

Supporting Information

Hydrogen Atom Transfer-Enabled Hydroacylation of Alkenes with Acyl Chlorides

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1. General remarks

All the manipulations were performed in an argon-filled glovebox, unless mentioned otherwise. Anhydrous solvent was purchased from commercial sources and transferred under argon atmosphere. Acyl chlorides were purchased from Adamas or TCI, and some are used after purification via distillation or recrystallization. Alkene substrates were prepared according to previously reported procedures.^[1] Other reagents were purchased from Leyan.com, Adamas-beta®, Energy Chemicals, TCI, Bidepharm and used directly without further purification unless otherwise specified.

¹H NMR, ¹³C NMR spectra were recorded using Bruker 400 MHz NMR spectrometer. ¹H NMR and ¹³C NMR spectra were referenced to resonances of the residual protons in the deuterated solvents. Multiplicities are recorded as: s = singlet, d = doublet, t = triplet and m = multiplet. GC-MS analysis was performed on Shimadzu GC-2010 gas chromatography coupled to a Shimadzu QP-2010 mass selective detector. Reactions carried out at elevated temperature were heated using oil bath.

Medium-sized screw-cap test tubes (4 mL) were used for a part of 0.20 mmol scale reactions:15
× 45 mm tubes



Large-sized screw-cap test tubes (10 mL) were used for a part of 0.20 mmol scale reactions:15
× 100 mm tubes

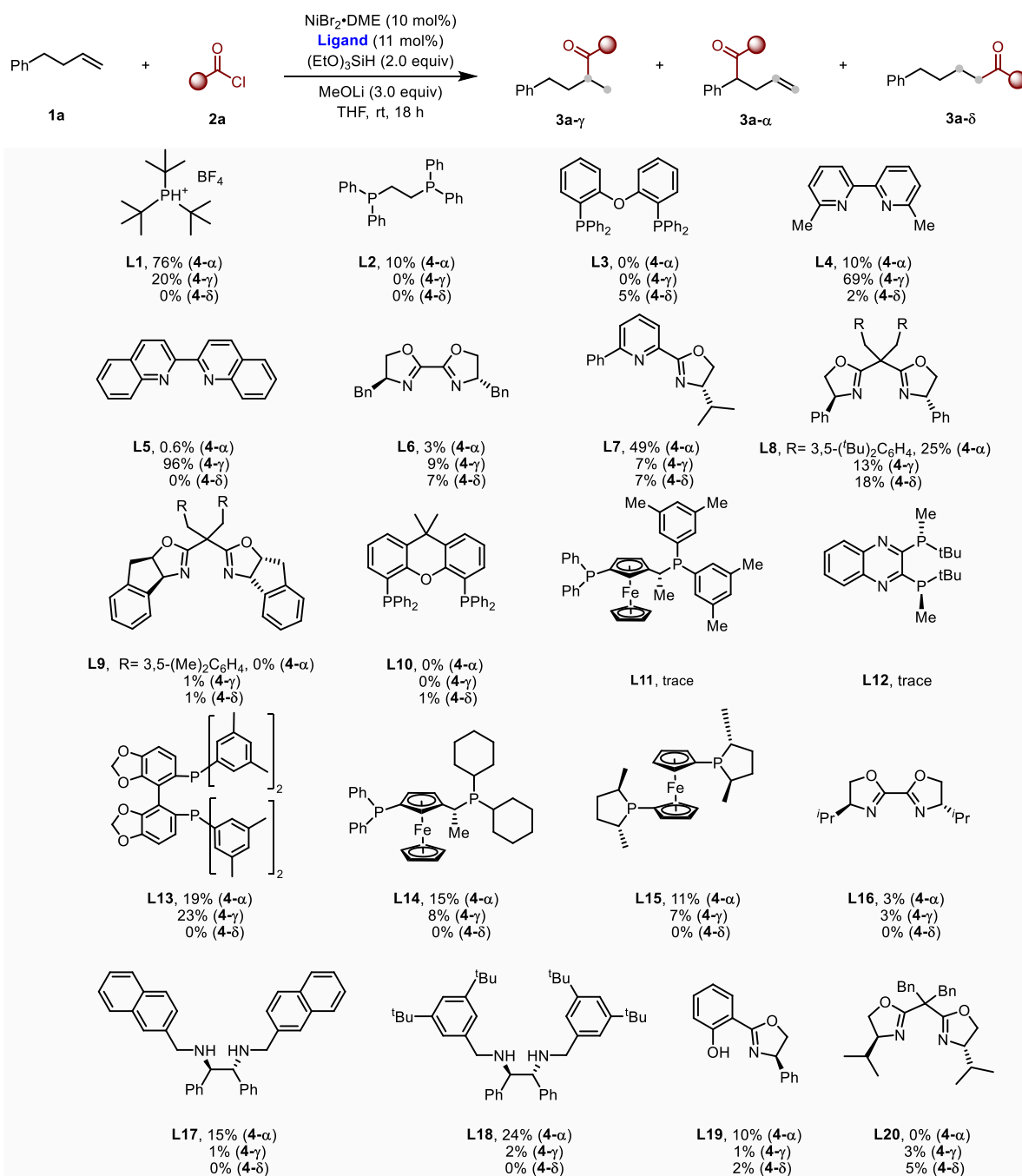


100 mL round bottom flask (synthware) was used for 5.0 mmol-scale reaction.

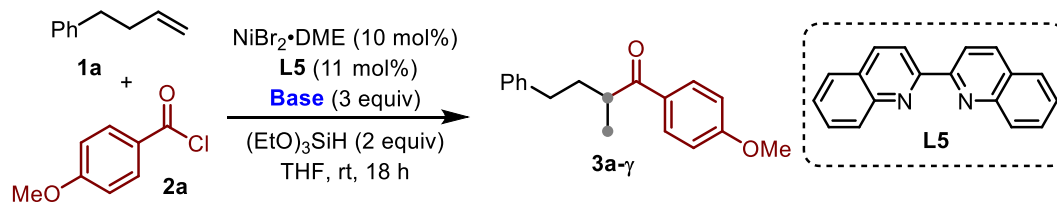


2. Conditional optimization

Table S1. Effect of ligand.



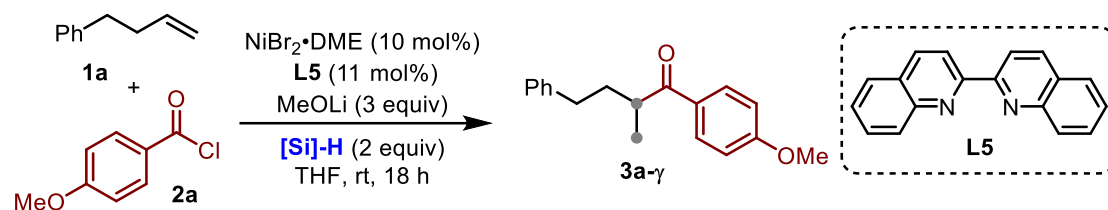
1a (0.2 mmol), **2a** (0.4 mmol), $\text{NiBr}_2 \cdot \text{DME}$ (10 mol%), Ligand (11 mol%), $(\text{EtO})_3\text{SiH}$ (2.0 equiv), MeOLi (3.0 equiv), THF (1.0 mL), rt, 18 h. The yield and regio-isomeric ratio (rr) were determined by GC-MS.

Table S2. Effect of base.

entry	Base	yield (%)	rr
1	MeOLi	94	> 99:1
2	K ₃ PO ₄	5	> 99:1
3	K ₂ HPO ₄	N.R	/
4	Na ₂ CO ₃	N.R	/
5	K ₂ CO ₃	3	> 99:1
6	Cs ₂ CO ₃	20	> 99:1
7	<i>t</i> BuOK	N.R	/
8	<i>t</i> BuONa	N.R	/
9	MeONa	N.R	/
10	MeOK	N.R	/
11	NaOH	63	86:14
12	KOH	45	94:6
13	LiOH	78	81:19
14	KOAc	N.R	/
15	CsF	27	93:7
16	NaF	N.R	/
17	KF	N.R	/
18	PhCO ₂ K	4	> 99:1

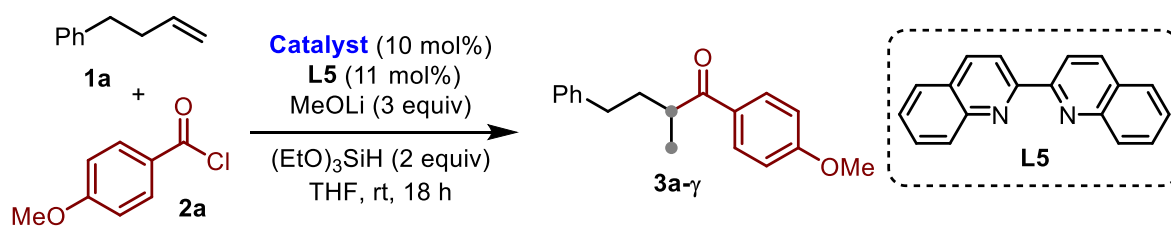
1a (0.2 mmol), **2a** (0.4 mmol), NiBr₂·DME (10 mol%), **L5** (11 mol%), (EtO)₃SiH (2.0 equiv), Base (3.0 equiv), THF (1.0 mL), rt, 18 h. The yield and regio-isomeric ratio (rr) were determined by GC-MS.

Table S3. Effect of silane.



entry	[Si]-H	yield (%)	rr
1	(MeO) ₃ SiH	88	88:12
2	(EtO) ₃ SiH	95	> 99:1
3	Me(EtO) ₂ SiH	87	87:13
4	Ph ₂ SiH ₂	63	63:37
5	PhSiH ₃	N.R	/
6	Me ₂ PhSiH	N.R	/
7	HBpin	N.R	/

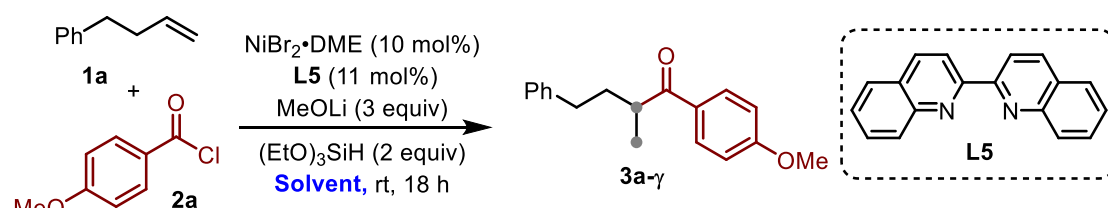
1a (0.2 mmol), **2a** (0.4 mmol), $\text{NiBr}_2 \cdot \text{DME}$ (10 mol%), **L5** (11 mol%), **[Si]-H** (2.0 equiv), MeOLi (3.0 equiv), THF (1.0 mL), rt, 18 h. The yield and regio-isomeric ratio (rr) were determined by GC-MS.

Table S4. Effect of catalyst.

entry	catalyst	yield (%)	rr
1	NiBr ₂	N.R	/
2	Ni(OTf) ₂	N.R	/
3	NiCl ₂ ·DME	69	82:18
4	NiBr ₂ ·DME	94	> 99:1
5	Ni(acac) ₂	85	88:12
6	Fe(OTf) ₂	N.R	/
7	Fe(OAc) ₂	N.R	/
8	Fe(acac) ₂	N.R	/
9	Fe(acac) ₃	N.R	/
10	FeBr ₂	N.R	/
11	CoBr ₂ ·DME	N.R	/
12	Co(acac) ₂	N.R	/
13	Cu(OAc) ₂	N.R	/
14	MnBr ₂	N.R	/
15	Mn(acac) ₂	N.R	/
16	Mn(dpm) ₃	N.R	/

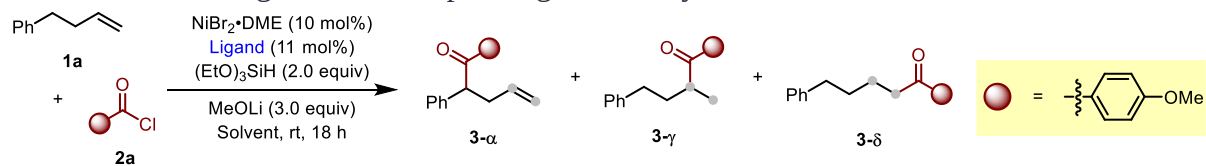
1a (0.2 mmol), **2a** (0.4 mmol), Catalyst (10 mol%), **L5** (11 mol%), (EtO)₃SiH (2.0 equiv), MeOLi (3.0 equiv), THF (1.0 mL), rt, 18 h. The yield and regio-isomeric ratio (rr) were determined by GC-MS.

Table S5. Effect of solvent.



entry	Solvent	yield (%)	rr
1	Toluene	7	> 99:1
2	DMA	42	71:29
3	Hexane	4	67:33
4	THF	95	> 99:1
5	CH_3CN	71	73:27
6	DMF	14	30:70
7	DMSO	N.R	/
8	DME	83	87:13
9	Et_2O	10	> 99:1
10	1,4-Dioxane	59	> 99:1
11	$t\text{BuOH}$	40	77:13
12	MeOH	N.R	/

1a (0.2 mmol), **2a** (0.4 mmol), $\text{NiBr}_2 \cdot \text{DME}$ (10 mol%), **L5** (11 mol%), $(\text{EtO})_3\text{SiH}$ (2.0 equiv), MeOLi (3.0 equiv), Solvent (1.0 mL), rt, 18 h. The yield and regio-isomeric ratio (rr) were determined by GC-MS.

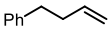
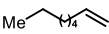
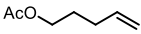
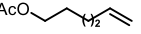
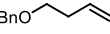
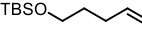
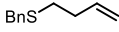
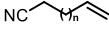
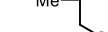
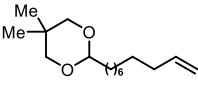
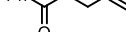
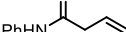
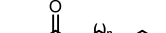
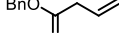
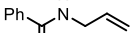
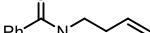
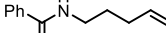
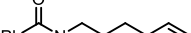
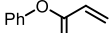
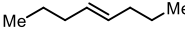
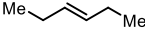
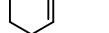
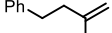
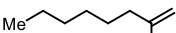
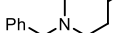
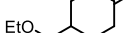
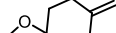
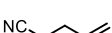
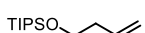
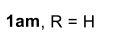
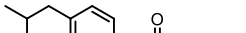
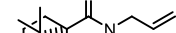
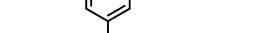
Table S6. Screening of the Corresponding Selectivity.

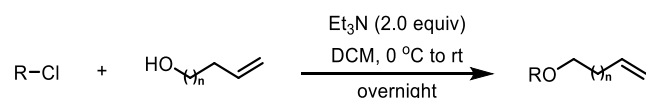
entry	ligand	yield of hydroacylation product (%)			ee (%)
		3-α	3-γ	3-δ	
1	L6	3	9	7	9
2	L8	25	13	18	9
3	L13	19	23	0	2
4	L14	15	8	0	5
5	L16	3	5	0	7
6	L20	29	8	21	36

1a (0.2 mmol), **2a** (0.4 mmol), NiBr₂·DME (10 mol%), Ligand (11 mol%), (EtO)₃SiH (2.0 equiv), MeOLi (3.0 equiv), THF (1.0 mL), rt, 18 h. Determined by GC or HPLC using chiral columns.

3. Preparation of substrates

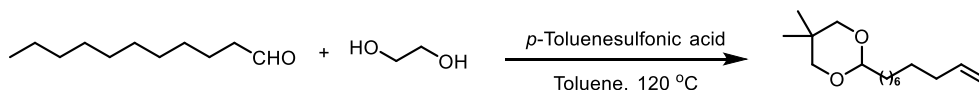
Table S7. Synthesis method of alkene substrate **1a-1aw**.

						
1a	1b	1c	1d	1e	1f	1g
						
1h	1i, n=0 1j, n=1	1k	1l	1m	1n	
						
1o, n=1 1p, n=0	1q	1r	1s	1t	1u	
						
1v	1w, E-alkene 1x, Z-alkene	1y, Z-alkene	1z	1aa	1ab	1ac
						
1ad	1ae	1af	1ag	1ah	1ai	
						
1aj	1ak	1al	1am, R = H 1an, R = 2-CF₃ 1ao, R = 4-^tBu 1ap, R = 4-Br	1aq		
						
1ar	1as	1at	1au			
						
1av	1aw					

General procedure for synthesizing olefinic substrates. (GP1):

Compounds **1d–1e** and **1g** were synthesized from the corresponding chlorides and the corresponding enols.

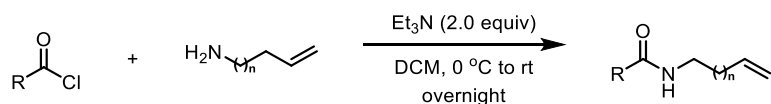
The corresponding enol (20 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (50 mL), Et_3N (40 mmol, 2.0 equiv) was added and the mixture was stirred for 10 min, then chloride (30 mmol, 1.5 equiv) was added dropwise after 15 min and the mixture was stirred for different reaction times at room temperature under Ar atmosphere. Then, the aqueous layer was extracted with NaOH solution (1 M, 30 mL) was added and stirred was stirred for 5 min, extracted with CH_2Cl_2 (3×50 mL), dried over sodium sulfate and the solvent was removed under reduced pressure. The residue was purified by using column chromatography (ethyl acetate: petroleum ether = 1:20) to provide the desired product.

General procedure for synthesizing olefinic substrates. (GP2):

Compound **1k** was synthesized from 10-undecenal and ethylene glycol.

10-Undecenal (20 mmol, 1.0 equiv) was dissolved in toluene (50 mL), *p*-toluenesulfonic acid (50 mmol, 2.5 equiv) was added and the mixture was stirred under Ar for 10 min, then ethylene glycol (40 mmol, 2.0 equiv) was added and stirred at reflux for 12 h at 120 °C. The toluene solvent was then removed under reduced pressure, extracted with CH_2Cl_2 (3×50 mL) and water, dried over sodium sulfate and the solvent removed under reduced pressure. The residue was purified by column chromatography (ethyl acetate: petroleum ether = 1:20) to give the desired product.

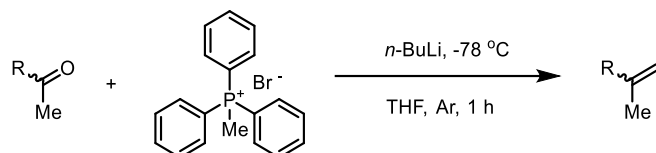
General procedure for synthesis of amide substrates. (GP3):



Compound **1r–1u**, **1ap–1ar** and **1at** -were synthesized from acyl chloride and amines.

Allylamine derivatives (20 mmol, 1.0 equiv) was dissolved in CH_2Cl_2 (20 mL), Et_3N (40 mmol, 2.0 equiv) was added and the mixture was stirred for 10 min, benzoyl chloride derivatives (20 mmol, 1.0 equiv) dissolve in CH_2Cl_2 (20 mL) was added dropwise over 15 min and the mixture was stirred for different reaction times at room temperature under Ar atmosphere. Then, the aqueous layer was extracted with NaOH solution (1 M, 30 mL) was added and stirred was stirred for 5 min, extracted with CH_2Cl_2 (3×50 mL), dried over sodium sulfate and the solvent was removed under reduced pressure. The residue was purified by using column chromatography (ethyl acetate: petroleum ether = 1:8) to provide the desired product. The residue was purified by using column chromatography (ethyl acetate: petroleum ether = 1:10) to provide the desired product.

General procedure for synthesizing olefinic substrates. (GP4):



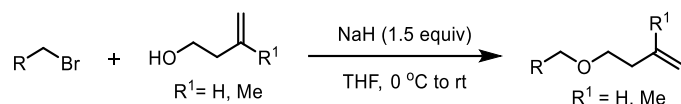
Compound **1ae–1ai** were synthesized from ketone.

The Wittig reaction was carried out by modifying the literature program:^[2]

$MePPh_3Br$ (2.0 equiv) and THF were added to a dry Schlenk flask, protected by Ar and cooled to $-78\text{ }^\circ\text{C}$ for 10 min in a cold trap, then $n-BuLi$ (2.0 equiv) was added. The reaction was stirred at $-78\text{ }^\circ\text{C}$ for 30 min and the corresponding ketone (1.0 equiv) was added dropwise. The reaction is transferred to room temperature and stirred for 1 h. When the ketone is consumed (as determined by TLC), the flask is vented to air and the reaction is quenched with sodium chloride. The reaction was quenched with water. The organic layer is separated and the aqueous layer is extracted three times with Et_2O . The aqueous layer was extracted three times with Et_2O .

The combined organic layers were filtered over Na₂SO₄. The filtrate was concentrated under reduced pressure to give the corresponding crude product. The residue was purified by column chromatography (ethyl acetate: petroleum ether = 1:50) to give the desired product.

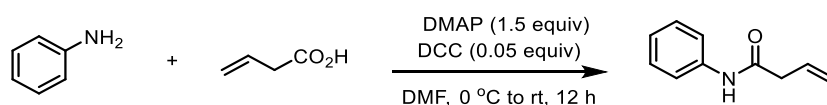
General procedure for synthesizing olefinic substrates. (GP5):



Compound **1ak–1ao** and **1f** were synthesized from the corresponding alcohol and the corresponding benzyl bromide

In a dry Schlenk flask, NaH (1.5 equiv) and THF are added and cooled to 0 °C in a cold trap under Ar protection and the corresponding alcohol (1.0 equiv) is added. The reaction was stirred at 0 °C for 15 min, then the corresponding benzyl bromide (1.1 equiv) was added. The reaction is brought to room temperature and stirred for 5 h. After the reaction is complete the reaction is quenched with saturated NH₄Cl at 0 °C. The reaction is extracted three times with EA and water. The combined organic layers were filtered over Na₂SO₄ and the filtrate concentrated under reduced pressure to give the corresponding crude product. The residue was purified by column chromatography (ethyl acetate: petroleum ether = 1:50) to give the desired product.

General procedure for synthesis of amide substrates or carboxylate substrate. (GP6):



Compound **1n** were synthesized from bromine and amines.

Relevant acid (10 mmol, 1.0 equiv), 4-dimethylaminopyridine (0.5 mmol, 0.05 equiv) and dicyclohexylcarbodiimide (15 mmol, 1.5 equiv) were added to DMF and aniline (11 mmol, 1.1 equiv) was added slowly to the mixture at 0 °C. Then the mixture was stirred for different reaction times at room temperature under Ar atmosphere. After that the mixture was extracted with CH₂Cl₂ and water (3 × 50 mL), dried over sodium sulfate and the solvent was removed

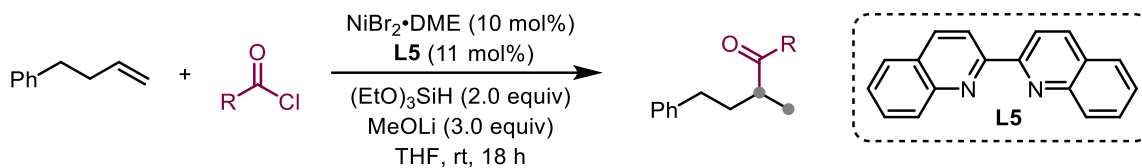
under reduced pressure. The residue was purified by using column chromatography (ethyl acetate: petroleum ether = 1:8) to provide the desired product.

Preparation of acyl chloride (GP7):

Acyl chlorides were purchased from Adamas or TCI, **1ap-1ar,1aw** are used after purification via distillation and **1ay-1az** are used after recrystallization.

Synthesis of compound **1r-1u** were according the literature,^[1] and the characterization data are consistent with the literature reported data. Other olefinic substrates have been reported or are available for direct purchase.

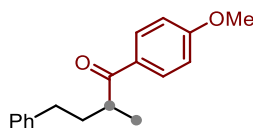
4. General procedure for hydroacylation of alkenes with acyl chlorides



General procedure: In an argon-filled glovebox, $NiBr_2 \cdot DME$ (6.2 mg, 0.02 mmol, 10 mol%), Ligand (5.6 mg, 0.022 mmol, 11 mol%), relevant alkene substrate (0.2 mmol, 1.0 equiv), $MeOLi$ (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then relevant acyl chlorides (0.4 mmol, 2.0 equiv), $(EtO)_3SiH$ (74 μL , 0.4 mmol, 2.0 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The conditions for flash chromatography and data for characterization of the products are listed below.

5. Analytical data of compounds

1-(4-methoxyphenyl)-2-methyl-4-phenylbutan-1-one (3a)



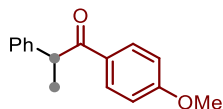
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 50.3 mg (94% yield) of **3a** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, J = 8.7 Hz, 2H), 7.26 – 7.21 (m, 2H), 7.17 (d, J = 7.1 Hz, 1H), 7.12 (d, J = 7.0 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 3.84 (s, 3H), 3.40 – 3.34 (m, 1H), 2.64 – 2.57 (m, 2H), 2.20 – 2.08 (m, 1H), 1.76 – 1.67 (m, 1H), 1.19 (d, J = 6.8 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 202.8, 163.5, 142.0, 130.7, 129.7, 128.6, 128.5, 126.0, 113.9, 55.6, 39.4, 35.5, 33.7, 17.6.

HRMS (ESI) m/z calcd for C₁₈H₂₁O₂⁺ [M+H⁺] 269.1536, found 269.1536..

1-(4-methoxyphenyl)-2-phenylpropan-1-one (3b)



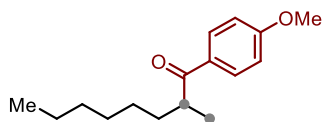
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 34.1 mg (71% yield) of **3b** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.94 (m, 2H), 7.34 – 7.29 (m, 4H), 7.27 – 7.20 (m, 1H), 6.93 – 6.86 (m, 2H), 4.83 – 4.56 (m, 1H), 3.86 (d, J = 1.2 Hz, 3H), 1.56 (dd, J = 6.9, 1.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 199.0, 163.3, 142.1, 131.2, 129.6, 129.1, 127.8, 126.9, 113.8, 55.6, 47.7, 19.7.

HRMS (ESI) m/z calcd for C₁₆H₁₇O₂⁺ [M+H⁺] 241.1223, found 241.1222.

1-(4-methoxyphenyl)-2-methyloctan-1-one (3c)



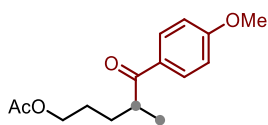
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 41.2 mg (83% yield) of **3c** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 3.47 – 3.36 (m, 1H), 1.83 – 1.68 (m, 1H), 1.48 – 1.36 (m, 1H), 1.31 – 1.22 (m, 8H), 1.17 (d, *J* = 6.8 Hz, 3H), 0.85 (t, *J* = 6.6 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.3, 163.4, 130.6, 129.9, 113.9, 55.6, 40.3, 34.1, 31.9, 29.6, 27.6, 22.8, 17.6, 14.2.

HRMS (ESI) *m/z* calcd for C₁₆H₂₅O₂⁺ [M+H⁺] 249.1849, found 249.1847.

5-(4-methoxyphenyl)-4-methyl-5-oxopentyl acetate (**3d**)



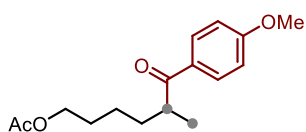
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 40.1 mg (76% yield) of **3d** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 7.6 Hz, 2H), 6.95 (d, *J* = 7.6 Hz, 2H), 4.08 – 4.01 (m, 2H), 3.87 (s, 3H), 3.46 (h, *J* = 6.9 Hz, 1H), 2.02 (d, *J* = 1.2 Hz, 3H), 1.93 – 1.82 (m, 1H), 1.68 – 1.60 (m, 2H), 1.55 – 1.45 (m, 1H), 1.20 (dd, *J* = 7.0, 1.2 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 202.6, 163.6, 130.7, 129.6, 119.8, 114.0, 64.5, 55.6, 39.8, 30.1, 26.6, 21.1, 17.9.

HRMS (ESI) *m/z* calcd for C₁₅H₂₁O₄⁺ [M+H⁺] 265.1434, found 265.1434.

5-(4-methoxyphenyl)-4-methyl-5-oxopentyl acetate (**3e**)



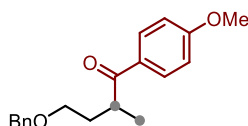
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 39.5 mg (71% yield) of **3e** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 (dd, J = 8.9, 2.3 Hz, 2H), 6.94 (dd, J = 8.9, 2.2 Hz, 2H), 4.06 – 3.98 (m, 2H), 3.87 (d, J = 2.1 Hz, 3H), 3.47 – 3.37 (m, 1H), 2.01 (d, J = 2.2 Hz, 3H), 1.88 – 1.77 (m, 1H), 1.65 – 1.53 (m, 2H), 1.49 – 1.41 (m, 1H), 1.39 – 1.30 (m, 2H), 1.18 (dd, J = 6.8, 2.2 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 202.9, 171.3, 163.5, 130.6, 129.7, 113.9, 64.5, 55.6, 40.2, 33.5, 28.9, 24.0, 21.1, 17.8.

HRMS (ESI) m/z calcd for C₁₆H₂₃O₄⁺ [M+H⁺] 279.1591, found 279.1593.

4-(benzyloxy)-1-(4-methoxyphenyl)-2-methylbutan-1-one (**3f**)



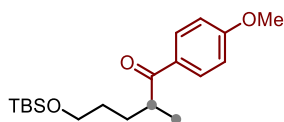
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 42.3 mg (71% yield) of **3f** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 (dd, J = 9.0, 2.3 Hz, 2H), 7.39–7.26 (m, 5H), 6.97 (dd, J = 9.1, 2.3 Hz, 2H), 4.48 (s, 2H), 3.92 (d, J = 2.1 Hz, 3H), 3.83–3.70 (m, 1H), 3.63–3.54 (m, 1H), 3.53–3.44 (m, 1H), 2.27–2.14 (m, 1H), 1.83–1.70 (m, 1H), 1.23 (dd, J = 6.8, 2.3 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.0, 163.5, 138.5, 130.8, 129.7, 128.5, 127.7, 127.7, 113.8, 73.1, 68.1, 55.6, 36.9, 33.9, 17.8.

HRMS (ESI) m/z calcd for C₁₉H₂₃O₃⁺ [M+H⁺] 299.1642, found 299.1645.

5-((tert-butyldimethylsilyl)oxy)-1-(4-methoxyphenyl)-2-methylpentan-1-one (**3g**)



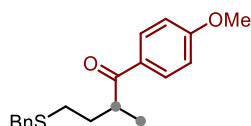
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 45.7 mg (68% yield) of **3g** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, J = 8.9 Hz, 2H), 6.97 (d, J = 8.9 Hz, 2H), 3.90 (s, 3H), 3.63 (t, J = 6.1 Hz, 2H), 3.49 (q, J = 6.7 Hz, 1H), 1.91 – 1.83 (m, 1H), 1.61 – 1.51 (m, 3H), 1.22 (d, J = 6.9 Hz, 3H), 0.91 (s, 8H), 0.06 (d, J = 3.9 Hz, 6H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.1, 163.4, 130.7, 129.8, 113.9, 63.2, 55.6, 40.0, 30.7, 30.3, 26.1, 18.5, 17.5, -5.2.

HRMS (ESI) m/z calcd for C₁₉H₃₃O₃Si⁺ [M+H⁺] 337.2193, found 337.2193.

4-(benzyloxy)-1-(4-methoxyphenyl)-2-methylbutan-1-one (**3h**)



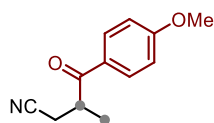
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 36.4 mg (58% yield) of **3h** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, J = 8.9 Hz, 2H), 7.36–7.29 (m, 4H), 7.29–7.22 (m, 1H), 6.98 (d, J = 8.9 Hz, 2H), 3.91 (s, 3H), 3.71 (s, 2H), 3.63 (h, J = 7.1 Hz, 1H), 2.48 (hept, J = 6.9 Hz, 2H), 2.15 (dq, J = 14.9, 7.8, 7.2 Hz, 1H), 1.69 (dq, J = 14.1, 7.8, 7.2 Hz, 1H), 1.18 (d, J = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.3, 163.5, 138.5, 130.8, 129.5, 129.0, 128.6, 127.1, 113.8, 55.6, 39.0, 36.2, 32.9, 29.3, 17.6.

HRMS (ESI) m/z calcd for C₁₉H₂₃O₂S⁺ [M+H⁺] 315.1413, found 315.1417.

4-(4-methoxyphenyl)-3-methyl-4-oxobutanenitrile (**3i**)



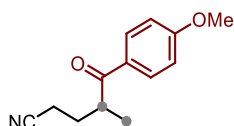
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 14.6 mg (36% yield) of **3i** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.9 Hz, 2H), 7.01 (d, *J* = 8.9 Hz, 2H), 3.93 (s, 3H), 3.84 – 3.76 (m, 1H), 2.76 (dd, *J* = 16.9, 5.9 Hz, 1H), 2.65 (dd, *J* = 16.9, 8.1 Hz, 1H), 1.43 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 201.1, 163.9, 130.9, 128.9, 119.7, 114.1, 55.7, 38.9, 28.6, 18.3, 15.4.

HRMS (ESI) *m/z* calcd for C₁₂H₁₄NO₂⁺ [*M*+H⁺] 204.1019, found 204.1018.

5-(4-methoxyphenyl)-4-methyl-5-oxopentanenitrile (**3j**)



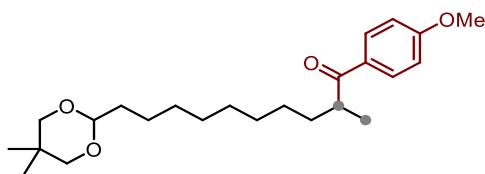
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 30.8 mg (71% yield) of **3j** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.9 Hz, 2H), 6.96 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H), 3.72–3.58 (m, 1H), 2.50–2.38 (m, 1H), 2.38–2.29 (m, 1H), 2.28–2.14 (m, 1H), 1.85–1.72 (m, 1H), 1.24 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 201.1, 163.9, 130.9, 128.9, 119.7, 114.1, 55.7, 38.9, 28.6, 18.3, 15.4.

HRMS (ESI) *m/z* calcd for C₁₃H₁₅NO₂⁺ [*M*+H⁺] 217.1103, found 217.1104.

10-(5,5-dimethyl-1,3-dioxan-2-yl)-1-(4-methoxyphenyl)-2-methyldecan-1-one (**3k**)



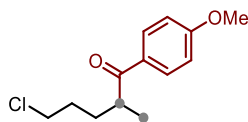
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 42.1 mg (54% yield) of **3k** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.9 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 4.45 – 4.40 (m, 1H), 3.91 (s, 3H), 3.66 – 3.59 (m, 2H), 3.48 – 3.40 (m, 3H), 1.86 – 1.73 (m, 1H), 1.69 – 1.59 (m, 2H), 1.47 – 1.35 (m, 3H), 1.33 – 1.25 (m, 10H), 1.23 – 1.19 (m, 6H), 0.75 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.3, 163.4, 130.6, 130.6, 129.9, 113.9, 102.4, 55.6, 40.3, 35.0, 34.1, 30.3, 29.8, 29.6, 29.5, 27.6, 24.1, 23.1, 22.0, 17.5.

HRMS (ESI) *m/z* calcd for C₂₄H₃₉O₄⁺ [M+H⁺] 391.2843, found 391.2845.

5-chloro-1-(4-methoxyphenyl)-2-methylpentan-1-one (**3l**)



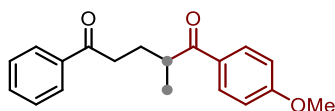
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 29.8 mg (62% yield) of **3l** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.9 Hz, 2H), 6.95 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 3.52 (t, *J* = 7.0 Hz, 2H), 3.49 – 3.41 (m, 1H), 1.99 – 1.88 (m, 1H), 1.83 – 1.73 (m, 2H), 1.65 – 1.59 (m, 1H), 1.20 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 202.4, 163.6, 130.7, 129.5, 114.0, 55.6, 45.1, 39.7, 31.0, 30.5, 17.9.

HRMS (ESI) *m/z* calcd for C₂₄H₃₉O₄⁺ [M+H⁺] 241.0990, found 241.0993.

