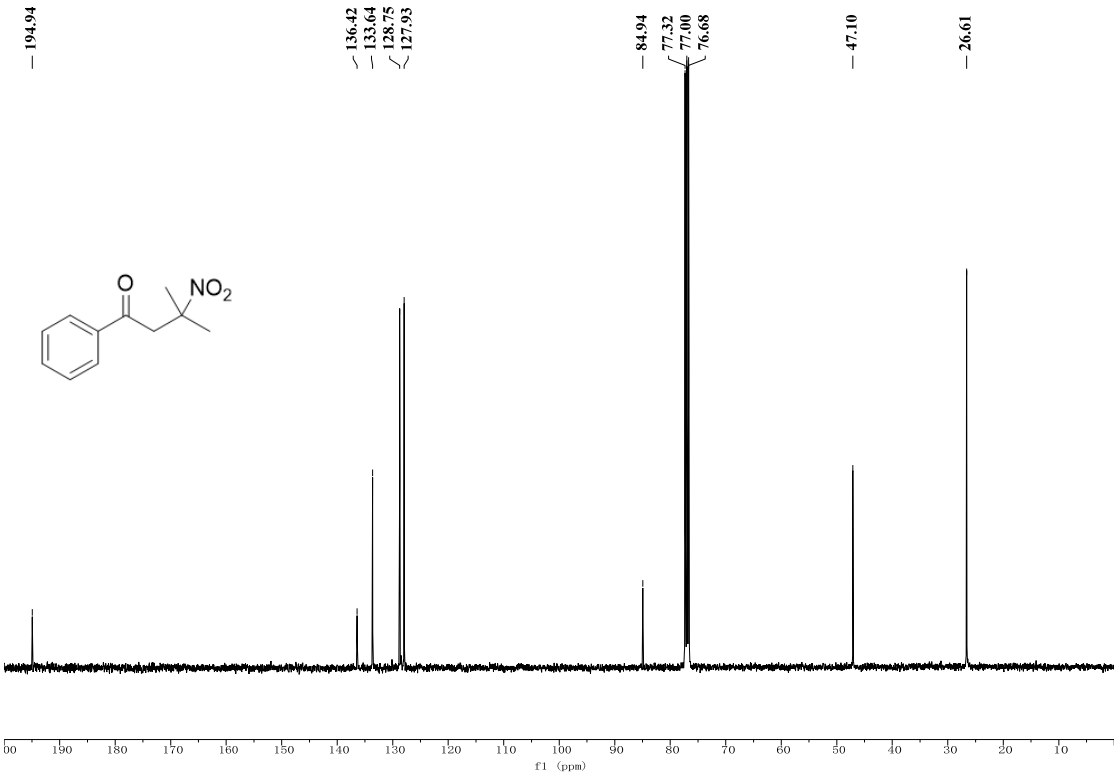

Br
Ph
NO2
132.803
131.391
129.154
128.210
80.367
77.319
77.000
76.684
f1 (ppm)

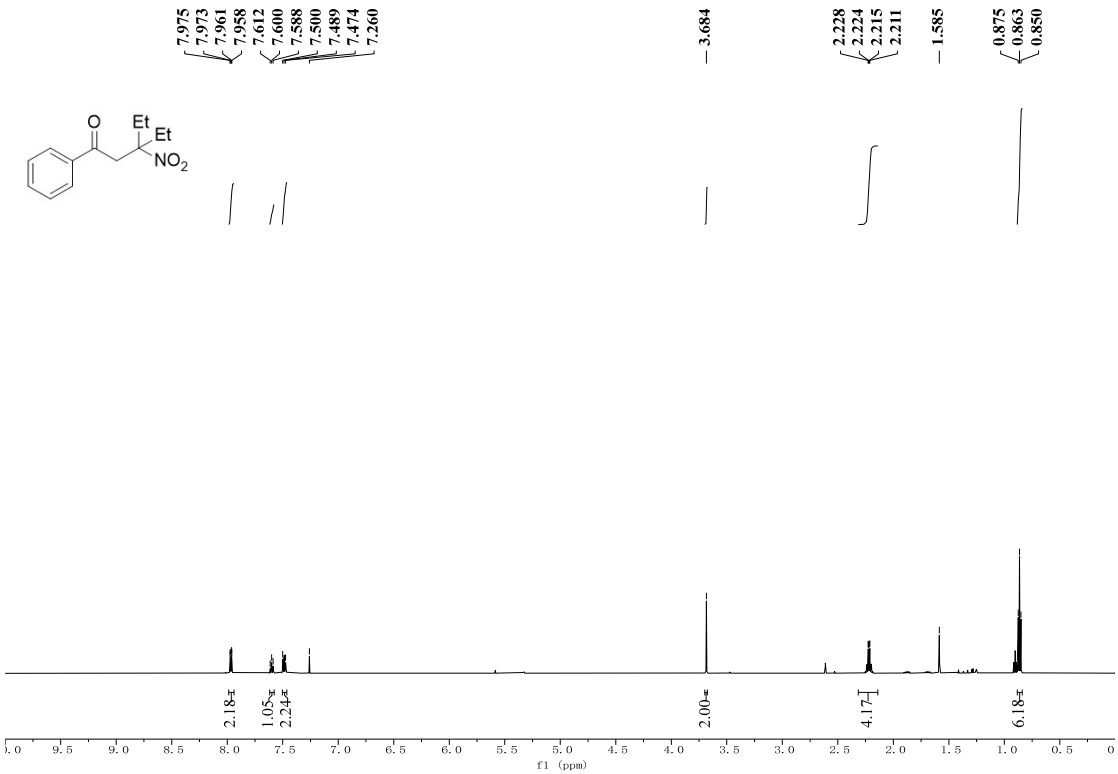

7.260
4.781
4.778
4.759
4.756
4.271
4.249
1.529
1.368
Br
NO2
O
O
2.00
2.04
3.32
3.04
f1 (ppm)

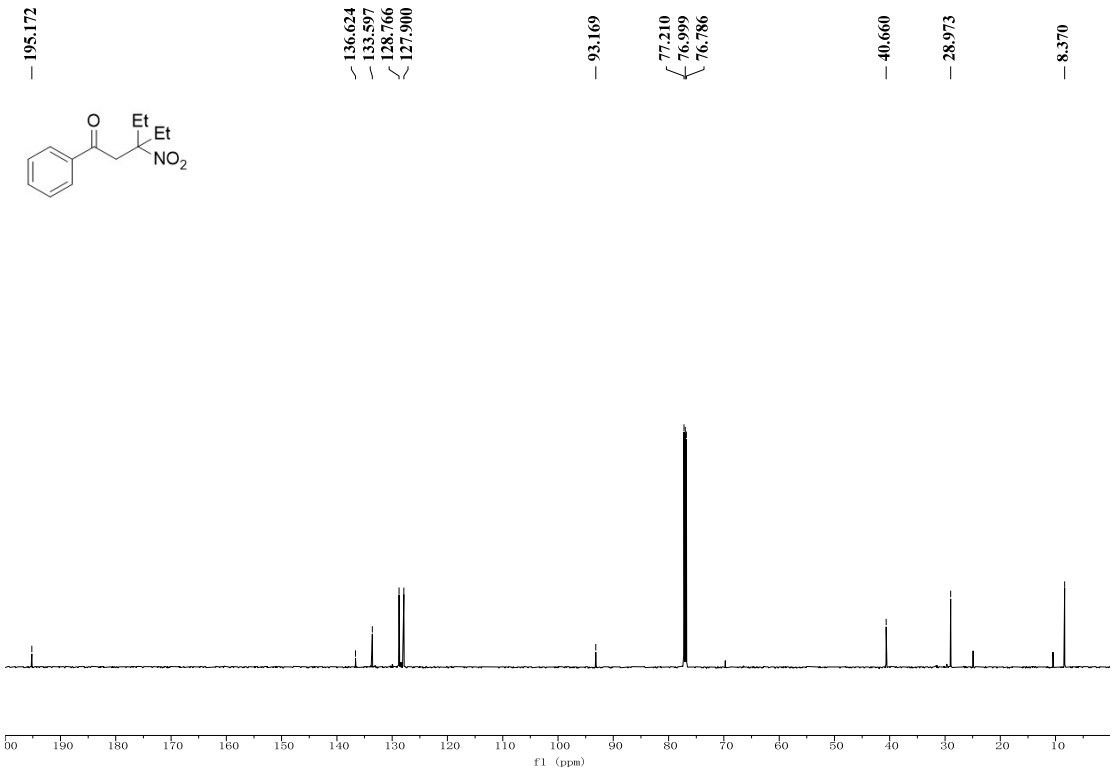

99.440
77.316
76.900
76.613
66.136
27.768
18.443
Br
NO2
O
O
f1 (ppm)

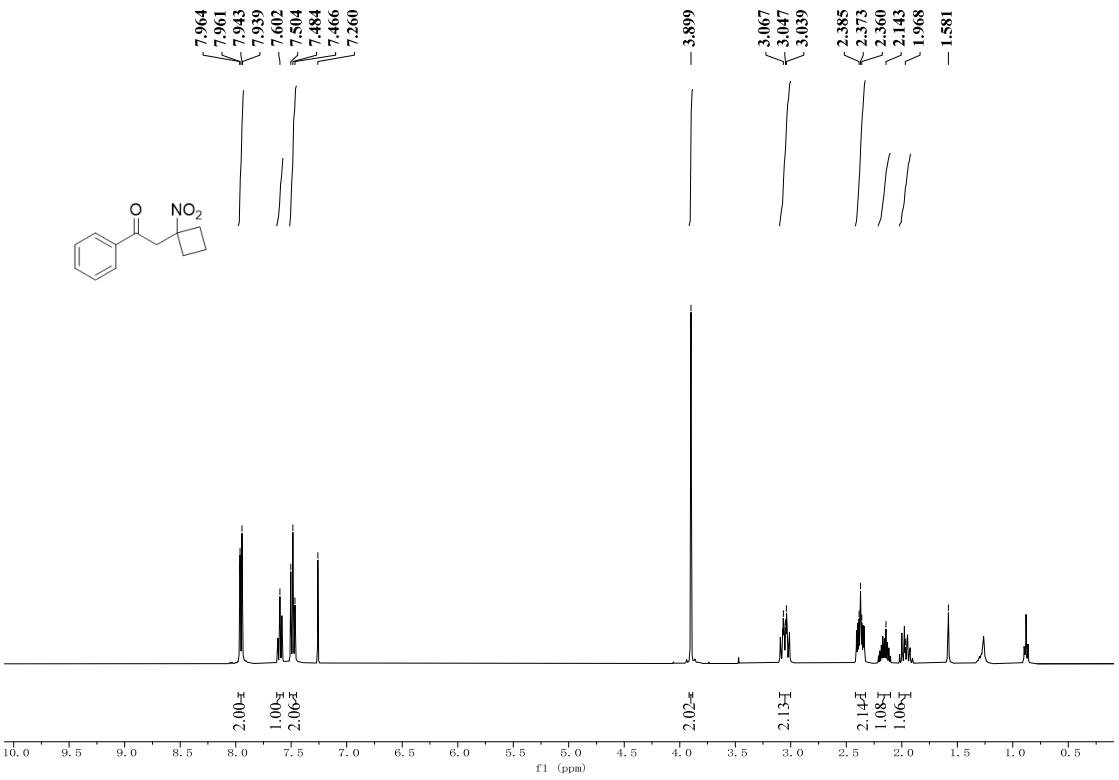

Br
Br
NO2
5.800
5.783
5.757
5.727
5.293
5.085
5.046
5.042
2.853
2.832
2.813
2.193
2.176
2.169
1.725
1.704
1.686
0.90
1.87
2.00
1.88
2.09
f1 (ppm)
137.018
116.198
87.658
77.218
77.006
76.793
48.296
32.081
26.306
f1 (ppm)

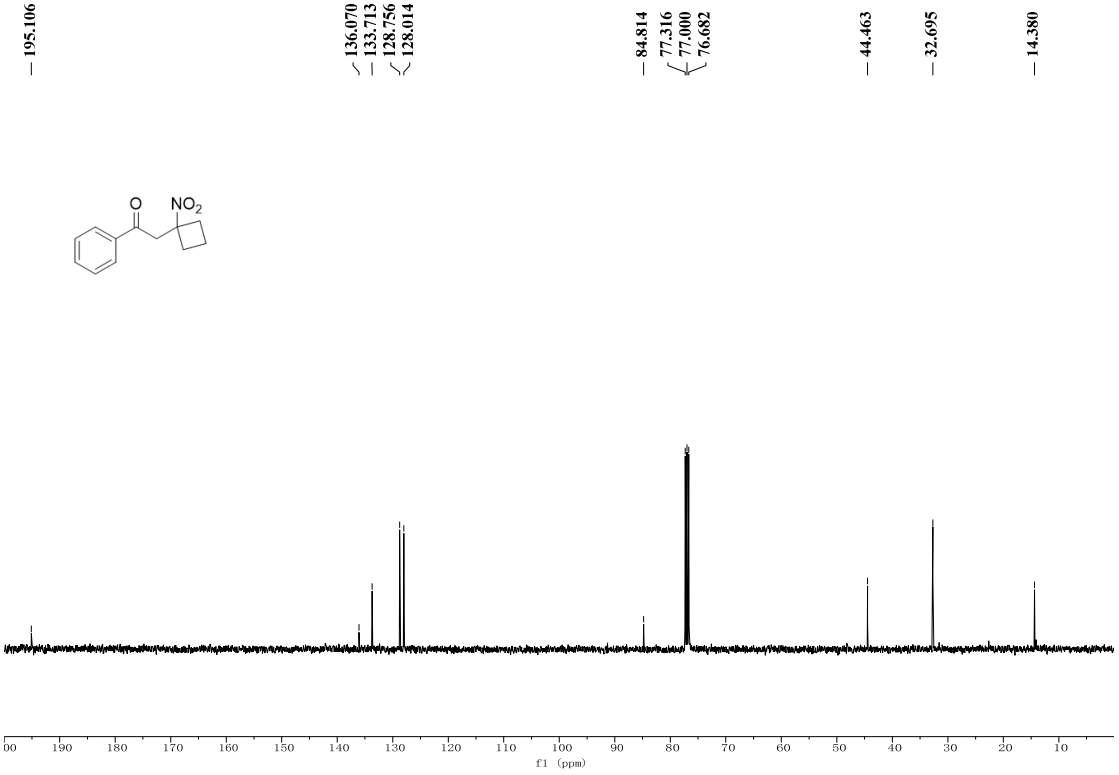

7.95
7.94
7.93
7.93
7.92
7.62
7.60
7.58
7.50
7.48
7.46
7.26
3.68
1.77
O
NO2
1.95
1.03
2.08
2.00
6.03
f1 (ppm)

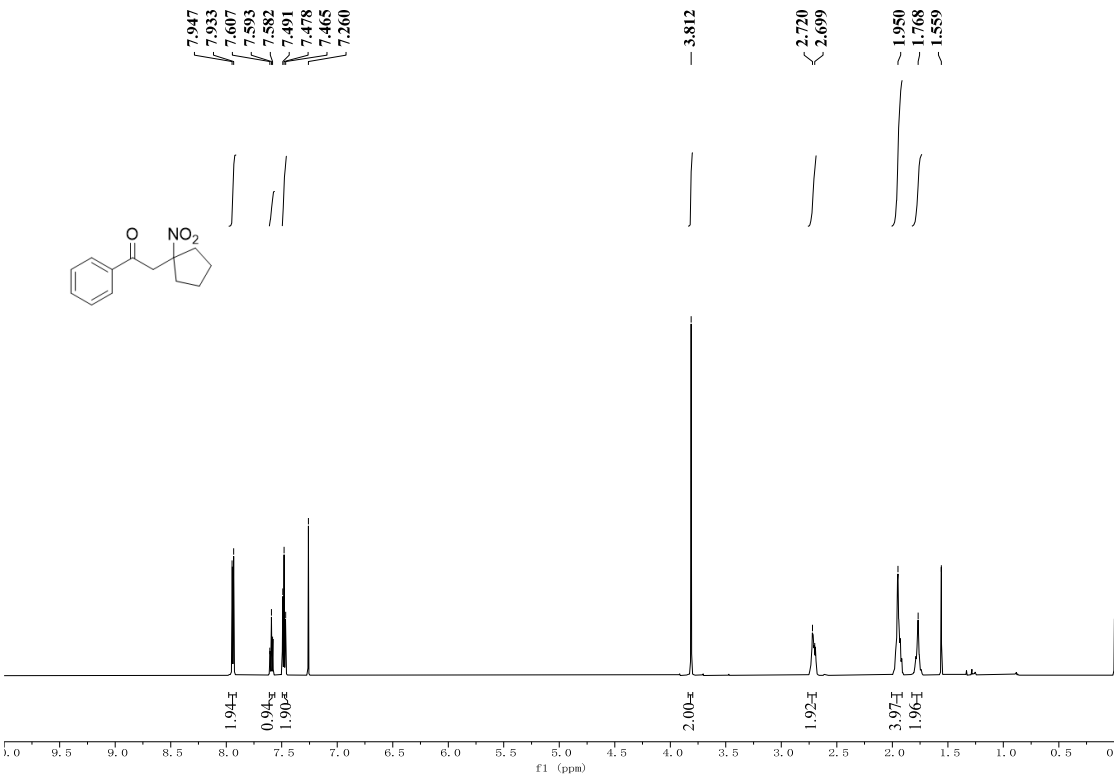

194.94
136.42
133.64
128.75
127.93
84.94
77.32
77.00
76.68
47.10
26.61
O
NO2
f1 (ppm)

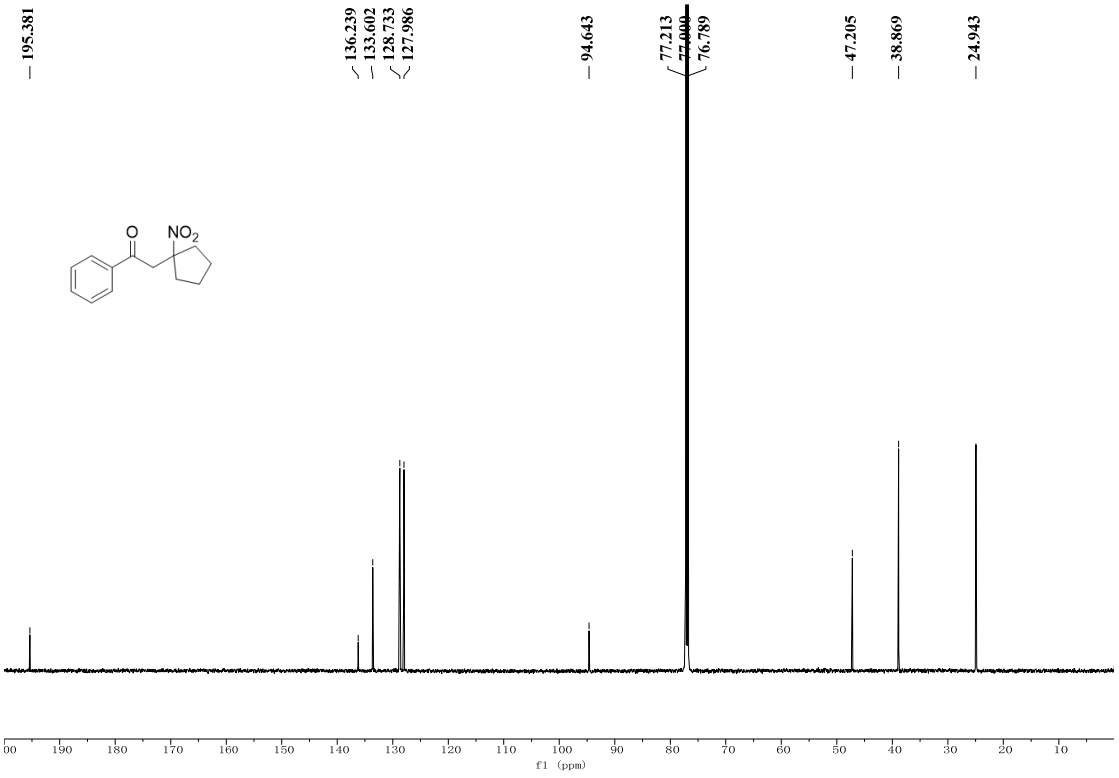

7.975
7.973
7.961
7.958
7.612
7.600
7.588
7.500
7.489
7.474
7.260
3.684
2.228
2.224
2.215
2.211
1.585
0.875
0.863
0.850
O
Et
Et
NO2
2.18
1.05
2.24
2.00
4.17
6.18
f1 (ppm)

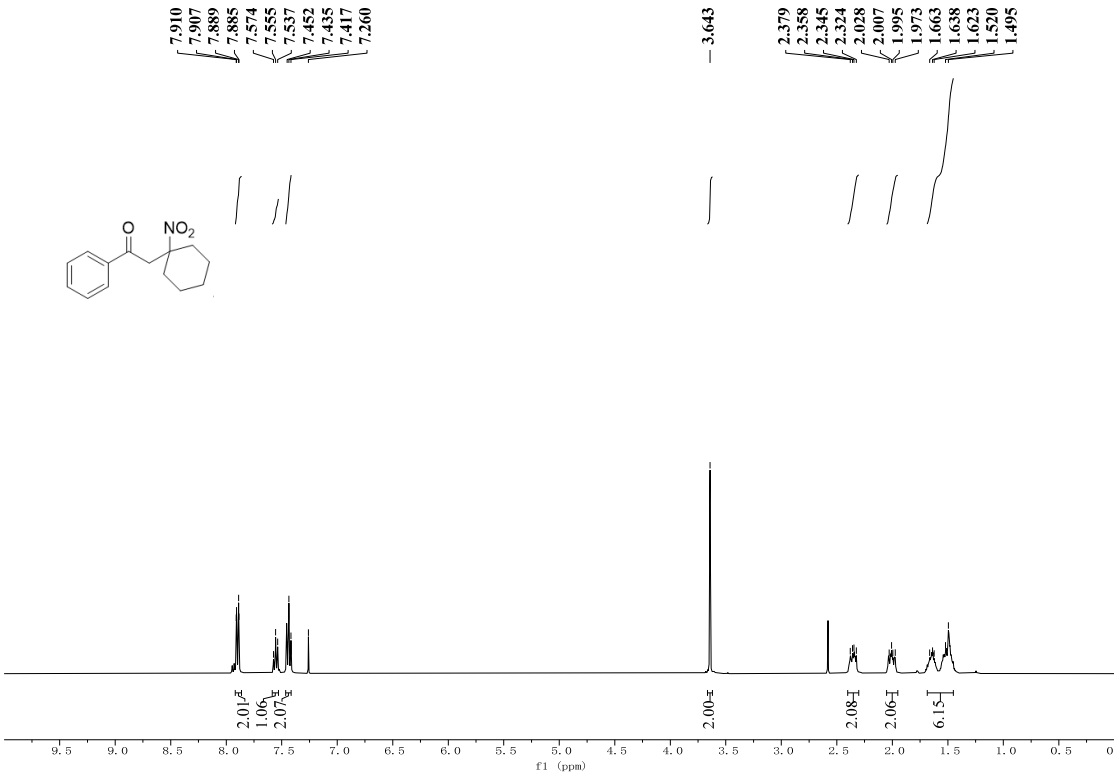

195.172
136.624
133.597
128.766
127.900
93.169
77.210
76.999
76.786
40.660
28.973
8.370
O
Et
Et
NO2
f1 (ppm)

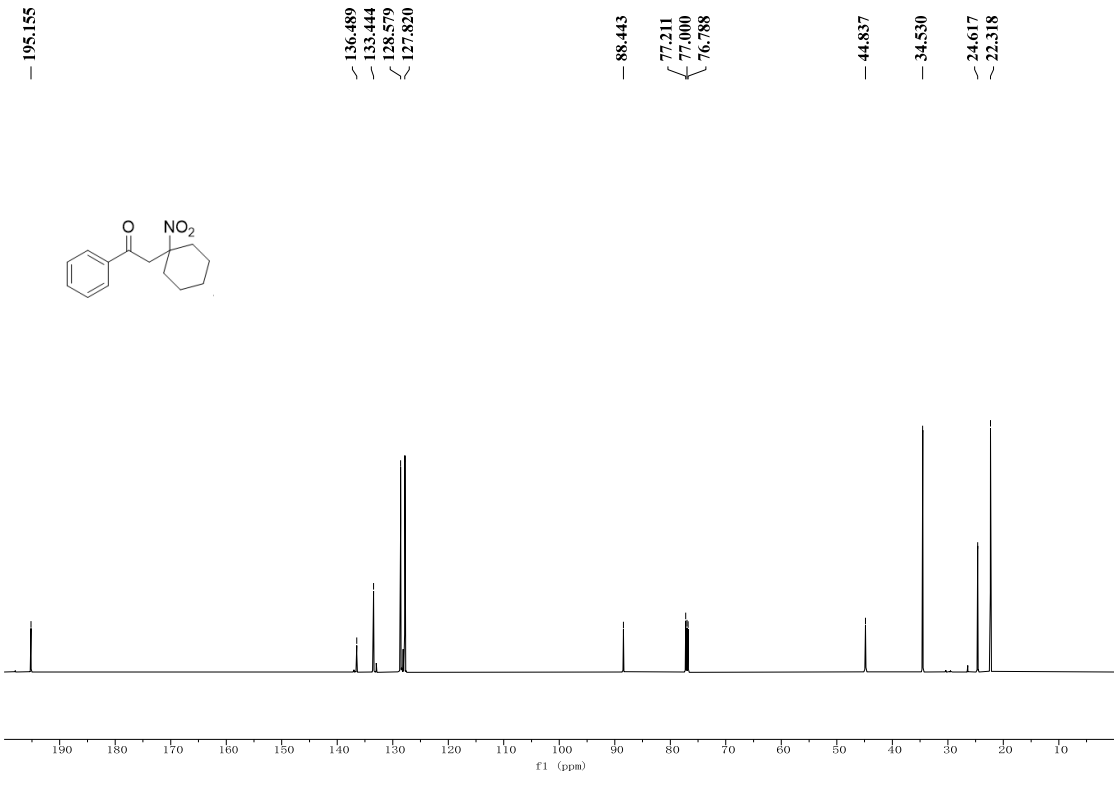

7.964
7.961
7.943
7.939
7.602
7.504
7.484
7.466
7.260
3.899
3.067
3.047
3.039
2.385
2.373
2.360
2.143
1.968
1.581
O
NO2
2.00
1.00
2.06
2.02
2.13
2.14
1.08
1.06
f1 (ppm)

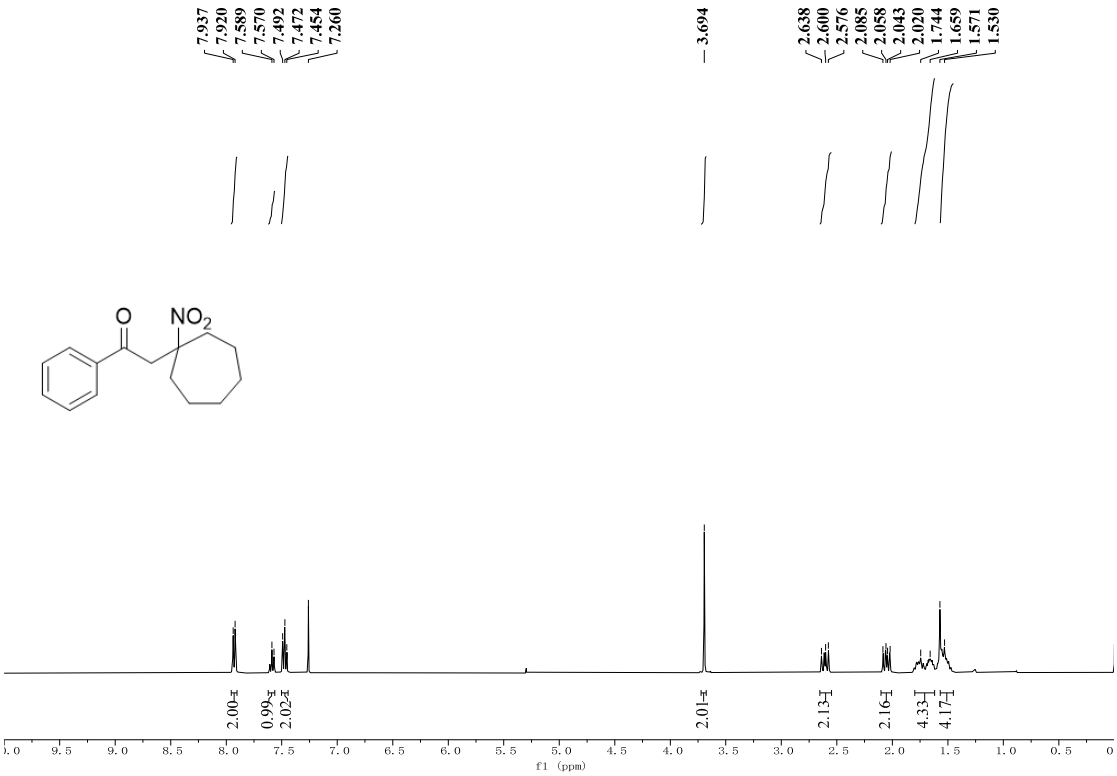

195.106
136.070
133.713
128.756
128.014
84.814
77.316
77.000
76.682
44.463
32.695
14.380
O
NO2
f1 (ppm)

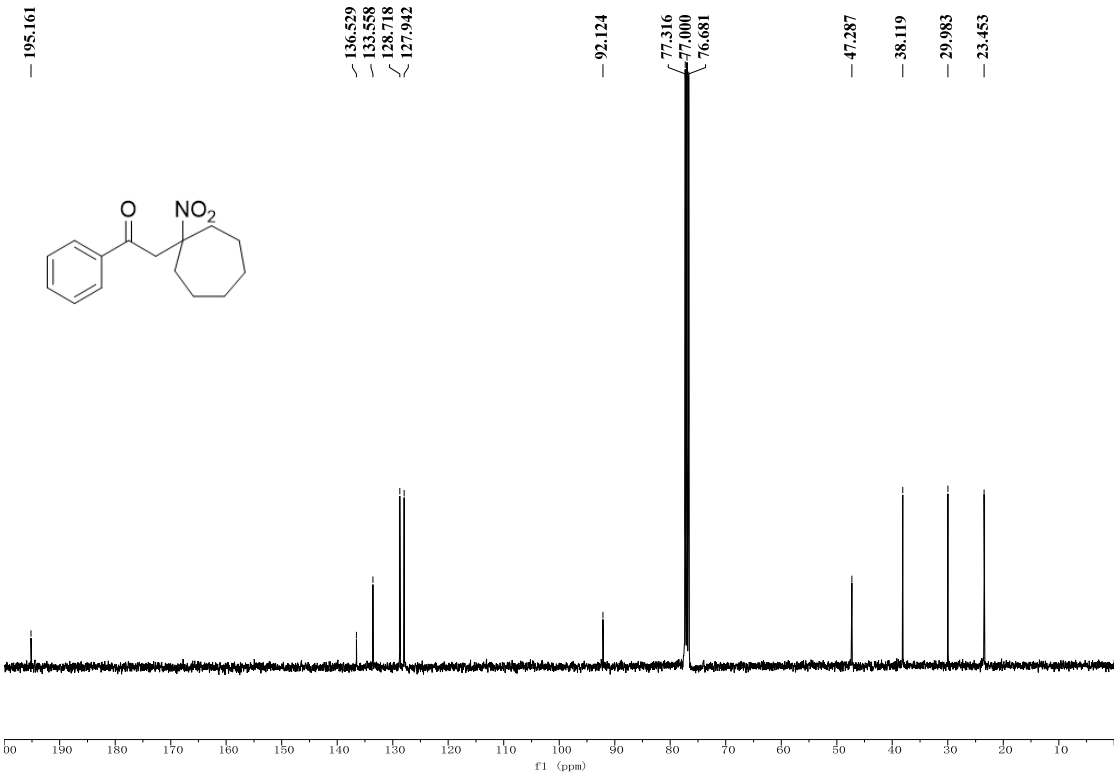

7.947
7.933
7.607
7.593
7.582
7.491
7.478
7.465
7.260
3.812
2.720
2.699
1.950
1.768
1.559
O
NO2
1.94
0.94
1.90
2.00
1.92
3.97
1.96
f1 (ppm)


195.381
136.239
133.602
128.733
127.986
94.643
77.213
77.000
76.789
47.205
38.869
24.943
O
NO2
f1 (ppm)


7.910
7.907
7.889
7.885
7.574
7.555
7.537
7.452
7.435
7.417
7.260
3.643
2.379
2.358
2.345
2.324
2.028
2.007
1.995
1.973
1.663
1.638
1.623
1.520
1.495
O
NO2
2.01
1.06
2.07
2.00
2.08
2.06
6.15
f1 (ppm)


195.155
136.489
133.444
128.579
127.820
88.443
77.211
77.000
76.788
44.837
34.530
24.617
22.318
O
NO2
f1 (ppm)


7.937
7.920
7.589
7.570
7.492
7.472
7.454
7.260
3.694
2.638
2.600
2.576
2.085
2.058
2.043
2.020
1.744
1.659
1.571
1.530
O
NO2
2.00
0.99
2.02
2.01
2.13
2.16
4.33
4.17
f1 (ppm)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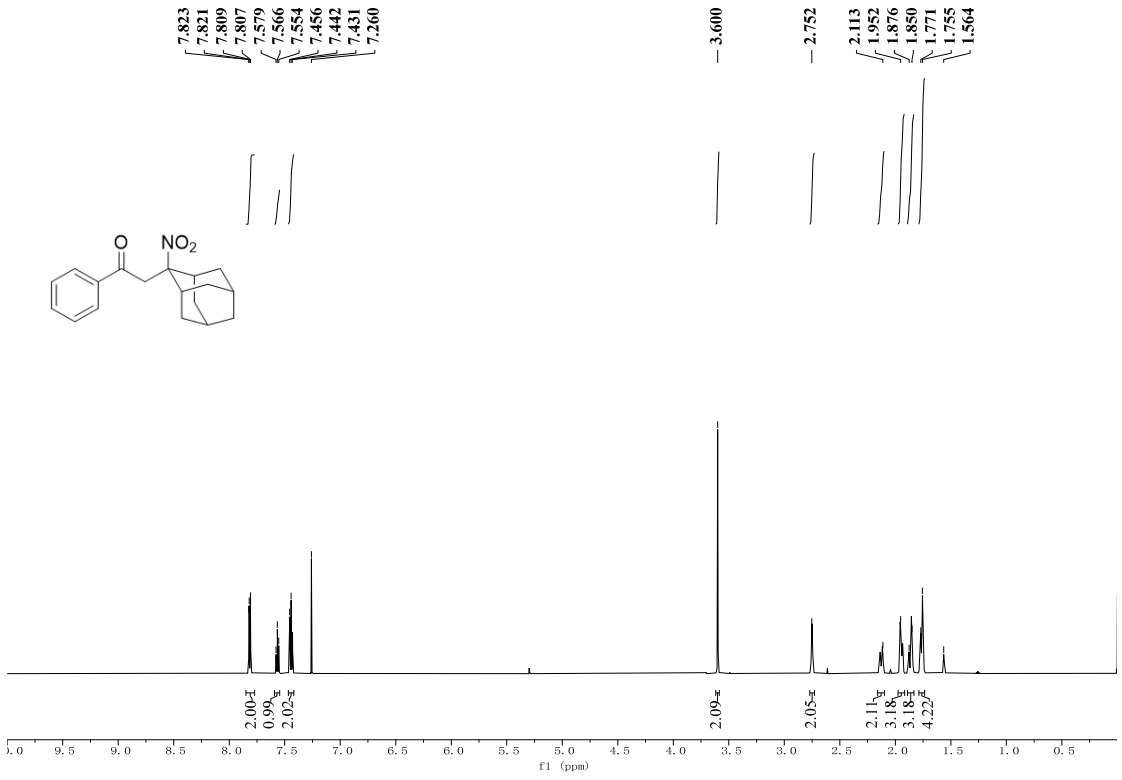
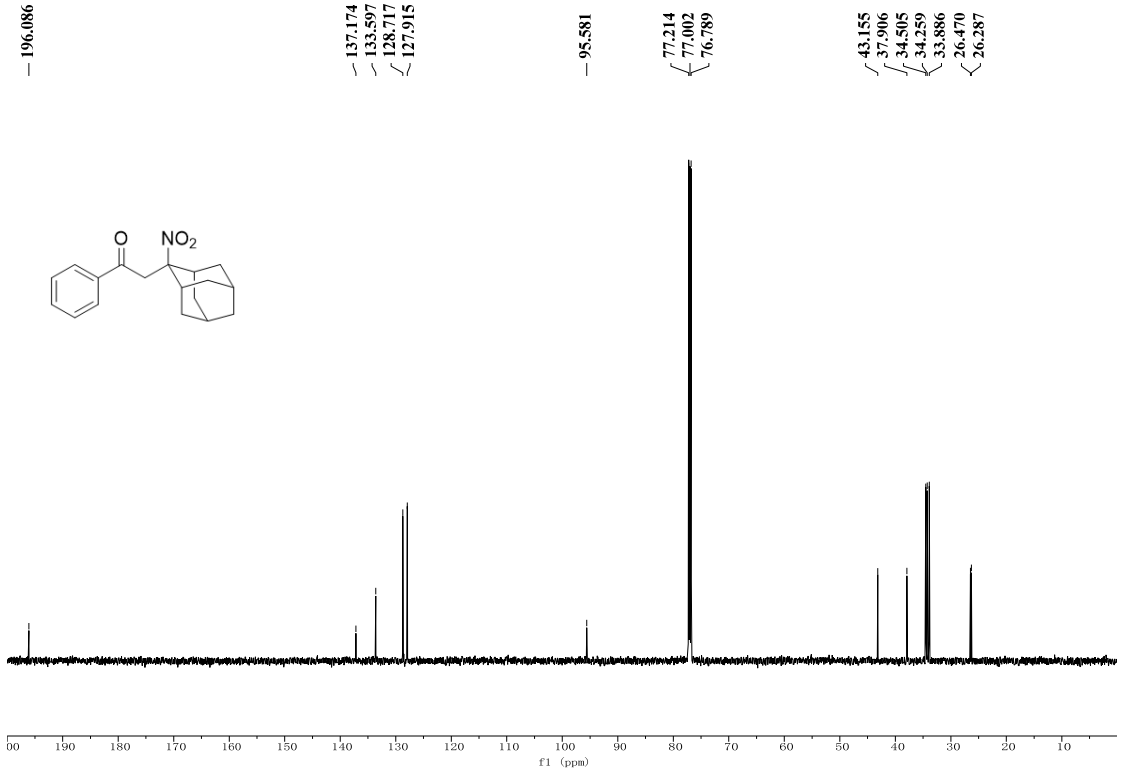
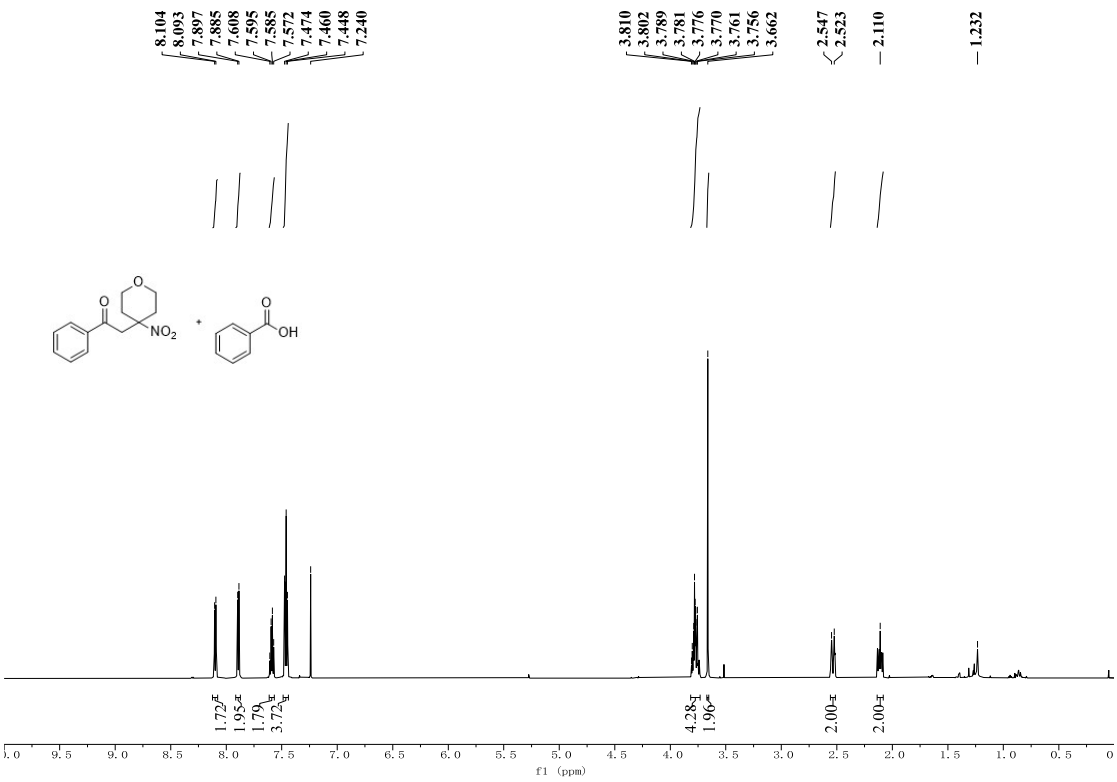
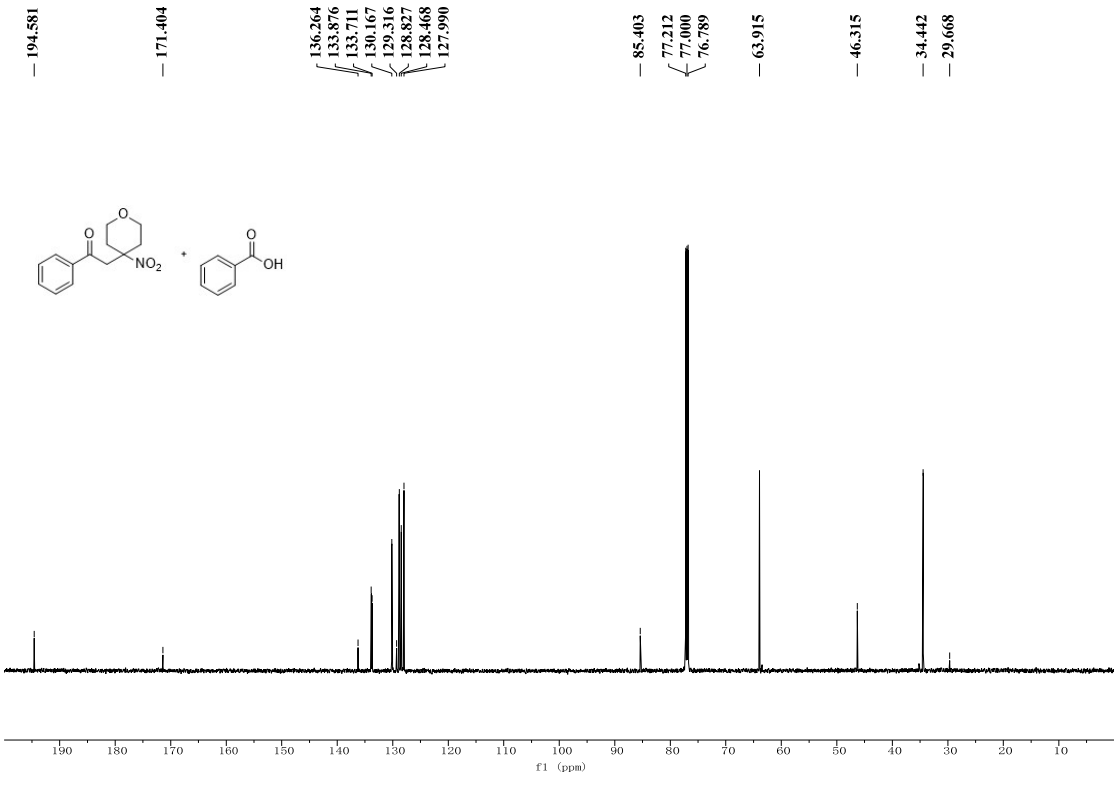
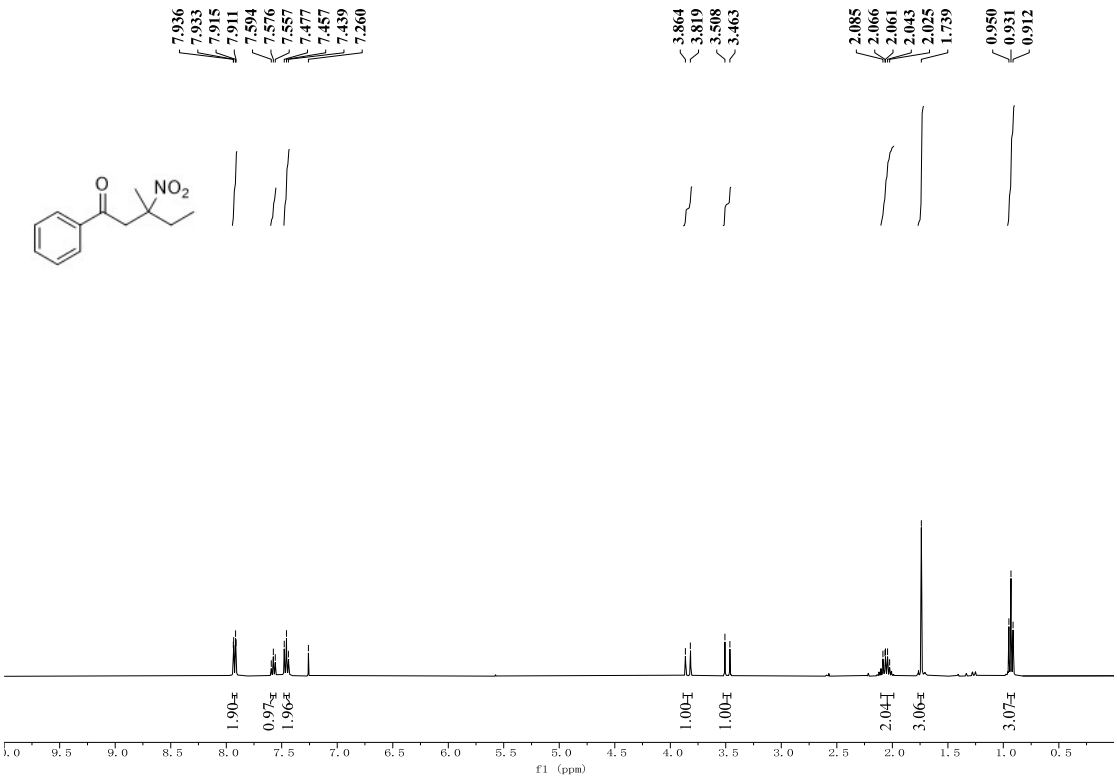
136.529
133.558
128.718
127.942
92.124
77.316
77.000
76.681
47.287
38.119
29.983
23.453
O
NO2
f1 (ppm)

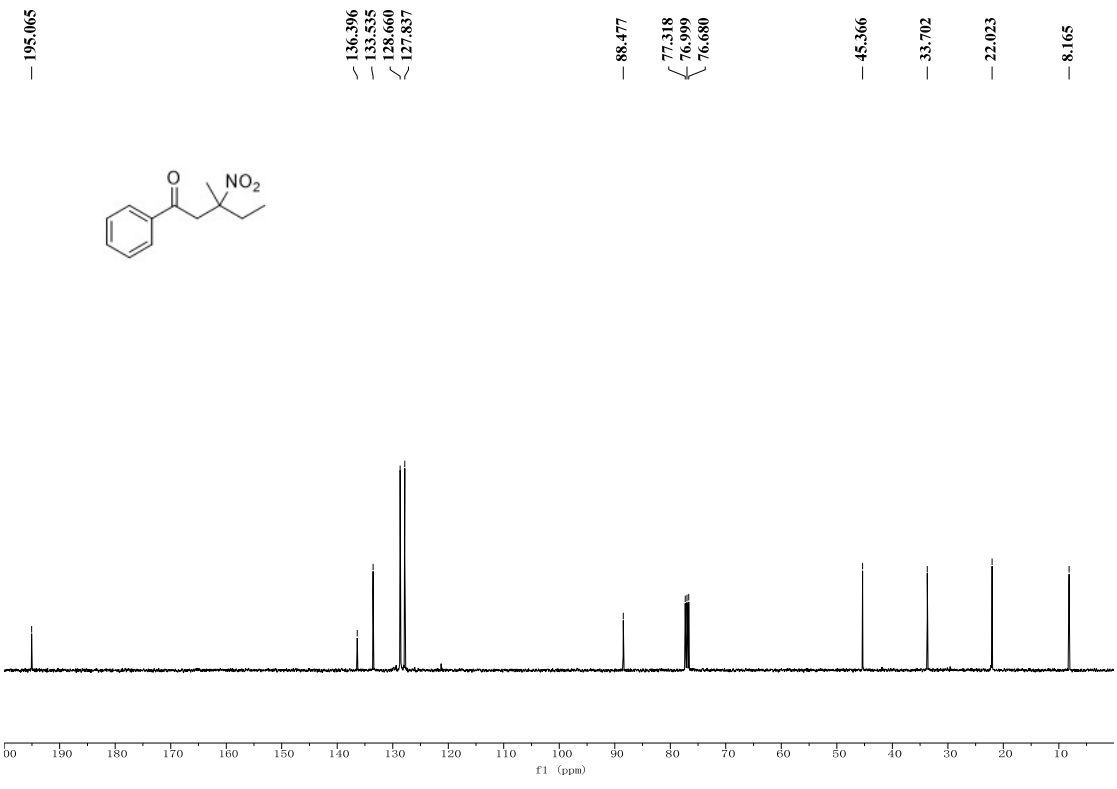

7.823
7.821
7.809
7.807
7.579
7.566
7.554
7.456
7.442
7.431
7.260
3.600
2.752
2.113
1.952
1.876
1.850
1.771
1.755
1.564
O
NO2
2.00
0.99
2.02
2.09
2.05
2.11
3.18
3.18
4.22
f1 (ppm)


196.086
137.174
133.597
128.717
127.915
95.581
77.214
77.002
76.789
43.155
37.906
34.505
34.259
33.886
26.470
26.287
O
NO2
f1 (ppm)


8.104
8.093
7.897
7.885
7.608
7.595
7.585
7.572
7.474
7.460
7.448
7.240
3.810
3.802
3.789
3.781
3.776
3.770
3.761
3.756
3.662
2.547
2.523
2.110
1.232
1.72
1.95
1.79
3.72
4.28
1.96
2.00
2.00
f1 (ppm)


194.581
171.404
136.264
133.876
133.711
130.167
129.316
128.827
128.468
127.990
85.403
77.212
77.000
76.789
63.915
46.315
34.442
29.668
f1 (ppm)


7.936
7.933
7.915
7.911
7.594
7.576
7.557
7.477
7.457
7.439
7.260
3.864
3.819
3.508
3.463
2.085
2.066
2.061
2.043
2.025
1.739
0.950
0.931
0.912
O
NO2
1.90
0.97
1.96
1.00
1.00
2.04
3.06
3.07
f1 (ppm)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136.396
133.535
128.660
127.837
88.477
77.318
76.999
76.680
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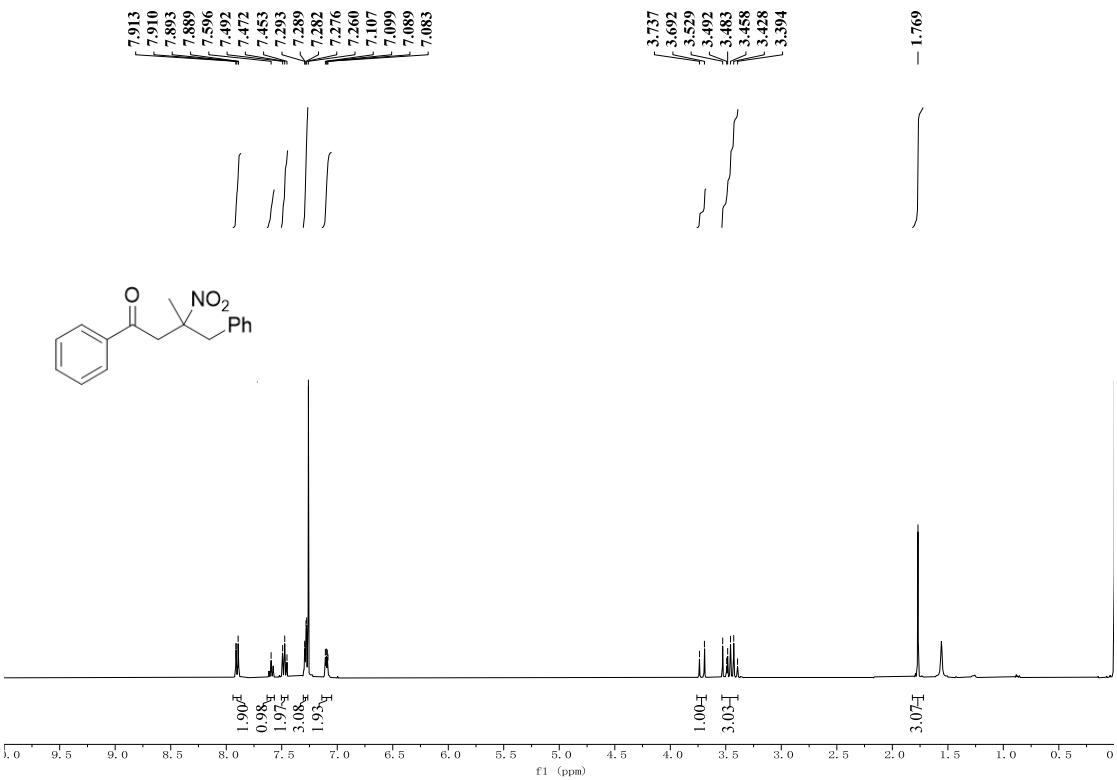
33.702
22.023
8.165
O
NO2
f1 (ppm)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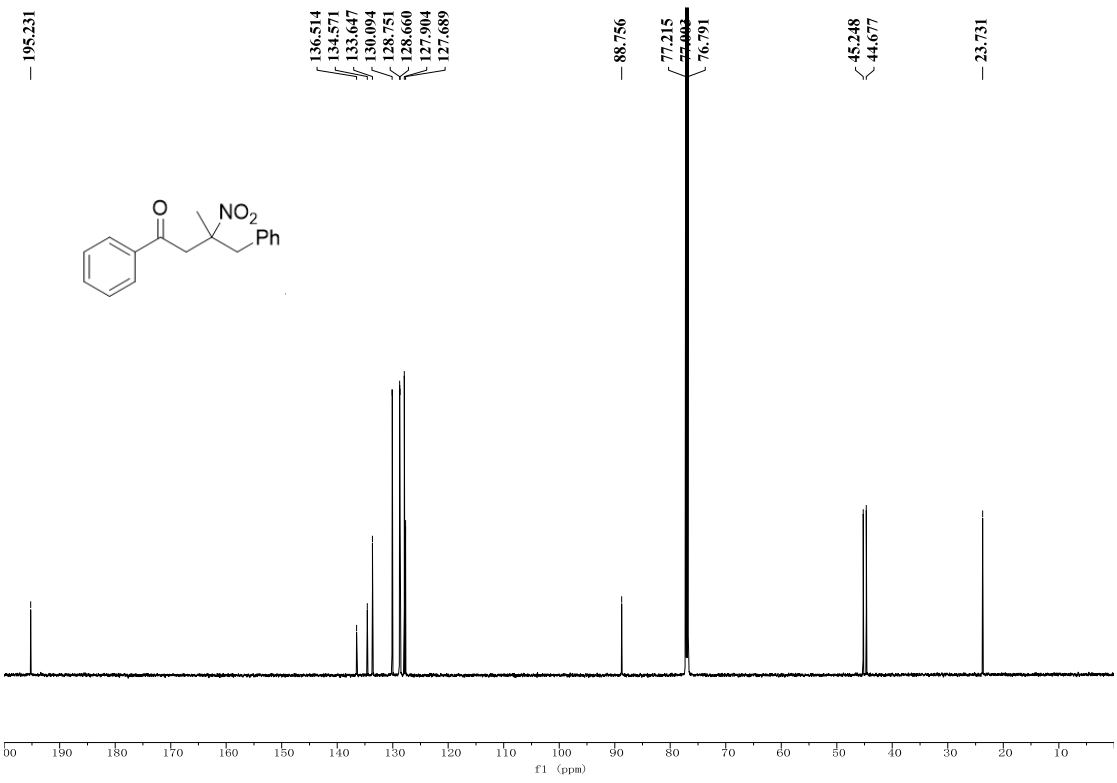
7.893
7.889
7.596
7.492
7.472
7.453
7.293
7.289
7.282
7.276
7.260
7.107
7.099
7.089
7.083
3.737
3.692
3.529
3.492
3.483
3.458
3.428
3.394
1.769
O
NO2
Ph
1.90
0.98
1.97
3.08
1.93
1.00
3.03
3.07
f1 (ppm)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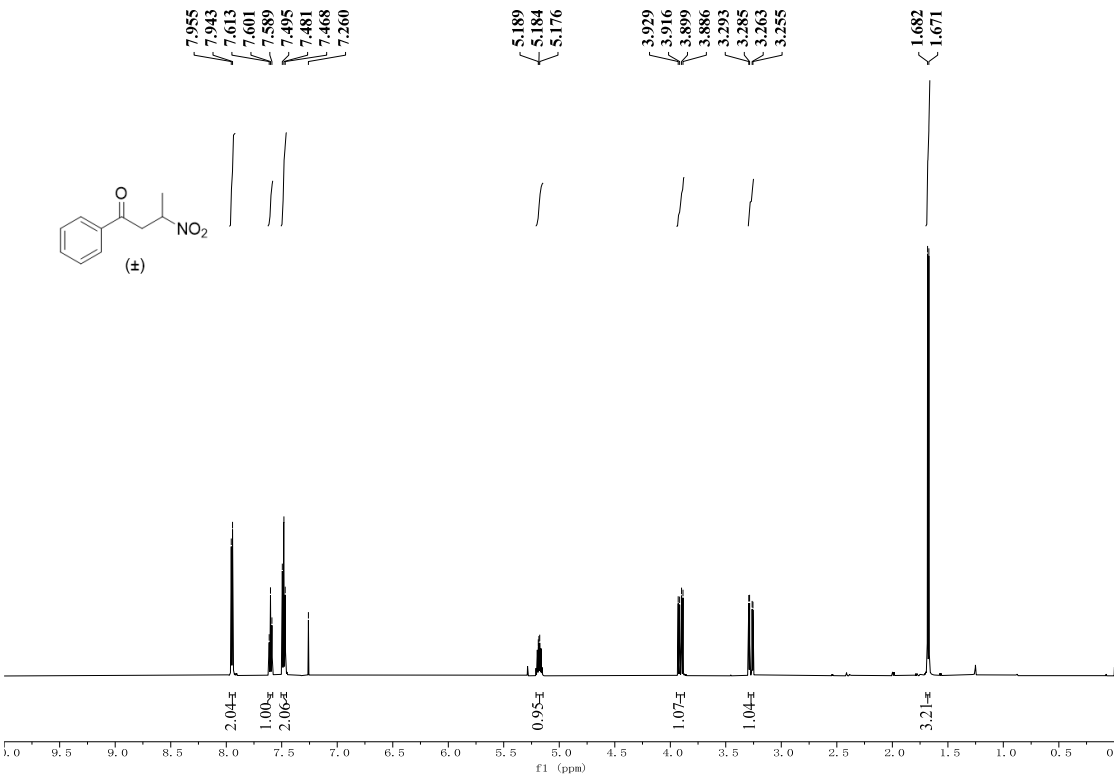
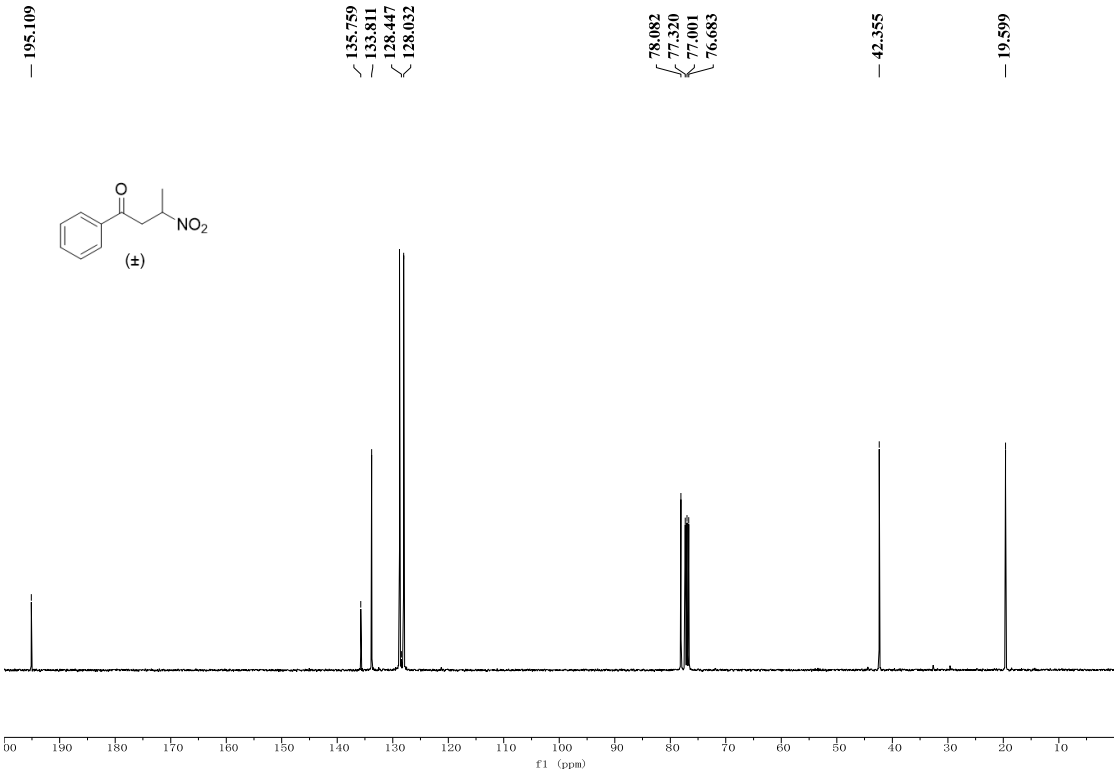
136.514
134.571
133.647
130.094
128.751
128.660
127.904
127.689
88.756
77.215
77.002
76.791
45.248
44.677
23.731
O
NO2
Ph
f1 (ppm)


7.955
7.943
7.613
7.601
7.589
7.495
7.481
7.468
7.260
5.189
5.184
5.176
3.929
3.916
3.899
3.886
3.293
3.285
3.263
3.255
1.682
1.671
O
NO2
(±)
2.04
1.00
2.06
0.95
1.07
1.04
3.21
f1 (ppm)


195.109
135.759
133.811
128.447
128.032
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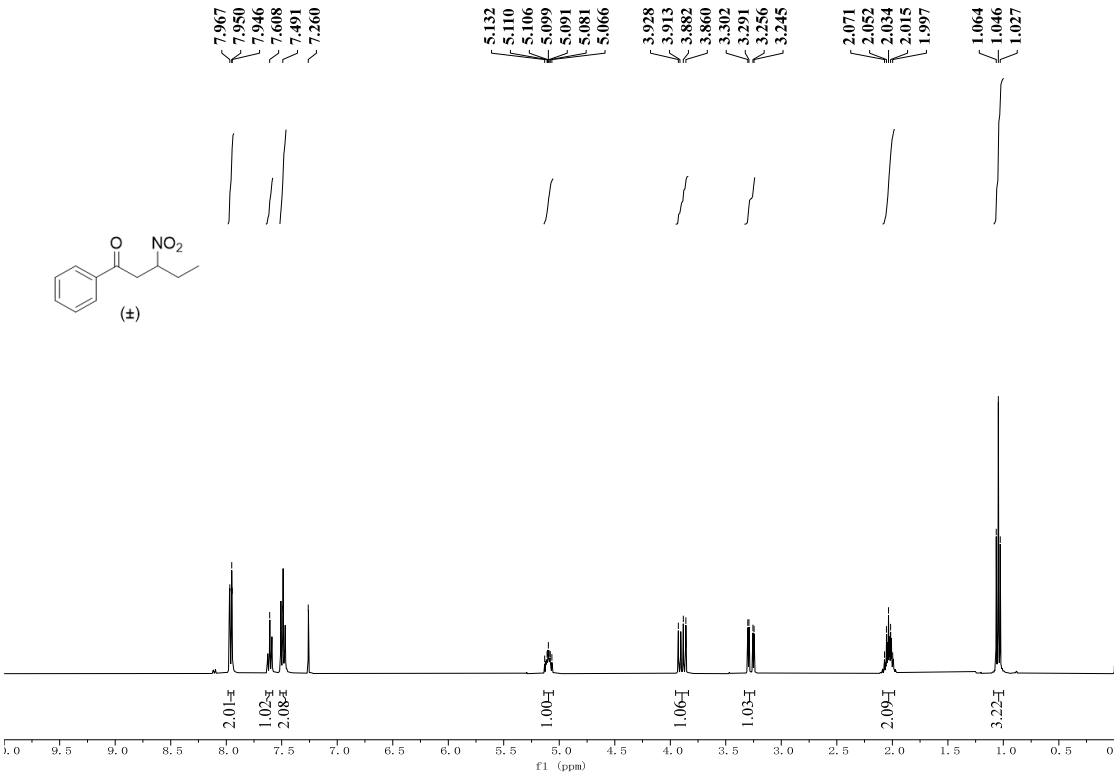
77.320
77.001
76.683
42.355
19.599
O
NO2
(±)
f1 (ppm)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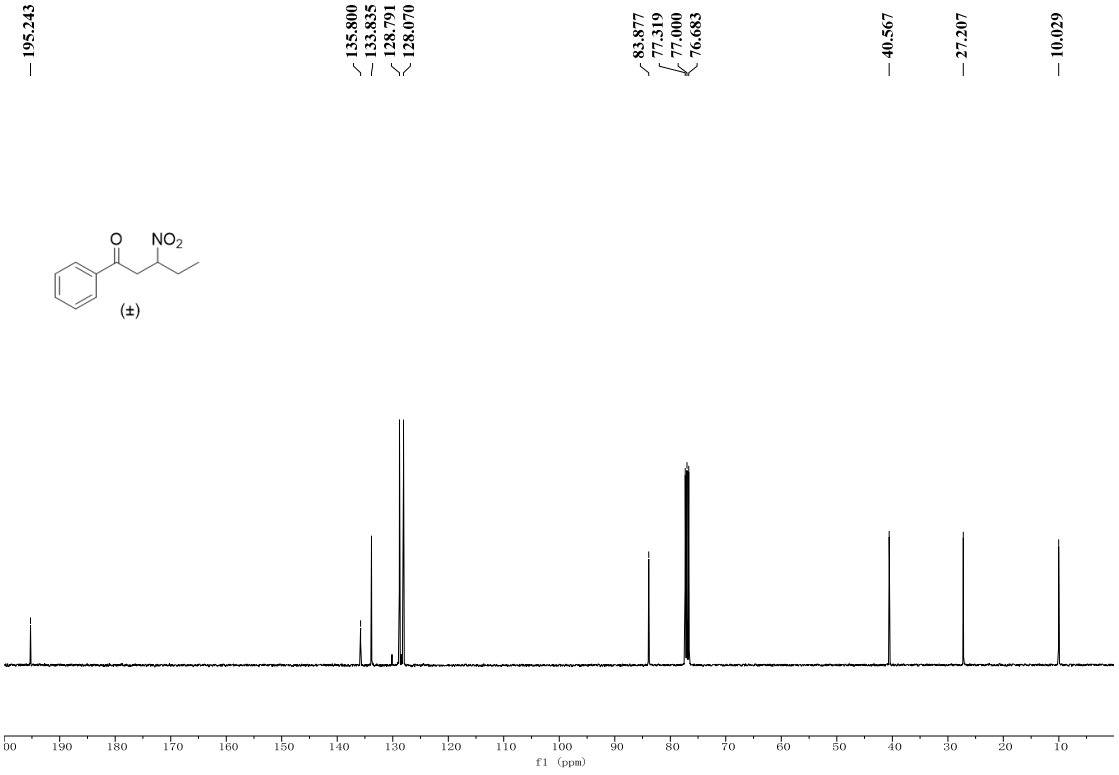
7.946
7.608
7.491
7.260
5.132
5.110
5.106
5.099
5.091
5.081
5.066
3.928
3.913
3.882
3.860
3.302
3.291
3.256
3.245
2.071
2.052
2.034
2.015
1.997
1.064
1.046
1.027
O
NO2
(±)
2.01
1.02
2.08
1.00
1.06
1.03
2.09
3.22
f1 (ppm)