1-(4-methoxyphenyl)-2-methyl-5-phenylpentane-1,5-dione (**3m**)



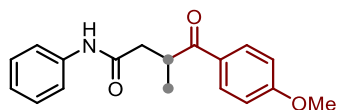
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 30.2 mg (51% yield) of **3m** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 8.9 Hz, 2H), 7.93 (d, *J* = 7.0 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 3.69–3.57 (m, 1H), 3.16–3.04 (m, 1H), 2.96–2.83 (m, 1H), 2.34–2.19 (m, 1H), 1.98–1.85 (m, 1H), 1.24 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.6, 200.2, 163.6, 136.9, 133.2, 130.8, 129.5, 128.7, 128.2, 114.0, 55.6, 39.4, 36.0, 28.0, 18.0.

HRMS (ESI) *m/z* calcd for C₁₉H₂₁O₃⁺ [M+H⁺] 297.1485, found 297.1488.

4-(4-methoxyphenyl)-3-methyl-4-oxo-N-phenylbutanamide (**3n**)



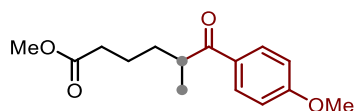
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 33.9 mg (57% yield) of **3n** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 8.9 Hz, 2H), 7.77 (s, 1H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 7.9 Hz, 2H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 8.9 Hz, 2H), 4.12–4.01 (m, 1H), 3.86 (s, 3H), 2.95 (dd, *J* = 14.6, 8.5 Hz, 1H), 2.51 (dd, *J* = 14.6, 5.0 Hz, 1H), 1.28 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.3, 170.1, 163.9, 138.0, 131.1, 129.0, 128.6, 124.3, 119.9, 114.0, 55.6, 40.9, 37.9, 18.7.

HRMS (ESI) *m/z* calcd for C₁₈H₂₀NO₃⁺ [M+H⁺] 298.1438, found 298.1436.

Methyl 6-(4-methoxyphenyl)-5-methyl-6-oxohexanoate (**3o**)



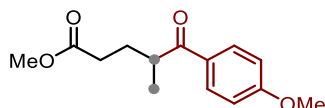
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 40.1 mg (76% yield) of **3o** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H), 3.64 (s, 3H), 3.43 (h, *J* = 6.7 Hz, 1H), 2.30 (td, *J* = 7.4, 2.2 Hz, 2H), 1.87 – 1.77 (m, 1H), 1.69 – 1.57 (m, 2H), 1.50 – 1.41 (m, 1H), 1.18 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.6, 174.0, 163.5, 130.7, 129.6, 113.9, 55.6, 51.6, 40.1, 34.2, 33.2, 23.0, 17.8.

HRMS (ESI) *m/z* calcd for C₁₅H₂₁O₄⁺ [M+H⁺] 265.1434, found 265.1434.

Methyl 5-(4-methoxyphenyl)-4-methyl-5-oxopentanoate (**3p**)



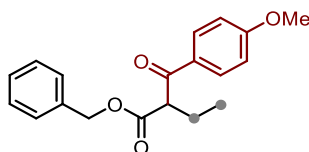
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 44.1 mg (88% yield) of **3p** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 3.65 (s, 3H), 3.58 – 3.46 (m, 1H), 2.43 – 2.24 (m, 2H), 2.20 – 2.08 (m, 1H), 1.81 – 1.70 (m, 1H), 1.19 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.1, 173.8, 163.5, 130.6, 129.3, 113.8, 55.5, 51.6, 39.1, 31.5, 28.4, 17.5.

HRMS (ESI) *m/z* calcd for C₁₄H₁₉O₄⁺ [M+H⁺] 251.1278, found 251.1276.

Benzyl 2-(4-methoxybenzoyl)butanoate (**3q**)



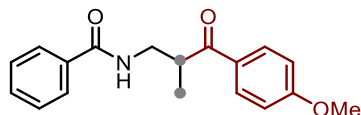
The general procedure was followed, (MeO)₃SiH was substituted for (EtO)₃SiH at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 21.0 mg (31% yield) of **3q** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.9 Hz, 2H), 7.32–7.26 (m, 2H), 7.25–7.19 (m, 2H), 6.90 (d, *J* = 8.9 Hz, 2H), 5.12 (s, 2H), 4.22 (t, *J* = 7.2 Hz, 1H), 3.87 (s, 3H), 2.05 (p, *J* = 7.3 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 193.5, 170.2, 163.9, 135.7, 131.1, 129.4, 128.6, 128.3, 128.2, 114.0, 67.0, 55.71, 55.66, 22.6, 12.3.

HRMS (ESI) *m/z* calcd for C₂₀H₂₅O₄⁺ [*M*+*H*⁺] 329.1747, found 329.1744.

***N*-(3-(4-methoxyphenyl)-2-methyl-3-oxopropyl)benzamide (3r)**



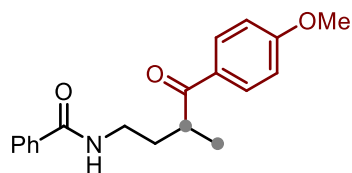
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 3/1) gave 44.6 mg (75% yield) of **3r** as a colorless oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 7.0 Hz, 2H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.43–7.35 (m, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 6.82 (s, 1H), 3.90–3.74 (m, 5H), 3.74–3.63 (m, 1H), 1.27 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.6, 167.8, 164.0, 134.5, 131.6, 131.0, 129.0, 127.0, 114.1, 55.7, 42.2, 40.6, 16.3.

HRMS (ESI) *m/z* calcd for C₁₈H₂₀NO₃⁺ [*M*+*H*⁺] 312.1594, found 312.1595.

***N*-(4-(4-methoxyphenyl)-3-methyl-4-oxobutyl)benzamide (3s)**



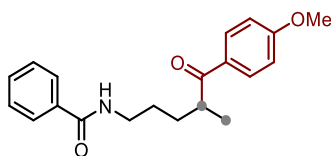
The general procedure was followed at rt for 18 h.. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 59.1 mg (95% yield) of **3s** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.9 Hz, 2H), 7.68 (d, *J* = 6.9 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 2H), 6.90 (d, *J* = 8.9 Hz, 2H), 6.47 (s, 1H), 3.85 (s, 3H), 3.62–3.52 (m, 1H), 3.49 (q, *J* = 6.6 Hz, 2H), 2.26–2.14 (m, 1H), 1.89–1.76 (m, 1H), 1.24 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.1, 167.5, 163.7, 134.6, 131.4, 130.8, 129.1, 128.6, 126.9, 114.0, 55.6, 38.8, 38.6, 32.8, 18.5.

HRMS (ESI) *m/z* calcd for C₁₉H₂₂NO₃⁺ [M+H⁺] 312.1600, found 312.1608.

N-(5-(4-methoxyphenyl)-4-methyl-5-oxopentyl)benzamide (3t)

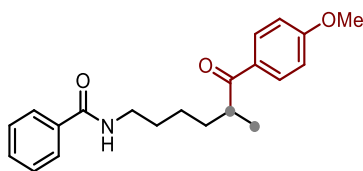


The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 52.0 mg (80% yield) of **3t** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.8 Hz, 2H), 7.81 (d, *J* = 7.1 Hz, 2H), 7.53 – 7.47 (m, 1H), 7.46 – 7.39 (m, 2H), 6.95 (d, *J* = 8.9 Hz, 2H), 6.52 (t, *J* = 5.8 Hz, 1H), 3.89 (s, 3H), 3.56 – 3.44 (m, 2H), 3.44 – 3.34 (m, 1H), 2.01 – 1.90 (m, 1H), 1.75 – 1.65 (m, 1H), 1.63 – 1.51 (m, 2H), 1.22 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.0, 167.6, 163.6, 134.7, 131.4, 130.7, 129.4, 128.6, 127.0, 113.9, 55.6, 40.0, 39.8, 30.6, 27.5, 18.2.

N-(6-(4-methoxyphenyl)-5-methyl-6-oxohexyl)benzamide (3u)



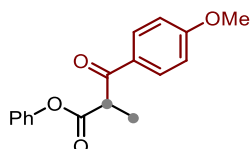
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 53.6 mg (79% yield) of **3u** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.9 Hz, 2H), 7.75 (d, *J* = 7.2 Hz, 2H), 7.49 – 7.43 (m, 1H), 7.42 – 7.35 (m, 2H), 6.92 (d, *J* = 8.9 Hz, 2H), 6.42 (t, *J* = 5.9 Hz, 1H), 3.85 (s,

3H), 3.47 – 3.35 (m, 3H), 1.91 – 1.80 (m, 1H), 1.64 – 1.53 (m, 2H), 1.51 – 1.43 (m, 1H), 1.42 – 1.31 (m, 2H), 1.17 (d, $J = 6.9$ Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 203.1, 167.6, 163.5, 134.8, 131.4, 130.6, 129.6, 128.6, 127.0, 113.9, 55.6, 40.2, 39.8, 33.2, 29.7, 24.8, 17.9.

Phenyl 3-(4-methoxyphenyl)-2-methyl-3-oxopropanoate (**3v**)



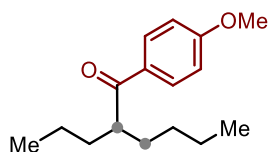
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 40.8 mg (72% yield) of **3v** as a yellow oil.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, $J = 8.9$ Hz, 2H), 7.34 (t, $J = 7.9$ Hz, 2H), 7.20 (t, $J = 7.4$ Hz, 1H), 7.00 (t, $J = 8.1$ Hz, 4H), 4.57 (q, $J = 7.1$ Hz, 1H), 3.89 (s, 3H), 1.61 (d, $J = 7.1$ Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 194.0, 169.8, 164.0, 150.5, 132.2, 131.1, 129.4, 128.5, 121.3, 114.1, 55.6, 48.2, 14.0.

HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{17}\text{O}_4^+$ [$\text{M}+\text{H}^+$] 284.3110, found 284.3117.

E-1-(4-methoxyphenyl)-2-propylhexan-1-one (**3w**)



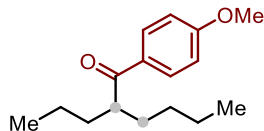
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 36.2 mg (73% yield) of **3w** as a white oil.

^1H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, $J = 8.9$ Hz, 2H), 6.94 (d, $J = 8.9$ Hz, 2H), 3.87 (s, 3H), 3.43 – 3.27 (m, 1H), 1.82 – 1.65 (m, 2H), 1.57 – 1.40 (m, 21H), 1.31 – 1.19 (m, 6H), 0.87 (t, $J = 5.0$ Hz, 3H), 0.84 (t, $J = 4.9$ Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 203.4, 163.3, 130.8, 130.4, 113.7, 55.4, 45.5, 35.0, 32.5, 29.9, 22.9, 20.9, 14.3, 13.9.

HRMS (ESI) m/z calcd for $C_{16}H_{25}O_2^+$ $[M+H]^+$ 249.1849, found 249.1847.

Z-1-(4-methoxyphenyl)-2-propylhexan-1-one (3x)



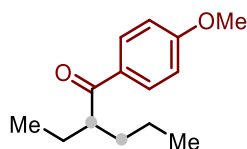
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 33.2 mg (67% yield) of **3x** as a white oil.

1H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 8.7 Hz, 2H), 6.94 (d, J = 8.7 Hz, 2H), 3.87 (s, 3H), 3.42 – 3.27 (m, 1H), 1.77 – 1.69 (m, 2H), 1.50 – 1.41 (m, 2H), 1.29 – 1.21 (m, 6H), 0.89 – 0.79 (m, 6H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 203.4, 163.3, 130.8, 130.4, 113.7, 55.4, 45.5, 35.0, 32.4, 29.8, 22.9, 20.8, 14.3, 13.9.

HRMS (ESI) m/z calcd for $C_{16}H_{25}O_2^+$ $[M+H]^+$ 249.1849, found 249.1853.

Z-2-ethyl-1-(4-methoxyphenyl)pentan-1-one (3y)



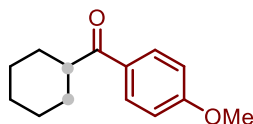
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 27.3 mg (62% yield) of **3y** as a yellow oil.

1H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.5 Hz, 2H), 6.94 (d, J = 8.6 Hz, 2H), 3.87 (s, 3H), 3.46 – 3.28 (m, 1H), 1.82 – 1.67 (m, 2H), 1.59 – 1.39 (m, 2H), 1.31 – 1.24 (m, 2H), 0.90 – 0.83 (m, 6H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 203.3, 163.3, 130.5, 130.4, 113.7, 55.4, 47.0, 34.5, 25.6, 20.8, 14.3, 12.0.

HRMS (ESI) m/z calcd for $C_{14}H_{21}O_2^+$ $[M+H]^+$ 221.1536, found 221.1535.

Cyclohexyl(4-methoxyphenyl)methanone (3z)



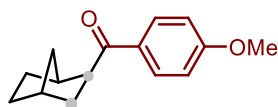
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 25.8 mg (59% yield) of **3z** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 3.22 (m, *J* = 11.2 Hz, 1H), 1.90 – 1.67 (m, 5H), 1.53 – 1.27 (m, 5H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.5, 163.2, 130.5, 129.2, 113.7, 55.4, 45.3, 29.5, 26.0, 25.9.

HRMS (ESI) *m/z* calcd for C₁₄H₁₉O₂⁺ [*M*+*H*⁺] 219.1380, found 219.1383.

((1*R*,2*R*,4*S*)-bicyclo[2.2.1]heptan-2-yl)(4-methoxyphenyl)methanone (3aa**)**



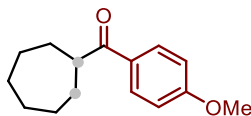
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 30.8 mg (67% yield) of **3aa** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H), 3.16 (dd, *J* = 8.7, 5.6 Hz, 1H), 2.50 (s, 1H), 2.33 (s, 1H), 2.04 – 1.98 (m, 1H), 1.64 – 1.58 (m, 2H), 1.50 – 1.41 (m, 3H), 1.34 – 1.29 (m, 1H), 1.14 (d, *J* = 9.7 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 200.1, 163.1, 130.6, 129.6, 113.6, 55.4, 49.2, 41.1, 36.2, 33.8, 29.8, 29.0.

HRMS (ESI) *m/z* calcd for C₁₅H₁₉O₂⁺ [*M*+*H*⁺] 231.1380, found 231.1389.

Cycloheptyl(4-methoxyphenyl)methanone (3ab**)**



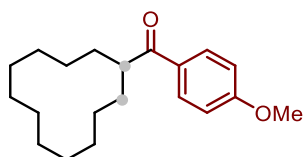
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 36.8 mg (79% yield) of **3ab** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H), 3.42 – 3.35 (m, 1H), 1.95 – 1.89 (m, 2H), 1.83 – 1.77 (m, 2H), 1.74 – 1.67 (m, 2H), 1.65 – 1.51 (m, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.0, 163.2, 130.5, 129.3, 113.7, 55.4, 46.3, 31.0, 28.3, 26.8.

HRMS (ESI) *m/z* calcd for C₁₅H₂₁O₂⁺ [*M*+*H*⁺] 233.1536, found 233.1538.

Cyclododecyl(4-methoxyphenyl)methanone (**3ac**)



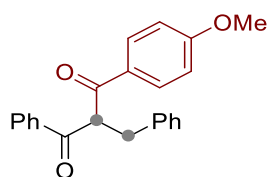
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 27.9 mg (46% yield) of **3ac** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 – 7.92 (m, 2H), 6.96 – 6.93 (m, 2H), 3.87 (s, 3H), 3.55 – 3.47 (m, 1H), 1.75 – 1.68 (m, 2H), 1.65 – 1.58 (m, 2H), 1.48 – 1.25 (m, 18H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.8, 163.2, 130.4, 130.0, 113.7, 55.4, 41.5, 26.7, 23.9, 23.5, 23.5, 22.6.

HRMS (ESI) *m/z* calcd for C₂₀H₃₁O₂⁺ [*M*+*H*⁺] 303.2319, found 303.2326.

2-benzyl-1-(4-methoxyphenyl)-3-phenylpropane-1,3-dione (**3ad**)



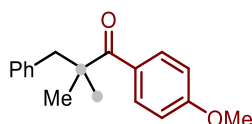
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 5/1) gave 46.8 mg (68% yield) of **3ad** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 7.94 (m, 4H), 7.55 (t, *J* = 6.7 Hz, 1H), 7.44 (t, *J* = 6.9 Hz, 2H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.31 (t, *J* = 6.9 Hz, 2H), 7.25 – 7.20 (m, 1H), 6.88 (d, *J* = 6.9 Hz, 2H), 5.30 (t, 1H), 4.20 (dd, *J* = 17.9, 10.0 Hz, 1H), 3.82 (s, 3H), 3.28 (dd, *J* = 17.9, 3.3 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 198.2, 197.3, 163.3, 139.2, 136.5, 133.2, 131.3, 129.3, 129.1, 128.5, 128.2, 127.2, 113.7, 55.4, 48.4, 43.8.

HRMS (ESI) m/z calcd for $C_{23}H_{21}O_3^+$ $[M+H]^+$ 345.1485, found 345.1482.

1-(4-methoxyphenyl)-2,2-dimethyl-3-phenylpropan-1-one (3ae)



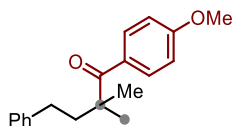
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 32.2 mg (60% yield) of **3ae** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, J = 8.7 Hz, 2H), 7.31 – 7.27 (m, 1H), 7.25 – 7.20 (m, 2H), 7.10 (d, J = 6.7 Hz, 2H), 6.92 (d, J = 8.7 Hz, 2H), 3.89 (s, 3H), 3.14 (s, 2H), 1.36 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 206.3, 161.8, 138.0, 131.0, 130.7, 130.4, 128.0, 126.3, 113.3, 55.4, 48.5, 46.6, 26.3.

HRMS (ESI) m/z calcd for $C_{18}H_{21}O_2^+$ $[M+H]^+$ 269.1536, found 269.1532.

1-(4-methoxyphenyl)-2-methyl-4-phenylbutan-1-one (3af)



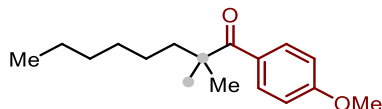
The general procedure was followed at rt for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 25.4 mg (45% yield) of **3af** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, J = 8.7 Hz, 2H), 7.26 – 7.21 (m, 2H), 7.17 (d, J = 7.1 Hz, 1H), 7.12 (d, J = 7.0 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 3.84 (s, 3H), 3.40 (h, J = 6.8 Hz, 1H), 2.64 – 2.57 (m, 2H), 2.20 – 2.08 (m, 1H), 1.76 – 1.67 (m, 1H), 1.19 (d, J = 6.8 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 202.8, 163.5, 142.0, 130.7, 129.7, 128.6, 128.5, 126.0, 113.9, 55.6, 39.4, 35.5, 33.7, 17.6.

HRMS (ESI) *m/z* calcd for C₁₉H₂₃O₂⁺ [M+H⁺] 283.1693, found 283.1691.

1-(4-methoxyphenyl)-2,2-dimethyloctan-1-one (3ag)



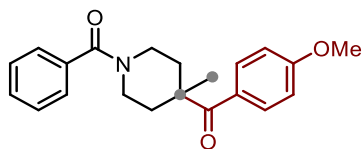
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 37.3 mg (71% yield) of **3ag** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 1.77 (t, 2H), 1.31 (s, 6H), 1.21 – 1.17 (m, 8H), 0.83 (t, *J* = 6.5 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 206.4, 161.9, 130.8, 130.5, 113.2, 55.3, 47.6, 41.5, 31.5, 29.9, 26.6, 24.7, 22.5, 14.0.

HRMS (ESI) *m/z* calcd for C₁₇H₂₇O₂⁺ [M+H⁺] 263.2006, found 263.2009.

(1-benzoyl-4-methylpiperidin-4-yl)(4-methoxyphenyl)methanone (3ah)



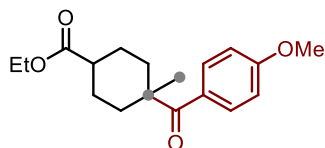
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 39.1 mg (58% yield) of **3ah** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.9 Hz, 2H), 7.40–7.32 (m, 5H), 6.90 (d, *J* = 9.0 Hz, 2H), 4.26–4.12 (m, 1H), 3.84 (s, 3H), 3.51 (q, *J* = 16.2, 12.6 Hz, 1H), 3.16 (t, *J* = 11.9 Hz, 2H), 2.50–2.24 (m, 2H), 1.82–1.60 (m, 1H), 1.49 (s, 4H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.3, 170.1, 163.9, 138.0, 131.1, 129.0, 128.6, 124.3, 119.9, 114.0, 55.6, 40.9, 37.9, 18.7.

HRMS (ESI) *m/z* calcd for C₂₁H₂₄NO₃⁺ [M+H⁺] 338.1756, found 338.1759.

Ethyl 4-(4-methoxybenzoyl)-4-methylcyclohexane-1-carboxylate (3ai)



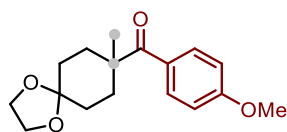
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 36.5 mg (60% yield) of **3ai** as a colorless oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 8.5 Hz, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 3.90 (s, 3H), 2.41 – 2.31 (m, 1H), 1.93 – 1.89 (m, 4H), 1.88 – 1.84 (m, 4H), 1.47 (s, 5H), 1.31 (t, *J* = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.9, 175.6, 161.9, 130.8, 130.4, 113.2, 60.1, 55.3, 47.8, 42.7, 36.2, 28.0, 26.0, 14.

HRMS (ESI) *m/z* calcd for C₁₈H₂₅O₄⁺ [*M*+*H*⁺] 305.1747, found 305.1745.

(4-methoxyphenyl)(8-methyl-1,4-dioxaspiro[4.5]decan-8-yl)methanone (**3aJ**)



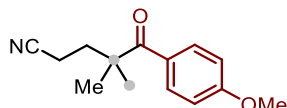
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 33.1 mg (57% yield) of **3aJ** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.81 (d, *J* = 8.9 Hz, 2H), 6.88 (d, *J* = 8.9 Hz, 2H), 3.91 (t, *J* = 2.8 Hz, 4H), 3.84 (s, 3H), 2.39 – 2.33 (m, 2H), 1.69 – 1.60 (m, 4H), 1.56 – 1.48 (m, 2H), 1.43 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.9, 161.9, 130.5, 113.2, 108.6, 100.0, 64.2, 55.4, 47.2, 34.0, 31.9, 25.8.

HRMS (ESI) *m/z* calcd for C₁₇H₂₃O₄⁺ [*M*+*H*⁺] 291.1591, found 291.1594.

5-(4-methoxyphenyl)-4,4-dimethyl-5-oxopentanenitrile (**3ak**)



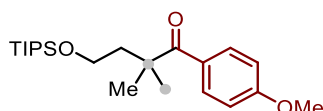
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 37.9 mg (82% yield) of **3ak** as a brown oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, J = 8.5 Hz, 2H), 7.04 (d, J = 8.6 Hz, 2H), 3.95 (s, 3H), 2.50 (t, J = 5.8 Hz, 2H), 1.85 (t, J = 6.9 Hz, 2H), 1.27 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 165.4, 162.2, 141.6, 128.6, 113.9, 110.0, 55.4, 44.4, 38.2, 28.0, 26.3.

HRMS (ESI) m/z calcd for C₁₄H₁₈NO₂⁺ [M+H⁺] 232.1332, found 232.1332.

1-(4-methoxyphenyl)-2,2-dimethyl-4-((triisopropylsilyl)oxy)butan-1-one (3al)



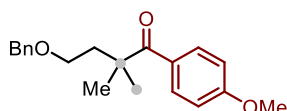
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 30/1) gave 54.5 mg (72% yield) of **3al** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, J = 8.3 Hz, 2H), 6.88 (d, J = 8.4 Hz, 2H), 3.84 (s, 3H), 3.66 (t, J = 7.2 Hz, 2H), 2.11 (t, J = 7.2 Hz, 2H), 1.35 (s, 6H), 0.98 (s, 21H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.4, 162.0, 130.8, 130.5, 113.2, 60.1, 55.3, 46.1, 43.9, 26.9, 17.9, 11.9.

HRMS (ESI) m/z calcd for C₂₂H₃₉O₃Si⁺ [M+H⁺] 379.2663, found 379.2666.

4-(benzyloxy)-1-(4-methoxyphenyl)-2,2-dimethylbutan-1-one (3am)



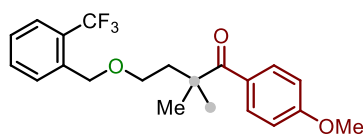
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 33.7 mg (54% yield) of **3am** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, J = 8.6 Hz, 2H), 7.34 – 7.20 (m, 5H), 6.89 (d, J = 8.6 Hz, 2H), 4.41 (s, 2H), 3.87 (s, 3H), 3.50 (t, J = 6.9 Hz, 2H), 2.19 (t, J = 6.9 Hz, 2H), 1.38 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.7, 161.9, 138.3, 130.7, 128.2, 127.5, 127.4, 113.2, 73.0, 67.1, 55.3, 46.2, 40.8, 26.8.

HRMS (ESI) m/z calcd for C₂₀H₂₅O₃⁺ [M+H⁺] 313.1798 found 313.1795.

1-(4-methoxyphenyl)-2,2-dimethyl-4-((2-(trifluoromethyl)benzyl)oxy)butan-1-one (3an)



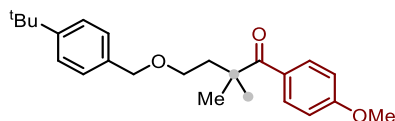
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 33.4 mg (44% yield) of **3an** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.79 (m, 2H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 3.6 Hz, 2H), 7.36 – 7.28 (m, 1H), 6.90 – 6.85 (m, 2H), 4.56 (s, 2H), 3.85 (s, 3H), 3.55 (t, *J* = 6.7 Hz, 2H), 2.21 (t, *J* = 6.7 Hz, 2H), 1.38 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.4, 161.9, 137.1, 131.8, 130.8, 130.5, 128.5, 127.0, 125.51 (q, *J* = 5.8 Hz), 113.20 (t, *J* = 6.5 Hz), 99.9, 68.7, 67.6, 55.37 (t, *J* = 8.2 Hz), 46.1, 40.8, 26.8.

HRMS (ESI) *m/z* calcd for C₂₁H₂₃F₃O₃⁺ [M+H⁺] 381.1672, found 381.1670.

4-((4-(tert-butyl)benzyl)oxy)-1-(4-methoxyphenyl)-2,2-dimethylbutan-1-one (3ao)



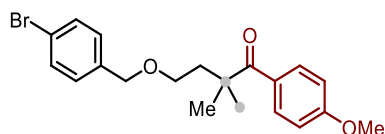
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 30.9 mg (42% yield) of **3ao** as a brown oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 4.35 (s, 2H), 3.85 (s, 3H), 3.47 (t, *J* = 7.0 Hz, 2H), 2.16 (t, *J* = 7.0 Hz, 2H), 1.36 (s, 6H), 1.30 (s, 12H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.7, 161.9, 150.4, 135.2, 130.7, 130.6, 127.4, 125.2, 113.2, 72.8, 67.0, 55.3, 46.2, 40.8, 34.5, 31.3, 26.8.

HRMS (ESI) *m/z* calcd for C₂₄H₃₃O₃⁺ [M+H⁺] 369.2424, found 369.2423.

4-((4-bromobenzyl)oxy)-1-(4-methoxyphenyl)-2,2-dimethylbutan-1-one (3ap)



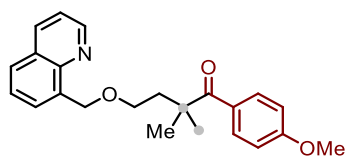
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 31.3 mg (40% yield) of **3ap** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 4.31 (s, 2H), 3.85 (s, 3H), 3.46 (t, *J* = 6.8 Hz, 2H), 2.16 (t, *J* = 6.9 Hz, 2H), 1.35 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 205.5, 161.9, 137.3, 131.3, 130.7, 130.6, 129.1, 121.2, 113.2, 72.2, 67.2, 55.4, 46.1, 40.9, 29.7, 26.9.

HRMS (ESI) *m/z* calcd for C₂₀H₂₄ Br O₃⁺ [M+H⁺] 391.0903, found 391.0906.

1-(4-methoxyphenyl)-2,2-dimethyl-4-(quinolin-8-ylmethoxy)butan-1-one (**3aq**)



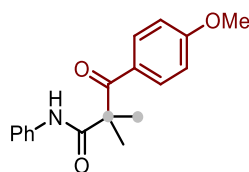
The general procedure was followed at 0 °C for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 26.9 mg (37% yield) of **3aq** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 9.03 (s, 1H), 8.17 (d, *J* = 25.5 Hz, 3H), 7.85 (d, *J* = 42.1 Hz, 2H), 7.51 (d, *J* = 29.9 Hz, 2H), 6.80 (s, 2H), 3.78 (s, 5H), 1.72 (t, 2H), 1.26 (t, 2H), 0.87 (d, *J* = 5.5 Hz, 3H), 0.83 (d, *J* = 5.3 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.1, 163.4, 150.1, 145.3, 135.5, 131.4, 128.7, 128.6, 128.5, 127.0, 121.5, 113.6, 69.0, 55.4, 38.8, 25.0, 22.7, 22.7.

HRMS (ESI) *m/z* calcd for C₂₃H₂₆NO₃⁺ [M+H⁺] 364.1907, found 364.1907.

3-(4-methoxyphenyl)-2,2-dimethyl-3-oxo-N-phenylpropanamide (**3ar**)



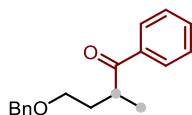
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 5/1) gave 44.6 mg (75% yield) of **3ar** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.9 Hz, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.25 (s, 1H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.82 (s, 3H), 1.60 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 199.0, 171.7, 163.4, 137.5, 131.5, 129.0, 127.9, 124.7, 120.0, 113.8, 55.5, 55.3, 24.5.

HRMS (ESI) *m/z* calcd for C₁₈H₂₀NO₃⁺ [*M*+*H*⁺] 298.1438, found 298.143.

4-(benzyloxy)-2-methyl-1-phenylbutan-1-one (**3as**)



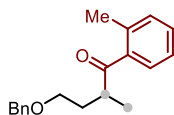
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 43.4 mg (81% yield) of **3as** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.89 (m, 2H), 7.51 – 7.45 (m, 1H), 7.40 – 7.35 (m, 2H), 7.23 – 7.17 (m, 5H), 4.36 (s, 2H), 3.73 – 3.64 (m, 1H), 3.51 – 3.45 (m, 1H), 3.42 – 3.36 (m, 1H), 2.15 – 2.07 (m, 1H), 1.71 – 1.62 (m, 1H), 1.13 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 204.3, 138.3, 136.6, 132.8, 128.6, 128.4, 128.3, 127.6, 127.5, 72.9, 67.9, 37.2, 33.6, 17.5.

HRMS (ESI) *m/z* calcd for C₁₈H₂₁O₂⁺ [*M*+*H*⁺] 269.1536, found 269.1538.

4-(benzyloxy)-2-methyl-1-(*o*-tolyl)butan-1-one (**3at**)



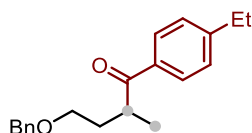
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 38.9 mg (69% yield) of **3at** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 7.6 Hz, 1H), 7.43 – 7.27 (m, 8H), 4.50 (s, 2H), 3.64 – 3.50 (m, 3H), 2.48 (s, 3H), 2.25 – 2.15 (m, 1H), 1.80 – 1.71 (m, 1H), 1.20 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 208.6, 138.6, 138.3, 137.8, 131.6, 130.8, 128.4, 128.0, 127.7, 127.6, 125.6, 73.0, 68.0, 40.6, 33.1, 20.8, 17.1.

HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{23}\text{O}_2^+$ $[M+H]^+$ 283.1693, found 283.1691.

4-(benzyloxy)-1-(4-ethylphenyl)-2-methylbutan-1-one (3au)



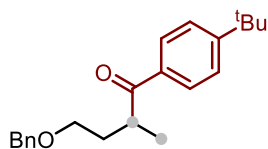
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 39.1 mg (66% yield) of **3au** as a yellow oil.

^1H NMR (400 MHz, Chloroform- d) δ 7.91 (d, J = 6.8 Hz, 2H), 7.32 – 7.22 (m, 7H), 4.43 (s, 2H), 3.80 – 3.66 (m, 1H), 3.58 – 3.49 (m, 1H), 3.49 – 3.40 (m, 1H), 2.70 (q, J = 7.3 Hz, 2H), 2.23 – 2.10 (m, 1H), 1.76 – 1.68 (m, 1H), 1.26 (t, J = 6.8 Hz, 3H), 1.18 (d, J = 5.4 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform- d) δ 204.0, 149.8, 138.4, 134.3, 128.6, 128.3, 128.1, 127.6, 127.5, 72.9, 68.0, 37.1, 33.7, 28.9, 17.6, 15.2.

HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{25}\text{O}_2^+$ $[M+H]^+$ 297.1849, found 297.1850.

4-(benzyloxy)-1-(4-(tert-butyl)phenyl)-2-methylbutan-1-one (3av)



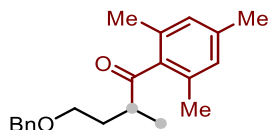
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 51.8 mg (80% yield) of **3av** as a white oil.

^1H NMR (400 MHz, Chloroform- d) δ 7.94 (d, J = 8.3 Hz, 2H), 7.47 (d, J = 8.3 Hz, 2H), 7.33 – 7.25 (m, 5H), 4.44 (s, 2H), 3.75 (m, J = 13.7, 6.9 Hz, 1H), 3.55 (m, J = 9.4, 6.1 Hz, 1H), 3.45 (m, J = 9.4, 6.6 Hz, 1H), 2.18 (m, J = 13.5, 6.9 Hz, 1H), 1.78 – 1.69 (m, 1H), 1.35 (s, 9H), 1.20 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform- d) δ 204.0, 156.6, 138.5, 134.0, 128.4, 128.4, 127.7, 127.6, 125.6, 73.0, 68.1, 37.2, 35.1, 33.7, 31.2, 17.7.

HRMS (ESI) m/z calcd for $C_{22}H_{29}O_2^+$ $[M+H]^+$ 325.2162, found 325.2165.

4-(benzyloxy)-1-mesityl-2-methylbutan-1-one (3aw)



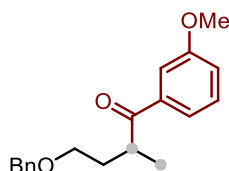
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 40.3 mg (65% yield) of **3aw** as a white solid.

1H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.27 (m, 5H), 6.83 (s, 2H), 4.47 (s, 2H), 3.56 (t, J = 6.0 Hz, 2H), 3.14 (m, J = 13.9, 7.0 Hz, 1H), 2.27 (s, 3H), 2.19 (s, 6H), 1.68 – 1.59 (m, 2H), 1.14 (d, J = 5.8 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 213.4, 138.7, 138.4, 133.5, 128.7, 128.3, 128.1, 127.6, 127.6, 72.9, 67.9, 44.2, 31.7, 21.0, 19.7, 15.6.

HRMS (ESI) m/z calcd for $C_{21}H_{27}O_2^+$ $[M+H]^+$ 311.2006, found 311.2002.

4-(benzyloxy)-1-(3-methoxyphenyl)-2-methylbutan-1-one (3ax)



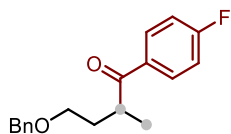
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 32.2 mg (54% yield) of **3ax** as a yellow oil.

1H NMR (400 MHz, Chloroform-*d*) δ 7.57 (d, J = 7.5 Hz, 1H), 7.50 (s, 1H), 7.39 – 7.26 (m, 6H), 7.10 (d, J = 8.2 Hz, 1H), 4.43 (s, 2H), 3.82 (s, 3H), 3.77 – 3.67 (m, 1H), 3.54 (m, J = 15.3, 6.1 Hz, 1H), 3.50 – 3.42 (m, 1H), 2.17 (m, J = 13.8, 6.8 Hz, 1H), 1.78 – 1.67 (m, 1H), 1.20 (d, J = 6.9 Hz, 3H).

^{13}C NMR (1004MHz, Chloroform-*d*) δ 204.1, 159.9, 138.3, 138.0, 129.5, 128.3, 127.6, 127.5, 120.9, 119.4, 112.6, 73.0, 67.9, 55.4, 37.4, 33.7, 17.5.

HRMS (ESI) m/z calcd for $C_{19}H_{23}O_3^+$ $[M+H]^+$ 299.1642, found 299.1647.

4-(benzyloxy)-1-(4-fluorophenyl)-2-methylbutan-1-one (3ay)



The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 28.1 mg (49% yield) of **3ay** as a white solid.

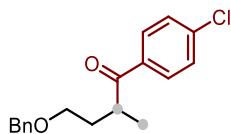
¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.97 (m, 2H), 7.33 – 7.27 (m, 4H), 7.24 (s, 1H), 7.10 (t, *J* = 8.4 Hz, 2H), 4.43 (s, 2H), 3.76 – 3.66 (m, 1H), 3.58 – 3.51 (m, 1H), 3.48 – 3.41 (m, 1H), 2.21 – 2.12 (m, 1H), 1.77 – 1.69 (m, 1H), 1.19 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.75 (s), 166.9, 138.3, 131.1, 131.0, 128.3, 127.6, 115.7, 115.5, 73.0, 67.8, 37.2, 33.7, 17.5.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -105.79 (s).

HRMS (ESI) *m/z* calcd for C₁₈H₂₀FO₂⁺ [*M*+*H*⁺] 287.1442, found 287.1446.

4-(benzyloxy)-1-(4-chlorophenyl)-2-methylbutan-1-one e (3az)



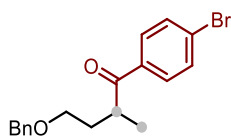
T The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 39.9 mg (66% yield) of **3az** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.6 Hz, 2H), 7.43 – 7.39 (m, 2H), 7.33 – 7.27 (m, 3H), 7.26 – 7.23 (m, 2H), 4.42 (s, 2H), 3.73 – 3.66 (m, 1H), 3.57 – 3.51 (m, 1H), 3.47 – 3.42 (m, 1H), 2.20 – 2.11 (m, 1H), 1.76 – 1.67 (m, 1H), 1.19 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.1, 139.2, 138.2, 134.9, 129.8, 128.9, 128.6, 128.3, 127.6, 73.0, 67.8, 37.3, 33.7, 17.4.

HRMS (ESI) *m/z* calcd for C₁₈H₂₀ClO₂⁺ [*M*+*H*⁺] 303.1146, found 303.1146.

4-(benzyloxy)-1-(4-bromophenyl)-2-methylbutan-1-one (3ba)



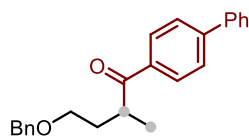
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 42.9 mg (62% yield) of **3ba** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.94 (m, 1H), 7.41 – 7.30 (m, 8H), 3.93 (s, 2H), 3.53 – 3.29 (m, 2H), 3.08 – 2.98 (m, 1H), 2.00 – 1.84 (m, 2H), 1.29 (d, *J* = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.1, 139.2, 138.2, 134.9, 129.9, 128.9, 128.6, 128.3, 127.6, 73.1, 67.8, 37.3, 33.7, 17.4.

HRMS (ESI) *m/z* calcd for C₁₈H₂₀BrO₂⁺ [*M*+*H*⁺] 347.0641, found 347.0643.

1-([1,1'-biphenyl]-4-yl)-4-(benzyloxy)-2-methylbutan-1-one (**3bb**)



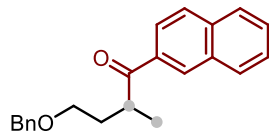
The general procedure was followed, DME was substituted for THF at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 52.2 mg (76% yield) of **3bb** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 7.1 Hz, 2H), 7.65 (dd, *J* = 14.6, 7.4 Hz, 4H), 7.48 (t, *J* = 7.0 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.27 (dd, *J* = 12.0, 4.5 Hz, 5H), 4.45 (s, 2H), 3.85 – 3.73 (m, 1H), 3.60 – 3.53 (m, 1H), 3.52 – 3.43 (m, 1H), 2.27 – 2.14 (m, 1H), 1.80 – 1.71 (m, 1H), 1.23 (d, *J* = 6.8 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 203.9, 145.5, 140.0, 138.4, 135.3, 129.0, 128.9, 128.3, 128.2, 127.6, 127.5, 127.2, 73.0, 68.0, 37.3, 33.7, 17.6.

HRMS (ESI) *m/z* calcd for C₂₄H₂₅O₂⁺ [*M*+*H*⁺] 345.1849, found 345.1849.

4-(benzyloxy)-2-methyl-1-(naphthalen-2-yl)butan-1-one (**3bc**)



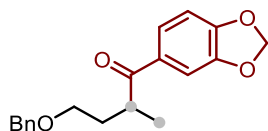
The general procedure was followed, DME was substituted for THF at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 52.8 mg (83% yield) of **3bc** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.60 – 8.56 (m, 1H), 8.12 – 8.07 (m, 1H), 7.96 – 7.90 (m, 3H), 7.68 – 7.55 (m, 2H), 7.30 (s, 5H), 4.48 (s, 2H), 4.04 – 3.95 (m, 1H), 3.67 – 3.61 (m, 1H), 3.57 – 3.50 (m, 1H), 2.34 – 2.23 (m, 1H), 1.89 – 1.80 (m, 1H), 1.31 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 204.3, 138.3, 135.5, 134.0, 132.6, 130.0, 129.6, 128.4, 128.3, 128.3, 127.7, 127.6, 127.5, 126.6, 124.3, 73.0, 68.0, 37.3, 33.9, 17.7.

HRMS (ESI) *m/z* calcd for C₂₂H₂₃O₂⁺ [*M*+H⁺] 319.1693, found 319.1692.

(1-(benzo[d][1,3]dioxol-5-yl)-4-(benzyloxy)-2-methylbutan-1-one (3bd)



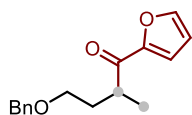
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 50.1 mg (80% yield) of **3bd** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.47 (d, *J* = 1.6 Hz, 1H), 7.33 – 7.27 (m, 5H), 6.83 (d, *J* = 8.2 Hz, 1H), 6.04 (s, 2H), 4.44 (s, 2H), 3.67 (m, *J* = 13.6, 6.9 Hz, 1H), 3.57 – 3.50 (m, 1H), 3.46 – 3.40 (m, 1H), 2.19 – 2.09 (m, 1H), 1.76 – 1.66 (m, 1H), 1.18 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.4, 151.6, 148.2, 138.4, 131.5, 128.3, 127.6, 127.5, 124.5, 108.3, 107.8, 101.8, 73.0, 68.0, 37.0, 33.9, 17.7.

HRMS (ESI) *m/z* calcd for C₁₉H₂₁O₄⁺ [*M*+H⁺] 313.1434, found 313.1433.

4-(benzyloxy)-1-(furan-2-yl)-2-methylbutan-1-one (3be)



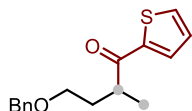
The general procedure was followed, without ligand addition at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 21.7 mg (42% yield) of **3be** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.59 (s, 1H), 7.38 – 7.25 (m, 5H), 7.21 (d, J = 3.4 Hz, 1H), 6.62 – 6.34 (m, 1H), 4.44 (s, 2H), 3.59 – 3.49 (m, 2H), 3.47 – 3.38 (m, 1H), 2.28 – 1.96 (m, 1H), 1.86 – 1.66 (m, 1H), 1.21 (d, J = 7.0 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 193.0, 152.4, 146.4, 138.3, 128.3, 127.6, 117.6, 112.1, 112.0, 72.9, 67.9, 38.3, 33.3, 17.3.

HRMS (ESI) m/z calcd for C₁₆H₁₉O₃⁺ [M+H⁺] 259.1329, found 259.1331.

4-(benzyloxy)-2-methyl-1-(thiophen-2-yl)butan-1-one (**3bf**)



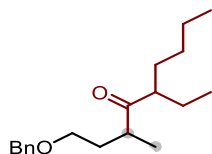
The general procedure was followed, without ligand addition at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 31.2 mg (57% yield) of **3bf** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, J = 3.5 Hz, 1H), 7.64 (d, J = 4.8 Hz, 1H), 7.34 – 7.25 (m, 5H), 7.12 (t, J = 4.3 Hz, 1H), 4.43 (s, 2H), 3.65 – 3.50 (m, 2H), 3.49 – 3.37 (m, 1H), 2.23 – 2.11 (m, 1H), 1.80 – 1.69 (m, 1H), 1.24 (d, J = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 197.2, 144.2, 138.3, 133.7, 131.9, 128.3, 128.1, 128.0, 127.6, 72.9, 67.9, 39.2, 33.9, 18.0.

HRMS (ESI) m/z calcd for C₁₆H₁₉O₂S⁺ [M+H⁺] 275.1100, found 275.1101.

1-(benzyloxy)-5-ethyl-3-methylnonan-4-one (**3bg**)



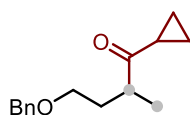
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 35.4 mg (61% yield) of **3bg** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.29 (m, 5H), 4.47 (s, 2H), 3.52 – 3.44 (m, 2H), 2.86 (dd, J = 13.9, 6.9 Hz, 1H), 2.55 – 2.39 (m, 1H), 2.07 – 1.96 (m, 1H), 1.70 – 1.61 (m, 2H), 1.57 – 1.51 (m, 1H), 1.39 – 1.27 (m, 4H), 1.24 – 1.16 (m, 2H), 1.05 (d, J = 7.0 Hz, 2H), 0.90 – 0.80 (m, 7H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 220.0, 128.3, 127.7, 127.6, 127.6, 73.0, 68.0, 52.3, 42.2, 32.3, 30.1, 29.7, 29.3, 22.9, 16.4, 13.9, 11.8.

HRMS (ESI) m/z calcd for C₁₉H₃₁O₂⁺ [M+H⁺] 291.2319, found 291.2317.

4-(benzyloxy)-1-cyclopropyl-2-methylbutan-1-one (3bh)



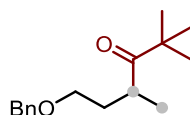
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 20/1) gave 35.3 mg (76% yield) of **3bh** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 (s, 5H), 4.49 (s, 2H), 3.53 – 3.43 (m, 2H), 2.96 – 2.85 (m, 1H), 2.13 – 2.03 (m, 1H), 1.71 – 1.60 (m, 2H), 1.14 (d, J = 7.0 Hz, 3H), 1.02 – 0.94 (m, 2H), 0.87 – 0.80 (m, 2H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 214.2, 138.4, 128.4, 127.7, 127.6, 73.0, 68.0, 43.7, 32.7, 19.4, 16.5, 10.8, 10.7.

HRMS (ESI) m/z calcd for C₁₅H₂₁O₂⁺ [M+H⁺] 233.1536, found 233.1536.

6-(benzyloxy)-2,2,4-trimethylhexan-3-one (3bi)



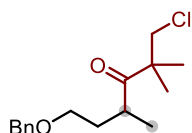
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 43.2 mg (87% yield) of **3bi** as a white oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, J = 8.1 Hz, 1H), 7.33 – 7.27 (m, 4H), 4.45 (d, J = 4.7 Hz, 2H), 3.49 – 3.41 (m, 1H), 3.37 – 3.23 (m, 2H), 2.01 – 1.91 (m, 1H), 1.65 – 1.55 (m, 1H), 1.14 (s, 9H), 1.04 (d, J = 6.8 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 219.7, 138.3, 128.4, 127.7, 127.6, 72.9, 68.1, 44.8, 36.2, 34.2, 26.1, 18.6.

HRMS (ESI) m/z calcd for C₁₆H₂₅O₂⁺ [M+H⁺] 249.1849, found 249.1848.

6-(benzyloxy)-1-chloro-2,2,4-trimethylhexan-3-one (3bJ)



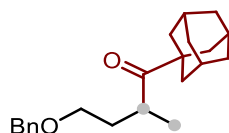
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 47.9 mg (85% yield) of **3bJ** as a brown oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.29 (m, 5H), 4.45 (d, J = 5.6 Hz, 2H), 3.67 – 3.57 (m, 2H), 3.50 – 3.43 (m, 1H), 3.42 – 3.35 (m, 1H), 3.24 (dd, J = 13.6, 6.8 Hz, 1H), 2.05 – 1.94 (m, 1H), 1.65 – 1.55 (m, 1H), 1.28 (s, 3H), 1.24 (s, 3H), 1.07 (d, J = 6.8 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 216.6, 138.2, 128.4, 127.7, 127.6, 72.9, 67.8, 51.8, 49.6, 36.9, 33.9, 22.5, 22.5, 18.1.

HRMS (ESI) m/z calcd for C₁₆H₂₄ClO₂⁺ [M+H⁺] 283.1459, found 283.1455.

1-((3R,5R)-adamantan-1-yl)-4-(benzyloxy)-2-methylbutan-1-one (3bk)



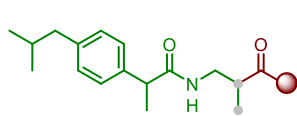
The general procedure was followed, DME was substituted for THF at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 50.8 mg (78% yield) of **3bk** as a brown solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.27 (m, 5H), 4.45 (s, 2H), 3.46 – 3.40 (m, 1H), 3.33 – 3.24 (m, 2H), 2.05 – 2.01 (m, 3H), 1.98 – 1.91 (m, 1H), 1.86 – 1.81 (m, 3H), 1.79 – 1.71 (m, 6H), 1.70 – 1.64 (m, 3H), 1.61 – 1.55 (m, 1H), 0.99 (d, J = 6.8 Hz, 3H).

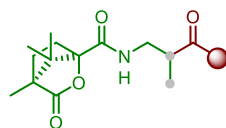
¹³C NMR (100 MHz, Chloroform-*d*) δ 219.2, 138.3, 128.4, 127.8, 127.6, 73.0, 68.2, 46.9, 37.7, 36.6, 35.4, 34.0, 27.9, 18.5.

HRMS (ESI) m/z calcd for $\text{C}_{22}\text{H}_{31}\text{O}_2^+$ $[\text{M}+\text{H}^+]$ 327.2319, found 327.2316.

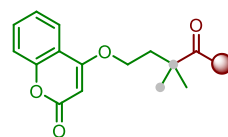
6. Modification of drug-relevant molecules



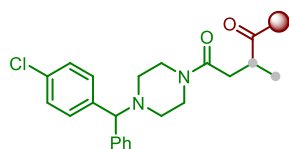
4a 72%
from *Ibuprofen* derivative



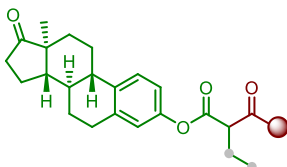
4b, 75%
from (1*S*)-(-)-*Camphanic acid* derivative



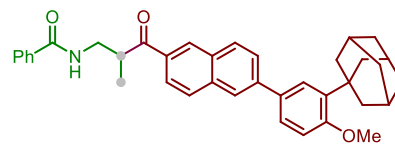
4c, 83%
from 4-Hydroxycoumarin derivative



4d, 52%, dr=1:1
from *Cetirizine* intermediate

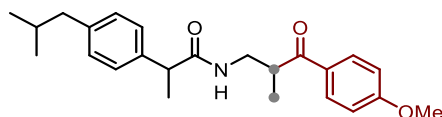


4e, 44%, dr=1:1
from *Estrone* intermediate



4f, 83%
from *Adapalene* derivative

2-(4-isobutylphenyl)-N-(3-(4-methoxyphenyl)-2-methyl-3-oxopropyl)propanamide (**4a**)



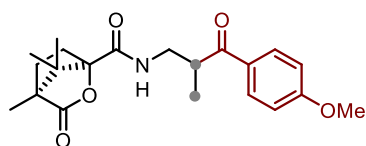
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 5/1) gave 64.8 mg (72% yield) of **4a** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.88 (dd, J = 24.0, 8.9 Hz, 2H), 7.12–7.08 (m, 1H), 7.06–6.98 (m, 2H), 6.95–6.90 (m, 3H), 5.97–5.83 (m, 1H), 3.85 (d, J = 6.6 Hz, 3H), 3.76–3.67 (m, 1H), 3.49–3.37 (m, 3H), 2.41 (d, J = 7.2 Hz, 1H), 2.35 (d, J = 7.2 Hz, 1H), 1.87–1.70 (m, 1H), 1.43 (dd, J = 8.0, 7.2 Hz, 3H), 1.08 (dd, J = 15.7, 7.1 Hz, 3H), 0.89–0.82 (m, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.2, 202.2, 174.9, 174.9, 163.8, 163.8, 140.7, 140.6, 138.6, 138.5, 130.9, 130.9, 129.7, 129.6, 129.1, 127.3, 127.2, 114.0, 113.9, 55.6, 55.6, 46.8, 46.8, 45.1, 45.1, 42.2, 42.2, 40.3, 40.2, 30.3, 30.2, 22.5, 18.4, 18.4, 16.0, 15.8.

HRMS (ESI) m/z calcd for $C_{24}H_{32}NO_3^+$ [$M+H^+$] 382.2377, found 382.2375.

(1*S*,4*S*)-N-(3-(4-methoxyphenyl)-2-methyl-3-oxopropyl)-4,7,7-trimethyl-3-oxo-2-oxabicyclo[2.2.1]heptane-1-carboxamide (**4b**)



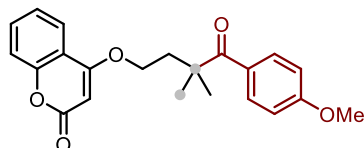
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 67.3 mg (75% yield) of **4b** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98–7.88 (m, 2H), 6.95–6.90 (m, 2H), 6.86 (q, *J* = 5.8 Hz, 1H), 3.85 (d, *J* = 1.8 Hz, 3H), 3.79–3.71 (m, 1H), 3.61–3.49 (m, 2H), 2.53–2.41 (m, 1H), 1.88–1.71 (m, 2H), 1.67–1.58 (m, 1H), 1.19 (d, *J* = 7.1 Hz, 3H), 1.08 (d, *J* = 7.1 Hz, 3H), 1.03 (d, *J* = 3.2 Hz, 3H), 0.88 (s, 1.5H), 0.64 (s, 1.5H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 201.2, 201.1, 178.2, 167.5, 167.4, 163.9, 163.8, 130.9, 130.8, 128.9, 128.9, 114.0, 92.5, 92.5, 55.6, 55.6, 55.3, 55.3, 53.9, 53.8, 41.7, 41.6, 40.5, 40.3, 30.4, 29.1, 16.9, 16.8, 16.7, 16.4, 16.1, 16.0, 9.8, 9.8.

HRMS (ESI) *m/z* calcd for C₂₁H₂₈NO₅⁺ [*M*+*H*⁺] 374.1962, found 374.1963.

4-((3,3-dimethyl-4-oxopentyl)oxy)-2H-chromen-2-one (**4c**)



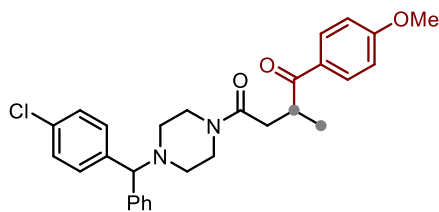
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 60.7 mg (83% yield) of **4c** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 8.9 Hz, 2H), 7.49 – 7.39 (m, 2H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 5.58 (s, 1H), 4.17 (t, *J* = 6.5 Hz, 2H), 3.83 (s, 3H), 2.41 (t, *J* = 6.5 Hz, 2H), 1.46 (s, 6H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 204.0, 165.3, 162.8, 162.4, 153.2, 132.2, 131.1, 129.5, 123.7, 123.1, 116.5, 115.5, 113.4, 90.5, 90.4, 66.3, 55.4, 55.4, 46.0, 39.6, 26.8, 26.8.

HRMS (ESI) *m/z* calcd for C₂₂H₂₃O₅⁺ [*M*+*H*⁺] 367.1540, found 367.1541.

4-(4-((4-chlorophenyl)(phenyl)methyl)piperazin-1-yl)-1-(4-methoxyphenyl)-2-methylbutane-1,4-dione (**4d**)



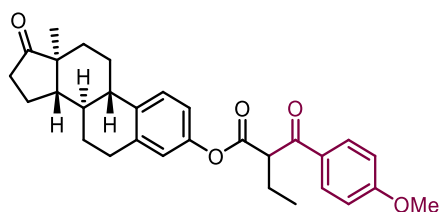
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 51.0 mg (52% yield) of **4d** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, *J* = 8.9 Hz, 2H), 7.38 (dd, *J* = 7.7, 3.0 Hz, 4H), 7.30 (dd, *J* = 16.6, 8.0 Hz, 4H), 7.23 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 8.9 Hz, 2H), 4.21 (d, *J* = 13.6 Hz, 1H), 4.14 – 4.00 (m, 1H), 3.87 (s, 3H), 3.63 – 3.50 (m, 4H), 3.06 (d, *J* = 9.1 Hz, 0.5H), 3.02 (d, *J* = 9.0 Hz, 0.5H), 2.43 – 2.30 (m, 5H), 1.21 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 202.4, 169.8, 163.4, 141.7, 140.9, 132.8, 130.9, 129.2, 129.1, 128.84, 128.78, 127.8, 127.4, 113.8, 75.2, 55.5, 51.9, 51.5, 45.5, 41.8, 36.9, 36.7, 18.3.

HRMS (ESI) *m/z* calcd for C₂₉H₃₂ClN₂O₃⁺ [*M*+*H*⁺] 491.2101, found 491.2101.

(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[*a*]phenanthren-3-yl 2-(4-methoxybenzoyl)butanoate (4e**)**



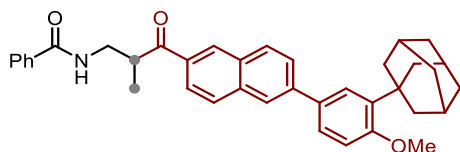
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 41.7 mg (44% yield) of **4e** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 8.9 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 1H), 7.04–6.99 (m, 2H), 6.83–6.75 (m, 2H), 4.45–4.41 (m, 1H), 3.93 (s, 3H), 2.95–2.87 (m, 2H), 2.57–2.55 (m, 1H), 2.45–2.38 (m, 1H), 2.33–2.25 (m, 1H), 2.22–2.11 (m, 3H), 2.07–1.97 (m, 2H), 1.67–1.61 (m, 2H), 1.59–1.53 (m, 2H), 1.51–1.45 (m, 2H), 1.33–1.27 (m, 1H), 1.12 (t, *J* = 7.4 Hz, 3H), 0.93 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 220.9, 193.5, 169.2, 164.0, 148.4, 138.1, 137.6, 131.1, 129.2, 126.4, 121.4, 118.5, 114.1, 55.6, 55.6, 50.4, 48.0, 44.2, 38.0, 35.9, 31.6, 29.4, 26.4, 25.8, 22.7, 21.6, 13.9, 12.3.

HRMS (ESI) *m/z* calcd for C₃₀H₃₅O₅⁺ [M+H⁺] 475.2479, found 475.2477.

***N*-(3-(6-(3-(adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)-2-methyl-3-oxopropyl)benzamide (4f)**



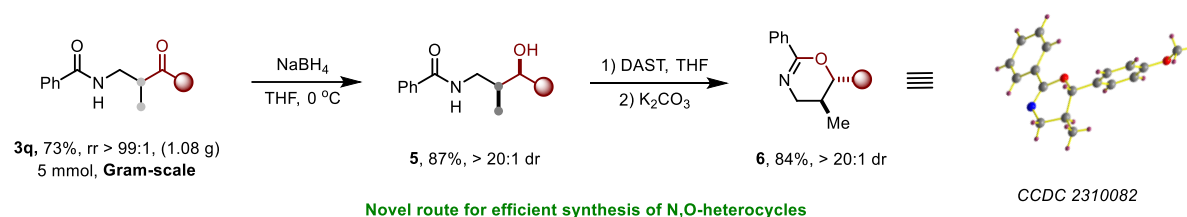
The general procedure was followed at rt for 18 h. Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 99.3 mg (83% yield) of **4f** as a yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (d, *J* = 1.8 Hz, 1H), 8.07–7.97 (m, 3H), 7.94 (d, *J* = 8.7 Hz, 1H), 7.81 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.75–7.71 (m, 2H), 7.60 (d, *J* = 2.4 Hz, 1H), 7.55 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.49–7.43 (m, 1H), 7.42–7.36 (m, 2H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.84 (t, *J* = 6.2 Hz, 1H), 4.15–4.06 (m, 1H), 3.90 (s, 3H), 3.89–3.84 (m, 1H), 3.81–3.72 (m, 1H), 2.20–2.16 (m, 6H), 2.13–2.08 (m, 3H), 1.82–1.78 (m, 6H), 1.36 (d, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 204.0, 167.8, 159.2, 142.0, 139.2, 136.3, 134.5, 132.8, 132.5, 131.6, 131.4, 130.4, 130.2, 128.9, 128.7, 127.0, 126.8, 126.1, 125.9, 124.8, 124.5, 112.3, 55.3, 42.3, 41.1, 40.7, 37.4, 37.3, 29.2, 16.4.

HRMS (ESI) *m/z* calcd for C₃₈H₄₀NO₃⁺ [M+H⁺] 558.3003, found 558.3002.

7. Gram-scale reaction and product derivatizations



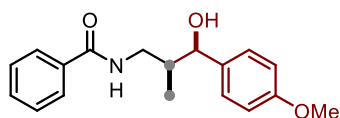
Gram-Scale Synthesis of 3q: In an argon-filled glovebox, $\text{NiBr}_2 \cdot \text{DME}$ (154 mg, 0.5 mmol, 10 mol%), Ligand (123.2 mg, 0.55 mmol, 11 mol%), relevant alkene substrate (805 mg, 5 mmol, 1.0 equiv), MeOLi (570 mg, 15 mmol, 3.0 equiv), THF (25 mL) were added to a 100 mL pressure flask. Then relevant acyl chlorides (1706 mg, 10 mmol, 2 equiv), $(\text{EtO})_3\text{SiH}$ (1850 μL , 10 mmol, 2 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The compound **3q** was isolated as a yellow oil (1.08 g, 73% yield, *rr* > 99:1) after chromatography on silica with ethyl acetate/petroleum ether (1/3).

Product Derivatizations Procedure for step 1 : In an argon atmosphere, sodium borohydride (3 equiv) and MeOH were added to a 50 mL pressure flask. Then the compound **3q** (1 equiv) were added to the mixture. The reaction mixture was stirred at rt for 5 h. After the reaction time, 1M HCl solution was added slowly under the ice bath. Then remove solvent under vacuum, and the resulting solution was extracted with CH_2Cl_2 (25 mL $\times$ 3). The combined organic extracts were then washed again with brine (10 mL), dried over Na_2SO_4 . Remaining liquid was removed solvent under vacuum and allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The compound **5** was isolated as a white solid. after chromatography on silica with ethyl acetate/petroleum ether (1:5).

Product Derivatizations Procedure for step 2: To a flame-dried flask was charged with a stir bar and the compound **5**. The flask was sealed, and then evacuated and back-filled with argon

(3 times). Then CH₂Cl₂ (50 mL) was added under argon. The flask was cooled to -78 °C in a dryice/acetone bath, and diethylaminosulfur trifluoride (3 equiv) was added dropwise. The reaction mixture was stirred for 1 h, then K₂CO₃ (4 equiv) was added slowly. The flask was removed from the cold bath and allowed to warm to room temperature. After the reaction time, water was added slowly to the mixture. The stirring was continued for an additional 1 h. Then the reaction mixture was diluted with CH₂Cl₂ (20 mL) and water (30 mL). The organic layer was washed with aqueous NaHCO₃ (20 mL). and brine (30 mL), dried over Na₂SO₄, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The compound **6** was isolated as a white solid. after chromatography on silica with ethyl acetate/petroleum ether (1:8).

***N*-((2*S*,3*R*)-3-hydroxy-3-(4-methoxyphenyl)-2-methylpropyl)benzamide (**5**)**



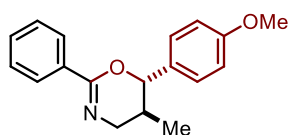
Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 52.1 mg (87% yield) of **5** as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.75–7.71 (m, 2H), 7.50–7.44 (m, 1H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.21 (d, *J* = 8.7 Hz, 2H), 7.15 (t, *J* = 5.9 Hz, 1H), 6.83 (d, *J* = 8.7 Hz, 2H), 4.76 (d, *J* = 3.6 Hz, 1H), 3.76 (s, 3H), 3.67 (s, 1H), 3.60–3.48 (m, 1H), 3.32 (dt, *J* = 13.8, 5.0 Hz, 1H), 2.13–1.99 (m, 1H), 0.80 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 168.4, 158.7, 134.7, 134.3, 131.6, 128.6, 127.2, 127.1, 113.6, 74.6, 55.3, 43.6, 40.2, 12.2.

HRMS (ESI) *m/z* calcd for C₁₈H₂₂NO₃⁺ [*M*+*H*⁺] 300.1594, found 300.1595.

(5*S*,6*S*)-6-(4-methoxyphenyl)-5-methyl-2-phenyl-5,6-dihydro-4*H*-1,3-oxazine (6**)**



Purification by column chromatography (petroleum ether/EtOAc = 10/1) gave 47.2 mg (84% yield) of **6** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, J = 8.0 Hz, 2H), 7.49–7.42 (m, 1H), 7.38 (t, J = 7.4 Hz, 2H), 7.36–7.28 (m, 2H), 6.98 (d, J = 8.7 Hz, 2H), 4.80 (dd, J = 9.9, 1.6 Hz, 1H), 3.88 (s, 3H), 3.75 (dd, J = 16.7, 4.8 Hz, 1H), 3.35 (dd, J = 17.4, 11.2 Hz, 1H), 2.16–2.00 (m, J = 6.1 Hz, 1H), 0.88 (d, J = 8.2 Hz, 3H).

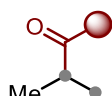
¹³C NMR (100 MHz, Chloroform-*d*) δ 159.8, 156.4, 133.8, 131.4, 130.5, 128.4, 128.2, 127.2, 114.0, 83.0, 55.4, 51.1, 33.0, 15.1.

HRMS (ESI) m/z calcd for C₁₈H₂₀NO₂⁺ [M+H⁺] 282.1489, found 282.1483.

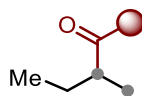
8. Hydrogenation of gaseous olefins



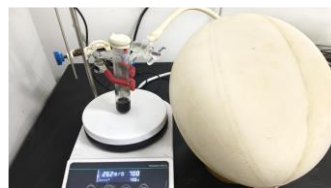
7a, 41%



7b, 62%, rr >99:1

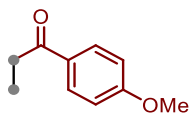


7c, 59%, rr >99:1



General procedure of upgrading gaseous olefins: In an argon-filled glovebox, NiBr₂•DME (0.02 mmol, 10 mol%), relevant ligand (0.022 mmol, 11 mol%), MeOLi (0.6 mmol, 3.0 equiv), THF (1 mL), **2a** (0.2 mmol, 1.0 equiv), (EtO)₃SiH (74 μL, 0.4 mmol, 2.0 equiv) were added to a 10 mL reaction flask. The flask moveout of the glove box. The reaction unit is connected to a balloon and replaced with gas. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent.

1-(4-methoxyphenyl)propan-1-one (**7a**)



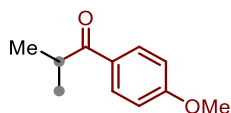
The general procedure was followed using the corresponding olefin (1 atm), **2a** (0.20 mmol) for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 13.5 mg (41% yield) of **7a** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 7.94 (m, 2H), 7.34 – 7.29 (m, 4H), 7.27 – 7.20 (m, 1H), 6.93 – 6.86 (m, 2H), 4.83 – 4.56 (m, 1H), 3.86 (d, *J* = 1.2 Hz, 3H), 1.56 (dd, *J* = 6.9, 1.1 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 199.0, 163.3, 142.1, 131.2, 129.6, 129.1, 127.8, 126.9, 113.8, 55.6, 47.7, 19.7.

HRMS (ESI) *m/z* calcd for C₁₀H₁₃O₂⁺ [*M*+*H*⁺] 165.0910, found 165.0912.

1-(4-methoxyphenyl)-2-methylpropan-1-one (**7b**)



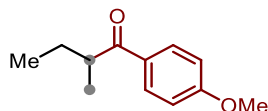
The general procedure was followed using the corresponding olefin (1 atm), **2a** (0.20 mmol) for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 22.1 mg (62% yield) of **7b** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 8.9 Hz, 2H), 6.94 (d, J = 8.9 Hz, 2H), 3.87 (s, 3H), 3.52 (hept, J = 6.8 Hz, 1H), 1.20 (d, J = 6.8 Hz, 6H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.2, 163.4, 130.7, 129.3, 113.9, 55.6, 35.1, 19.4.

HRMS (ESI) m/z calcd for C₁₁H₁₅O₂⁺ [M+H⁺] 179.1067, found 179.1064.

1-(4-methoxyphenyl)-2-methylbutan-1-one (7c)



The general procedure was followed using the corresponding olefin (1 atm), **2a** (0.20 mmol) for 18 h. Purification by column chromatography (Petroleum ether is used for column chromatography) gave 22.7 mg (59% yield) of **7c** as a yellow oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 8.6 Hz, 2H), 6.94 (d, J = 8.6 Hz, 2H), 3.87 (s, 3H), 3.35 (h, J = 6.7 Hz, 1H), 1.90 – 1.74 (m, 1H), 1.55 – 1.42 (m, 1H), 1.17 (d, J = 6.8 Hz, 3H), 0.90 (t, J = 7.4 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 203.1, 163.3, 130.5, 129.8, 113.7, 55.5, 41.7, 26.8, 17.0, 11.8.

HRMS (ESI) m/z calcd for C₁₂H₁₇O₂⁺ [M+H⁺] 193.1223, found 193.1224.

9. Mechanistic studies

9.1 Hydroacylation with various acyl electrophiles

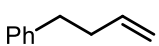
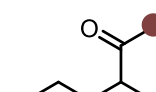
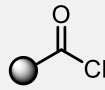
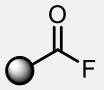
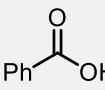
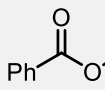
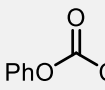
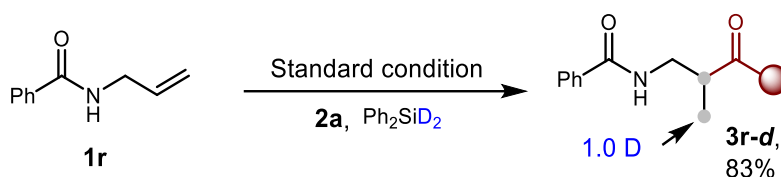
	Standard condition Acyl electrophiles			
1a			3a	
				
2a	2b'	2c'	2d'	2e'
Yield of 3a				
96%	0%	2%	0%	0%

Table S8. Hydroacylation with various acyl electrophiles

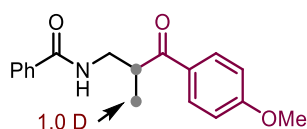
Standard condition: In an argon-filled glovebox, NiBr₂•DME (6.2 mg, 0.02 mmol, 10 mol%), L5 (0.022 mmol, 11 mol%), relevant alkene substrate (0.2 mmol, 1.0 equiv), MeOLi (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then relevant acyl compounds (0.4 mmol, 2.0 equiv), (EtO)₃SiH (74 μL, 0.4 mmol, 2.0 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h and yield and regio-isomeric ratio (rr) were determined by GC-MS.

9.2 Isotopic labeling experiment



Procedure: In an argon-filled glovebox, $\text{NiBr}_2 \cdot \text{DME}$ (6.2 mg, 0.02 mmol, 10 mol%), Ligand (5.6 mg, 0.022 mmol, 11 mol%), **1r** (32.2 mg, 0.2 mmol, 1.0 equiv), MeOLi (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then relevant acyl chlorides (68.2 mg, 0.4 mmol, 2 equiv), Ph_2SiD_2 (74 μL , 0.4 mmol, 2 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The conditions for flash chromatography and data for characterization of the products are listed below.

N-(3-(4-methoxyphenyl)-2-methyl-3-oxopropyl)benzamide (**3r-d**)



The title compound was isolated as a white solid after chromatography on silica with ethyl acetate/petroleum ether (1:8), gave 49.3 mg (83% yield) of **3r-d**.