195.243
135.800
133.835
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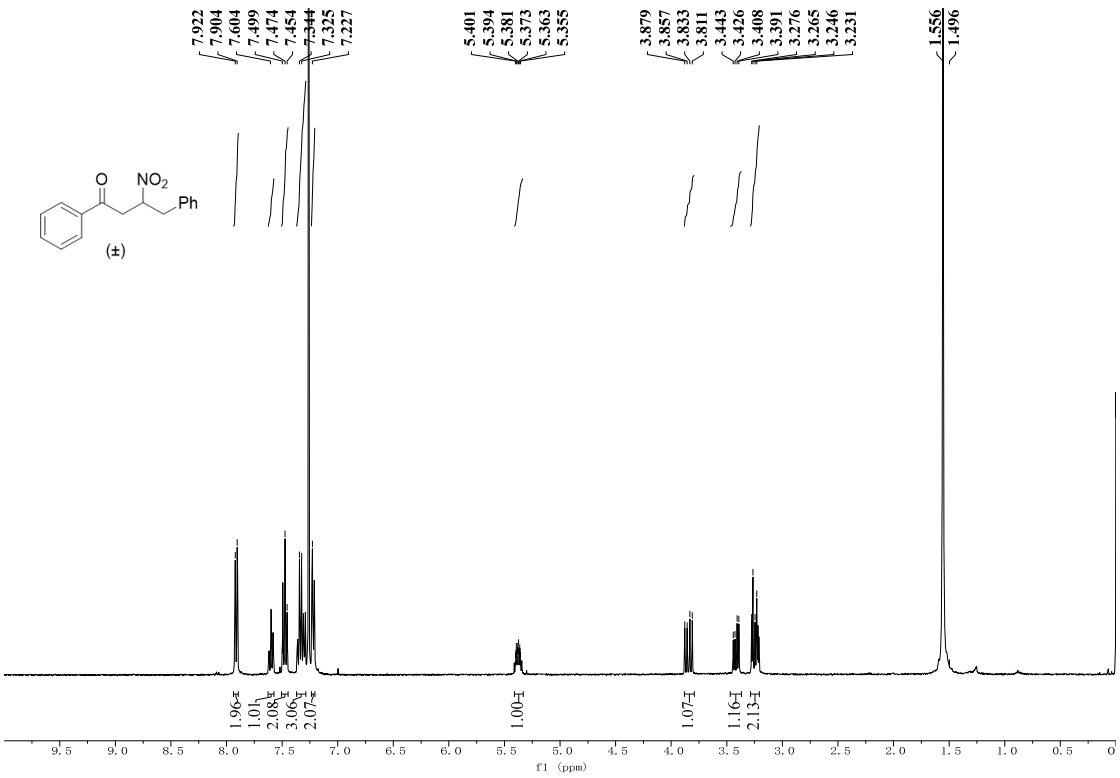
77.319
77.000
76.683
40.567
27.207
10.029
O
NO2
(±)
f1 (ppm)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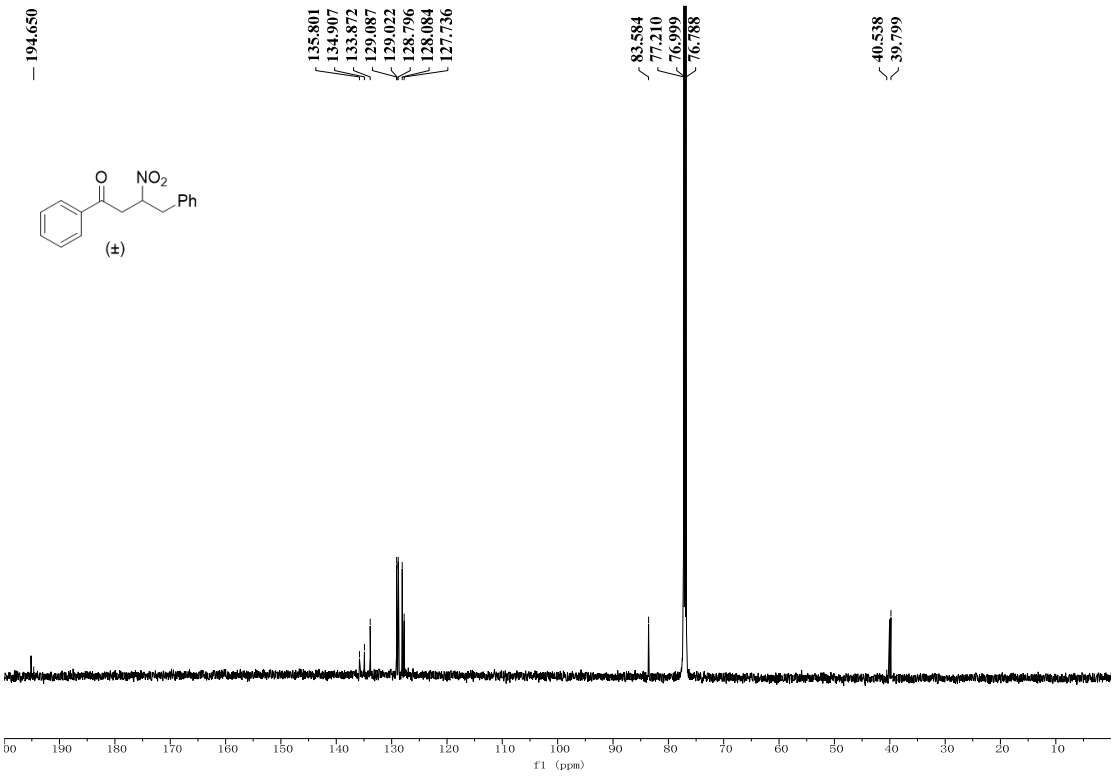
7.904
7.604
7.499
7.474
7.454
7.344
7.325
7.227
5.401
5.394
5.381
5.373
5.363
5.355
3.879
3.857
3.833
3.811
3.443
3.426
3.408
3.391
3.276
3.265
3.246
3.231
1.556
1.496
O
NO2
Ph
(±)
1.96
1.01
2.08
3.06
2.07
1.00
1.07
1.16
2.13
f1 (ppm)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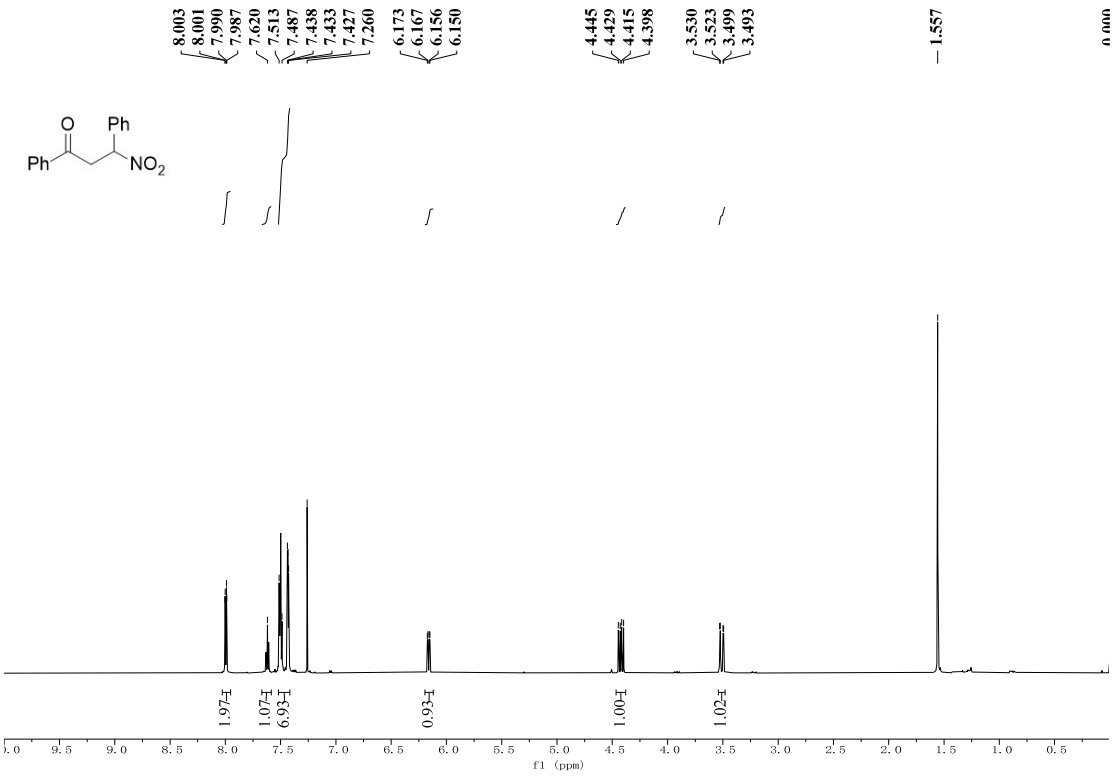
129.022
128.796
128.084
127.736
83.584
77.210
76.999
76.788
40.538
39.799
O
NO2
Ph
(±)
f1 (ppm)


8.003
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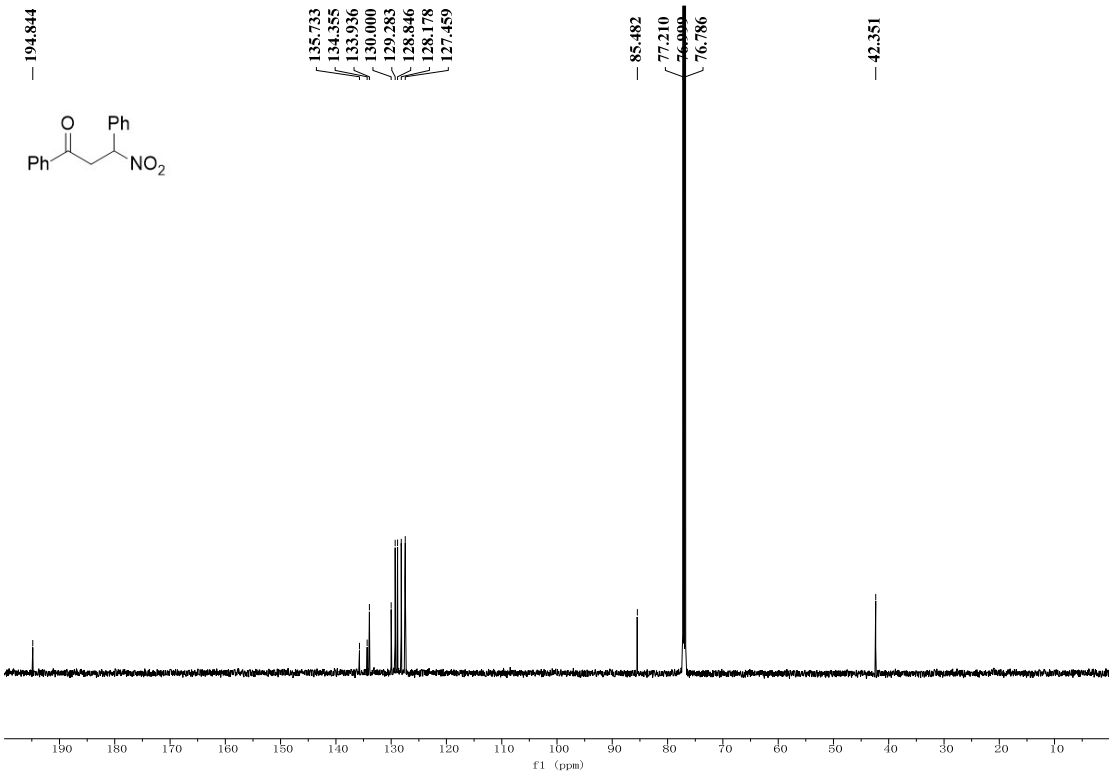
7.990
7.987
7.620
7.513
7.487
7.438
7.433
7.427
7.260
6.173
6.167
6.156
6.150
4.445
4.429
4.415
4.398
3.530
3.523
3.499
3.493
1.557
0.000
O
Ph
Ph
NO2
1.97
1.07
6.93
0.93
1.00
1.02
f1 (ppm)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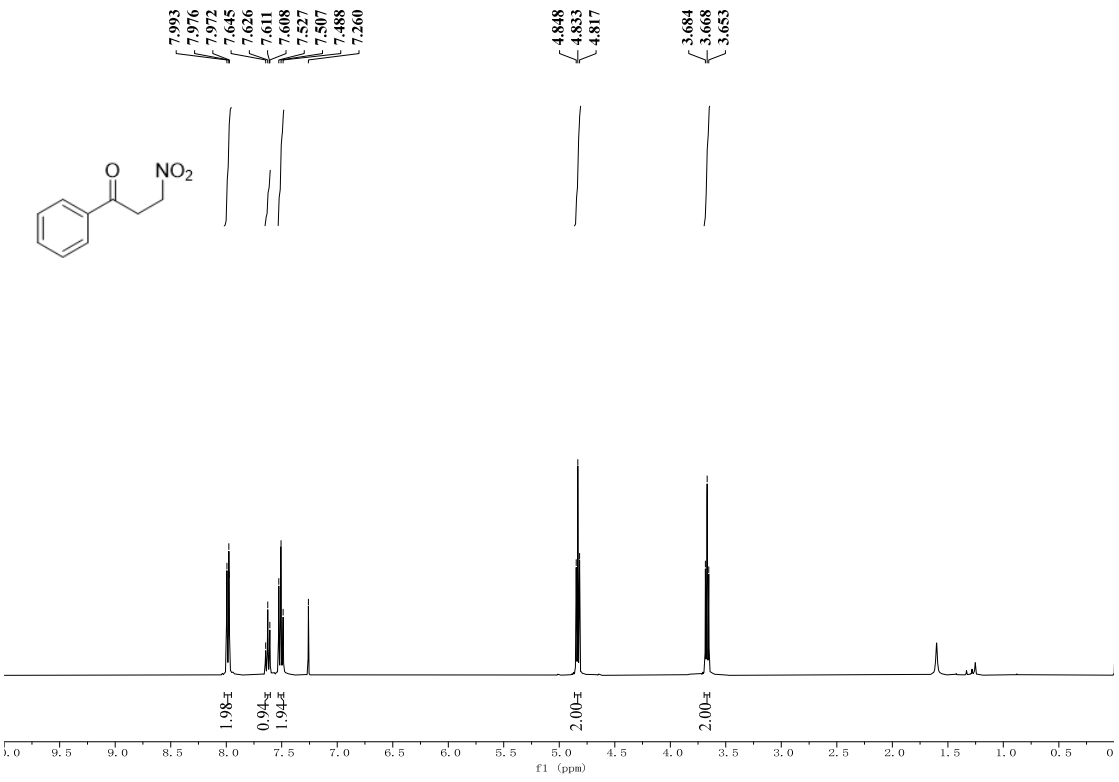
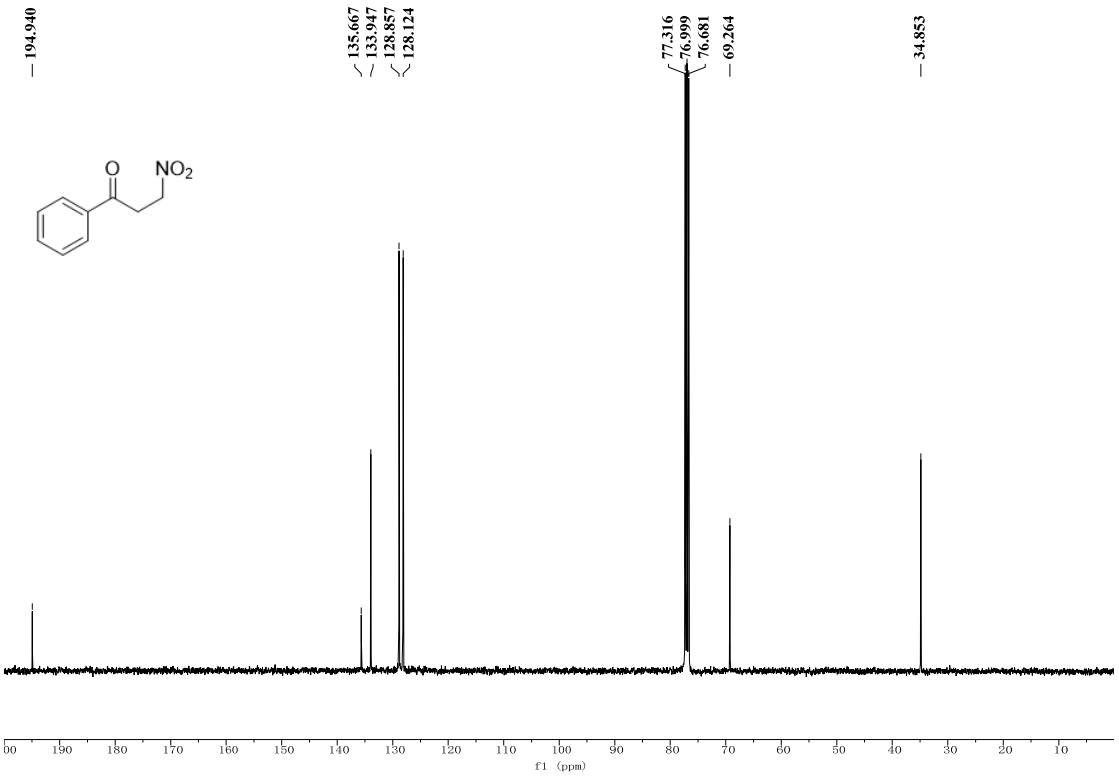
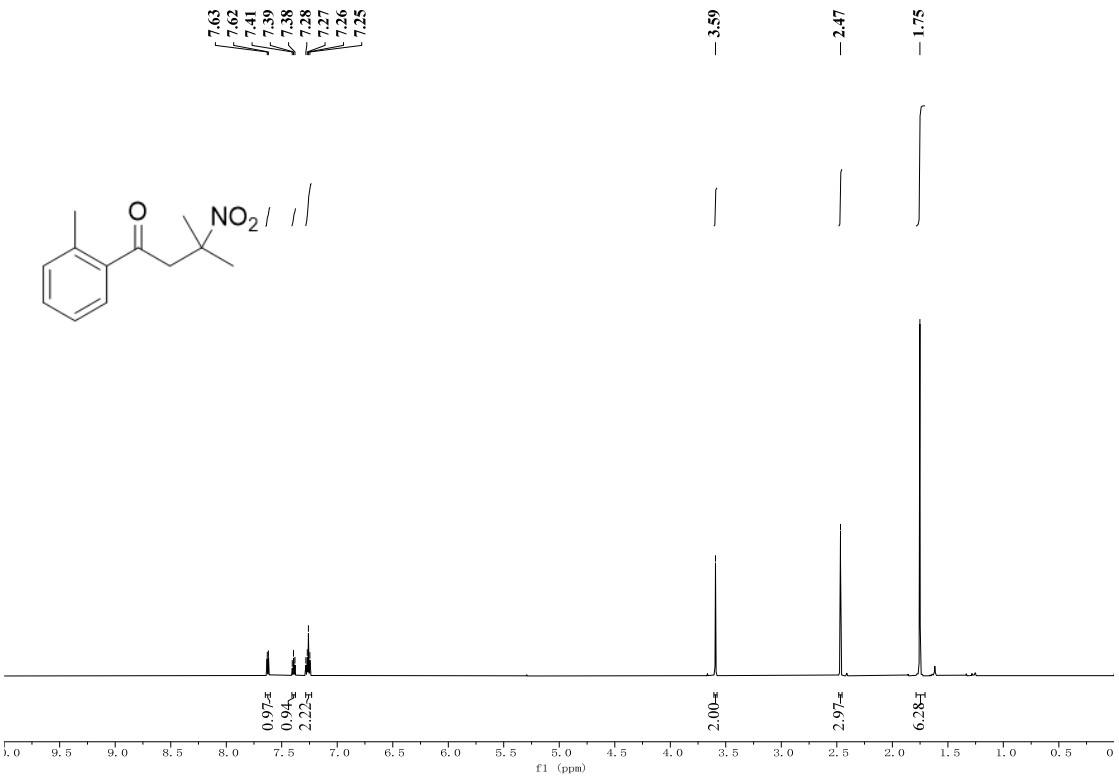
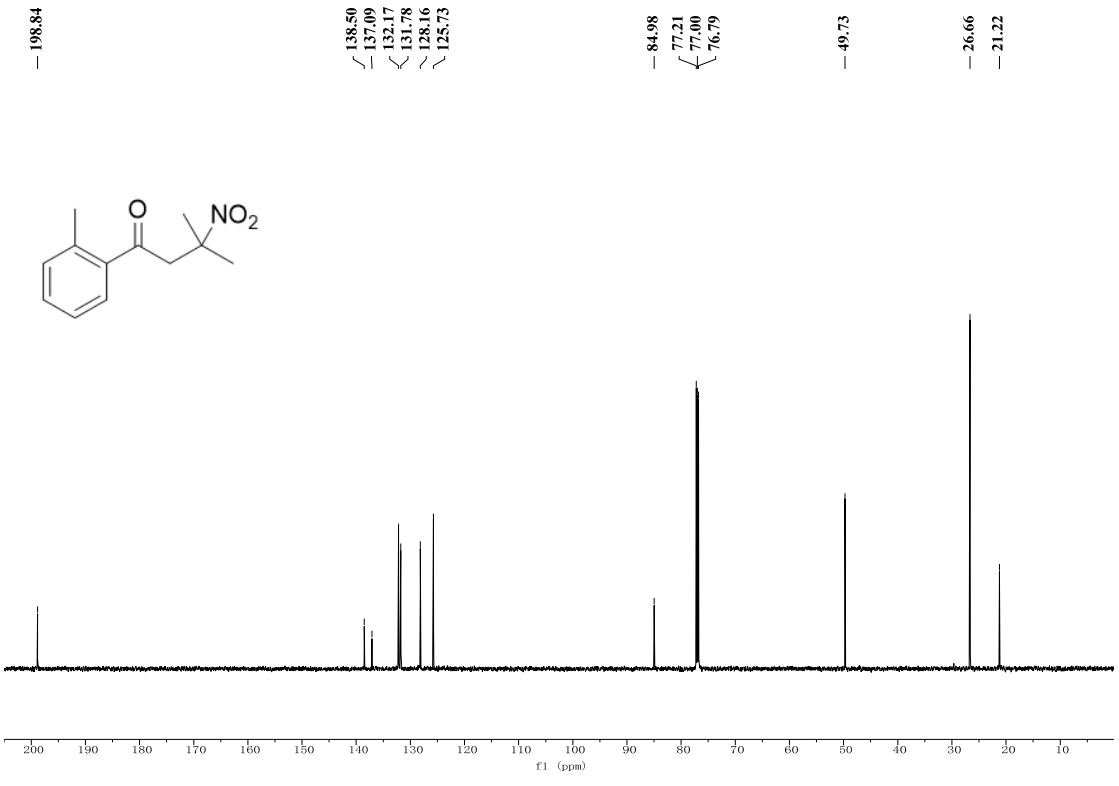
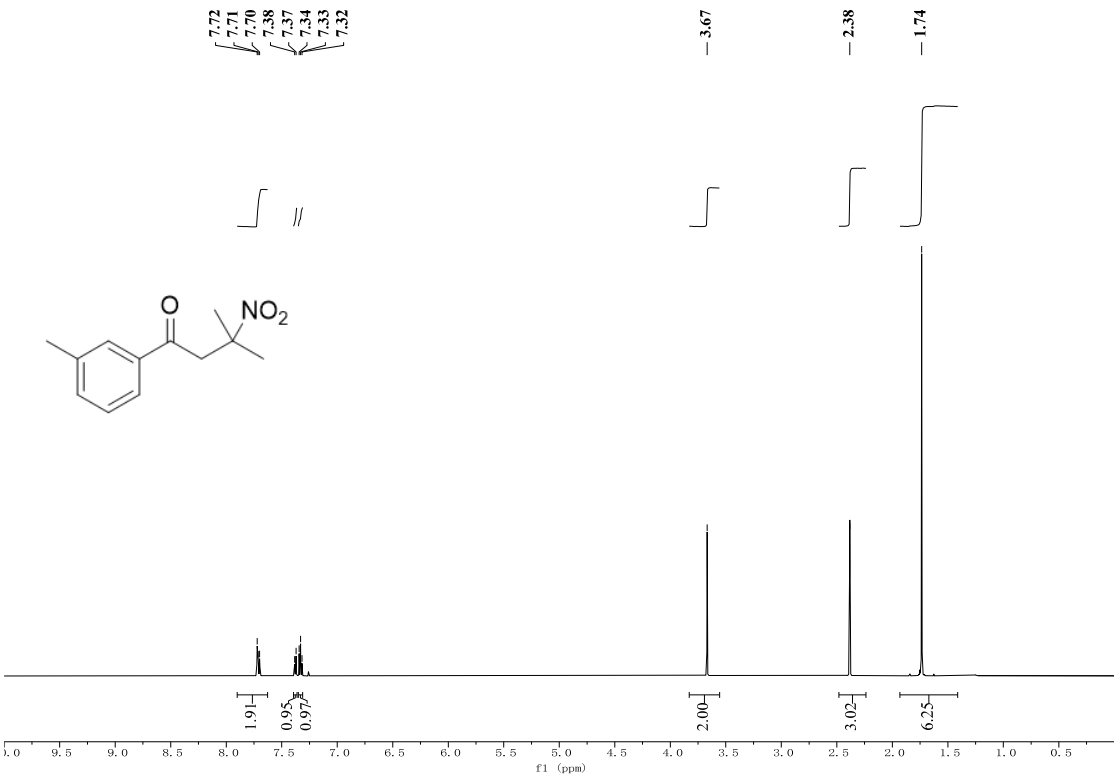
134.355
133.936
130.000
129.283
128.846
128.178
127.459
85.482
77.210
76.690
76.786
42.351
O
Ph
Ph
NO2
f1 (ppm)

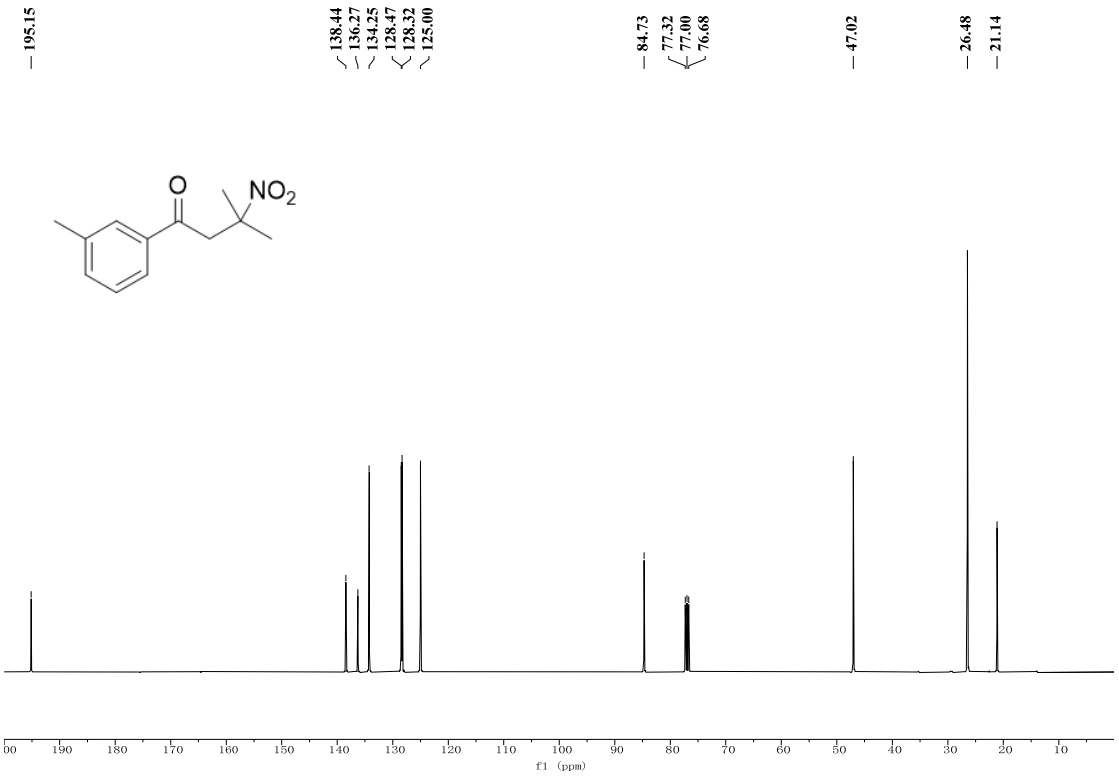

7.993
7.976
7.972
7.645
7.626
7.611
7.608
7.527
7.507
7.488
7.260
4.848
4.833
4.817
3.684
3.668
3.653
O
NO2
1.98
0.94
1.94
2.00
2.00
f1 (ppm)

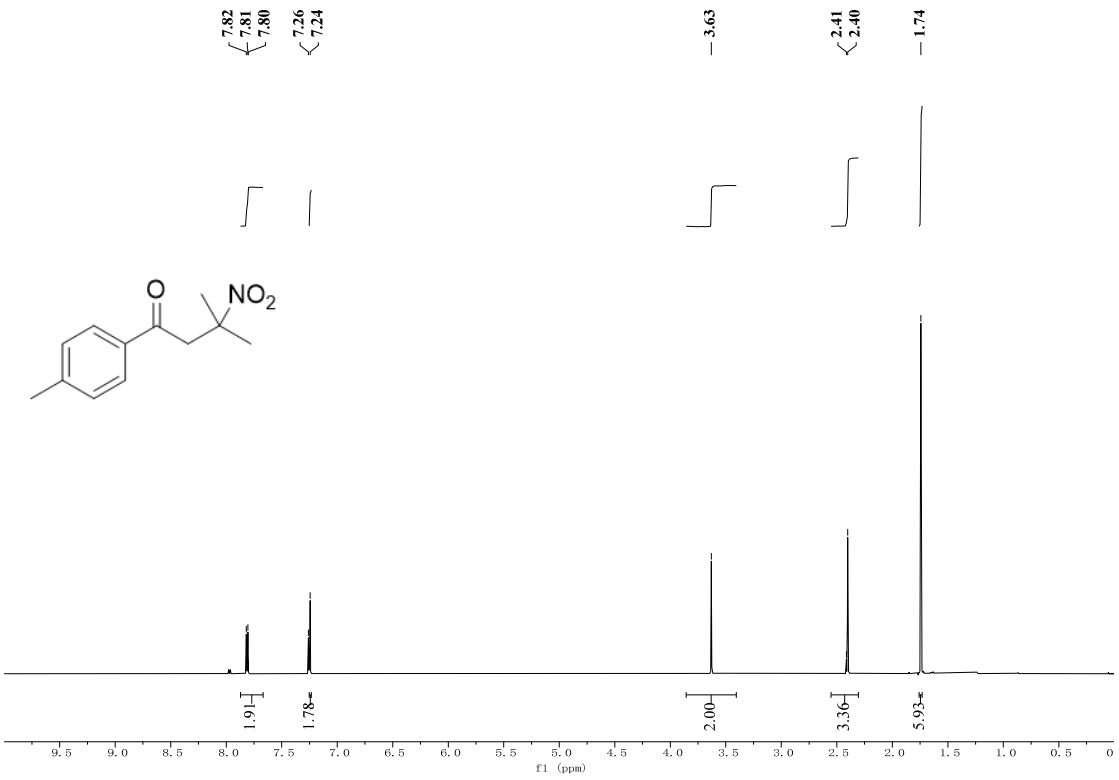

194.940
135.667
133.947
128.857
128.124
77.316
76.999
76.681
69.264
34.853
O
NO2
f1 (ppm)

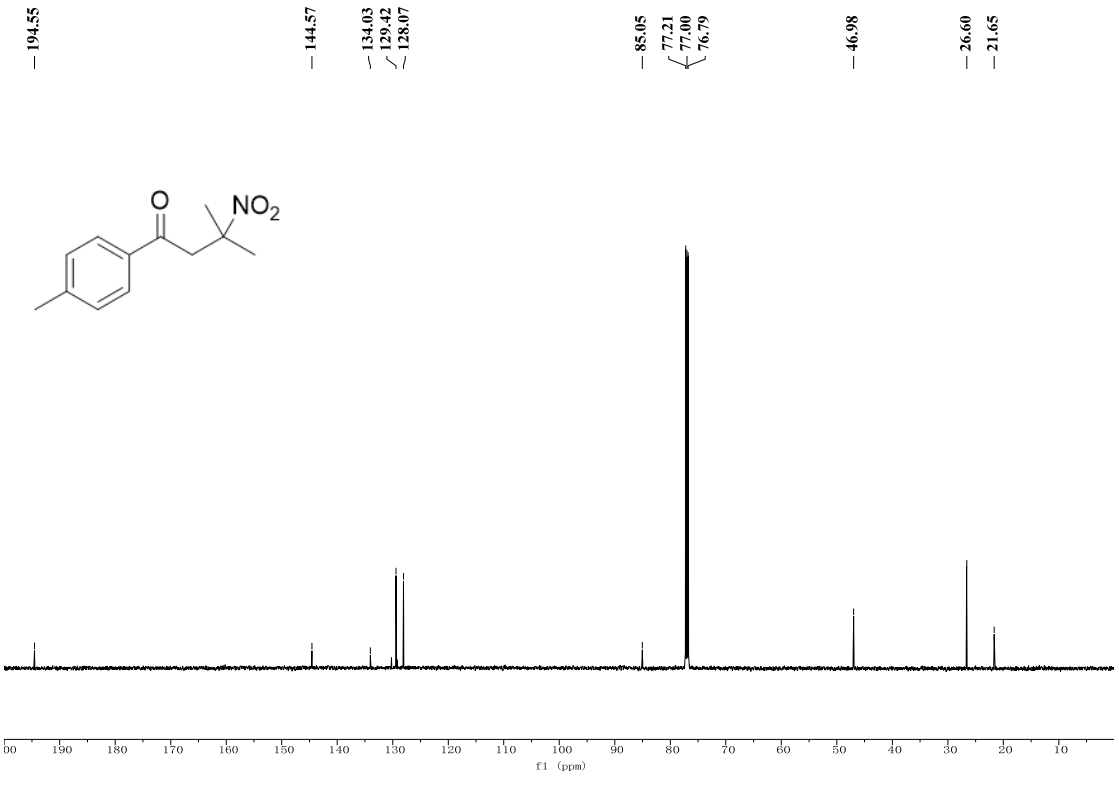

7.63
7.62
7.41
7.39
7.38
7.28
7.27
7.26
7.25
3.59
2.47
1.75
O
NO2
0.97
0.94
2.22
2.00
2.97
6.28
f1 (ppm)

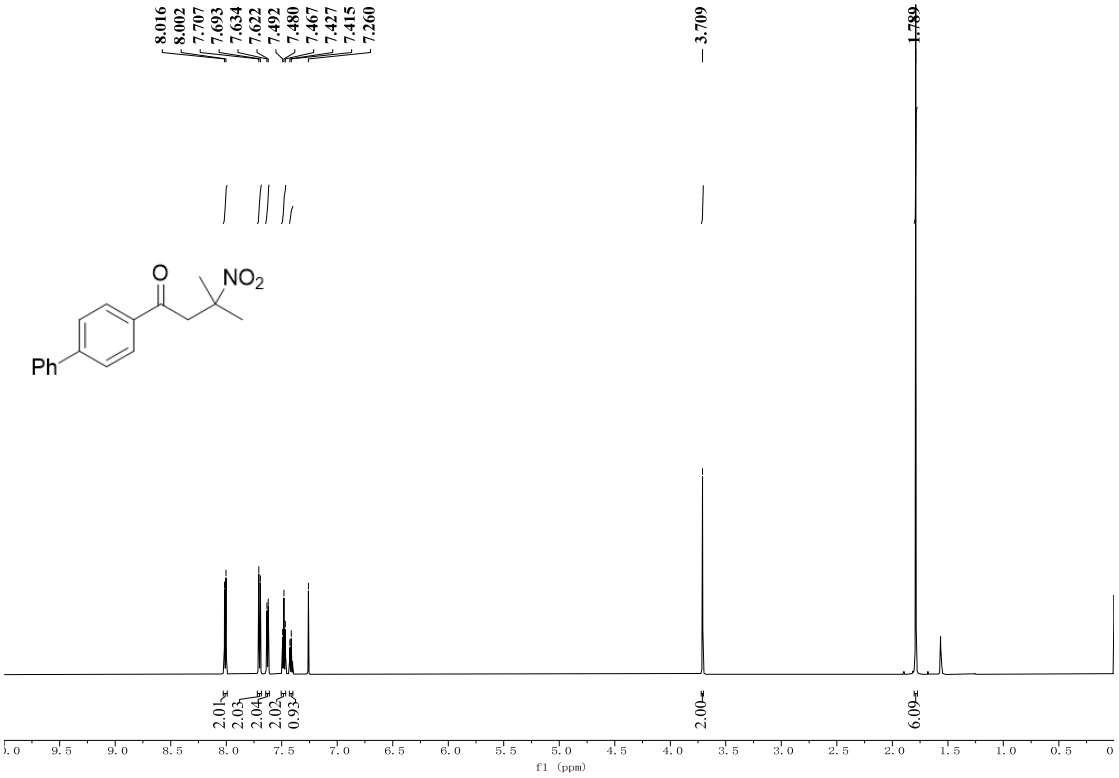

198.84
138.50
137.09
132.17
131.78
128.16
125.73
84.98
77.21
77.00
76.79
49.73
26.66
21.22
O
NO2
f1 (ppm)

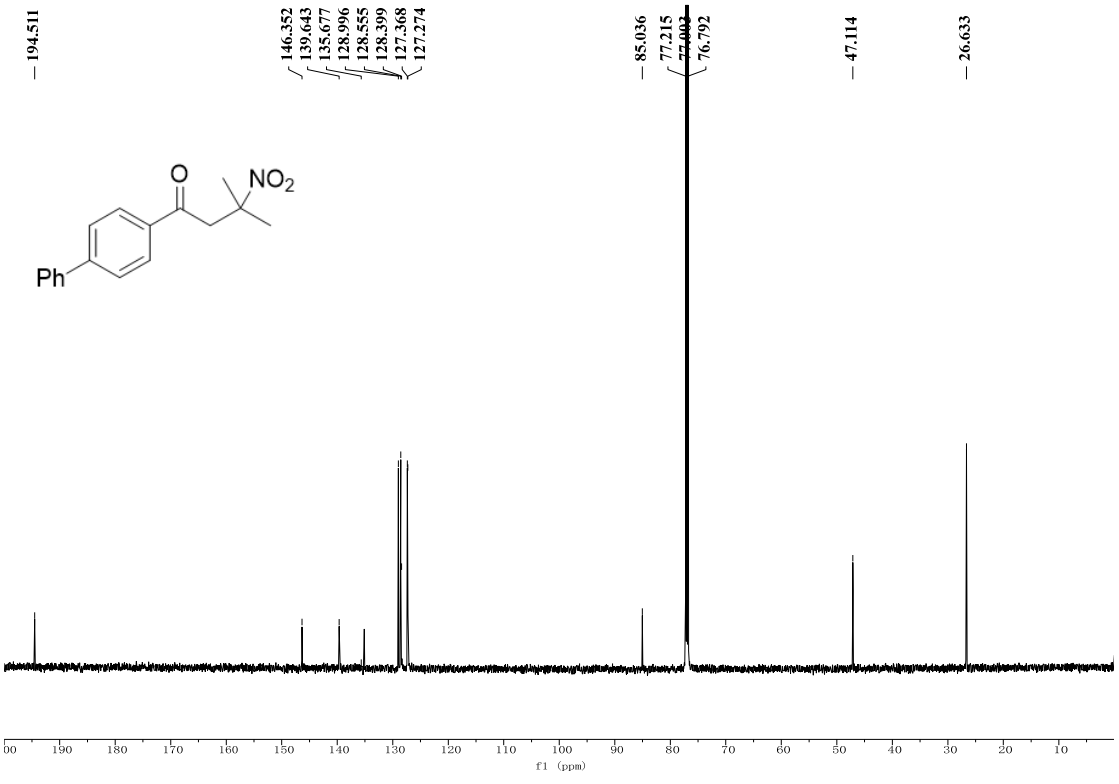

7.72
7.71
7.70
7.38
7.37
7.34
7.33
7.32
3.67
2.38
1.74
O
NO2
1.91
0.95
0.97
2.00
3.02
6.25
f1 (ppm)

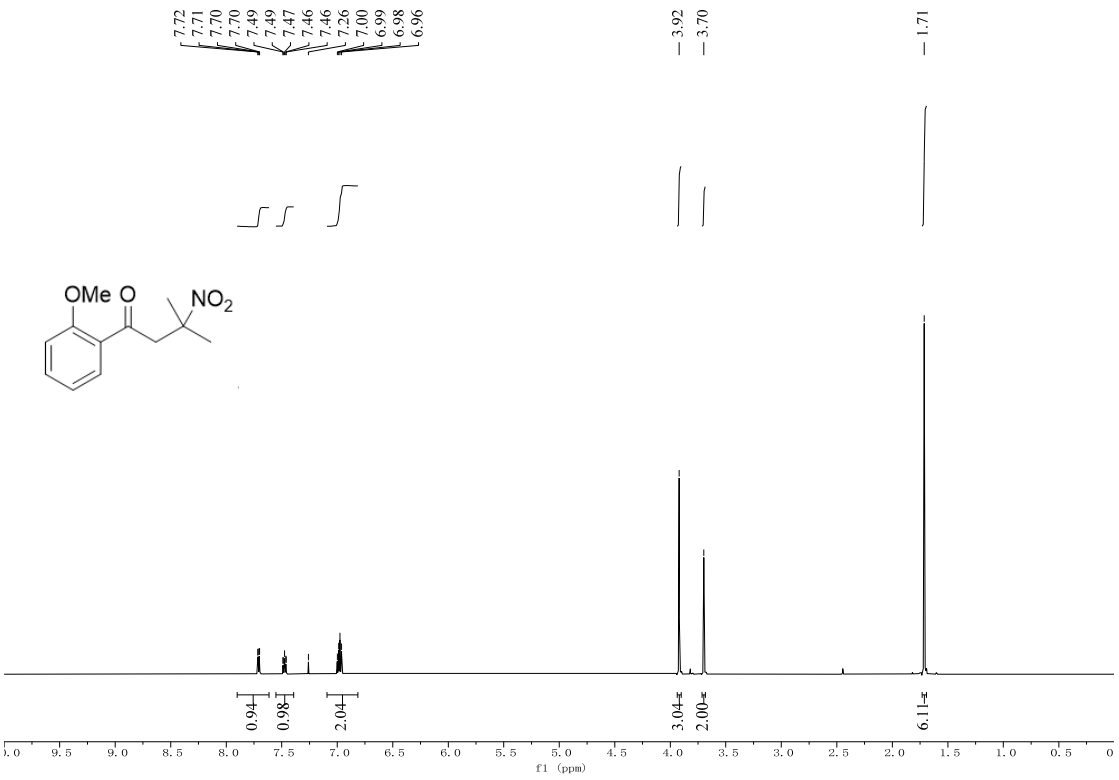

195.15
138.44
136.27
134.25
128.47
128.32
125.00
84.73
77.32
77.00
76.68
47.02
26.48
21.14
O
NO2
f1 (ppm)

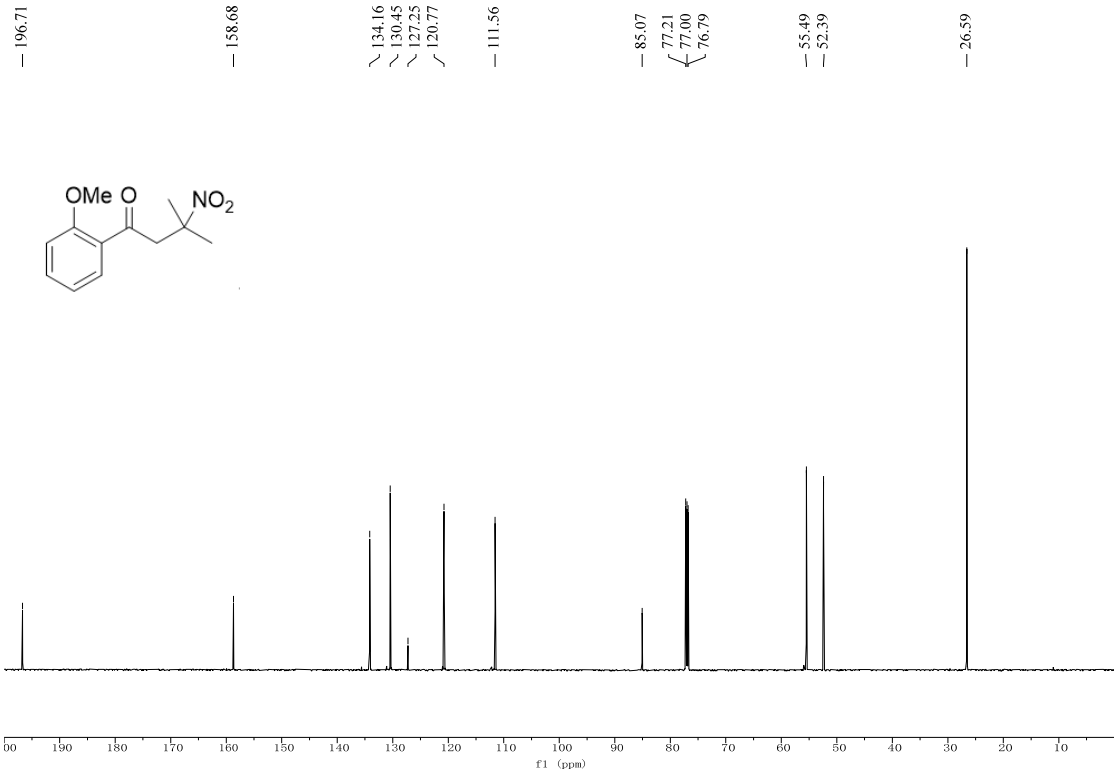

7.82
7.81
7.80
7.26
7.24
3.63
2.41
2.40
1.74
O
NO2
1.91
1.78
2.00
3.36
5.93
f1 (ppm)

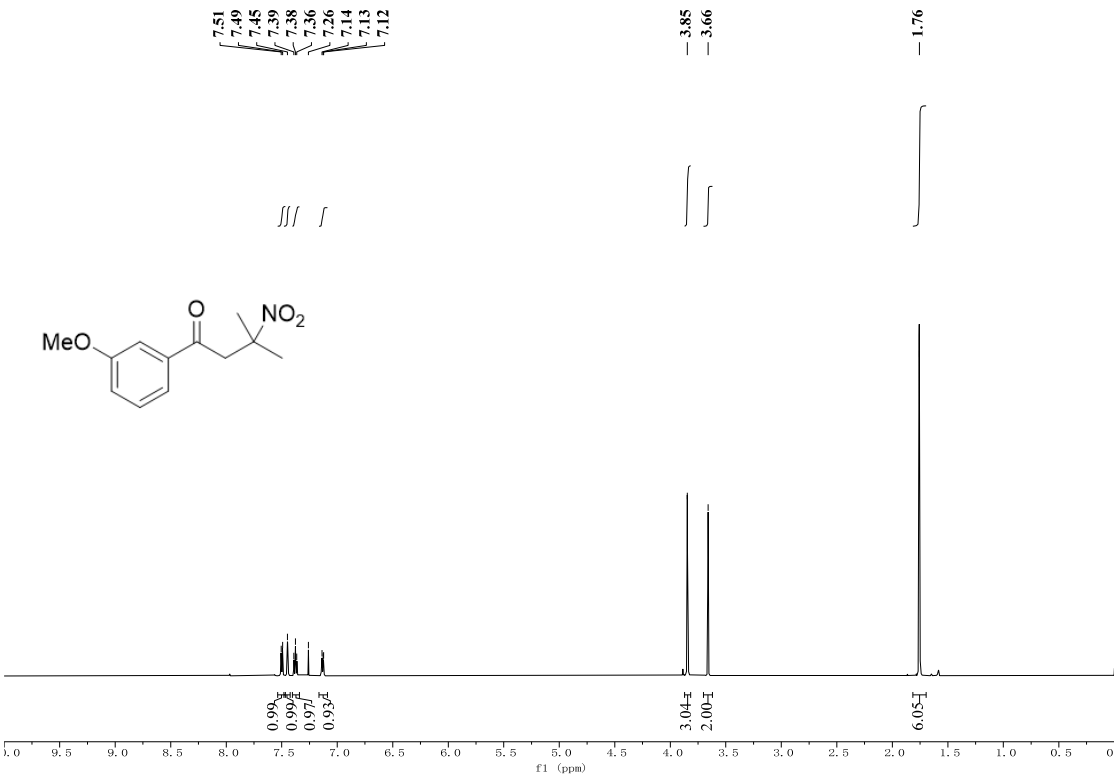

194.55
144.57
134.03
129.42
128.07
85.05
77.21
77.00
76.79
46.98
26.60
21.65
O
NO2
f1 (ppm)

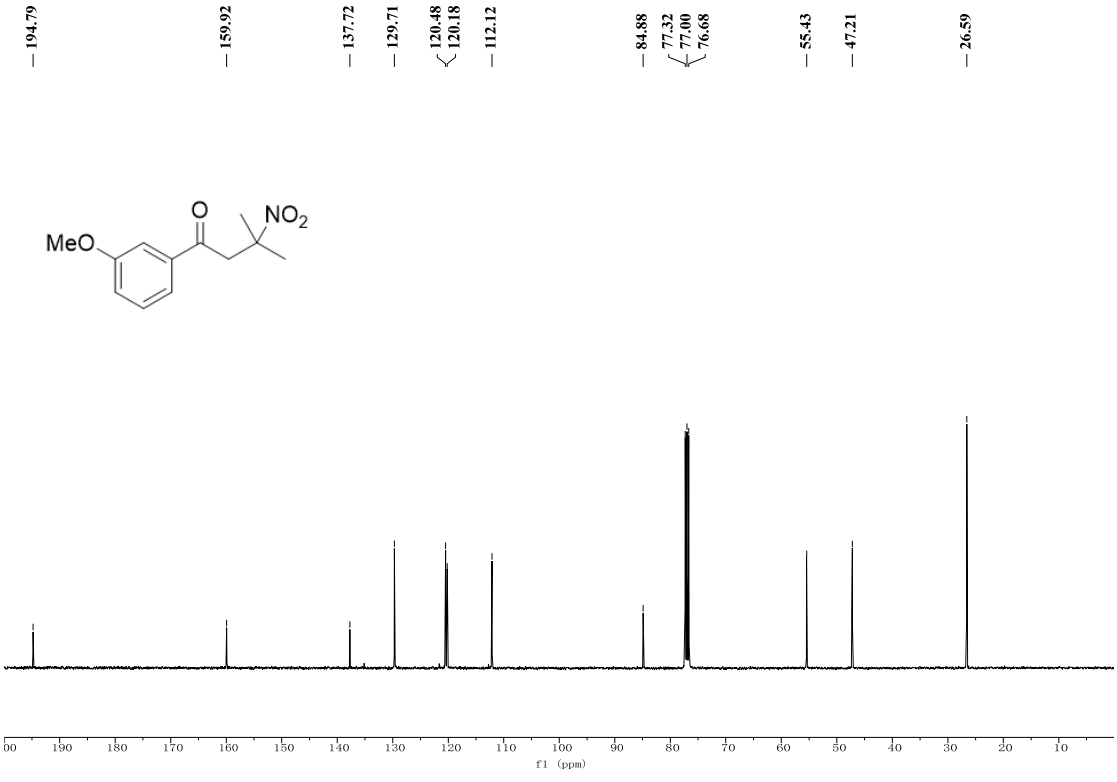

8.016
8.002
7.707
7.693
7.634
7.622
7.492
7.480
7.467
7.427
7.415
7.260
3.709
1.789
O
NO2
Ph
2.01
2.03
2.04
2.02
0.93
2.00
6.09
f1 (ppm)

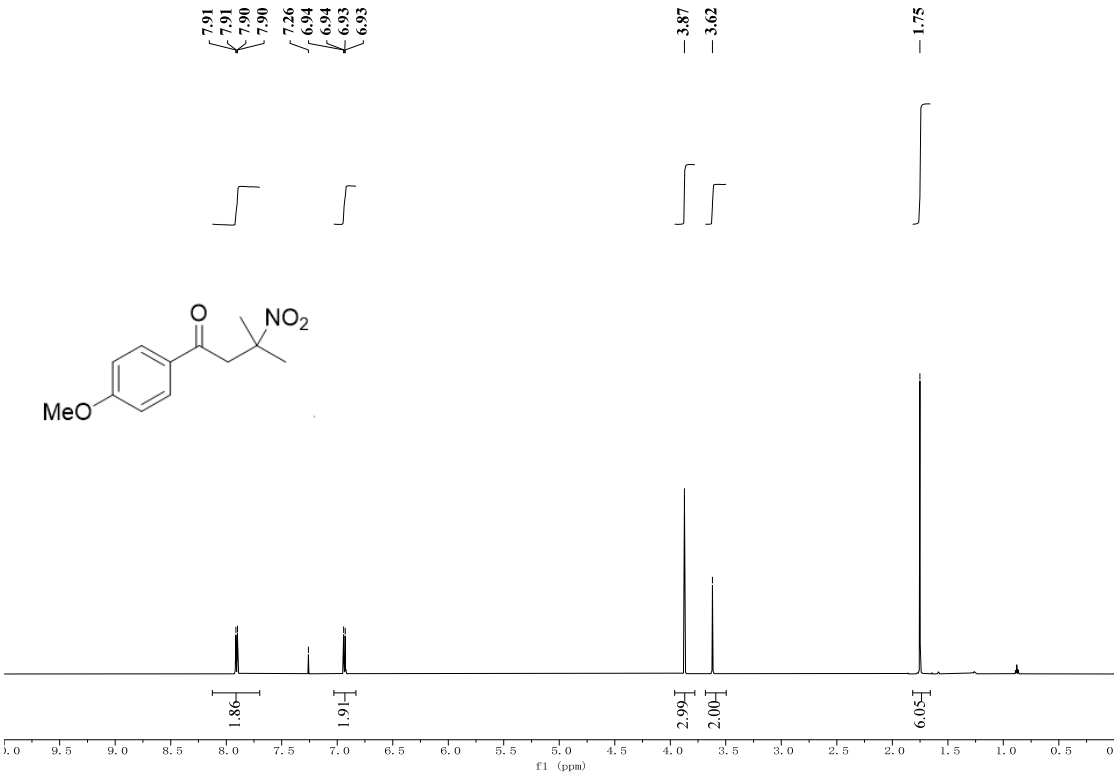

194.511
146.352
139.643
135.677
128.996
128.555
128.399
127.368
127.274
85.036
77.215
77.003
76.792
47.114
26.633
O
NO2
Ph
f1 (ppm)

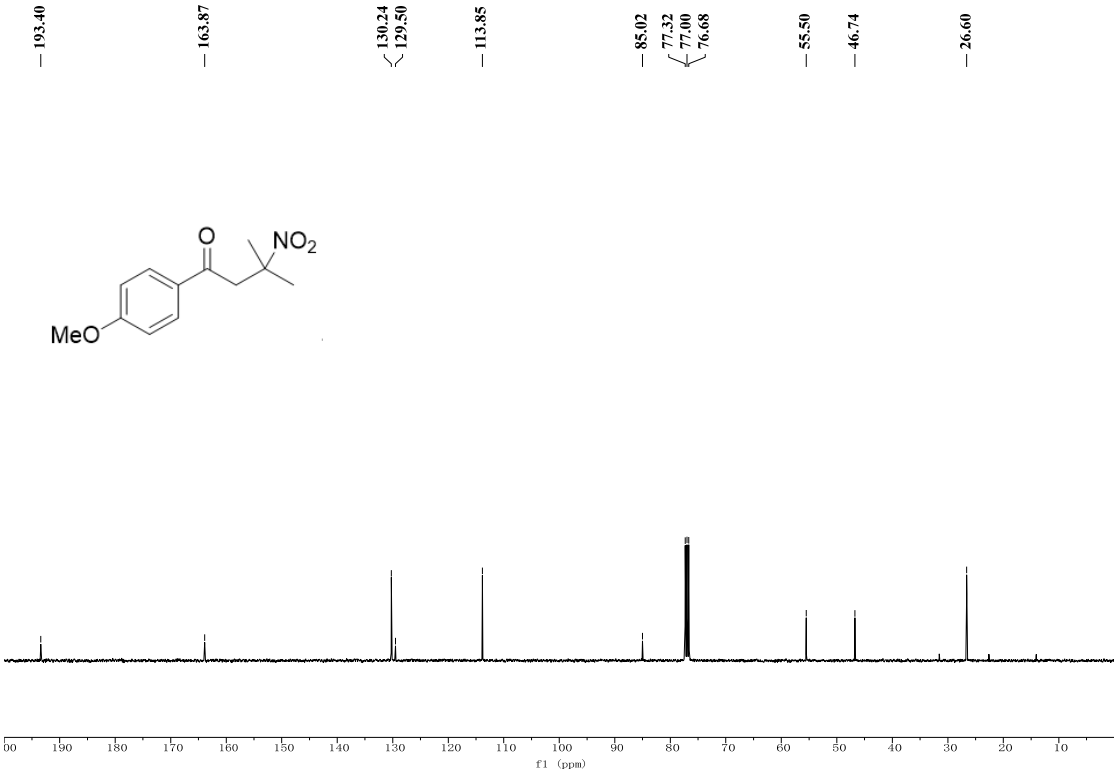

7.72
7.71
7.70
7.70
7.49
7.49
7.47
7.46
7.46
7.26
7.00
6.99
6.98
6.96
3.92
3.70
1.71
OMe O
NO2
0.94
0.98
2.04
3.04
2.00
6.11
f1 (ppm)

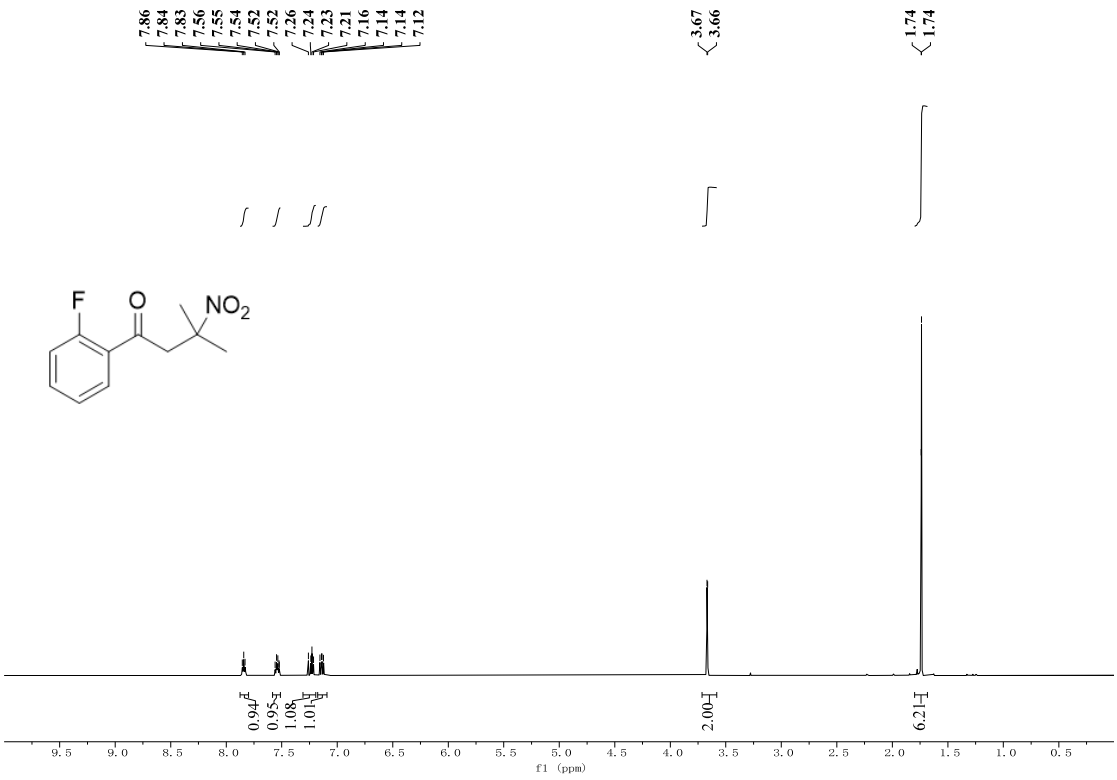

196.71
158.68
134.16
130.45
127.25
120.77
111.56
85.07
77.21
77.00
76.79
55.49
52.39
26.59
OMe O
NO2
f1 (ppm)

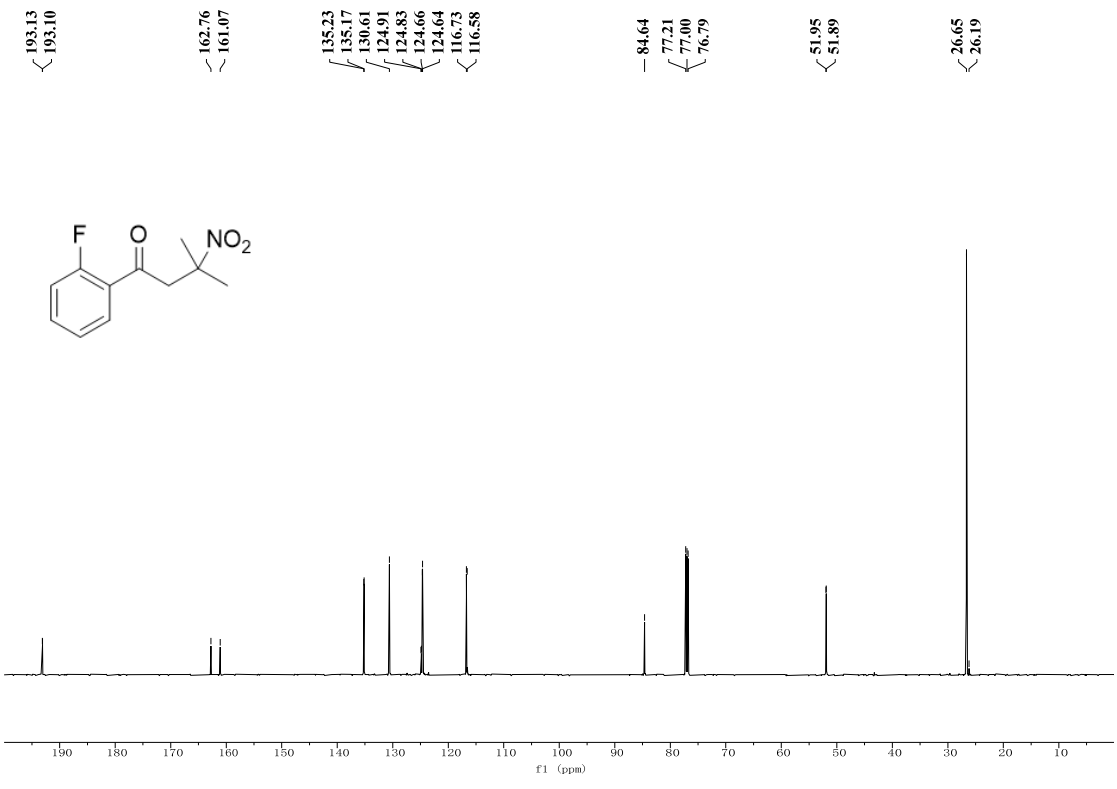

7.51
7.49
7.45
7.39
7.38
7.36
7.26
7.14
7.13
7.12
3.85
3.66
1.76
MeO
O
NO2
0.99
0.99
0.97
0.93
3.04
2.00
6.05
f1 (ppm)