^1H NMR (400 MHz, Chloroform- d) δ 8.01–7.92 (m, 2H), 7.82–7.75 (m, 2H), 7.47–7.42 (m, 1H), 7.40–7.34 (m, 2H), 6.96–6.87 (m, 2H), 5.72 (td, J = 7.4, 4.6 Hz, 1H), 3.82 (s, 3H), 1.97–1.92 (m, 1H), 1.68–1.62 (m, 1H), 1.37–1.35 (m, 1H), 1.25–1.23 (m, 1H), 0.82–0.78 (m, 2H)

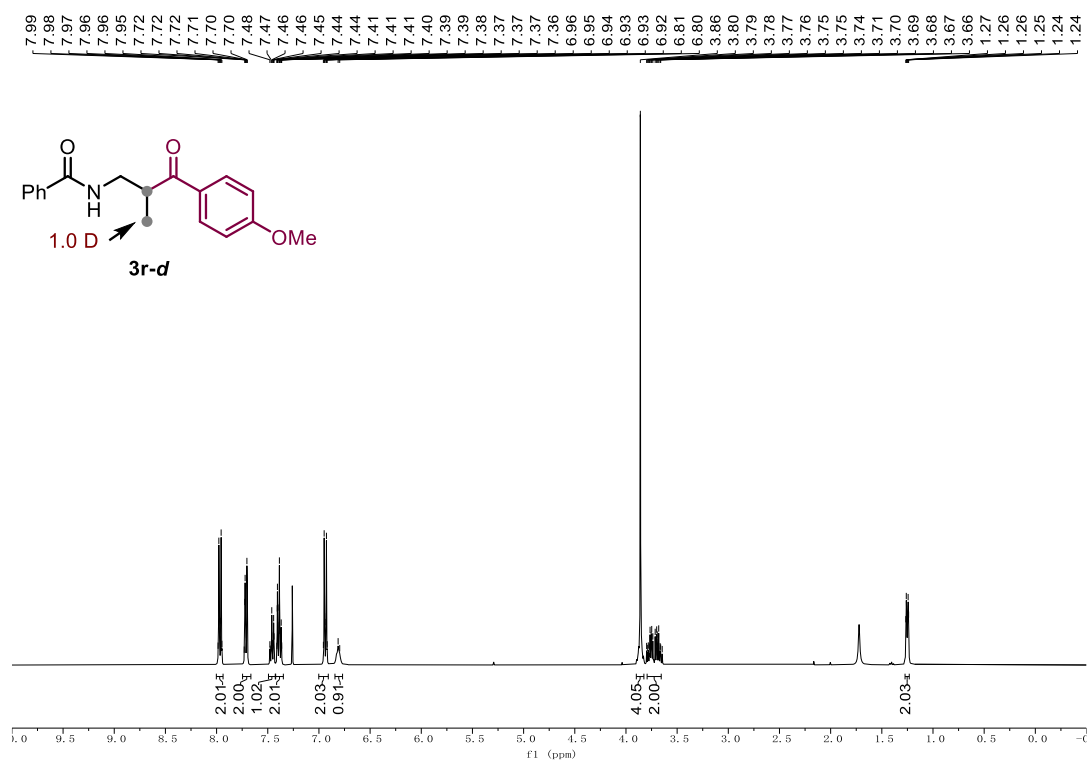
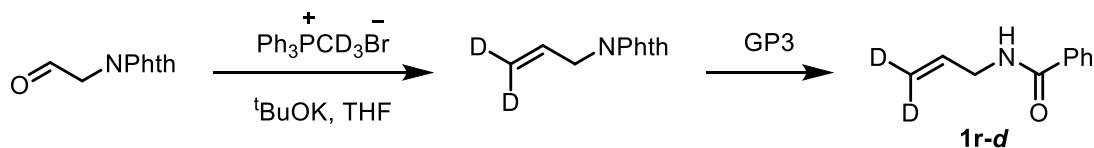
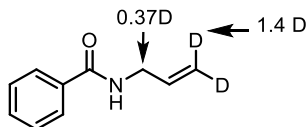


Figure S1. ^1H NMR (400 MHz, CDCl_3) spectra of **3r-d**



Procedure for synthesis **1r-d**'was according the report literature.^[3]

***N*-(allyl-3,3-d₂)benzamide (**1r-d**)**



The title compound was isolated as a yellow oil after chromatography on silica with ethyl acetate/petroleum ether (1:8).

^1H NMR (400 MHz, CDCl_3) δ 7.83–7.75 (m, 2H), 7.56–7.48 (m, 1H), 7.47–7.41 (m, 2H), 6.19 (s, 0.93H), 5.99–5.91 (m, 1H), 5.48–5.05 (m, 0.59H), 4.10 (t, J = 5.7 Hz, 1.63H).

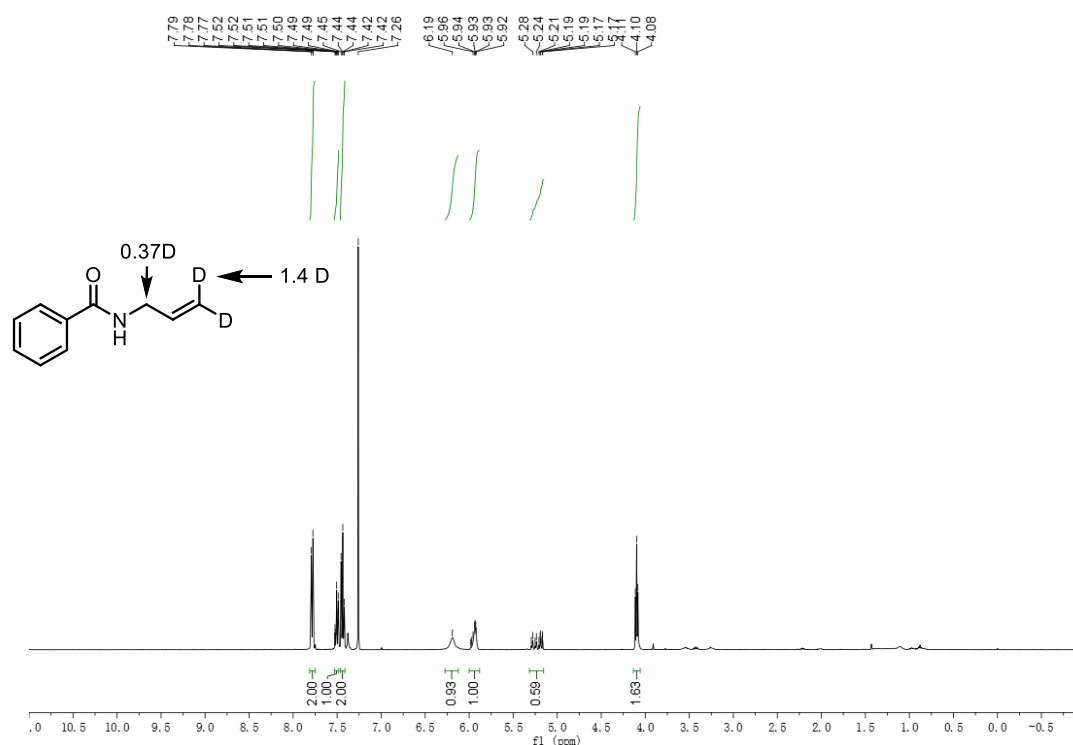
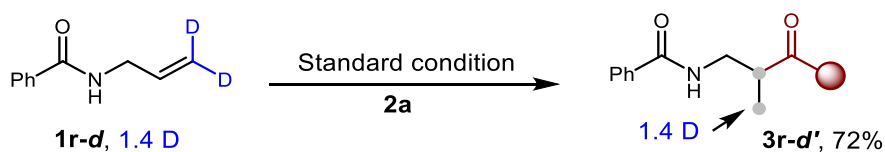
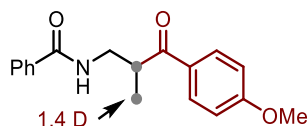


Figure S2. ^1H NMR (400 MHz, CDCl_3) spectra of **1r-d**



Procedure: In an argon-filled glovebox, $\text{NiBr}_2 \cdot \text{DME}$ (6.2 mg, 0.02 mmol, 10 mol%), Ligand (5.6 mg, 0.022 mmol, 11 mol%), deuterated alkene substrate (32.6 mg, 0.2 mmol, 1.0 equiv), MeOLi (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then relevant acyl chlorides (68.2 mg, 0.4 mmol, 2 equiv), $(\text{EtO})_3\text{SiH}$ (74 μL , 0.4 mmol, 2 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The conditions for flash chromatography and data for characterization of the products are listed below.

***N*-(3-(4-methoxyphenyl)-2-methyl-3-oxopropyl)benzamide (3r-d')**



The title compound was isolated as a white solid after chromatography on silica with ethyl acetate/petroleum ether (1:8), gave 50.5 mg (85% yield) of **3r-d'**.

¹H NMR (400 MHz, Chloroform-d) δ 7.90–7.88 (m, 2H), 7.65–7.63 (m, 2H), 7.41–7.35 (m, 1H), 7.38–7.30 (m, 2H), 6.88–6.82 (m, 2H), 6.81 (d, J = 6.3 Hz, 1H), 3.78 (s, 4H), 3.71–3.55 (m, 2H), 1.18 (t, J = 6.7 Hz, 2H).

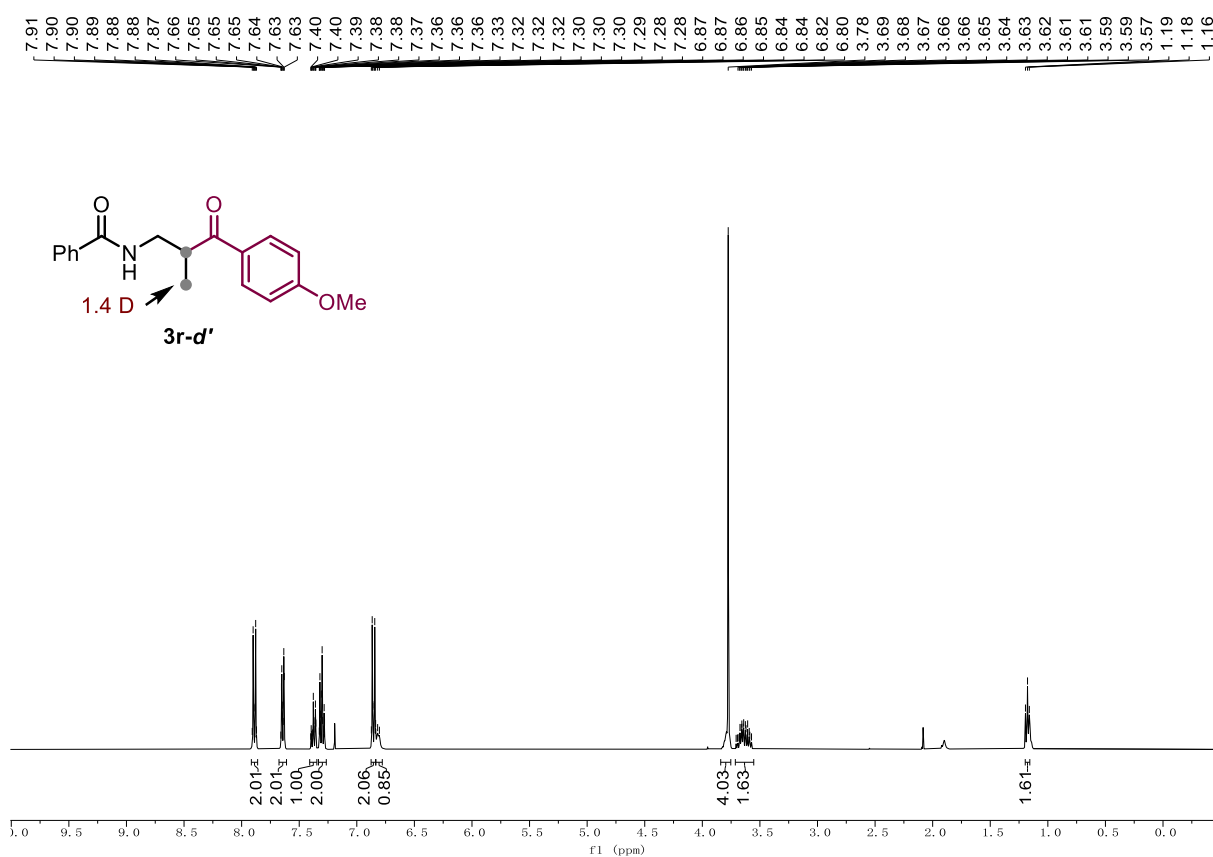
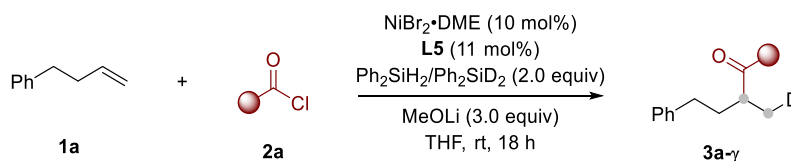


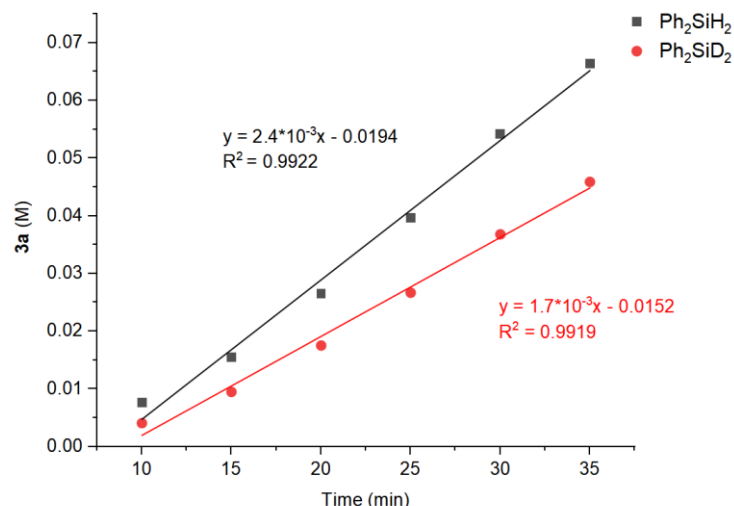
Figure S3. ¹H NMR (400 MHz, CDCl₃) spectra of **3r-d'**

9.3 Kinetic isotope effect for hydroacylation

KIEs with Ph₂SiD₂/Ph₂SiH₂ based on initial rates. ^[4]



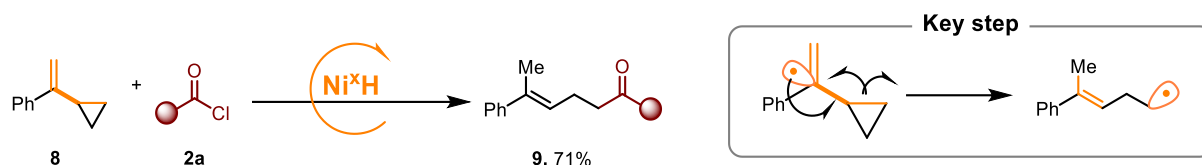
Procedure: According to General Procedure, NiBr₂·DME (6.2 mg, 0.02 mmol, 10 mol%), **L5** (5.6 mg, 0.022 mmol, 11 mol%), **1a** (0.2 mmol, 1.0 equiv), MeOLi (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then **2a** (68.2 mg, 0.4 mmol, 2 equiv) were used. Using Ph₂SiH₂ or Ph₂SiD₂ instead of (EtO)₃SiH. The reaction mixture was stirred at rt. The reaction samples were extracted at 10, 15, 20, 25, 30 and 35 minutes respectively and yields were determined by GC-MS. After that, the yield was converted into a concentration map.



Determination of the kinetic isotope effect of [Si]-H.

Comment: A linear trendline was drawn between 10-35 min of each reaction progress curve to obtain the initial rates of the reaction. Dividing the slope of the trendline for the reaction using Ph₂SiH₂ by the slope of the trendline for the reaction using Ph₂SiD₂ gave $K_H/K_D = 2.4/1.7 = 1.41$.

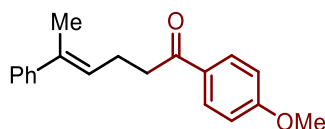
9.4 Evidence for radical intermediates



Procedure for synthesis **8** was according the report literature.^[5]

Procedure: In an argon-filled glovebox, $\text{NiBr}_2\cdot\text{DME}$ (6.2 mg, 0.02 mmol, 10 mol%), **L5** (5.6 mg, 0.022 mmol, 11 mol%), relevant alkene substrate (0.2 mmol, 1.0 equiv), MeOLi (22.8 mg, 0.6 mmol, 3.0 equiv), THF (1 mL) were added to a 4 mL reaction flask. Then **2a** (68.2 mg, 0.4 mmol, 2.0 equiv), $(\text{EtO})_3\text{SiH}$ (74 μL , 0.4 mmol, 2 equiv) were added to the mixture. The reaction mixture was stirred at rt for 18 h. After the reaction time, remove solvent under vacuum. Remaining liquid was allowed to silica gel column chromatography. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and petroleum ether as eluent. The conditions for flash chromatography and data for characterization of the products are listed below.

(E)-1-(4-methoxyphenyl)-5-phenylhex-4-en-1-one (**9**)



Purification by column chromatography (petroleum ether/ EtOAc = 10/1) gave 39.8 mg (71% yield) of **9** as a colorless oil.

^1H NMR (400 MHz, $\text{Chloroform-}d$) δ 7.97 (d, J = 8.7 Hz, 2H), 7.37 (d, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.25 – 7.18 (m, 1H), 6.94 (d, J = 8.7 Hz, 2H), 5.82 (t, J = 7.2 Hz, 1H), 3.87 (s, 3H), 3.08 (t, J = 7.5 Hz, 2H), 2.64 (q, J = 7.4 Hz, 2H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, $\text{Chloroform-}d$) δ 198.3, 163.4, 143.7, 135.8, 130.3, 128.1, 126.8, 126.6, 125.6, 113.9, 113.7, 55.5, 38.0, 23.7, 15.8.

HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{21}\text{O}_2^+$ $[\text{M}+\text{H}^+]$ 281.1536, found 281.1536

10. X-ray crystallographic data

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **6** in a mixture of petroleum ether and Tetrahydrofuran at room temperature. X-Ray structural analysis of single crystal was obtained to confirm the absolute configuration. The X-ray data of single crystal is deposited in the Cambridge Crystallographic Data Centre with a number of **CCDC 2310082**.

Crystal Data for $C_{18}H_{19}NO_2$ ($M = 281.34$ g/mol): monoclinic, space group P21/c (no. 14), $a = 20.8991(8)$ Å, $b = 5.68754(17)$ Å, $c = 13.0519(4)$ Å, $\beta = 103.846(3)^\circ$, $V = 1506.32(9)$ Å³, $Z = 4$, $T = 296.00(10)$ K, $\mu(\text{CuK}\alpha) = 0.640$ mm⁻¹, $D_{\text{calc}} = 1.241$ g/cm³, 4818 reflections measured ($4.354^\circ \leq 2\theta \leq 134.146^\circ$), 2686 unique ($R_{\text{int}} = 0.0245$, $R_{\text{sigma}} = 0.0307$) which were used in all calculations. The final R_1 was 0.0427 ($I > 2\sigma(I)$) and wR_2 was 0.1176 (all data).

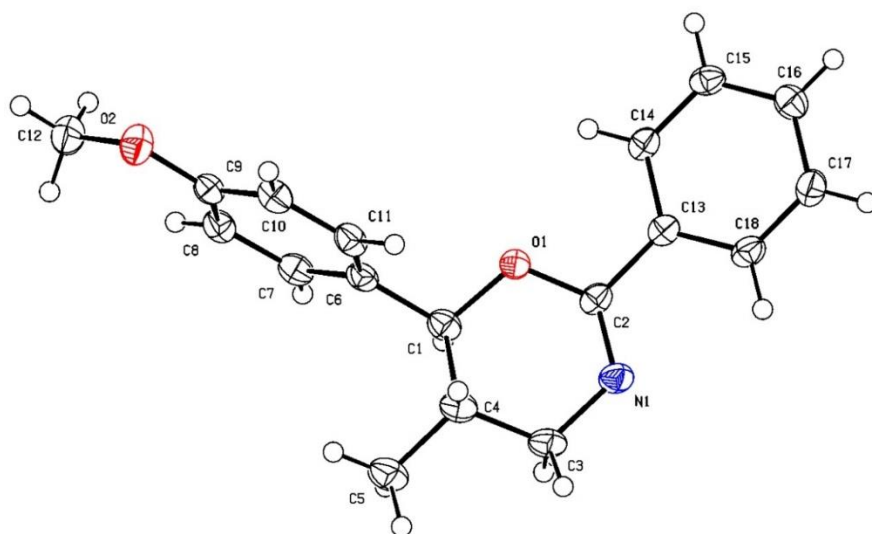


Figure S4. X-ray structure of compound **6** (The thermal ellipsoid was drawn at the 50% probability level).

Table S9 Crystal data and structure refinement for compound 6.

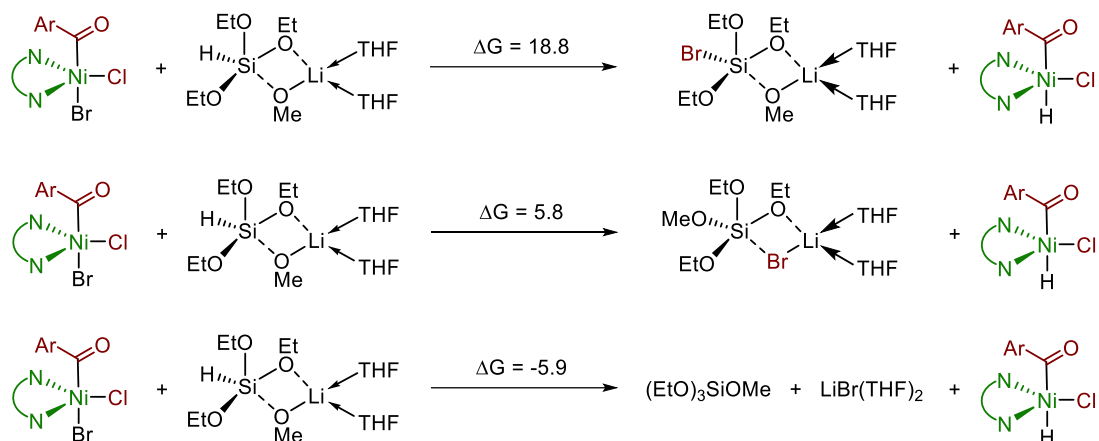
Identification code	3u'
Empirical formula	C ₁₃ H ₁₅ NO
Formula weight	281.34
Temperature/K	296.00(10)
Crystal system	monoclinic
Space group	P21/c
a/Å	20.8991(8)
b/Å	5.68754(17)
c/Å	13.0519(4)
α /°	90
β /°	103.846(3)
γ /°	90
Volume/Å ³	1506.32(9)
Z	4
ρ_{calc} /cm ³	1.241
μ /mm ⁻¹	0.640
F(000)	600.0
Crystal size/mm ³	0.25 × 0.23 × 0.22
Radiation	GaK α (λ = 1.54184)
2 θ range for data collection/°	4.354 to 134.146
Index ranges	-24 ≤ h ≤ 24, -6 ≤ k ≤ 4, -13 ≤ l ≤ 15
Reflections collected	4818
Independent reflections	2686 [R _{int} = 0.0245, R _{sigma} = 0.0307]
Data/restraints/parameters	2686/0/193
Goodness-of-fit on F ²	1.080
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0427, wR ₂ = 0.1113
Final R indexes [all data]	R ₁ = 0.0478, wR ₂ = 0.1176
Largest diff. peak/hole / e Å ⁻³	0.26/-0.25

11. DFT calculations

11.1 Computational Details

All the calculations were performed using Gaussian 09 package.^[6] The geometry optimizations were carried out using (u)B3LYP-D3(BJ)^[7] functional with a mixed basis set: SDD for Ni, Br, and Cl, and 6-31G(*d*) for all other atoms. Frequencies were computed analytically at the same level of theory to confirm whether the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Selected transition-state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations.^[8] To obtain better accuracy, solution-phase single-point energies for the optimized geometries were recalculated using (u)TPSS-D3(BJ)^[9] functional with a larger basis set of def2-TZVPP.^[10] Solvation effects (solvent=THF) were taken into account by performing single-point calculations with the SMD model.^[11] The final free energies reported in the article are the large basis set single-point energies corrected by gas-phase Gibbs free energy correction (at 298.15 K). The 3D diagrams of molecules were generated using CYLView.^[12]

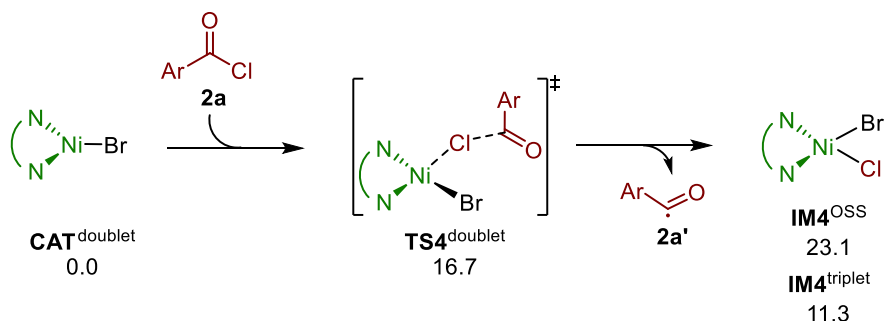
11.2 Formation of Ni-H species



Scheme S1. Gibbs free energy of the formation of the Ni-H species. The energies are given in kcal/mol.

11.3 C-Cl bond cleavage via halogen-atom abstraction

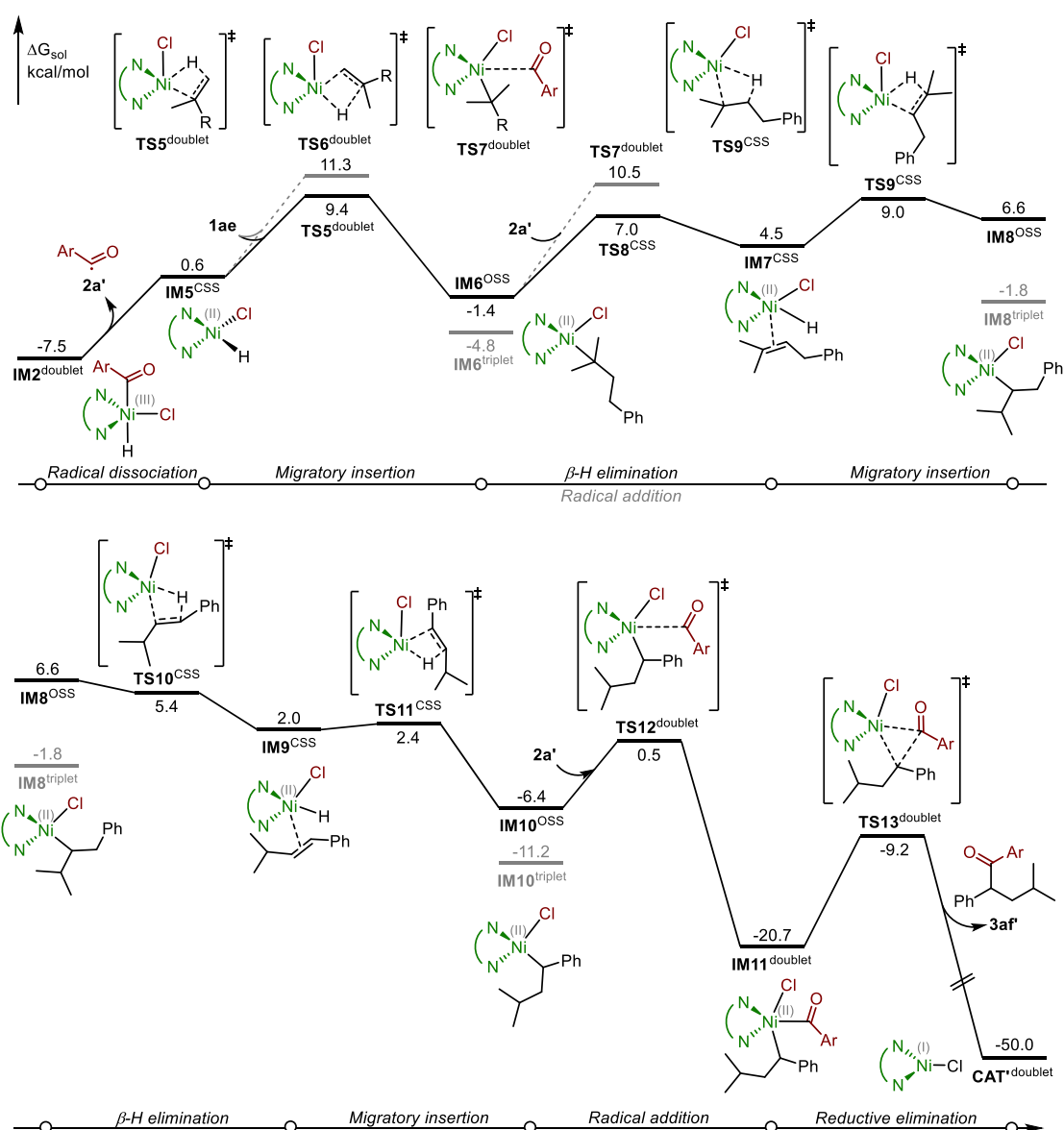
The C-Cl bond cleavage via the halogen-atom abstraction was found to occur via transition state **TS4**^{doublet}, which is 10.2 kcal/mol higher in energy compared with the three-membered transition state **TS1**^{doublet}.



Scheme S2. C-Cl bond cleavage via the halogen-atom abstraction transition state. The energies are given in kcal/mol.

11.4 Formation of remote hydroacylation product

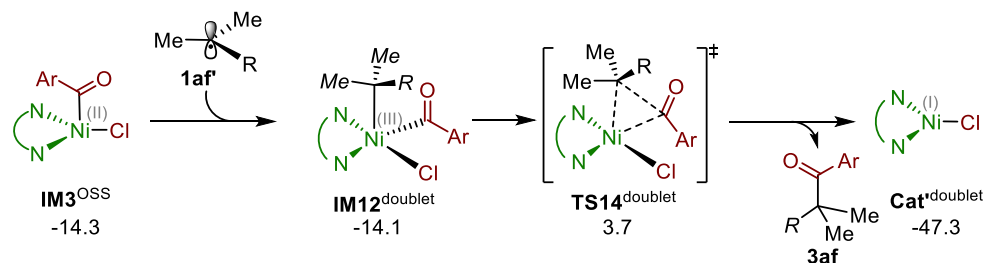
The dissociation of the acyl radical from the Ni(III) center is required to form a Ni(II)-H intermediate. Subsequently, the Ni-H intermediate undergoes migratory insertion with substrate **1af** to form **IM6^{OSS}**, which then undergoes chain walking to generate **IM10^{OSS}**. The ensuing direct addition of radical **2a'** to the Ni center of **IM10^{OSS}** via transition state **TS12^{doublet}**, results in the formation of Ni(III) intermediate **IM11^{doublet}**. Finally, the catalytic cycle is closed by reductive elimination through transition state **TS13^{doublet}**, giving rise to the remote hydroacylation product, along with the Ni(I) species **CAT^{doublet}**. To be noted, the migratory insertion via **TS5^{doublet}** was found to be higher than the HAT step via **TS2^{doublet}** by as much as 7.0 kcal/mol, thus ruling out this possibility.



Scheme S3. The Gibbs free energy surface for the formation of remote hydroacylation product via chain transfer of the Ni(II)-H species.

11.5 C-C bond formation via radical addition/C-C reductive elimination

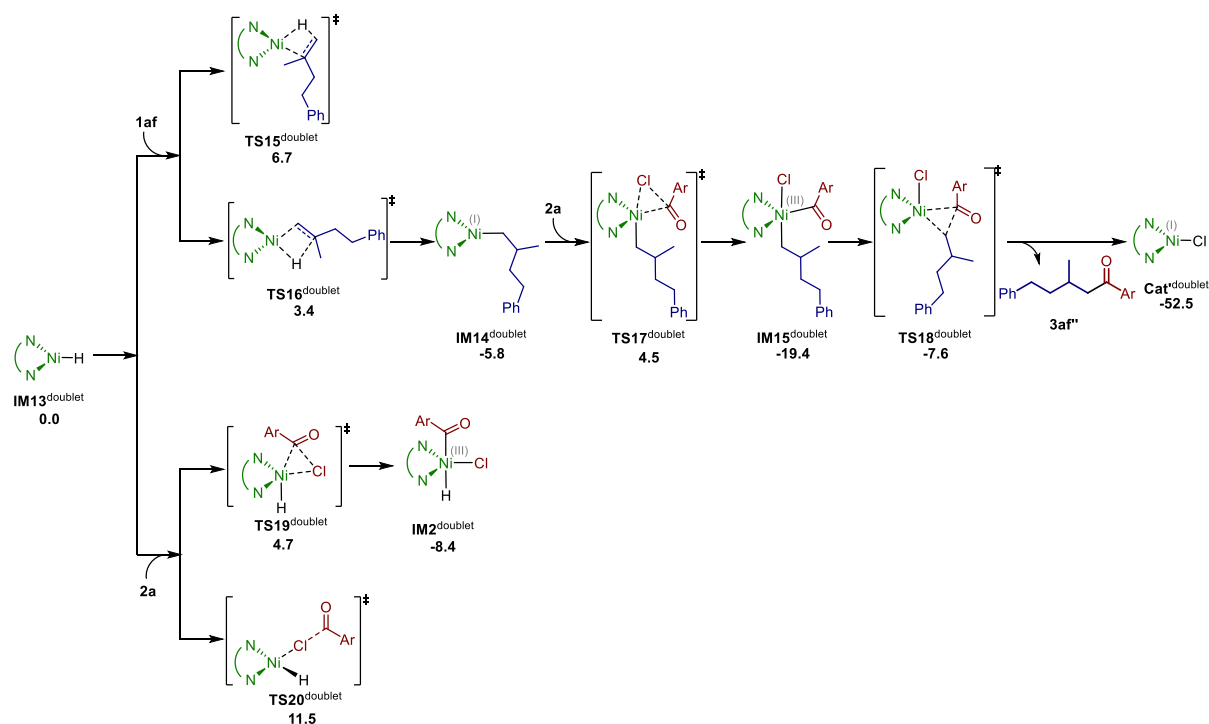
The C-C bond formation via the radical addition to the Ni(II) center followed by the C-C reductive elimination, was also explored but was calculated to be kinetically less favorable than the direct outer-sphere reductive elimination.



Scheme S4. C-C bond formation via radical addition/C-C reductive elimination. The energies are given in kcal/mol.

11.6 The catalytic pathway involving Ni(I)-H

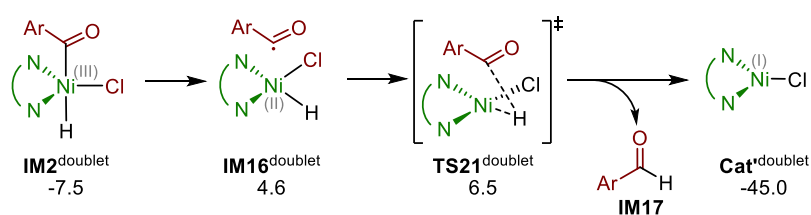
The Ni(I)-H intermediate undergoes a 2,1-migratory insertion with alkene **1af** through transition state **TS16**^{doublet}, forming intermediate **IM14**^{doublet}. The energy of the 1,2-migratory insertion transition state **TS15**^{doublet} is 3.3 kcal/mol higher than that of **TS16**^{doublet}. Subsequently, intermediate **IM14**^{doublet} undergoes oxidative addition with substrate **2a** via transition state **TS17**^{doublet}, leading to the formation of intermediate **IM15**^{doublet}. Finally, the terminal carbon-functionalized product is generated through transition state **TS18**^{doublet}, accompanied by the formation of a Ni(I)-Cl species, thereby completing the catalytic cycle. Additionally, the transition states for the two-electron oxidative addition transition state **TS19**^{doublet} of the Ni(I)-H intermediate with substrate **2a** and the chlorine atom transfer transition state **TS20**^{doublet} were calculated, with energy barriers of 4.7 kcal/mol and 11.5 kcal/mol, respectively. These results indicate that the Ni(I)-H intermediate is more likely to promote the formation of terminal carbon-functionalized products, which is inconsistent with the experimental observations.



Scheme S5. Catalytic pathway involving Ni(I)-H intermediate.

Furthermore, our calculations show that the reductive elimination to form the aldehyde proceeds via transition state TS21^{doublet}, which is approximately 4 kcal/mol higher in energy than the hydrogen atom transfer via TS2^{doublet}. Consequently, only a small amount of aldehyde was observed in the experiments.

11.7 Potential for Reductive Elimination to Form Aldehyde



Scheme S6. Reductive elimination from IM2^{doublet} to form aldehyde. The energies are given in kcal/mol.

11.6 Table of Calculated Energies and Energy Corrections

Stationary point	Single-point energy- (u)TPSS-D3(BJ)-SMD def2- TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1af	-427.861672	0.181135
1af	-428.434507	0.188406
2a	-920.043879	0.097883
2a'	-459.735780	0.096427
3af	-888.279084	0.315722
3af	-888.284539	0.316841
3af'	-888.286357	0.315978
Cat ^{doublet}	-4885.779037	0.206088
Cat ^{doublet}	-2771.946889	0.20715
LiBr(THF) ₂	-3046.937199	0.196046
(EtO) ₃ SiOMe	-868.541796	0.211485
[Si]-H	-1341.947788	0.448056
IM1 ^{doublet}	-5805.848878	0.327364
IM2 ^{doublet}	-3232.296409	0.337167
IM3 ^{OSS}	-3231.733079	0.328663
IM4 ^{OSS}	-5345.842782	0.204439
IM4 ^{triplet}	-5345.861617	0.203272
IM5 ^{OSS}	-2772.525064	0.218107
IM6 ^{OSS}	-3200.413071	0.422448
IM6 ^{triplet}	-3200.418678	0.422691
IM7 ^{OSS}	-3200.406301	0.425115
IM8 ^{OSS}	-3200.403062	0.425183
IM8 ^{triplet}	-3200.415076	0.423795
IM9 ^{OSS}	-3200.412140	0.426883
IM10 ^{OSS}	-3200.424678	0.426034
IM10 ^{triplet}	-3200.431603	0.425383
IM11 ^{doublet}	-3660.211623	0.550933
IM12 ^{doublet}	-3660.197583	0.547417
IM13 ^{doublet}	-2312.212803	0.212912
IM14 ^{doublet}	-2740.118043	0.428359
IM15 ^{doublet}	-3660.205278	0.547928
IM16 ^{doublet}	-3232.277669	0.337744
IM17	-460.388661	0.109416
TS1 ^{doublet}	-5805.834934	0.326404
TS2 ^{doublet}	-3660.163892	0.539959
TS2 ^{doublet}	-3660.156265	0.537763
TS3 ^{doublet}	-3660.175478	0.544421
TS4 ^{doublet}	-5805.817919	0.325511

TS5 ^{CSS}	-3200.397581	0.424123
TS6 ^{CSS}	-3200.393775	0.423369
TS7 ^{doublet}	-3660.152907	0.541814
TS8 ^{OSS}	-3200.399347	0.42213
TS9 ^{CSS}	-3200.395593	0.421473
TS10 ^{CSS}	-3200.401200	0.42137
TS11 ^{CSS}	-3200.406139	0.421603
TS12 ^{doublet}	-3660.171516	0.544523
TS13 ^{doublet}	-3660.191783	0.549344
TS14 ^{doublet}	-3660.171453	0.549543
TS15 ^{doublet}	-2740.092887	0.423192
TS16 ^{doublet}	-2740.099107	0.424061
TS17 ^{doublet}	-3660.163329	0.544139
TS18 ^{doublet}	-3660.185686	0.547215
TS19 ^{doublet}	-3232.272415	0.333983
TS20 ^{doublet}	-3232.261082	0.333442
TS21 ^{doublet}	-3232.274544	0.337631

11.7 Cartesian coordinates

1af

C	-2.53184300	1.68042200	0.28892000
H	-2.23599100	0.64364700	0.42939300
H	-2.22860300	2.15125600	-0.64298100
C	-3.23544200	2.33961200	1.21460400
C	-3.64587800	1.68021400	2.51085300
H	-3.43442700	0.60579200	2.46716300
H	-4.73108100	1.78294600	2.65572200
C	-2.93603900	2.27201600	3.75273500
H	-3.16296400	3.34148000	3.83081200
H	-1.85236700	2.18583200	3.60814200
C	-3.35163500	1.57098900	5.02374300
C	-2.69373000	0.40943200	5.44735600
C	-4.43638700	2.03545100	5.77774900
C	-3.10603800	-0.27006800	6.59359600
H	-1.84760200	0.03862100	4.87308400
C	-4.85336300	1.36002600	6.92515200
H	-4.95541800	2.93798400	5.46235900
C	-4.18877400	0.20365900	7.33686200
H	-2.57975300	-1.16694800	6.90901600
H	-5.69449200	1.73885000	7.49951700
H	-4.50976100	-0.32211700	8.23169300
C	-3.65500300	3.77579500	1.02417400
H	-4.74472400	3.87996900	1.11664100

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H	-3.21259900	4.42999200	1.78665500
H	-3.35709400	4.15574900	0.04243000
1af'			
C	-3.41181500	2.31212200	1.18088800
C	-3.79613400	1.68089200	2.48169300
H	-3.71896100	0.58695100	2.41821000
H	-4.84124200	1.91259800	2.72906100
C	-2.91096800	2.15082200	3.67749400
H	-2.98467900	3.24168700	3.76231000
H	-1.86312900	1.91680700	3.45400500
C	-3.32274200	1.49978300	4.97364900
C	-2.77090100	0.27372400	5.36675000
C	-4.31057400	2.07552900	5.78300200
C	-3.19060200	-0.35949200	6.53664400
H	-2.00136600	-0.18448900	4.74927300
C	-4.73419800	1.44687300	6.95391200
H	-4.74746000	3.02817900	5.49149200
C	-4.17502600	0.22573900	7.33503100
H	-2.74627200	-1.30773300	6.82713900
H	-5.49820400	1.91219700	7.57097600
H	-4.50135800	-0.26398100	8.24819800
C	-3.86383400	3.70855800	0.88853300
H	-4.85980700	3.90750600	1.30308400
H	-3.18376400	4.46723800	1.31950500
H	-3.89598100	3.90560400	-0.19107900
C	-2.24154200	1.76718900	0.42375500
H	-2.30633800	2.00424500	-0.64635200
H	-1.28195100	2.19115800	0.77480400
H	-2.16152200	0.67827000	0.52920700
2a			
C	-5.51527200	-0.96461000	2.27128400
C	-4.13871400	-1.06534500	2.24672300
C	-3.43570300	-0.98577200	1.02497200
C	-4.15284400	-0.80316700	-0.16346100
C	-5.53959200	-0.70088400	-0.14718500
C	-6.22904400	-0.78136400	1.07224700
H	-6.07175100	-1.02358400	3.20040500
H	-3.58004400	-1.20672400	3.16518100
H	-3.62042400	-0.74089000	-1.10415000
H	-6.07097500	-0.55984500	-1.08000600
O	-7.57200000	-0.69458900	1.19997300

C	-8.35662400	-0.50978000	0.02749400
H	-9.39198600	-0.47006700	0.36741000
H	-8.10080400	0.42931000	-0.47805600
H	-8.23175700	-1.34672900	-0.67021900
C	-1.97800500	-1.10383600	1.10407000
O	-1.30454800	-1.26067600	2.07221900
Cl	-1.09479000	-0.98453100	-0.57907300

2a'

C	-4.61703700	5.24033500	-5.57927000
C	-4.40645800	3.88511400	-5.41017400
C	-5.30131200	3.11799300	-4.63528600
C	-6.40181600	3.74289200	-4.04055400
C	-6.62455500	5.10776300	-4.20371800
C	-5.72863000	5.86093400	-4.97659500
H	-3.94436100	5.85321900	-6.17045000
H	-3.55437900	3.39309100	-5.86863500
H	-7.08591400	3.14563400	-3.44512800
H	-7.48298000	5.57175700	-3.73409100
O	-5.84459900	7.19203600	-5.20377100
C	-6.94366600	7.88364600	-4.62640300
H	-6.83612800	8.92393900	-4.93594700
H	-7.89974700	7.48980200	-4.99314200
H	-6.92163800	7.82380700	-3.53114800
C	-5.09622200	1.67444400	-4.44296500
O	-4.21745500	0.98522700	-4.87462100

3af

H	-7.62860800	-4.05551000	5.86106600
C	-7.78116800	-5.13336300	5.76435800
C	-7.03806600	-5.69362600	4.53875200
H	-8.85422500	-5.33267100	5.68216100
C	-7.51172000	-4.94626900	3.26007400
H	-7.41717000	-5.59784600	6.68487700
H	-6.87517200	-5.19347500	2.40634700
H	-7.37663700	-3.86992000	3.42675100
C	-8.97444200	-5.20019400	2.84658700
H	-9.64936700	-4.92216000	3.66312300
H	-9.12403300	-6.26964000	2.65910600
C	-9.32714500	-4.41556800	1.60457800
C	-9.77432400	-3.09168000	1.69816800
C	-9.16078800	-4.97516200	0.33199800
C	-10.04898100	-2.34615300	0.55183300

H	-9.90873400	-2.64430700	2.68047800
C	-9.43420700	-4.23443700	-0.81828700
H	-8.81630000	-6.00348000	0.24459700
C	-9.87933100	-2.91587500	-0.71145800
H	-10.39858900	-1.32149600	0.64457000
H	-9.30345000	-4.68768100	-1.79726900
H	-10.09539800	-2.33755500	-1.60533500
C	-7.29919000	-7.21701300	4.47931900
H	-8.37130100	-7.41685200	4.57446500
H	-6.95625400	-7.68625000	3.55533800
H	-6.79760300	-7.72115200	5.31283600
C	-2.08304900	-6.05020900	3.34055100
C	-3.13831600	-5.64423400	4.13513800
C	-4.47782200	-5.91619200	3.78474900
C	-4.70261100	-6.61417600	2.59012800
C	-3.65005600	-7.02832200	1.77398700
C	-2.33041900	-6.74833600	2.14686000
H	-1.05397000	-5.84108900	3.61411400
H	-2.95872500	-5.10104000	5.05578000
H	-5.70591000	-6.84595400	2.26112500
H	-3.87084100	-7.56133600	0.85718100
O	-1.23360000	-7.10403600	1.42990500
C	-1.42713500	-7.80655200	0.21168200
H	-0.42954300	-7.98552400	-0.19195800
H	-1.93069500	-8.76720200	0.37915100
H	-2.00944400	-7.21268200	-0.50432000
C	-5.52663300	-5.41421700	4.73509500
O	-5.16665500	-4.76014200	5.70631900

3af'

C	0.24849100	1.89088000	1.43976300
C	0.59580500	2.14112600	-0.05400900
H	1.07287500	3.12473100	-0.14051200
C	-4.22251600	-0.37017900	0.90857400
C	-2.87337600	-0.40191000	1.20742900
C	-2.09766800	0.77384300	1.20394400
C	-2.73132000	1.98246200	0.88950800
C	-4.09121800	2.03208500	0.58462400
C	-4.84390800	0.85086400	0.59274800
H	-4.82678900	-1.27149300	0.90894100
H	-2.37884100	-1.33544200	1.45273400
H	-2.17015200	2.91046600	0.87692200
H	-4.54917700	2.98459100	0.34685400

O	-6.17052400	0.78156100	0.31181200
C	-6.85097500	1.98303500	-0.01794800
H	-6.43023500	2.44661800	-0.91934400
H	-7.88693300	1.69779300	-0.20634800
H	-6.81554200	2.70316700	0.80946600
C	-0.64687600	0.65461900	1.53466400
O	-0.17119500	-0.43437300	1.83478000
C	1.49671800	1.07137600	-0.67719300
H	1.06942200	0.07068200	-0.55824000
H	1.63215700	1.26032500	-1.74761700
H	2.48913700	1.06148100	-0.21410000
C	1.47872800	1.73323500	2.34475600
H	2.02688800	0.82732400	2.07125800
H	1.13911200	1.56963200	3.37467100
C	2.42492200	2.94578300	2.32086300
H	1.86056200	3.85543100	2.56640500
H	2.82345100	3.08722700	1.30917000
C	3.57047200	2.77579900	3.29093600
C	4.71692400	2.06211700	2.91933100
C	3.49110600	3.27703100	4.59553500
C	5.75662900	1.85405600	3.82527000
H	4.79288400	1.66690400	1.90857900
C	4.52847600	3.07288900	5.50617400
H	2.60688500	3.83354000	4.89839500
C	5.66545800	2.35969700	5.12351500
H	6.63900900	1.29961100	3.51725100
H	4.44960600	3.47269800	6.51359000
H	6.47509600	2.20083700	5.83026500
H	-0.33860000	2.20471100	-0.62413800
H	-0.32019200	2.76245600	1.78926600

3af''

C	-0.08834600	2.20467000	0.82535300
C	1.43464200	2.14745600	0.99953300
H	1.80988200	1.36232500	0.33129600
C	-4.25527800	-0.59431400	0.71782200
C	-2.87855800	-0.47989500	0.76793200
C	-2.25448600	0.78233000	0.77102500
C	-3.06305000	1.92391600	0.71975400

C	-4.45282900	1.82587200	0.66682700
C	-5.05520500	0.56089600	0.66655900
H	-4.74634000	-1.56194900	0.71626800
H	-2.24723600	-1.36106700	0.80571800
H	-2.61583600	2.91233800	0.71768300
H	-5.04996200	2.72881300	0.62741400
O	-6.39528500	0.34727800	0.61893300
C	-7.25405700	1.47628500	0.56210100
H	-7.06759700	2.07575900	-0.33804800
H	-8.26919400	1.07819500	0.52917100
H	-7.13956900	2.11121600	1.44988000
C	-0.76645500	0.83673500	0.82051200
O	-0.10565800	-0.19467700	0.83688200
H	-0.34517200	2.69993200	-0.12295700
H	-0.53616300	2.82750800	1.61254800
C	2.06266000	3.48725400	0.59543100
H	1.70355100	4.29872900	1.24209100
H	3.15450800	3.46181600	0.67040400
H	1.80966300	3.74815900	-0.43913100
C	1.79771400	1.74936300	2.44074200
H	1.19771100	0.88224200	2.73409300
H	1.53003200	2.56792600	3.12516100
C	3.28108000	1.39049600	2.63981700
H	3.91503300	2.24907400	2.38978000
H	3.54260900	0.58689400	1.93917800
C	3.56743200	0.94991300	4.05608200
C	3.30676600	-0.36657300	4.45890800
C	4.04874500	1.85526600	5.00906900
C	3.52297400	-0.76787200	5.77685700

H	2.93164300	-1.08044700	3.72904100
C	4.26656600	1.45947200	6.32956000
H	4.25680700	2.88035500	4.71015400
C	4.00408000	0.14500100	6.71780900
H	3.31902300	-1.79451100	6.06925200
H	4.64457000	2.17652000	7.05352800
H	4.17567800	-0.16700500	7.74428900

Cat^{doublet}

C	-1.72822500	-2.73480600	-3.90854000
C	-1.01293200	-1.56064600	-3.82350800
C	-1.59530500	-0.40835800	-3.24116400
C	-2.93379700	-0.48140000	-2.74373700
C	-3.65029900	-1.69938500	-2.84184300
C	-3.05306500	-2.80122900	-3.41433900
H	0.10306500	0.91453200	-3.49343400
H	-1.27719400	-3.61539000	-4.35590200
H	0.00458000	-1.49959400	-4.20003300
C	-0.91489400	0.82914300	-3.12350600
H	-4.66609400	-1.74144700	-2.46006800
H	-3.60615400	-3.73257900	-3.48706500
C	-2.86996600	1.76641500	-2.07313300
C	-1.54265000	1.90525500	-2.54664600
H	-1.02661700	2.85300600	-2.45521100
C	-7.78801300	4.05969500	0.54153100
C	-6.97786300	3.12261100	-0.06166200
C	-5.66548200	3.47781500	-0.45945100
C	-5.19436800	4.80800100	-0.22985100
C	-6.05442100	5.74535000	0.39292700
C	-7.32714600	5.37826000	0.77120700
H	-8.79301000	3.78280000	0.84472700
H	-7.32310800	2.10888600	-0.24189500
C	-3.87544700	5.12089800	-0.64342400
H	-5.69155100	6.75506200	0.56515200
H	-7.98256400	6.10074900	1.24810000
C	-3.09796300	4.16069400	-1.24215400
C	-3.62522500	2.86129700	-1.44054600
H	-3.49032000	6.12384800	-0.48162500
H	-2.08969600	4.39509000	-1.56039000
N	-3.53713900	0.60828300	-2.17249400

N	-4.86857800	2.53832900	-1.05908700
Ni	-5.37721300	0.66341300	-1.44540800
Br	-7.21360400	-0.75347500	-1.17638600

Cat^{doublet}

C	-1.73961000	-2.73350200	-3.90585600
C	-1.01932000	-1.56178600	-3.82312500
C	-1.59581700	-0.40671900	-3.24113800
C	-2.93335900	-0.47459700	-2.74176700
C	-3.65568400	-1.68925300	-2.83692200
C	-3.06355700	-2.79434400	-3.40955500
H	0.10735700	0.91032600	-3.49717400
H	-1.29256800	-3.61619000	-4.35316500
H	-0.00218400	-1.50558500	-4.20153800
C	-0.91033400	0.82933400	-3.12554700
H	-4.67127100	-1.72607100	-2.45289300
H	-3.62031700	-3.72367800	-3.48051700
C	-2.86039000	1.77512000	-2.07328900
C	-1.53307500	1.90837100	-2.54900900
H	-1.01377700	2.85467000	-2.45924600
C	-7.78637100	4.05059200	0.53444400
C	-6.97156200	3.11683800	-0.06881300
C	-5.65970000	3.47758800	-0.46262600
C	-5.19290400	4.80819700	-0.23012100
C	-6.05722400	5.74134400	0.39237000
C	-7.33002800	5.36969900	0.76739500
H	-8.79121800	3.77014000	0.83493800
H	-7.31319000	2.10188000	-0.25175400
C	-3.87308300	5.12586700	-0.64090300
H	-5.69817800	6.75199600	0.56732000
H	-7.98845200	6.08956700	1.24417300
C	-3.09169900	4.16917400	-1.23989000
C	-3.61433800	2.86834300	-1.44165400
H	-3.49145200	6.12969500	-0.47643200
H	-2.08331700	4.40657800	-1.55602600
N	-3.53162200	0.61815300	-2.17064100
N	-4.85844400	2.54116500	-1.06221900
Ni	-5.36650800	0.67278300	-1.44211400
Cl	-7.08569700	-0.68623700	-1.18803300

LiBr(THF)₂

Li	2.43329400	-6.45699800	-2.43152800
C	3.25481700	-7.69049000	-0.06421800

C	5.19808800	-6.31178800	-0.08050700
C	4.47522300	-7.35017400	0.78960900
H	2.90496600	-8.71991100	0.04791000
H	2.43159400	-6.99205600	0.12480600
H	6.25841300	-6.20537300	0.16522000
H	4.70894400	-5.33650700	0.00241400
H	5.10228700	-8.23697700	0.93767300
H	4.19035900	-6.96088200	1.77053100
C	4.98216100	-6.86865900	-1.48334700
O	3.67929600	-7.51625400	-1.44980200
C	3.45268900	-7.24485500	-4.98820700
C	3.04202500	-4.88584000	-5.44616000
C	4.16651600	-5.95932900	-5.44281800
H	3.14111000	-7.85890000	-5.84306300
H	4.02384700	-7.86707200	-4.29561800
H	2.92697900	-4.40197500	-6.41977200
H	3.24191000	-4.11579700	-4.69725700
H	4.62825300	-6.09053300	-6.42535500
H	4.95767900	-5.68405800	-4.73931500
C	1.78162900	-5.66440600	-5.04967100
O	2.27383500	-6.79708500	-4.29111200
H	1.10818500	-5.10774400	-4.39701400
H	1.23570400	-6.04825600	-5.92112300
H	5.73050600	-7.62259400	-1.75635700
H	4.95096900	-6.08951400	-2.25097800
Br	2.15855800	-4.29752000	-1.58558700

(EtO)₃SiOMe

Si	-1.15927300	-0.00717700	-0.07166100
O	-0.61377500	0.68463500	1.31584700
O	-2.49050000	-0.88514500	0.31726300
C	-2.99269000	-1.97426500	-0.46301100
C	-2.41612600	-3.29518200	0.02411200
H	-2.76217600	-1.82535300	-1.52547400
H	-4.08271600	-1.96133900	-0.35385700
H	-2.85004800	-4.13390000	-0.53323700
H	-1.33122000	-3.30497600	-0.11531700
H	-2.63528600	-3.43512300	1.08809700
C	-0.47964700	-0.03263900	2.54592100
C	0.76725800	-0.90822900	2.54922200
H	-1.37767800	-0.63797200	2.71924800
H	-0.42221100	0.72031900	3.33909900
H	0.88124400	-1.41127500	3.51665000

H	0.70717700	-1.67092000	1.76614800
H	1.65980600	-0.29987900	2.36772900
O	-0.09647600	-1.03736400	-0.79387500
O	-1.41784600	1.21393500	-1.13852500
C	-2.14105200	2.40411400	-0.81073400
H	-1.78668100	2.79770400	0.14964100
H	-3.20663800	2.16090100	-0.70261200
C	-1.93533600	3.42117600	-1.91985400
H	-2.48870200	4.34208600	-1.70345500
H	-0.87305700	3.66770100	-2.01883000
H	-2.28538600	3.02051600	-2.87684400
C	1.11209400	-0.57677300	-1.38764900
H	1.78380900	-0.15362000	-0.62996900
H	1.60480000	-1.43327300	-1.85652400
H	0.91143300	0.18479500	-2.14944600

[Si]-H

Si	-0.42307100	-0.24945100	-0.07392300
O	0.61095600	0.01091400	1.25812400
O	-1.16264400	-1.83748200	-0.26691800
C	-2.43927300	-2.18442600	0.23906400
C	-3.37139200	-2.63822800	-0.87707600
H	-2.86917500	-1.32605400	0.76930500
H	-2.31750900	-2.99509800	0.97307500
H	-4.33344700	-2.96529800	-0.46474400
H	-3.56133600	-1.81900700	-1.57894500
H	-2.93476000	-3.47379500	-1.43635600
C	0.17376800	0.57128200	2.47801600
C	-0.14920300	-0.51937300	3.49486300
H	-0.71263700	1.20350200	2.32726700
H	0.97743900	1.21618100	2.85895200
H	-0.45389700	-0.08982400	4.45732300
H	-0.96547700	-1.14989300	3.12330000
H	0.72628000	-1.15697900	3.66236600
O	0.94539500	-1.01813600	-0.93457900
Li	0.22978400	-2.70875900	-1.20560800
O	-0.53284400	0.87377500	-1.35388000
C	-1.52930400	1.87174800	-1.42915700
H	-1.07290500	2.76635600	-1.87430200
H	-1.88908100	2.14941800	-0.42820200
C	-2.70772000	1.40725900	-2.27979700
H	-3.44918700	2.20637900	-2.40370600
H	-2.36343300	1.09619400	-3.27273900

H	-3.20137600	0.55140100	-1.80524600
C	0.62480300	-4.31004000	1.09339800
C	2.57693100	-2.94038400	1.38513200
C	1.64681900	-3.88804300	2.15963800
H	0.35897600	-5.37042600	1.14562100
H	-0.28224200	-3.70419400	1.14001400
H	3.57222400	-2.85964600	1.83231800
H	2.12995200	-1.94464800	1.30639600
H	2.20194100	-4.75782000	2.52895000
H	1.16411000	-3.40393900	3.01233900
C	2.60068600	-3.60438000	0.01483500
O	1.24280500	-4.05310400	-0.19897700
C	1.01653800	-3.19773600	-3.92395800
C	0.03970700	-0.97679200	-4.18916300
C	1.34323500	-1.78137500	-4.43914800
H	0.77177300	-3.87998800	-4.74924100
H	1.80531900	-3.65269100	-3.31892000
H	-0.32299400	-0.47798200	-5.09280800
H	0.18078500	-0.22769100	-3.40831700
H	1.62241000	-1.80803600	-5.49655600
H	2.17681500	-1.34329600	-3.88582700
C	-0.95318500	-2.03178800	-3.69166900
O	-0.13952300	-3.05664800	-3.08161000
H	-1.63329800	-1.66372300	-2.92575900
H	-1.52804800	-2.48587200	-4.51088700
H	3.27317500	-4.47314600	-0.01198400
H	2.85380300	-2.92883600	-0.80396700
H	-1.66240400	0.28494200	0.63974600
C	2.10445800	-0.26657600	-1.20609700
H	2.52863800	0.14668200	-0.28326000
H	2.85478300	-0.91923500	-1.67392800
H	1.88849500	0.56243500	-1.89145400

IM1^{doublet}

C	-1.58700600	-2.83162200	-3.75225500
C	-0.81300100	-1.70596200	-3.58574900
C	-1.40594200	-0.49126200	-3.15978100
C	-2.81363900	-0.45483200	-2.91518700
C	-3.58960500	-1.62751700	-3.08396100
C	-2.98027300	-2.79057500	-3.49510000
H	0.39982200	0.70186200	-3.12521200
H	-1.13053300	-3.76210000	-4.07553000
H	0.25723700	-1.73143200	-3.77059400
C	-0.67287200	0.70135700	-2.95273000

H	-4.65100000	-1.59816600	-2.86493300
H	-3.57359100	-3.69094900	-3.61791800
C	-2.70965400	1.81132300	-2.31430700
C	-1.31043700	1.84209400	-2.52761400
H	-0.74818200	2.74987600	-2.34939100
C	-7.73685500	4.41249100	-0.26729800
C	-6.90675300	3.40624900	-0.70685300
C	-5.57192100	3.71174200	-1.07169100
C	-5.08645200	5.04913500	-0.93531300
C	-5.97366600	6.06176400	-0.49269700
C	-7.27661600	5.74964900	-0.17313500
H	-8.75836700	4.17720200	0.01487400
H	-7.24872700	2.38039800	-0.78224700
C	-3.73107900	5.29434800	-1.25732100
H	-5.60292000	7.07875800	-0.39721500
H	-7.95215300	6.52595800	0.17394200
C	-2.92659400	4.26362200	-1.67603300
C	-3.48716200	2.97348800	-1.83541000
H	-3.33583100	6.30205300	-1.16504500
H	-1.88568200	4.44218800	-1.91366000
N	-3.41397300	0.69981500	-2.51326500
N	-4.76858200	2.72993100	-1.56847600
Ni	-5.38436000	0.87265000	-2.16965800
C	-4.87261800	4.93123500	-5.04791100
C	-4.77582100	3.55087300	-4.98044600
C	-5.80184700	2.79914600	-4.37765500
C	-6.94017400	3.44953700	-3.89406300
C	-7.05707300	4.83256700	-3.99243800
C	-6.00762900	5.58332900	-4.53759200
H	-4.08144300	5.53193700	-5.48414500
H	-3.89563200	3.04482800	-5.36480400
H	-7.72423500	2.86295400	-3.43212600
H	-7.94625600	5.31298800	-3.60464600
O	-5.99088900	6.93951100	-4.60905600
C	-7.08011500	7.64908400	-4.03428900
H	-6.84445900	8.70720500	-4.15688600
H	-8.02175800	7.42445000	-4.55066800
H	-7.18513500	7.41330000	-2.96783500
C	-5.52979100	1.36576200	-4.14311600
O	-5.16204100	0.53708400	-4.92133800
Cl	-7.58927100	0.40168500	-2.58302900
Br	-5.12686200	-0.10046200	0.08950600

IM2^{doublet}

C	-1.62068200	-2.85987100	-3.86799300
C	-0.81263800	-1.78155700	-3.58130800
C	-1.37204900	-0.58550300	-3.06946700
C	-2.78263200	-0.51853400	-2.85730700
C	-3.59435000	-1.63878300	-3.15332800
C	-3.01722700	-2.78669300	-3.64956500
H	0.47528900	0.53511300	-2.89895900
H	-1.18706800	-3.77445500	-4.26091100
H	0.26092600	-1.83171400	-3.74082100
C	-0.60079700	0.56159700	-2.75245600
H	-4.66365000	-1.57802500	-2.98127400
H	-3.64127000	-3.64509800	-3.87706700
C	-2.61807300	1.70216800	-2.09556700
C	-1.21202500	1.69143500	-2.26871300
H	-0.62728100	2.56906700	-2.02282900
C	-7.69432200	4.41530200	-0.34365700
C	-6.86375000	3.39024200	-0.73924500
C	-5.49688800	3.65430500	-0.99785300
C	-4.98418300	4.97428700	-0.81170300
C	-5.87054200	6.00790800	-0.42375800
C	-7.20257300	5.73447800	-0.19854700
H	-8.74165300	4.20870200	-0.14549000
H	-7.23419400	2.37972700	-0.87200300
C	-3.59861800	5.18446900	-1.02469800
H	-5.47825600	7.01322500	-0.29669800
H	-7.87617800	6.52914500	0.10888400
C	-2.79596000	4.13568900	-1.39242700
C	-3.37830200	2.86324600	-1.61670400
H	-3.18478700	6.17970400	-0.89004100
H	-1.73530100	4.28518800	-1.55140800
N	-3.35721900	0.62338800	-2.37519200
N	-4.68598200	2.64783500	-1.44199300
Ni	-5.28628900	0.84440900	-2.13083100
C	-4.74622000	5.09649600	-4.71188000
C	-4.58809600	3.71781800	-4.72084600
C	-5.62796600	2.88053600	-4.28186100
C	-6.84026500	3.44928200	-3.88351700
C	-7.02086100	4.83128200	-3.91579700
C	-5.96138700	5.66217200	-4.29746400
H	-3.94372500	5.75959300	-5.01886600
H	-3.64780800	3.27815900	-5.04045700
H	-7.63576800	2.80202400	-3.53219200

H	-7.97001200	5.24546200	-3.59952000
O	-6.00875800	7.02538900	-4.29142500
C	-7.19982200	7.64273600	-3.83157500
H	-7.02016400	8.71802200	-3.88462300
H	-8.05755200	7.38735500	-4.46732600
H	-7.42111100	7.35696400	-2.79513000
C	-5.31683400	1.44087000	-4.06414900
O	-4.94490700	0.66922200	-4.91394700
Cl	-7.45396600	0.24966600	-2.41000400
H	-5.21134600	0.23691900	-0.71031400

IM3^{OSS}

C	-3.75930800	-1.98382500	4.98964100
C	-3.50479300	-0.66782500	5.32254600
C	-3.67781200	0.36136700	4.36862400
C	-4.13683700	0.02705000	3.05778500
C	-4.37291200	-1.32936100	2.73315900
C	-4.18858100	-2.31217700	3.68483300
H	-3.07338200	2.01081500	5.64495000
H	-3.61646500	-2.76960500	5.72598600
H	-3.16208400	-0.40327200	6.31961600
C	-3.41561000	1.72897200	4.65332200
H	-4.72155400	-1.57162900	1.73508900
H	-4.37667900	-3.34985700	3.42547300
C	-4.09076100	2.28355100	2.40729500
C	-3.60219800	2.67434800	3.67878900
H	-3.42030600	3.72148900	3.88966200
C	-6.72138500	3.82740300	-2.78824200
C	-6.34406600	3.02571400	-1.73023700
C	-5.54675600	3.55810800	-0.69154900
C	-5.15097800	4.92874500	-0.73874100
C	-5.55668900	5.72328100	-1.83569900
C	-6.32785500	5.18269000	-2.84454200
H	-7.33383700	3.41206500	-3.58257400
H	-6.65375900	1.98678500	-1.67787000
C	-4.35905300	5.42562400	0.33328500
H	-5.25021000	6.76543700	-1.86843300
H	-6.63772600	5.79908000	-3.68292900
C	-4.00122400	4.59830400	1.36668000
C	-4.41610900	3.24269700	1.35777000
H	-4.03883200	6.46367600	0.31868000
H	-3.38386800	4.96732100	2.17685500
N	-4.36282900	0.99482000	2.10947400

N	-5.16361400	2.75150700	0.34938800
Ni	-5.76309900	0.90285800	0.59745700
C	-7.36407300	1.97419600	5.04161600
C	-7.52517500	2.22617700	3.68897100
C	-7.49964100	1.16258600	2.76768300
C	-7.34189300	-0.14901100	3.22661600
C	-7.22460300	-0.40884400	4.58865000
C	-7.20382300	0.65546400	5.49915900
H	-7.35511600	2.77919100	5.76907600
H	-7.64850800	3.24292300	3.32929500
H	-7.29969900	-0.95997700	2.50801100
H	-7.09815600	-1.43114600	4.92062200
O	-7.02423700	0.51540100	6.83926200
C	-6.82377900	-0.79492700	7.35045400
H	-6.68103400	-0.67655000	8.42576200
H	-5.93486000	-1.25991900	6.90747000
H	-7.69783600	-1.43303900	7.16806800
C	-7.47108200	1.49247200	1.32469100
O	-8.22473400	2.18510900	0.70151900
Cl	-6.48285600	-1.08340700	-0.15825300

IM4^{OSS}

C	-1.72112000	-2.74030300	-3.91525500
C	-1.01695600	-1.56073600	-3.83582600
C	-1.60983000	-0.41545500	-3.24794800
C	-2.94444200	-0.50588300	-2.74219800
C	-3.64960800	-1.73125200	-2.83332300
C	-3.04313600	-2.82330700	-3.41017000
H	0.06515700	0.93028900	-3.50770000
H	-1.26539800	-3.61629600	-4.36635000
H	-0.00326500	-1.48849900	-4.21972200
C	-0.94907800	0.82977100	-3.13137400
H	-4.65954200	-1.78868600	-2.44294800
H	-3.58375100	-3.76185400	-3.47963500
C	-2.90704600	1.74056500	-2.06919000
C	-1.58433000	1.89988500	-2.54842000
H	-1.07862100	2.85283400	-2.46015200
C	-7.84067300	4.00535900	0.55317600
C	-7.02814600	3.07486300	-0.05272900
C	-5.71709400	3.44069900	-0.44540500
C	-5.25019400	4.77138300	-0.20896600
C	-6.11472100	5.70322500	0.41800100
C	-7.38464400	5.32637400	0.79068900

H	-8.84504100	3.72463500	0.85379500
H	-7.37073100	2.06284400	-0.23703100
C	-3.93389800	5.08618200	-0.62030700
H	-5.75697800	6.71338400	0.59625500
H	-8.04541100	6.04186500	1.27024700
C	-3.14947500	4.13286500	-1.22393600
C	-3.67465700	2.83397900	-1.42806500
H	-3.55074000	6.08908700	-0.45367100
H	-2.14208700	4.37328000	-1.53840900
N	-3.54416500	0.57623900	-2.17380600
N	-4.91177300	2.52175300	-1.04654900
Ni	-5.42792900	0.62368900	-1.45183100
Br	-6.78435000	0.79775500	-3.39835500
Cl	-5.32733900	-0.44742700	0.52251100

IM4^{triplet}

C	-1.75494300	-2.75416300	-3.92124900
C	-1.04074700	-1.58086300	-3.83922800
C	-1.62597300	-0.43037300	-3.25385300
C	-2.96338500	-0.50859700	-2.75380500
C	-3.67864700	-1.72808700	-2.84643500
C	-3.07931000	-2.82551300	-3.42062700
H	0.06214100	0.89992100	-3.50691100
H	-1.30529300	-3.63423000	-4.37047800
H	-0.02494600	-1.51752200	-4.21905000
C	-0.95444100	0.80867200	-3.13456700
H	-4.68934000	-1.77945200	-2.45708600
H	-3.62757000	-3.75953600	-3.49090700
C	-2.90834900	1.73804600	-2.08112100
C	-1.58203700	1.88455200	-2.55376400
H	-1.06764200	2.83255800	-2.46304500
C	-7.82676000	4.04941400	0.52837000
C	-7.02141500	3.11131200	-0.07541000
C	-5.70649700	3.46534800	-0.46641300
C	-5.22802200	4.79167400	-0.22895200
C	-6.08538800	5.73178500	0.39549500
C	-7.35951300	5.36660000	0.76548000
H	-8.83384800	3.77761000	0.82805700
H	-7.37274400	2.10149600	-0.25588200
C	-3.90771300	5.09383000	-0.63671200
H	-5.71888600	6.73871900	0.57418300
H	-8.01488700	6.08827800	1.24315400
C	-3.13025500	4.13258600	-1.23700800

C	-3.66786400	2.83914200	-1.44294400
H	-3.51573000	6.09326900	-0.46973900
H	-2.11963500	4.36350800	-1.54816700
N	-3.55673000	0.57964700	-2.18907900
N	-4.90942200	2.53822400	-1.06634300
Ni	-5.45598200	0.64533600	-1.50912200
Br	-6.78439100	0.85279400	-3.48248100
Cl	-5.49484600	-0.50287700	0.43104200