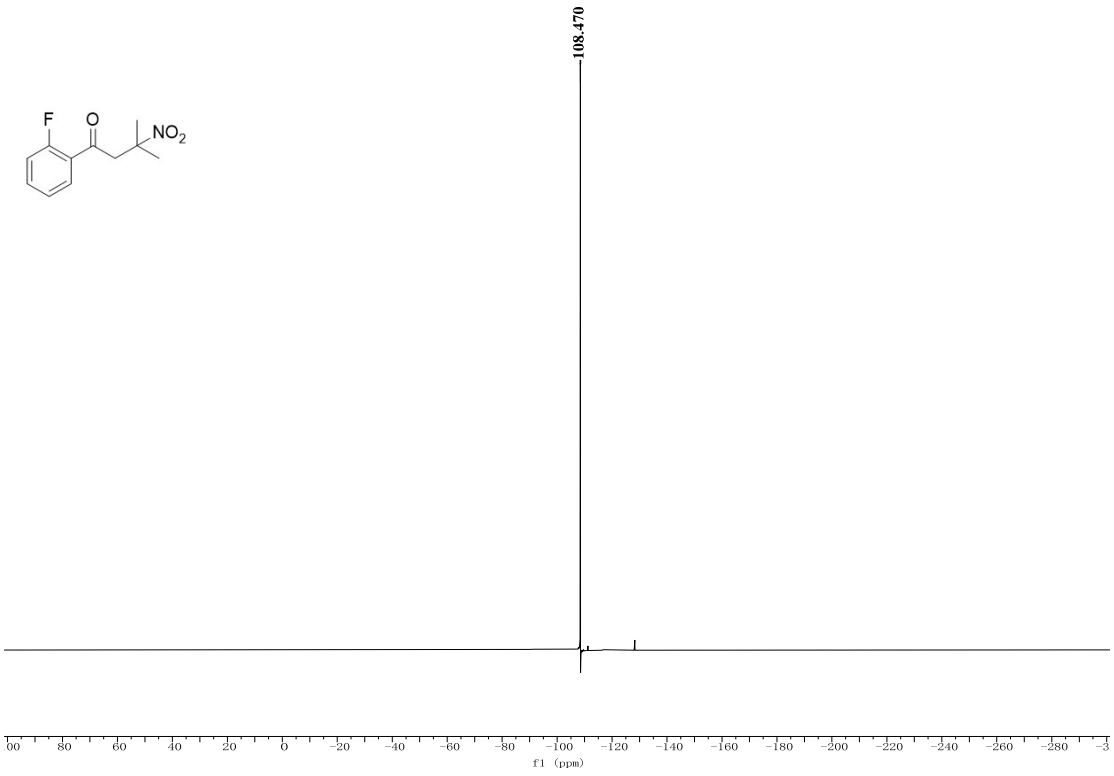

194.79
159.92
137.72
129.71
120.48
120.18
112.12
84.88
77.32
77.00
76.68
55.43
47.21
26.59
MeO
O
NO2
f1 (ppm)

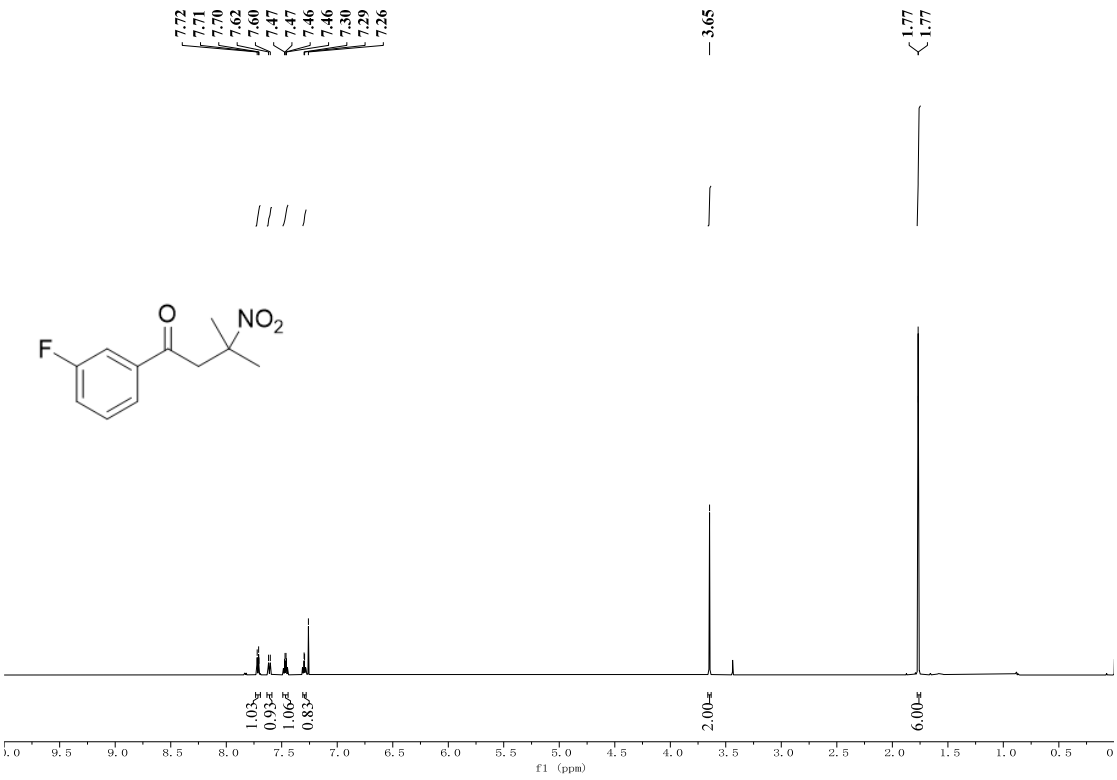

7.91
7.91
7.90
7.90
7.26
6.94
6.94
6.93
6.93
3.87
3.62
1.75
O
NO2
MeO
1.86
1.91
2.99
2.00
6.05
f1 (ppm)


193.40
163.87
130.24
129.50
113.85
85.02
77.32
77.00
76.68
55.50
46.74
26.60
O
NO2
MeO
f1 (ppm)


7.86
7.84
7.83
7.56
7.55
7.54
7.52
7.52
7.26
7.24
7.23
7.21
7.16
7.14
7.14
7.12
3.67
3.66
1.74
1.74
F
O
NO2
0.94
0.95
1.08
1.01
2.00
6.21
f1 (ppm)


193.13
193.10
162.76
161.07
135.23
135.17
130.61
124.91
124.83
124.66
124.64
116.73
116.58
84.64
77.21
77.00
76.79
51.95
51.89
26.65
26.19
F
O
NO2
f1 (ppm)


F
O
NO2
-108.470
f1 (ppm)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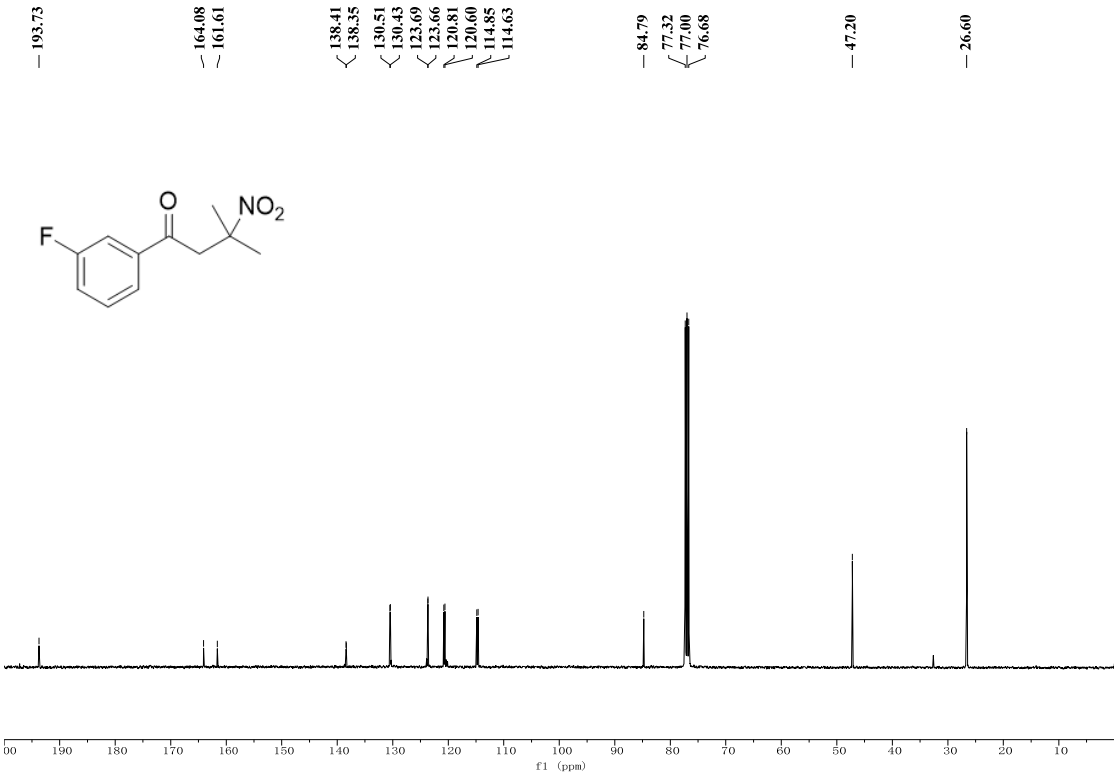
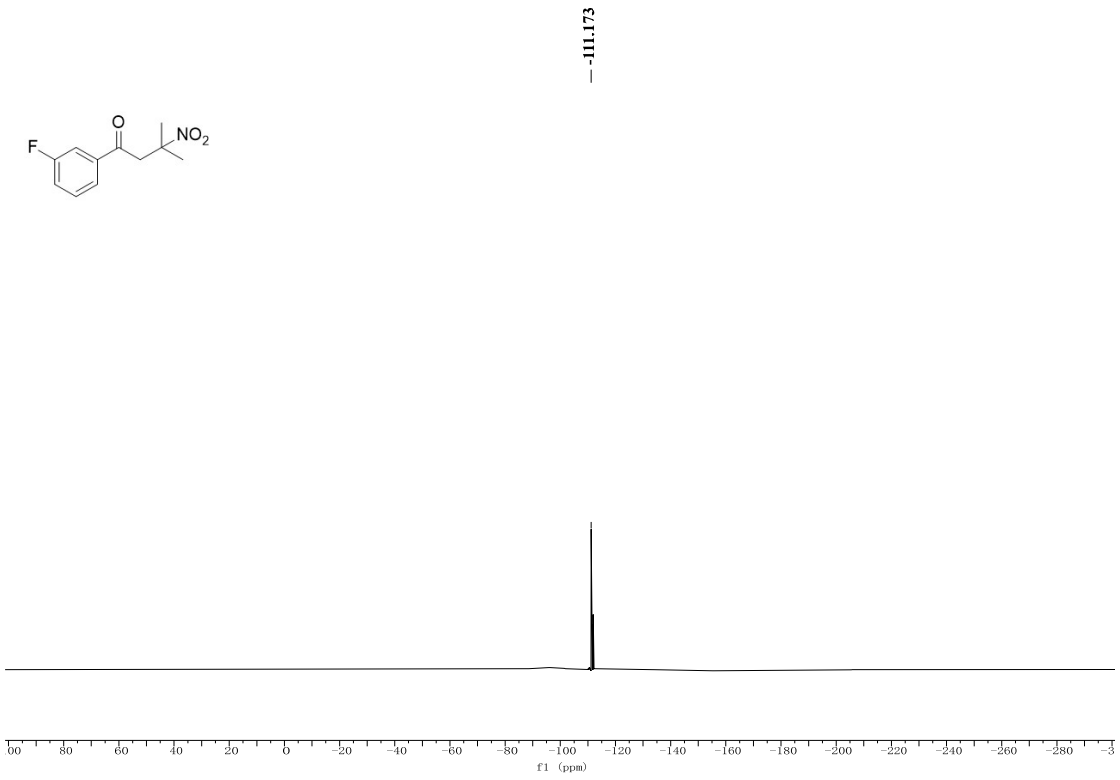
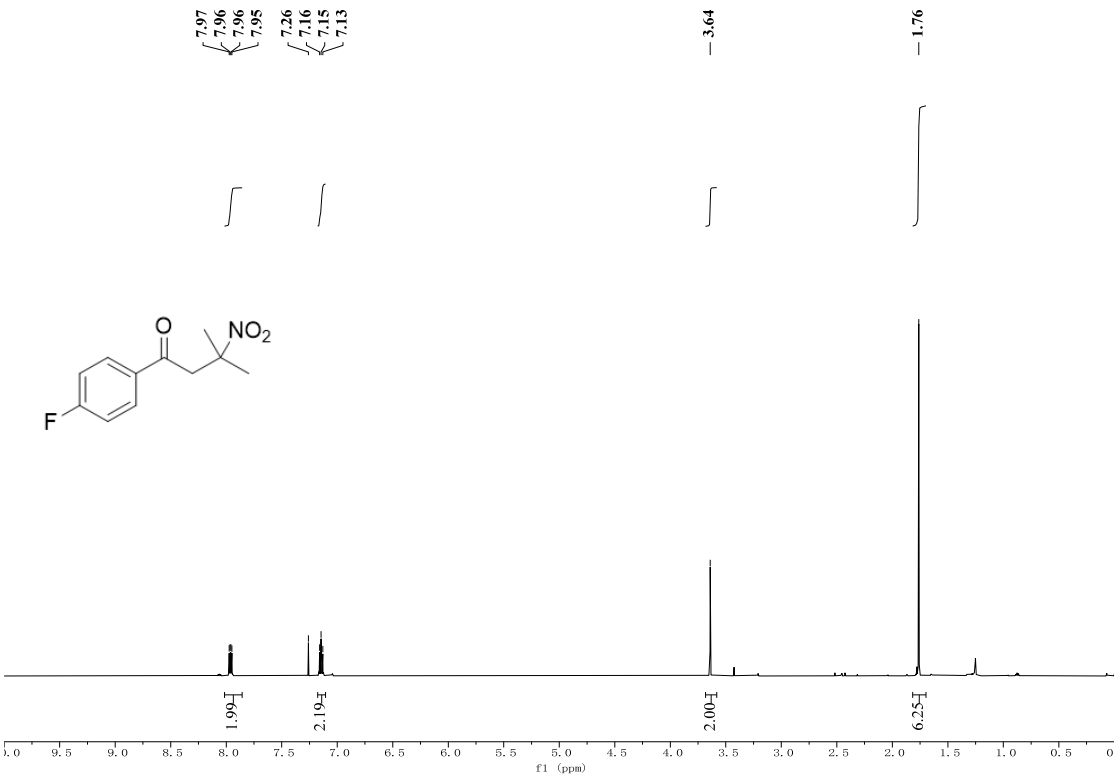
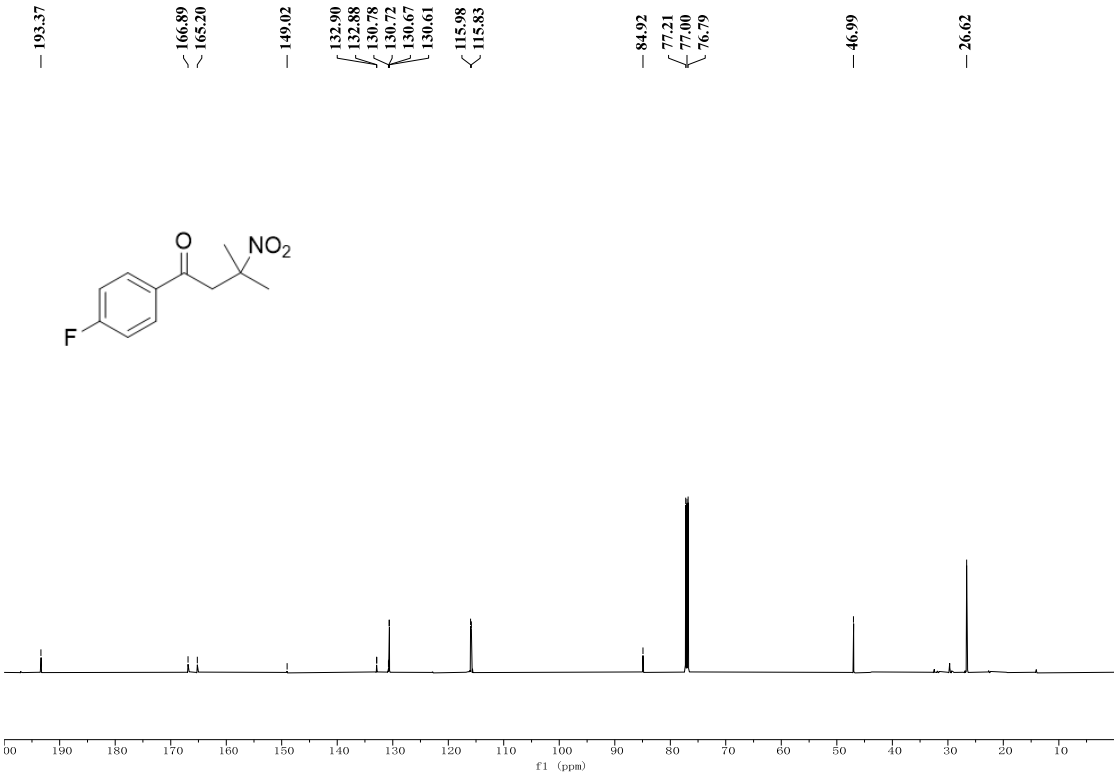
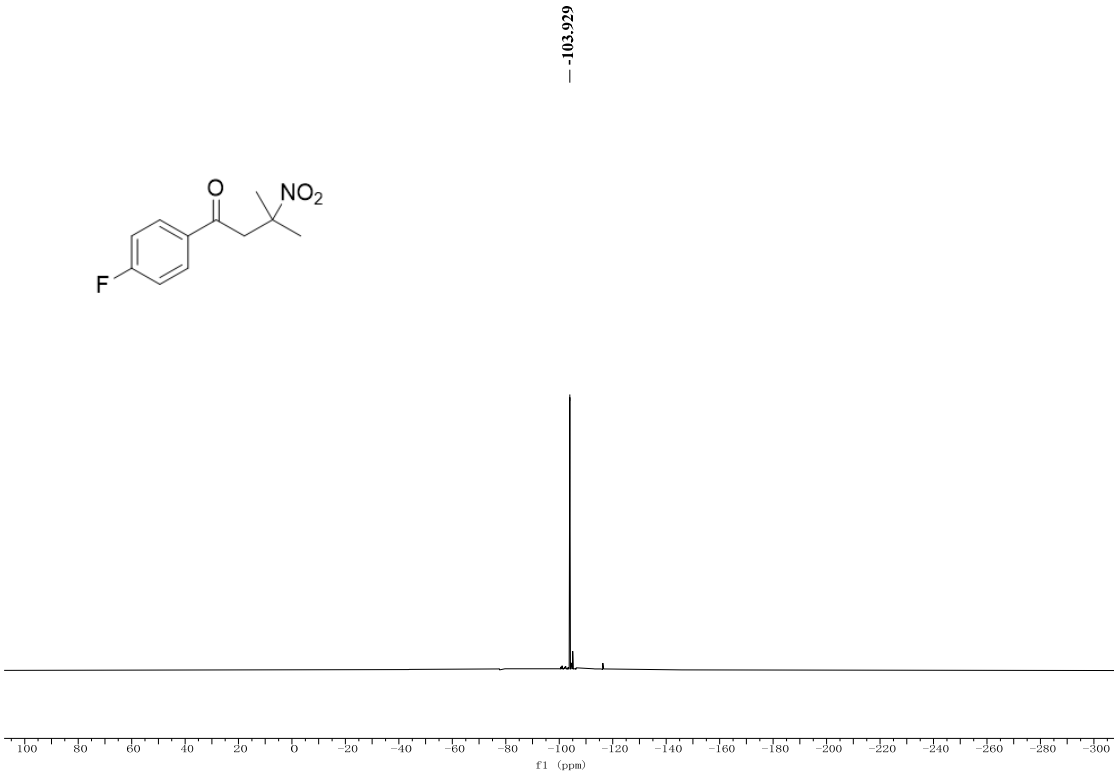
7.71
7.70
7.62
7.60
7.47
7.47
7.46
7.46
7.30
7.29
7.26
3.65
1.77
1.77
O
NO2
F
1.03
0.93
1.06
0.83
2.00
6.00
f1 (ppm)

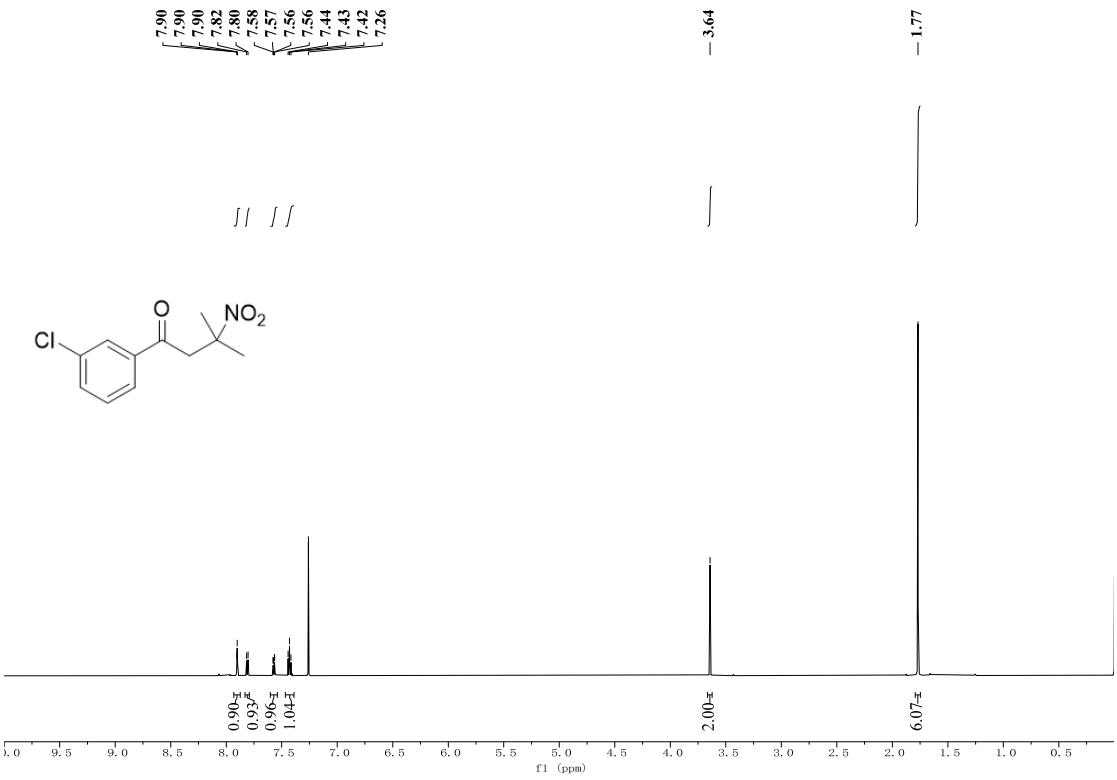

193.73
164.08
161.61
138.41
138.35
130.51
130.43
123.69
123.66
120.81
120.60
114.85
114.63
84.79
77.32
77.00
76.68
47.20
26.60
O
NO2
F
f1 (ppm)

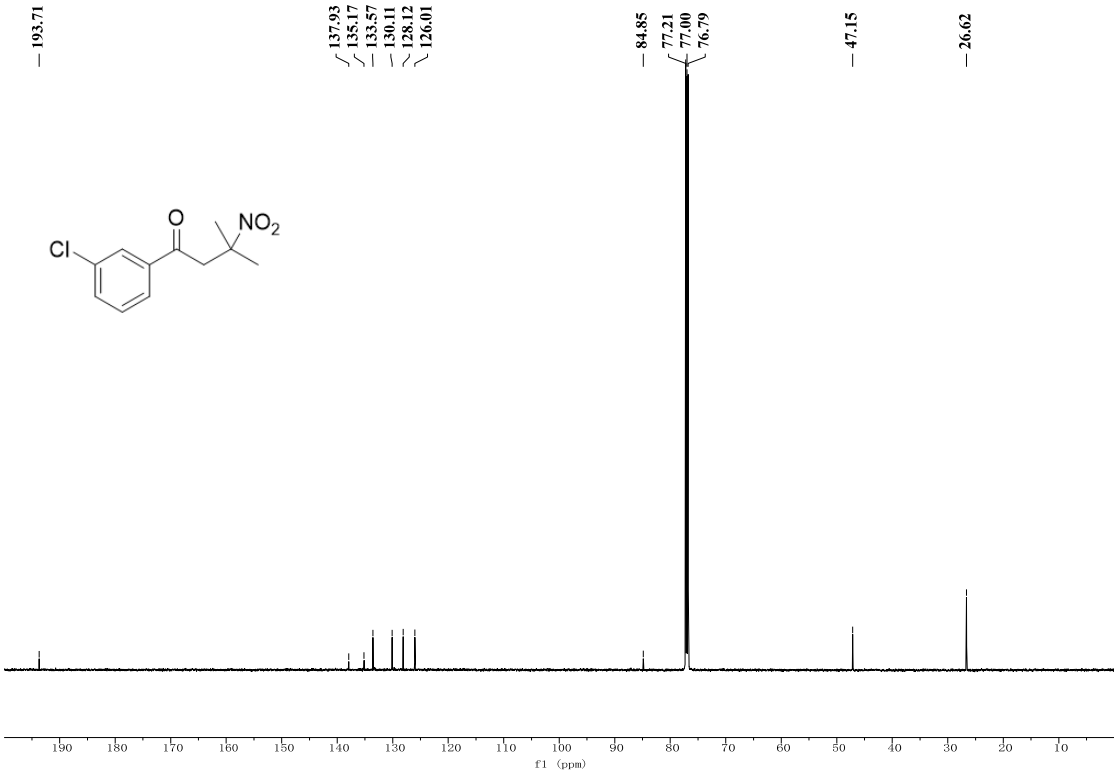

-111.173
O
F
NO2
00
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−220
−240
−260
−280
−3
f1 (ppm)

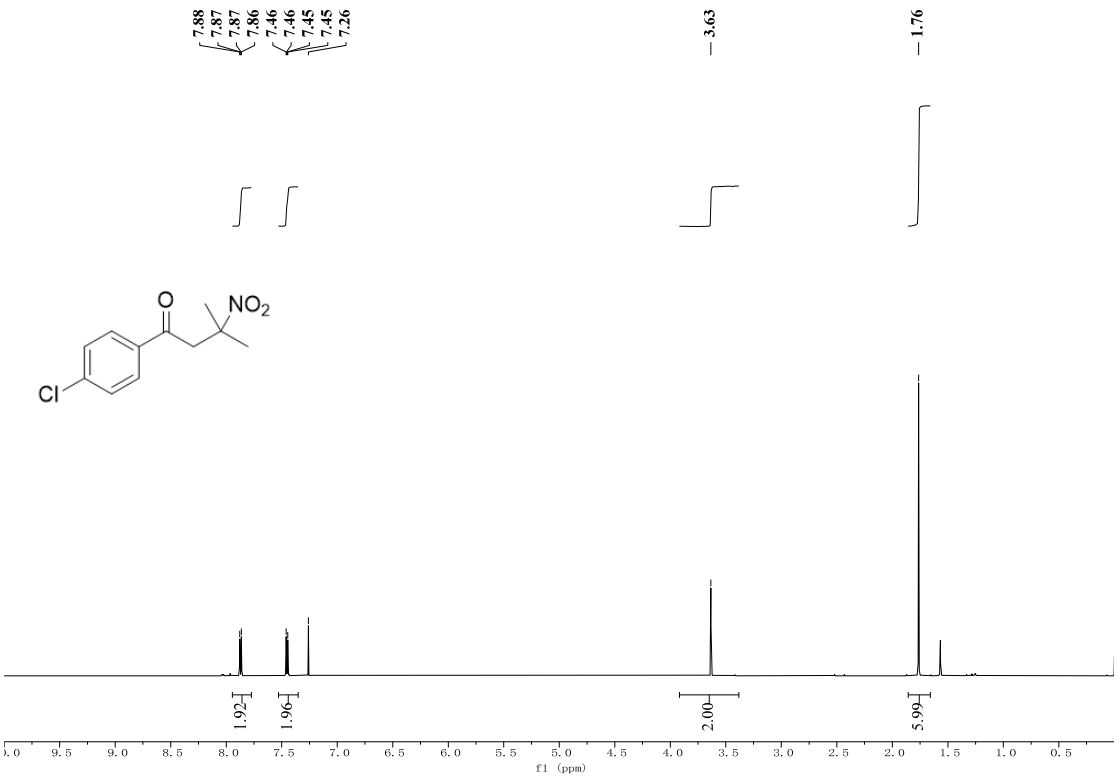

7.97
7.96
7.96
7.95
7.26
7.16
7.15
7.13
3.64
1.76
O
NO2
F
1.99
2.19
2.00
6.25
f1 (ppm)

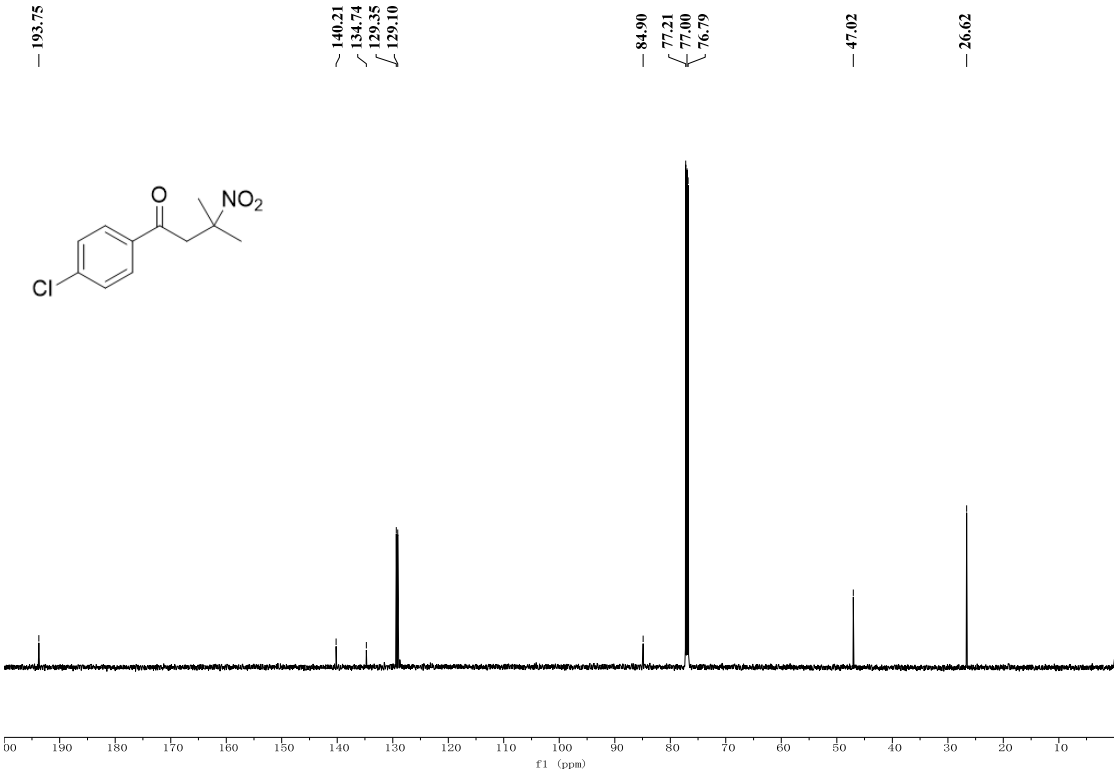

193.37
166.89
165.20
149.02
132.90
132.88
130.78
130.72
130.67
130.61
115.98
115.83
84.92
77.21
77.00
76.79
46.99
26.62
O
NO2
F
f1 (ppm)


-103.929
O
NO2
F
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)


7.90
7.90
7.90
7.82
7.80
7.58
7.57
7.56
7.56
7.44
7.43
7.42
7.26
3.64
1.77
Cl
O
NO2
0.90
0.93
0.96
1.04
2.00
6.07
f1 (ppm)


193.71
137.93
135.17
133.57
130.11
128.12
126.01
84.85
77.21
77.00
76.79
47.15
26.62
Cl
O
NO2
f1 (ppm)


7.88
7.87
7.87
7.86
7.46
7.46
7.45
7.45
7.26
3.63
1.76
O
NO2
Cl
1.92
1.96
2.00
5.99
f1 (ppm)


193.75
140.21
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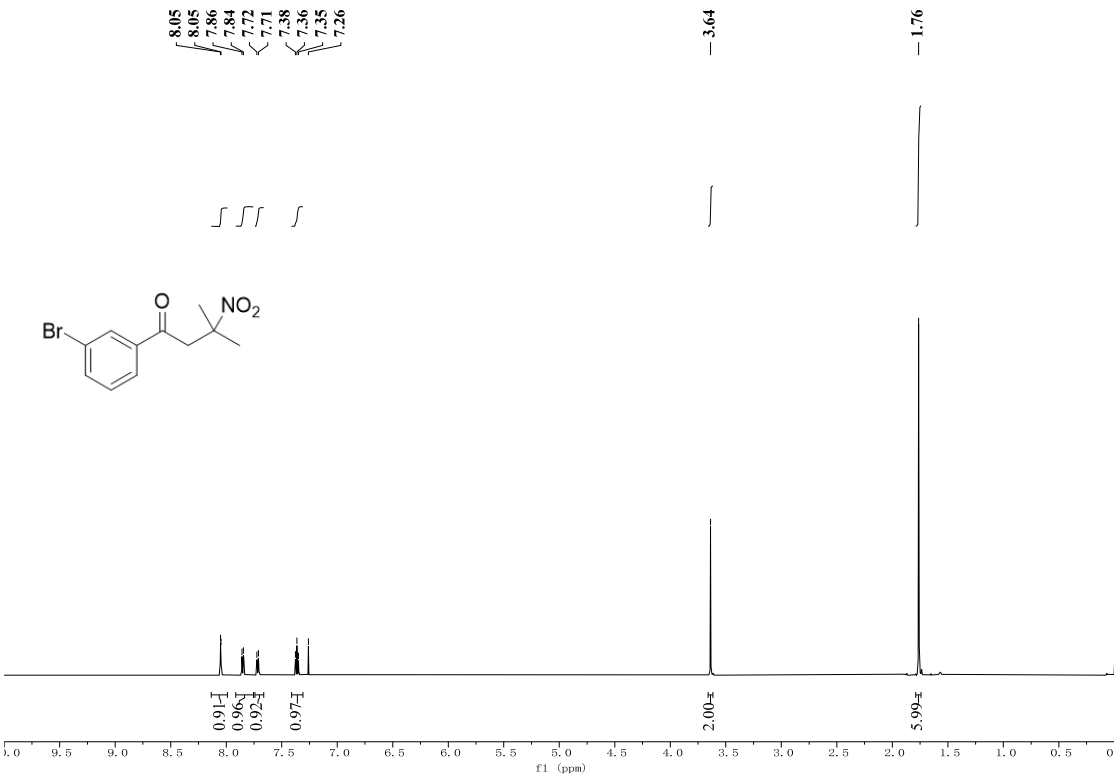
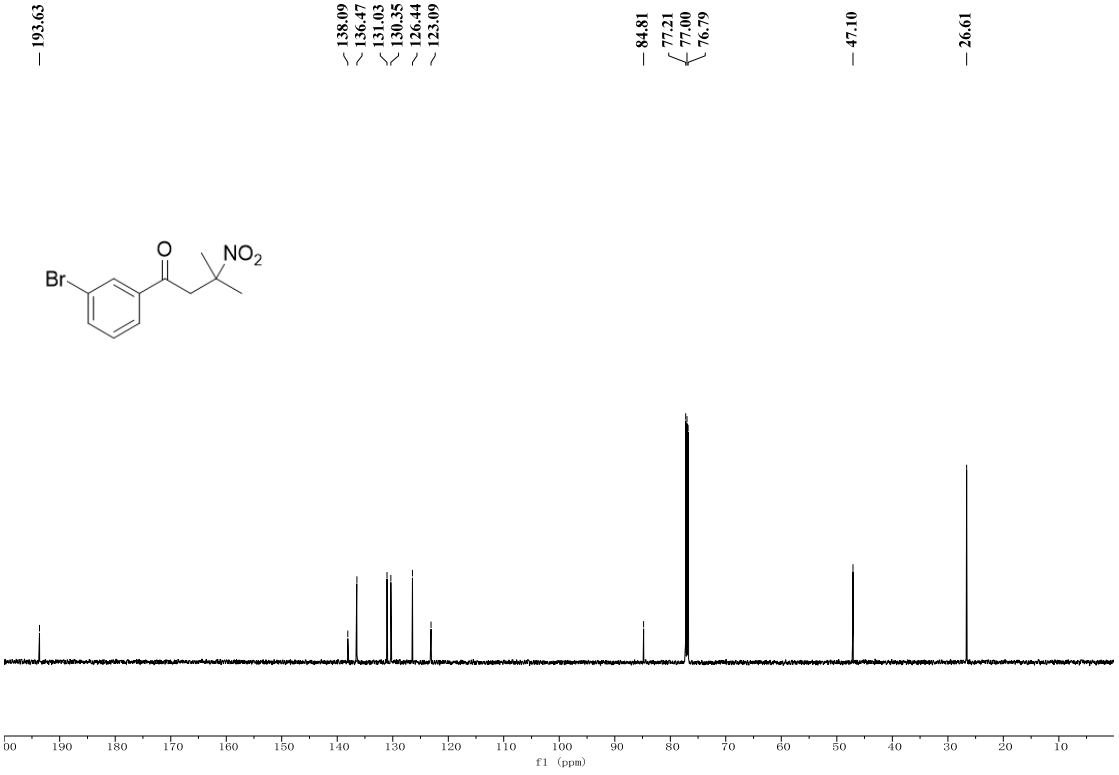
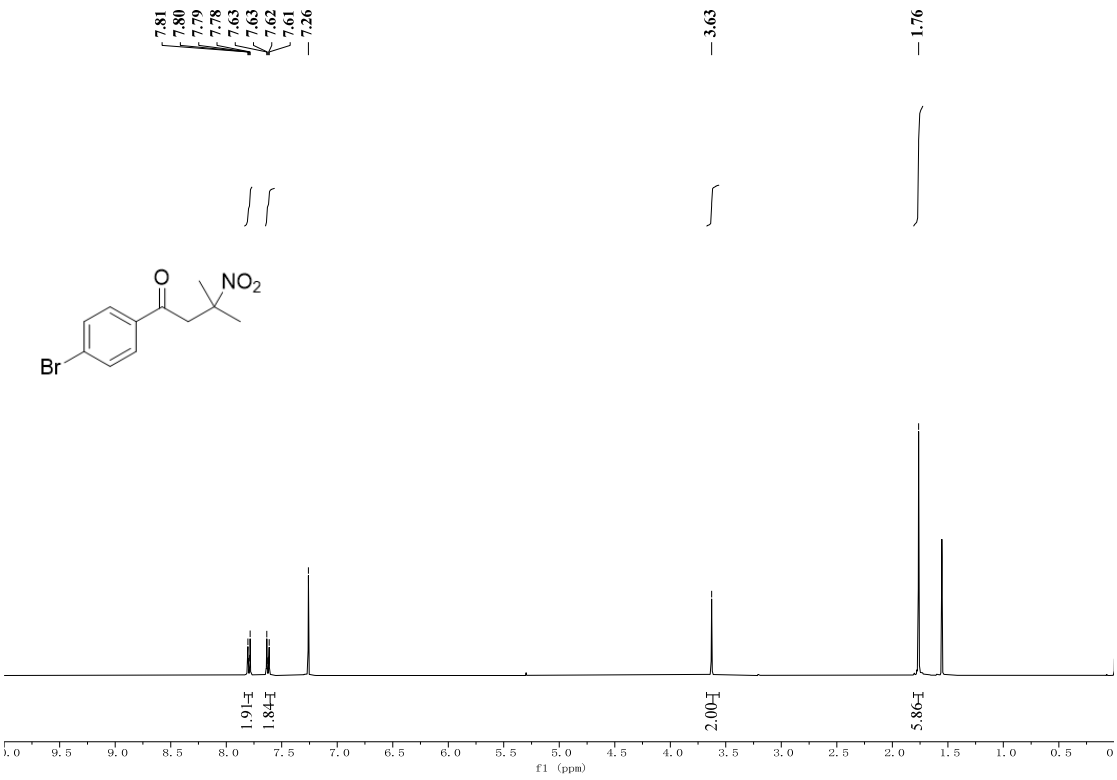
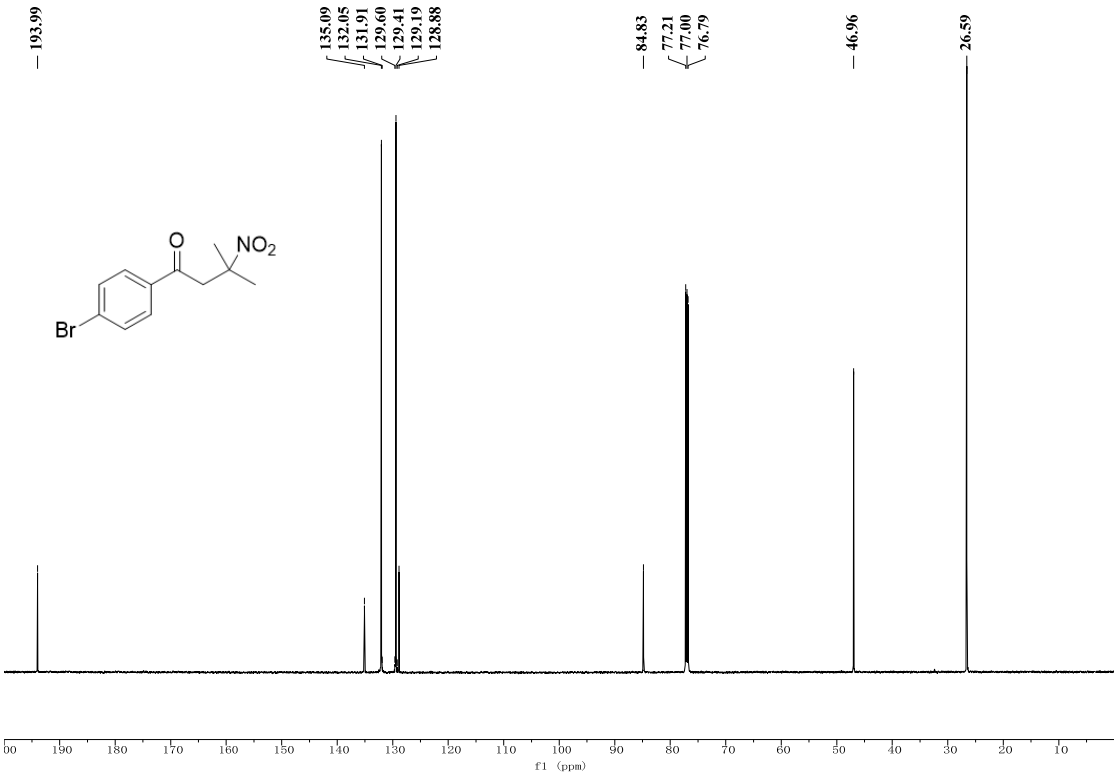
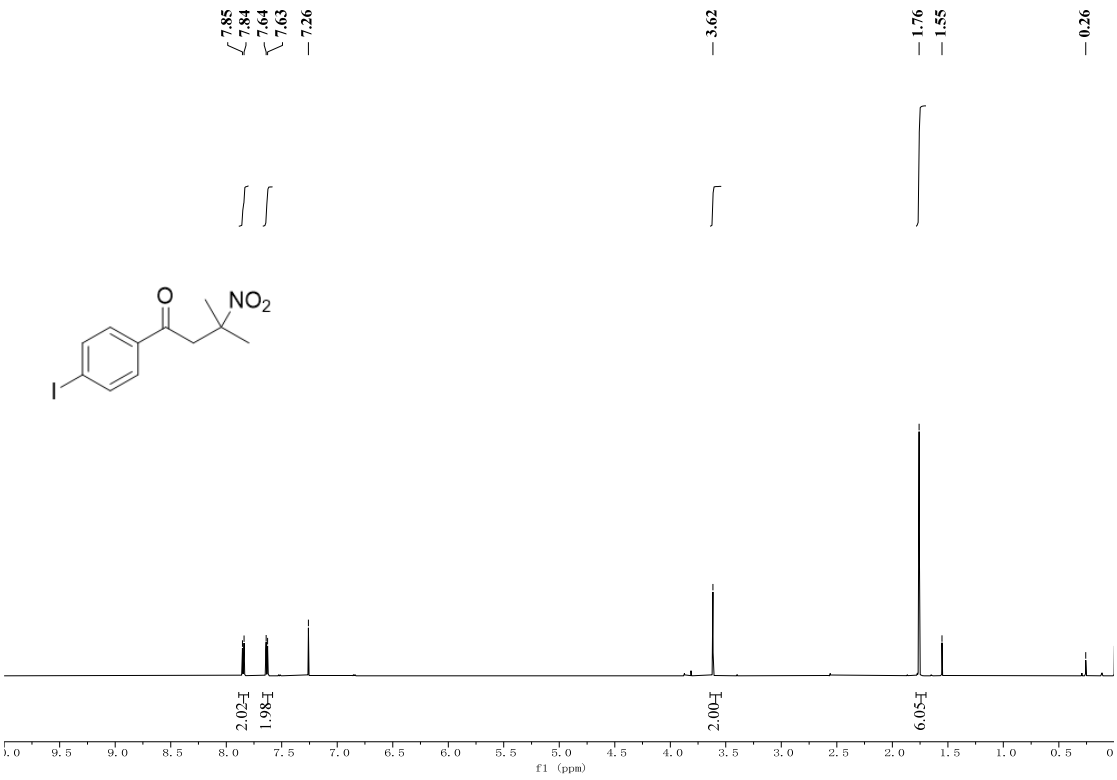
129.35
129.10
84.90
77.21
77.00
76.79
47.02
26.62
O
NO2
Cl
f1 (ppm)

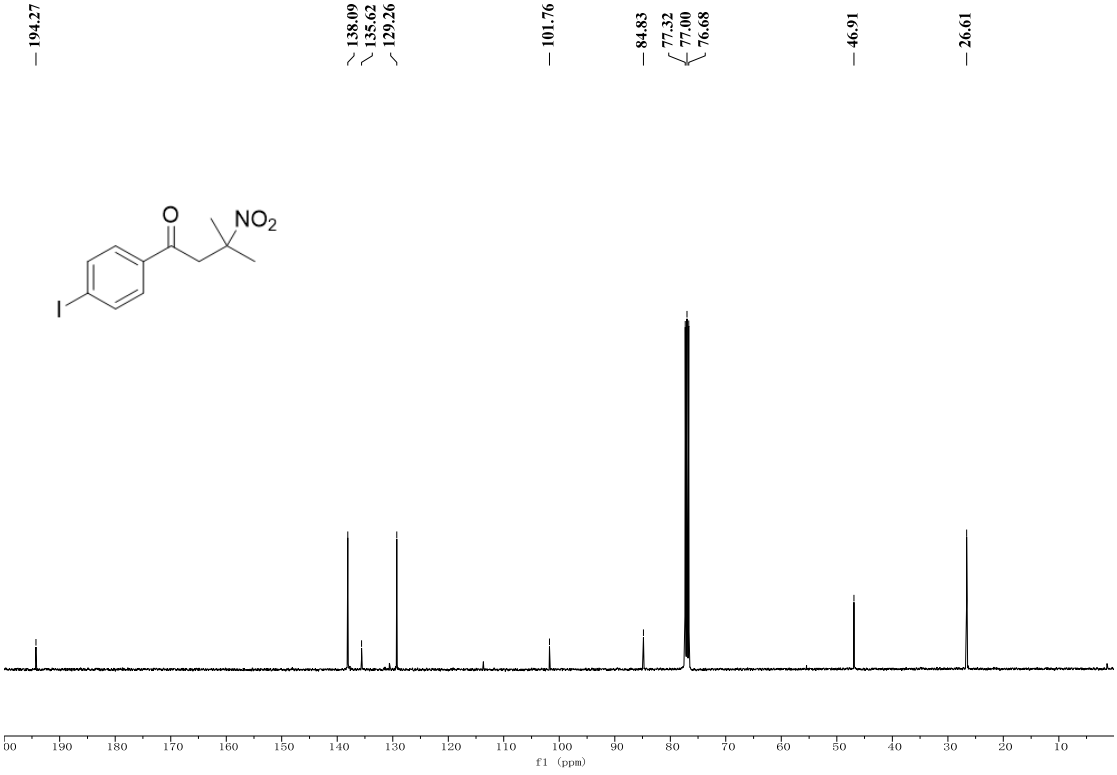

8.05
8.05
7.86
7.84
7.72
7.71
7.38
7.36
7.35
7.26
3.64
1.76
O
NO2
Br
0.91
0.96
0.92
0.97
2.00
5.99
f1 (ppm)


193.63
138.09
136.47
131.03
130.35
126.44
123.09
84.81
77.21
77.00
76.79
47.10
26.61
O
NO2
Br
f1 (ppm)


7.81
7.80
7.79
7.78
7.63
7.63
7.62
7.61
7.26
3.63
1.76
O
NO2
Br
1.91
1.84
2.00
5.86
f1 (ppm)


193.99
135.09
132.05
131.91
129.60
129.41
129.19
128.88
84.83
77.21
77.00
76.79
46.96
26.59
O
NO2
Br
f1 (ppm)


7.85
7.84
7.64
7.63
7.26
3.62
1.76
1.55
0.26
O
NO2
I
2.02
1.98
2.00
6.05
f1 (ppm)


194.27
138.09
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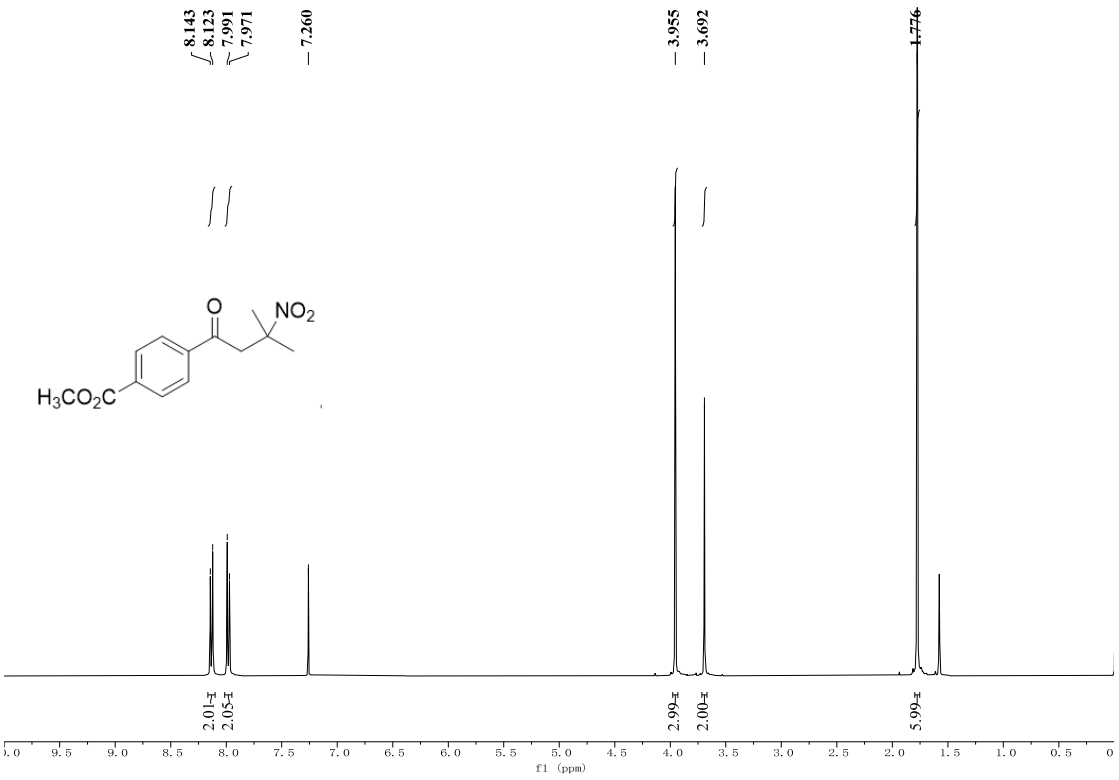
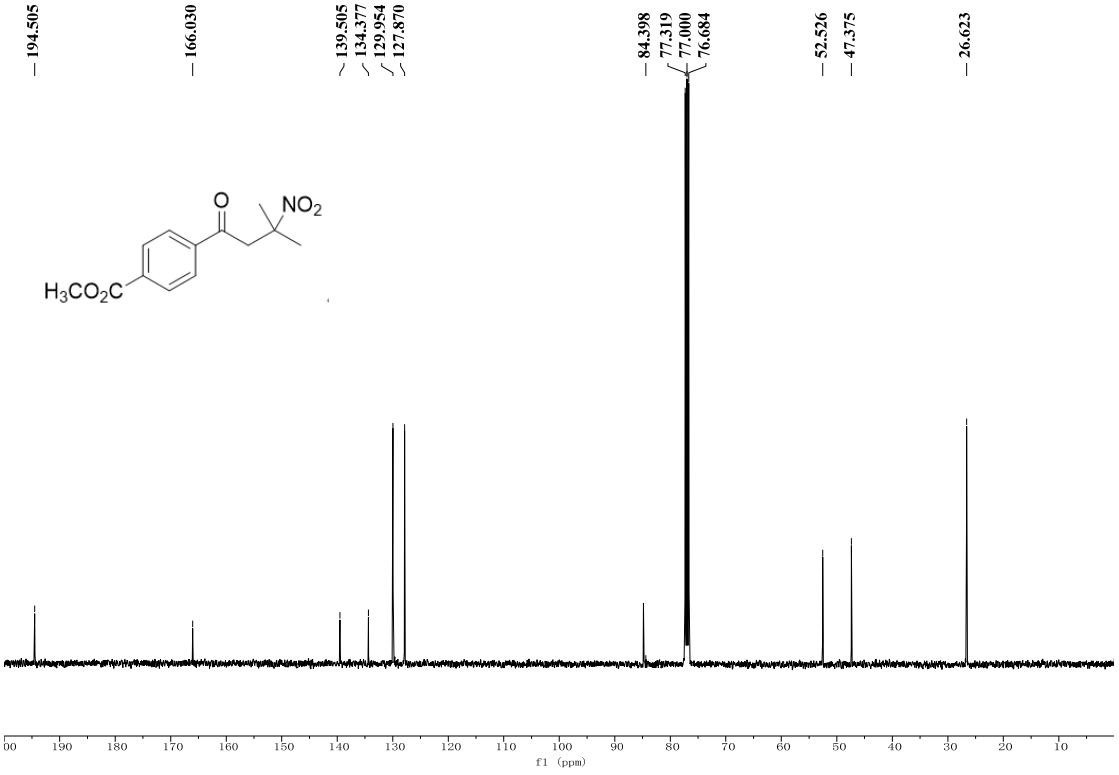
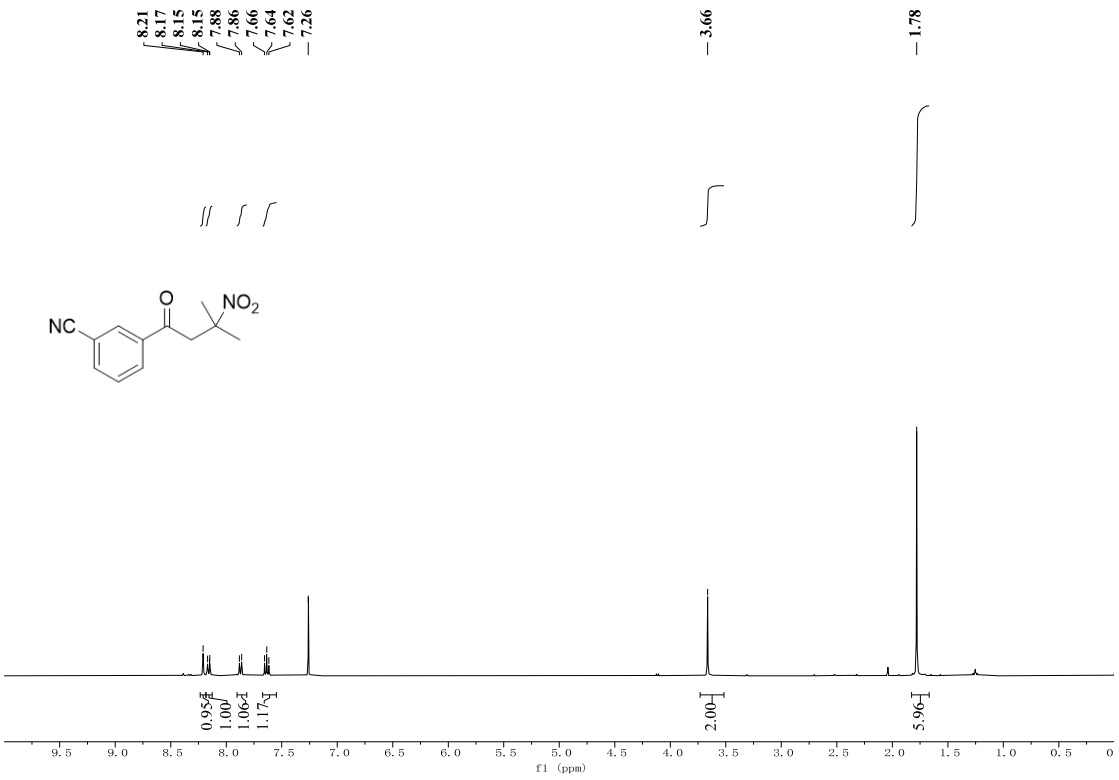
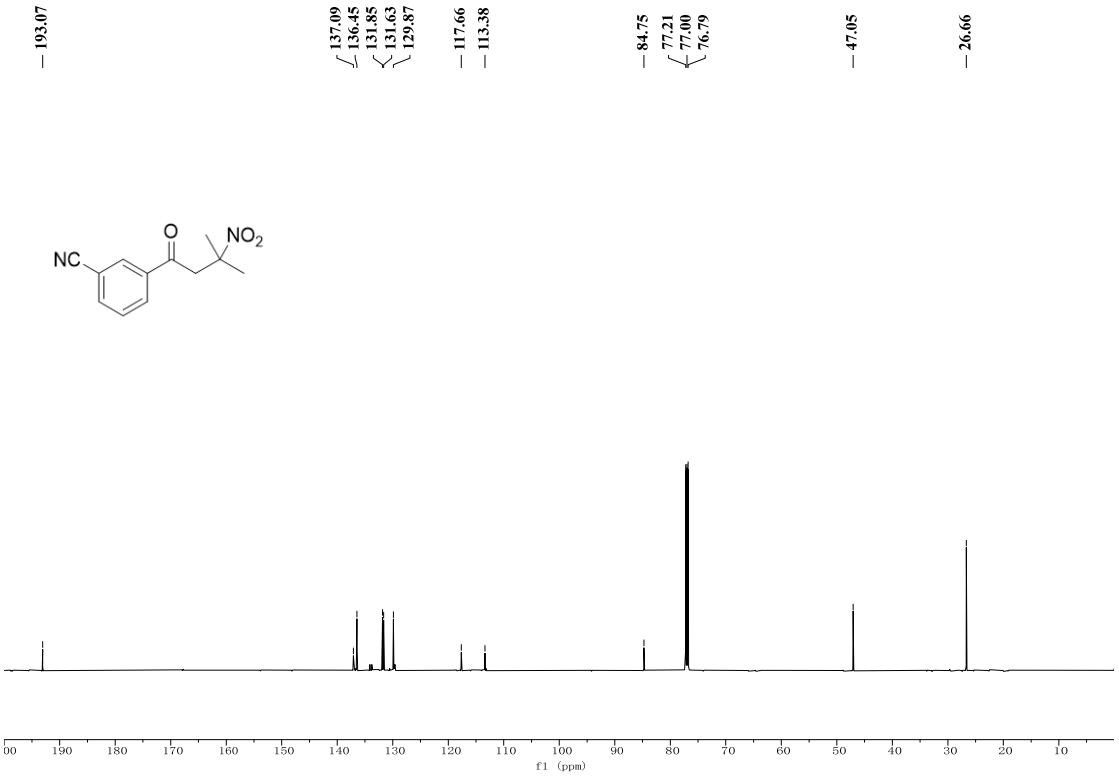
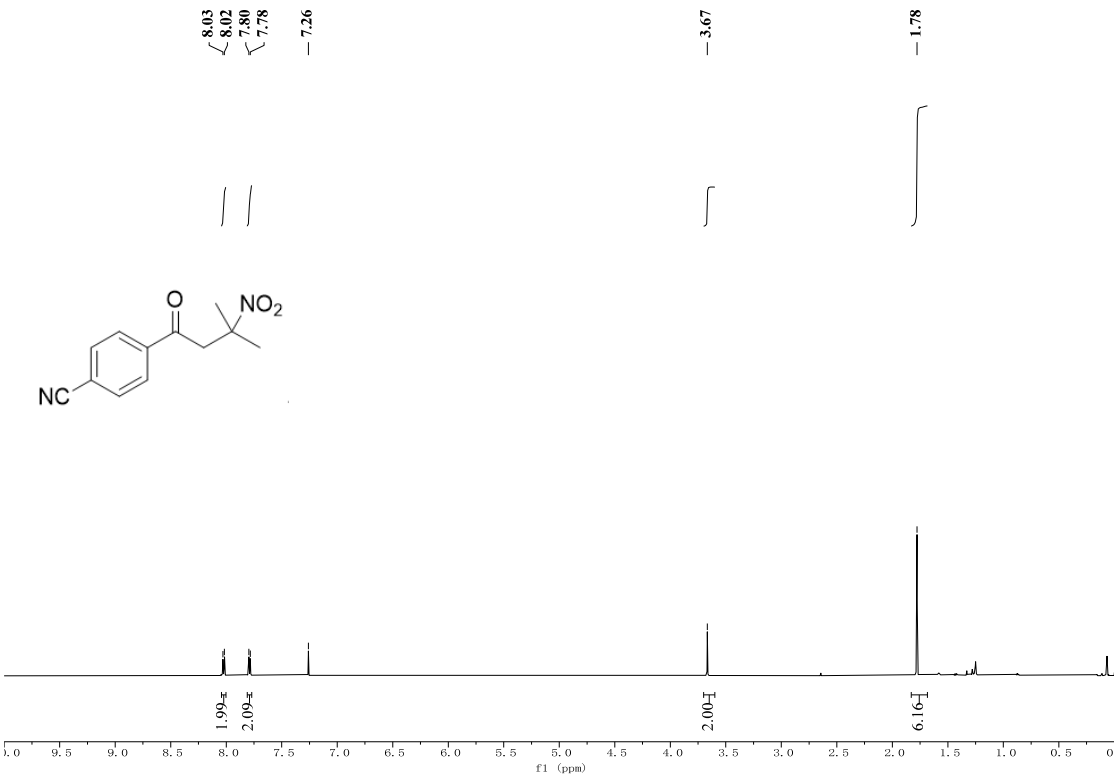
129.26
101.76
84.83
77.32
77.00
76.68
46.91
26.61
O
NO2
I
f1 (ppm)

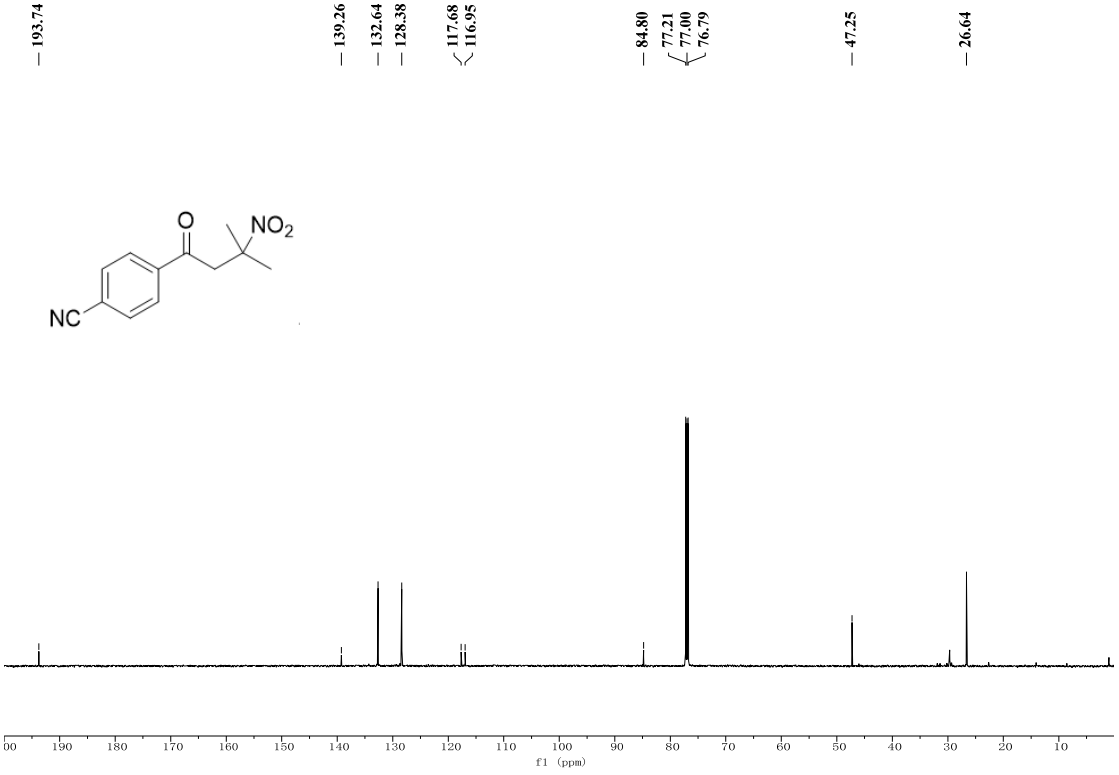

8.143
8.123
7.991
7.971
7.260
3.955
3.692
1.776
O
NO2
H3CO2C
2.01
2.05
2.99
2.00
5.99
f1 (ppm)