IM5^{CSS}

C	-1.79413100	-2.59314300	-4.24893300
C	-1.06386700	-1.45444200	-4.00129200
C	-1.62812100	-0.38424300	-3.26217200
C	-2.95954100	-0.50404200	-2.75048700
C	-3.69263700	-1.68345900	-3.03250600
C	-3.12019000	-2.69846000	-3.76651300
H	0.09144700	0.92575200	-3.39095100
H	-1.35959500	-3.40937400	-4.81787700
H	-0.04784000	-1.35073800	-4.37203000
C	-0.92412000	0.81804800	-3.02059600
H	-4.70403300	-1.76108700	-2.65555500
H	-3.69696700	-3.59395100	-3.97674300
C	-2.85825900	1.67228300	-1.87014500
C	-1.53894700	1.84360300	-2.34937800
H	-1.02217400	2.78146900	-2.19301700
C	-7.95946800	4.24489600	0.00916900
C	-7.12416800	3.24057100	-0.42596200
C	-5.73255300	3.48377000	-0.54634800
C	-5.22333500	4.78752800	-0.23746900
C	-6.11086100	5.79211400	0.22195900
C	-7.45470100	5.52433500	0.34594000
H	-9.02406000	4.05107700	0.09773800
H	-7.49920700	2.25421800	-0.66038100
C	-3.84162600	5.01942800	-0.42701500
H	-5.71156000	6.77437700	0.45964800
H	-8.13455300	6.29658900	0.69330600
C	-3.04464700	4.02864500	-0.94377600
C	-3.61665600	2.76572600	-1.23217800
H	-3.42544100	5.99226800	-0.17968100
H	-1.99010700	4.20720100	-1.11064600
N	-3.53065900	0.51869500	-2.02464000
N	-4.90203800	2.49071700	-0.98956700
Ni	-5.09686900	0.43524300	-0.94579400

H	-5.03992100	-1.00135700	-0.86376600
Cl	-6.69680300	0.20063900	0.54859800

IM6^{OSS}

C	-1.94223200	-2.90709100	-3.97518700
C	-1.09378800	-1.86715500	-3.64926700
C	-1.59654700	-0.68717500	-3.05608000
C	-2.99566100	-0.58418300	-2.79005000
C	-3.85012600	-1.65472500	-3.14384200
C	-3.32645500	-2.79382700	-3.72420700
H	0.29531300	0.37012800	-2.90108300
H	-1.54762600	-3.81006900	-4.43117700
H	-0.02722900	-1.93921900	-3.84619600
C	-0.77253800	0.42145900	-2.70789500
H	-4.91639100	-1.55525900	-2.96388100
H	-3.99082300	-3.60910600	-3.99465500
C	-2.72315000	1.58139600	-1.88733400
C	-1.32771200	1.53841100	-2.14125900
H	-0.70397300	2.38469700	-1.88015600
C	-7.62460100	4.36284800	0.25075100
C	-6.87189500	3.38397300	-0.36948800
C	-5.47136900	3.53955200	-0.49258700
C	-4.85032000	4.72208500	0.01057600
C	-5.64887700	5.70259600	0.64123900
C	-7.01340500	5.52645200	0.76447300
H	-8.69952300	4.23601900	0.33774200
H	-7.33892100	2.49422900	-0.78218500
C	-3.44104100	4.85168400	-0.15496100
H	-5.16885000	6.59897000	1.02534000
H	-7.61917500	6.28561900	1.24992100
C	-2.73048100	3.86467000	-0.78577200
C	-3.39719800	2.70414200	-1.25514200
H	-2.94169000	5.73933400	0.22277800
H	-1.65893100	3.96097900	-0.91130600
N	-3.52466600	0.53691400	-2.19974800
N	-4.73245600	2.55162000	-1.09523300
Ni	-5.34915700	0.71038700	-1.43898600
Cl	-7.29829200	-0.23022800	-2.07158100
H	-4.11012600	-1.85708400	-0.41335100
C	-5.00145800	-1.62825800	0.17906000
C	-5.11596000	-0.15186400	0.49002000
H	-4.92282000	-2.19531000	1.12209400
C	-3.85755600	0.48031600	1.05049300

H	-5.88183800	-1.99391800	-0.35364600
H	-4.00561200	1.55523700	1.18828500
H	-3.02204700	0.35878700	0.35523300
C	-3.39834200	-0.10490800	2.41533000
H	-3.18843100	-1.17439200	2.30552900
H	-4.20257100	-0.00360200	3.15261100
C	-2.16380300	0.62271700	2.88464000
C	-0.89208200	0.21491800	2.46186900
C	-2.26735400	1.77001500	3.68082700
C	0.24734800	0.93117300	2.82820200
H	-0.79775600	-0.67272800	1.84005300
C	-1.13091000	2.48967300	4.05045500
H	-3.24931400	2.10006900	4.01250800
C	0.13134900	2.07221200	3.62455900
H	1.22622500	0.59621000	2.49563800
H	-1.23073900	3.37432700	4.67358400
H	1.01798300	2.62934400	3.91394100
C	-6.38300600	0.24112600	1.21791300
H	-6.35440200	-0.16717200	2.24279600
H	-6.48229500	1.32754600	1.30829700
H	-7.27165900	-0.15363200	0.72238300

IM6^{triplet}

C	-2.01393000	-2.96395600	-4.02249600
C	-1.15353500	-1.93597100	-3.70066800
C	-1.64529000	-0.75159500	-3.10170500
C	-3.04319300	-0.64009900	-2.82889000
C	-3.91157700	-1.70316900	-3.17743900
C	-3.39894200	-2.84137900	-3.76296200
H	0.25018300	0.29264800	-2.95509400
H	-1.63103600	-3.87024900	-4.48179300
H	-0.08888500	-2.01757500	-3.90267200
C	-0.81664000	0.34866900	-2.75735200
H	-4.97513700	-1.59618300	-2.98617300
H	-4.06858600	-3.65305800	-4.03027700
C	-2.75625300	1.51430800	-1.92863500
C	-1.36260900	1.46961100	-2.18559600
H	-0.73353900	2.31183100	-1.92582700
C	-7.62554900	4.33760800	0.21964300
C	-6.88454300	3.35670700	-0.40512500
C	-5.48094100	3.50363000	-0.52312200
C	-4.84645300	4.67387100	-0.00630000
C	-5.63745900	5.65888100	0.63201700

C	-7.00146300	5.49278000	0.74569500
H	-8.70152500	4.22216400	0.30662400
H	-7.35652200	2.47088900	-0.82049100
C	-3.43968300	4.78543600	-0.16565500
H	-5.15024200	6.54576200	1.02814500
H	-7.60273900	6.25202400	1.23651400
C	-2.73869700	3.79414100	-0.80383500
C	-3.42534500	2.65171300	-1.28560200
H	-2.92834200	5.66102300	0.22405300
H	-1.66521400	3.87408700	-0.92012200
N	-3.55712100	0.48203500	-2.23700000
N	-4.75214500	2.51813600	-1.13165000
Ni	-5.39473400	0.64221000	-1.43332100
Cl	-7.34305700	-0.17151600	-2.26393900
H	-3.96552300	-1.85170200	-0.33164500
C	-4.88527800	-1.61019200	0.21446900
C	-5.03471700	-0.11022500	0.44329100
H	-4.84914800	-2.15961400	1.17115300
C	-3.79863500	0.52435800	1.06422100
H	-5.73226000	-2.01291900	-0.35160200
H	-3.96598800	1.59855900	1.20883300
H	-2.93795300	0.43451100	0.38872100
C	-3.34533900	-0.05020700	2.43269500
H	-3.09888500	-1.11217400	2.32376900
H	-4.16860000	0.01887400	3.15299300
C	-2.14692100	0.71167600	2.93749800
C	-0.84841500	0.32484600	2.58065600
C	-2.30732700	1.87740600	3.69813200
C	0.25874000	1.07710200	2.97422900
H	-0.70861600	-0.57752300	1.98921700
C	-1.20433300	2.63340800	4.09491000
H	-3.30985500	2.19168400	3.98010600
C	0.08453400	2.23584300	3.73339000
H	1.25830300	0.75571100	2.69294300
H	-1.35024600	3.53081800	4.69056500
H	0.94550800	2.82066100	4.04524000
C	-6.30556200	0.21933300	1.22044700
H	-6.28048700	-0.22634200	2.23051600
H	-6.43306400	1.30072900	1.35235300
H	-7.19615100	-0.16911200	0.71684100

IM7^{CSS}

C	-5.85984300	-1.57834100	-0.14548600
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C	-5.59386200	-0.55240600	-1.02370700
C	-4.36276800	0.14685200	-0.95357500
C	-3.39139200	-0.24545900	0.02118400
C	-3.69987000	-1.28891200	0.93102200
C	-4.91121500	-1.93724900	0.84406200
H	-4.74923600	1.54387200	-2.56439000
H	-6.80578400	-2.10895700	-0.19955700
H	-6.32233200	-0.25776800	-1.77441500
C	-4.03970700	1.23301800	-1.80235600
H	-2.97131900	-1.52877100	1.69662000
H	-5.14752500	-2.72960500	1.54782000
C	-1.93092000	1.44513600	-0.65839700
C	-2.84683500	1.89405700	-1.64427800
H	-2.59989000	2.73360400	-2.28237200
C	3.30499600	2.11144900	2.25599600
C	2.13604100	1.50362800	1.85704900
C	1.33261500	2.10710600	0.85652000
C	1.73037500	3.36900900	0.30986600
C	2.94968300	3.95665500	0.73094400
C	3.72710500	3.33508500	1.68113400
H	3.90804200	1.64985300	3.03207100
H	1.77168000	0.59650900	2.32341600
C	0.86094600	3.98757900	-0.61895400
H	3.24769800	4.90848700	0.29958100
H	4.65774300	3.79017100	2.00675900
C	-0.33001800	3.38826600	-0.94172000
C	-0.64481000	2.12239800	-0.38708700
H	1.13293800	4.94901500	-1.04634300
H	-1.02670900	3.88059700	-1.60820600
N	-2.18199600	0.38350200	0.10782600
N	0.18541400	1.48540600	0.44268100
Ni	-0.42335400	-0.44653200	0.83665300
C	0.18841700	-1.30982600	-0.95359300
C	1.02092200	-1.68774500	0.11666000
H	-1.00405100	-1.69773200	1.14847100
Cl	-0.46144700	-0.29505200	3.15014800
C	0.63962100	-0.32927100	-2.01383500
H	1.36349900	0.40088500	-1.64890200
H	1.10700800	-0.87990500	-2.84257500
H	-0.21174600	0.21936900	-2.43382100
C	-0.87469200	-2.26707400	-1.45666900
H	-1.15255400	-3.00376400	-0.69884000
H	-1.78453800	-1.73991100	-1.76571500

H	-0.49565400	-2.80621000	-2.33800300
H	0.81901400	-2.65846000	0.56500600
C	2.46798800	-1.26358500	0.28526000
H	2.62220700	-0.22475900	-0.01074400
H	2.73820700	-1.33603100	1.34400600
C	3.36768900	-2.16466000	-0.53946200
C	3.88931600	-1.73454000	-1.76537000
C	3.65931500	-3.46560800	-0.10857500
C	4.67978500	-2.58136000	-2.54400200
H	3.67839700	-0.72506100	-2.10847300
C	4.44786200	-4.31543200	-0.88325900
H	3.26637800	-3.81040800	0.84515400
C	4.96000600	-3.87622700	-2.10625700
H	5.07942200	-2.22764800	-3.49080600
H	4.66658900	-5.31981200	-0.53067200
H	5.57598500	-4.53678400	-2.71002300

IM8^{OSS}

C	5.80162400	0.72943200	0.32562600
C	5.36129600	-0.45973300	0.87536500
C	3.99300200	-0.65670500	1.16473300
C	3.06521000	0.38999000	0.88025900
C	3.53650600	1.60326600	0.32643800
C	4.88242200	1.76394300	0.05433900
H	4.16540100	-2.66998200	1.96470700
H	6.85545100	0.87111600	0.10610000
H	6.06192700	-1.26145300	1.09399300
C	3.48060000	-1.85851200	1.73520800
H	2.82678100	2.40251300	0.13105600
H	5.23385700	2.69971300	-0.36981000
C	1.25981600	-0.91261700	1.68033900
C	2.14064900	-1.98091900	1.99227700
H	1.75146100	-2.89110400	2.43263600
C	-4.25327800	1.52285200	1.48196500
C	-2.87699000	1.45011500	1.37123800
C	-2.20204900	0.25022400	1.69663700
C	-2.95425900	-0.87096500	2.16194900
C	-4.35891200	-0.76298100	2.26288900
C	-5.00161100	0.41246800	1.92395100
H	-4.76131100	2.44796800	1.22695300
H	-2.29578700	2.30577600	1.03946200
C	-2.23629200	-2.05482700	2.50274400

H	-4.92484500	-1.62253400	2.61262100
H	-6.08203300	0.48498700	2.00248100
C	-0.87218700	-2.09044200	2.37942800
C	-0.17567100	-0.95395500	1.89246200
H	-2.78370000	-2.92207600	2.86093900
H	-0.32550900	-2.98905900	2.63913800
N	1.72502000	0.23728200	1.13369100
N	-0.83812800	0.18049600	1.55389100
Ni	0.28089600	1.40335600	0.44692900
C	0.00141600	0.34667700	-1.28358800
C	1.19515600	0.54381300	-2.21132400
H	2.06348200	0.80383600	-1.59247600
H	0.04159900	-0.63220700	-0.80054700
Cl	0.03589700	3.50412500	-0.27312400
C	1.54723000	-0.80373400	-2.88237400
H	0.72200000	-1.16094500	-3.50650500
H	2.43573700	-0.68809300	-3.51422500
H	1.76275400	-1.57202800	-2.13098900
C	1.03292200	1.65917000	-3.24797600
H	1.98050000	1.81217800	-3.77656600
H	0.27788700	1.40276900	-3.99968000
H	0.74725900	2.60077400	-2.77131400
C	-1.40608300	0.65665600	-1.77134600
H	-2.05676100	0.89299300	-0.92415100
H	-1.40492700	1.53667100	-2.41620900
C	-1.98039000	-0.55425500	-2.48434500
C	-2.07492800	-0.60787100	-3.87906800
C	-2.39708800	-1.66529300	-1.73718500
C	-2.57216800	-1.74644200	-4.51637200
H	-1.76222200	0.24999000	-4.46846300
C	-2.89379500	-2.80281700	-2.37046100
H	-2.33648600	-1.63134500	-0.65205200
C	-2.98033500	-2.84858200	-3.76419300
H	-2.64242600	-1.77018800	-5.60046900
H	-3.21805300	-3.65324600	-1.77652200
H	-3.36696400	-3.73498500	-4.25911000
IM8 ^{triplet}			
C	5.78618800	0.79218700	0.30099800
C	5.37494700	-0.37062300	0.91759800
C	4.00969100	-0.57066000	1.23255000
C	3.06554400	0.44809000	0.90043800
C	3.50940000	1.63714800	0.27150700
C	4.84739500	1.79985700	-0.02004900

H	4.21431500	-2.53198900	2.13598700
H	6.83483900	0.93854300	0.06065200
H	6.09007800	-1.14904100	1.16958100
C	3.51900100	-1.74084100	1.86989900
H	2.78228700	2.40793900	0.03201500
H	5.18311600	2.71243200	-0.50276900
C	1.29206800	-0.82128200	1.78502000
C	2.18053300	-1.86511700	2.14575900
H	1.80496100	-2.75505600	2.63559200
C	-4.24533700	1.53906400	1.51755000
C	-2.87498900	1.46731500	1.37814100
C	-2.18863300	0.29144600	1.76981900
C	-2.92202600	-0.80375400	2.32104800
C	-4.32781000	-0.69675200	2.44511500
C	-4.97817800	0.45224300	2.04777900
H	-4.76713700	2.44172900	1.21520200
H	-2.30403500	2.29981800	0.97667600
C	-2.18902400	-1.95118100	2.72431300
H	-4.88216900	-1.53444200	2.85956600
H	-6.05696300	0.52749200	2.14434100
C	-0.82437300	-1.98101600	2.58344200
C	-0.15535200	-0.86816200	2.01498600
H	-2.72022700	-2.79927400	3.14710600
H	-0.26304400	-2.85355400	2.89421400
N	1.73464100	0.29208200	1.17717100
N	-0.83076400	0.22192600	1.61251000
Ni	0.25861000	1.40165800	0.39867000
C	-0.01021700	0.19324800	-1.20792200
C	1.17154100	0.30902800	-2.18098400
H	2.08370000	0.41888200	-1.57721100
H	-0.00148200	-0.80442300	-0.74949500
Cl	0.05718700	3.59775100	-0.07044300
C	1.37272200	-0.98435800	-3.00060000
H	0.52593300	-1.17092200	-3.66750600
H	2.28159800	-0.91284300	-3.61216700
H	1.47677200	-1.85416700	-2.34102600
C	1.10572400	1.53145300	-3.10538700
H	2.05138800	1.64587000	-3.64855300
H	0.31311300	1.42312300	-3.85488500
H	0.91738700	2.45040200	-2.54134700
C	-1.41078800	0.49419000	-1.75404100
H	-2.10367800	0.64537800	-0.91776800
H	-1.40337300	1.43405300	-2.31314900

C	-1.97427000	-0.62408400	-2.61024400
C	-2.13880100	-0.48485800	-3.99271200
C	-2.32856800	-1.84383800	-2.01668800
C	-2.63049400	-1.53852700	-4.76617500
H	-1.87699700	0.45789900	-4.46648200
C	-2.82188700	-2.89787600	-2.78306200
H	-2.21570300	-1.96088400	-0.94060300
C	-2.97108500	-2.75046000	-4.16461200
H	-2.74940900	-1.41048300	-5.83892500
H	-3.09349600	-3.83512000	-2.30382500
H	-3.35380000	-3.57140400	-4.76461500

IM9^{CSS}

C	-6.06281700	-1.40441300	0.04734500
C	-5.82631600	-0.28544000	-0.71843300
C	-4.55060600	0.33243900	-0.70365200
C	-3.51034800	-0.23644800	0.09752400
C	-3.78331200	-1.37679700	0.89566500
C	-5.03818800	-1.94247800	0.86573100
H	-5.00787700	1.94248200	-2.07914200
H	-7.04210000	-1.87363000	0.03605000
H	-6.60971600	0.14302300	-1.33781500
C	-4.24382000	1.49746600	-1.44750500
H	-2.99512700	-1.75095700	1.53991500
H	-5.24995600	-2.80896300	1.48488800
C	-2.01825000	1.45209500	-0.53184400
C	-2.99852400	2.06857900	-1.34849300
H	-2.76834400	2.97615000	-1.89287500
C	3.06915800	1.81388900	2.61589800
C	1.91692000	1.25476100	2.11608300
C	1.22848900	1.90154700	1.05941300
C	1.71444700	3.15180200	0.55659400
C	2.92602300	3.67761400	1.07224400
C	3.59128900	3.01703400	2.07901300
H	3.59111000	1.32087800	3.42905800
H	1.48689900	0.34903400	2.52662000
C	0.93238600	3.81641400	-0.41495500
H	3.30172100	4.61702400	0.67546400
H	4.51395600	3.42682100	2.47957200
C	-0.27988700	3.29215800	-0.79769000
C	-0.68700100	2.04279400	-0.27206000
H	1.27985400	4.76133700	-0.82438600
H	-0.91206900	3.82646500	-1.49596600

N	-2.26181500	0.31391600	0.11999200
N	0.08866500	1.34164000	0.56084200
Ni	-0.51249200	-0.63821100	0.60295200
C	0.26985800	-1.07852000	-1.21164200
C	1.08655400	-1.62107600	-0.19978600
H	-1.09314900	-1.93068500	0.56314800
Cl	-0.59025800	-1.03091600	2.89818200
C	-0.51235200	-1.96598200	-2.16433500
H	-0.90840400	-2.81859100	-1.59792700
H	0.92078200	-2.66606300	0.05498700
H	0.58297300	-0.13494700	-1.66384000
C	0.45954600	-2.50965800	-3.23086000
H	0.89469300	-1.68803600	-3.81460700
H	1.28295100	-3.06323500	-2.76775800
H	-0.05835500	-3.17850400	-3.92893800
C	-1.68131200	-1.23805400	-2.83602900
H	-2.14557100	-1.87098600	-3.60092200
H	-2.45019300	-0.96369600	-2.11360600
H	-1.33475100	-0.32057800	-3.32981100
C	2.41516100	-1.12632000	0.20394200
C	3.11279400	-0.14278400	-0.51793300
C	3.04477600	-1.70292700	1.32097800
C	4.38987100	0.25564100	-0.13215500
H	2.65709800	0.30217000	-1.39685800
C	4.32224900	-1.30702900	1.70530500
H	2.50318000	-2.44757900	1.89718800
C	5.00150300	-0.32368400	0.98092200
H	4.90941600	1.02066000	-0.70240600
H	4.78879600	-1.76352400	2.57410200
H	5.99943600	-0.01478300	1.27922600

IM10^{OSS}

C	-1.49210000	-5.60146100	-0.95660900
C	-0.14921700	-5.69818500	-0.65477900
C	0.64502800	-4.53370700	-0.53539800
C	0.03669000	-3.25532500	-0.72631300
C	-1.33950100	-3.17829800	-1.05201600
C	-2.08488900	-4.33501200	-1.16054200
H	2.52456500	-5.52410000	-0.09143900
H	-2.09580300	-6.49959300	-1.04555700
H	0.31806700	-6.66794800	-0.50496000
C	2.03436700	-4.56539700	-0.23636200
H	-1.78297500	-2.20176800	-1.22449100

H	-3.13926900	-4.26954300	-1.41132700
C	2.08004700	-2.15554900	-0.32153200
C	2.74327300	-3.39551700	-0.13707800
H	3.80348500	-3.41648000	0.08434100
C	2.03314200	3.86206500	-0.34229000
C	1.56877000	2.57666900	-0.51917800
C	2.42983000	1.47910800	-0.28667000
C	3.78464100	1.71113100	0.09929100
C	4.23113300	3.04348500	0.26401200
C	3.36867700	4.09949100	0.05497800
H	1.36269200	4.70029400	-0.50246900
H	0.54202100	2.38509600	-0.81449900
C	4.61210600	0.57672300	0.31407400
H	5.26164000	3.21813400	0.56214900
H	3.71558100	5.11936100	0.19197500
C	4.10059800	-0.68876600	0.16348500
C	2.73999300	-0.85514900	-0.19629900
H	5.64864700	0.72286300	0.60501100
H	4.72945800	-1.55446300	0.33308800
N	0.76407600	-2.10090000	-0.60253900
N	1.94070200	0.20690200	-0.41136200
Ni	0.00901400	-0.25172200	-0.43088100
C	-0.21727000	-0.33845500	1.61904500
C	-1.56680000	-0.98734300	1.85241400
H	-1.70664800	-1.80757700	1.13923700
H	0.60542800	-1.01004500	1.88215900
Cl	-1.93059700	0.59283000	-1.21443000
C	-1.72740700	-1.58896300	3.27083500
H	-0.88235000	-2.27552200	3.43577000
C	0.04490500	1.03460900	2.05066800
C	1.30773400	1.36829800	2.59054200
C	-0.90705500	2.07006200	1.91961500
C	1.59997700	2.66307900	3.00136500
H	2.05841600	0.58736100	2.68428500
C	-0.61017800	3.36536500	2.32924400
H	-1.86317700	1.85429800	1.45661800
C	0.64097400	3.67170400	2.87424400
H	2.58048300	2.89059700	3.40979500
H	-1.35741600	4.14595700	2.21428000
H	0.86802600	4.68603900	3.18949400
H	-2.37753000	-0.27803700	1.65905900
C	-1.70135000	-0.52372100	4.37241400
H	-2.49999000	0.21286600	4.21755000

H	-1.85322400	-0.98077600	5.35769500
H	-0.75351100	0.02109700	4.39333100
C	-3.02214000	-2.40986500	3.33188900
H	-3.02948700	-3.19702200	2.56872700
H	-3.14488100	-2.88408900	4.31279800
H	-3.89559400	-1.76824100	3.15892900

IM10^{triplet}

C	-1.49603500	-5.61359700	-1.01375200
C	-0.15224800	-5.71419200	-0.72220600
C	0.64053600	-4.54926400	-0.58848400
C	0.02743800	-3.26905800	-0.75343200
C	-1.35200900	-3.18804500	-1.06700300
C	-2.09366500	-4.34416300	-1.19159300
H	2.52448400	-5.54111100	-0.17658600
H	-2.09930900	-6.51075200	-1.11422100
H	0.31766400	-6.68534100	-0.59186000
C	2.03037400	-4.58163800	-0.30195500
H	-1.79940900	-2.21009700	-1.21923500
H	-3.14996300	-4.27767000	-1.43341100
C	2.06953200	-2.17197600	-0.35042100
C	2.73852600	-3.41167700	-0.19061300
H	3.80070200	-3.43359200	0.01978600
C	2.02231000	3.84454800	-0.29121500
C	1.56074100	2.56329900	-0.49360700
C	2.42246600	1.46335400	-0.27014700
C	3.77644500	1.68988300	0.12734800
C	4.22036000	3.02097000	0.31581700
C	3.35640700	4.07640000	0.11912300
H	1.35217900	4.68475500	-0.43957300
H	0.53629600	2.37710500	-0.79892700
C	4.60085200	0.55449000	0.32729600
H	5.24829000	3.19278300	0.62371800
H	3.69917300	5.09464400	0.27672800
C	4.09016100	-0.71048900	0.15637200
C	2.73246600	-0.86902500	-0.21090900
H	5.63590000	0.69551700	0.62594500
H	4.71806500	-1.57811300	0.31802200
N	0.75455700	-2.11843200	-0.61511500
N	1.93867100	0.19461200	-0.41507400
Ni	-0.00849100	-0.26057200	-0.41770900
C	-0.17209800	-0.35214000	1.62840600
C	-1.52100600	-1.00884000	1.89092800

H	-1.65406700	-1.85674300	1.20665400
H	0.64944900	-1.00591000	1.94381500
Cl	-1.87223900	0.55037400	-1.40678600
C	-1.70268000	-1.55916200	3.32594200
H	-0.85645300	-2.23492300	3.52714300
C	0.05992700	1.03266900	2.06318600
C	1.30519100	1.40396400	2.61880500
C	-0.90056500	2.05436900	1.88950600
C	1.57185700	2.71481000	2.99926100
H	2.06464500	0.63685400	2.75287900
C	-0.63058100	3.36556300	2.26840400
H	-1.85067200	1.81382600	1.42475600
C	0.60481300	3.70811100	2.82683300
H	2.54100000	2.96509000	3.42238000
H	-1.38935100	4.12976900	2.12022000
H	0.81045900	4.73317900	3.12155200
H	-2.33897800	-0.31496700	1.66447800
C	-1.69442100	-0.45575000	4.38975800
H	-2.49520400	0.27037500	4.20026900
H	-1.85438800	-0.87819000	5.38943400
H	-0.74999600	0.09471000	4.39998100
C	-2.99482700	-2.38282800	3.40450400
H	-2.99358500	-3.19661400	2.66932100
H	-3.12698500	-2.82336600	4.40001000
H	-3.86888700	-1.75084000	3.20063800

IM11^{doublet}

C	-1.97741400	-3.47360000	-4.11644300
C	-1.28434300	-2.44568100	-3.51886500
C	-1.97821200	-1.32374600	-2.99709400
C	-3.40662100	-1.29870000	-3.04336000
C	-4.08850600	-2.34742600	-3.71082700
C	-3.38736400	-3.40773800	-4.23506800
H	-0.23946900	-0.18434000	-2.38713500
H	-1.44472000	-4.32912700	-4.52064500
H	-0.19954200	-2.46502100	-3.45700600
C	-1.32430800	-0.19491800	-2.45036600
H	-5.16304200	-2.29457800	-3.79452700
H	-3.92310700	-4.20941700	-4.73160100
C	-3.47669400	0.82049400	-2.07411000
C	-2.05960900	0.88730100	-2.03544500
H	-1.56463400	1.76479800	-1.64001500
C	-8.60910900	3.25442400	-0.05643300

C	-7.77061200	2.29966900	-0.58035100
C	-6.44152300	2.64079200	-0.93192100
C	-5.97577400	3.97228500	-0.69356100
C	-6.87358400	4.93978200	-0.17586200
C	-8.16709600	4.58669200	0.13290100
H	-9.62622700	2.98240700	0.20434800
H	-8.11292200	1.28422000	-0.72176400
C	-4.61715200	4.24989900	-0.96851500
H	-6.51531200	5.95238700	-0.01143400
H	-8.85124100	5.32661800	0.53756400
C	-3.78645600	3.24691400	-1.40429200
C	-4.32242100	1.95445900	-1.63241200
H	-4.23518000	5.25480200	-0.80987600
H	-2.74056100	3.44912300	-1.59687700
N	-4.11604500	-0.26989300	-2.49086400
N	-5.61494000	1.69319500	-1.46268200
Ni	-6.16297300	-0.28547900	-1.78283200
Cl	-5.92197600	-0.47505900	0.54753300
C	-7.03669500	-0.10414300	-3.63833600
C	-6.04615300	0.39785500	-4.68512000
H	-5.21075100	-0.30219800	-4.76911500
H	-5.59937200	1.34849500	-4.36598100
C	-6.62615900	0.57285400	-6.10847200
H	-7.46389200	1.27983300	-6.05983900
C	-5.37068200	-5.52734800	-2.21604900
C	-6.25963500	-4.46485900	-2.16486700
C	-5.91030600	-3.26649300	-1.51625400
C	-4.67398200	-3.18772500	-0.86731400
C	-3.78846200	-4.26155600	-0.88200400
C	-4.11979500	-5.42524000	-1.58616200
H	-5.61562500	-6.44800400	-2.73623000
H	-7.22884700	-4.53589600	-2.64825700
H	-4.41612900	-2.28140600	-0.33429100
H	-2.84027800	-4.17091700	-0.36631900
O	-3.29981100	-6.50455100	-1.71895400
C	-1.99602300	-6.41475900	-1.16735800
H	-1.49788700	-7.35233300	-1.42000200
H	-1.43929400	-5.57322800	-1.60022400
H	-2.02690900	-6.30285500	-0.07602200
C	-6.85702800	-2.11409200	-1.65377500
O	-8.05607700	-2.29785600	-1.69316100
C	-8.21281700	0.77713300	-3.40613400
C	-8.17586200	2.16492100	-3.65787200

C	-9.42331900	0.24173300	-2.91657900
C	-9.28918900	2.97255900	-3.44457300
H	-7.26112900	2.61861700	-4.02360000
C	-10.52823900	1.05598600	-2.67779300
H	-9.47074400	-0.81948200	-2.70277900
C	-10.47311200	2.42621200	-2.94653200
H	-9.22608200	4.03742200	-3.65336300
H	-11.44360900	0.61359600	-2.29298100
H	-11.34115300	3.05694500	-2.77566600
H	-7.38050200	-1.10850700	-3.88441900
C	-5.55470700	1.16084600	-7.03435600
H	-4.69330400	0.48386500	-7.11251000
H	-5.94475300	1.32132000	-8.04655500
H	-5.18744700	2.12366000	-6.65794400
C	-7.15958500	-0.75263200	-6.66457200
H	-7.51477900	-0.63285900	-7.69484500
H	-6.37014700	-1.51710300	-6.67043800
H	-7.99355900	-1.13353200	-6.06678400

IM12^{doublet}

C	-0.88662200	-2.00032400	-3.32104600
C	-0.59293200	-0.74135400	-2.84736400
C	-1.62356600	0.09855900	-2.35654000
C	-2.97214700	-0.37841900	-2.34530000
C	-3.24588300	-1.66736900	-2.86036500
C	-2.22526600	-2.46158900	-3.33020900
H	-0.38311900	1.81270200	-1.89093100
H	-0.09336700	-2.64052600	-3.69521700
H	0.42847200	-0.37056100	-2.84584000
C	-1.39316500	1.41228100	-1.88801100
H	-4.26787400	-2.01141100	-2.86703100
H	-2.45427700	-3.45386000	-3.70664200
C	-3.75556000	1.62535500	-1.45199400
C	-2.44651700	2.17304900	-1.45030900
H	-2.27735000	3.18696600	-1.11289200
C	-9.59815300	2.26531000	-0.13433500
C	-8.45430800	1.67060700	-0.61543600
C	-7.23214400	2.39089200	-0.61058300
C	-7.19749500	3.71380200	-0.07066500
C	-8.39781400	4.30089500	0.40205300
C	-9.57621300	3.59108200	0.36572500
H	-10.52893900	1.70677500	-0.12947100
H	-8.47065200	0.64638000	-0.97137200

C	-5.94177900	4.36374000	-0.01739100
H	-8.36585400	5.31035900	0.80293000
H	-10.49352100	4.03980600	0.73479200
C	-4.81174800	3.71565200	-0.45071800
C	-4.92534700	2.40836400	-0.98954400
H	-5.87984300	5.36966900	0.38879600
H	-3.84764900	4.20130000	-0.37712200
N	-3.99880600	0.38543400	-1.87227500
N	-6.10236200	1.80366300	-1.09652400
Ni	-6.08155800	-0.16481800	-1.74780900
Cl	-5.82582100	-0.72279000	0.53727200
H	-8.04687900	1.64014000	-3.31897200
C	-7.96589800	0.64837700	-3.77705300
C	-6.53030500	0.13035700	-3.76800900
H	-8.34103100	0.73326700	-4.80956600
C	-5.54297500	1.20780200	-4.23554300
H	-8.63897600	-0.03436200	-3.25022200
H	-4.53019000	0.79474000	-4.27967600
H	-5.51620200	2.03255800	-3.51807800
C	-5.82995500	1.85137000	-5.61760200
H	-6.82260500	2.31471200	-5.61117500
H	-5.83376900	1.08763800	-6.40271500
C	-4.77720500	2.89007200	-5.91297300
C	-4.89361400	4.18872400	-5.39856200
C	-3.61905900	2.56071900	-6.62827300
C	-3.88540300	5.13213100	-5.59529000
H	-5.78725500	4.45873600	-4.83967500
C	-2.60729500	3.50043100	-6.82903900
H	-3.51241700	1.55569500	-7.03041200
C	-2.73664700	4.79071300	-6.31229000
H	-3.99845800	6.13601500	-5.19402400
H	-1.71911700	3.22585200	-7.39214500
H	-1.95179100	5.52516800	-6.47080200
C	-6.41552400	-1.10853000	-4.65755400
H	-6.60769000	-0.84566600	-5.71010100
H	-5.41878700	-1.55945100	-4.61852300
H	-7.14601600	-1.87590000	-4.39223700
C	-6.37896000	-5.48891000	-2.83111400
C	-6.94234500	-4.22869300	-2.71395900
C	-6.32643200	-3.23712700	-1.92869100
C	-5.15900500	-3.55520100	-1.22975600
C	-4.59769400	-4.82852400	-1.31980800
C	-5.20005100	-5.79715700	-2.13280900

H	-6.83363200	-6.25909200	-3.44574600
H	-7.86585500	-3.99179200	-3.23236300
H	-4.71378100	-2.80627500	-0.58492100
H	-3.70342500	-5.05231700	-0.75073600
O	-4.72518900	-7.06189800	-2.30585200
C	-3.55269800	-7.43464600	-1.60102500
H	-3.35619400	-8.47295000	-1.87329300
H	-2.69452600	-6.81353900	-1.89044800
H	-3.69663100	-7.36307800	-0.51532000
C	-6.95361000	-1.88799300	-1.87467200
O	-8.16668000	-1.75442500	-1.84721000

IM13^{doublet}

C	-1.69723000	-2.73825100	-3.91652000
C	-0.99357900	-1.55538500	-3.82749200
C	-1.58352500	-0.40830100	-3.24560700
C	-2.92023400	-0.49000100	-2.75000700
C	-3.62206000	-1.71387600	-2.85254700
C	-3.01963900	-2.81524500	-3.42513100
H	0.10932600	0.92772100	-3.49646100
H	-1.23686600	-3.61367100	-4.36459000
H	0.02407700	-1.48547000	-4.20254800
C	-0.90808600	0.83574200	-3.12725800
H	-4.63866400	-1.76512100	-2.47255000
H	-3.56729500	-3.74988600	-3.49865200
C	-2.87245800	1.76230900	-2.07544600
C	-1.54597900	1.90454400	-2.54970600
H	-1.03570300	2.85551300	-2.45747800
C	-7.78555700	4.05651900	0.54101000
C	-6.97814100	3.11717800	-0.06421400
C	-5.66450100	3.46895800	-0.46309200
C	-5.19301400	4.79971400	-0.23171500
C	-6.04949300	5.73788000	0.39223700
C	-7.32343800	5.37342900	0.77213700
H	-8.79144200	3.78208900	0.84489700
H	-7.31100100	2.10175500	-0.25287700
C	-3.87296100	5.11099800	-0.64688100
H	-5.68413300	6.74688800	0.56471600
H	-7.97666300	6.09730800	1.25033600
C	-3.09778100	4.15186400	-1.24631200
C	-3.62712300	2.85002400	-1.44531100
H	-3.48666900	6.11368600	-0.48445200
H	-2.08959100	4.38636800	-1.56477200