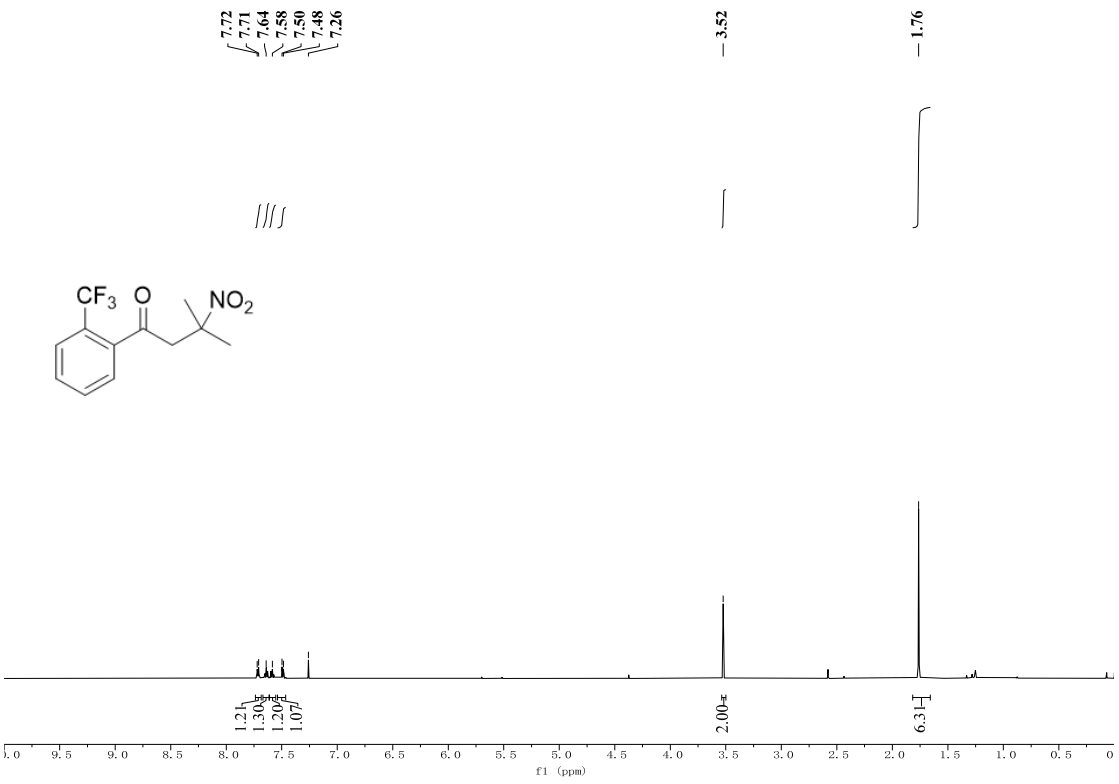

194.505
166.030
139.505
134.377
129.954
127.870
84.398
77.319
77.000
76.684
52.526
47.375
26.623
O
NO2
H3CO2C
f1 (ppm)

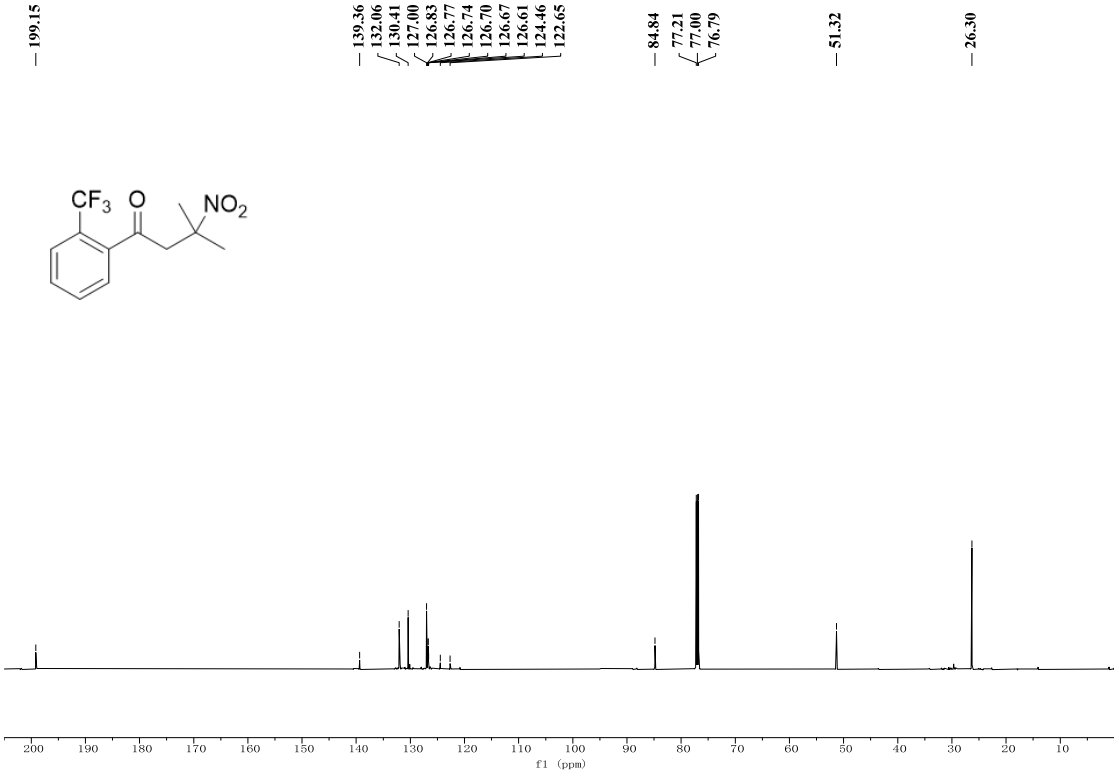

8.21
8.17
8.15
8.15
7.88
7.86
7.66
7.64
7.62
7.26
3.66
1.78
NC
O
NO2
0.95
1.00
1.06
1.17
2.00
5.96
f1 (ppm)

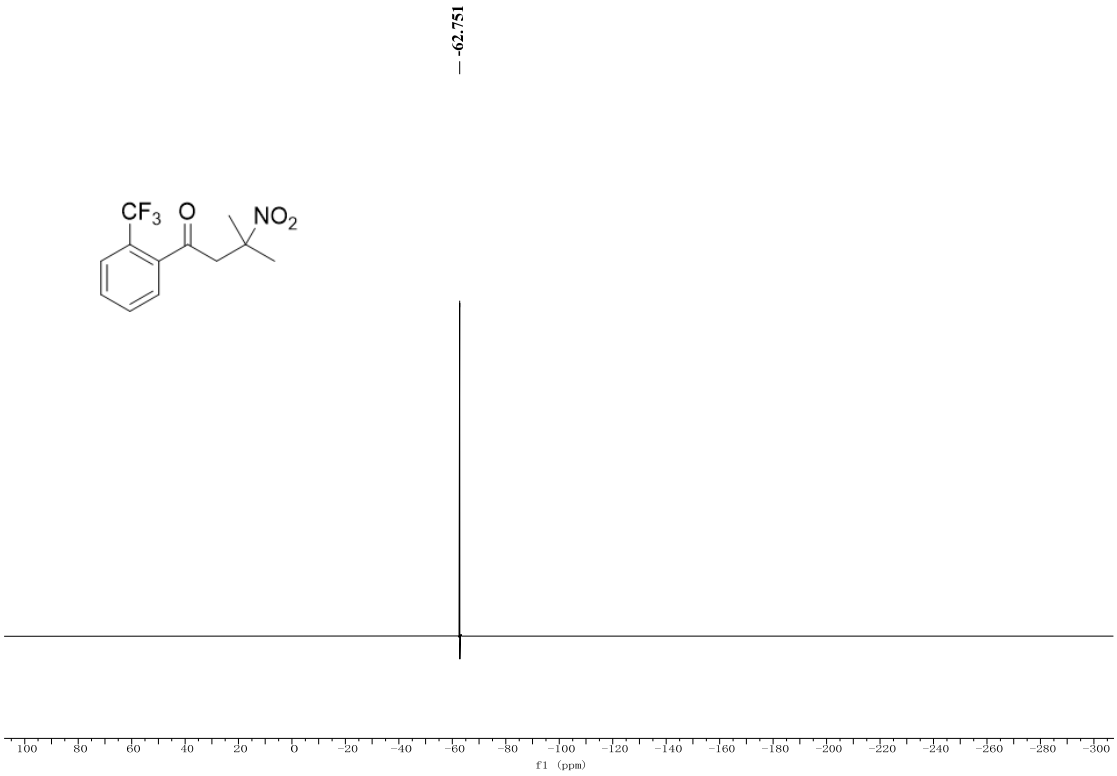

193.07
137.09
136.45
131.85
131.63
129.87
117.66
113.38
84.75
77.21
77.00
76.79
47.05
26.66
NC
O
NO2
f1 (ppm)

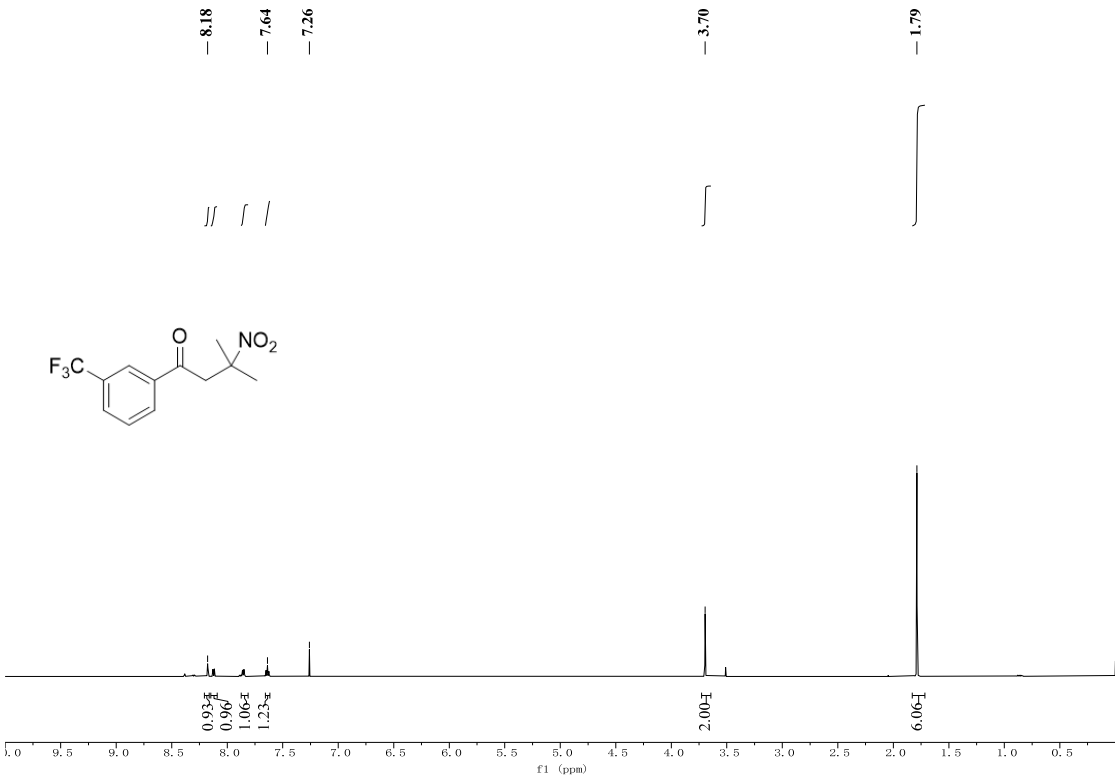

8.03
8.02
7.80
7.78
7.26
3.67
1.78
O
NO2
NC
1.99
2.09
2.00
6.16
f1 (ppm)

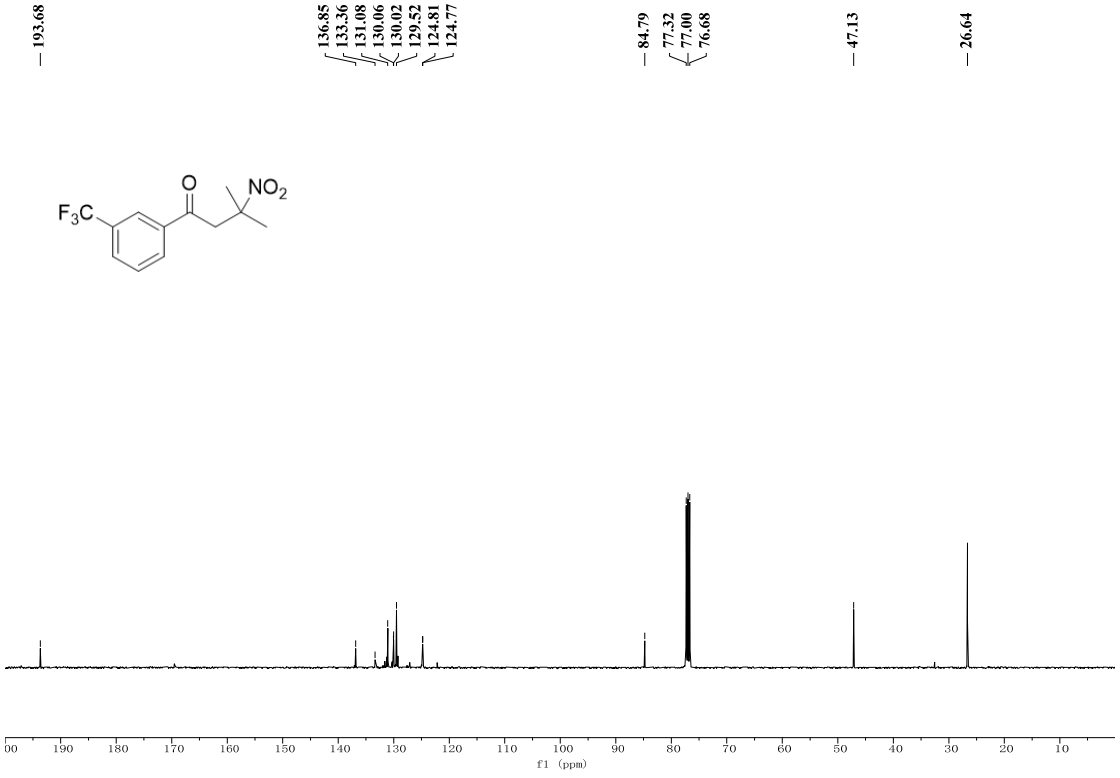

193.74
139.26
132.64
128.38
117.68
116.95
84.80
77.21
77.00
76.79
47.25
26.64
O
NO2
NC
f1 (ppm)

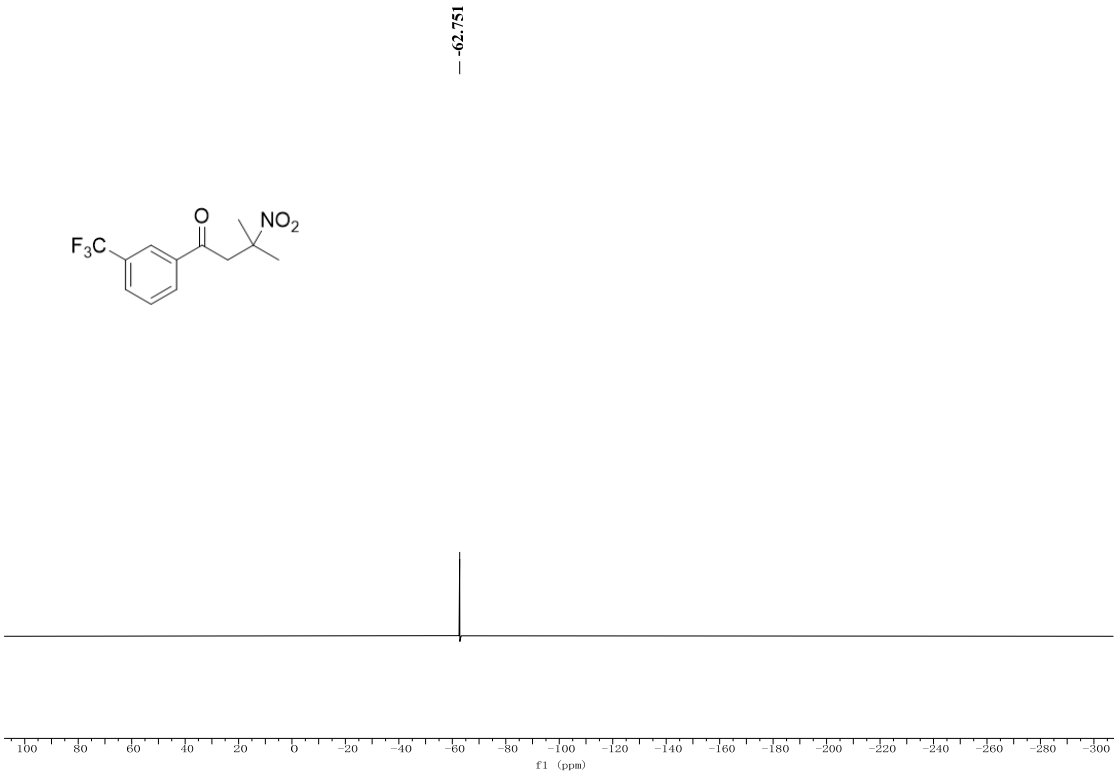

7.72
7.71
7.64
7.58
7.50
7.48
7.26
3.52
1.76
CF3
O
NO2
1.21
1.30
1.20
1.07
2.00
6.31
f1 (ppm)

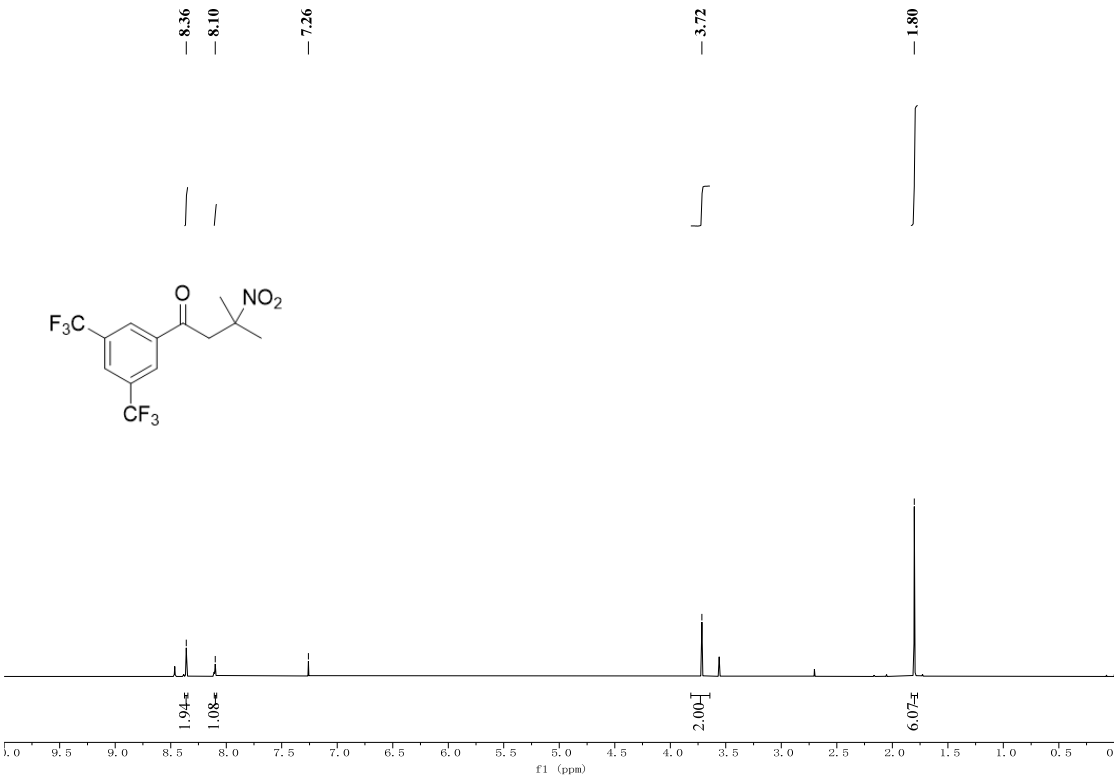

199.15
139.36
132.06
130.41
127.00
126.83
126.77
126.74
126.70
126.67
126.61
124.46
122.65
84.84
77.21
77.00
76.79
51.32
26.30
CF3
O
NO2
f1 (ppm)

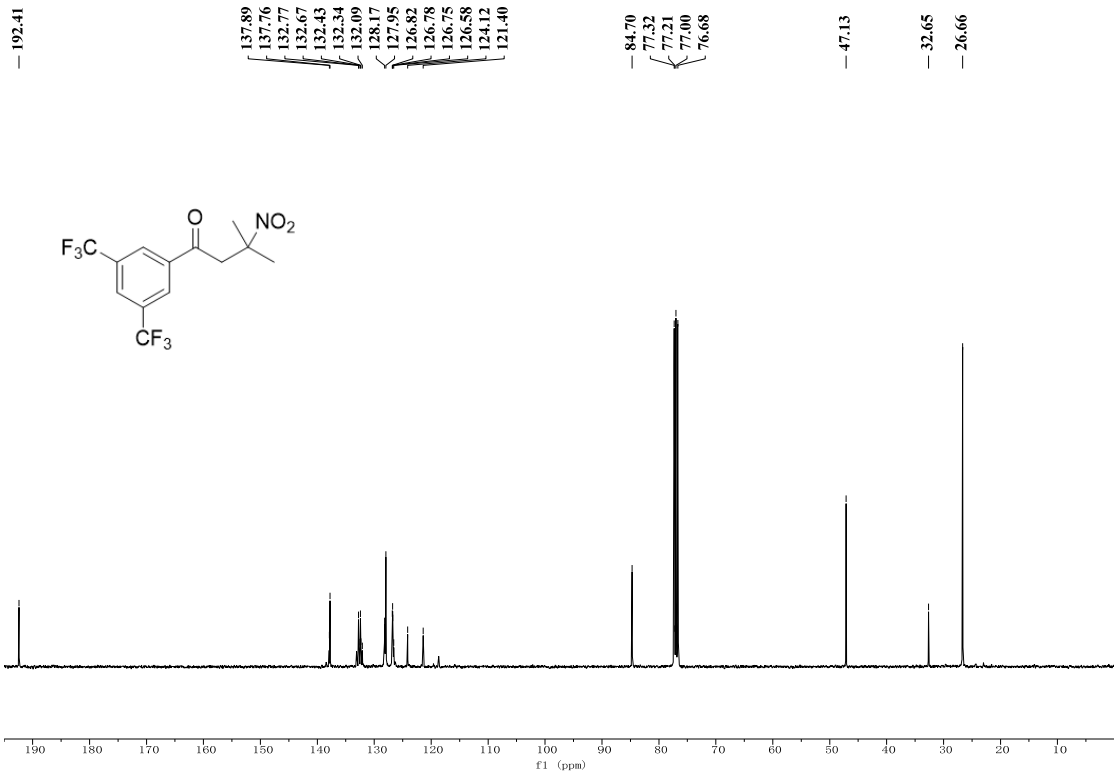

-62.751
CF3
O
NO2
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

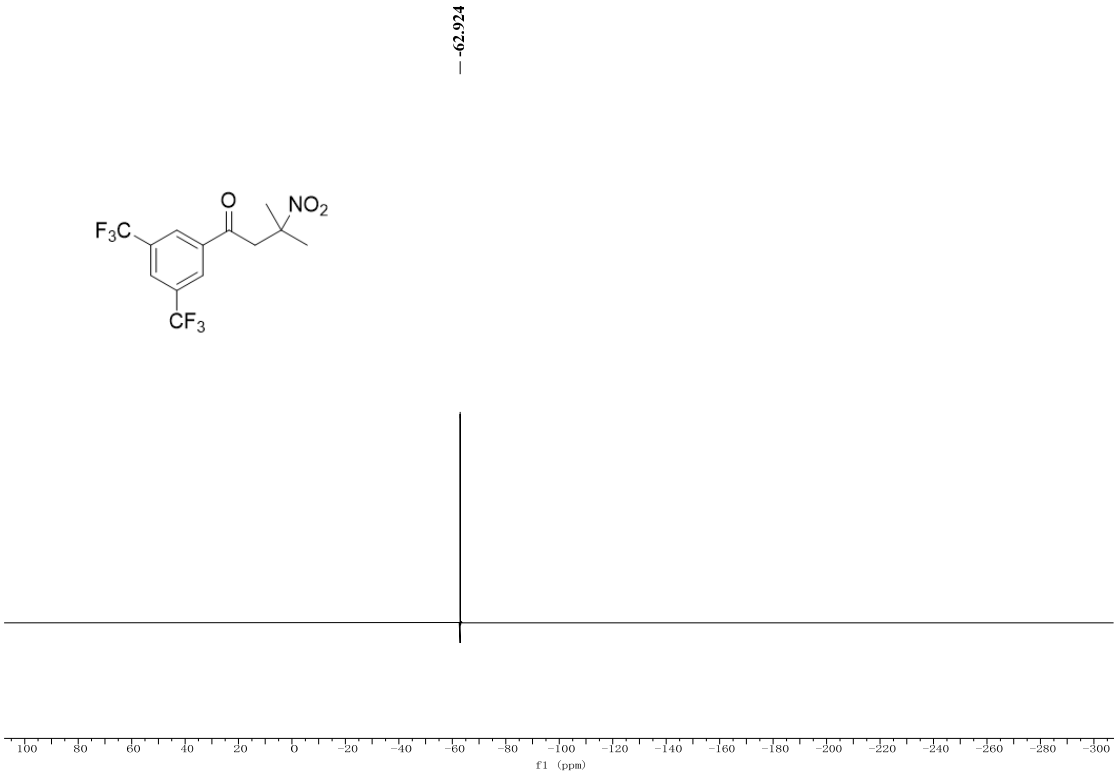

8.18
7.64
7.26
3.70
1.79
O
NO2
F3C
0.93
0.96
1.06
1.23
2.00
6.06
f1 (ppm)

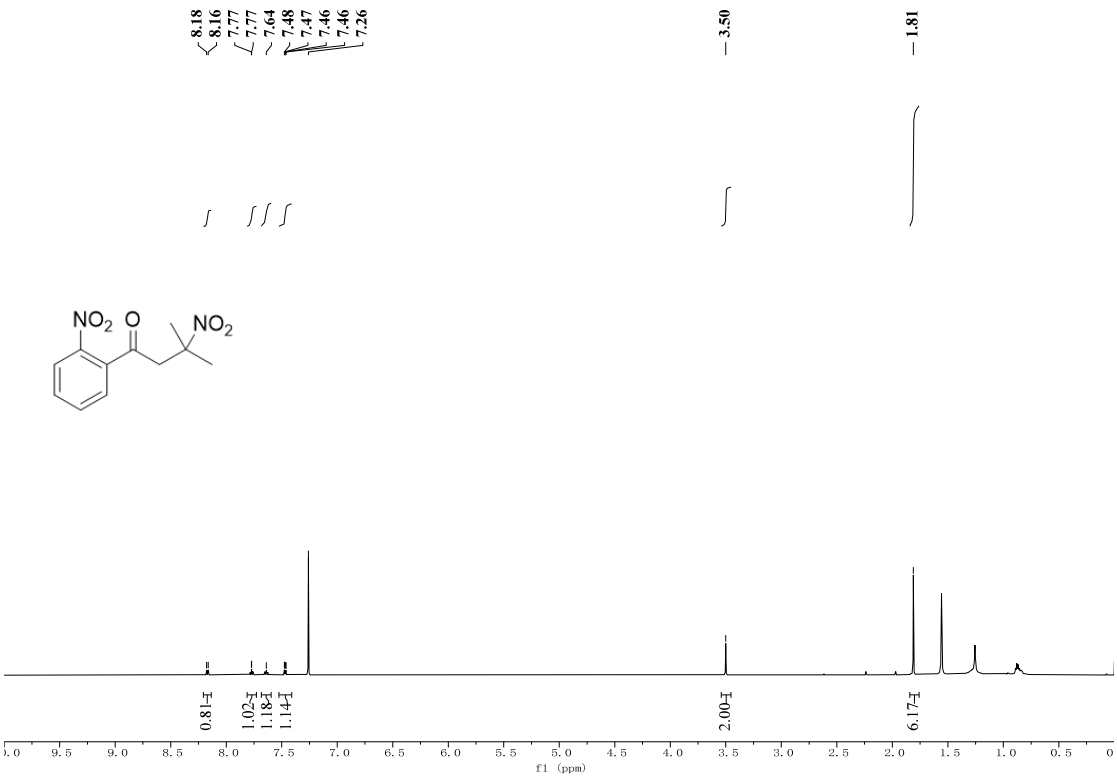

193.68
136.85
133.36
131.08
130.06
130.02
129.52
124.81
124.77
84.79
77.32
77.00
76.68
47.13
26.64
O
NO2
F3C
f1 (ppm)

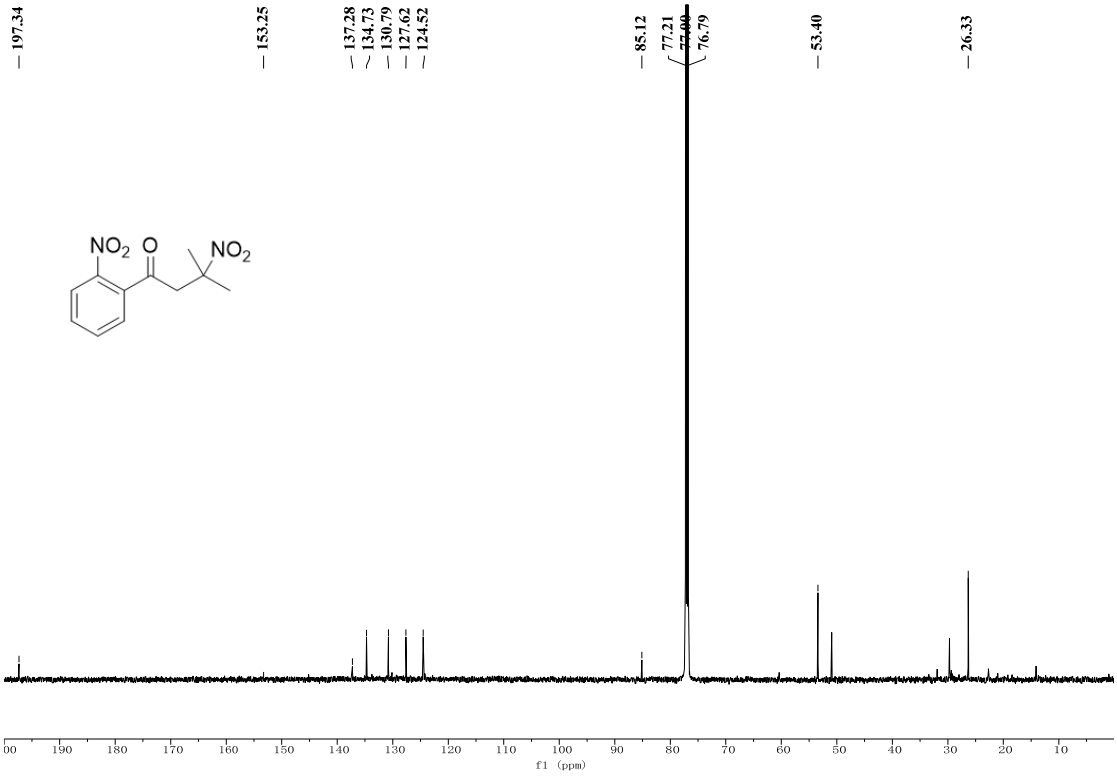

-62.751
O
NO2
F3C
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

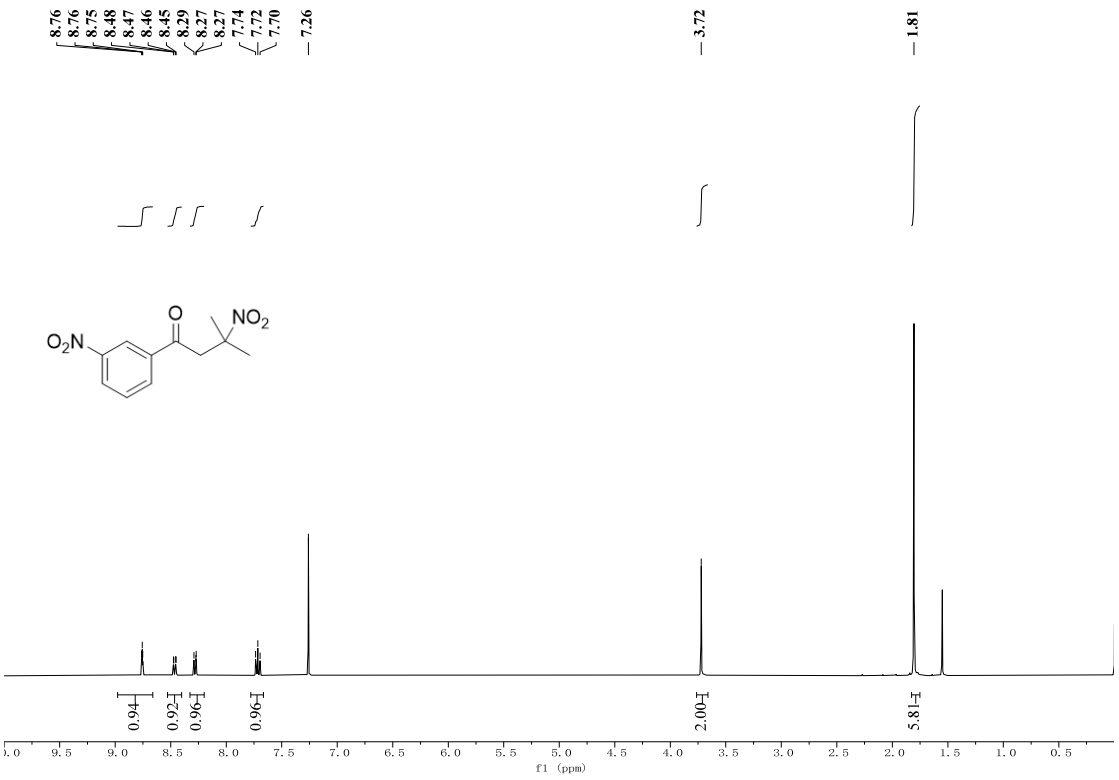

8.36
8.10
7.26
3.72
1.80
O
NO2
F3C
CF3
1.94
1.08
2.00
6.07
f1 (ppm)

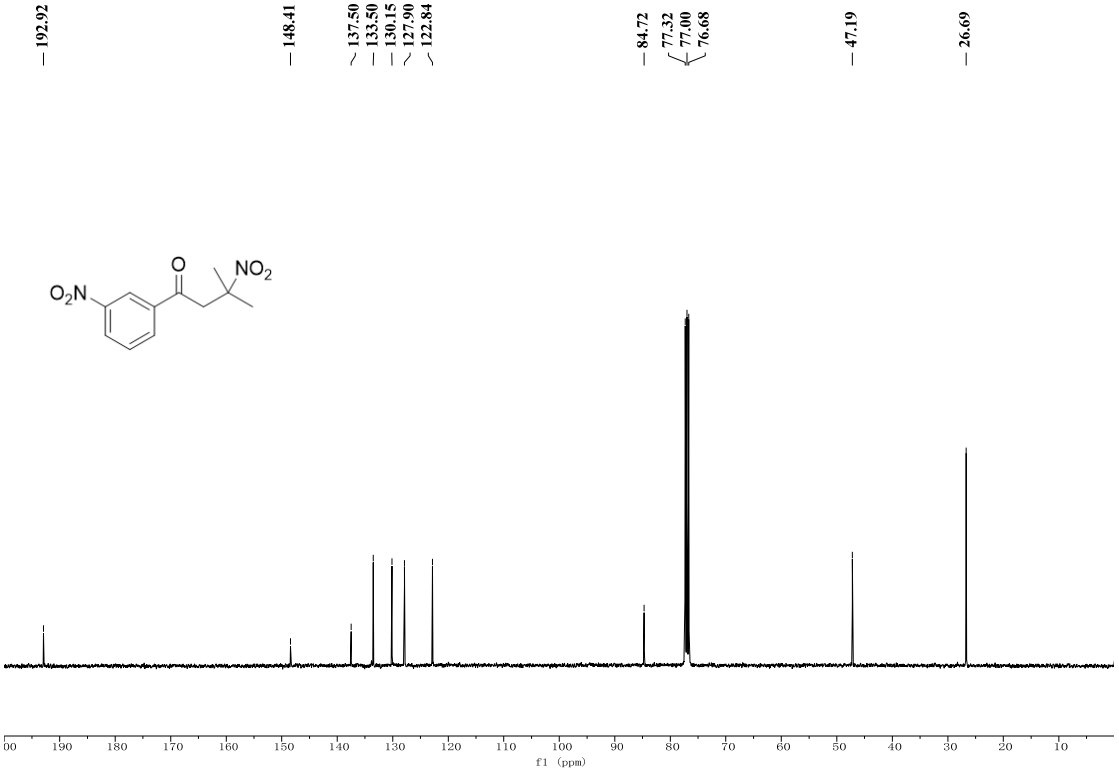

192.41
137.89
137.76
132.77
132.67
132.43
132.34
132.09
128.17
127.95
126.82
126.78
126.75
126.58
124.12
121.40
84.70
77.32
77.21
77.00
76.68
47.13
32.65
26.66
O
NO2
F3C
CF3
f1 (ppm)

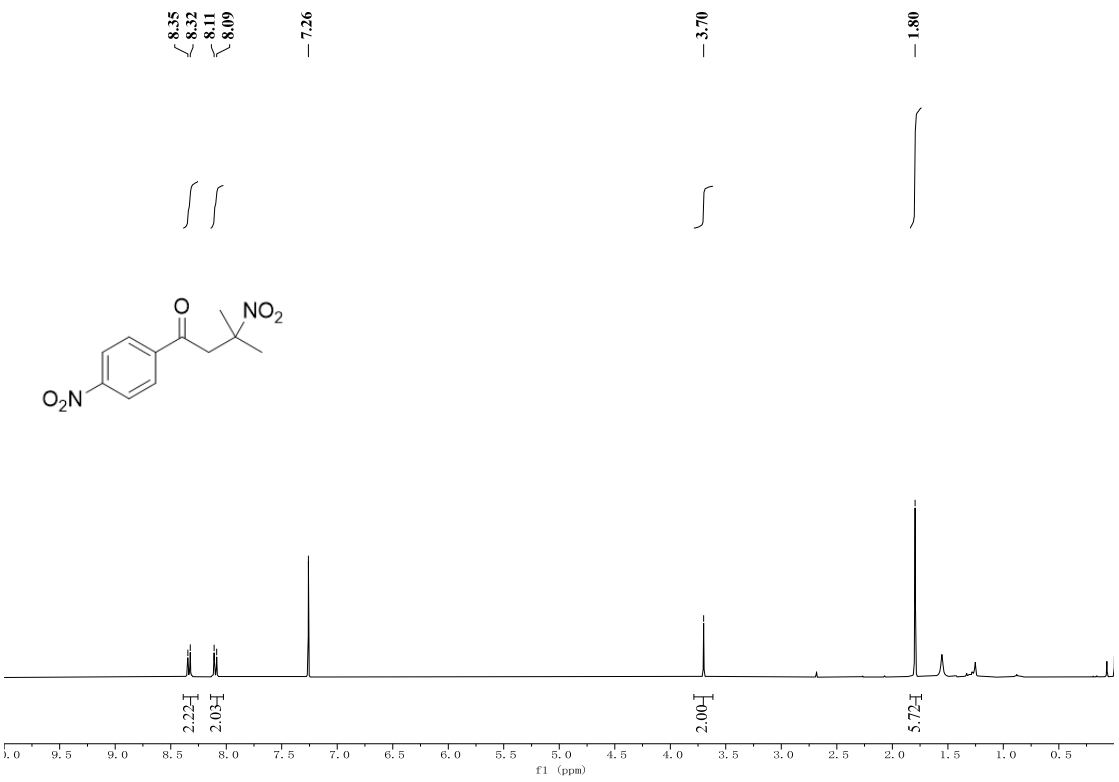

-62.924
O
NO2
F3C
CF3
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

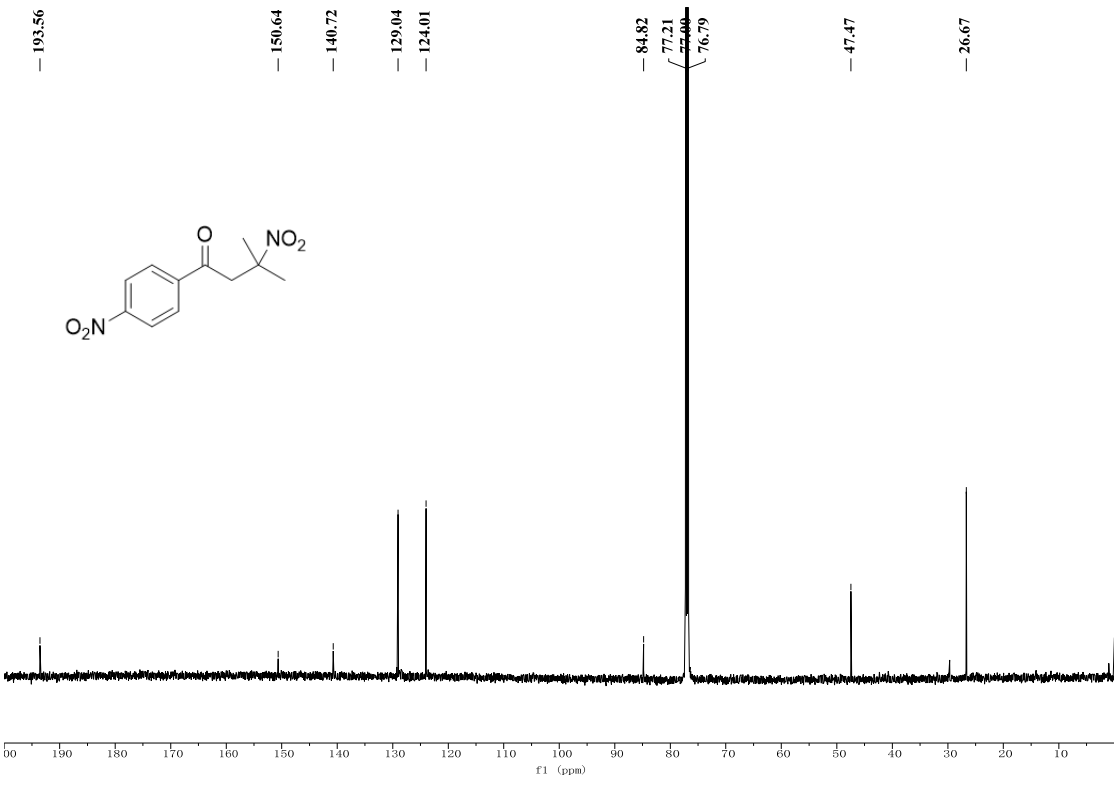

8.18
8.16
7.77
7.77
7.64
7.48
7.47
7.46
7.46
7.26
3.50
1.81
NO2
O
NO2
0.81
1.02
1.18
1.14
2.00
6.17
f1 (ppm)

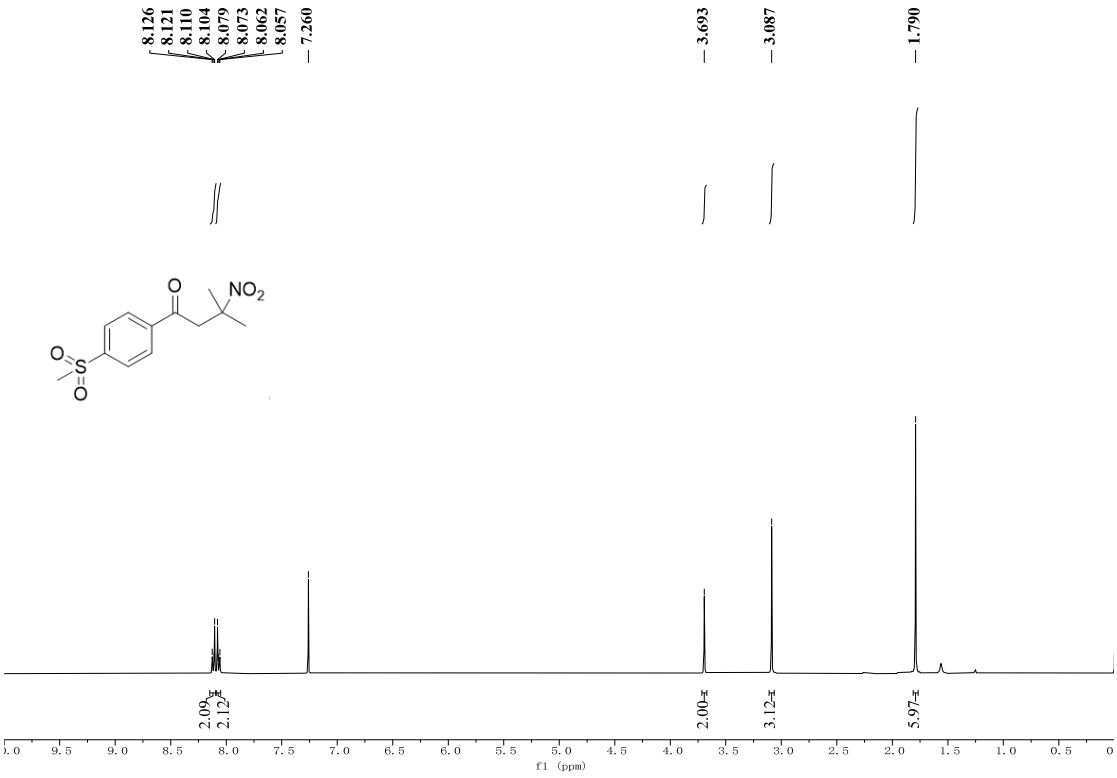

197.34
153.25
137.28
134.73
130.79
127.62
124.52
85.12
77.21
77.00
76.79
53.40
26.33
NO2
O
NO2
f1 (ppm)

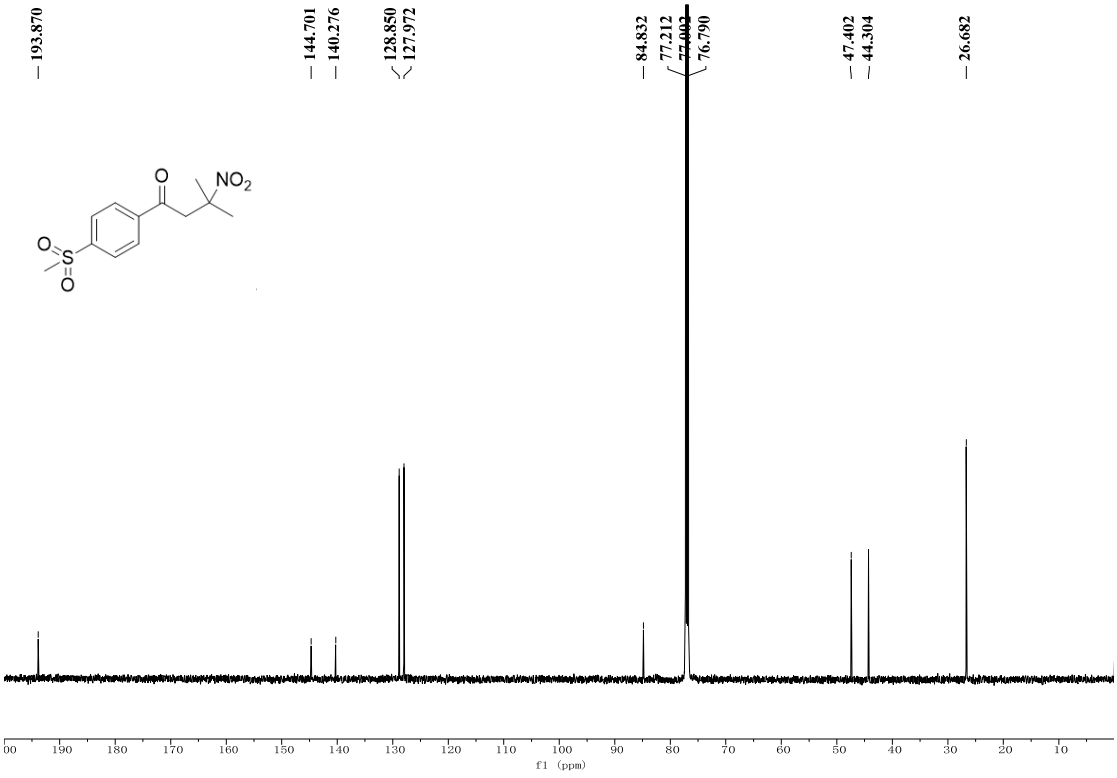

8.76
8.76
8.75
8.48
8.47
8.46
8.45
8.29
8.27
8.27
7.74
7.72
7.70
7.26
3.72
1.81
O
NO2
O2N
0.94
0.92
0.96
0.96
2.00
5.81
f1 (ppm)

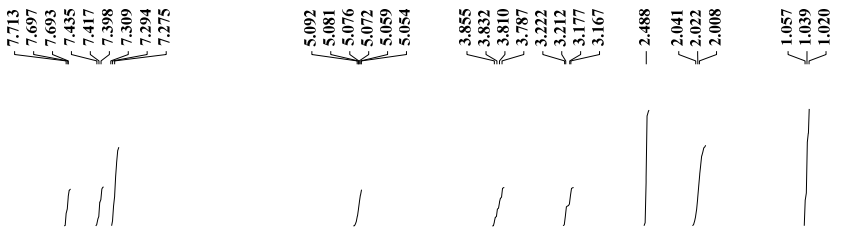

192.92
148.41
137.50
133.50
130.15
127.90
122.84
84.72
77.32
77.00
76.68
47.19
26.69
O
NO2
O2N
f1 (ppm)

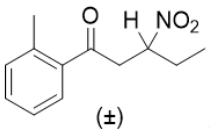

8.35
8.32
8.11
8.09
7.26
3.70
1.80
O
NO2
O2N
2.22
2.03
2.00
5.72
f1 (ppm)


193.56
150.64
140.72
129.04
124.01
84.82
77.21
77.00
76.79
47.47
26.67
O
NO2
O2N
f1 (ppm)

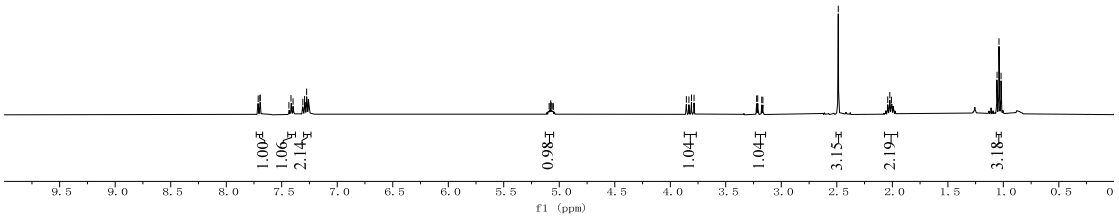

8.126
8.121
8.110
8.104
8.079
8.073
8.062
8.057
7.260
3.693
3.087
1.790
O
NO2
O
S
O
2.09
2.12
2.00
3.12
5.97
f1 (ppm)


193.870
144.701
140.276
128.850
127.972
84.832
77.212
77.003
76.790
47.402
44.304
26.682
O
NO2
O
S
O
f1 (ppm)

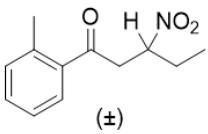

7.713
7.697
7.693
7.435
7.417
7.398
7.309
7.294
7.275
5.092
5.081
5.076
5.072
5.059
5.054
3.855
3.832
3.810
3.787
3.222
3.212
3.177
3.167
2.488
2.041
2.022
2.008
1.057
1.039
1.020


O
H
NO2

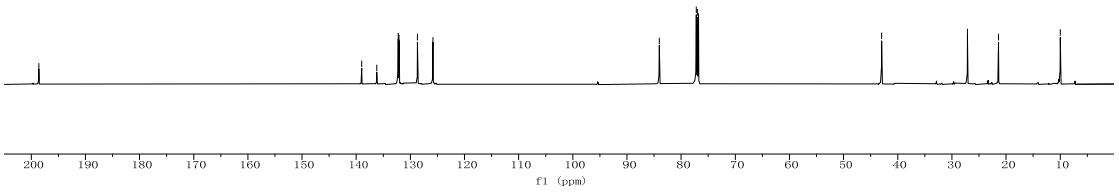
(±)

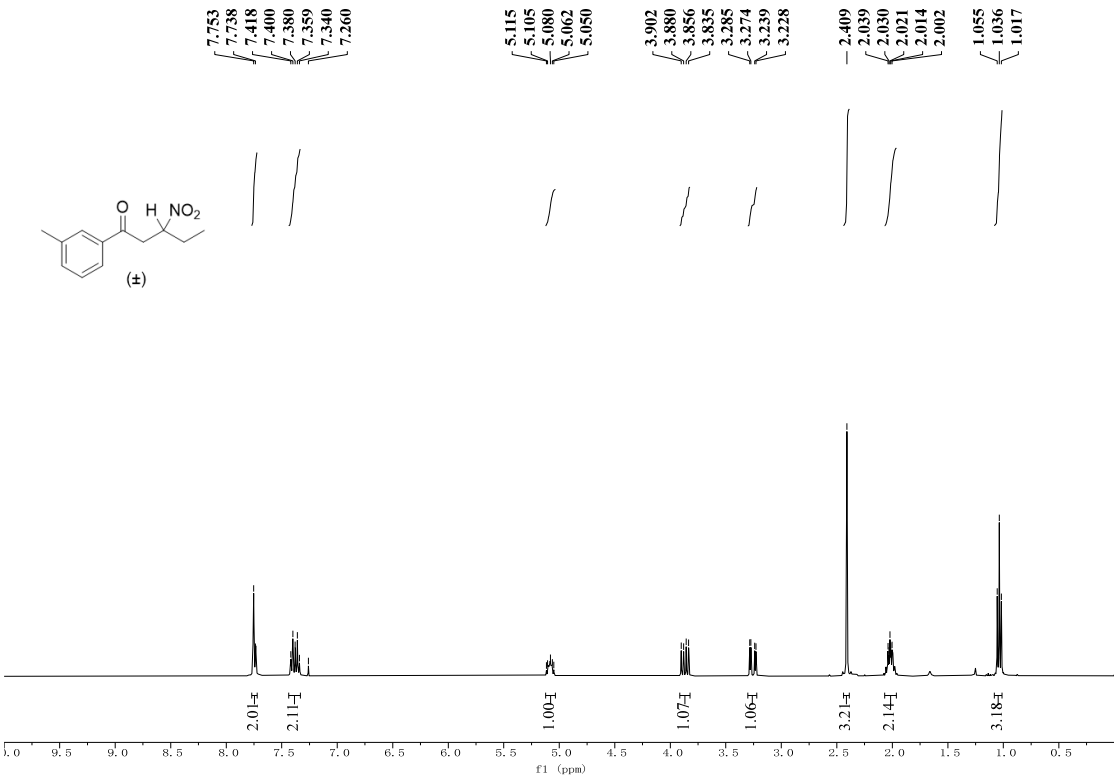

1.00
1.06
2.14
0.98
1.04
1.04
3.15
2.19
3.18
f1 (ppm)

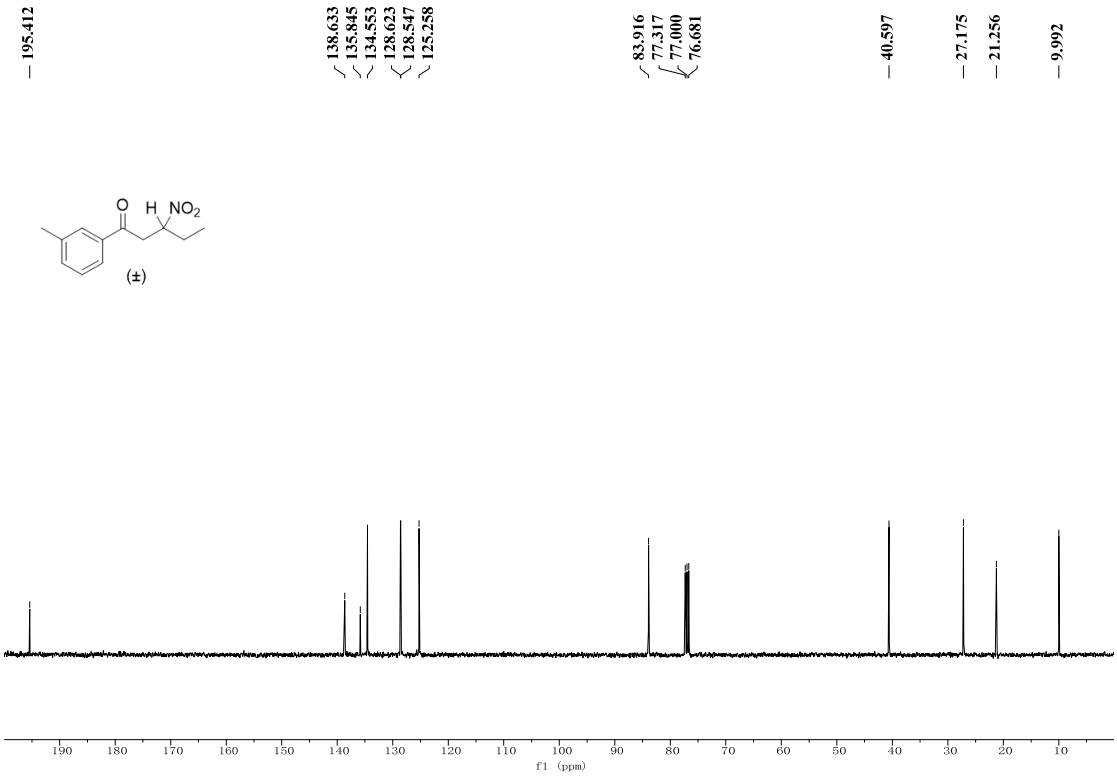

198.604
138.977
136.205
132.254
132.107
128.680
125.820
84.026
77.211
76.999
76.789
42.978
27.121
21.384
9.994

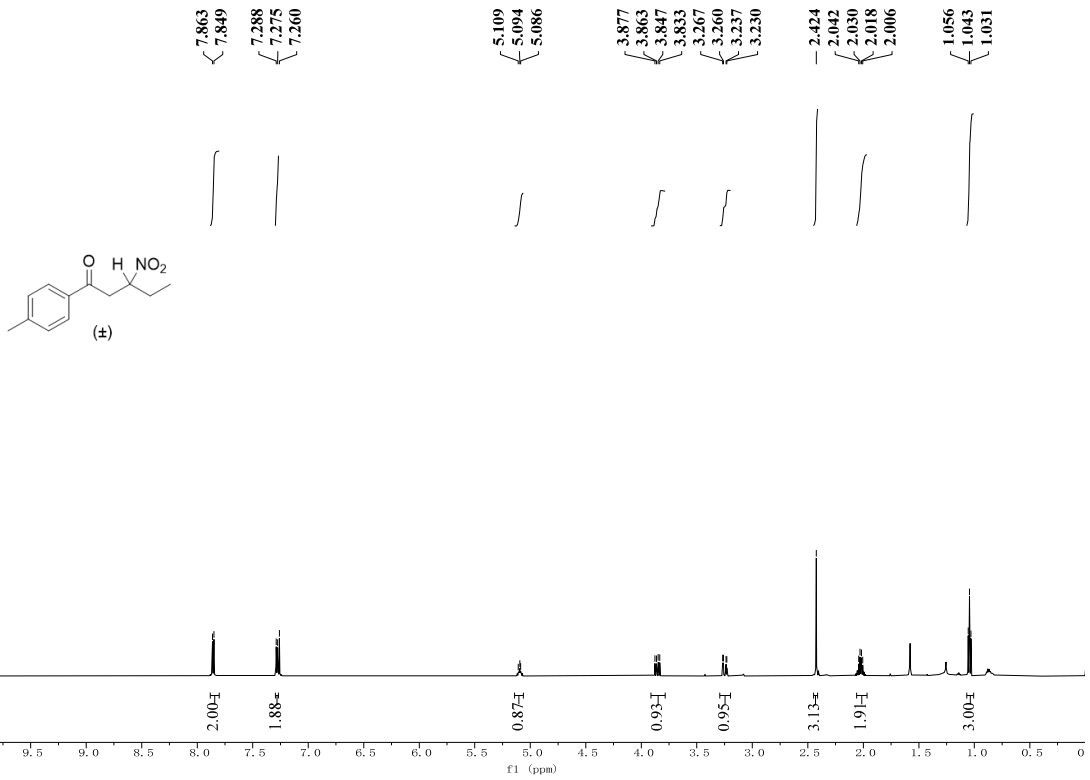

O
H
NO2

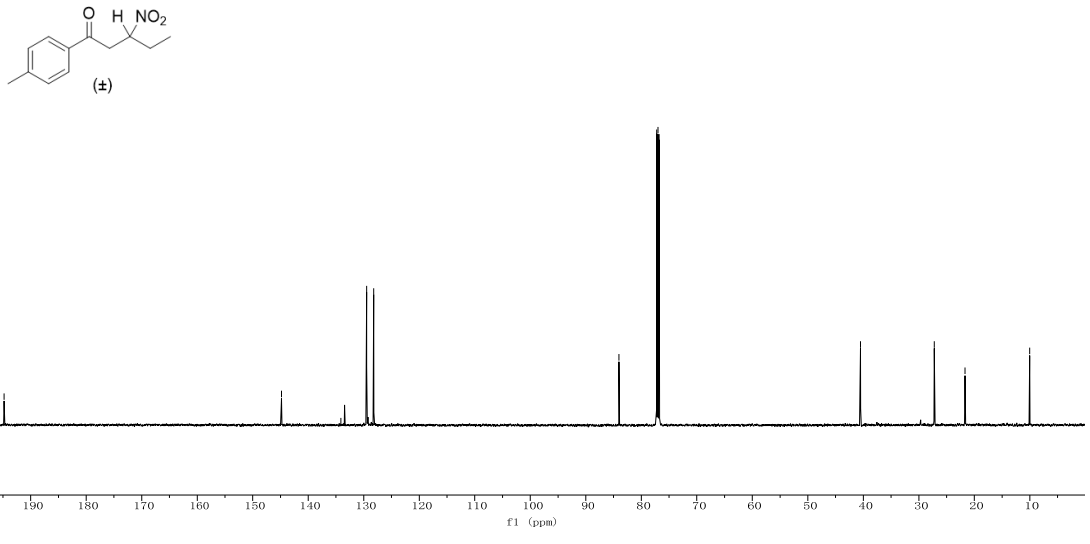
(±)

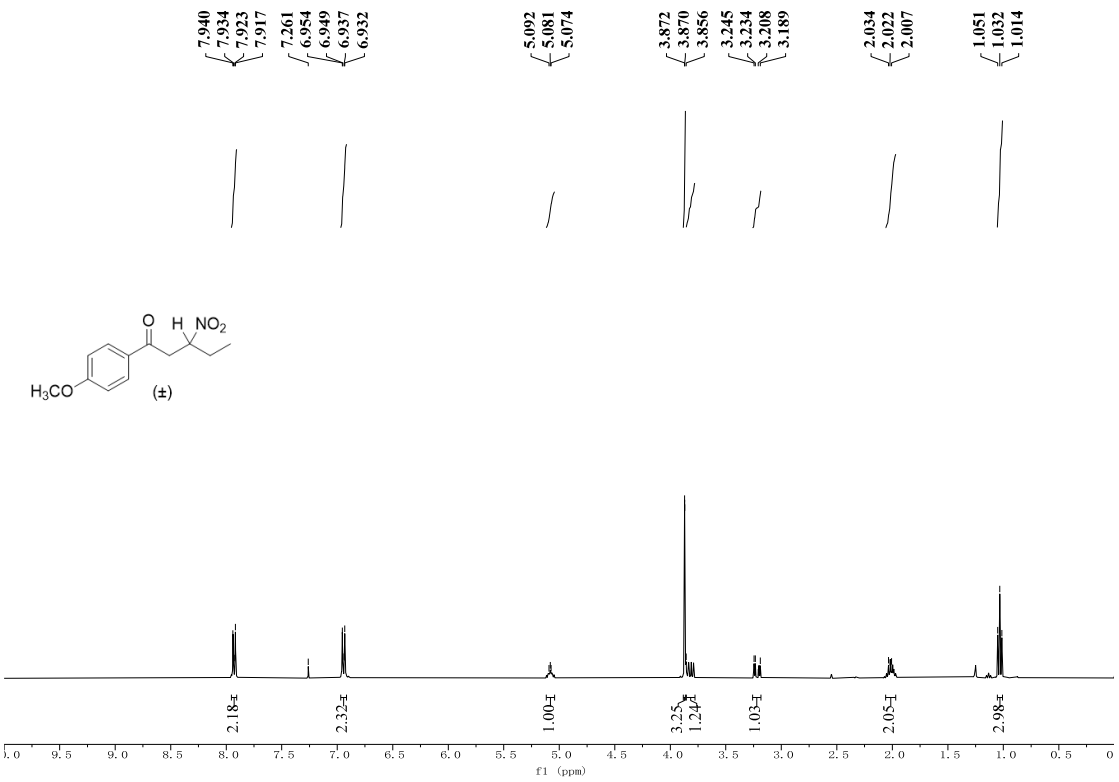

f1 (ppm)

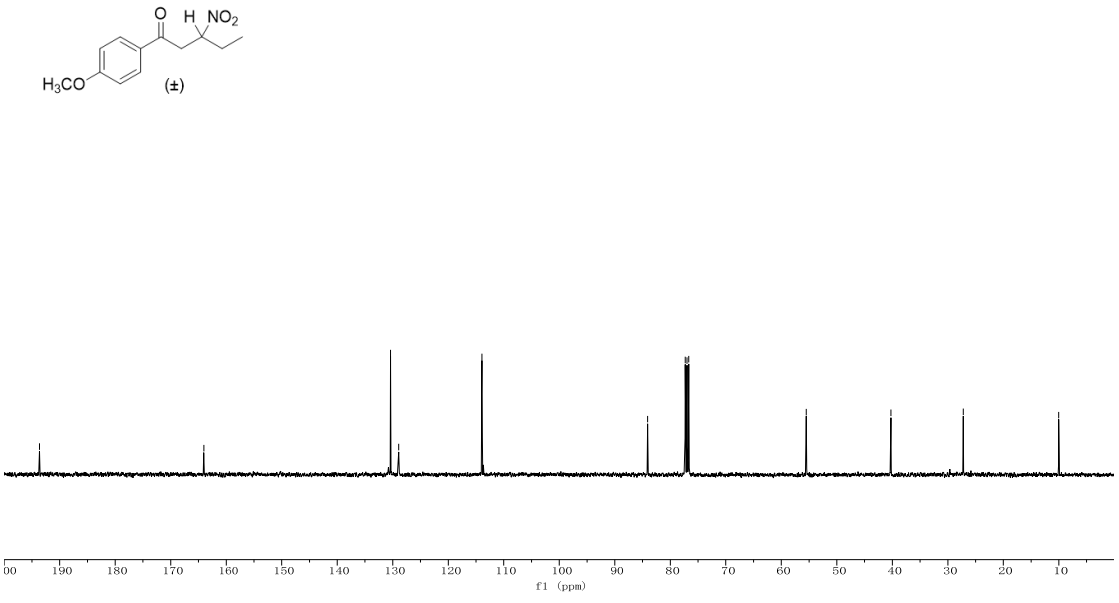

7.753
7.738
7.418
7.400
7.380
7.359
7.340
7.260
5.115
5.105
5.080
5.062
5.050
3.902
3.880
3.856
3.835
3.285
3.274
3.239
3.228
2.409
2.039
2.030
2.021
2.014
2.002
1.055
1.036
1.017
O
H
NO2
(±)
2.01
2.11
1.00
1.07
1.06
3.21
2.14
3.18
f1 (ppm)