N	-3.54053300	0.59530500	-2.17503300
N	-4.87066200	2.52919100	-1.06279100
Ni	-5.37805200	0.58064400	-1.47654700
H	-6.81756200	0.03773000	-1.11016500

IM14^{doublet}

C	5.12725200	-1.95310600	-1.18592100
C	4.26703500	-3.03438600	-1.06921400
C	2.88726600	-2.85162100	-0.85997500
C	2.35109100	-1.52657500	-0.76881100
C	3.25331700	-0.44385900	-0.88417000
C	4.60829200	-0.65256800	-1.08916000
H	2.36069700	-4.96302700	-0.80277300
H	6.18946200	-2.10985700	-1.34625900
H	4.64849800	-4.05043200	-1.13669200
C	1.97849600	-3.94859300	-0.73186700
H	2.87377800	0.56512600	-0.80014600
H	5.27214600	0.20385800	-1.17044200
C	0.16522000	-2.38040000	-0.41353200
C	0.65270900	-3.71240300	-0.50772700
H	-0.03210400	-4.54361400	-0.39026400
C	-4.23795100	1.40075600	1.26156800
C	-2.98670500	1.01077000	0.81552200
C	-2.72612000	-0.33038300	0.46281300
C	-3.77974400	-1.28471000	0.62420500
C	-5.04737800	-0.85655100	1.06628900
C	-5.28584700	0.47135000	1.37756900
H	-4.40249400	2.43996300	1.53344200
H	-2.17815900	1.72066500	0.76253000
C	-3.49224000	-2.65755000	0.34944900
H	-5.83571700	-1.59840700	1.16926500
H	-6.26603400	0.78808900	1.72122300
C	-2.22454500	-3.02934500	0.00940900
C	-1.19940900	-2.05366900	-0.12997300
H	-4.28451800	-3.39479200	0.44451400
H	-1.99341000	-4.07317700	-0.16547500
N	1.00777700	-1.31002500	-0.57277200
N	-1.47855900	-0.71621000	0.01769300
Ni	-0.05523900	0.33764700	-0.66660800
C	-0.84267900	1.93618200	-1.31442200
C	0.54710800	2.10332800	-1.84093900
H	1.17693700	1.19895700	-1.43965200
H	-1.15386900	2.69477900	-0.60044500

C	1.32246000	3.33574200	-1.31288400
H	2.11701300	3.58453200	-2.02764400
H	0.63156000	4.18662700	-1.30721900
H	-1.61428200	1.73978400	-2.06279200
C	0.67196200	1.94540800	-3.36225400
H	1.71635300	1.82213000	-3.67112900
H	0.10483500	1.07631100	-3.70928100
H	0.27062400	2.83666300	-3.85813400
C	1.98407100	3.19820500	0.07710700
H	2.81659700	2.48897600	0.00765900
H	2.43284100	4.16864100	0.32520300
C	1.05948000	2.76409300	1.19082000
C	1.13090500	1.46869500	1.71809700
C	0.08604200	3.63774600	1.69449000
C	0.24316500	1.05002600	2.71412800
H	1.89822800	0.78537800	1.36706500
C	-0.79624700	3.22609800	2.69176900
H	0.02116600	4.64949500	1.29998400
C	-0.72425600	1.92565000	3.20081800
H	0.30600200	0.03478000	3.09403400
H	-1.54433700	3.91711000	3.07083200
H	-1.42408600	1.59917600	3.96396300

IM15^{doublet}

C	0.35438600	-0.18915600	-2.35115300
C	0.21533000	1.17959000	-2.40234300
C	-1.07496000	1.76770500	-2.43605700
C	-2.22753500	0.92478900	-2.40904600
C	-2.05527300	-0.48021200	-2.36017700
C	-0.79129400	-1.02174000	-2.33219200
H	-0.43671700	3.83654800	-2.51375100
H	1.34365100	-0.63573900	-2.32860600
H	1.08691100	1.82798500	-2.42189300
C	-1.29072700	3.16499900	-2.50066900
H	-2.92975600	-1.11897900	-2.34411800
H	-0.67409600	-2.10038700	-2.29719700
C	-3.66631800	2.75947800	-2.49621300
C	-2.56986000	3.66018400	-2.53682200
H	-2.73911000	4.72889400	-2.55905400
C	-9.61584100	2.12507900	-1.64476900
C	-8.29046800	1.75455200	-1.69663800
C	-7.30991400	2.69923600	-2.08850600
C	-7.71929100	4.03336700	-2.41643500

C	-9.09251300	4.37741400	-2.35416800
C	-10.02532700	3.43956800	-1.97573500
H	-10.35834300	1.39402000	-1.33928000
H	-7.98902400	0.74721000	-1.43367000
C	-6.71842900	4.95454000	-2.79824200
H	-9.38911600	5.39175500	-2.60715900
H	-11.07705700	3.70545800	-1.92605300
C	-5.40493300	4.56101000	-2.82504700
C	-5.07190500	3.22652500	-2.48031400
H	-6.99998300	5.96850400	-3.06932900
H	-4.63285700	5.25446100	-3.13261000
N	-3.48711000	1.44635600	-2.43550100
N	-5.99569600	2.32848000	-2.14158600
Ni	-5.18325300	0.35828800	-1.86927400
Cl	-4.59249000	0.79107000	0.34804900
C	-5.89727300	-0.27756200	-3.63167000
C	-5.36118400	0.51041700	-4.83397300
H	-5.16348500	1.54869800	-4.53792600
C	-5.25274300	-4.74170800	-1.70982600
C	-5.98545300	-3.56610000	-1.69063600
C	-5.44344500	-2.39140700	-1.13579600
C	-4.16467300	-2.43707200	-0.57308200
C	-3.42750700	-3.62273300	-0.56896100
C	-3.96481800	-4.77743300	-1.15018400
H	-5.65241900	-5.65131900	-2.14641300
H	-6.98560800	-3.53586100	-2.11070200
H	-3.76207400	-1.54708000	-0.10169900
H	-2.44973700	-3.63339000	-0.10201500
O	-3.32569100	-5.97772000	-1.21705800
C	-2.02211900	-6.06924600	-0.66754000
H	-1.69822400	-7.09812400	-0.83229300
H	-1.32603200	-5.38364300	-1.16924400
H	-2.02323900	-5.85514900	0.40903000
C	-6.25587000	-1.13617000	-1.25176600
O	-7.45640800	-1.14555300	-1.08474900
H	-5.70571400	-1.34900300	-3.76981700
H	-6.97911300	-0.14454300	-3.53263500
C	-4.04489100	-0.09184400	-5.34984500
H	-4.26317000	-0.99596300	-5.93601300
H	-3.43475700	-0.42290800	-4.50557900
C	-3.19595700	0.86966400	-6.19982500
H	-3.77192100	1.20749800	-7.07003400
H	-2.97334500	1.76319400	-5.60081900

C	-1.90788200	0.22454900	-6.65174100
C	-1.84342300	-0.50084500	-7.84779100
C	-0.76501800	0.27974200	-5.84520200
C	-0.66997400	-1.15335900	-8.22779300
H	-2.72315100	-0.55474300	-8.48537100
C	0.40943100	-0.37289500	-6.21742700
H	-0.79751300	0.83901800	-4.91632500
C	0.46190600	-1.09275900	-7.41242500
H	-0.63886700	-1.70829400	-9.16171600
H	1.28242000	-0.31612200	-5.57234500
H	1.37628700	-1.59996500	-7.70770200
C	-6.42214800	0.56389400	-5.94819900
H	-6.05716100	1.10040700	-6.83313800
H	-6.70564000	-0.44881100	-6.26113300
H	-7.32775700	1.07221300	-5.59793200

IM16^{doublet}

C	2.22534600	-4.92526700	-0.75780700
C	2.99511700	-3.79043400	-0.85256100
C	2.49883900	-2.54478700	-0.39381000
C	1.17081000	-2.46188600	0.13228300
C	0.41148500	-3.65326100	0.24393200
C	0.93165700	-4.85237300	-0.18927600
H	4.28204500	-1.40756000	-0.84830800
H	2.60726400	-5.87745800	-1.11273900
H	3.99196900	-3.82359800	-1.28178400
C	3.27811700	-1.36715400	-0.43772100
H	-0.58150200	-3.59224300	0.66877600
H	0.33513100	-5.75496000	-0.09749900
C	1.42750500	-0.15938600	0.51384800
C	2.75721100	-0.19159500	0.03499300
H	3.35221000	0.71135100	0.02612300
C	-2.88385400	2.89157000	3.41603600
C	-2.24942600	1.80956800	2.84636500
C	-1.02498700	1.99154100	2.15619000
C	-0.43971100	3.29746200	2.11142900
C	-1.12833800	4.39054000	2.69237300
C	-2.33382200	4.19265700	3.32693900
H	-3.82263100	2.74279600	3.94076200
H	-2.67610200	0.81794200	2.89368400
C	0.82535000	3.43384300	1.49515000
H	-0.67937600	5.37864900	2.63992700
H	-2.85797800	5.03115600	3.77572600

C	1.46555800	2.32898200	0.99674300
C	0.81142000	1.07351400	1.04014600
H	1.28637000	4.41583700	1.43614000
H	2.43804700	2.42361300	0.53320000
N	0.64735700	-1.25169600	0.53481700
N	-0.40872900	0.92194600	1.56156500
Ni	-1.19684100	-0.84099400	0.82824200
C	0.70455400	2.07792600	-2.20917200
C	1.40679800	1.01218900	-2.73671000
C	0.78513800	-0.24737400	-2.88362800
C	-0.55595500	-0.39331600	-2.51051900
C	-1.27451000	0.67307700	-1.97643200
C	-0.63569300	1.90925700	-1.80161500
H	1.16122400	3.05342900	-2.07706700
H	2.44444600	1.12167300	-3.03655100
H	-1.03193300	-1.36356100	-2.60728200
H	-2.29439500	0.51711200	-1.65070900
O	-1.20593900	2.99045500	-1.22704000
C	-2.57917000	2.90879900	-0.82735300
H	-2.78995000	3.85526900	-0.32818700
H	-3.22690800	2.79880200	-1.70526100
H	-2.75321900	2.07699900	-0.13958000
C	1.53832900	-1.40055100	-3.38029600
O	2.70473800	-1.46895500	-3.65607900
Cl	-3.37157400	-0.36855100	0.78629300
H	-1.63162500	-2.04604400	0.17255300

IM17^{doublet}

C	-1.80377100	4.88787900	0.03827500
C	-1.13931700	3.70329200	-0.21440600
C	-1.80206700	2.46986600	-0.07072400
C	-3.14085900	2.45868000	0.33075800
C	-3.82506200	3.64466900	0.58920500
C	-3.15303800	4.86647500	0.44212800
H	-1.31451400	5.85076200	-0.06546400
H	-0.09998200	3.69781200	-0.52691800
H	-3.65693500	1.50768500	0.44313900
H	-4.86229600	3.61161500	0.89932400
O	-3.71350900	6.08148300	0.66471000
C	-5.07415100	6.13344500	1.06872700
H	-5.31098400	7.19207500	1.18276300
H	-5.73277900	5.69107700	0.31076300
H	-5.22648900	5.61984300	2.02636900

C	-1.09771700	1.20637100	-0.33904600
O	0.06449100	1.11700200	-0.69253600
H	-1.71817100	0.29312100	-0.19319200

TS1^{doublet}

C	-1.51157600	-2.35170300	-4.04746400
C	-0.91615700	-1.10877700	-4.02692900
C	-1.58125100	-0.00743800	-3.43700600
C	-2.88043700	-0.20122800	-2.87444800
C	-3.46616200	-1.48907100	-2.89294200
C	-2.78921600	-2.54118200	-3.47115600
H	-0.02953200	1.46808000	-3.78019500
H	-0.99593900	-3.19394300	-4.49883400
H	0.07086900	-0.95687100	-4.45530700
C	-1.01859300	1.29331000	-3.36598500
H	-4.43587500	-1.63346900	-2.42914200
H	-3.24113500	-3.52797200	-3.47937800
C	-3.01407300	2.06506400	-2.25824100
C	-1.71831600	2.31413100	-2.77314600
H	-1.28870200	3.30611900	-2.71202000
C	-8.09243100	4.00996600	0.33530400
C	-7.18891300	3.11564700	-0.19730100
C	-5.93011000	3.57516400	-0.65460200
C	-5.59479600	4.95779000	-0.52506300
C	-6.54661600	5.84889200	0.02684700
C	-7.77648400	5.38535400	0.44191100
H	-9.05582300	3.65242500	0.68523900
H	-7.41641500	2.05791100	-0.26533700
C	-4.31436200	5.36965800	-0.97363300
H	-6.28673700	6.90009200	0.12228100
H	-8.50287100	6.07244000	0.86530300
C	-3.45009000	4.45450100	-1.51726100
C	-3.85464800	3.10187600	-1.64506000
H	-4.02798200	6.41397400	-0.88257200
H	-2.47363800	4.76610300	-1.86479600
N	-3.56946300	0.84524800	-2.32179500
N	-5.06138400	2.69193400	-1.23252900
Ni	-5.42096900	0.75904400	-1.61350200
C	-4.23153600	4.17795000	-5.03959300
C	-4.56895100	2.84306900	-4.91053900
C	-5.77151800	2.47026100	-4.26921600
C	-6.63503300	3.47119100	-3.80407800
C	-6.30220600	4.81162800	-3.93951400

C	-5.08429600	5.17338500	-4.53509400
H	-3.30130500	4.47941000	-5.50931000
H	-3.90190500	2.07014200	-5.27545200
H	-7.55780400	3.19273000	-3.31310300
H	-6.98146700	5.56139400	-3.55448300
O	-4.64283200	6.45025400	-4.66005800
C	-5.44924600	7.49130600	-4.12552900
H	-4.89966000	8.41625900	-4.30492600
H	-6.42257900	7.54197600	-4.62887600
H	-5.60567800	7.35796900	-3.04771700
C	-5.96792700	1.04338600	-4.07359800
O	-5.52896100	0.08655500	-4.62645700
Cl	-7.63607300	0.65674400	-2.87179600
Br	-5.77954000	-0.69943100	0.23901300

TS2^{doublet}

C	6.23018000	-0.02475700	-0.67937400
C	5.50528200	0.45885000	-1.75050900
C	4.09220500	0.44287000	-1.72586400
C	3.42871300	-0.07735200	-0.57503200
C	4.18667500	-0.57401700	0.50928000
C	5.56592200	-0.54458100	0.45317700
H	3.76551800	1.35293200	-3.66970400
H	7.31549700	-0.00768400	-0.70573900
H	6.00920200	0.86059900	-2.62547400
C	3.28508400	0.94218000	-2.78629500
H	3.67140400	-0.97620500	1.37534100
H	6.14456300	-0.92732400	1.28809800
C	1.31119900	0.37555300	-1.52188000
C	1.91694200	0.89884200	-2.69102400
H	1.29837900	1.28110500	-3.49405800
C	-3.48959600	-0.30957000	2.03433700
C	-2.15995700	-0.28031100	1.66984300
C	-1.80084300	-0.01639300	0.32703500
C	-2.82194700	0.25267900	-0.63263400
C	-4.17570300	0.19624900	-0.23003300
C	-4.50723800	-0.08604800	1.07933500
H	-3.75633400	-0.51125200	3.06762400
H	-1.37292400	-0.46214900	2.39380700
C	-2.42468900	0.59003600	-1.95300500
H	-4.94709200	0.39960300	-0.96759200
H	-5.54966000	-0.11549100	1.38326400
C	-1.09382300	0.65526900	-2.26879400

C	-0.12608500	0.33735400	-1.28417600
H	-3.18465800	0.81047500	-2.69637300
H	-0.77842600	0.92365200	-3.26967500
N	2.06202600	-0.07768400	-0.50095000
N	-0.47940400	-0.01026300	-0.03197000
Ni	1.07208900	-0.68923400	1.04512100
C	-1.78658800	-3.42889800	-2.01764200
C	-0.49963200	-3.22200100	-1.54135000
C	-0.27342400	-3.05163600	-0.16465900
C	-1.34967900	-3.13929600	0.72215200
C	-2.63713700	-3.39398500	0.25387000
C	-2.86497000	-3.50398800	-1.12284500
H	-1.98676400	-3.53154500	-3.07944500
H	0.33681900	-3.16043800	-2.23119800
H	-1.17401600	-2.99023900	1.78192800
H	-3.45381400	-3.45212200	0.96227000
O	-4.09423600	-3.67389400	-1.68871900
C	-5.22346100	-3.65620900	-0.83082000
H	-6.09495900	-3.75716400	-1.48024100
H	-5.20396600	-4.49308700	-0.12036300
H	-5.28420700	-2.71168300	-0.27487800
C	1.05801900	-2.56299000	0.28026900
O	2.11674000	-3.10830600	0.08258000
Cl	0.93015900	-1.43351100	3.17204100
H	1.40878500	0.77556200	1.61807700
C	2.19923800	1.96617400	2.46752500
H	1.40793600	1.91444600	3.21133500
H	3.06444200	1.33937400	2.66604600
C	2.29254900	3.03124400	1.61699100
C	1.07965500	3.88331400	1.35946400
H	1.34265700	4.93803400	1.20704700
H	0.40518000	3.83784800	2.22059200
C	0.33871700	3.33914500	0.10379000
H	0.45743500	2.25556800	0.12814600
H	0.83832200	3.69224900	-0.80503600
C	-1.13923700	3.63265900	0.03000900
C	-1.99669200	3.19397400	1.04982000
C	-1.70171400	4.26242200	-1.08487200
C	-3.37403400	3.37510200	0.95509500
H	-1.58344700	2.67896200	1.91228800
C	-3.08275400	4.44426700	-1.18711900
H	-1.05049500	4.60342600	-1.88650800
C	-3.92374100	3.99905900	-0.16743600

H	-4.01973000	3.00848700	1.74723400
H	-3.49949600	4.93418100	-2.06328500
H	-4.99879500	4.13583900	-0.24540200
C	3.46453700	3.20661500	0.69527400
H	4.28010400	2.51858600	0.93501800
H	3.17607500	3.02350500	-0.35134300
H	3.84821300	4.23567100	0.73452800

TS2'^{doublet}

C	-3.41718800	-1.30430800	5.50683000
C	-3.31597800	0.07199800	5.56941000
C	-3.59718100	0.86532100	4.43374500
C	-4.01725600	0.22388300	3.22982100
C	-4.08827700	-1.18810300	3.17623900
C	-3.79083700	-1.93383400	4.29885600
H	-3.16236200	2.79433000	5.32979900
H	-3.19175300	-1.90644500	6.38224300
H	-3.00909700	0.56481500	6.48818500
C	-3.47865200	2.28273300	4.42537200
H	-4.38836200	-1.66159000	2.24733500
H	-3.84876000	-3.01720900	4.25219900
C	-4.20708700	2.29820000	2.12828200
C	-3.75014800	2.98562800	3.28139200
H	-3.64792100	4.06400500	3.26294000
C	-6.24718500	2.17668100	-3.52887200
C	-5.94158500	1.71489700	-2.26661200
C	-5.41476300	2.60242600	-1.29987700
C	-5.24258400	3.98170600	-1.62359100
C	-5.57889800	4.42492500	-2.92403300
C	-6.06191100	3.53648700	-3.86223100
H	-6.61671000	1.48595900	-4.27893900
H	-6.08068200	0.67147400	-2.00455600
C	-4.72782000	4.84007000	-0.61304400
H	-5.44100200	5.47425200	-3.17100800
H	-6.29843900	3.87830900	-4.86473300
C	-4.39975300	4.33546000	0.61933400
C	-4.55915400	2.95016600	0.87518700
H	-4.59842400	5.89653700	-0.83053500
H	-4.00821400	4.98611000	1.39202500
N	-4.36284300	0.96076600	2.12926100
N	-5.04162400	2.12180400	-0.07253100
Ni	-5.30420300	0.28189600	0.52418600

C	-7.55162800	2.03291400	4.57704400
C	-7.61932300	1.98076100	3.19169100
C	-7.39684600	0.76783100	2.51748700
C	-7.15520400	-0.39288100	3.25796300
C	-7.13167500	-0.35586100	4.65027900
C	-7.29420100	0.86666600	5.31354300
H	-7.68848000	2.96538100	5.11544200
H	-7.81535600	2.88109200	2.61703900
H	-6.96710900	-1.32419500	2.73424100
H	-6.93445000	-1.26815500	5.19908700
O	-7.20868700	1.02534200	6.66536300
C	-6.86251900	-0.10980700	7.44222300
H	-6.80190500	0.24045500	8.47424500
H	-5.89263700	-0.52081500	7.13379900
H	-7.62643600	-0.89527400	7.37174600
C	-7.19204800	0.80229200	1.04394600
O	-7.96567900	1.25276500	0.23483700
Cl	-5.87372000	-1.83929400	0.02599400
H	-3.82323200	-0.14627500	0.07640900
C	-2.30109000	-1.80258000	-0.36083700
H	-2.81889000	-2.56516300	-0.93295200
H	-1.76911200	-2.12509800	0.53007500
C	-2.45744000	-0.47183600	-0.65229600
C	-3.02382400	-0.05136800	-2.00050400
H	-3.85358500	-0.71492900	-2.26578000
H	-3.44379900	0.95222800	-1.90852400
C	-2.01075400	-0.02512200	-3.16409500
H	-1.12662000	0.55720800	-2.87788000
H	-1.67000600	-1.04425500	-3.38062400
C	-2.66723600	0.59710000	-4.37409100
C	-3.46748800	-0.17093600	-5.22932500
C	-2.57839700	1.97546600	-4.60378200
C	-4.15791600	0.42084100	-6.28743400
H	-3.55236800	-1.24180400	-5.05939800
C	-3.26490000	2.57241300	-5.66070600
H	-1.97008200	2.58635400	-3.94053000
C	-4.05852200	1.79633500	-6.50701200
H	-4.77091700	-0.19261800	-6.94231500
H	-3.18352500	3.64407700	-5.82022500
H	-4.59315300	2.25836000	-7.33244900
C	-1.61180100	0.56636800	0.06584900
H	-2.12239100	1.53371000	0.09583600
H	-0.65502400	0.70989800	-0.45207300

H	-1.39793300	0.25884600	1.09393600
TS3 ^{doublet}			
C	-4.55234200	-3.18172100	-0.80112400
C	-3.50754000	-3.88073800	-0.23974500
C	-2.18395200	-3.38332000	-0.33347500
C	-1.95366200	-2.15067300	-1.01714500
C	-3.03818900	-1.46562000	-1.61769500
C	-4.31207100	-1.97257100	-1.49860500
H	-1.20355100	-4.97881800	0.75522300
H	-5.56709600	-3.55820700	-0.71521400
H	-3.68083300	-4.81466500	0.28796700
C	-1.06211800	-4.03671400	0.23253000
H	-2.84098600	-0.54339800	-2.15395300
H	-5.14470500	-1.43649500	-1.94298100
C	0.34031600	-2.23244500	-0.52546300
C	0.18916400	-3.47911600	0.12695700
H	1.04625100	-3.97449800	0.56519500
C	3.74912200	2.46239800	-2.14073300
C	2.63205800	1.66147500	-2.05747500
C	2.70056500	0.43459500	-1.35165700
C	3.94199500	0.01114100	-0.78868300
C	5.06594200	0.86824500	-0.87612200
C	4.96781000	2.07554700	-1.53097100
H	3.69417200	3.40514100	-2.67667900
H	1.69185400	1.94278800	-2.52211000
C	3.97825100	-1.26005900	-0.16669000
H	5.99517200	0.56029100	-0.40711300
H	5.82942600	2.73354000	-1.59004900
C	2.84170200	-2.02715900	-0.09908900
C	1.62621500	-1.51137100	-0.60979000
H	4.91106000	-1.61329100	0.25977100
H	2.86962300	-3.00313600	0.36887400
N	-0.70408800	-1.60285000	-1.07212700
N	1.57060300	-0.31672600	-1.20385900
Ni	-0.33270600	0.37178300	-1.36486100
Cl	-1.17744400	1.60246000	-3.08870700
H	-0.94273700	2.61222900	2.64538700
C	-0.90716600	3.36465100	1.85341300
C	0.05894800	3.01376300	0.75911100
H	-0.61716500	4.32231000	2.32360700
C	1.47391600	2.62694700	1.11011600
H	-1.92098200	3.49171200	1.46299500

H	2.15465700	3.44018900	0.80337500
H	1.76769600	1.77189900	0.49774100
C	1.76440000	2.26465400	2.57670300
H	0.99881500	1.57340100	2.93337800
H	1.71865500	3.16516500	3.20269400
C	3.11830900	1.60690000	2.70322700
C	3.21754800	0.21724100	2.84221600
C	4.30018700	2.35609100	2.62962300
C	4.46404900	-0.40448900	2.92891900
H	2.30552900	-0.37184900	2.86585100
C	5.54833500	1.73742400	2.70030500
H	4.23891000	3.43621100	2.51657600
C	5.63515500	0.35172900	2.85585500
H	4.52006200	-1.48325500	3.05292200
H	6.45333800	2.33688300	2.64443700
H	6.60626700	-0.13114600	2.92823800
C	-0.09729300	3.79798800	-0.51099100
H	-1.10446700	3.72662200	-0.93035500
H	0.10013900	4.86845100	-0.31244800
H	0.60219200	3.47863600	-1.28604900
C	-4.20175800	-0.27029700	1.89333000
C	-2.82456200	-0.19544900	1.77470100
C	-2.22771000	0.64553600	0.81791400
C	-3.05326900	1.42279100	0.00061100
C	-4.44135200	1.37858600	0.12599600
C	-5.02049900	0.51587000	1.06463100
H	-4.67790500	-0.93253700	2.60971900
H	-2.17693300	-0.80010800	2.40189600
H	-2.60840500	2.05047300	-0.76375000
H	-5.05315000	1.99567400	-0.52105700
O	-6.36241400	0.36113800	1.24493700
C	-7.23445200	1.11573700	0.42033100
H	-7.08868500	0.87793800	-0.64176200
H	-8.24662200	0.83772300	0.71897300
H	-7.09475200	2.19447900	0.56737100
C	-0.74723400	0.56276100	0.59746200
O	-0.03002000	0.04191500	1.45213600

TS4^{doublet}

C	-2.34508200	-1.89960100	-4.59660000
C	-1.97699000	-0.57899600	-4.77029100
C	-2.66516400	0.45140700	-4.09165700
C	-3.74926700	0.11042900	-3.22416900

C	-4.09176400	-1.24991500	-3.03739700
C	-3.40087500	-2.23250000	-3.72127300
H	-1.52660500	2.11768200	-4.88767800
H	-1.81388000	-2.68601300	-5.12414400
H	-1.15558400	-0.31362700	-5.43062700
C	-2.35144200	1.82914800	-4.24196300
H	-4.89165000	-1.50558800	-2.35178700
H	-3.67401000	-3.27314900	-3.57750300
C	-4.17177400	2.38116300	-2.76367200
C	-3.08591100	2.78054700	-3.58260800
H	-2.85519600	3.83102500	-3.70670600
C	-8.92671900	3.72714900	0.68399500
C	-8.01367100	2.94421100	0.00912900
C	-6.94896400	3.55319100	-0.69725700
C	-6.82177200	4.97589400	-0.69101400
C	-7.77572800	5.74893900	0.01118600
C	-8.81197300	5.13651200	0.68507600
H	-9.73858300	3.25427700	1.22779500
H	-8.08709900	1.86103800	0.02228300
C	-5.72225000	5.54020600	-1.39423500
H	-7.67312400	6.83086500	0.01475200
H	-9.53916700	5.73472200	1.22537600
C	-4.84592600	4.72923500	-2.06928000
C	-5.04128400	3.32388000	-2.05848800
H	-5.58591900	6.61823200	-1.38891700
H	-4.00773300	5.15706200	-2.60461200
N	-4.47986400	1.08424500	-2.60341100
N	-6.06020300	2.77246600	-1.37994900
Ni	-5.99829600	0.77377300	-1.32953600
Cl	-7.52645400	-0.92376800	-1.78949600
C	-5.47322800	2.07038300	-5.86782400
C	-5.72542600	0.74170900	-5.65129800
C	-6.75527600	0.35092700	-4.73266300
C	-7.47831300	1.35858700	-4.03377700
C	-7.23641700	2.69803600	-4.30473600
C	-6.22431100	3.06888400	-5.19638900
H	-4.69404500	2.38564800	-6.55213700
H	-5.13820300	-0.01871000	-6.15405400
H	-8.25107100	1.06745100	-3.33685200
H	-7.81459000	3.44546800	-3.77634900
O	-5.89680500	4.34620700	-5.50647400
C	-6.75797200	5.38709200	-5.05085600
H	-6.35544400	6.30889700	-5.47274400

H	-7.78129000	5.23135500	-5.41337400
H	-6.75870300	5.45420000	-3.95878100
C	-6.88658700	-1.00547200	-4.49527200
O	-6.97318300	-2.14501700	-4.71092500
Br	-4.93688600	0.45389300	0.80236600

TS5^{CSS}

C	4.27427400	1.83246700	-1.14030500
C	3.79505600	2.08232500	0.12506000
C	2.43397200	1.83986500	0.43199900
C	1.57296200	1.30845000	-0.57821800
C	2.08464400	1.08800700	-1.88221900
C	3.40965900	1.34606400	-2.15180000
H	2.50180200	2.46788700	2.50239600
H	5.32050900	2.01086800	-1.36939500
H	4.45223400	2.44977100	0.90742000
C	1.87062500	2.08095100	1.70771500
H	1.39640600	0.73317000	-2.64115500
H	3.79875600	1.17809600	-3.15166900
C	-0.23666000	1.25532200	0.88372800
C	0.54288800	1.81360000	1.93221700
H	0.10862100	1.98612000	2.90946000
C	-5.40912000	-1.33802300	-0.84015700
C	-4.08400300	-0.97083500	-0.89605200
C	-3.51175500	-0.21562000	0.15845200
C	-4.33397700	0.17916900	1.25850300
C	-5.69384600	-0.22139000	1.28850900
C	-6.22030000	-0.97098100	0.26190100
H	-5.84301100	-1.90598200	-1.65750800
H	-3.46394000	-1.20039800	-1.75350000
C	-3.74189400	0.97273600	2.26953100
H	-6.30946400	0.08024700	2.13164300
H	-7.26286300	-1.27350400	0.28643400
C	-2.42306100	1.33556900	2.16699700
C	-1.65887800	0.88513700	1.06011000
H	-4.34475100	1.30217100	3.11148600
H	-1.97185200	1.97646200	2.91404800
N	0.27299700	0.99674000	-0.31525200
N	-2.18721200	0.11990400	0.10546900
Ni	-0.98318800	-0.38421300	-1.43411900
H	-0.25179400	-0.71421500	-2.62676200
C	-0.66513000	-2.26602700	-2.08721200
C	-0.30896500	-2.16038600	-0.71325900

H	0.10014200	-2.52382700	-2.81945000
C	1.18287900	-2.16881000	-0.39684000
H	-1.65197400	-2.63404100	-2.36429100
H	1.69010600	-1.49037500	-1.08987700
H	1.58413100	-3.17482800	-0.60318400
Cl	-2.02147300	1.06812200	-2.88617300
C	1.53703000	-1.78825600	1.04494800
H	1.26217600	-2.61472000	1.71477600
H	0.91840300	-0.94318300	1.35985900
C	2.98682000	-1.41941400	1.29591400
C	3.33330200	-0.84721900	2.52948700
C	3.99968300	-1.60578500	0.35031100
C	4.64253200	-0.46388700	2.80726600
H	2.55588400	-0.69024600	3.27389700
C	5.31612400	-1.22473100	0.62380800
H	3.76672000	-2.04223600	-0.61494100
C	5.64390300	-0.65007700	1.84977200
H	4.88386200	-0.01971800	3.76963500
H	6.08415800	-1.37420600	-0.13029200
H	6.66692400	-0.35115900	2.06064500
C	-1.21704200	-2.76566100	0.33782400
H	-0.90380300	-3.79833400	0.55624000
H	-1.18888000	-2.21385800	1.28293000
H	-2.25621100	-2.79855300	0.00134700

TS6^{CSS}

C	-0.42208100	-6.30597500	0.08140300
C	0.88055600	-6.03138600	0.43353900
C	1.37456900	-4.70459600	0.36400600
C	0.50064100	-3.65726800	-0.06775500
C	-0.83386400	-3.96855600	-0.43678700
C	-1.28113500	-5.26824600	-0.36002500
H	3.39034300	-5.11031600	1.05159000
H	-0.79602000	-7.32413600	0.13527600
H	1.54562900	-6.82379500	0.76693900
C	2.70121500	-4.34392700	0.70671600
H	-1.46287400	-3.15700000	-0.78596200
H	-2.30135400	-5.50574600	-0.64639500
C	2.17051900	-2.05574400	0.16870000
C	3.10402700	-3.03496200	0.60447500
H	4.11244800	-2.75104600	0.88061600
C	0.88990200	3.82808600	-0.41278400
C	0.66105900	2.47510800	-0.31064100

C	1.74610000	1.57473800	-0.17404000
C	3.08017900	2.08934200	-0.17257900
C	3.28394000	3.48869800	-0.27804800
C	2.20966000	4.34215000	-0.38916100
H	0.04402400	4.49933800	-0.52485900
H	-0.33833400	2.07107600	-0.37856000
C	4.14240800	1.16047300	-0.07167800
H	4.30160900	3.86991600	-0.27184600
H	2.37127200	5.41307100	-0.46903100
C	3.86893400	-0.18006300	0.02990700
C	2.52070600	-0.62056800	0.05173900
H	5.16838000	1.51843200	-0.08691900
H	4.67484400	-0.90212200	0.07302500
N	0.91690000	-2.36380800	-0.13849700
N	1.50066200	0.23403800	-0.04170500
Ni	-0.35817400	-0.53560900	-0.00641300
C	-0.39026100	-0.53578200	2.00094300
C	-1.72938800	-0.32008700	1.64314400
H	-1.69271400	-1.06620200	-0.05863000
H	0.23298500	0.30809200	2.28503900
C	-2.26179400	1.09839800	1.55702000
H	-2.74688100	1.33587400	2.51724300
H	-1.41966000	1.78895400	1.46383600
H	-0.08810600	-1.50278000	2.39929900
Cl	-0.83489000	-0.01855500	-2.18632800
C	-2.76761400	-1.39053900	1.93532900
H	-3.16477600	-1.23219500	2.94820000
H	-3.60951400	-1.35000800	1.23796600
H	-2.33028000	-2.39201500	1.89064100
C	-3.26651800	1.35588200	0.40604400
H	-2.98110200	0.74467500	-0.45406400
H	-4.27145700	1.04355800	0.71649500
C	-3.26943800	2.80957800	-0.00673100
C	-2.66804500	3.19522500	-1.21262700
C	-3.80926200	3.80172500	0.82263800
C	-2.60184500	4.54303800	-1.57408800
H	-2.24268400	2.43083400	-1.85866900
C	-3.74299300	5.14812100	0.46428500
H	-4.28597300	3.51558000	1.75787800
C	-3.13546600	5.52419200	-0.73624800
H	-2.13562400	4.82334600	-2.51518500
H	-4.16832400	5.90402200	1.11935500
H	-3.08632000	6.57246300	-1.01845900