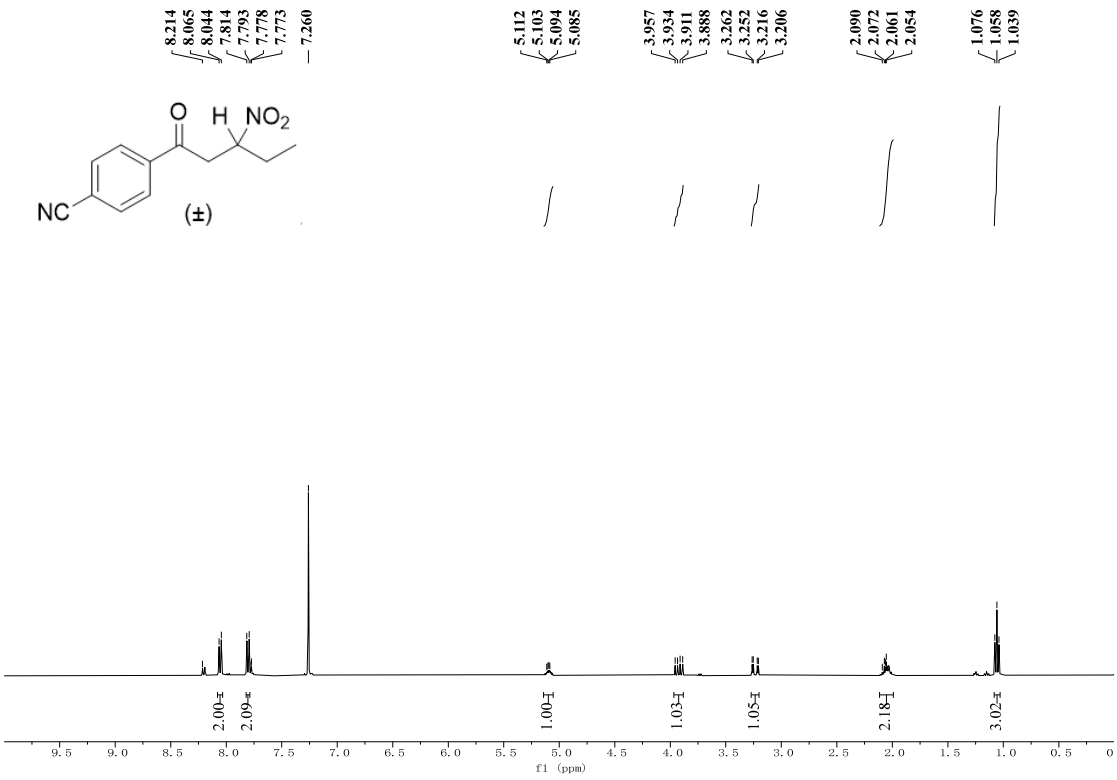

195.412
138.633
135.845
134.553
128.623
128.547
125.258
83.916
77.317
77.000
76.681
40.597
27.175
21.256
9.992
O
H
NO2
(±)
f1 (ppm)

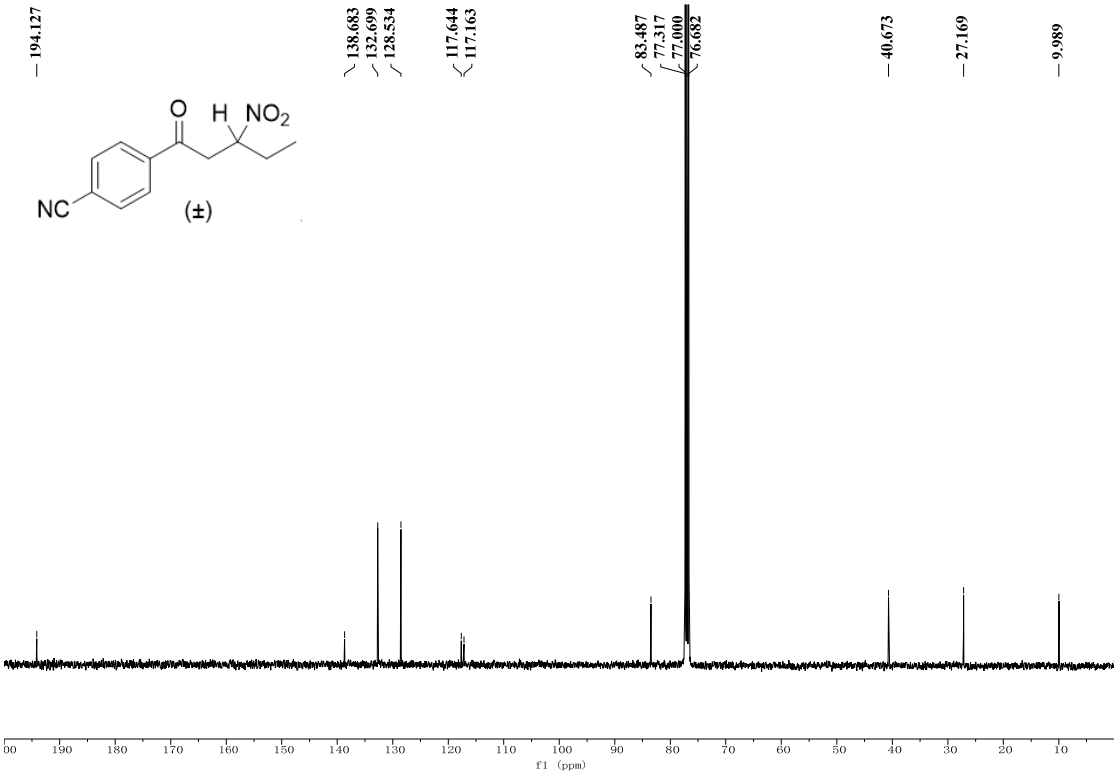

7.863
7.849
7.288
7.275
7.260
5.109
5.094
5.086
3.877
3.863
3.847
3.833
3.267
3.260
3.237
3.230
2.424
2.042
2.030
2.018
2.006
1.056
1.043
1.031
O
H
NO2
(±)
2.00
1.88
0.87
0.93
0.95
3.13
1.91
3.00
f1 (ppm)

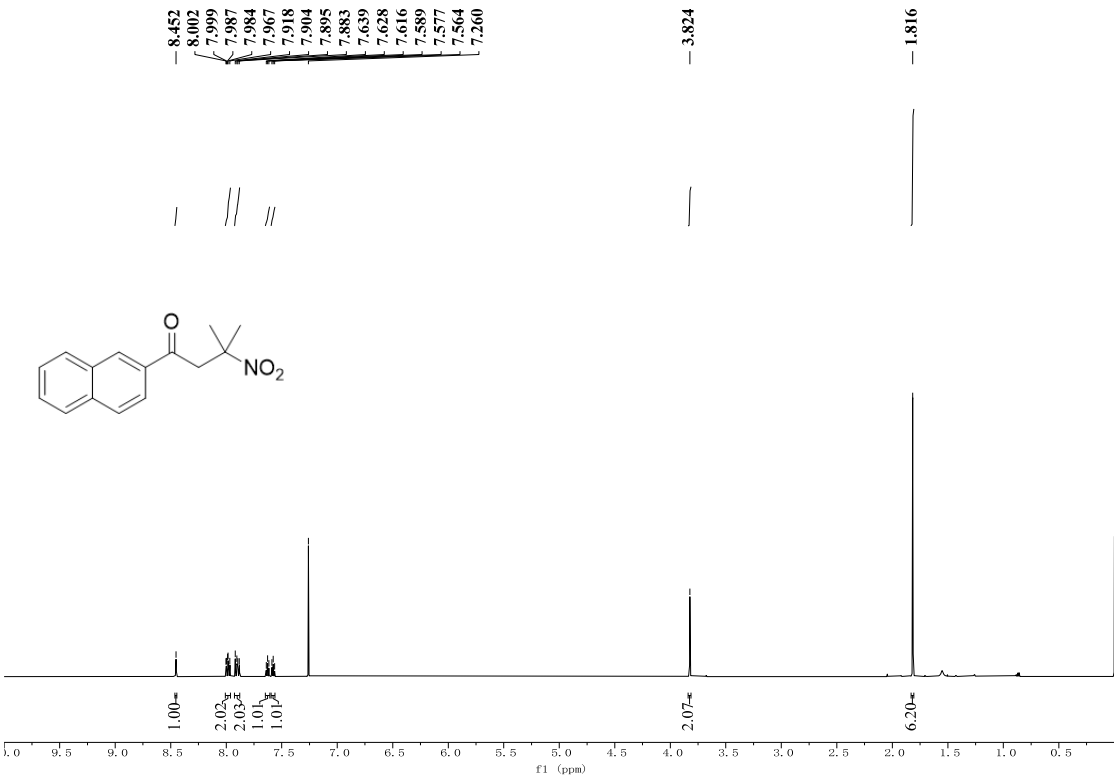

194.799
144.811
134.122
129.474
128.207
84.019
77.211
77.000
76.789
40.507
27.226
21.676
10.042
O
H
NO2
(±)
f1 (ppm)


7.940
7.934
7.923
7.917
7.261
6.954
6.949
6.937
6.932
5.092
5.081
5.074
3.872
3.870
3.856
3.245
3.234
3.208
3.189
2.034
2.022
2.007
1.051
1.032
1.014
O
H
NO2
H3CO
(±)
2.18
2.32
1.00
3.25
1.24
1.03
2.05
2.98
f1 (ppm)


193.635
164.037
130.400
128.929
113.929
84.095
77.321
77.001
76.684
55.507
40.254
27.219
10.036
O
H
NO2
H3CO
(±)
f1 (ppm)


8.214
8.065
8.044
7.814
7.793
7.778
7.773
7.260
5.112
5.103
5.094
5.085
3.957
3.934
3.911
3.888
3.262
3.252
3.216
3.206
2.090
2.072
2.061
2.054
1.076
1.058
1.039
O
H
NO2
NC
(±)
2.00
2.09
1.00
1.03
1.05
2.18
3.02
f1 (ppm)


194.127
138.683
132.699
128.534
117.644
117.163
83.487
77.317
77.000
76.682
40.673
27.169
9.989
O
H
NO2
NC
(±)
f1 (ppm)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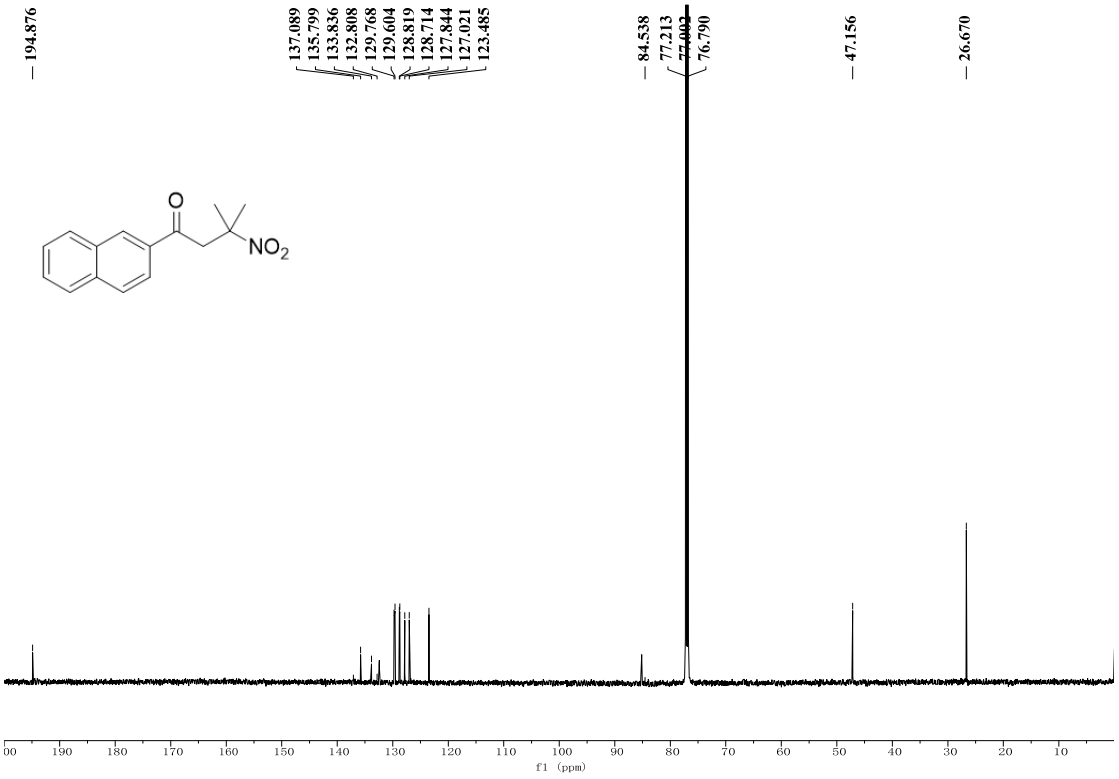
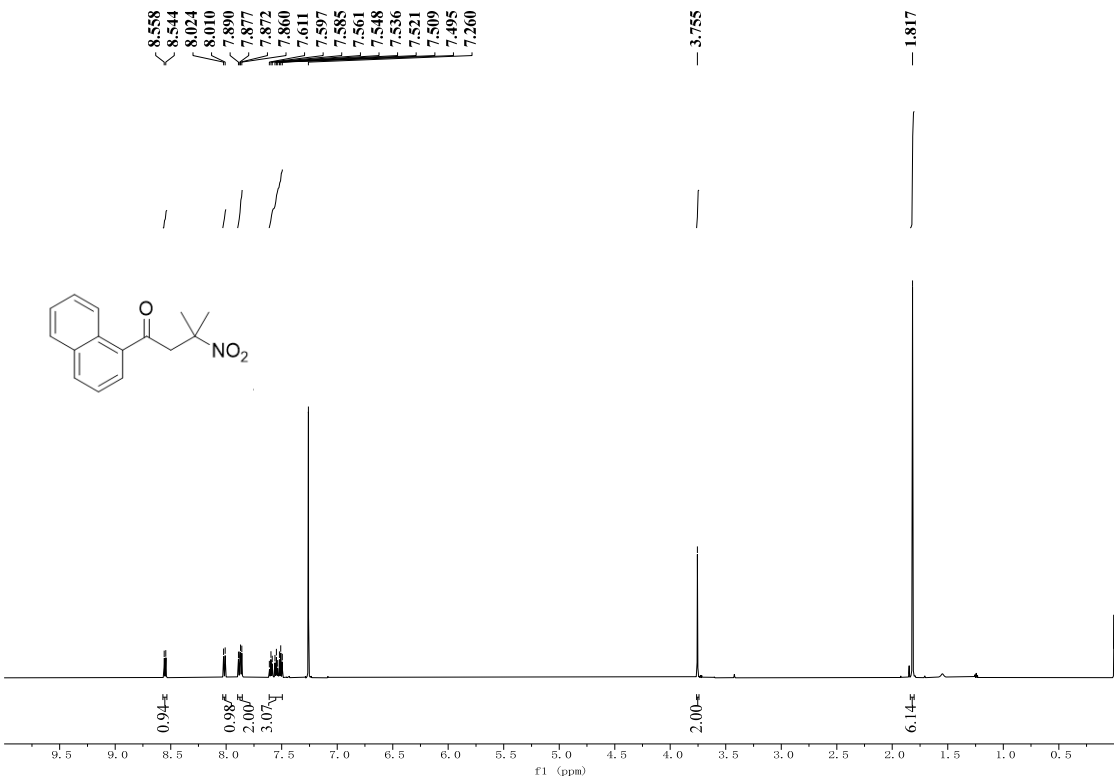
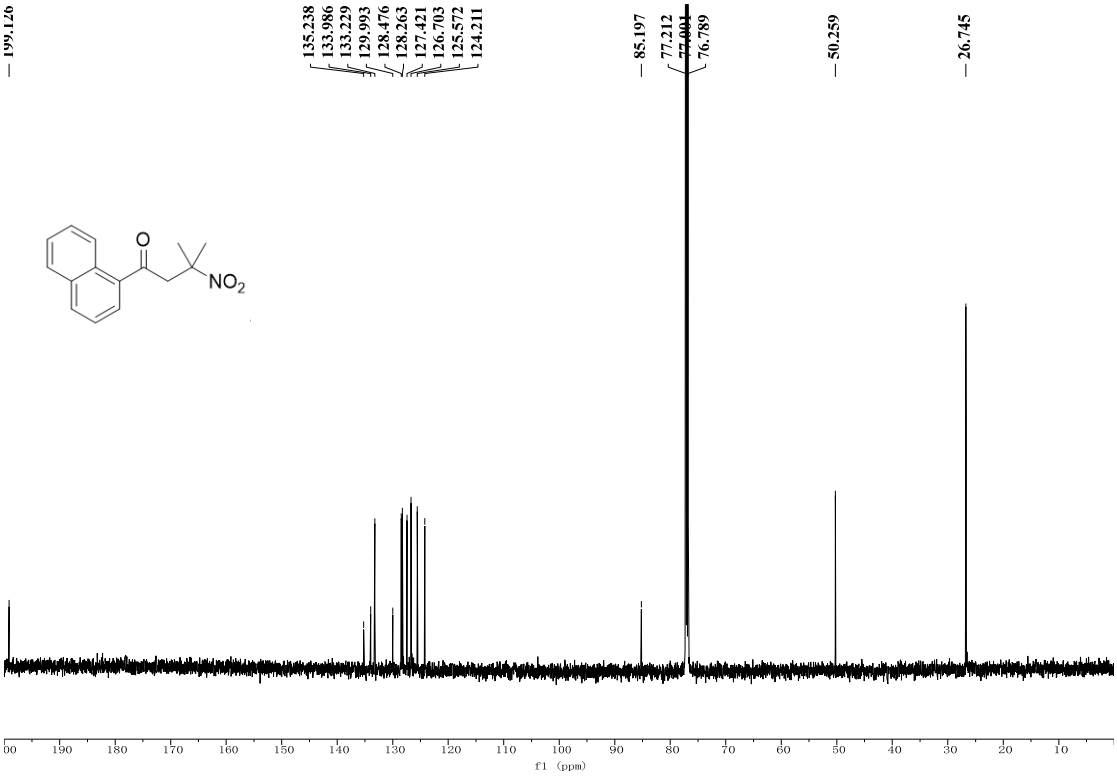
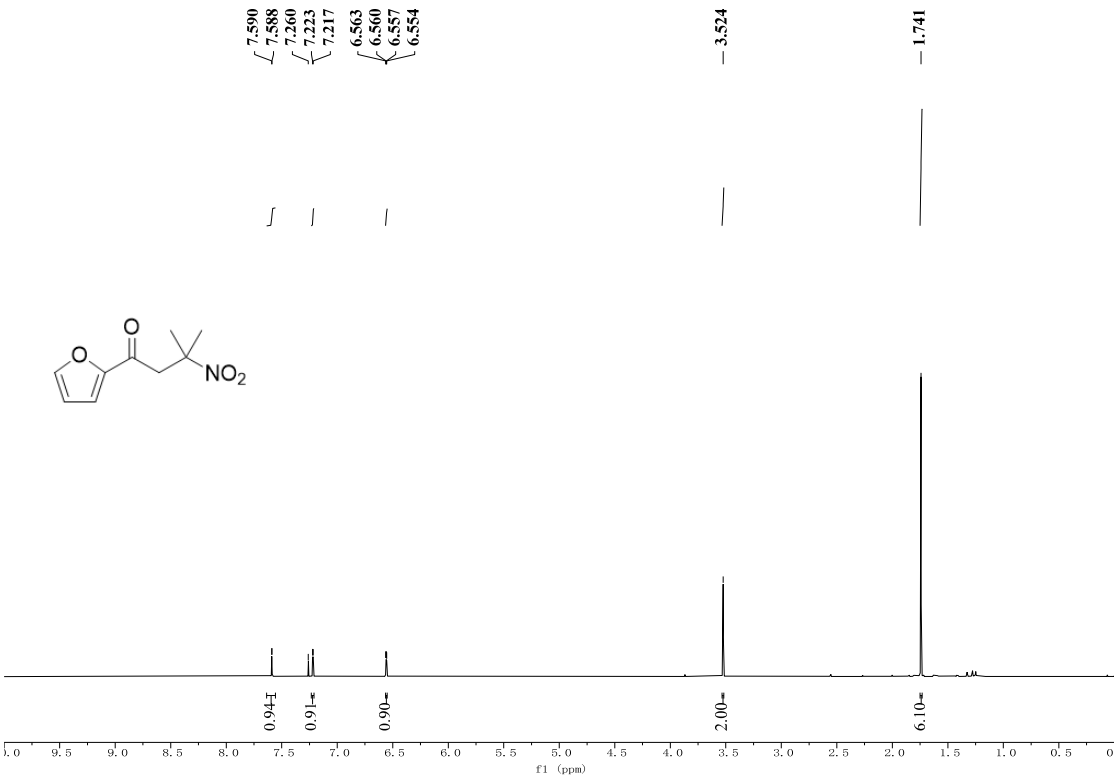
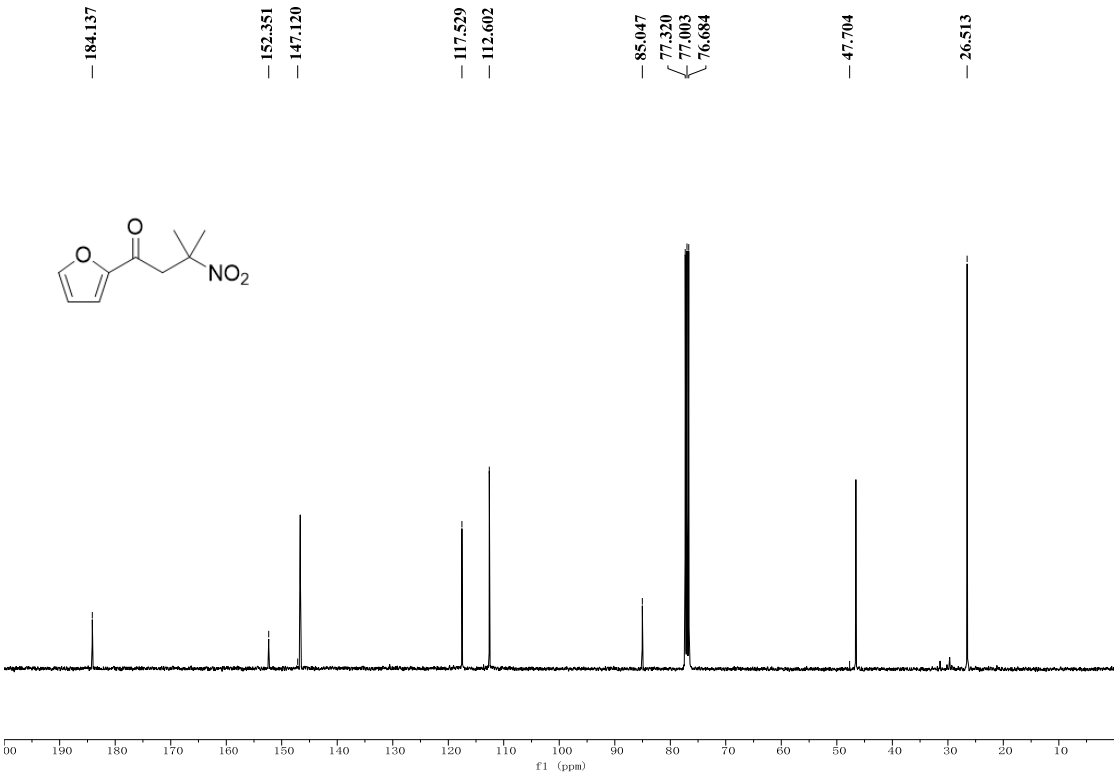
8.002
7.999
7.987
7.984
7.967
7.918
7.904
7.895
7.883
7.639
7.628
7.616
7.589
7.577
7.564
7.260
3.824
1.816
O
NO2
1.00
2.02
2.03
1.01
1.01
2.07
6.20
f1 (ppm)

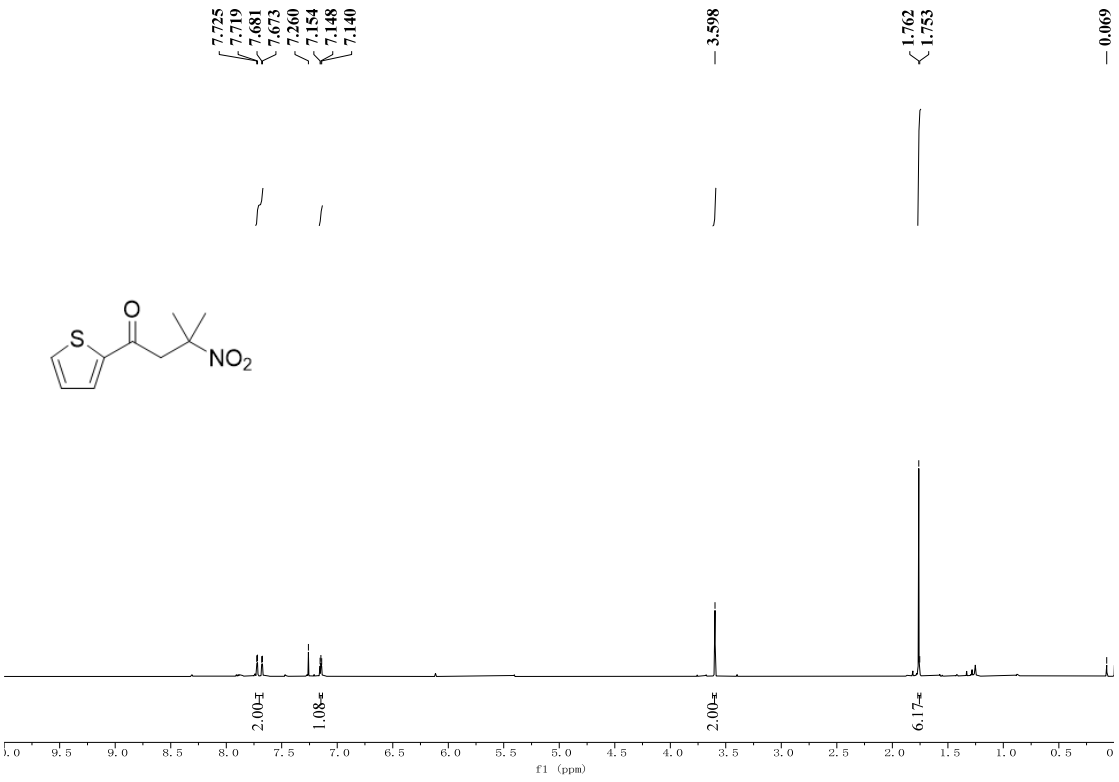

194.876
137.089
135.799
133.836
132.808
129.768
129.604
128.819
128.714
127.844
127.021
123.485
84.538
77.213
77.002
76.790
47.156
26.670
O
NO2
f1 (ppm)

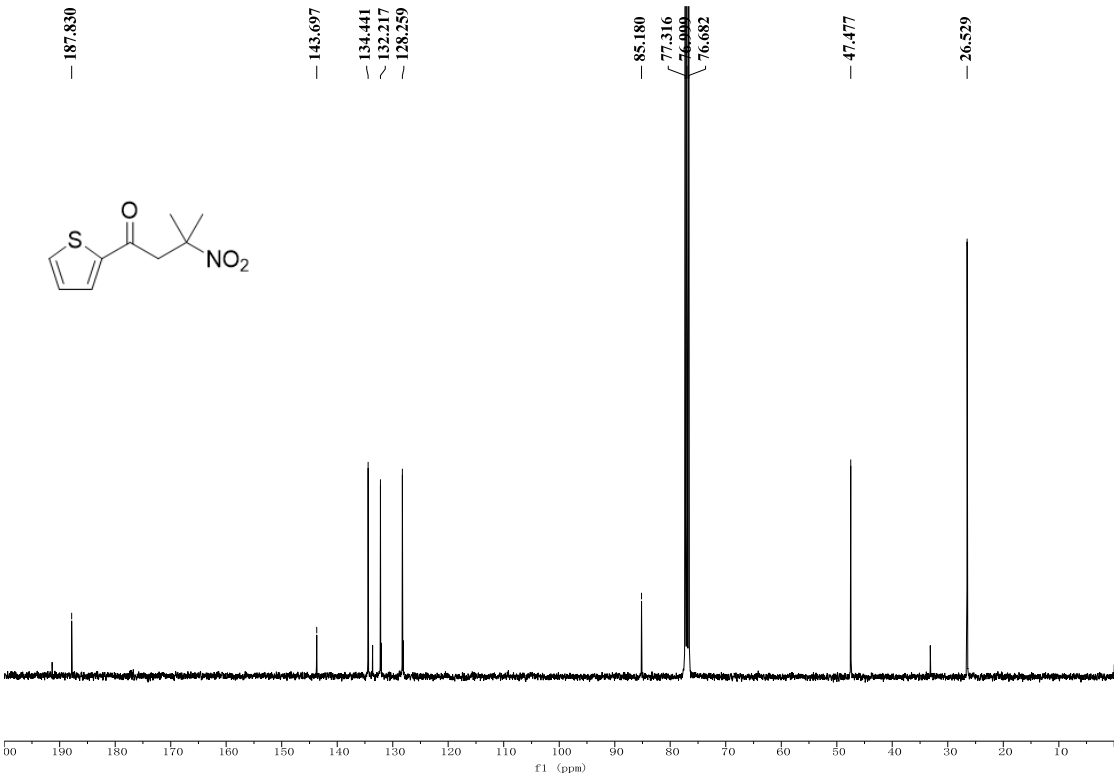

8.558
8.544
8.024
8.010
7.890
7.877
7.872
7.860
7.611
7.597
7.585
7.561
7.548
7.536
7.521
7.509
7.495
7.260
3.755
1.817
O
NO2
0.94
0.98
2.00
3.07
2.00
6.14
f1 (ppm)

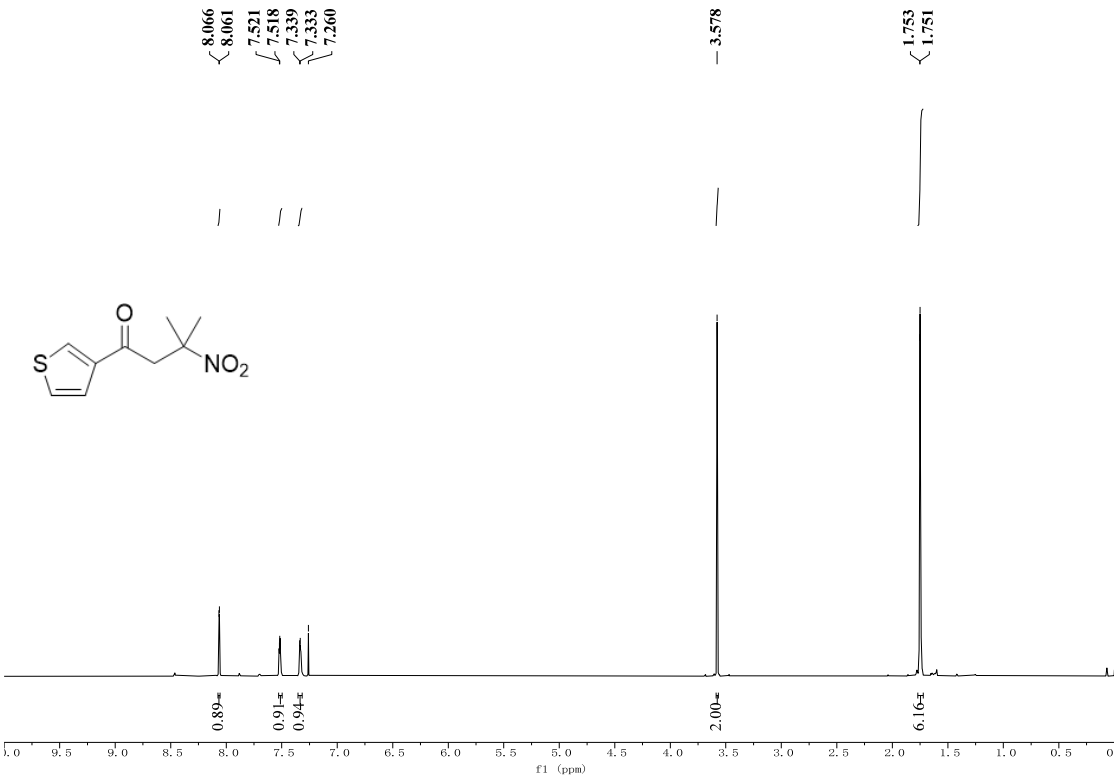

199.126
135.238
133.986
133.229
129.993
128.476
128.263
127.421
126.703
125.572
124.211
85.197
77.212
77.001
76.789
50.259
26.745
O
NO2
f1 (ppm)

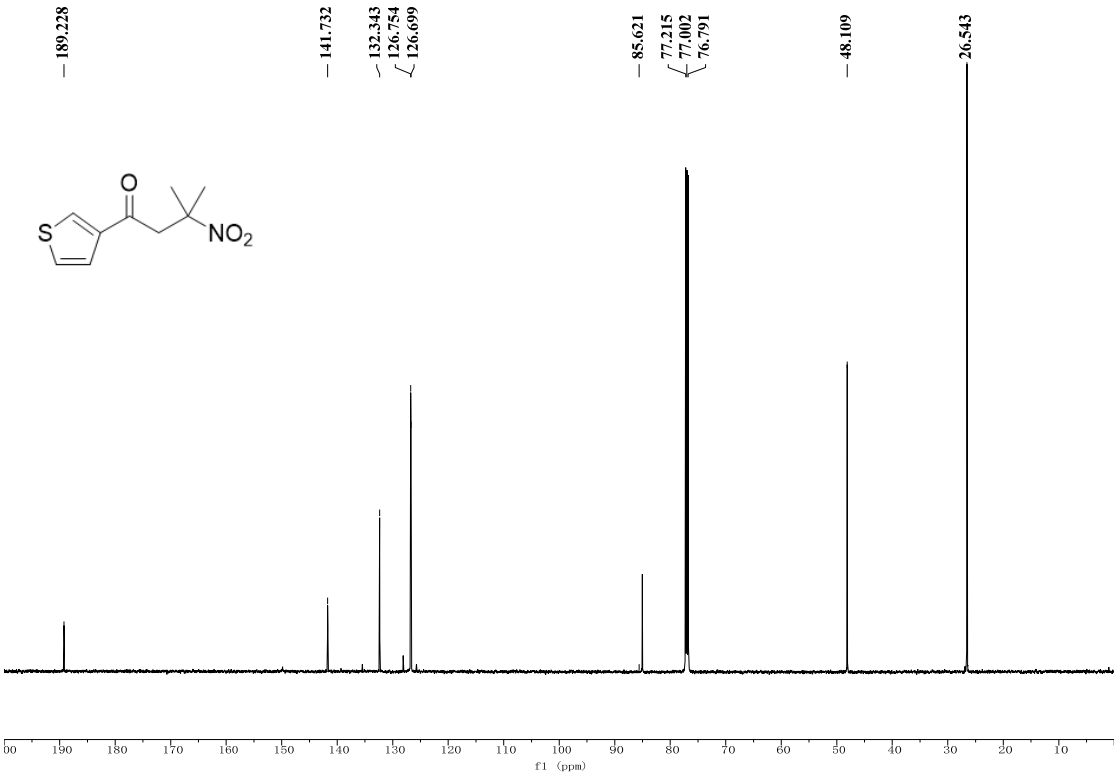

7.590
7.588
7.260
7.223
7.217
6.563
6.560
6.557
6.554
3.524
1.741
O
O
NO2
0.94
0.91
0.90
2.00
6.10
f1 (ppm)

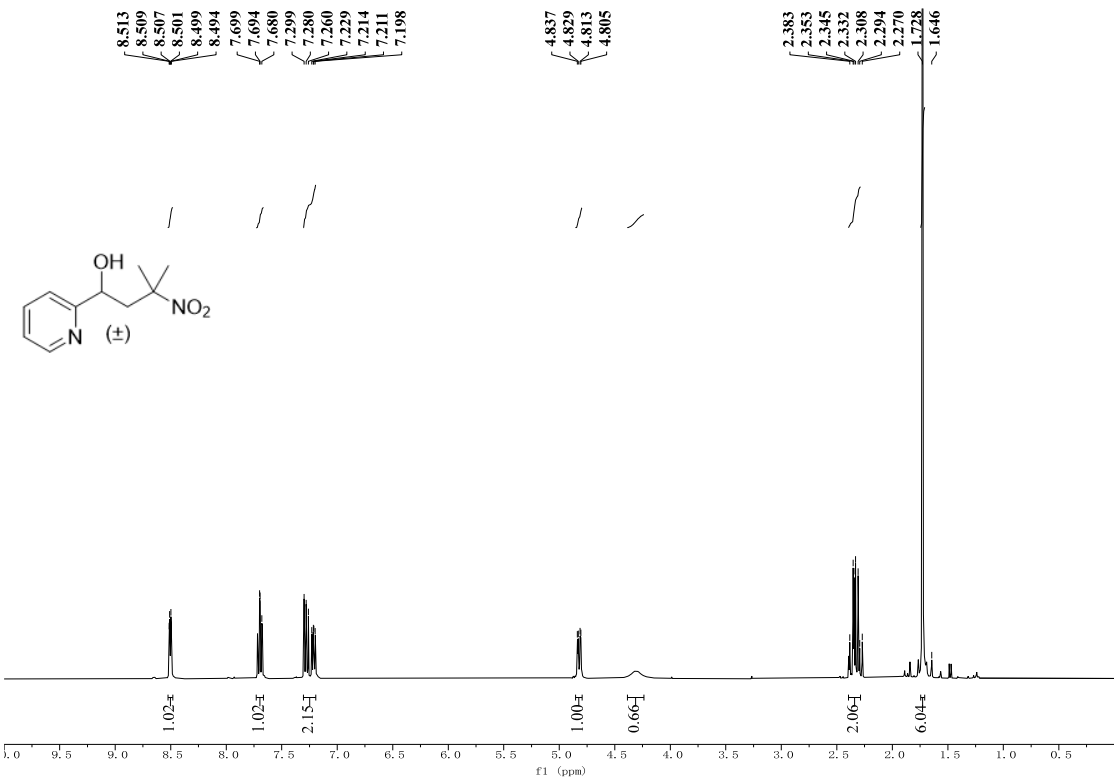

184.137
152.351
147.120
117.529
112.602
85.047
77.320
77.003
76.684
47.704
26.513
O
O
NO2
f1 (ppm)

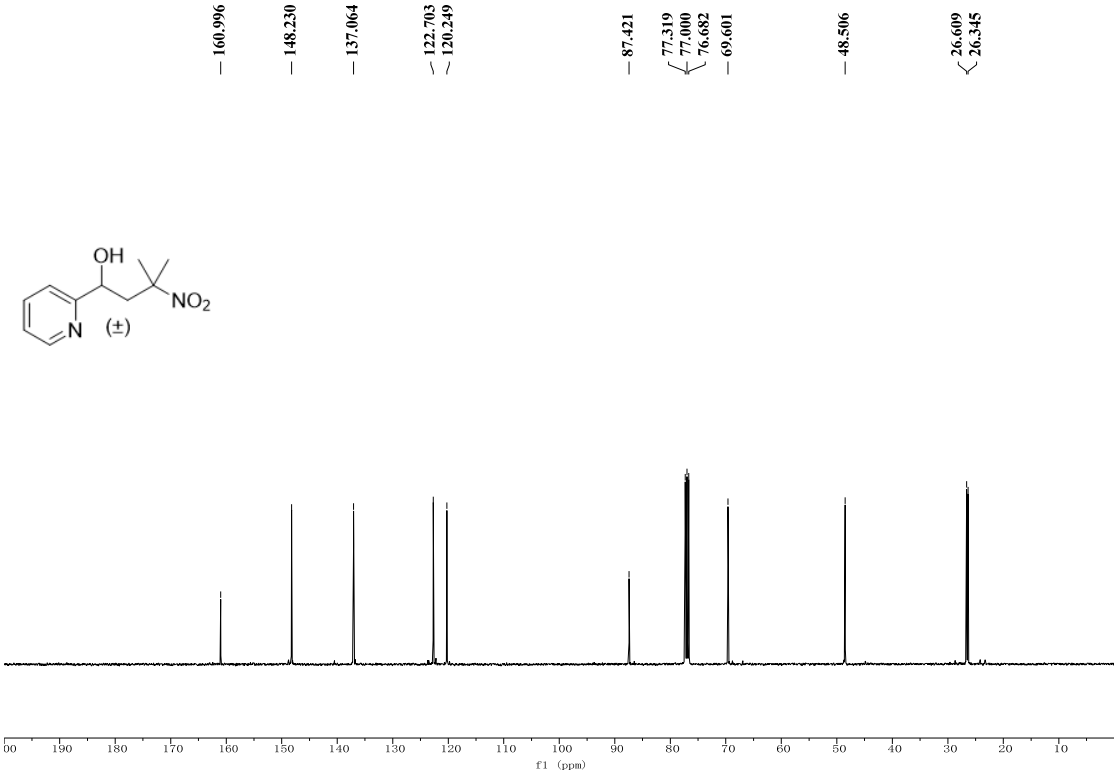

7.725
7.719
7.681
7.673
7.260
7.154
7.148
7.140
3.598
1.762
1.753
0.069
O
S
NO2
2.00
1.08
2.00
6.17
f1 (ppm)

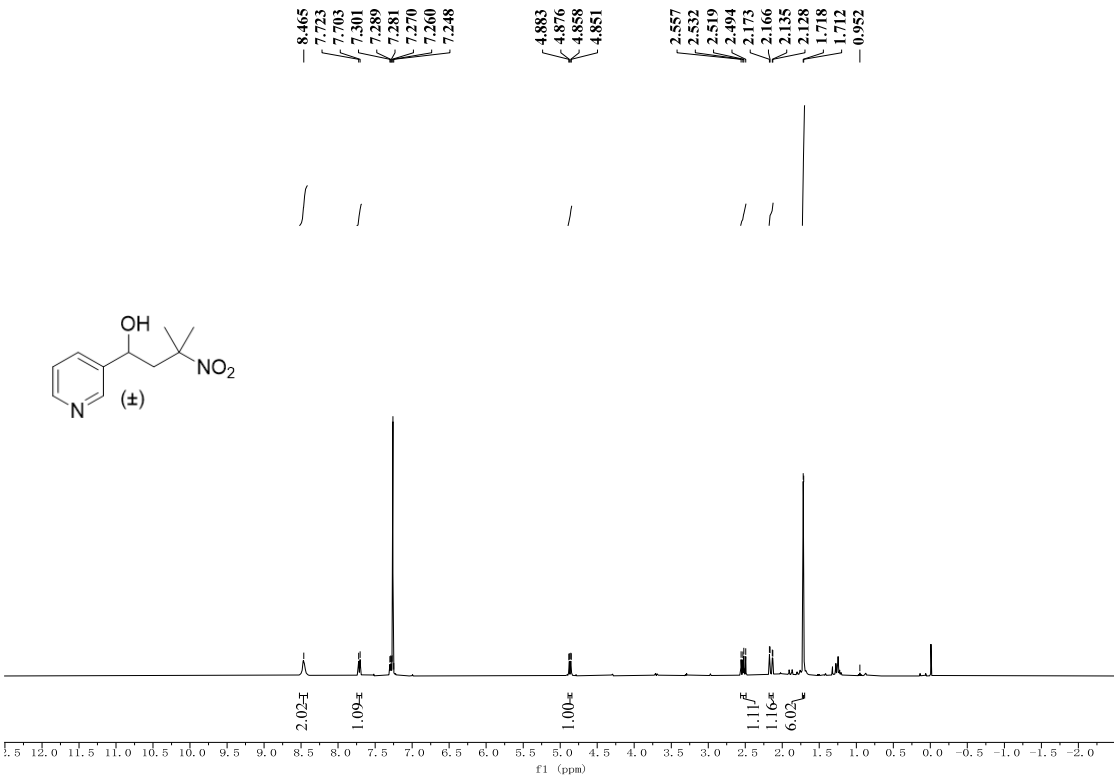

187.830
143.697
134.441
132.217
128.259
85.180
77.316
76.000
76.682
47.477
26.529
O
S
NO2
f1 (ppm)

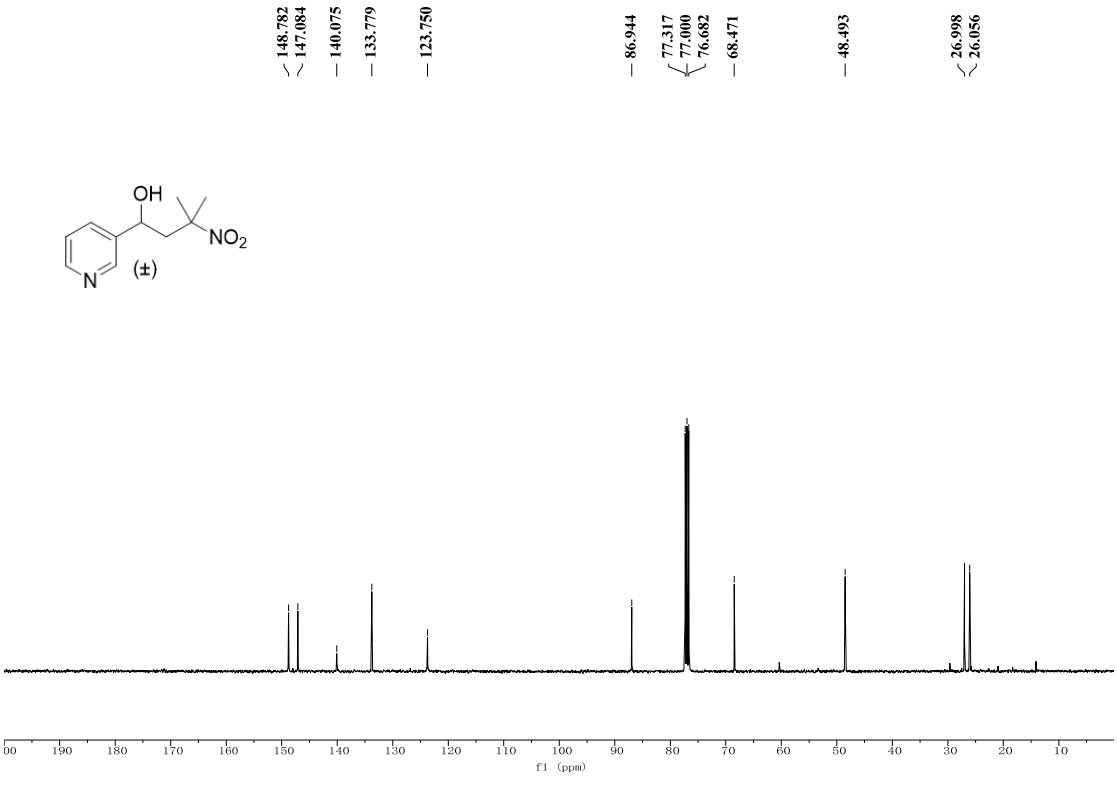

8.066
8.061
7.521
7.518
7.339
7.333
7.260
3.578
1.753
1.751
O
S
NO2
0.89
0.91
0.94
2.00
6.16
f1 (ppm)


189.228
141.732
132.343
126.754
126.699
85.621
77.215
77.002
76.791
48.109
26.543
O
S
NO2
f1 (ppm)


8.513
8.509
8.507
8.501
8.499
8.494
7.699
7.694
7.680
7.299
7.280
7.260
7.229
7.214
7.211
7.198
4.837
4.829
4.813
4.805
2.383
2.353
2.345
2.332
2.308
2.294
2.270
1.728
1.646
OH
NO2
N
(±)
1.02
1.02
2.15
1.00
0.66
2.06
6.04
f1 (ppm)


160.996
148.230
137.064
122.703
120.249
87.421
77.319
77.000
76.682
69.601
48.506
26.609
26.345
OH
NO2
N
(±)
f1 (ppm)


8.465
7.723
7.703
7.301
7.289
7.281
7.270
7.260
7.248
4.883
4.876
4.858
4.851
2.557
2.532
2.519
2.494
2.173
2.166
2.135
2.128
1.718
1.712
0.952
OH
NO2
N
(±)
2.02
1.09
1.00
1.11
1.16
6.02
f1 (ppm)


148.782
147.084
140.075
133.779
123.750
86.944
77.317
77.000
76.682
68.471
48.493
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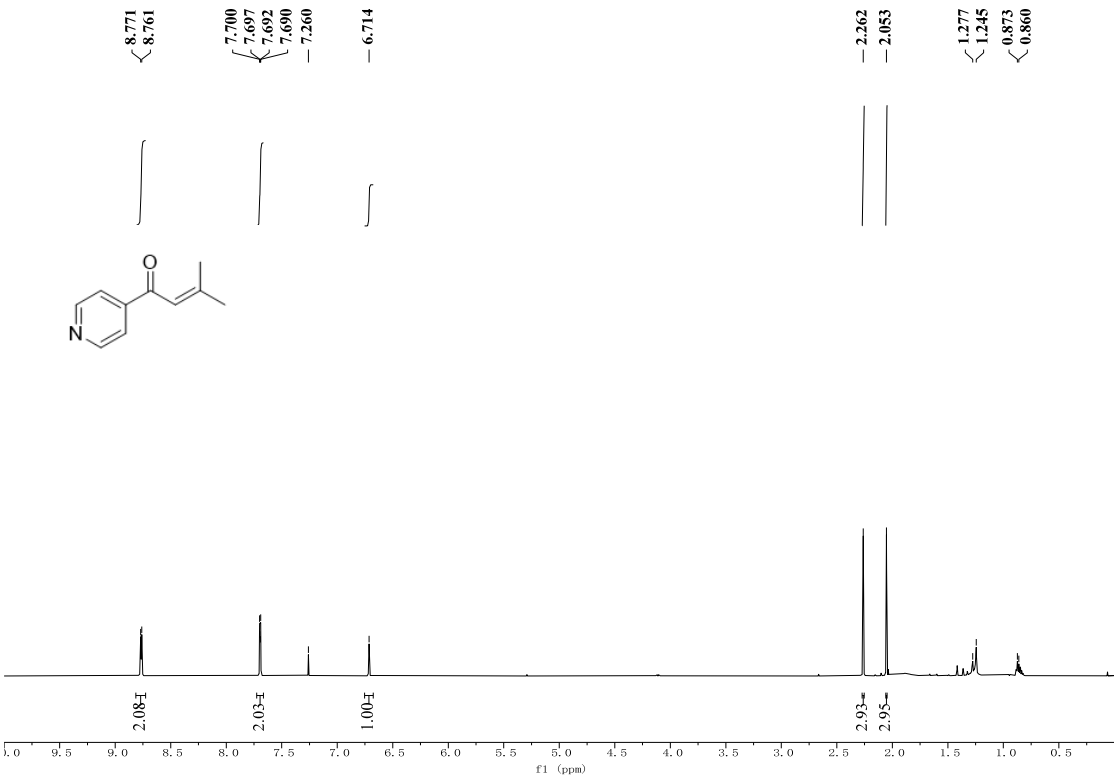
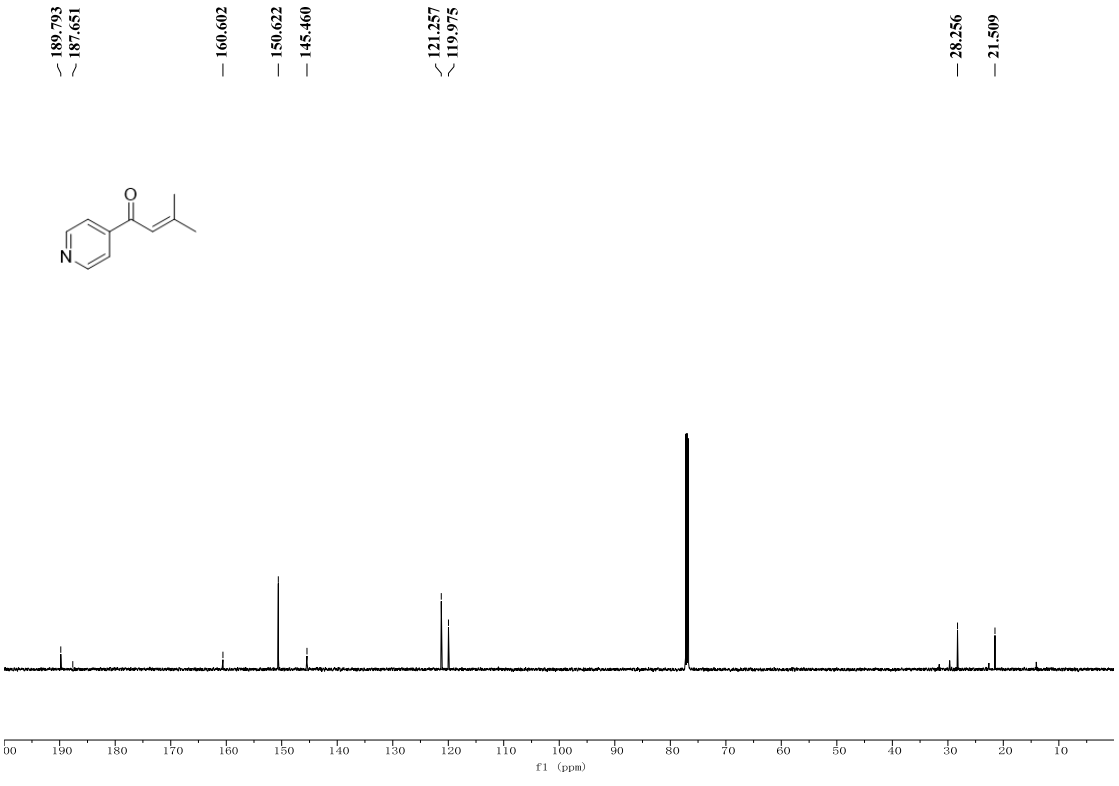
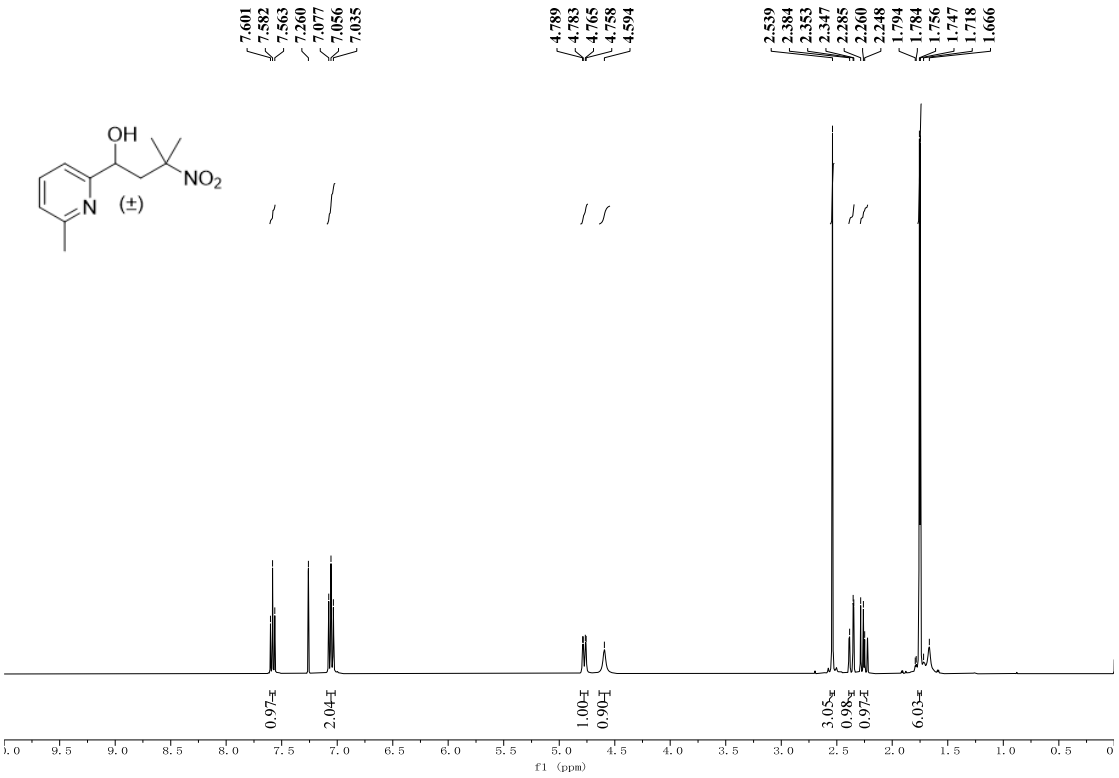
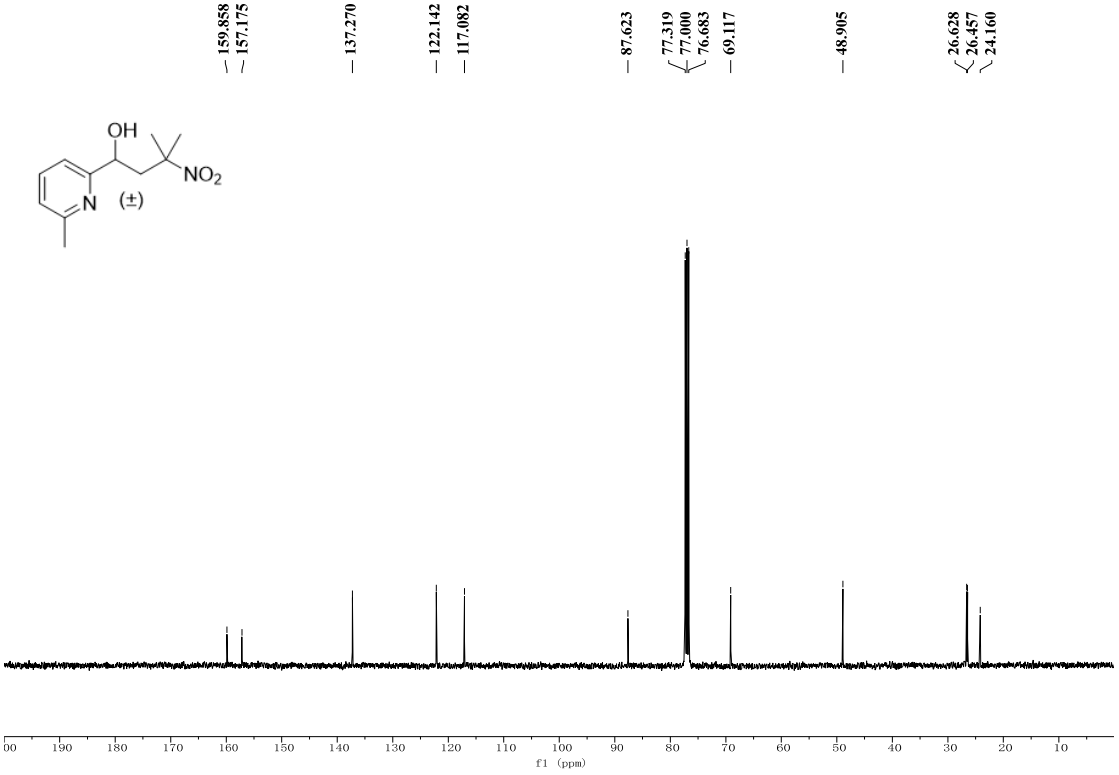
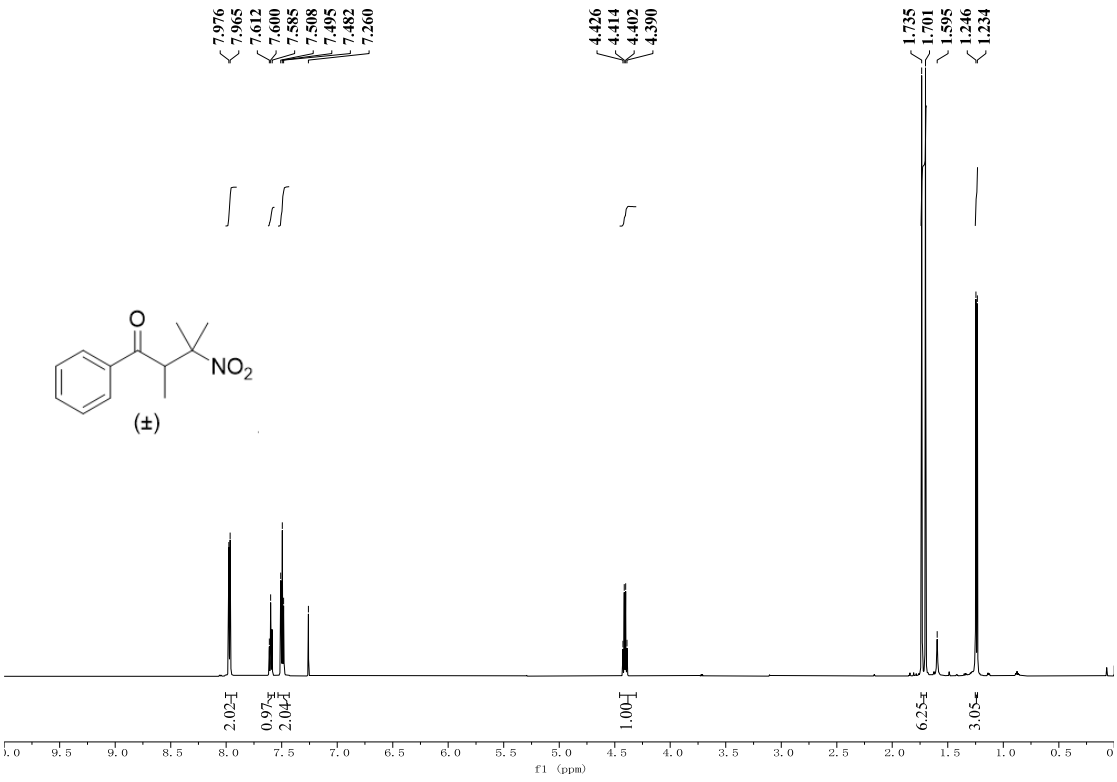
26.056
OH
NO2
N
(±)
f1 (ppm)

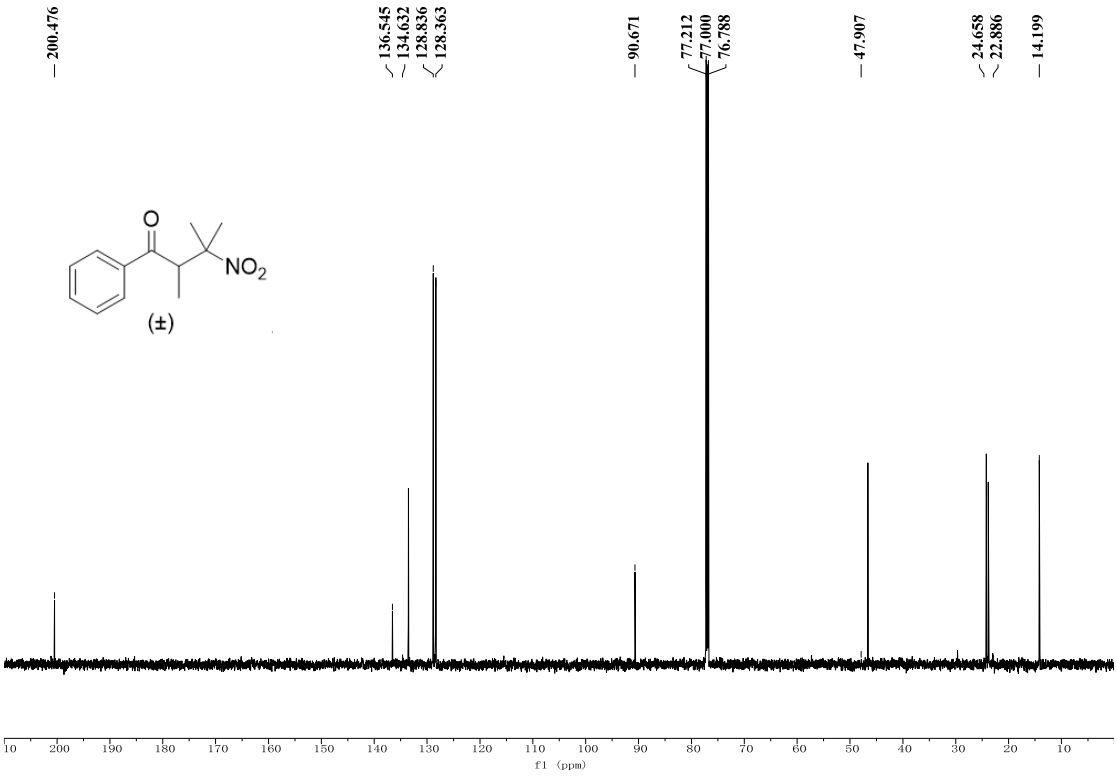

8.771
8.761
7.700
7.697
7.692
7.690
7.260
6.714
2.262
2.053
1.277
1.245
0.873
0.860
O
N
2.08
2.03
1.00
2.93
2.95
f1 (ppm)


189.793
187.651
160.602
150.622
145.460
121.257
119.975
28.256
21.509
O
N
f1 (ppm)


7.601
7.582
7.563
7.260
7.077
7.056
7.035
4.789
4.783
4.765
4.758
4.594
2.539
2.384
2.353
2.347
2.285
2.260
2.248
1.794
1.784
1.756
1.747
1.718
1.666
OH
NO2
N
(±)
0.97
2.04
1.00
0.90
3.05
0.98
0.97
6.03
f1 (ppm)


159.858
157.175
137.270
122.142
117.082
87.623
77.319
77.000
76.683
69.117
48.905
26.628
26.457
24.160
OH
NO2
N
(±)
f1 (ppm)


7.976
7.965
7.612
7.600
7.585
7.508
7.495
7.482
7.260
4.426
4.414
4.402
4.390
1.735
1.701
1.595
1.246
1.234
O
NO2
(±)
2.02
0.97
2.04
1.00
6.25
3.05
f1 (ppm)


200.476
136.545
134.632
128.836
128.363
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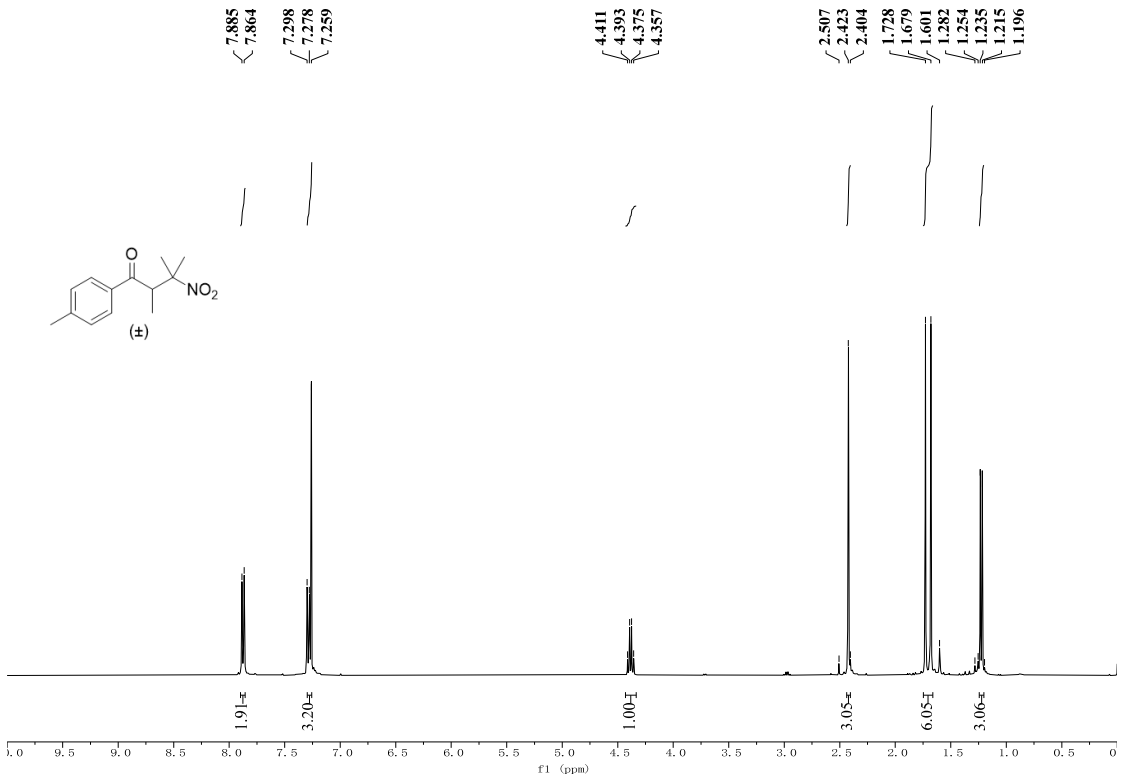
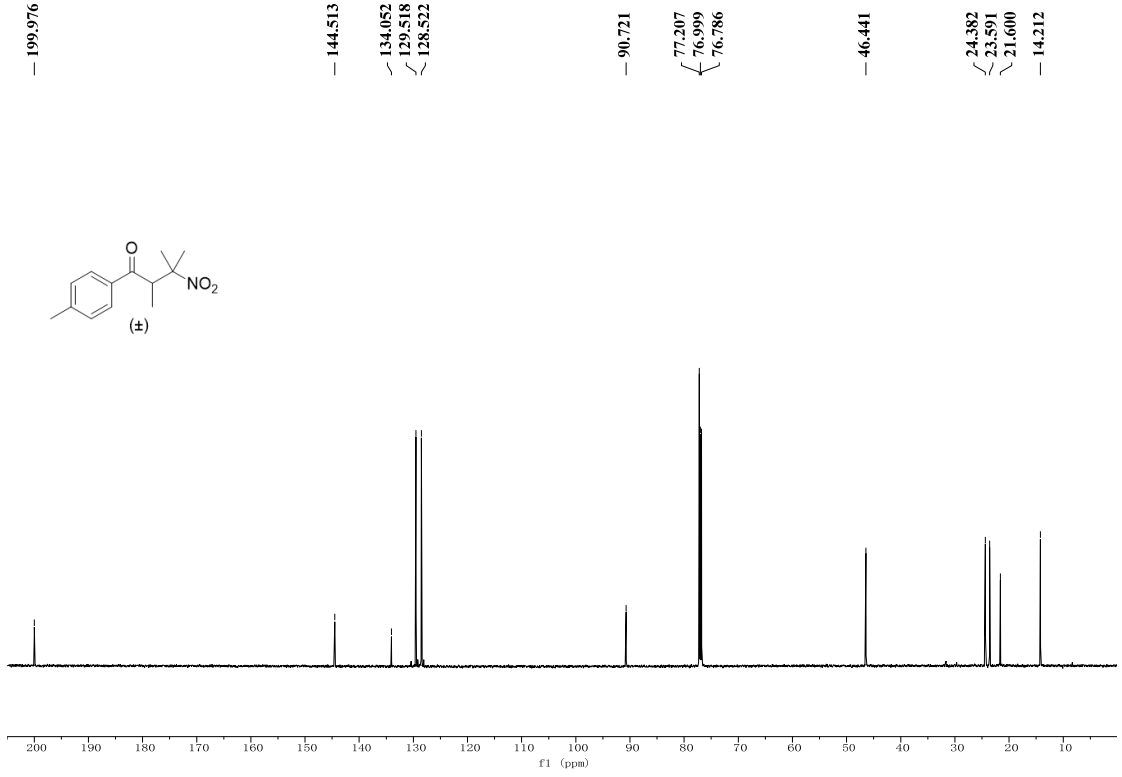
77.212
77.000
76.788
47.907
24.658
22.886
14.199
O
NO2
(±)
f1 (ppm)


7.885
7.864
7.298
7.278
7.259
4.411
4.393
4.375
4.357
2.507
2.423
2.404
1.728
1.679
1.601
1.282
1.254
1.235
1.215
1.196
O
NO2
(±)
1.91
3.20
1.00
3.05
6.05
3.06
f1 (ppm)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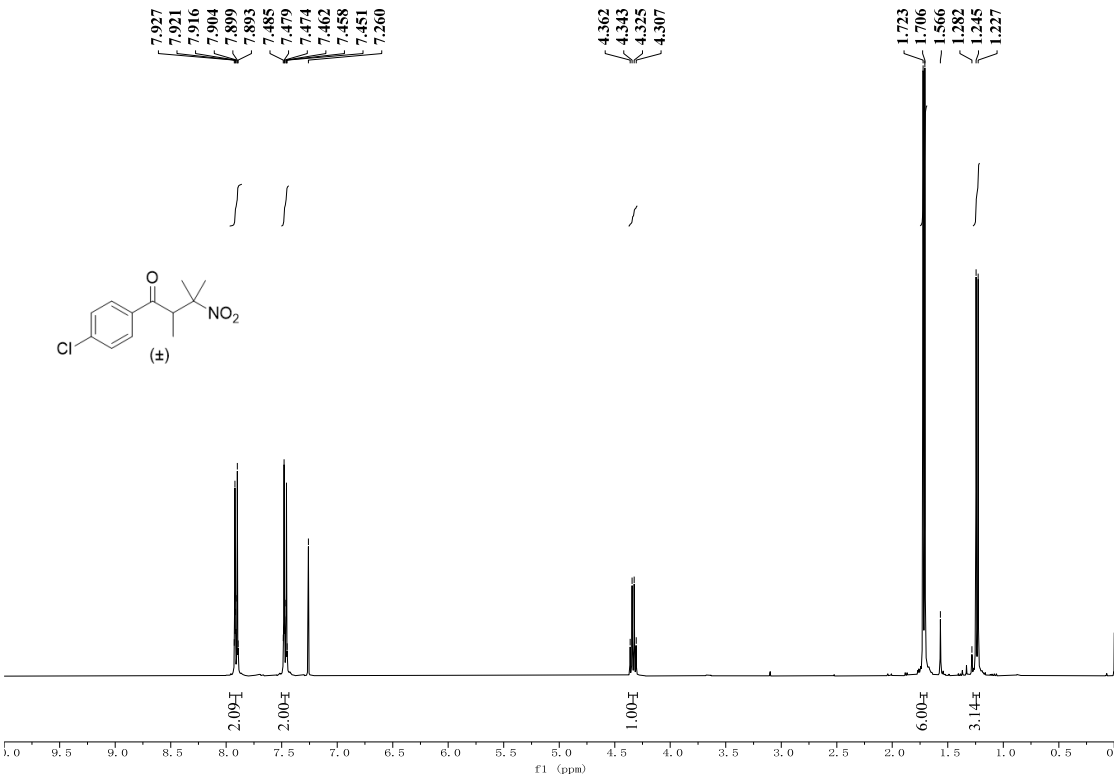
134.052
129.518
128.522
90.721
77.207
76.999
76.786
46.441
24.382
23.591
21.600
14.212
O
NO2
(±)
f1 (ppm)


7.927
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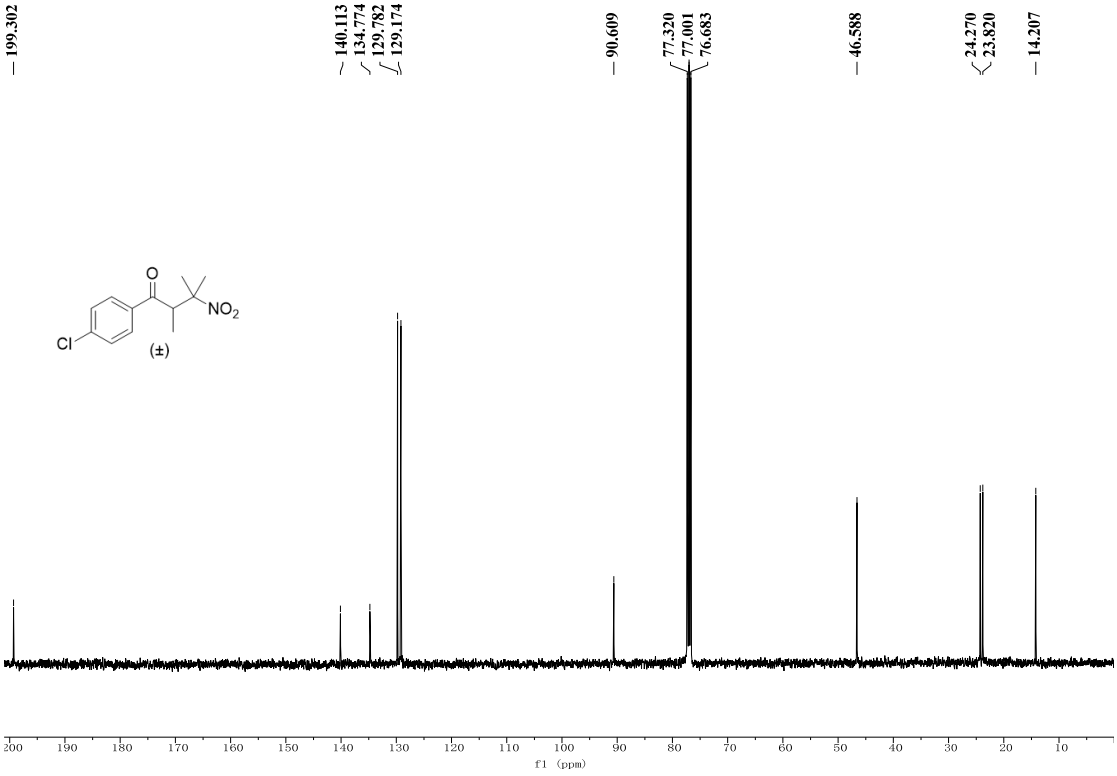
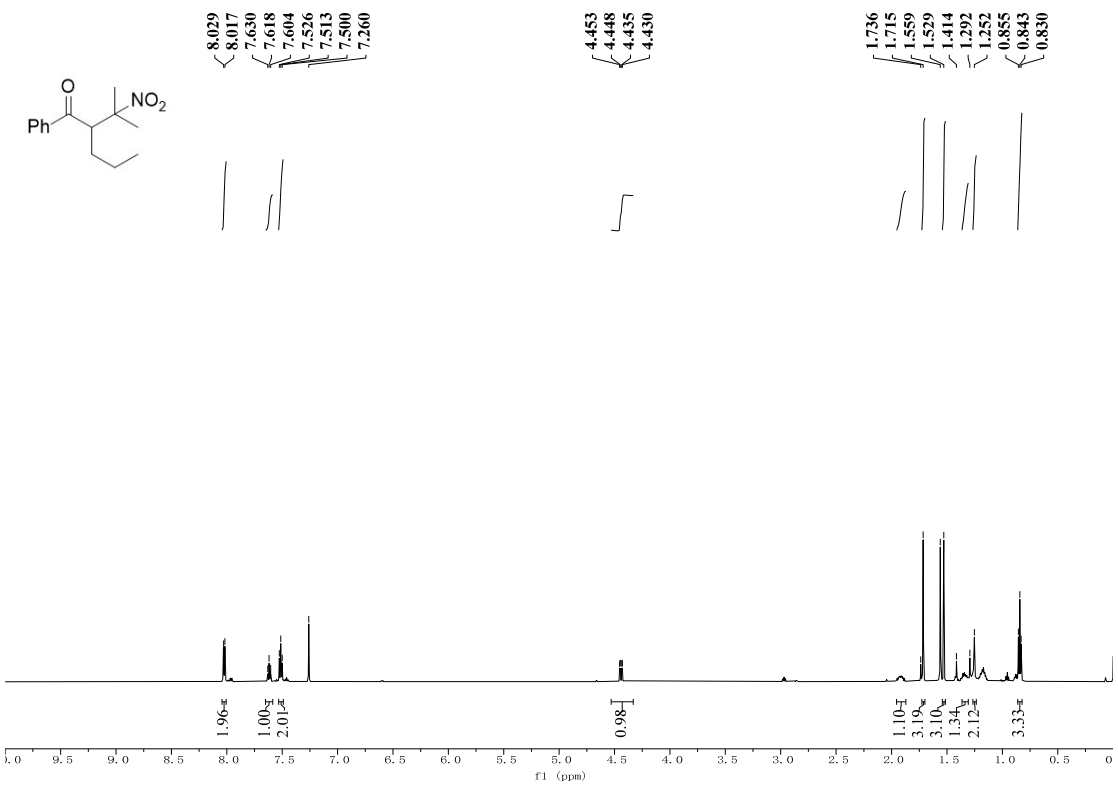
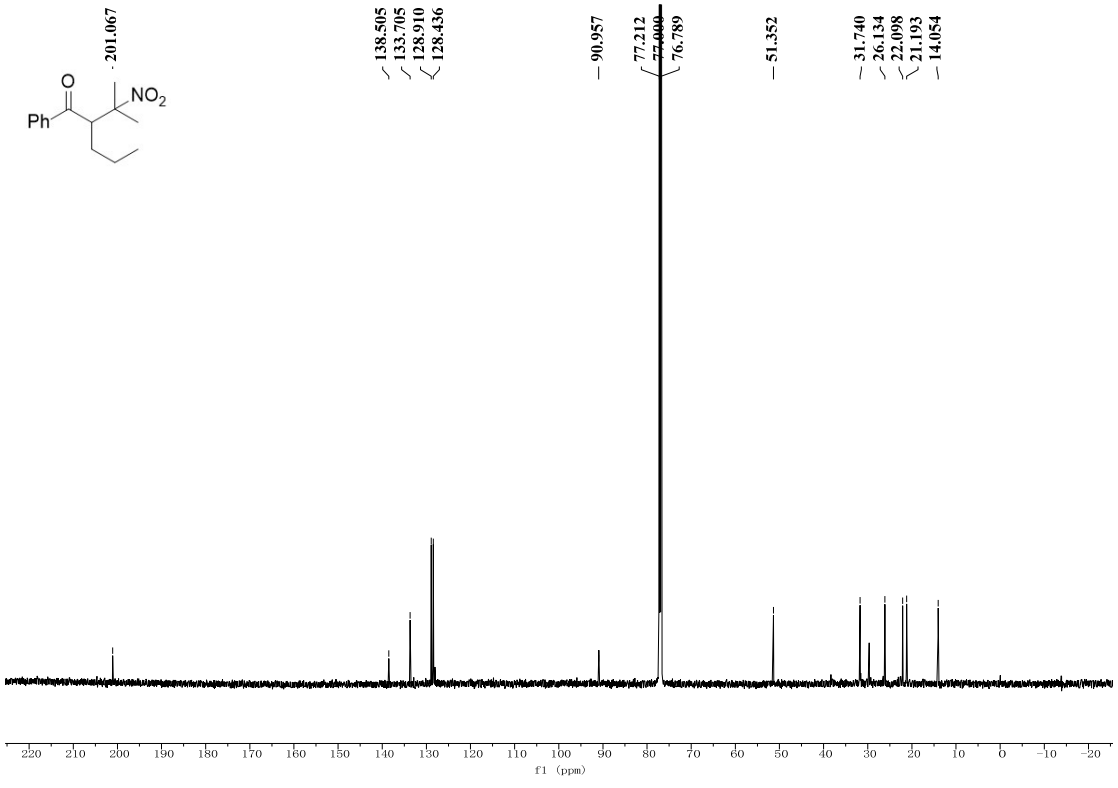
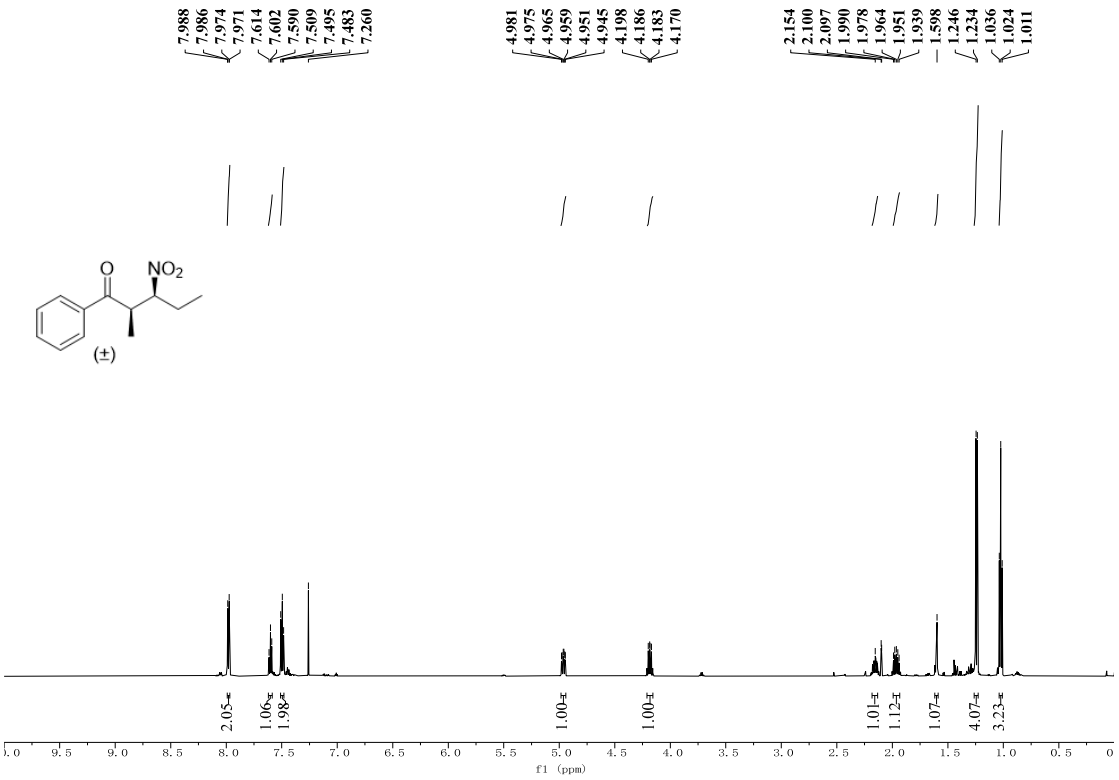
7.916
7.904
7.899
7.893
7.485
7.479
7.474
7.462
7.458
7.451
7.260
4.362
4.343
4.325
4.307
1.723
1.706
1.566
1.282
1.245
1.227
O
NO2
Cl
(±)
2.09
2.00
1.00
6.00
3.14
f1 (ppm)


199.302
140.113
134.774
129.782
129.174
90.609
77.320
77.001
76.683
46.588
24.270
23.820
14.207
O
NO2
Cl
(±)
f1 (ppm)


8.029
8.017
7.630
7.618
7.604
7.526
7.513
7.500
7.260
4.453
4.448
4.435
4.430
1.736
1.715
1.559
1.529
1.414
1.292
1.252
0.855
0.843
0.830
O
Ph
NO2
1.96
1.00
2.01
0.98
1.10
3.19
3.10
1.34
2.12
3.33
f1 (ppm)


201.067
138.505
133.705
128.910
128.436
90.957
77.212
77.000
76.789
51.352
31.740
26.134
22.098
21.193
14.054
O
Ph
NO2
f1 (ppm)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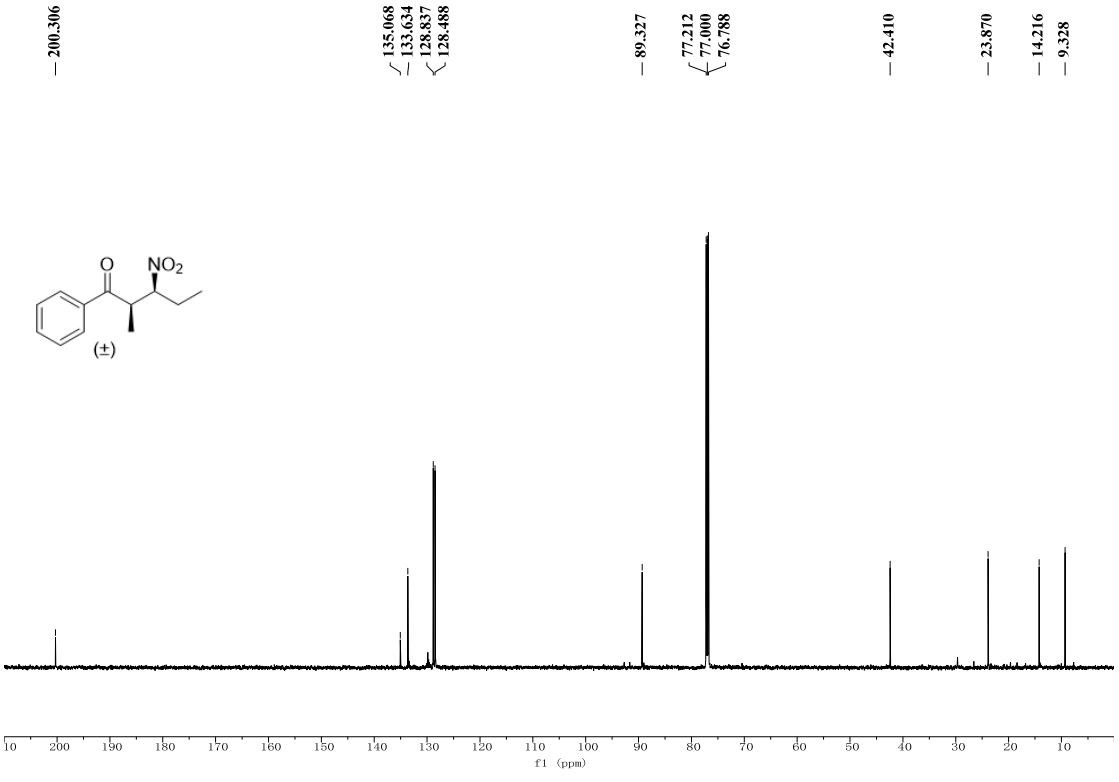
7.974
7.971
7.614
7.602
7.590
7.509
7.495
7.483
7.260
4.981
4.975
4.965
4.959
4.951
4.945
4.198
4.186
4.183
4.170
2.154
2.100
2.097
1.990
1.978
1.964
1.951
1.939
1.598
1.246
1.234
1.036
1.024
1.011
O
NO2
(±)
2.05
1.06
1.98
1.00
1.00
1.01
1.12
1.07
4.07
3.23
f1 (ppm)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135.068
133.634
128.837
128.488
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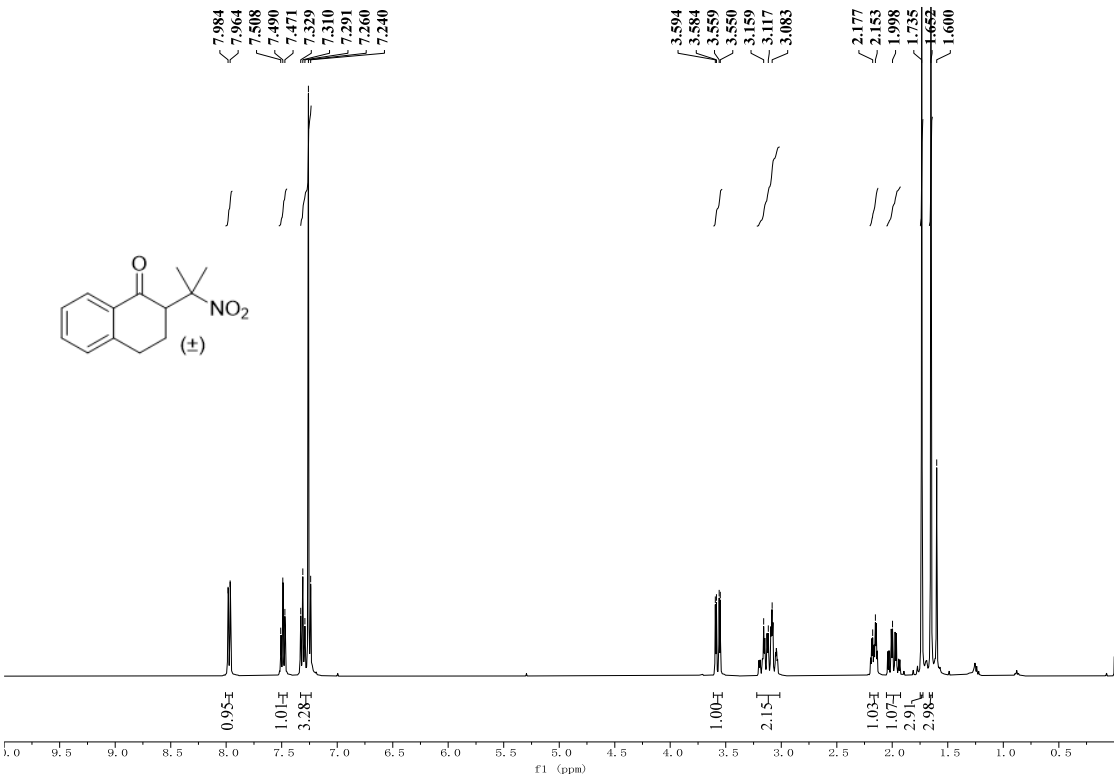
77.212
77.000
76.788
42.410
23.870
14.216
9.328
O
NO2
(±)
f1 (ppm)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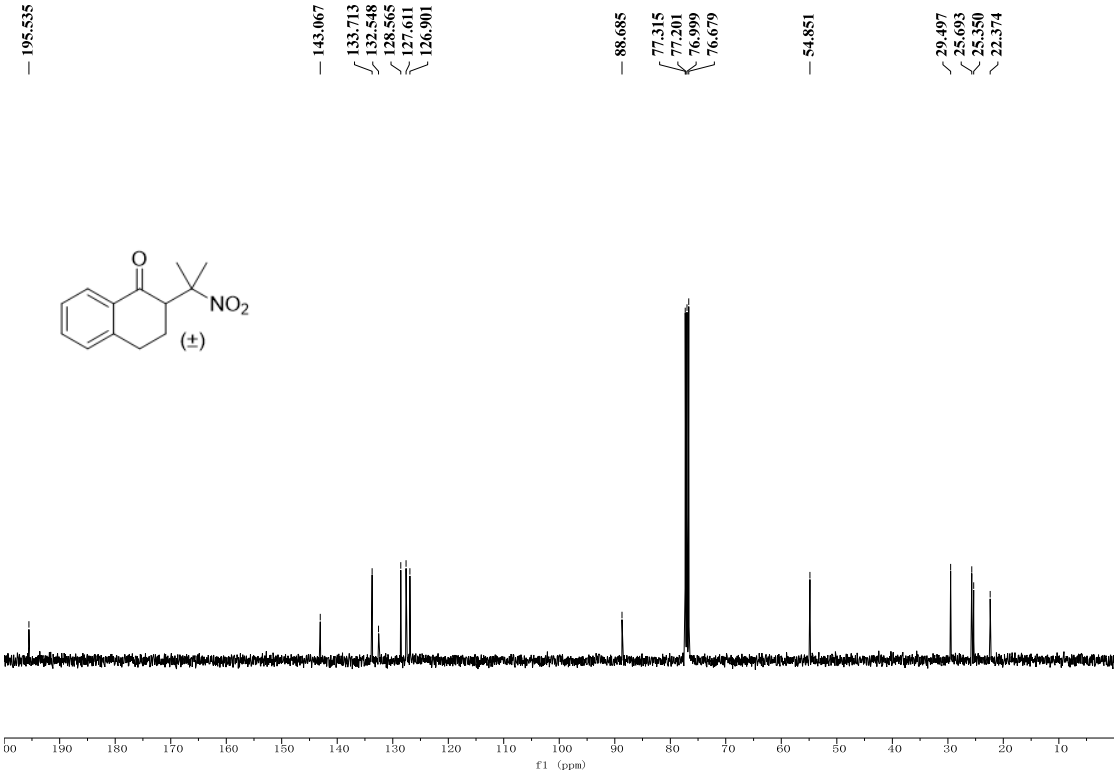
7.508
7.490
7.471
7.329
7.310
7.291
7.260
7.240
3.594
3.584
3.559
3.550
3.159
3.117
3.083
2.177
2.153
1.998
1.735
1.652
1.600
O
NO2
(±)
0.95
1.01
3.28
1.00
2.15
1.03
1.07
2.91
2.98
f1 (ppm)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132.548
128.565
127.611
126.901
88.685
77.315
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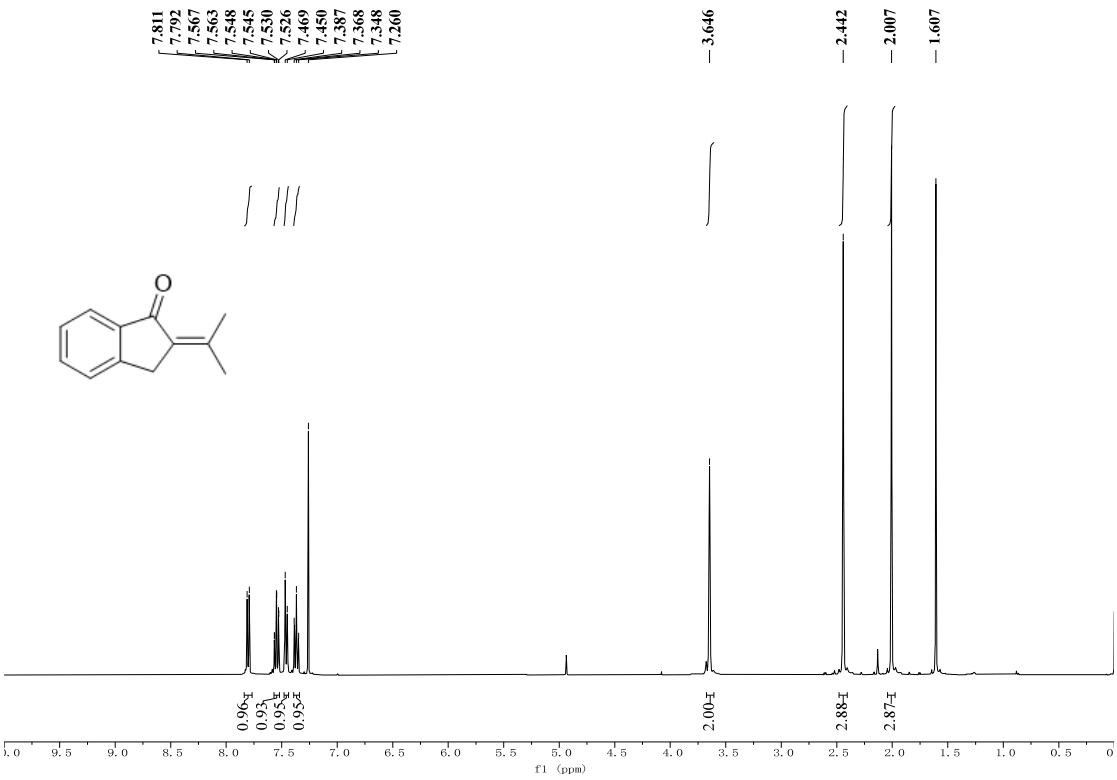
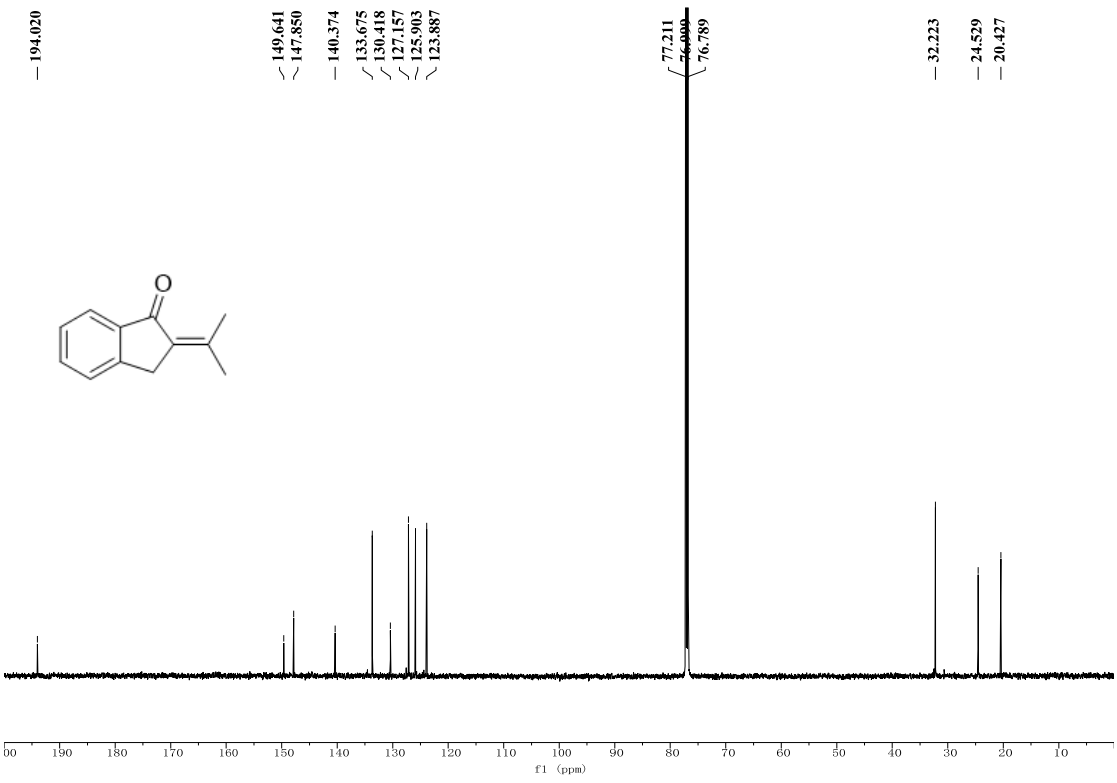
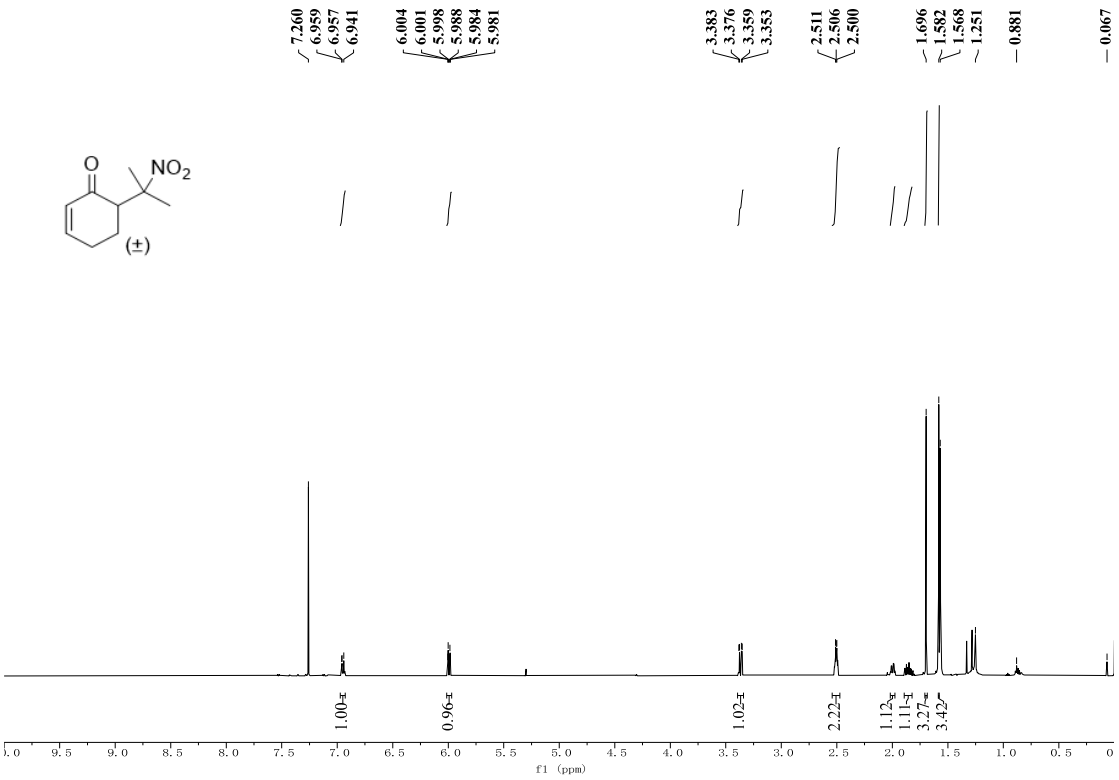
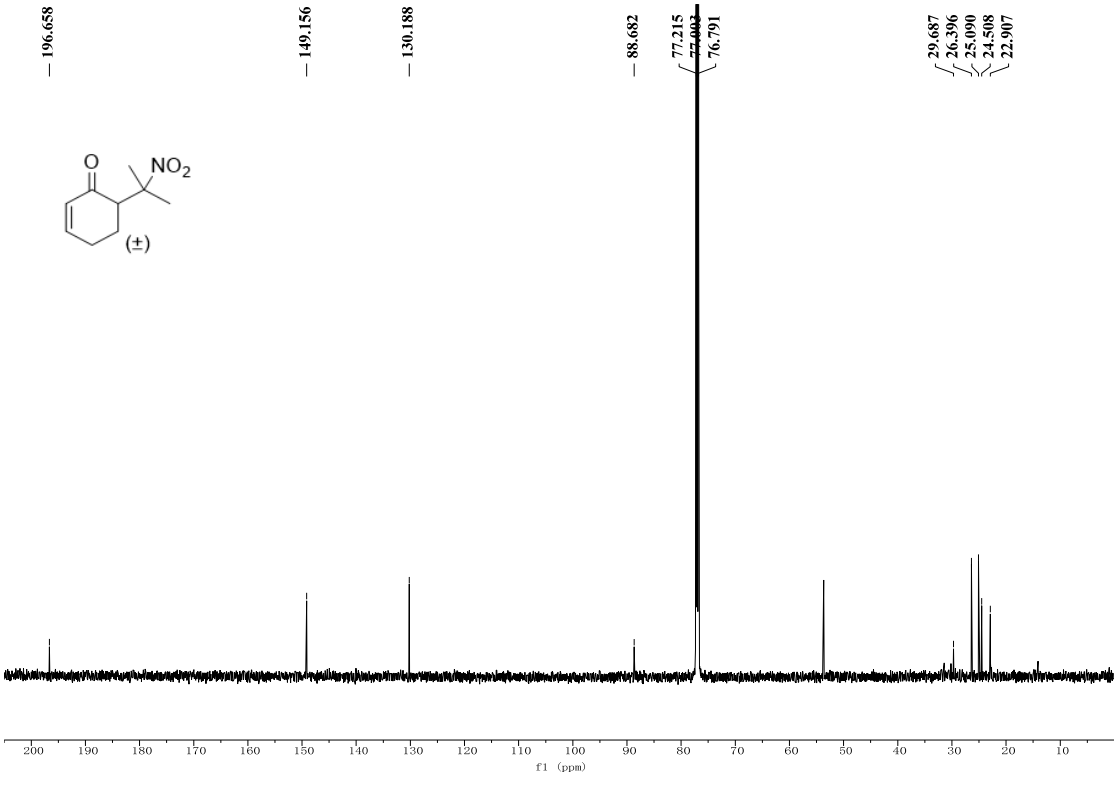
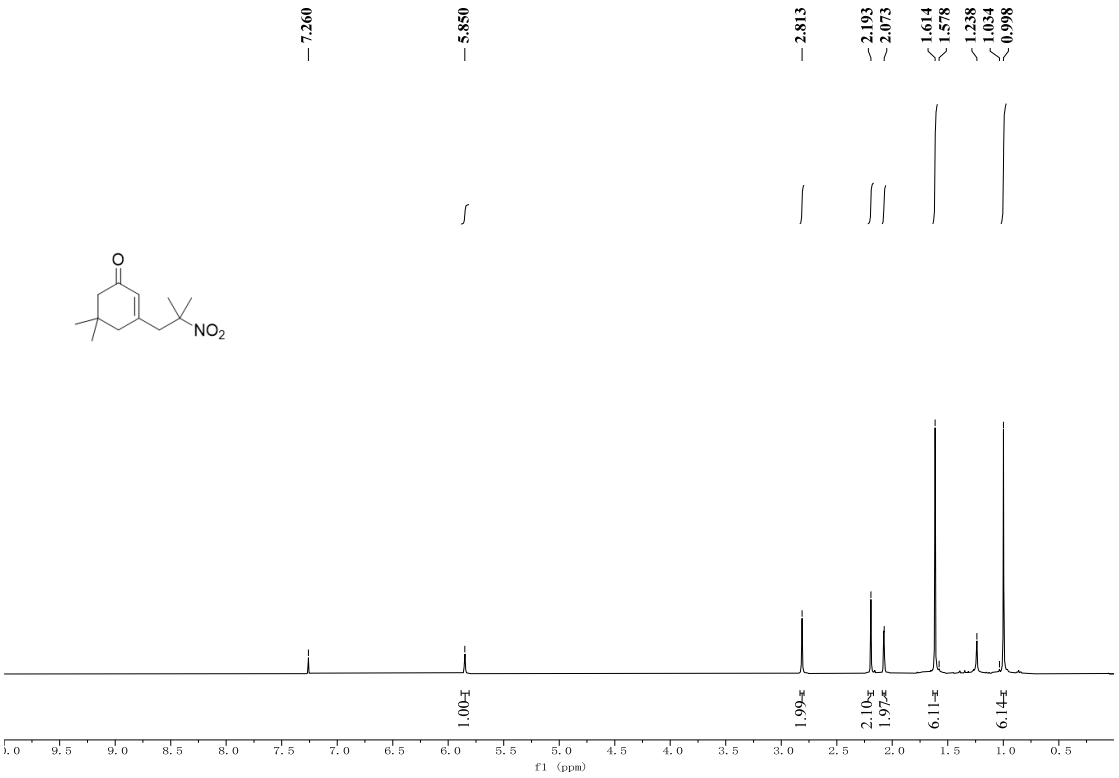
76.999
76.679
54.851
29.497
25.693
25.350
22.374
O
NO2
(±)
f1 (ppm)

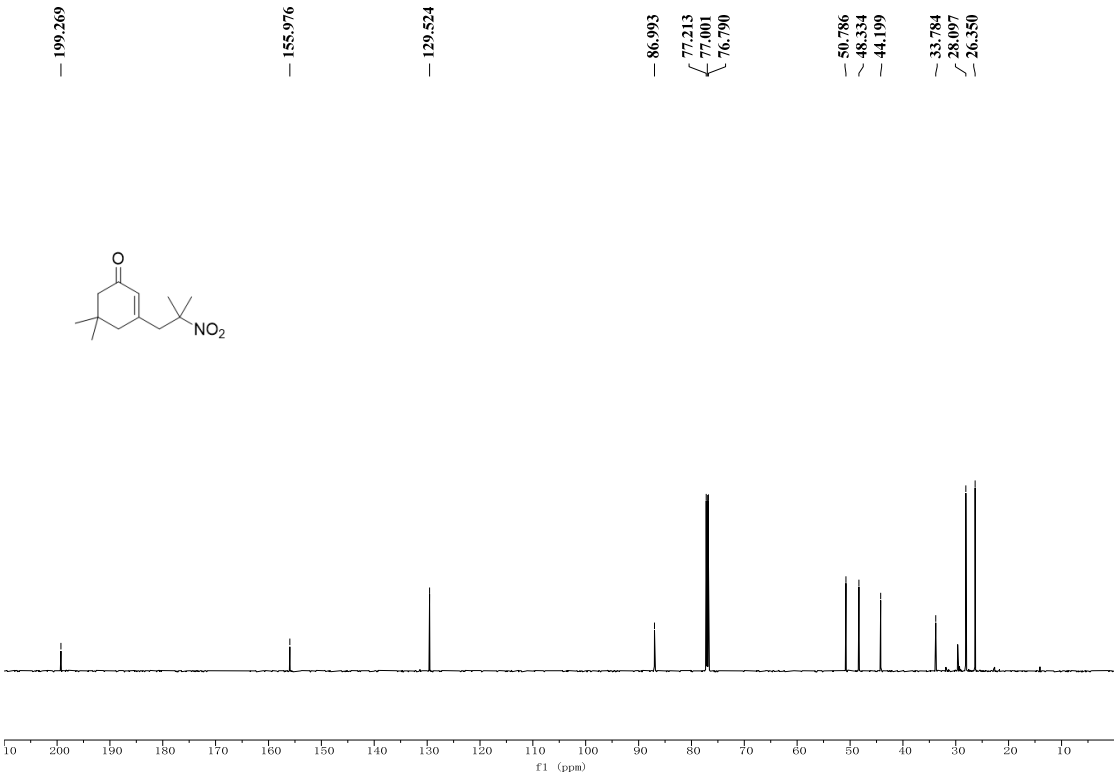

7.811
7.792
7.567
7.563
7.548
7.545
7.530
7.526
7.469
7.450
7.387
7.368
7.348
7.260
3.646
2.442
2.007
1.607
O
0.96
0.93
0.95
0.95
2.00
2.88
2.87
f1 (ppm)

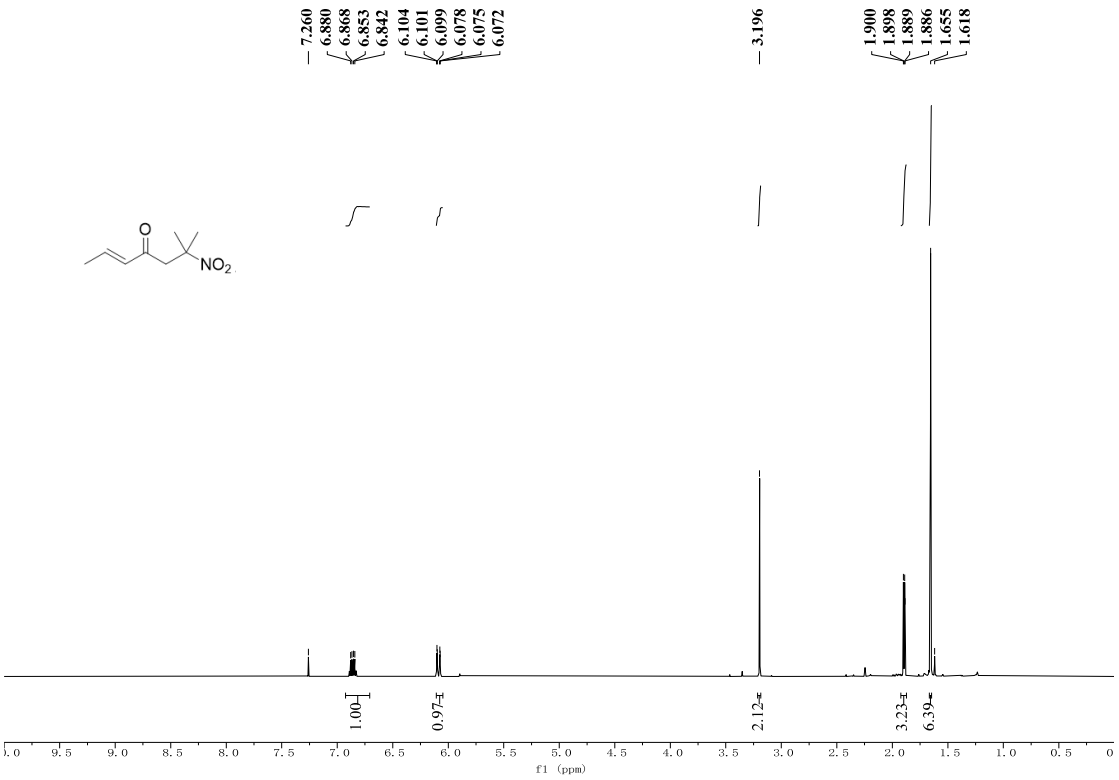

194.020
149.641
147.850
140.374
133.675
130.418
127.157
125.903
123.887
77.211
76.000
76.789
32.223
24.529
20.427
O
f1 (ppm)

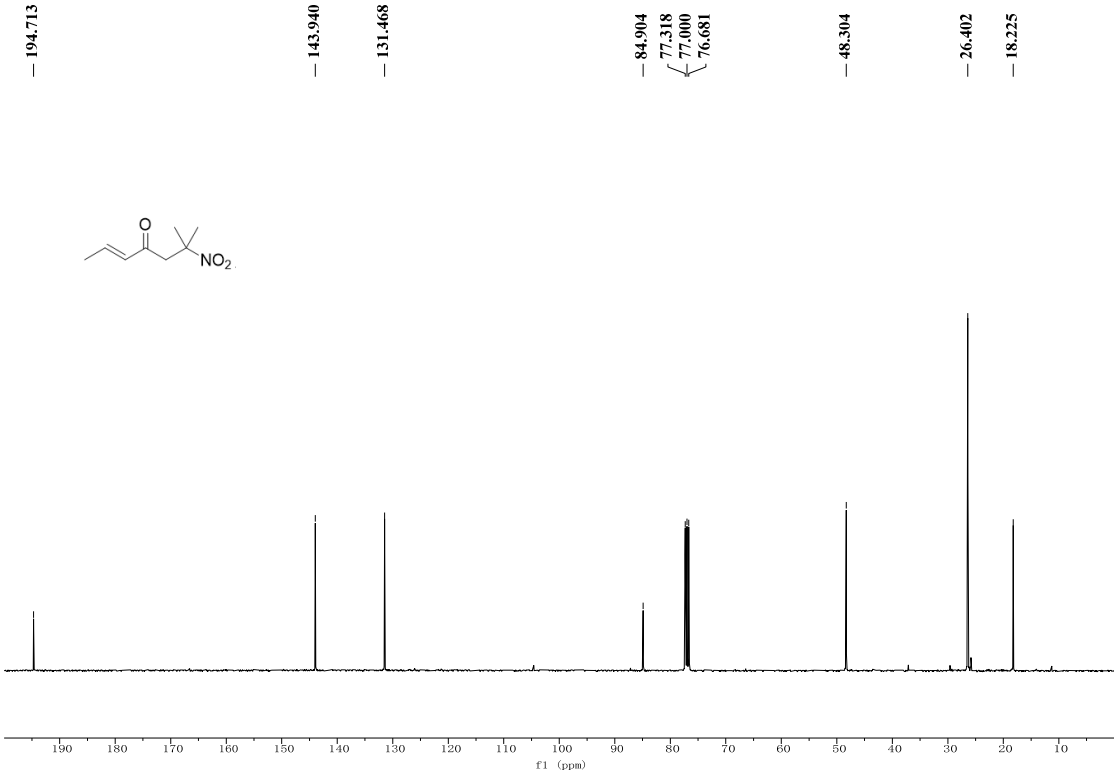

7.260
6.959
6.957
6.941
6.004
6.001
5.998
5.988
5.984
5.981
3.383
3.376
3.359
3.353
2.511
2.506
2.500
1.696
1.582
1.568
1.251
0.881
0.067
O
NO2
(±)
1.00
0.96
1.02
2.22
1.12
1.11
3.27
3.42
f1 (ppm)

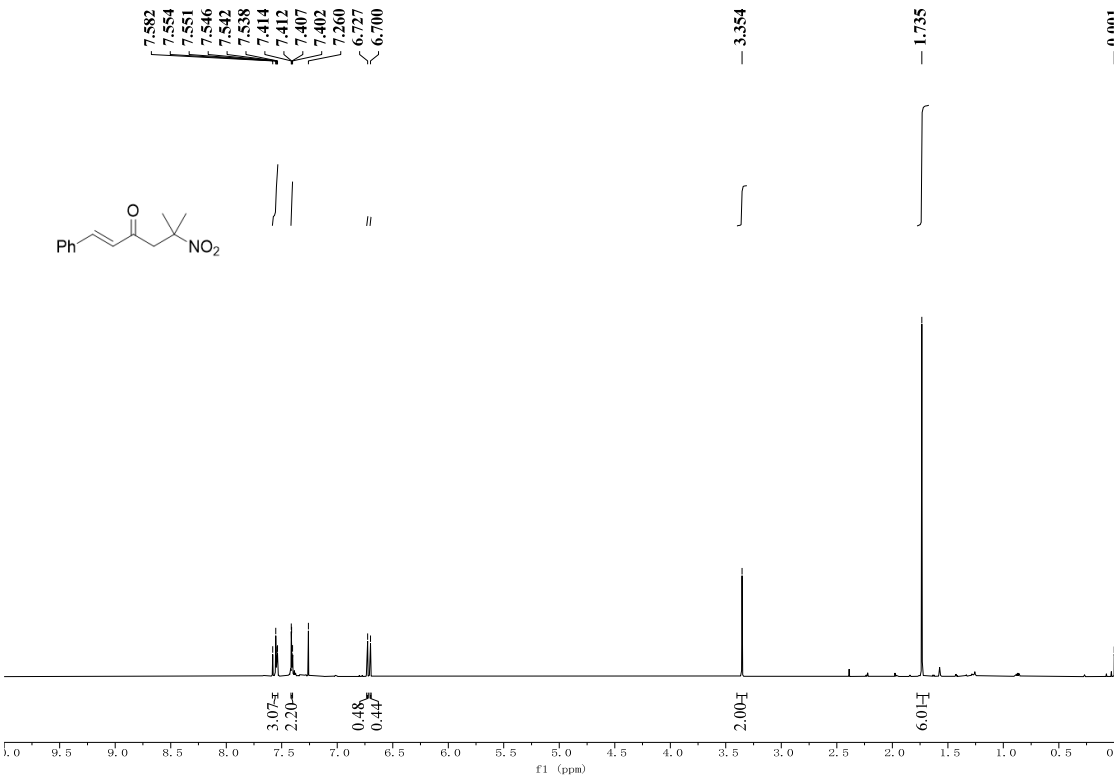

196.658
149.156
130.188
88.682
77.215
77.003
76.791
29.687
26.396
25.090
24.508
22.907
O
NO2
(±)
f1 (ppm)

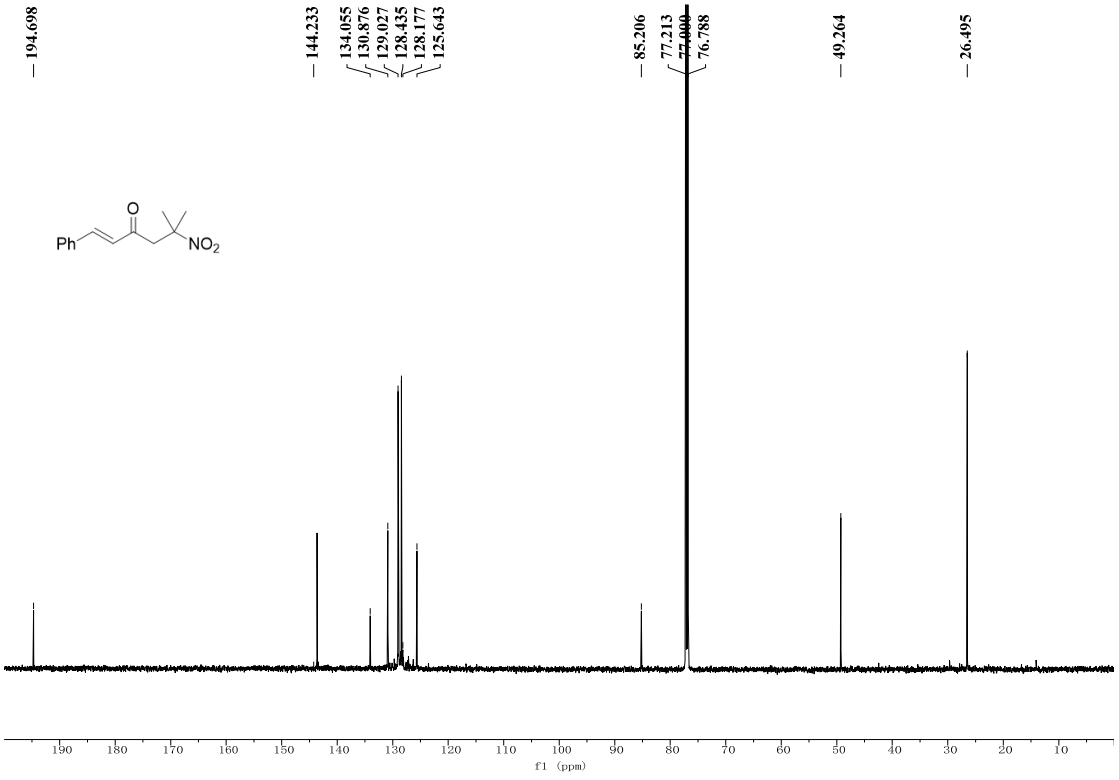

7.260
5.850
2.813
2.193
2.073
1.614
1.578
1.238
1.034
0.998
O
NO2
1.00
1.99
2.10
1.97
6.11
6.14
f1 (ppm)

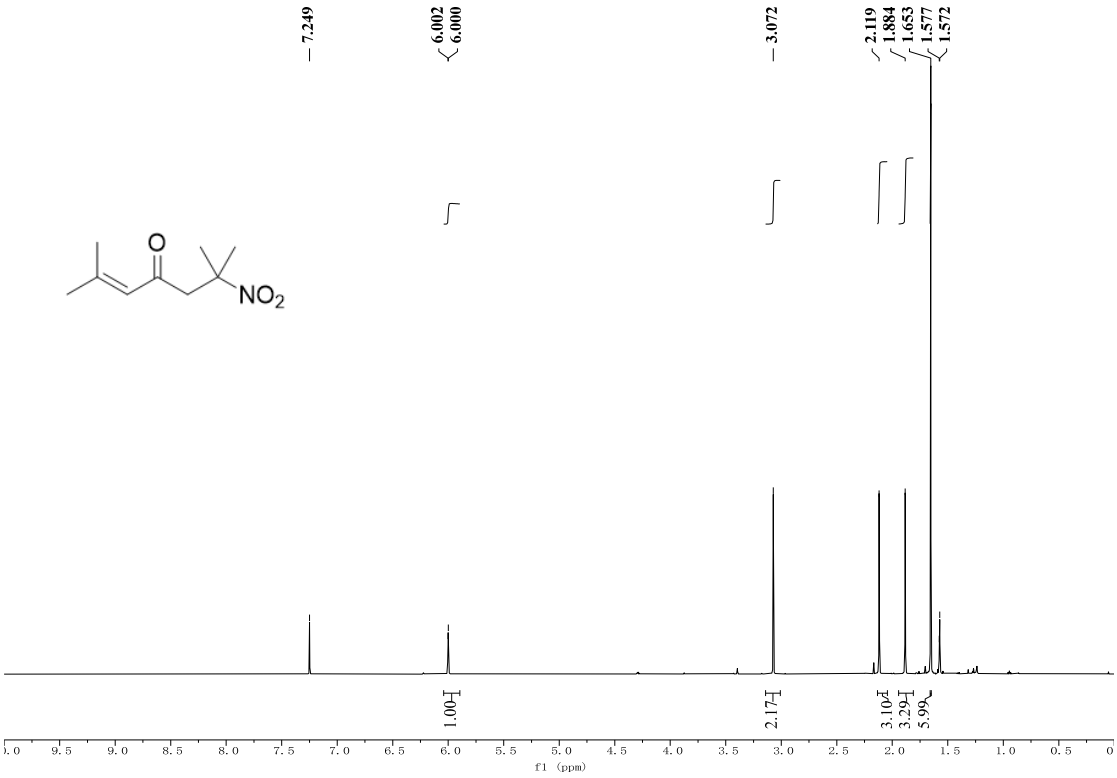

199.269
155.976
129.524
86.993
77.213
77.001
76.790
50.786
48.334
44.199
33.784
28.097
26.350
O
NO2
f1 (ppm)

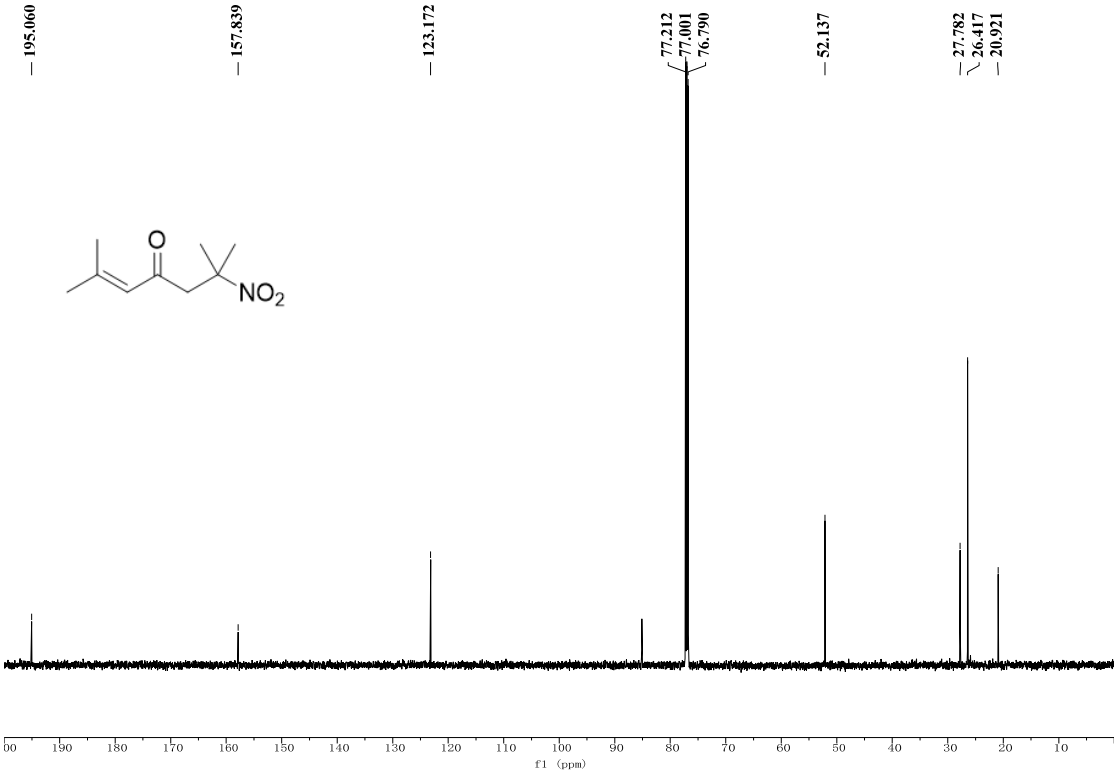

7.260
6.880
6.868
6.853
6.842
6.104
6.101
6.099
6.078
6.075
6.072
3.196
1.900
1.898
1.889
1.886
1.655
1.618
O
NO2
1.00
0.97
2.12
3.23
6.39
f1 (ppm)

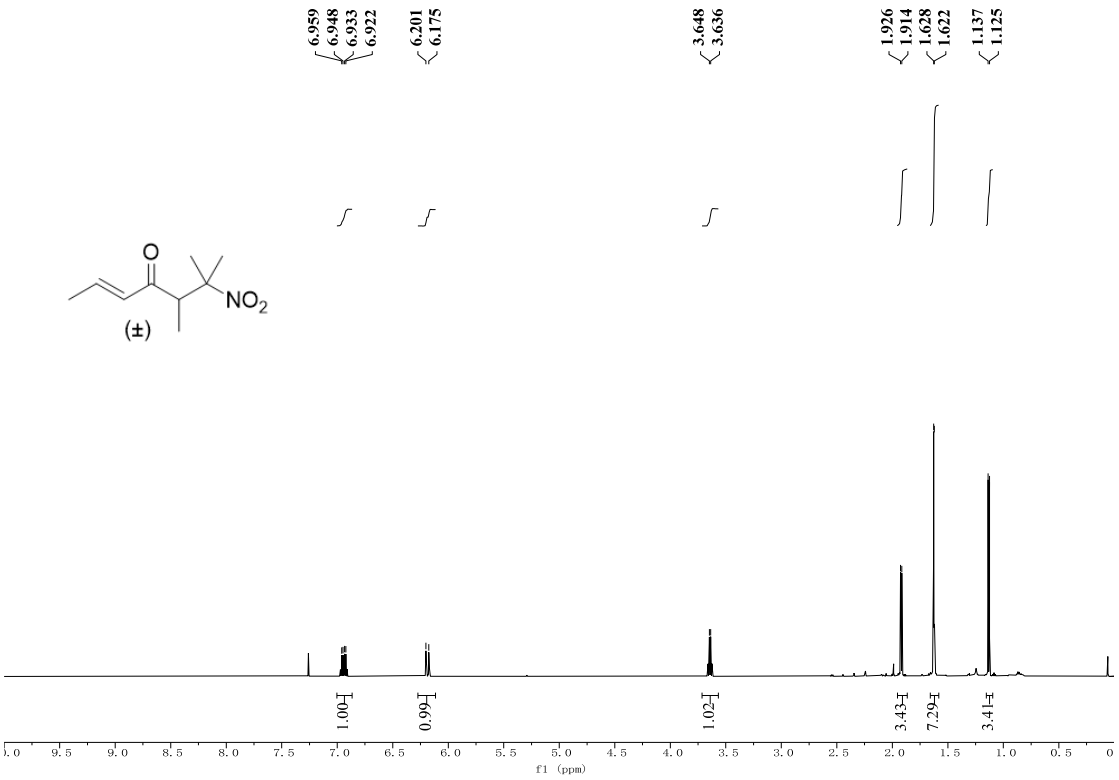

194.713
143.940
131.468
84.904
77.318
77.000
76.681
48.304
26.402
18.225
O
NO2
f1 (ppm)

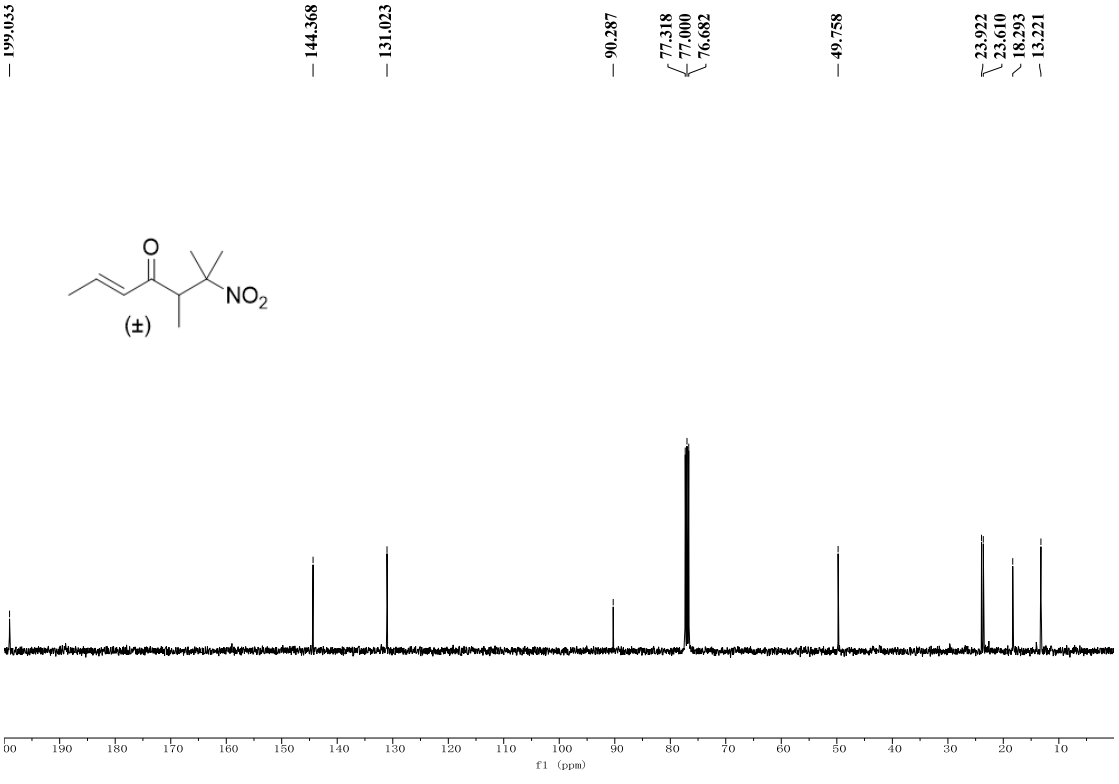

7.582
7.554
7.551
7.546
7.542
7.538
7.414
7.412
7.407
7.402
7.260
6.727
6.700
3.354
1.735
Ph
O
NO2
3.07
2.20
0.48
0.44
2.00
6.01
f1 (ppm)

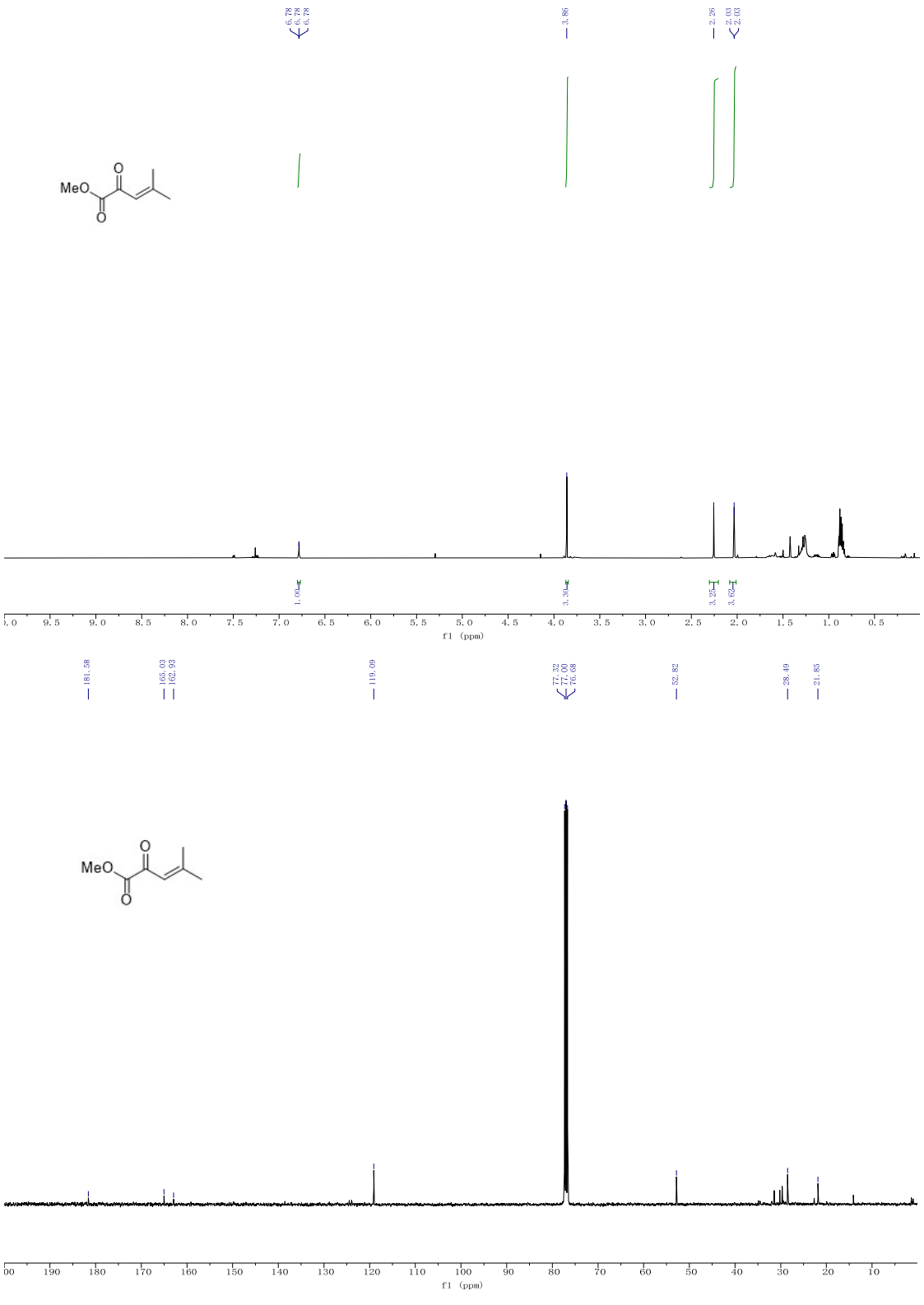

194.698
144.233
134.055
130.876
129.027
128.435
128.177
125.643
85.206
77.213
77.000
76.788
49.264
26.495
Ph
O
NO2
f1 (ppm)

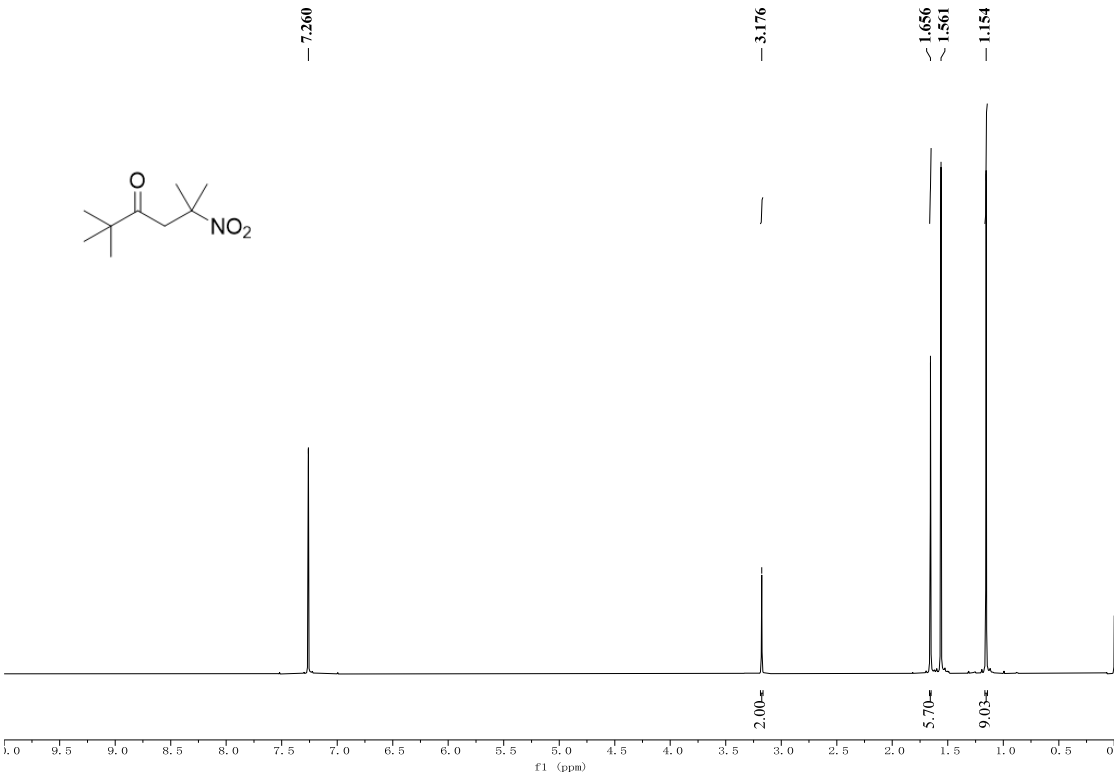

7.249
6.002
6.000
3.072
2.119
1.884
1.653
1.577
1.572
O
NO2
1.00
2.17
3.10
3.29
5.99
f1 (ppm)

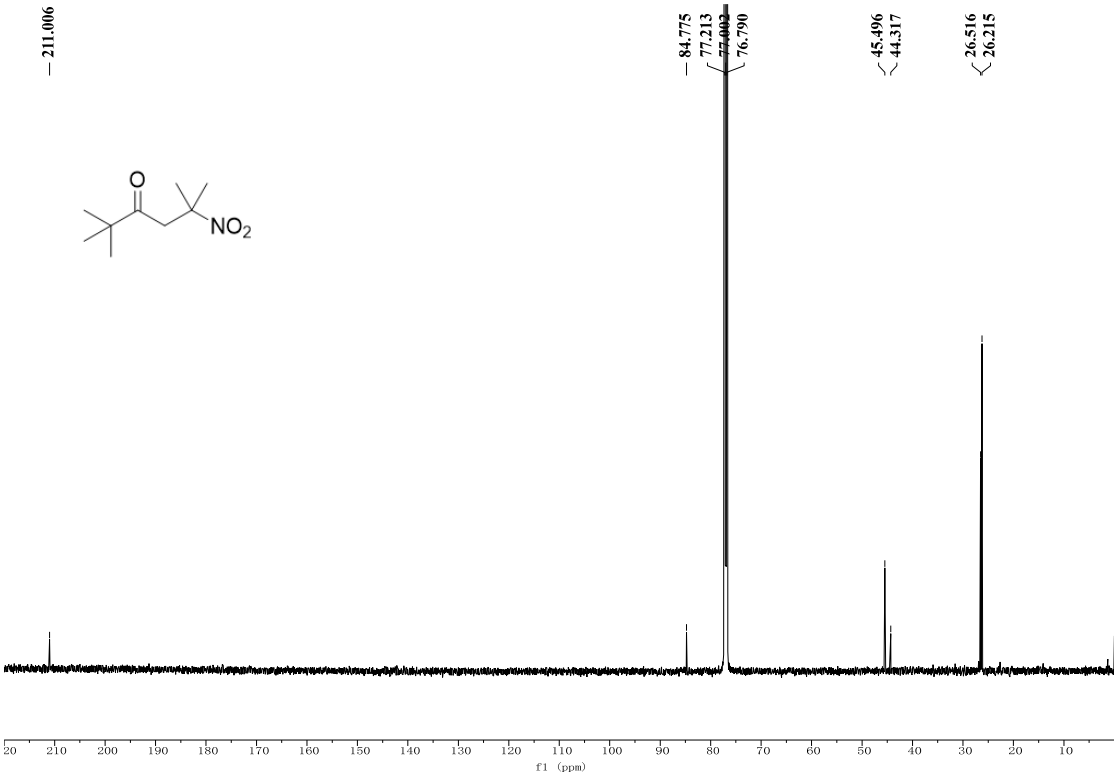

195.060
157.839
123.172
77.212
77.001
76.790
52.137
27.782
26.417
20.921
O
NO2
f1 (ppm)

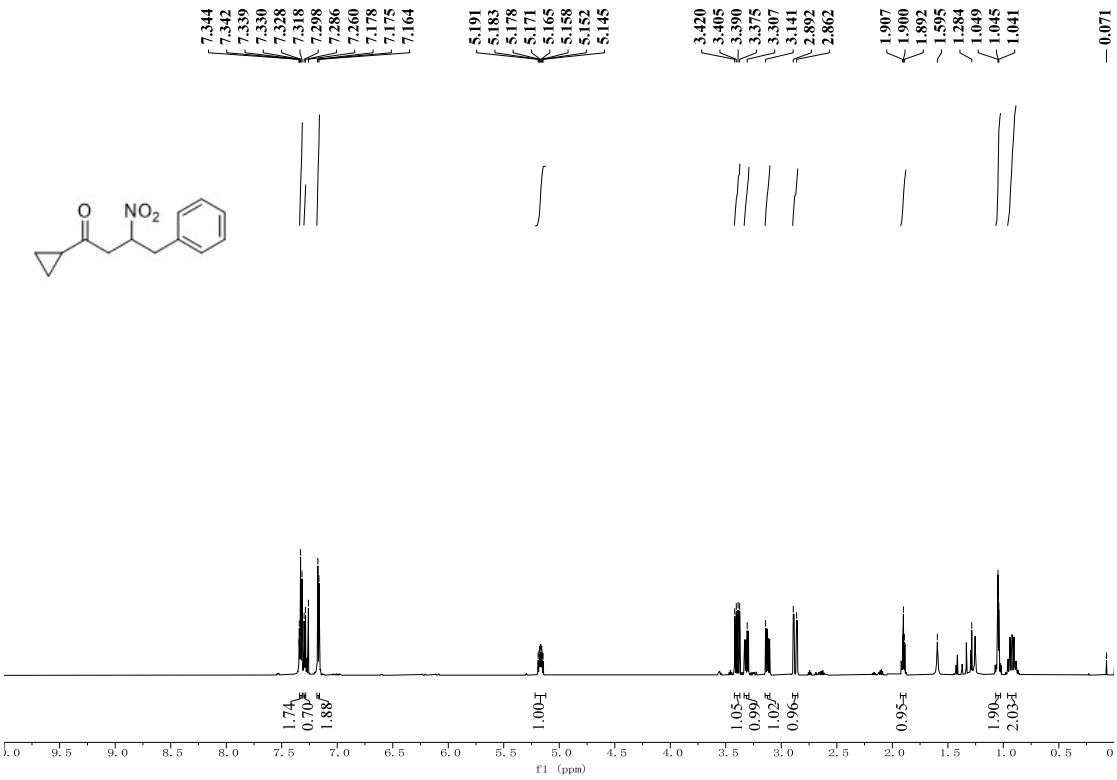

6.959
6.948
6.933
6.922
6.201
6.175
3.648
3.636
1.926
1.914
1.628
1.622
1.137
1.125
O
NO2
(±)
1.00
0.99
1.02
3.43
7.29
3.41
f1 (ppm)

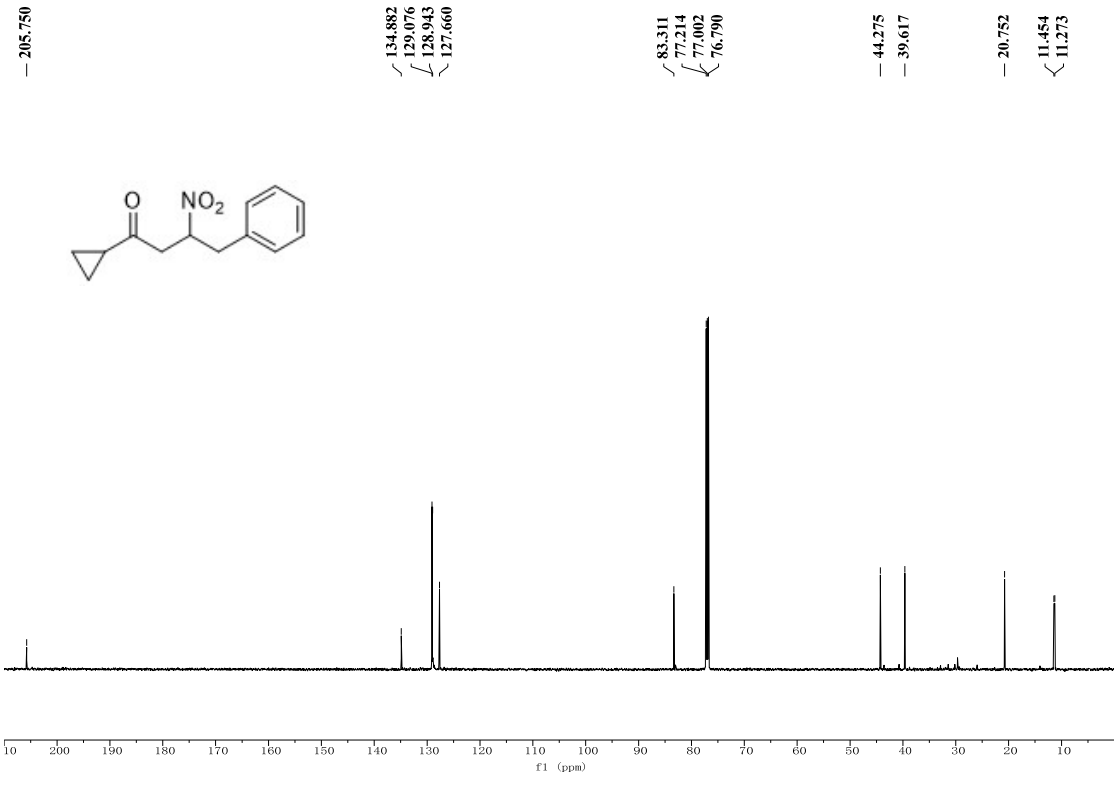

199.053
144.368
131.023
90.287
77.318
77.000
76.682
49.758
23.922
23.610
18.293
13.221
O
NO2
(±)
f1 (ppm)

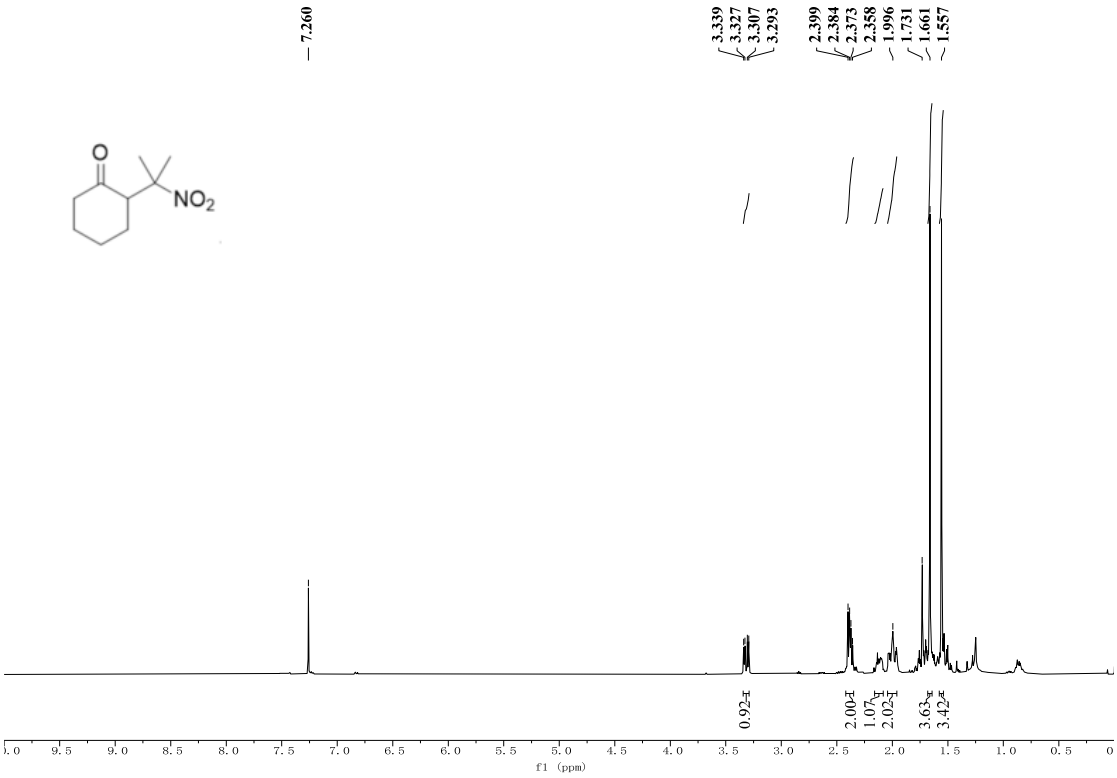

6.78
6.78
6.78
3.86
2.26
2.03
2.03
MeO
O
O
O
1.00
3.30
3.25
3.62
f1 (ppm)
181.58
165.03
162.93
119.09
77.32
77.00
76.68
52.82
28.49
21.85
MeO
O
O
O
f1 (ppm)

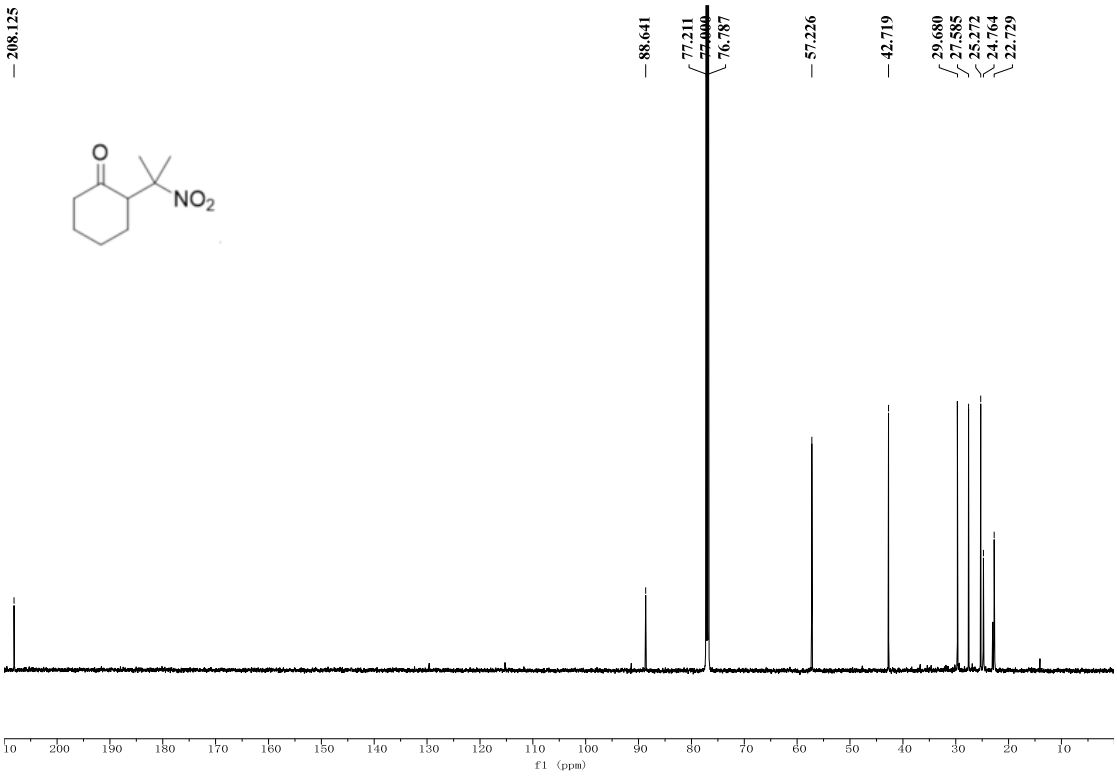

7.260
3.176
1.656
1.561
1.154
O
NO2
2.00
5.70
9.03
f1 (ppm)

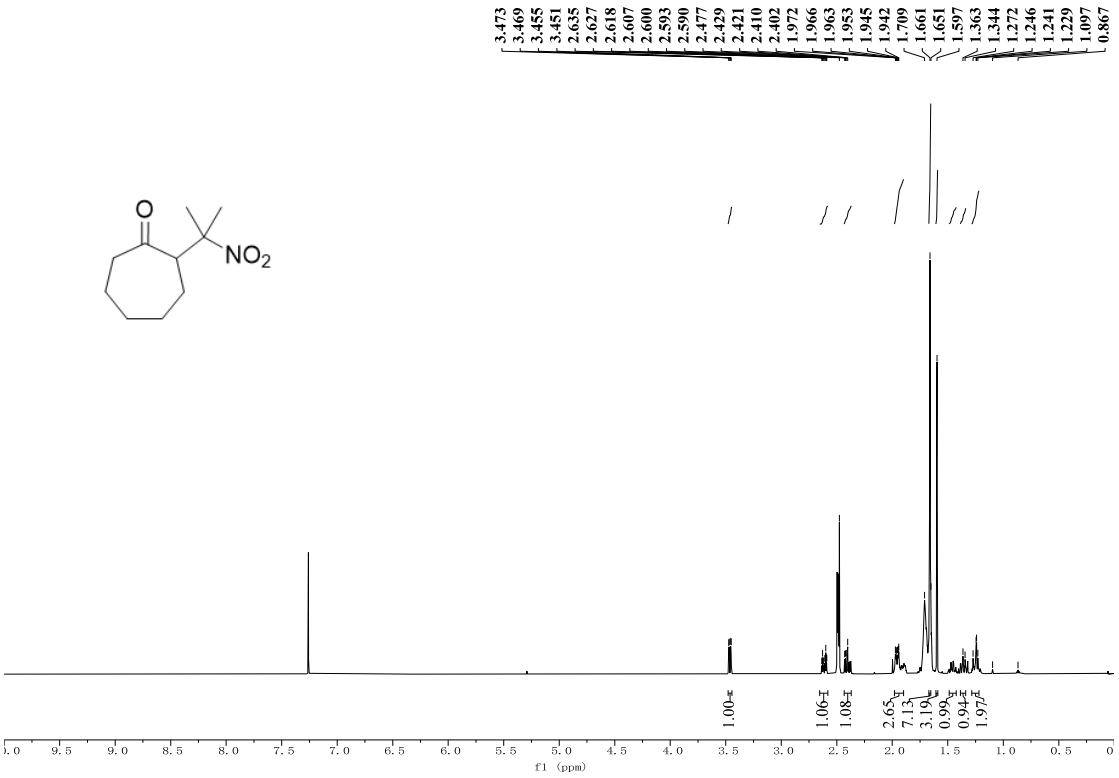

211.006
84.775
77.213
77.002
76.790
45.496
44.317
26.516
26.215
O
NO2
f1 (ppm)

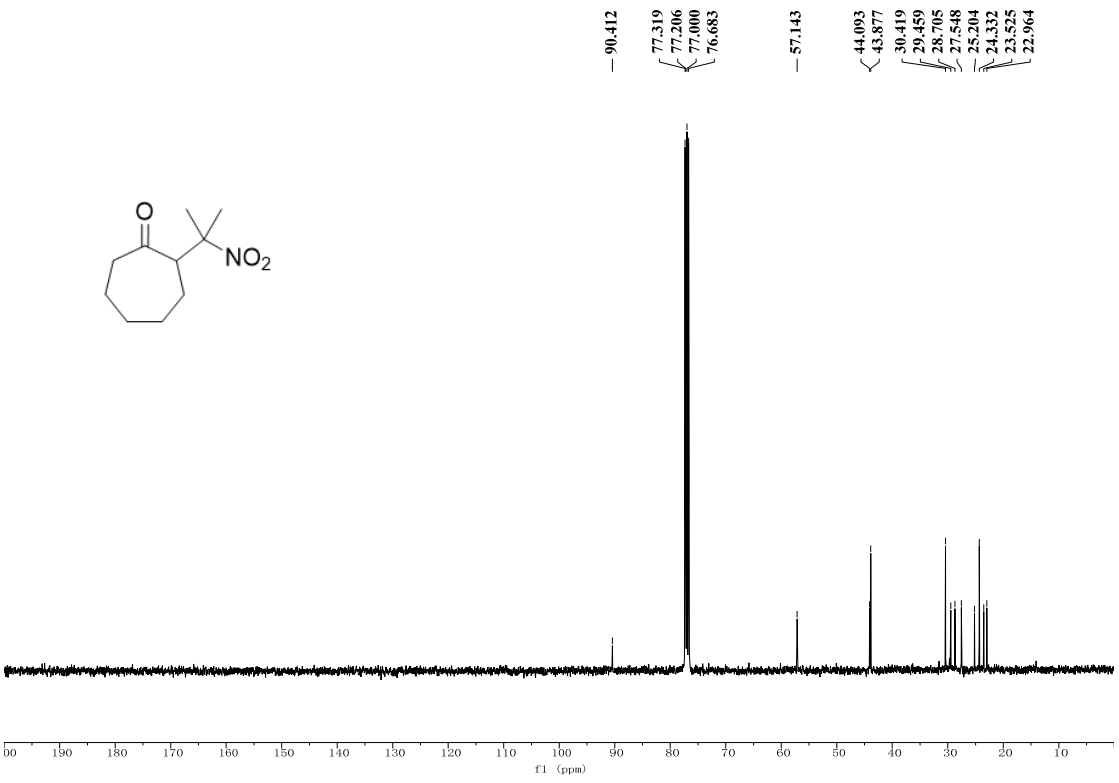

7.344
7.342
7.339
7.330
7.328
7.318
7.298
7.286
7.260
7.178
7.175
7.164
5.191
5.183
5.178
5.171
5.165
5.158
5.152
5.145
3.420
3.405
3.390
3.375
3.307
3.141
2.892
2.862
1.907
1.900
1.892
1.595
1.284
1.049
1.045
1.041
0.071
O
NO2
1.74
0.70
1.88
1.00
1.05
0.99
1.02
0.96
0.95
1.90
2.03
f1 (ppm)

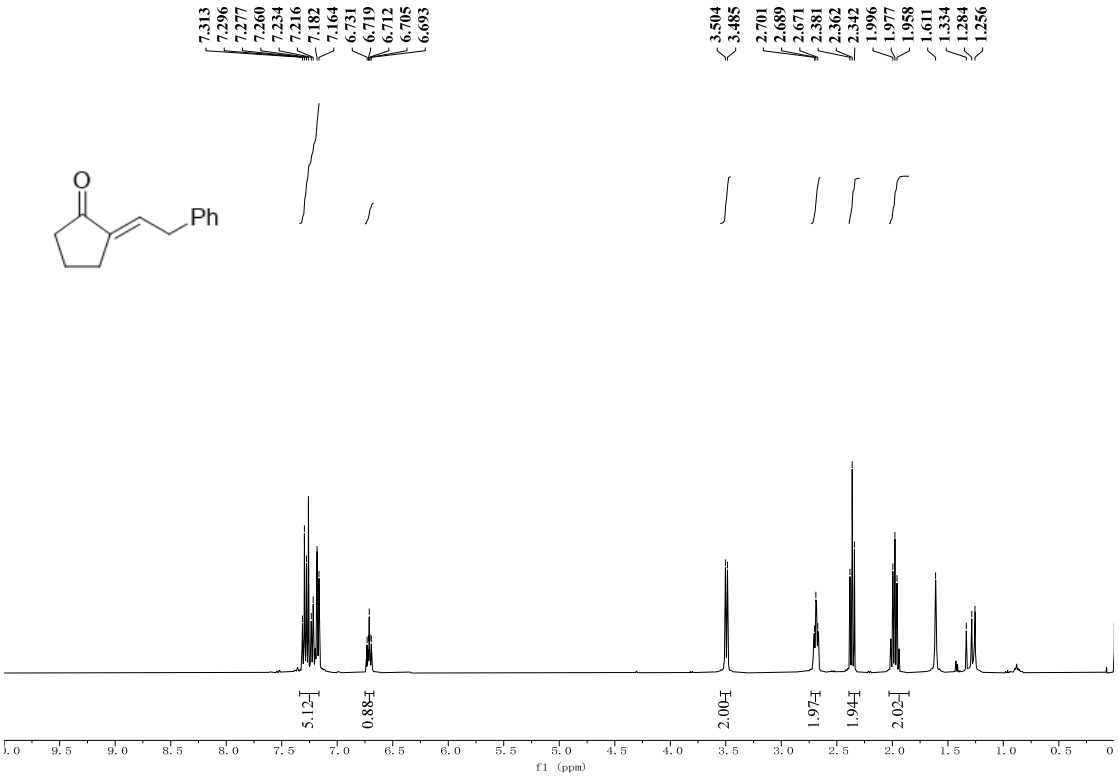

205.750
134.882
129.076
128.943
127.660
83.311
77.214
77.002
76.790
44.275
39.617
20.752
11.454
11.273
O
NO2
f1 (ppm)

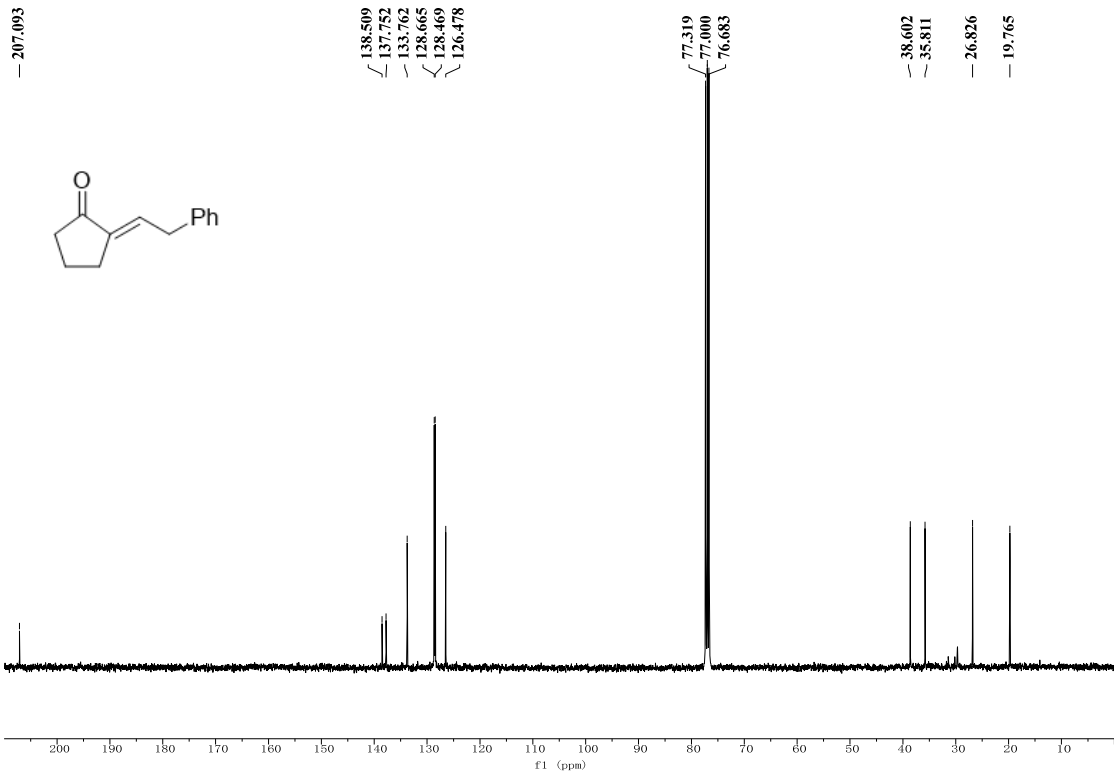

7.260
3.339
3.327
3.307
3.293
2.399
2.384
2.373
2.358
1.996
1.731
1.661
1.557
O
NO2
0.92
2.00
1.07
2.02
3.63
3.42
f1 (ppm)

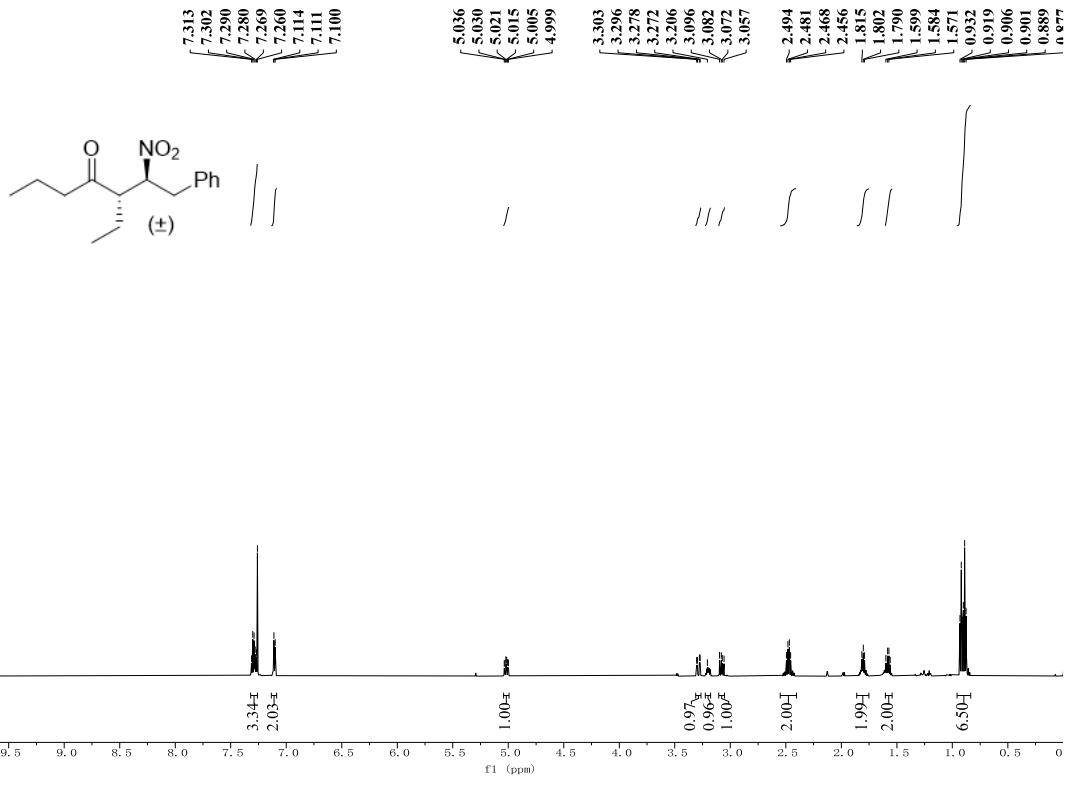

208.125
88.641
77.211
77.000
76.787
57.226
42.719
29.680
27.585
25.272
24.764
22.729
O
NO2
f1 (ppm)

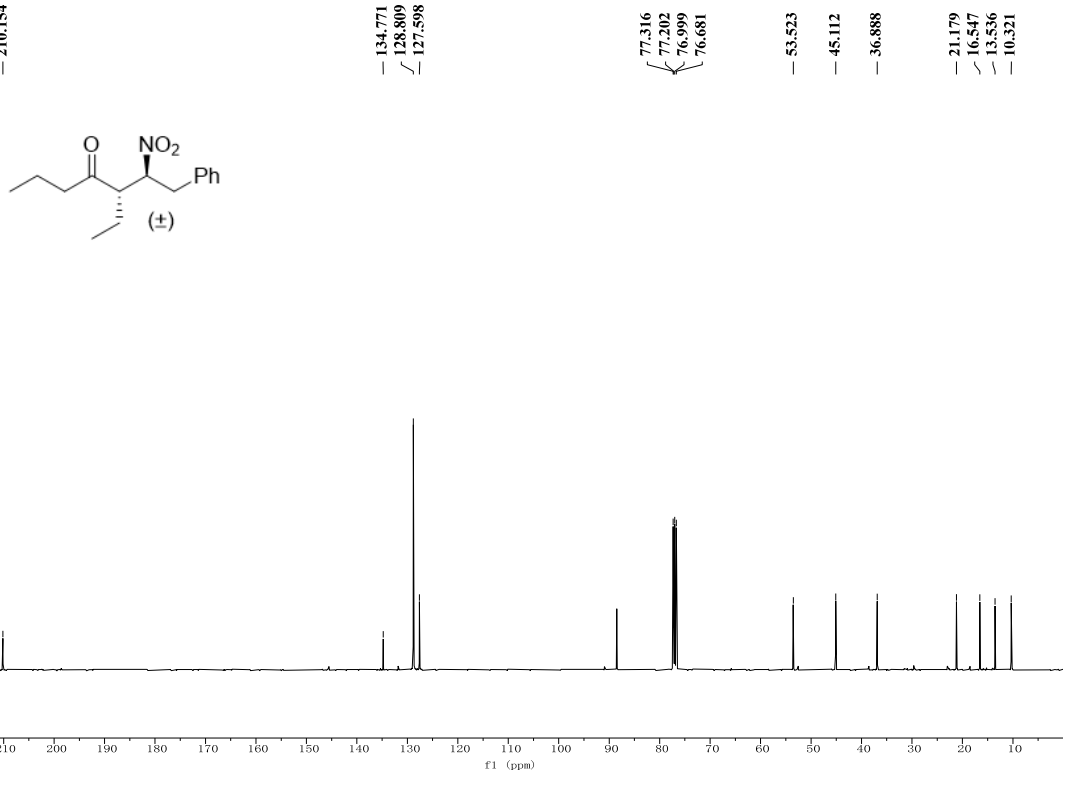

3.473
3.469
3.455
3.451
2.635
2.627
2.618
2.607
2.600
2.593
2.590
2.477
2.429
2.421
2.410
2.402
1.972
1.966
1.963
1.953
1.945
1.942
1.709
1.661
1.651
1.597
1.363
1.344
1.272
1.246
1.241
1.229
1.097
0.867
O
NO2
1.00
1.06
1.08
2.65
7.13
3.19
0.99
0.94
1.97
f1 (ppm)

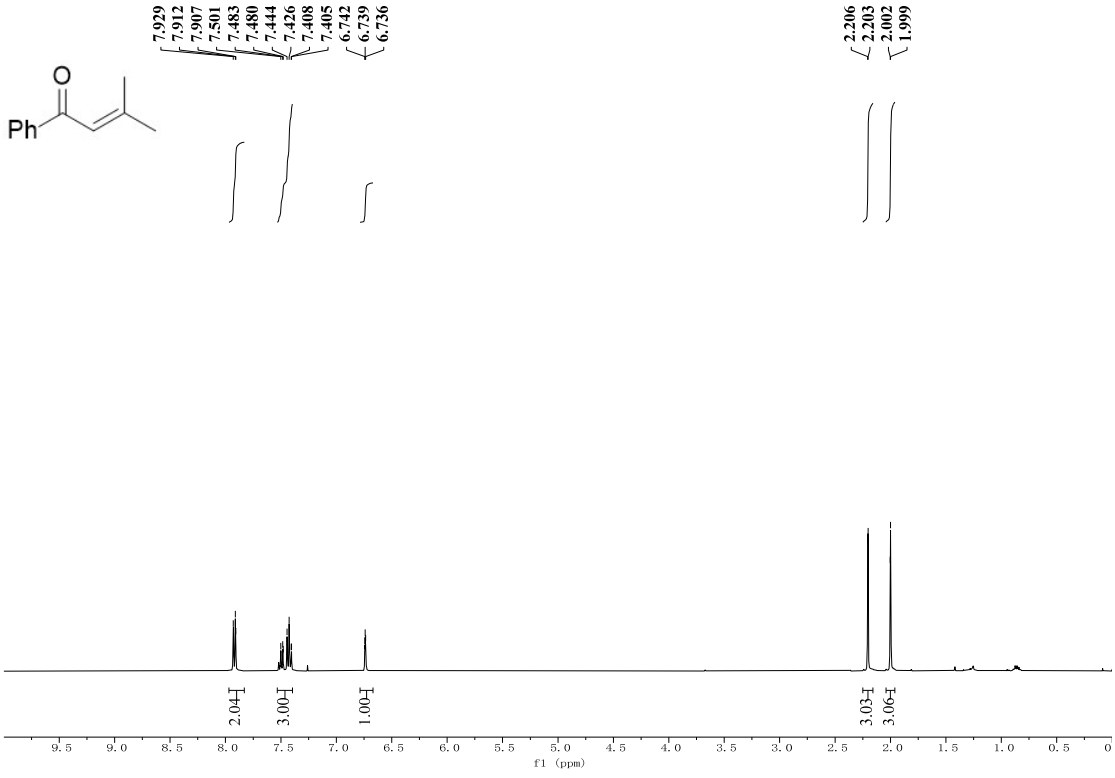

90.412
77.319
77.206
77.000
76.683
57.143
44.093
43.877
30.419
29.459
28.705
27.548
25.204
24.332
23.525
22.964
O
NO2
f1 (ppm)

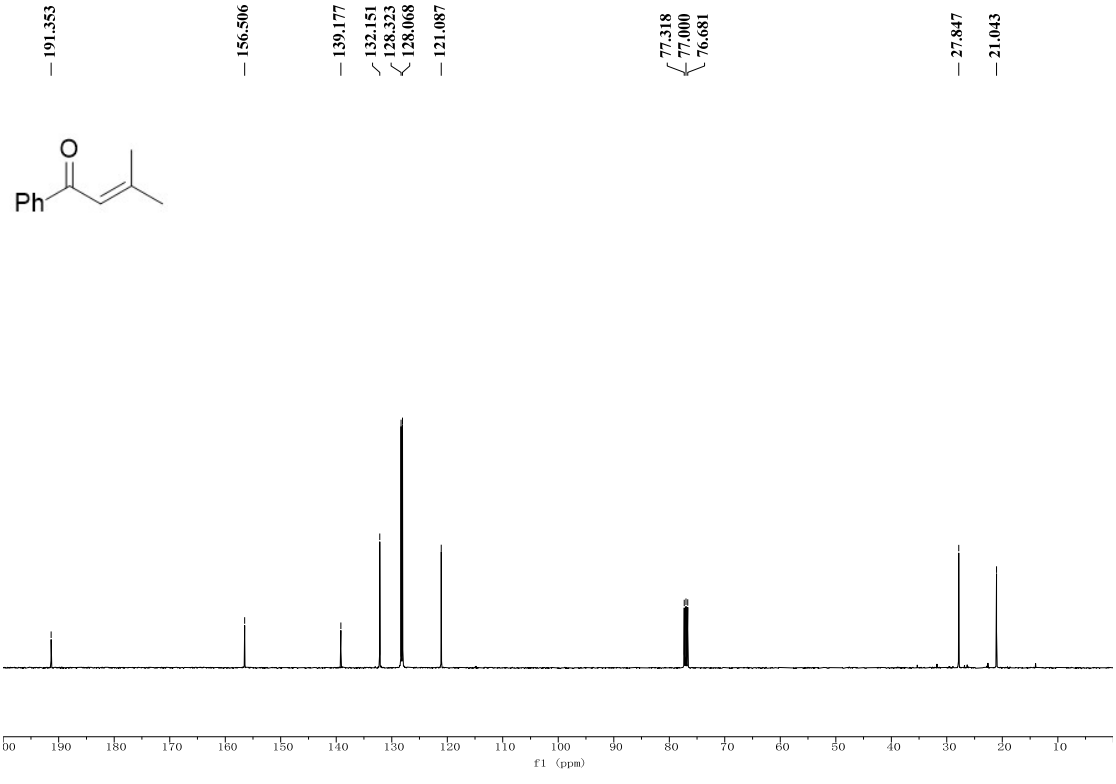

7.313
7.296
7.277
7.260
7.234
7.216
7.182
7.164
6.731
6.719
6.712
6.705
6.693
3.504
3.485
2.701
2.689
2.671
2.381
2.362
2.342
1.996
1.977
1.958
1.611
1.334
1.284
1.256
O
Ph
5.12
0.88
2.00
1.97
1.94
2.02
f1 (ppm)

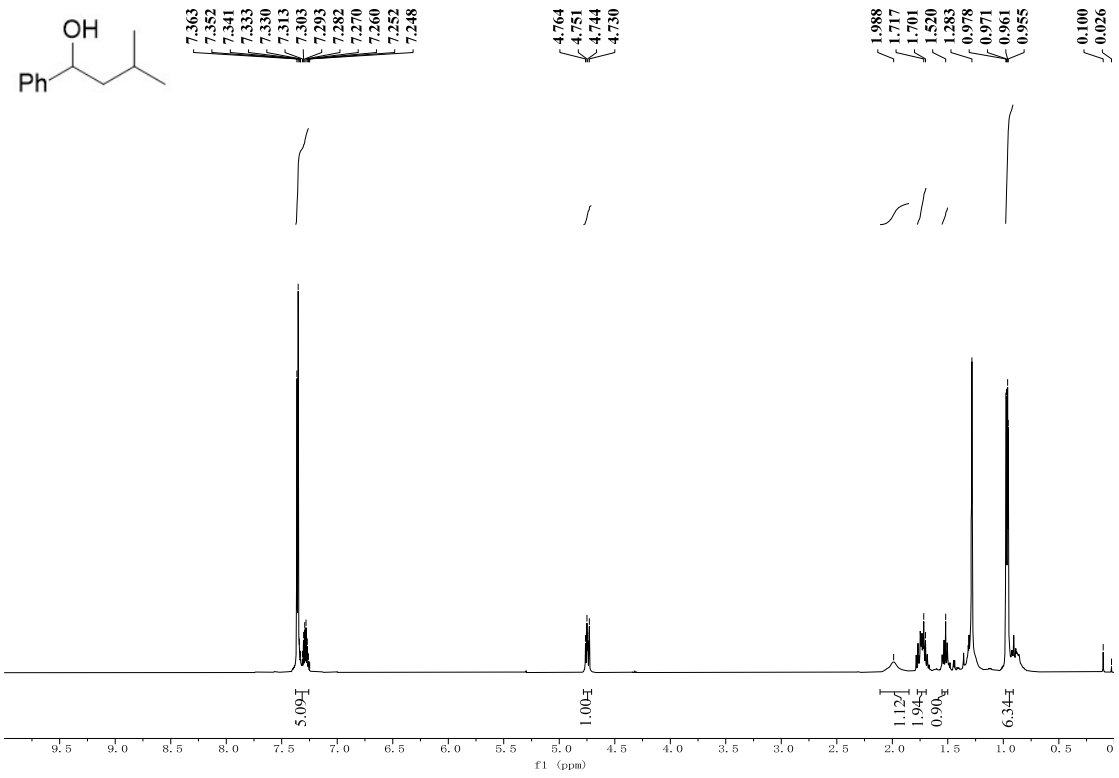

207.093
138.509
137.752
133.762
128.665
128.469
126.478
77.319
77.000
76.683
38.602
35.811
26.826
19.765
O
Ph
f1 (ppm)

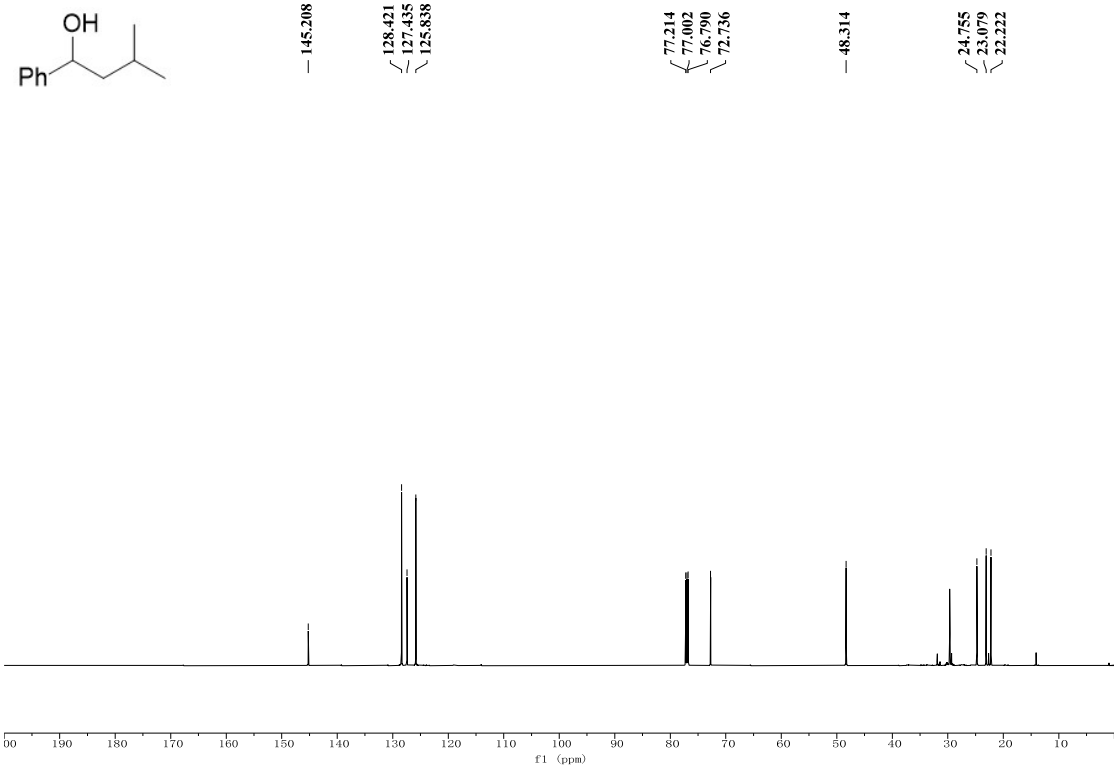

7.313
7.302
7.290
7.280
7.269
7.260
7.114
7.111
7.100
5.036
5.030
5.021
5.015
5.005
4.999
3.303
3.296
3.278
3.272
3.206
3.096
3.082
3.072
3.057
2.494
2.481
2.468
2.456
1.815
1.802
1.790
1.599
1.584
1.571
0.932
0.919
0.906
0.901
0.889
O
NO2
Ph
(±)
3.34
2.03
1.00
0.97
0.96
1.00
2.00
1.99
2.00
6.50
f1 (ppm)


210.154
134.771
128.809
127.598
77.316
77.202
76.999
76.681
53.523
45.112
36.888
21.179
16.547
13.536
10.321
O
NO2
Ph
(±)
f1 (ppm)


7.929
7.912
7.907
7.501
7.483
7.480
7.444
7.426
7.408
7.405
6.742
6.739
6.736
2.206
2.203
2.002
1.999
O
Ph
2.04
3.00
1.00
3.03
3.06
f1 (ppm)


191.353
156.506
139.177
132.151
128.323
128.068
121.087
77.318
77.000
76.681
27.847
21.043
O
Ph
f1 (ppm)


OH
Ph
7.363
7.352
7.341
7.333
7.330
7.313
7.303
7.293
7.282
7.270
7.260
7.252
7.248
4.764
4.751
4.744
4.730
1.988
1.717
1.701
1.520
1.283
0.978
0.971
0.961
0.955
0.100
0.026
5.09
1.00
1.12
1.94
0.90
6.34
f1 (ppm)


OH
Ph
145.208
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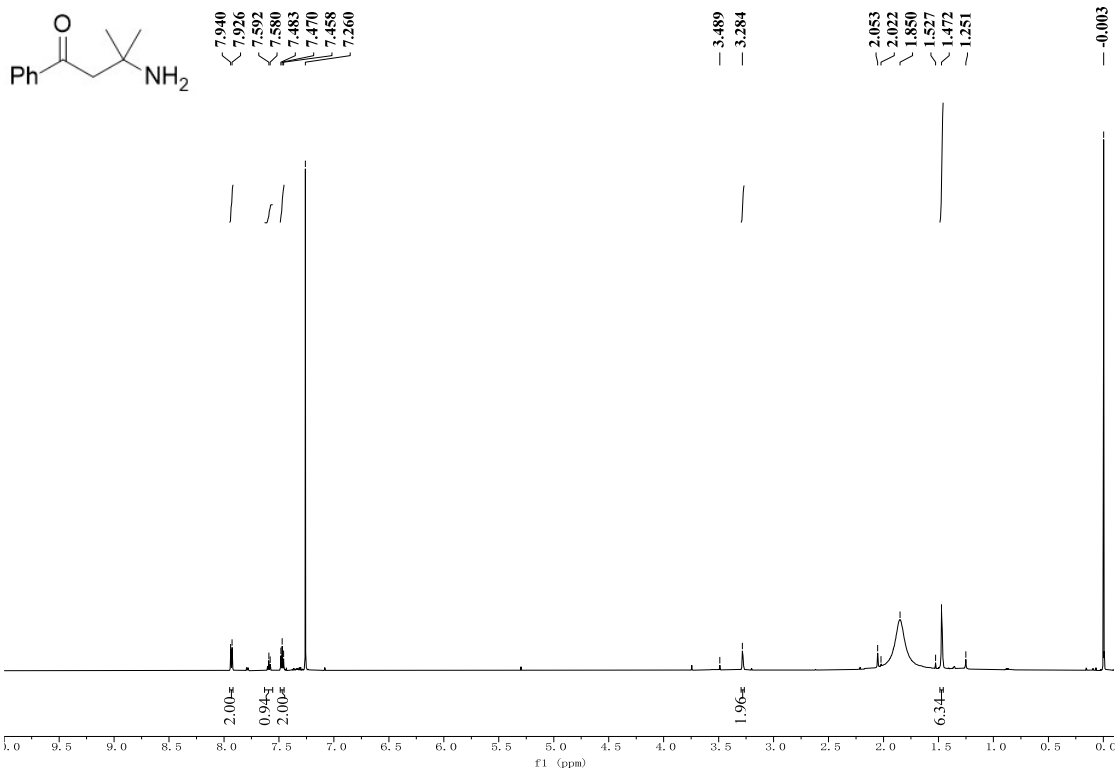
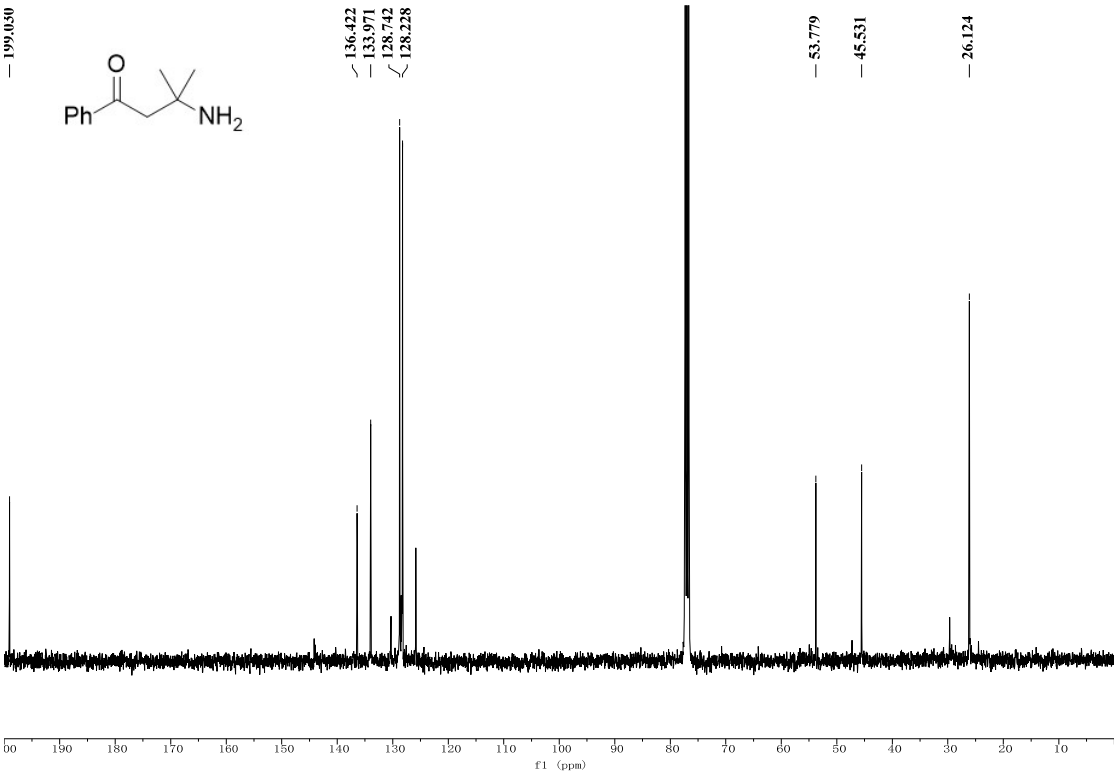
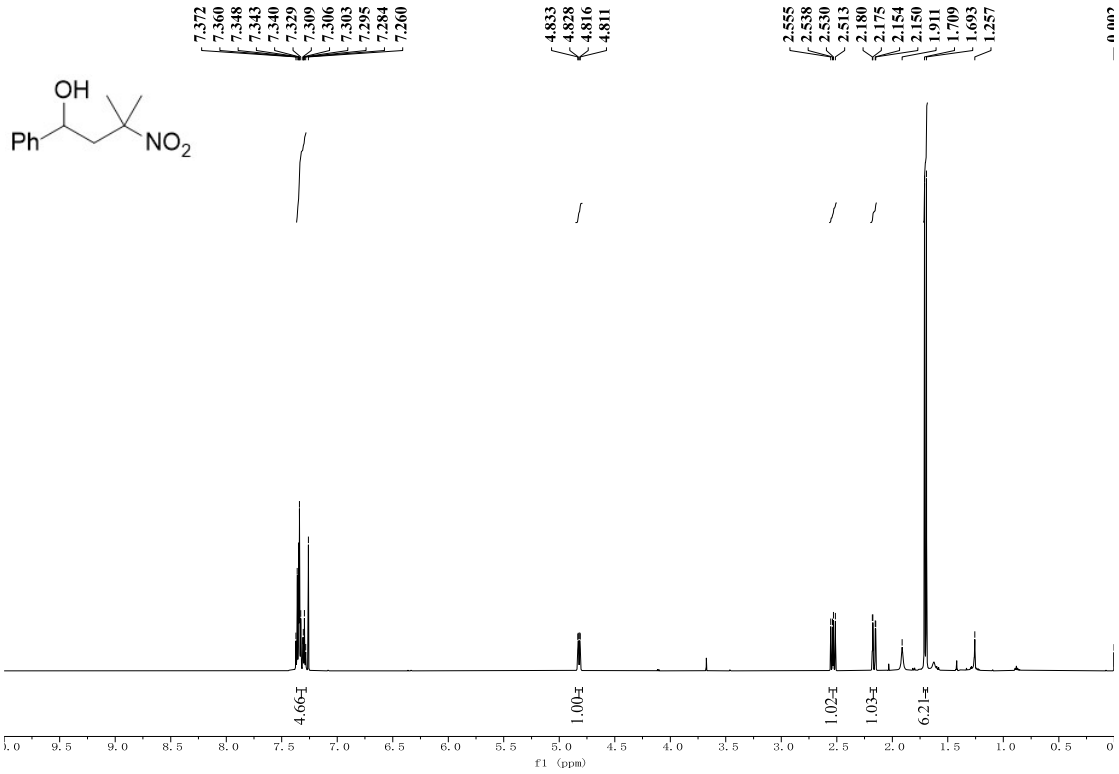
125.838
77.214
77.002
76.790
72.736
48.314
24.755
23.079
22.222
f1 (ppm)


Ph
NH2
7.940
7.926
7.592
7.580
7.483
7.470
7.458
7.260
3.489
3.284
2.053
2.022
1.850
1.527
1.472
1.251
-0.003
2.00
0.94
2.00
1.96
6.34
f1 (ppm)


Ph
NH2
199.050
136.422
133.971
128.742
128.228
53.779
45.531
26.124
f1 (ppm)


7.372
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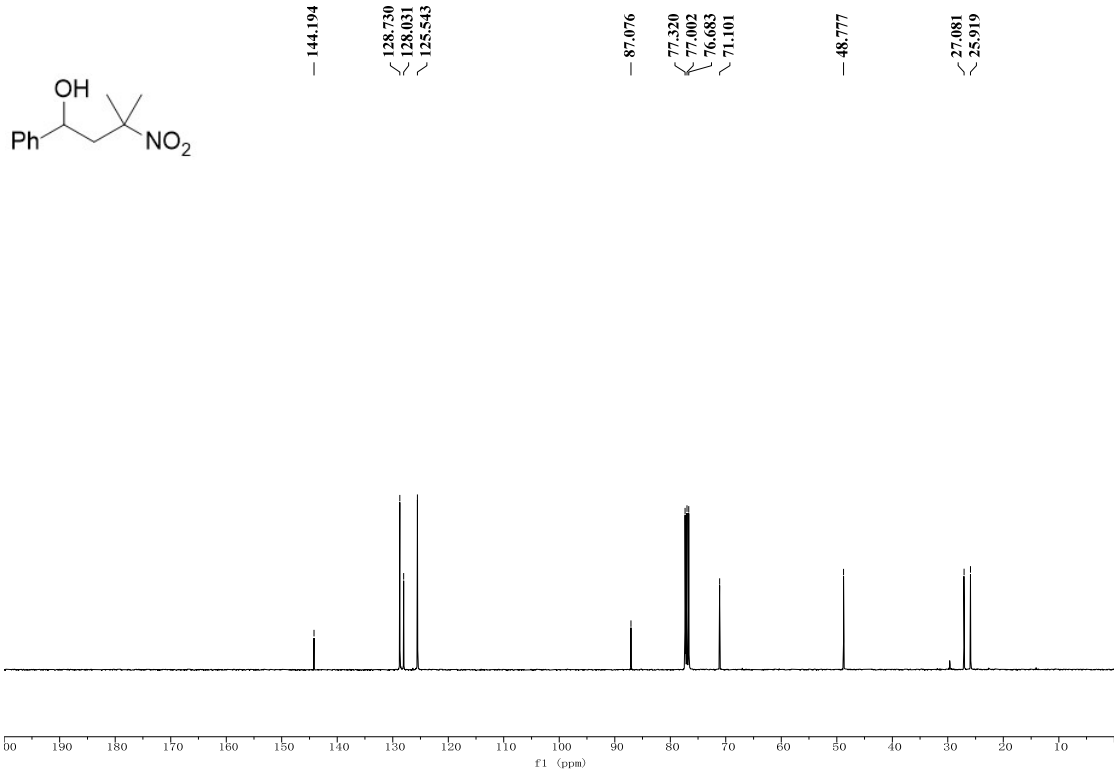
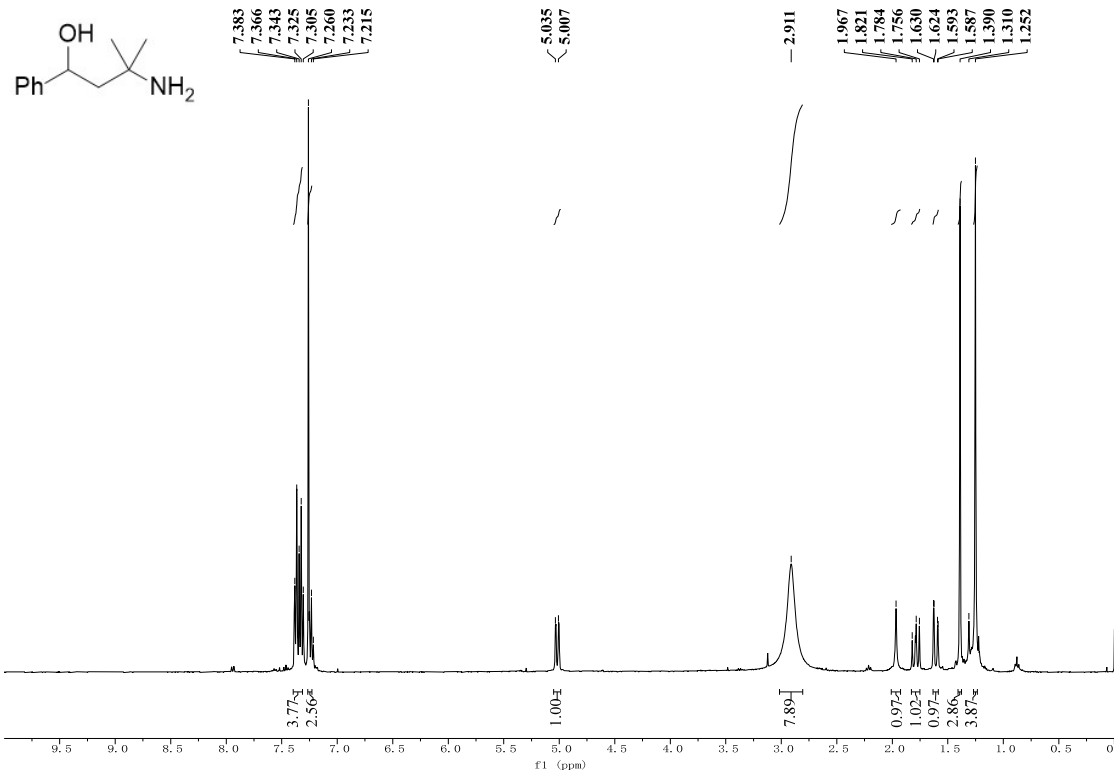
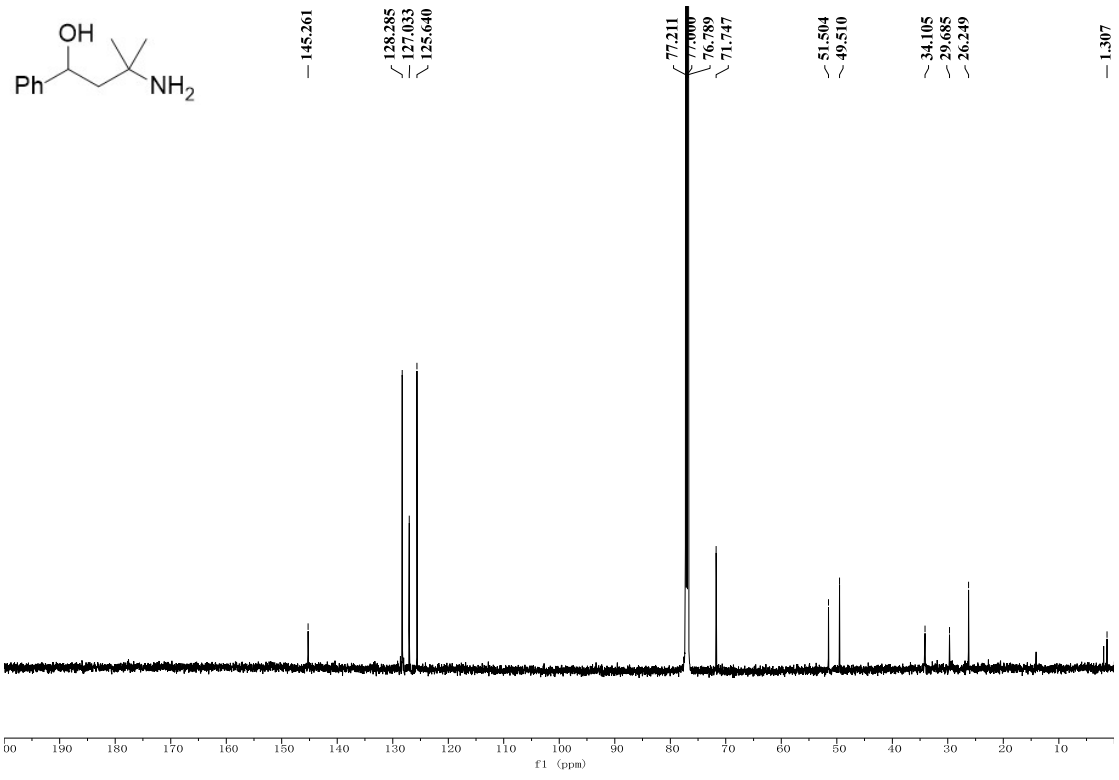
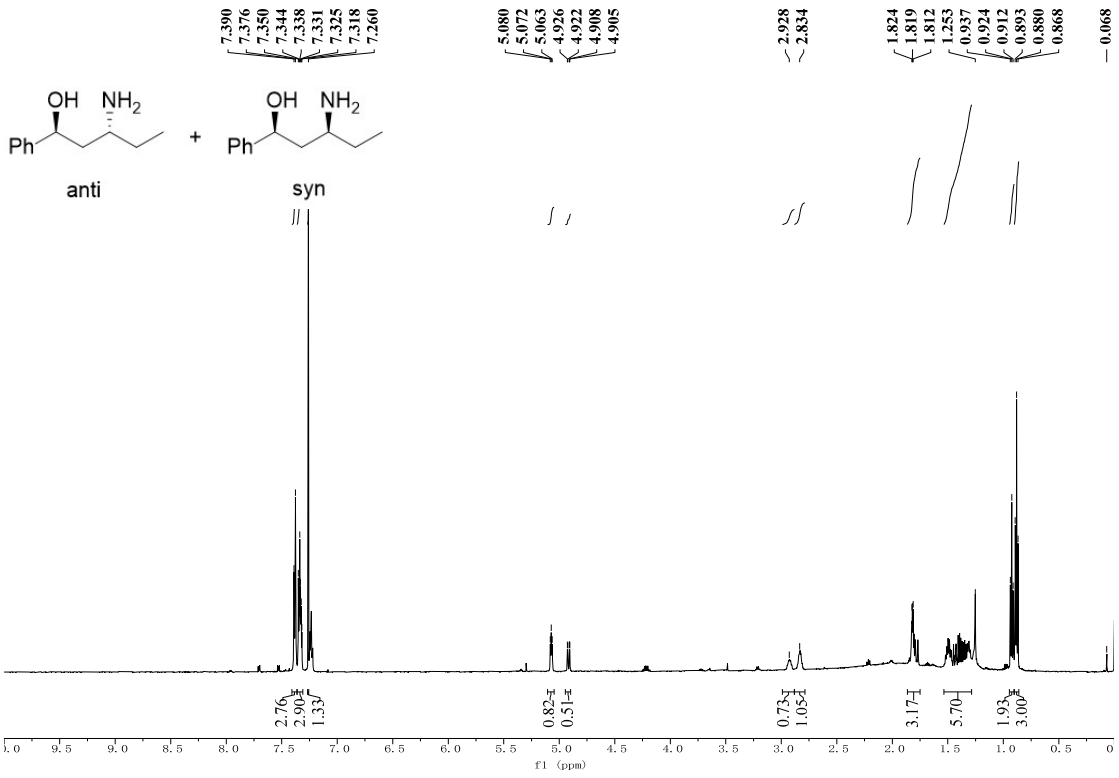
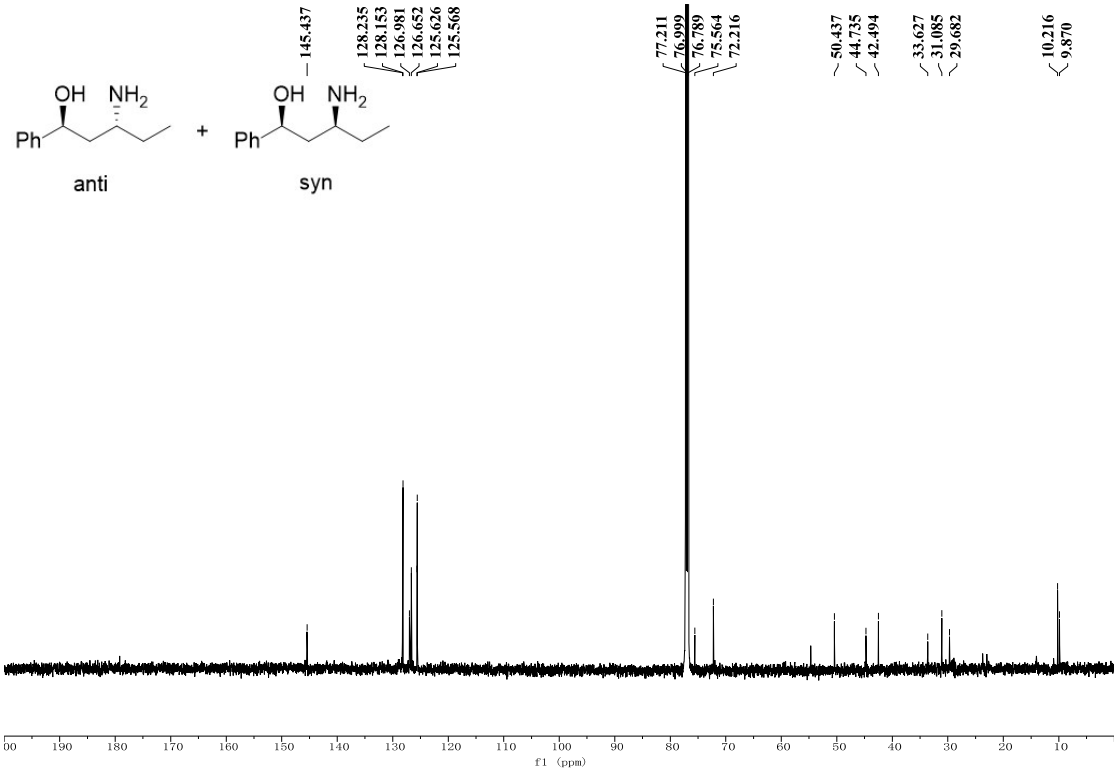
7.348
7.343
7.340
7.329
7.309
7.306
7.303
7.295
7.284
7.260
4.833
4.828
4.816
4.811
2.555
2.538
2.530
2.513
2.180
2.175
2.154
2.150
1.911
1.709
1.693
1.257
OH
Ph
NO2
4.66
1.00
1.02
1.03
6.21
f1 (ppm)

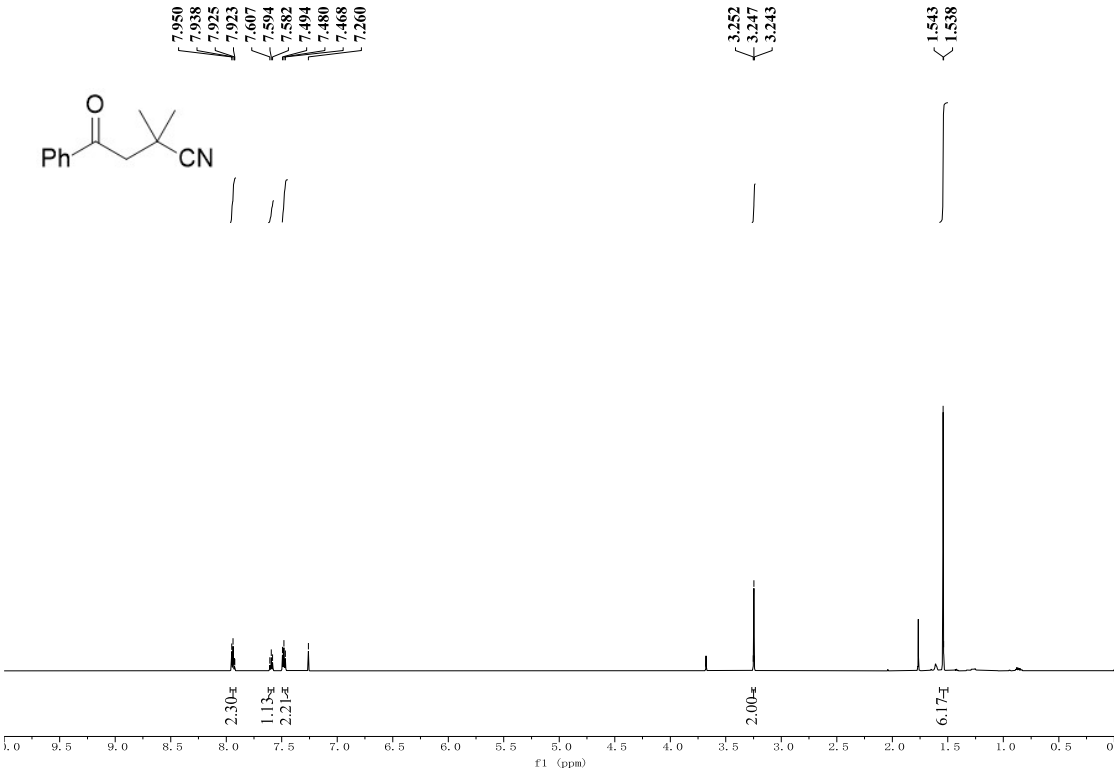

144.194
128.730
128.031
125.543
87.076
77.320
77.002
76.683
71.101
48.777
27.081
25.919
OH
Ph
NO2
f1 (ppm)

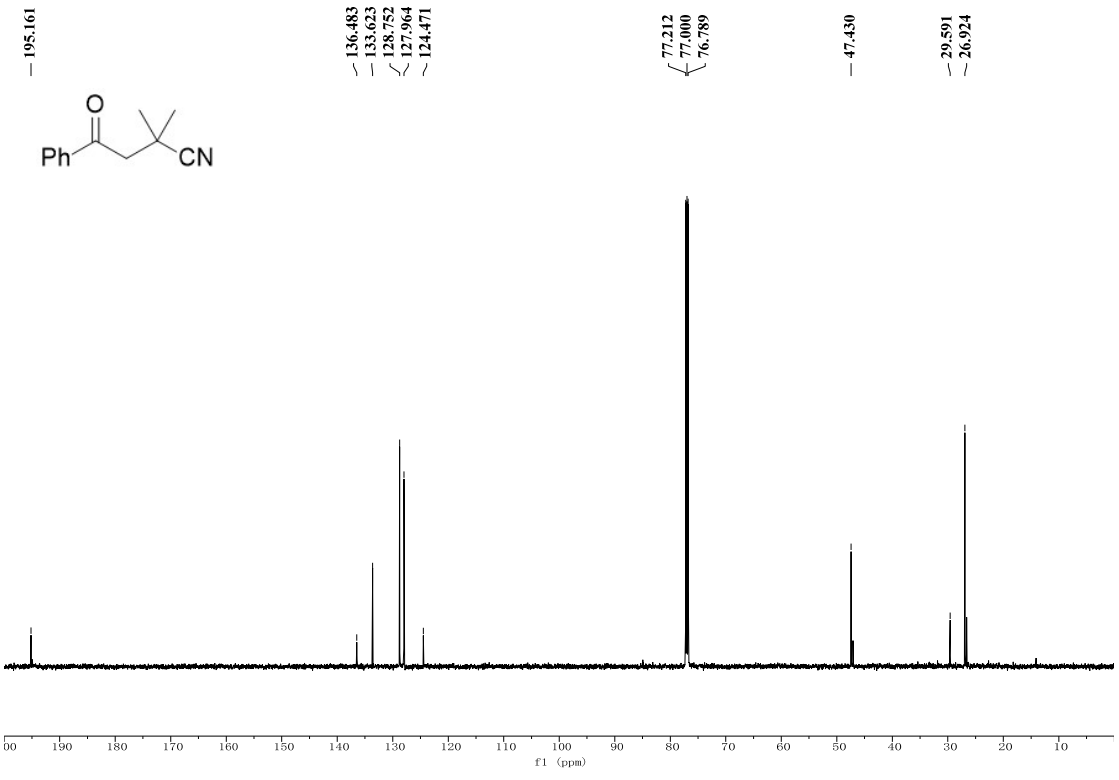

OH
Ph
NH2
7.383
7.366
7.343
7.325
7.305
7.260
7.233
7.215
5.035
5.007
2.911
1.967
1.821
1.784
1.756
1.630
1.624
1.593
1.587
1.390
1.310
1.252
3.77
2.56
1.00
7.89
0.97
1.02
0.97
2.86
3.87
f1 (ppm)

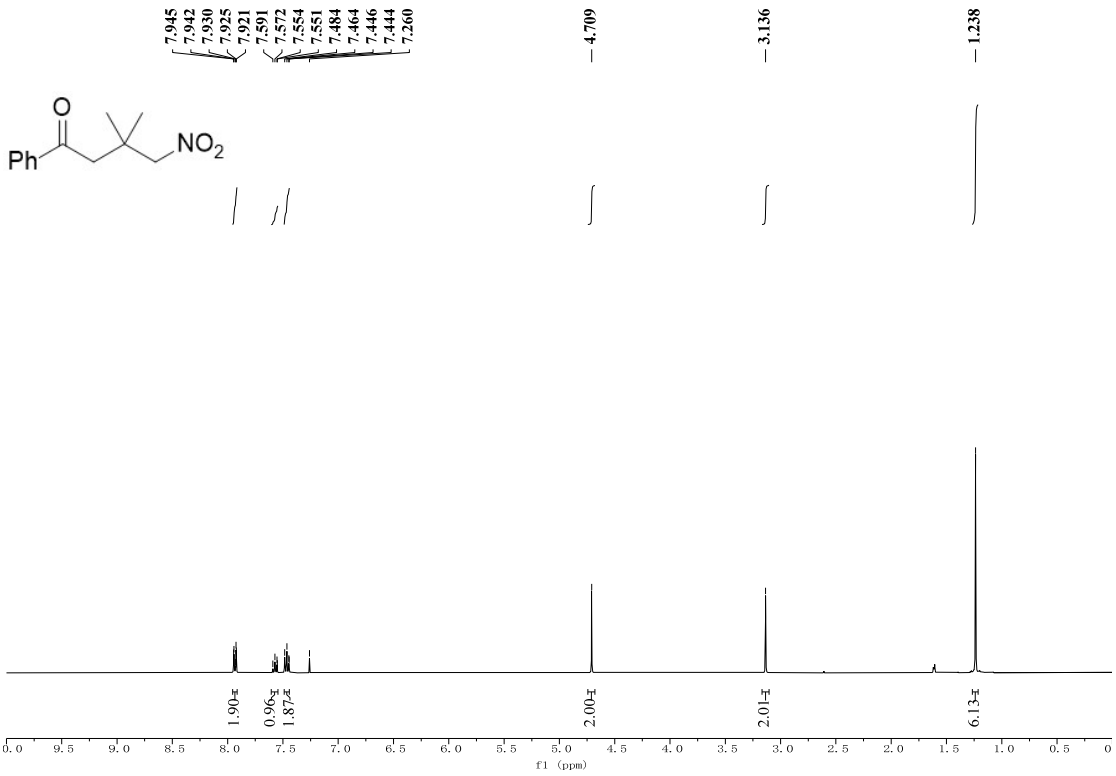

OH
Ph
NH2
145.261
128.285
127.033
125.640
77.211
77.000
76.789
71.747
51.504
49.510
34.105
29.685
26.249
1.307
f1 (ppm)

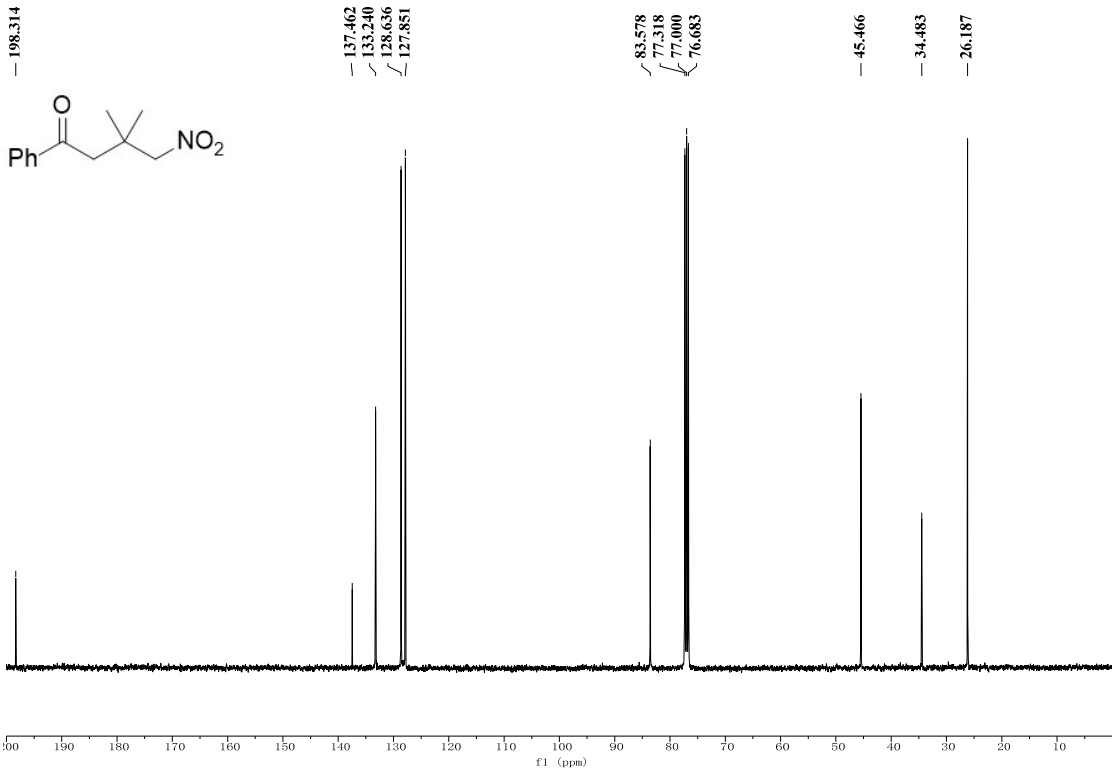

7.390
7.376
7.350
7.344
7.338
7.331
7.325
7.318
7.260
5.080
5.072
5.063
4.926
4.922
4.908
4.905
2.928
2.834
1.824
1.819
1.812
1.253
0.937
0.924
0.912
0.893
0.880
0.868
0.068
OH NH2
Ph
anti
+
OH NH2
Ph
syn
2.76
2.90
1.33
0.82
0.51
0.73
1.05
3.17
5.70
1.93
3.00
f1 (ppm)

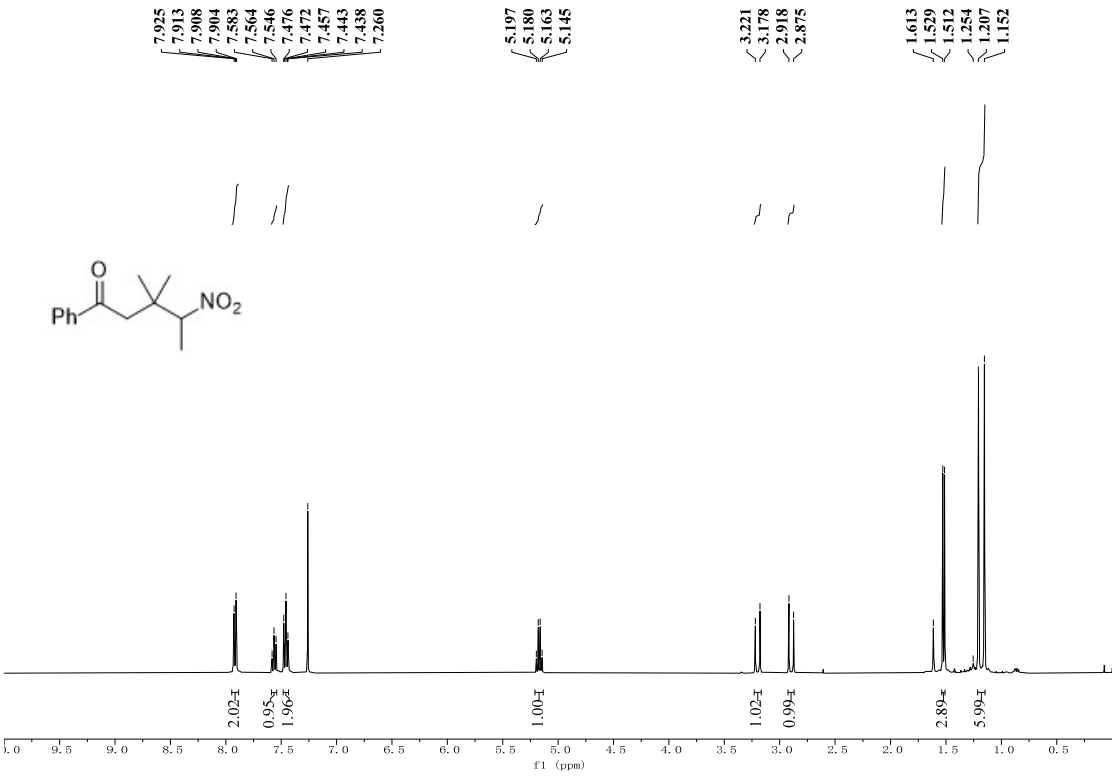

145.437
128.235
128.153
126.981
126.652
125.626
125.568
77.211
76.999
76.789
75.564
72.216
50.437
44.735
42.494
33.627
31.085
29.682
10.216
9.870
OH NH2
Ph
anti
+
OH NH2
Ph
syn
f1 (ppm)

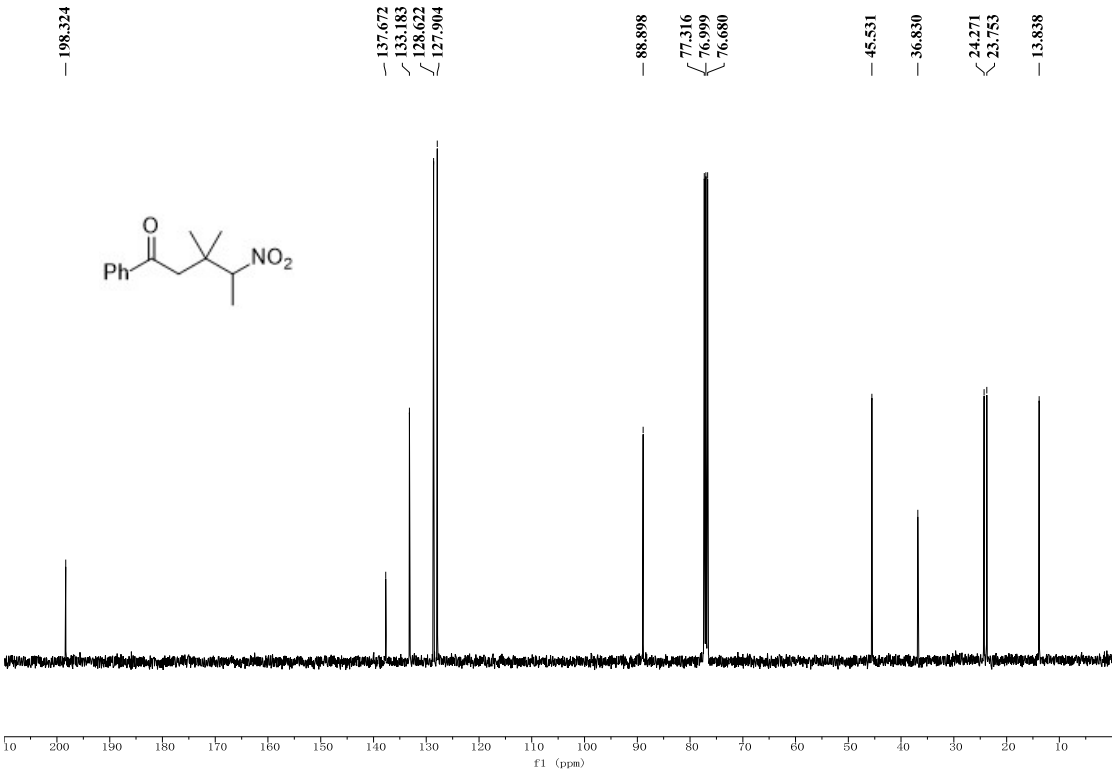

7.950
7.938
7.925
7.923
7.607
7.594
7.582
7.494
7.480
7.468
7.260
3.252
3.247
3.243
1.543
1.538
O
Ph
CN
2.30
1.13
2.21
2.00
6.17
f1 (ppm)

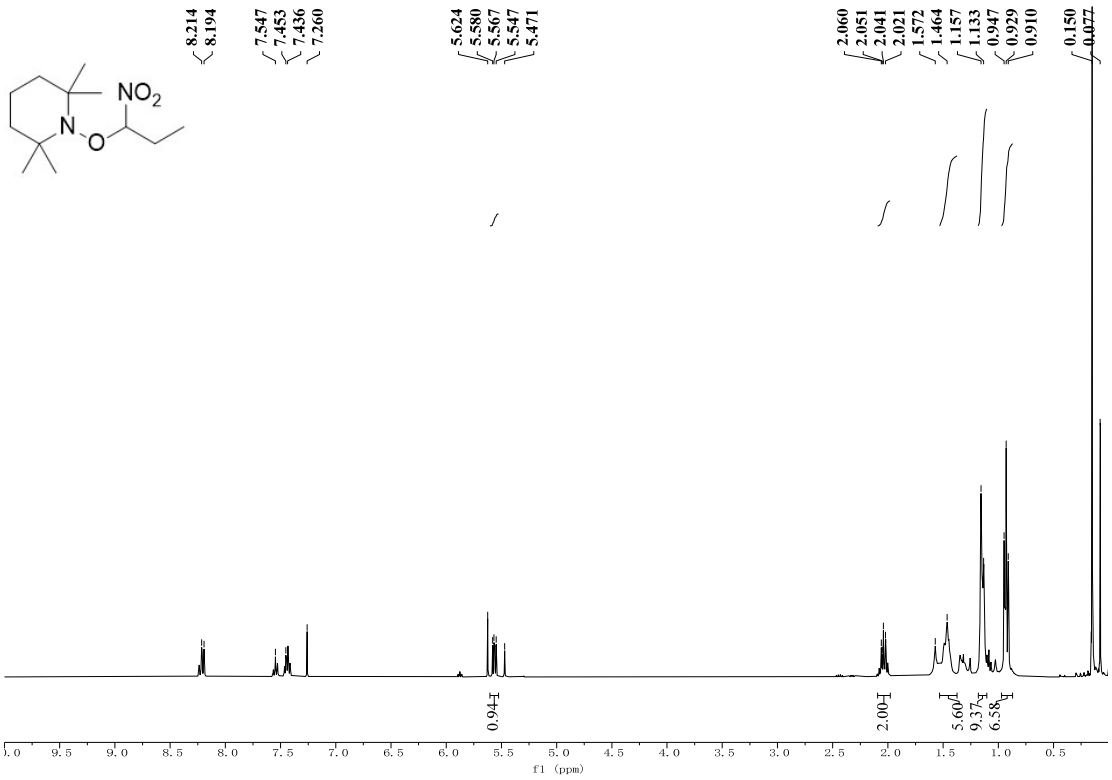

195.161
136.483
133.623
128.752
127.964
124.471
77.212
77.000
76.789
47.430
29.591
26.924
O
Ph
CN
f1 (ppm)

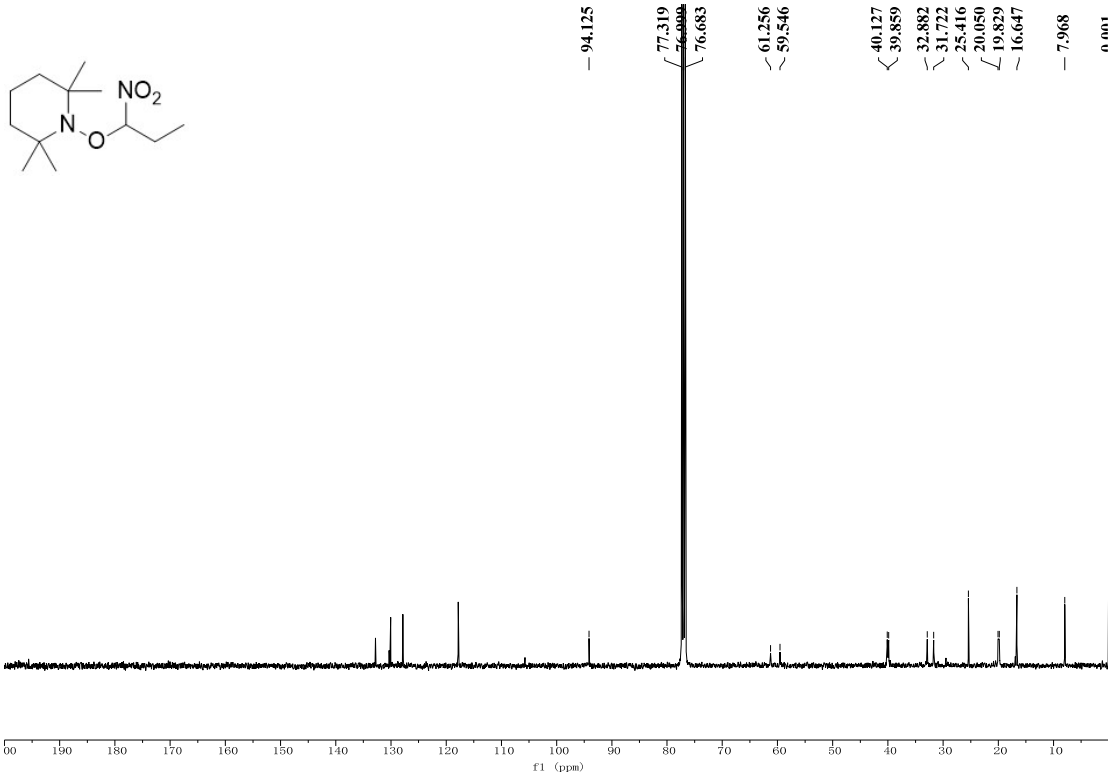

7.945
7.942
7.930
7.925
7.921
7.591
7.572
7.554
7.551
7.484
7.464
7.446
7.444
7.260
4.709
3.136
1.238
O
Ph
NO2
1.90
0.96
1.87
2.00
2.01
6.13
f1 (ppm)

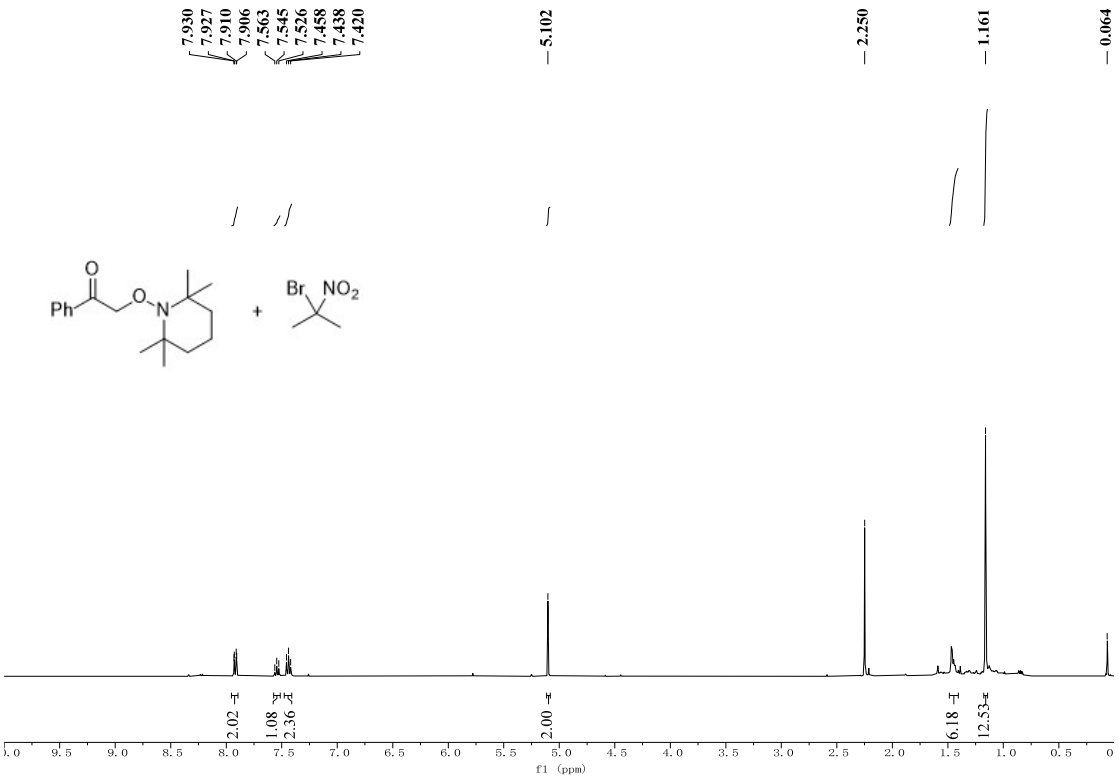

198.314
137.462
133.240
128.636
127.851
83.578
77.318
77.000
76.683
45.466
34.483
26.187
O
Ph
NO2
f1 (ppm)

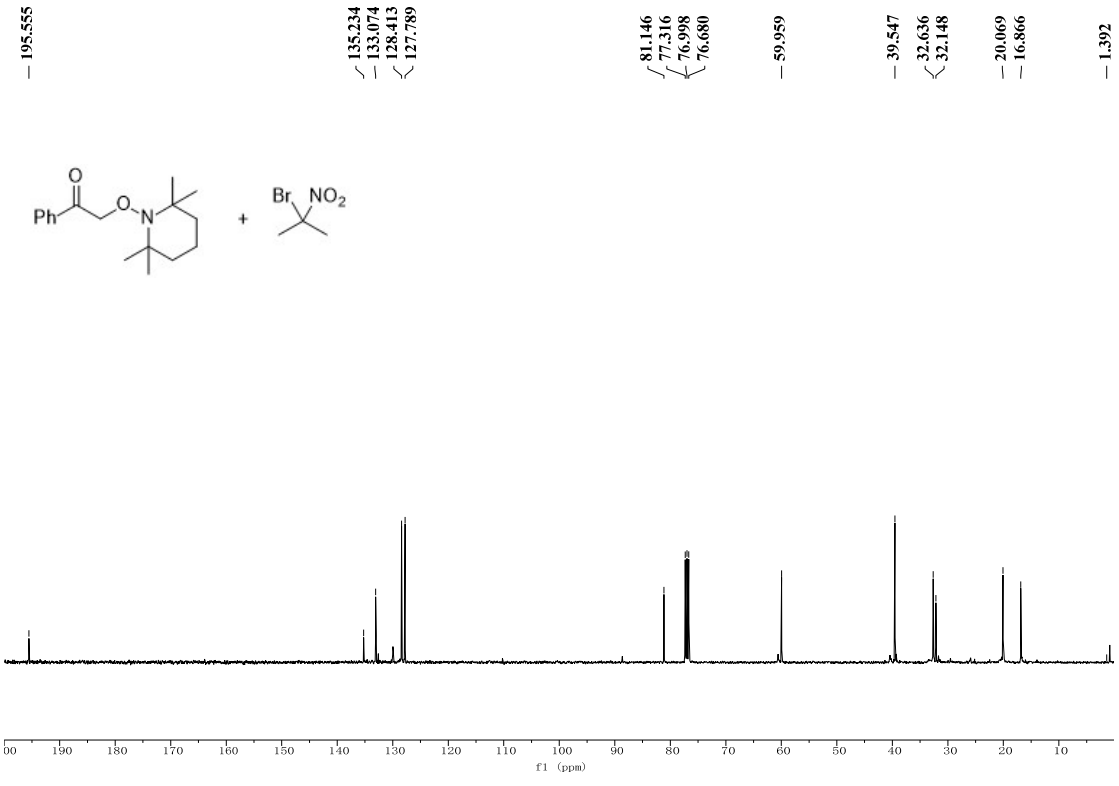

7.925
7.913
7.908
7.904
7.583
7.564
7.546
7.476
7.472
7.457
7.443
7.438
7.260
5.197
5.180
5.163
5.145
3.221
3.178
2.918
2.875
1.613
1.529
1.512
1.254
1.207
1.152
O
Ph
NO2
2.02
0.95
1.96
1.00
1.02
0.99
2.89
5.99
f1 (ppm)

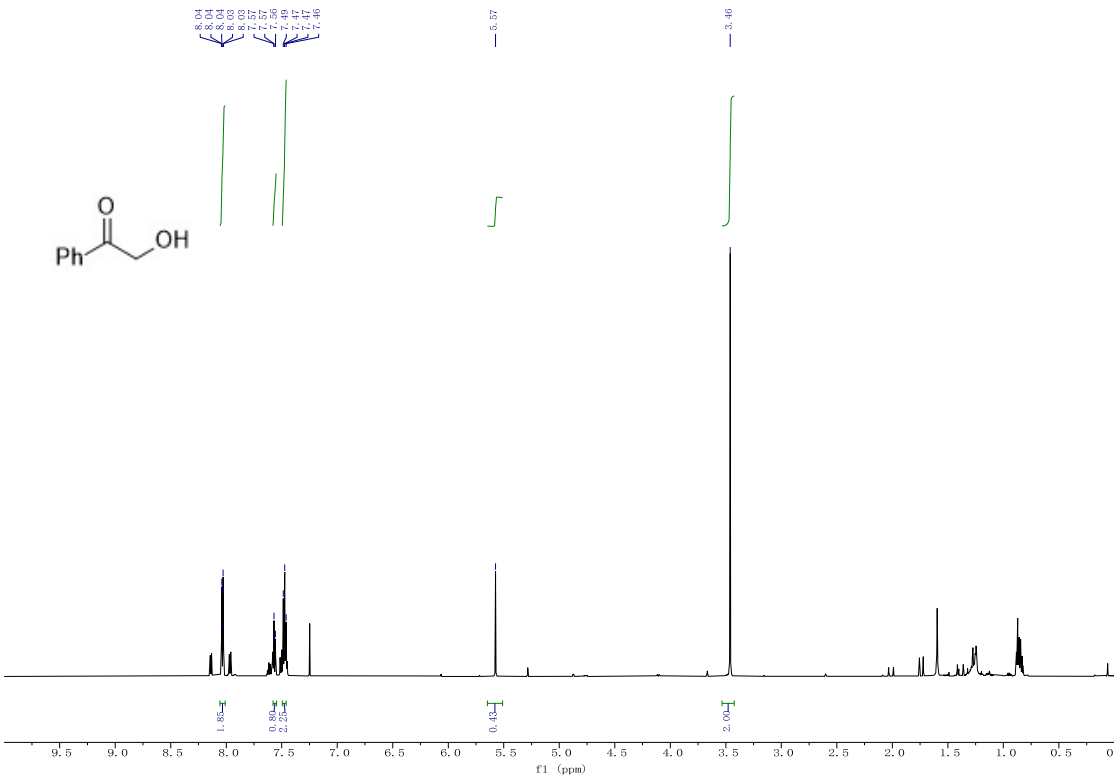

198.324
137.672
133.183
128.622
127.904
88.898
77.316
76.999
76.680
45.531
36.830
24.271
23.753
13.838
O
Ph
NO2
f1 (ppm)

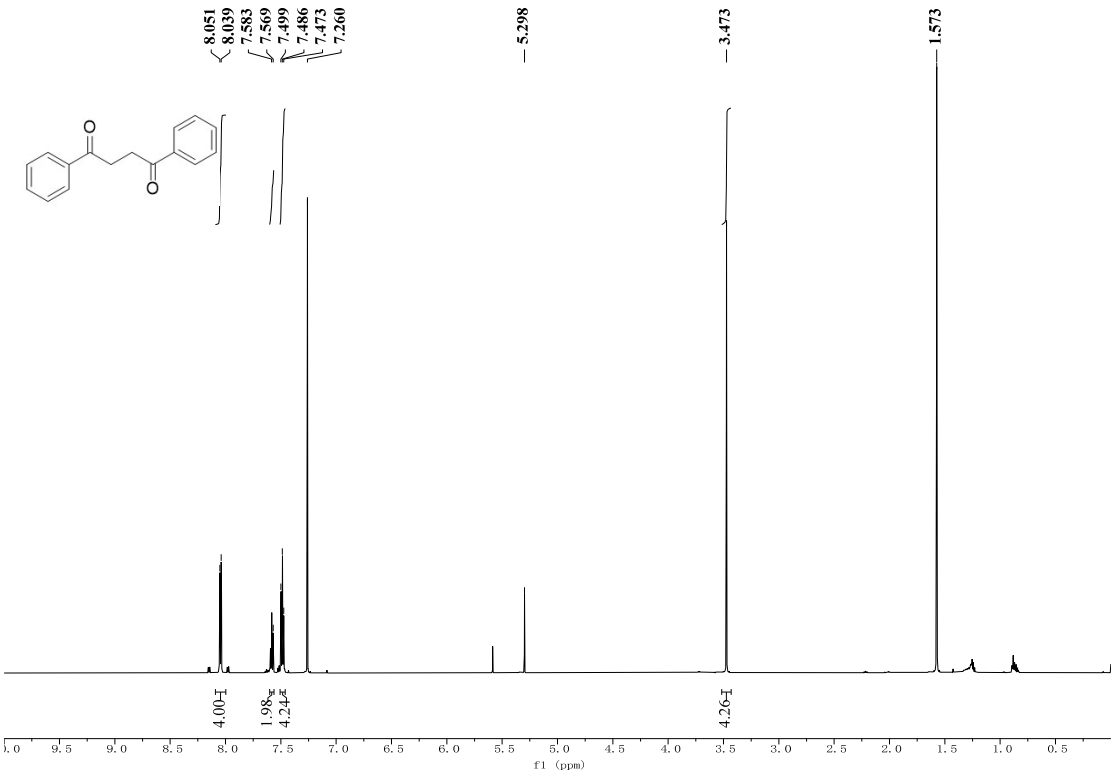

8.214
8.194
7.547
7.453
7.436
7.260
5.624
5.580
5.567
5.547
5.471
2.060
2.051
2.041
2.021
1.572
1.464
1.157
1.133
0.947
0.929
0.910
0.150
0.077
NO2
N
O
0.94
2.00
5.60
9.37
6.58
f1 (ppm)

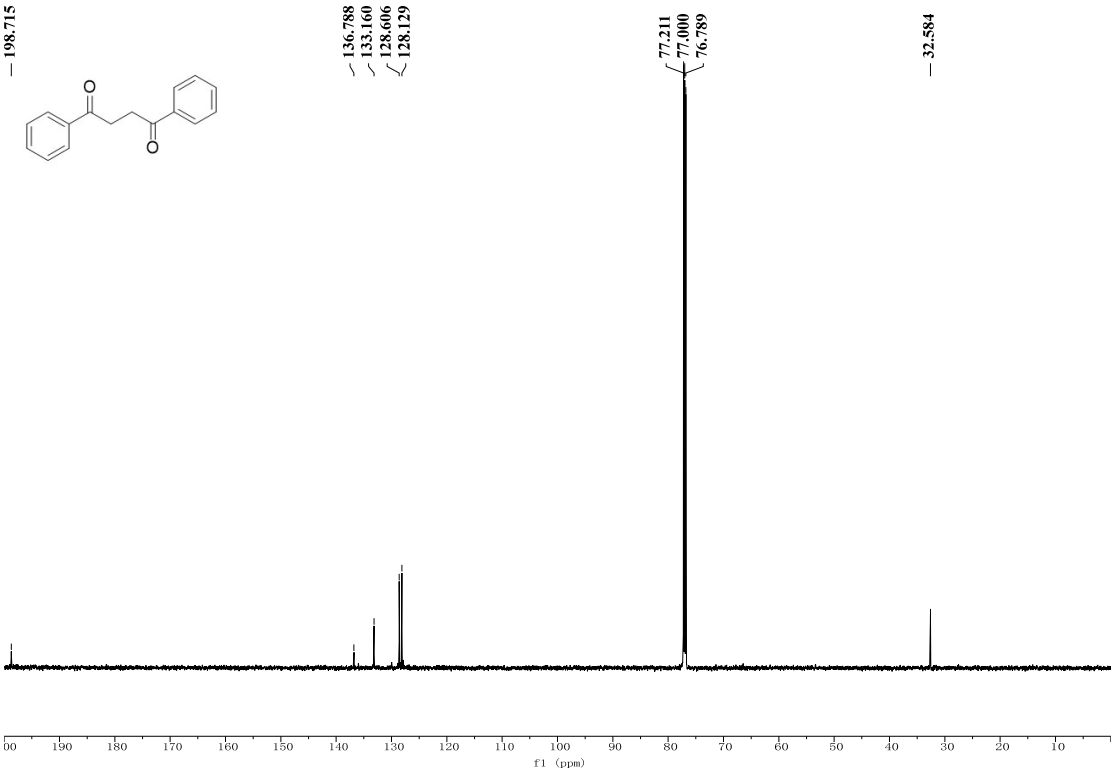

94.125
77.319
76.683
61.256
59.546
40.127
39.859
32.882
31.722
25.416
20.050
19.829
16.647
7.968
NO2
N
O
f1 (ppm)

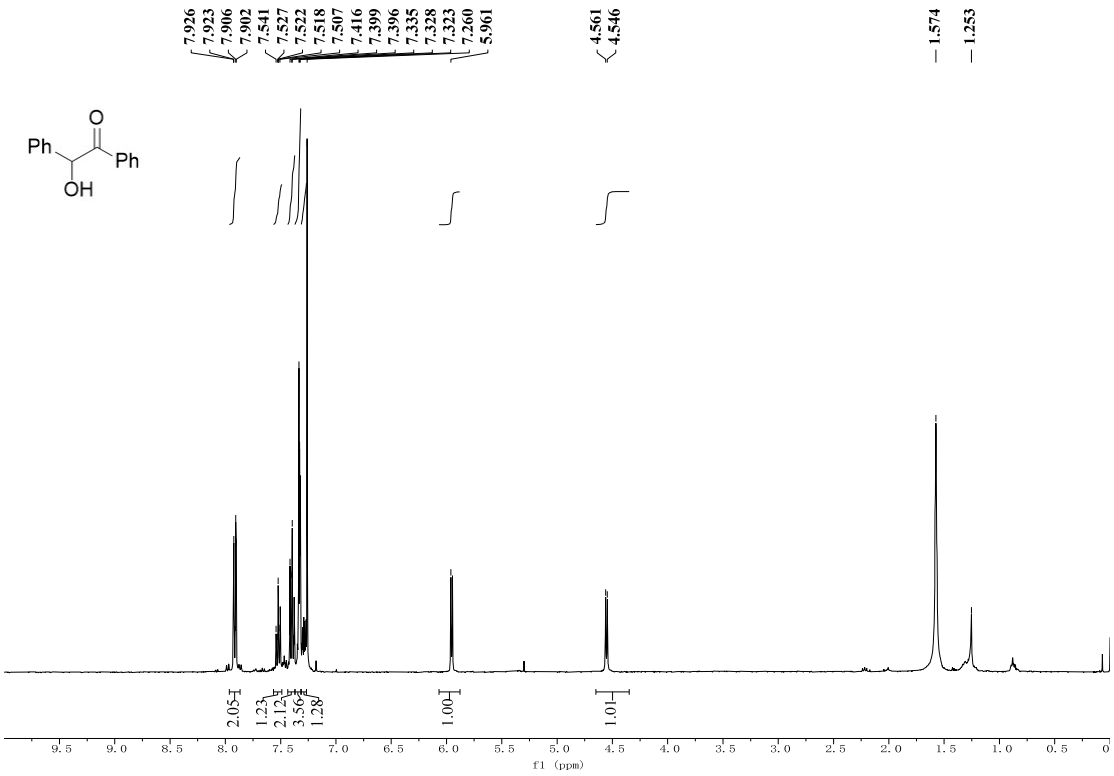

7.930
7.927
7.910
7.906
7.563
7.545
7.526
7.458
7.438
7.420
5.102
2.250
1.161
0.064
Ph
O
N
Br
NO2
2.02
1.08
2.36
2.00
6.18
12.53
f1 (ppm)

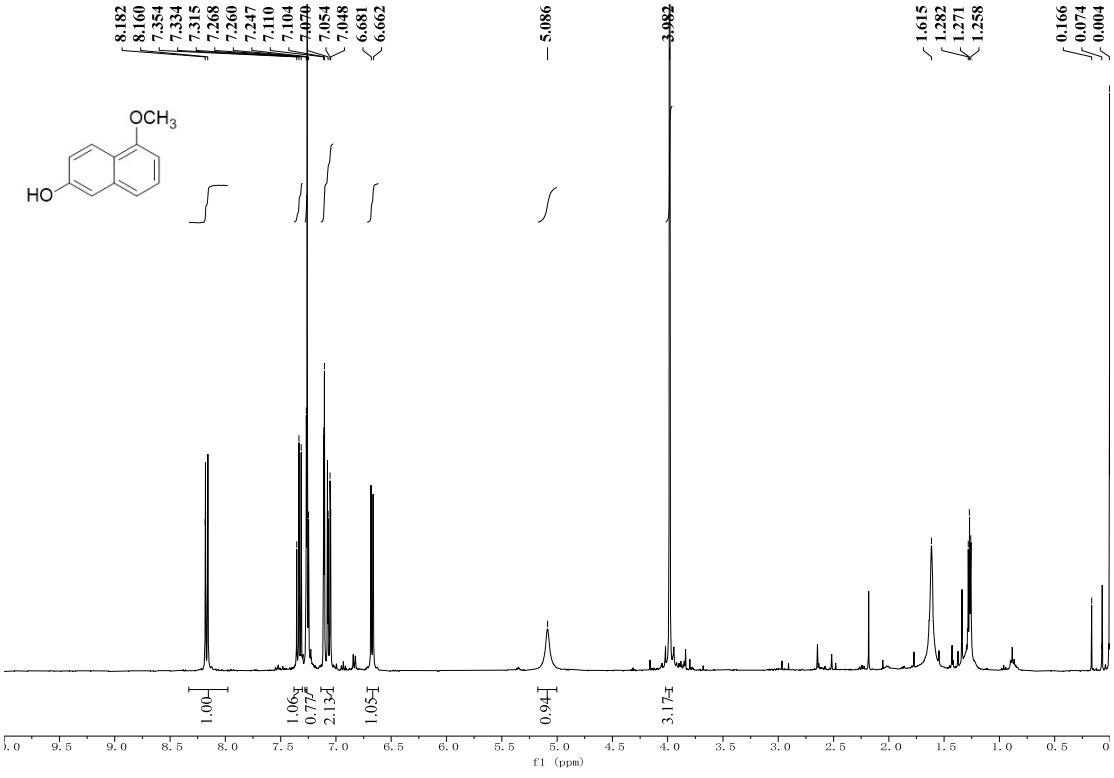

195.555
135.234
133.074
128.413
127.789
81.146
77.316
76.998
76.680
59.959
39.547
32.636
32.148
20.069
16.866
1.392
Ph
O
N
Br
NO2
f1 (ppm)

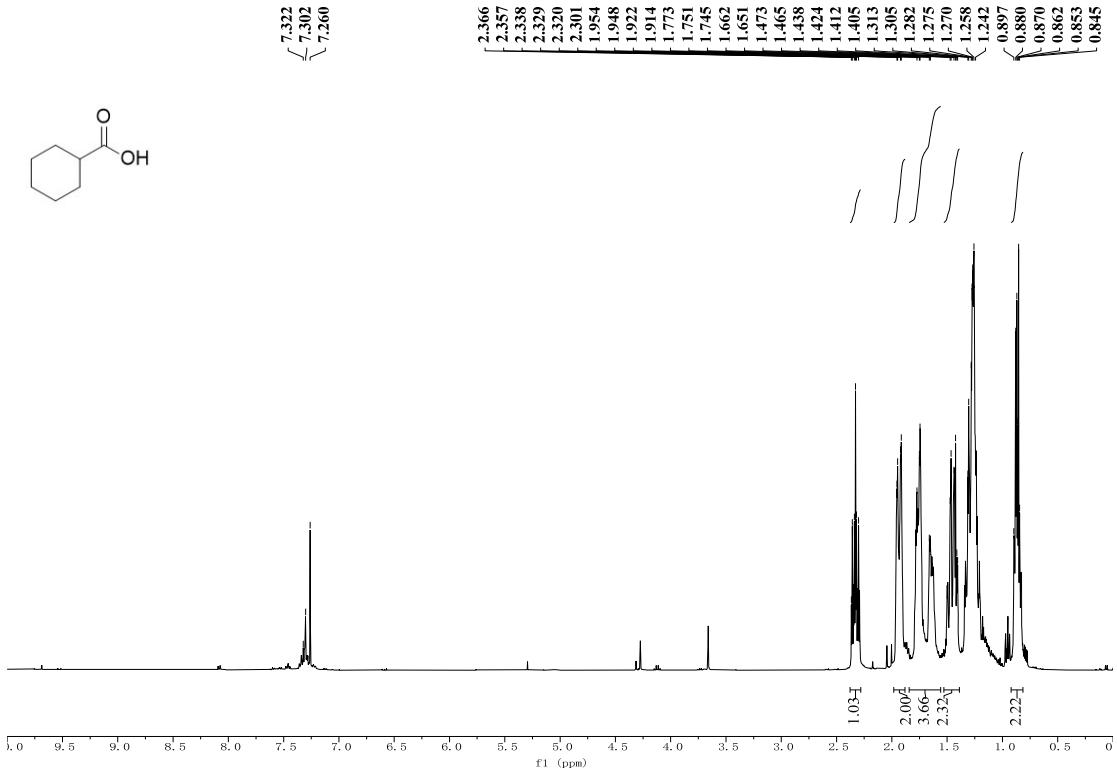

8.04
8.04
8.04
8.03
8.03
7.57
7.56
7.49
7.47
7.46
5.57
3.46
O
Ph
OH
1.85
0.80
2.25
0.43
2.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

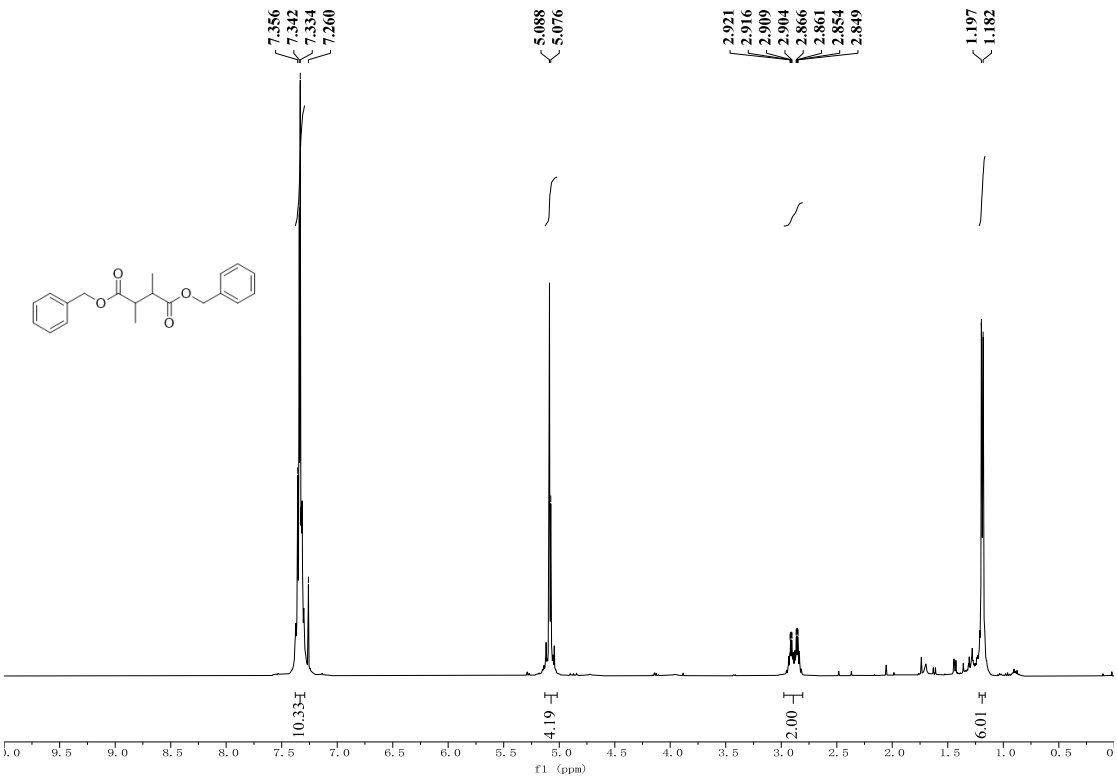

8.051
8.039
7.583
7.569
7.499
7.486
7.473
7.260
5.298
3.473
1.573
4.00
1.98
4.24
4.26
f1 (ppm)

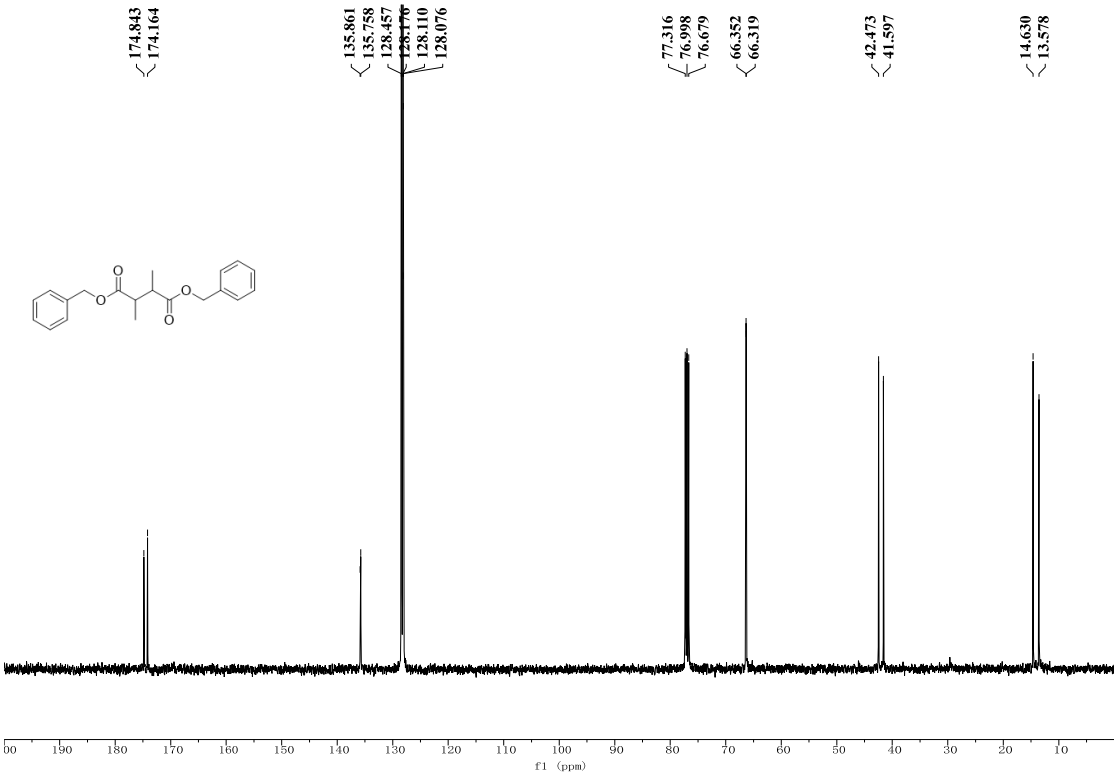

198.715
136.788
133.160
128.606
128.129
77.211
77.000
76.789
32.584
f1 (ppm)


7.926
7.923
7.906
7.902
7.541
7.527
7.522
7.518
7.507
7.416
7.399
7.396
7.335
7.328
7.323
7.260
5.961
4.561
4.546
1.574
1.253
Ph
O
Ph
OH
2.05
1.23
2.12
3.56
1.28
1.00
1.01
f1 (ppm)


8.182
8.160
7.354
7.334
7.315
7.268
7.260
7.247
7.110
7.104
7.070
7.054
7.048
6.681
6.662
5.086
3.982
1.615
1.282
1.271
1.258
0.166
0.074
0.004
OCH3
HO
1.00
1.06
0.77
2.13
1.05
0.94
3.17
f1 (ppm)


7.322
7.302
7.260
2.366
2.357
2.338
2.329
2.320
2.301
1.954
1.948
1.922
1.914
1.773
1.751
1.745
1.662
1.651
1.473
1.465
1.438
1.424
1.412
1.405
1.313
1.305
1.282
1.275
1.270
1.258
1.242
0.897
0.880
0.870
0.862
0.853
0.845
O
OH
1.03
2.00
3.66
2.32
2.22
f1 (ppm)


7.356
7.342
7.334
7.260
5.088
5.076
2.921
2.916
2.909
2.904
2.866
2.861
2.854
2.849
1.197
1.182
10.33
4.19
2.00
6.01
f1 (ppm)


174.843
174.164
135.861
135.758
128.457
128.176
128.110
128.076
77.316
76.998
76.679
66.352
66.319
42.473
41.597
14.630
13.578
f1 (ppm)