TS7^{doublet}

C	-1.27912500	-3.18087100	-3.09025600
C	-0.72729100	-1.93014900	-2.90967000
C	-1.54831400	-0.82366600	-2.58058100
C	-2.95468800	-1.02512300	-2.44020600
C	-3.49685700	-2.31444000	-2.64095600
C	-2.67478600	-3.37339600	-2.95436000
H	0.01241700	0.67883400	-2.47391500
H	-0.64231600	-4.02353500	-3.34244400
H	0.34278600	-1.77419300	-3.01708700
C	-1.05290600	0.48918700	-2.37609400
H	-4.56532600	-2.44652700	-2.54274000
H	-3.10650700	-4.35923400	-3.09627900
C	-3.30326600	1.23387400	-1.91832300
C	-1.91672100	1.50553700	-2.05398500
H	-1.53990200	2.50739500	-1.89136200
C	-8.88797700	3.10863500	-0.62964000
C	-7.86876000	2.22459800	-0.90876200
C	-6.55196800	2.70899700	-1.10907700
C	-6.29180300	4.10982800	-0.99088800
C	-7.36365200	4.98956300	-0.70354000
C	-8.63937000	4.49854000	-0.53276900
H	-9.89473200	2.73196100	-0.47817100
H	-8.04297800	1.15552200	-0.94620500
C	-4.95572100	4.54809600	-1.17053400
H	-7.16004500	6.05384100	-0.62120700
H	-9.45891500	5.17681800	-0.31516900
C	-3.96547700	3.63991700	-1.44534400
C	-4.29495700	2.26609300	-1.57029200
H	-4.72767000	5.60713700	-1.08702700
H	-2.94482400	3.97359100	-1.58393800
N	-3.79196200	0.00325000	-2.11045800
N	-5.54978500	1.83214700	-1.41835700
Ni	-5.81635200	-0.07645000	-2.08065500
Cl	-6.73754700	-1.09290700	-0.20711900
H	-8.05374000	1.26246200	-3.42901100
C	-7.71489700	0.39558100	-4.01155900
C	-6.18033000	0.36848800	-4.03997700
C	-5.60074200	1.70895400	-4.48021100
H	-8.10637800	-0.49484600	-3.50639800
H	-4.51534700	1.75862500	-4.31942900
H	-6.05665800	2.55216400	-3.94905400

C	-5.61390800	-0.74113700	-4.92648500
H	-5.79544300	-0.53273600	-5.99516300
H	-4.52726600	-0.83240300	-4.80973300
H	-6.05839700	-1.71625700	-4.71218900
C	-5.70785300	-6.53053400	-2.85321500
C	-6.43694400	-5.40947000	-3.20820000
C	-6.45612400	-4.27825600	-2.36537700
C	-5.74530100	-4.30375500	-1.15910200
C	-5.03519600	-5.44061500	-0.78288700
C	-5.00466000	-6.55475000	-1.63425400
H	-5.66815800	-7.40840100	-3.48992800
H	-6.99109800	-5.38376800	-4.14127700
H	-5.76936700	-3.42560300	-0.52110300
H	-4.50461700	-5.44416300	0.16138700
O	-4.32345200	-7.69998300	-1.37569700
C	-3.59277600	-7.78680200	-0.16031200
H	-3.13154300	-8.77536000	-0.16005000
H	-2.81138300	-7.01803500	-0.10848300
H	-4.25276200	-7.69084000	0.71064300
C	-7.13990600	-3.05900100	-2.81540000
O	-8.05045800	-2.95572100	-3.58533300
C	-8.41944100	0.46429800	-5.39341500
H	-8.06572800	1.33970300	-5.95064100
H	-8.14500900	-0.42297000	-5.97534200
C	-9.91665100	0.52562100	-5.22820200
C	-10.61800800	1.72596100	-5.39142700
C	-10.63096100	-0.61881500	-4.84254600
C	-11.99719500	1.78625800	-5.18295800
H	-10.07521600	2.62146200	-5.68661000
C	-12.00784400	-0.56231200	-4.63230600
H	-10.09496800	-1.55327600	-4.69660300
C	-12.69751600	0.64087400	-4.80293400
H	-12.52410800	2.72727800	-5.31972700
H	-12.54459500	-1.45935200	-4.33453600
H	-13.77123300	0.68401400	-4.64107800
H	-5.75813300	1.88153700	-5.55800800

TS8^{CSS}

C	-5.51045800	-2.06785200	-0.09447600
C	-5.44828000	-0.95080900	-0.89717400
C	-4.33740900	-0.07398400	-0.81499700
C	-3.28024400	-0.37497600	0.10032000
C	-3.37559400	-1.52229800	0.92916100

C	-4.47148100	-2.34933800	0.82834500
H	-4.98319100	1.35047400	-2.31622700
H	-6.36407600	-2.73608300	-0.15965400
H	-6.24662800	-0.72480700	-1.59922400
C	-4.20621100	1.09840600	-1.59943100
H	-2.57527000	-1.69986400	1.63948300
H	-4.54732600	-3.22486700	1.46620500
C	-2.09758400	1.53043700	-0.51942100
C	-3.10512500	1.90599600	-1.44676100
H	-2.99490600	2.80082800	-2.04780000
C	3.42659800	2.46248200	1.73300900
C	2.26089600	1.78745900	1.44900000
C	1.24539100	2.41813800	0.68636700
C	1.43553300	3.76656500	0.25074400
C	2.65110900	4.42999100	0.55607100
C	3.63197800	3.78758500	1.27606800
H	4.19449500	1.97655100	2.32736300
H	2.06320500	0.79782400	1.84154000
C	0.38316000	4.38106600	-0.46823500
H	2.78877800	5.45240500	0.21447600
H	4.56115200	4.29911200	1.50868600
C	-0.76979400	3.68135100	-0.72010400
C	-0.87697300	2.33527300	-0.28806800
H	0.49271800	5.40999300	-0.80014500
H	-1.59897600	4.15423300	-1.23163400
N	-2.17847600	0.41756100	0.20136800
N	0.10905000	1.72445500	0.37122900
Ni	-0.17291100	-0.23918500	0.75399800
C	0.43739900	-0.86668400	-1.08404000
C	0.90510500	-1.76394800	-0.08634100
H	-0.37536100	-1.61826300	1.08601900
Cl	-0.14682400	-0.09926700	3.05334900
C	1.36740200	0.10308500	-1.78247700
H	2.14374600	0.50457800	-1.12883100
H	1.86566100	-0.40410700	-2.62173900
H	0.81118300	0.95048900	-2.19852800
C	-0.70625400	-1.33590500	-1.96351800
H	-1.37995000	-2.01167300	-1.42853400
H	-1.29937300	-0.49340800	-2.33633400
H	-0.31509500	-1.87131800	-2.84216400
H	0.46308300	-2.76132200	-0.11222900
C	2.31640200	-1.80061300	0.47947400
H	2.76135800	-0.80363000	0.48435100

H	2.26415700	-2.12868100	1.52336500
C	3.17494600	-2.74871000	-0.33346900
C	4.02113900	-2.27170400	-1.34174900
C	3.09638600	-4.13191500	-0.12465800
C	4.76843800	-3.15289500	-2.12437600
H	4.09658600	-1.20079000	-1.50984600
C	3.83962600	-5.01645600	-0.90559500
H	2.45069200	-4.51491800	0.66254600
C	4.67793600	-4.52906600	-1.91049100
H	5.42340800	-2.76392100	-2.89948200
H	3.76920600	-6.08592400	-0.72617100
H	5.25968600	-5.21651400	-2.51814600

TS9^{CSS}

C	5.77659700	-0.52508900	0.10208700
C	5.11143900	-1.54000200	0.75325600
C	3.75447700	-1.37790600	1.12965100
C	3.08749400	-0.15117100	0.81765100
C	3.79857600	0.88390400	0.15690800
C	5.11634700	0.69419100	-0.19344700
H	3.47238200	-3.32531300	2.04068700
H	6.81620700	-0.65378900	-0.18436300
H	5.61433400	-2.47481300	0.98686600
C	3.00301000	-2.37516200	1.79974000
H	3.27042800	1.80984100	-0.04340400
H	5.66080500	1.48741700	-0.69699200
C	1.10611200	-0.89013200	1.78321200
C	1.69205500	-2.13641300	2.13350400
H	1.10493900	-2.90009800	2.62987300
C	-4.02773500	2.21683500	1.05749100
C	-2.70914300	1.87008800	0.86824000
C	-2.14831500	0.79035900	1.59622800
C	-2.96176100	0.08989600	2.54046600
C	-4.31717300	0.47119900	2.70825400
C	-4.84262000	1.51080200	1.97622900
H	-4.44609900	3.05171700	0.50343700
H	-2.05999000	2.43351600	0.21038400
C	-2.36333600	-0.96163700	3.27383800
H	-4.92759500	-0.07108300	3.42531800
H	-5.88087500	1.80037800	2.10770600
C	-1.04773600	-1.28152300	3.05474800
C	-0.30844000	-0.56725000	2.07786600
H	-2.95108100	-1.49888500	4.01323200

H	-0.56669200	-2.06043900	3.63366400
N	1.78091100	0.05323300	1.13832000
N	-0.84700000	0.42896800	1.37293200
Ni	0.33722000	1.34253300	0.01467900
C	0.08982000	-0.08873700	-1.38767400
C	0.15656000	1.13214500	-2.08979700
H	1.19910400	2.08322200	-0.84727300
H	1.00151900	-0.68798100	-1.41860300
Cl	0.35763500	3.35678700	1.09453400
C	1.35626400	1.38374000	-2.99197800
H	1.14308400	0.95750200	-3.98309700
H	1.55518400	2.45279200	-3.12083700
H	2.25989300	0.90573200	-2.60287600
C	-1.07765300	1.89066500	-2.52432100
H	-0.89344200	2.96911800	-2.49245400
H	-1.32363500	1.62111100	-3.56221800
H	-1.95032000	1.67846300	-1.90459700
C	-1.16660100	-0.93356700	-1.24901200
H	-1.05493600	-1.61079300	-0.39460200
H	-2.04305800	-0.31339600	-1.04462800
C	-1.39185900	-1.74440900	-2.50985400
C	-2.33154200	-1.34465900	-3.46724300
C	-0.62392600	-2.88824900	-2.76428400
C	-2.49838300	-2.06576700	-4.65060800
H	-2.93994400	-0.46374300	-3.28013300
C	-0.78608500	-3.61162000	-3.94510700
H	0.10635600	-3.21302000	-2.02596300
C	-1.72430500	-3.20079400	-4.89473900
H	-3.23567200	-1.74197100	-5.38037500
H	-0.18294500	-4.49786400	-4.12360000
H	-1.85328200	-3.76362100	-5.81491700

TS10^{CSS}

C	-5.65307300	-2.09288600	-0.14627900
C	-5.73559300	-0.78277000	-0.56050800
C	-4.60601500	0.06836000	-0.46950900
C	-3.37672500	-0.45018200	0.04724000
C	-3.32434700	-1.80052200	0.47942300
C	-4.43996300	-2.60045400	0.38177200
H	-5.53970900	1.85688200	-1.26021600
H	-6.52125700	-2.74150200	-0.21529300
H	-6.66440200	-0.38175200	-0.95764400
C	-4.62313600	1.42739100	-0.86467800

H	-2.39296900	-2.16021400	0.90042400
H	-4.39489600	-3.63142100	0.71983500
C	-2.30232500	1.59579200	-0.23525600
C	-3.48959700	2.19084100	-0.74136000
H	-3.50465600	3.23103500	-1.04053100
C	3.49926000	2.20972200	1.33960900
C	2.28899500	1.58523400	1.13938400
C	1.20875600	2.29973000	0.56652700
C	1.37854000	3.68352700	0.24745600
C	2.63930800	4.29506000	0.45963300
C	3.68293600	3.56893900	0.98804500
H	4.31697900	1.64744800	1.77850500
H	2.12837600	0.56184500	1.44553300
C	0.25679900	4.38201900	-0.25665000
H	2.76106100	5.34467800	0.20567000
H	4.64700300	4.04166200	1.15116400
C	-0.94106100	3.73148100	-0.40779700
C	-1.03320300	2.34964000	-0.09821100
H	0.35059600	5.43585300	-0.50473500
H	-1.80854700	4.27130000	-0.76419700
N	-2.25816000	0.32089900	0.13348900
N	0.01995200	1.66005600	0.33975600
Ni	-0.23807700	-0.30721200	0.66652900
C	0.49925400	-0.88934600	-1.10202300
C	0.93165800	-1.81263100	-0.11580700
H	-0.35446100	-1.70462300	1.00833700
Cl	-0.38130800	-0.06791700	2.94406800
C	-0.44767000	-1.31829200	-2.21087000
H	-1.31114900	-1.82245400	-1.75492400
H	0.52274100	-2.82280700	-0.18446200
H	1.20013500	-0.10089300	-1.37876500
C	0.25150800	-2.32545000	-3.14492300
H	1.12870900	-1.86739600	-3.61956100
H	0.59336600	-3.20895700	-2.59548200
H	-0.42495200	-2.65939000	-3.94127900
C	-0.95707800	-0.12183400	-3.02292100
H	-1.61567800	-0.45222500	-3.83430100
H	-1.51352900	0.58251100	-2.40267600
H	-0.11606700	0.41883500	-3.47676100
C	2.27739200	-1.74980900	0.52504600
C	3.39823300	-1.36907700	-0.22643300
C	2.44879800	-2.06341900	1.88237700
C	4.65846400	-1.28327000	0.36646100

H	3.27870900	-1.13788300	-1.28042600
C	3.70686900	-1.97553400	2.47362700
H	1.57861400	-2.30267200	2.48433700
C	4.81706500	-1.58243900	1.71999000
H	5.51477000	-0.98218900	-0.23116100
H	3.81782800	-2.19865300	3.53093300
H	5.79657200	-1.51232600	2.18508200

TS11^{CSS}

C	-0.18504700	-6.21960900	0.37765000
C	1.13267900	-5.87226100	0.57651400
C	1.55104100	-4.52925400	0.40331000
C	0.58603600	-3.54139500	0.03113700
C	-0.76250200	-3.92727000	-0.18152100
C	-1.13514000	-5.24135500	-0.00899000
H	3.64634700	-4.81625000	0.88086100
H	-0.50107100	-7.25009500	0.51010400
H	1.86739000	-6.61915400	0.86570800
C	2.88784100	-4.09611400	0.58558900
H	-1.46305700	-3.16130700	-0.49603000
H	-2.16665300	-5.53633600	-0.17683700
C	2.19312200	-1.85690700	0.02691100
C	3.21381600	-2.77650900	0.39066900
H	4.23147200	-2.43772300	0.54159900
C	0.51319000	3.91357300	-0.52485300
C	0.37507400	2.54676800	-0.44914100
C	1.52541800	1.72218900	-0.36879700
C	2.82032700	2.32416000	-0.40385800
C	2.92708500	3.73561000	-0.47381700
C	1.79516500	4.51662300	-0.52408100
H	-0.37185500	4.53929100	-0.59106800
H	-0.59532500	2.06636600	-0.48241300
C	3.94506000	1.46797400	-0.35801900
H	3.91629700	4.18522100	-0.48847200
H	1.88093200	5.59794100	-0.57651900
C	3.76653700	0.11197500	-0.25826500
C	2.45300700	-0.41143900	-0.16469000
H	4.94312200	1.89514100	-0.40462400
H	4.62037200	-0.55358700	-0.24618100
N	0.92952700	-2.23371100	-0.12685100
N	1.37783100	0.37251800	-0.22234700
Ni	-0.41624400	-0.50943800	0.05249000
C	-0.35292700	-0.54479800	2.08143900

C	-1.64598300	-0.14744200	1.64918900
H	-1.72848400	-1.05688000	0.18918700
H	-0.26127400	-1.58708700	2.39108700
Cl	-1.19876100	-0.11481900	-2.05569700
C	-2.89600900	-0.91435500	2.07491300
H	-2.65806700	-1.98755500	2.05802400
C	0.69884500	0.33255800	2.61805300
C	1.91608300	-0.24080100	3.02885200
C	0.56872200	1.72967800	2.70700000
C	2.97447100	0.55057700	3.46775000
H	2.02997000	-1.32108900	2.98140900
C	1.62739600	2.52182400	3.14244100
H	-0.36334800	2.20240400	2.41714700
C	2.84029400	1.93963300	3.51738200
H	3.90758100	0.08199300	3.76973100
H	1.50552900	3.60067500	3.18223700
H	3.66564200	2.55987600	3.85487800
H	-1.83883000	0.92192000	1.54187300
C	-3.23954100	-0.52172600	3.52137100
H	-3.45842400	0.55150300	3.59060300
H	-4.12381400	-1.06601300	3.87269700
H	-2.40694500	-0.73870200	4.19894700
C	-4.07920300	-0.65349400	1.13682400
H	-3.84379700	-0.94131600	0.10685400
H	-4.96613600	-1.20885900	1.46192800
H	-4.33595500	0.41360100	1.12909400

TS12^{doublet}

C	-1.40562600	-2.91343500	-4.08757600
C	-1.02241700	-1.60576900	-4.29718000
C	-1.79414500	-0.53797500	-3.77586900
C	-2.97805400	-0.83800000	-3.03754200
C	-3.34208600	-2.18579300	-2.82622600
C	-2.57350000	-3.20462600	-3.34189600
H	-0.56078900	1.09600400	-4.49339800
H	-0.80936300	-3.72546300	-4.49274300
H	-0.12421400	-1.37431800	-4.86342100
C	-1.45604000	0.82915200	-3.93856200
H	-4.22931200	-2.38754600	-2.24541000
H	-2.86874800	-4.23540800	-3.16984200
C	-3.42605000	1.43076500	-2.67958000
C	-2.25464600	1.80053500	-3.39117500
H	-1.99442900	2.84513700	-3.50462200

C	-8.34991600	2.97961600	0.42407900
C	-7.38941500	2.15857800	-0.11944200
C	-6.31492900	2.72276700	-0.84934500
C	-6.21499000	4.14509400	-0.97459100
C	-7.22096300	4.95955500	-0.39916900
C	-8.27298700	4.38580800	0.27829900
H	-9.18094300	2.54211100	0.96739500
H	-7.43029400	1.08366600	0.00214000
C	-5.10790700	4.66617400	-1.68366900
H	-7.14622200	6.03855400	-0.50489400
H	-9.04704800	5.01291700	0.71078700
C	-4.17538700	3.81590000	-2.22778200
C	-4.34948700	2.41741200	-2.09077200
H	-5.00473700	5.74227800	-1.79382700
H	-3.32597300	4.21397100	-2.76827100
N	-3.77137000	0.14937700	-2.52417800
N	-5.39476000	1.90298400	-1.43543400
Ni	-5.69078100	-0.08118700	-1.83747900
Cl	-5.79852400	-0.99264500	0.28944100
C	-6.67425700	0.22522800	-3.61450200
C	-5.83997600	0.82208000	-4.73672900
H	-4.96382300	0.18195600	-4.90888300
H	-5.43678200	1.80355000	-4.44712900
C	-6.56957700	0.98371000	-6.08999500
H	-7.46082900	1.60317000	-5.92424100
C	-5.44128900	-6.52591300	-2.40402300
C	-6.12043300	-5.38054600	-2.77460700
C	-6.02987600	-4.21326300	-1.98539500
C	-5.25843600	-4.22706300	-0.81694800
C	-4.58810900	-5.38411200	-0.42906900
C	-4.67116000	-6.53598000	-1.22480700
H	-5.48838500	-7.43303600	-2.99772100
H	-6.72071400	-5.36127800	-3.67866000
H	-5.19960700	-3.32416000	-0.21569700
H	-4.00607100	-5.37638300	0.48424300
O	-4.04577200	-7.70635900	-0.94805500
C	-3.25822300	-7.78668600	0.23286600
H	-2.85810700	-8.80116800	0.25468500
H	-2.43077900	-7.06669900	0.21004900
H	-3.86555700	-7.61290200	1.12950200
C	-6.69084100	-2.98702200	-2.45076300
O	-7.55598700	-2.89390800	-3.27334500
C	-7.89235800	0.95524200	-3.20755300

C	-8.04501300	2.35036500	-3.37053400
C	-8.95206500	0.26350500	-2.57705100
C	-9.19193100	3.01146800	-2.93943600
H	-7.25048600	2.92169100	-3.84096000
C	-10.09150400	0.92795900	-2.13514100
H	-8.86612300	-0.81178500	-2.44974400
C	-10.22290400	2.30873300	-2.31332000
H	-9.27360800	4.08631200	-3.07885800
H	-10.88698400	0.36364600	-1.65465900
H	-11.11518800	2.82665800	-1.97318100
H	-6.91694600	-0.81674100	-3.82445200
C	-5.66379200	1.70507300	-7.09470200
H	-4.74988200	1.12468700	-7.28099300
H	-6.16721700	1.85020700	-8.05811800
H	-5.36044300	2.69122500	-6.72103600
C	-7.03126200	-0.37016900	-6.64061300
H	-7.53225800	-0.25250300	-7.60895000
H	-6.17324600	-1.04087900	-6.78665100
H	-7.72866700	-0.86428500	-5.95731100

TS13^{doublet}

C	0.36286500	-1.65548600	2.33528500
C	0.33757800	-0.40081500	2.89835400
C	-0.83832200	0.38849600	2.82311600
C	-2.00375100	-0.15227200	2.19462900
C	-1.94471400	-1.43837000	1.60011100
C	-0.77952200	-2.16525300	1.66757400
H	-0.05580400	2.14227600	3.82107000
H	1.26626900	-2.25615800	2.38579100
H	1.21550200	0.01068300	3.38910000
C	-0.91676500	1.70913100	3.31891600
H	-2.81743300	-1.81014800	1.07834600
H	-0.73350300	-3.14570800	1.20382800
C	-3.18120700	1.84048600	2.51789100
C	-2.06313700	2.44416600	3.14020800
H	-2.11836500	3.46276300	3.49947600
C	-8.75523600	2.35067900	0.27536600
C	-7.56039000	1.75516400	0.61127500
C	-6.56230800	2.50848100	1.28099500
C	-6.79335700	3.89027300	1.56306800
C	-8.03751900	4.46947200	1.20943200
C	-9.00285400	3.71111800	0.58551100
H	-9.51666700	1.77390400	-0.24089000

H	-7.33701900	0.72653100	0.34831100
C	-5.74165700	4.61124100	2.18061500
H	-8.21134300	5.51862500	1.43327000
H	-9.95511800	4.15775000	0.31583300
C	-4.56225100	3.98060700	2.48682400
C	-4.42719800	2.59241500	2.22075100
H	-5.87708700	5.66698600	2.40014500
H	-3.75345500	4.53337100	2.94603800
N	-3.15954800	0.56730500	2.12384500
N	-5.40279200	1.89502900	1.65090900
Ni	-5.04635200	-0.24757100	1.78499500
Cl	-5.27082100	-1.01097100	-0.34970500
C	-6.01475500	-0.64496300	3.94310600
C	-7.41224700	-0.22328400	3.48419900
H	-7.39291300	0.78982200	3.08007200
H	-7.74428900	-0.86410400	2.66164900
C	-8.48724700	-0.30400800	4.58949300
H	-8.08410900	0.17147400	5.49531700
C	-6.83510300	-5.23562100	3.34044400
C	-5.94829800	-4.17709300	3.45241400
C	-6.06297100	-3.03953400	2.63218100
C	-7.07965100	-3.01463900	1.67518600
C	-7.97190800	-4.08012300	1.54076000
C	-7.85964500	-5.19218100	2.38243300
H	-6.75771000	-6.11049000	3.97810500
H	-5.14835100	-4.20747400	4.18546000
H	-7.14556900	-2.18571600	0.98178300
H	-8.73503300	-4.03504000	0.77294500
O	-8.68289600	-6.27774600	2.34545000
C	-9.72881600	-6.28517000	1.38892800
H	-10.25815700	-7.22916800	1.52950200
H	-9.33752900	-6.23603700	0.36441300
H	-10.42469100	-5.45053200	1.54739100
C	-5.10190100	-1.91468200	2.92256200
O	-3.97420100	-2.18443200	3.34824100
C	-8.84050200	-1.76080600	4.91822800
H	-9.25414400	-2.26530000	4.03623000
H	-9.58449400	-1.81225400	5.72150200
H	-7.96696100	-2.33894400	5.23764400
C	-9.73538200	0.47303100	4.15438100
H	-10.51885500	0.43283700	4.92007300
H	-10.15006800	0.05103400	3.22942000
H	-9.50252200	1.52720000	3.96084200

H	-6.14043100	-1.49828700	4.61395300
C	-5.20433600	0.36974100	4.70292300
C	-5.61907200	1.70186000	4.86321100
C	-4.01034200	-0.02161800	5.34300400
C	-4.87032900	2.60964800	5.61412100
H	-6.53874800	2.04442300	4.40314000
C	-3.25516700	0.88950300	6.07523600
H	-3.67148400	-1.04357900	5.23492300
C	-3.67930200	2.21333600	6.21873700
H	-5.22637900	3.63103900	5.72063200
H	-2.33167100	0.55990800	6.54387600
H	-3.09576000	2.91942100	6.80328800

TS14^{doublet}

C	-0.82194900	-0.55116100	-4.15554300
C	-0.85512400	0.81112000	-3.96880200
C	-1.96434600	1.42171600	-3.33236200
C	-3.05342300	0.61154700	-2.88548800
C	-2.99456300	-0.78576700	-3.09990900
C	-1.90418000	-1.35268300	-3.71744500
H	-1.27146000	3.46630200	-3.49218300
H	0.02993500	-1.01500800	-4.64365700
H	-0.04038000	1.44181400	-4.31203400
C	-2.06207500	2.81620200	-3.12968600
H	-3.82584600	-1.38868900	-2.77093600
H	-1.87755400	-2.42761800	-3.87009400
C	-4.19664900	2.46398900	-2.06228200
C	-3.15679500	3.33263600	-2.48551800
H	-3.24484300	4.40091600	-2.33631300
C	-9.74609000	2.01374900	0.28219400
C	-8.61409600	1.62744200	-0.39988600
C	-7.54136300	2.54098100	-0.55770300
C	-7.64791200	3.85053800	0.00767100
C	-8.83024700	4.21605400	0.69787100
C	-9.86140300	3.31435600	0.83083300
H	-10.56052000	1.30663800	0.40654000
H	-8.52082100	0.62737600	-0.80801500
C	-6.54064200	4.71848600	-0.13819200
H	-8.90166200	5.21348500	1.12323700
H	-10.76489300	3.59472800	1.36403000
C	-5.41958300	4.29388600	-0.80575200
C	-5.39195200	2.98688000	-1.35809800
H	-6.58226800	5.71369100	0.29628800

H	-4.55590900	4.94125200	-0.88378300
N	-4.15734200	1.15150600	-2.28830800
N	-6.42119200	2.15446600	-1.23963800
Ni	-6.06216100	0.17170800	-1.82191100
Cl	-5.30581600	-0.55131400	0.24092100
H	-7.59479900	1.84861600	-3.56325100
C	-8.01017700	0.90897900	-3.93842300
C	-6.94027200	-0.14611800	-4.17369500
H	-8.54713200	1.12776000	-4.87547300
C	-5.65536600	0.39294600	-4.77918900
H	-8.75141400	0.54537600	-3.21967300
H	-4.85626900	-0.34801200	-4.68867800
H	-5.33480100	1.27210100	-4.22368600
C	-5.69432300	0.83672300	-6.26639900
H	-6.54385500	1.50877000	-6.43704400
H	-5.81971500	-0.02625700	-6.92875500
C	-4.39574400	1.54818900	-6.56251500
C	-4.26976900	2.92504500	-6.33503300
C	-3.25546300	0.83108100	-6.94574700
C	-3.04340300	3.56995500	-6.49427700
H	-5.14406300	3.49313100	-6.02472700
C	-2.02692300	1.47105600	-7.10809000
H	-3.33211900	-0.24131000	-7.10802800
C	-1.91582900	2.84431400	-6.88349100
H	-2.96923800	4.63998300	-6.31835800
H	-1.15485500	0.89513400	-7.40484500
H	-0.96015300	3.34492300	-7.01363200
C	-7.51305000	-1.27562700	-5.02214500
H	-7.78200600	-0.87467400	-6.01095300
H	-6.80232700	-2.09196400	-5.17764500
H	-8.42907600	-1.68439500	-4.58805800
C	-6.71287100	-5.12349200	-3.26900200
C	-7.17714700	-3.82231900	-3.15557700
C	-6.38697100	-2.82154800	-2.56106500
C	-5.16114000	-3.19271200	-2.00257500
C	-4.68970200	-4.50350300	-2.09386800
C	-5.45685300	-5.47186200	-2.74948900
H	-7.31138500	-5.89628600	-3.74055700
H	-8.16384300	-3.57517200	-3.52930400
H	-4.61633500	-2.47125300	-1.40525700
H	-3.74613100	-4.75729700	-1.62555500
O	-5.08855700	-6.77392500	-2.91224100
C	-3.85045500	-7.18625500	-2.35849800

H	-3.75306500	-8.24684300	-2.59654500
H	-3.00887100	-6.63546200	-2.79942800
H	-3.83340600	-7.05408400	-1.26893900
C	-6.91429300	-1.43060600	-2.40702000
O	-8.01319000	-1.21765300	-1.87935200

TS15^{doublet}

C	5.32287500	0.47504300	-3.10776600
C	4.96389400	1.55837100	-2.32888100
C	3.65219500	1.68466200	-1.82189300
C	2.68444400	0.67307700	-2.10934600
C	3.06919500	-0.40819800	-2.93531200
C	4.36109400	-0.50724400	-3.41653900
H	3.95772600	3.57953900	-0.79930800
H	6.33376200	0.38874700	-3.49470600
H	5.68689000	2.33647600	-2.09676100
C	3.24134900	2.79528400	-1.02749600
H	2.31715400	-1.14047600	-3.20030600
H	4.63209900	-1.34533600	-4.05247900
C	1.03952900	1.81340400	-0.85771900
C	1.95622700	2.86328200	-0.57107300
H	1.63643100	3.70760100	0.02746900
C	-4.47924000	-0.58261600	-0.43618300
C	-3.14726600	-0.47449100	-0.79423500
C	-2.36632000	0.61236400	-0.34964600
C	-2.98748300	1.62819000	0.43713300
C	-4.34529600	1.48967400	0.79461700
C	-5.08294000	0.39715400	0.37411400
H	-5.06220600	-1.42963300	-0.78579900
H	-2.67895900	-1.21679800	-1.43159100
C	-2.19449400	2.75161000	0.82194900
H	-4.80439400	2.26538800	1.40251300
H	-6.12721500	0.30167700	0.65583000
C	-0.89134500	2.83334100	0.41322400
C	-0.31431600	1.79140600	-0.36087200
H	-2.64120400	3.53720600	1.42441200
H	-0.29382300	3.69582300	0.68274200
N	1.40480600	0.73481800	-1.60089700
N	-1.03213900	0.67960600	-0.69270700
Ni	0.01915900	-0.70854900	-1.52547200
H	0.37545200	-1.51731700	-2.76207300
C	0.44886300	-2.73478700	-1.58409800
C	0.09979900	-2.36690000	-0.25635800

H	1.49349300	-2.92543300	-1.82287500
C	1.24414200	-2.13728000	0.72372000
H	-0.24707900	-3.34918600	-2.15241700
H	2.16271100	-1.94891300	0.15529000
H	1.40839300	-3.08064900	1.27240000
C	1.10185600	-1.00086300	1.75965000
H	1.01214200	-0.04641900	1.23418800
H	2.04264800	-0.96035300	2.32642400
C	-0.05667400	-1.16041100	2.71711200
C	-0.13828100	-2.26548000	3.57508900
C	-1.09503900	-0.22401800	2.74013100
C	-1.24297700	-2.44521600	4.40656600
H	0.66510600	-2.99865600	3.58280400
C	-2.20815700	-0.40269500	3.56212000
H	-1.03525300	0.64553600	2.09741400
C	-2.28875200	-1.51860700	4.39545800
H	-1.29101000	-3.31147800	5.06125400
H	-3.01426100	0.32523800	3.53745400
H	-3.15521300	-1.66496200	5.03447300
C	-1.22038800	-2.84399300	0.31049300
H	-1.87791100	-3.21749700	-0.48177500
H	-1.04696600	-3.66885400	1.01743600
H	-1.76018900	-2.07139600	0.86196700

TS16^{doublet}

C	5.27782600	-2.46968000	-1.28349000
C	4.34874700	-3.28394000	-1.90935100
C	2.96579000	-3.07748800	-1.73864800
C	2.50424500	-1.99602800	-0.92131600
C	3.47402900	-1.19975800	-0.26985300
C	4.82789400	-1.42969000	-0.45296900
H	2.32087900	-4.74222200	-2.98306900
H	6.34110000	-2.64134800	-1.42096300
H	4.67313700	-4.10684900	-2.54175500
C	1.98902600	-3.92287300	-2.35158300
H	3.13463600	-0.41245100	0.39151600
H	5.54777300	-0.80090400	0.06383500
C	0.24116900	-2.63396800	-1.29219700
C	0.66130900	-3.71446800	-2.11289900
H	-0.08100900	-4.37377200	-2.54691700
C	-3.95049400	-0.04636000	2.15607200
C	-2.71179300	-0.23865900	1.56590500
C	-2.54693600	-1.16603200	0.51189600

C	-3.67706100	-1.94739900	0.11463100
C	-4.92549800	-1.72485400	0.72765900
C	-5.07175300	-0.77889200	1.72982500
H	-4.04928100	0.67128700	2.96582100
H	-1.84254500	0.30238500	1.92002200
C	-3.47310600	-2.95535300	-0.88073600
H	-5.77474100	-2.32319500	0.40637800
H	-6.03909700	-0.61928300	2.19642500
C	-2.21654800	-3.19398200	-1.36125500
C	-1.12303000	-2.39326200	-0.93176700
H	-4.31930700	-3.55045200	-1.21262600
H	-2.05003600	-3.99246400	-2.07487100
N	1.15612500	-1.75678100	-0.76072800
N	-1.32063900	-1.33028100	-0.08855800
Ni	0.26157400	-0.15682000	-0.18374400
C	-0.80870000	1.59522300	-0.06685000
C	0.12488700	1.78743300	-1.07454900
H	1.53706700	0.50325700	-0.17564100
H	-0.69089400	2.08449000	0.89213100
C	1.29221000	2.75745100	-0.98239700
H	2.11248100	2.37047900	-1.59798600
H	0.95332700	3.67680200	-1.48522100
H	-1.81261000	1.27491400	-0.32103500
C	-0.21567900	1.40425600	-2.50025800
H	0.63471700	0.92286500	-2.99491900
H	-1.07395700	0.72866200	-2.54574700
H	-0.46008300	2.31004000	-3.07462500
C	1.85554600	3.11976900	0.40089300
H	2.16655900	2.19817900	0.90486600
H	2.77075400	3.70342500	0.23067400
C	0.93847300	3.90592400	1.31512800
C	0.67922000	3.45706200	2.61635700
C	0.34009800	5.10026800	0.89338500
C	-0.16480100	4.17019700	3.46909500
H	1.13685800	2.53133700	2.95767600
C	-0.50465800	5.81646400	1.74074100
H	0.53518900	5.47497300	-0.10839800
C	-0.76315000	5.35238900	3.03214700
H	-0.35589400	3.79986900	4.47259100
H	-0.96154300	6.73892600	1.39270900
H	-1.42334500	5.90866000	3.69142500

TS17^{doublet}

C	0.27599000	-0.38771300	-2.24800800
C	0.17288100	0.91154400	-2.70571500
C	-1.07856400	1.56695000	-2.74520500
C	-2.24003000	0.87718200	-2.28738300
C	-2.11515100	-0.45985100	-1.84965900
C	-0.88107400	-1.07822700	-1.82776100
H	-0.39177400	3.42891000	-3.63016800
H	1.24148400	-0.88408500	-2.22886600
H	1.05044400	1.44289500	-3.06328900
C	-1.25266200	2.88593000	-3.25151300
H	-3.00868300	-0.99257600	-1.54850200
H	-0.80718600	-2.10913800	-1.49294700
C	-3.61474500	2.72838600	-2.75923300
C	-2.50113500	3.44946600	-3.26704600
H	-2.63782200	4.44970500	-3.65916300
C	-9.50014700	2.40946900	-1.47909900
C	-8.18356400	2.00321600	-1.56202800
C	-7.20649800	2.86941600	-2.10721100
C	-7.60510100	4.15725200	-2.58093100
C	-8.96108700	4.54319900	-2.47941700
C	-9.89592500	3.68553500	-1.93590700
H	-10.23962500	1.73490100	-1.05795700
H	-7.88889800	1.02148900	-1.21267800
C	-6.60329700	4.99060200	-3.15150700
H	-9.25274200	5.52535700	-2.84255900
H	-10.93645700	3.98747800	-1.86304700
C	-5.30875500	4.55209500	-3.22566400
C	-4.96759000	3.26957000	-2.71769500
H	-6.88023900	5.97038300	-3.53086900
H	-4.54723300	5.18037200	-3.67089700
N	-3.47646000	1.47151200	-2.28043100
N	-5.89932500	2.46119600	-2.17255800
Ni	-5.23889700	0.57114800	-1.95869100
Cl	-5.55789100	0.18192100	0.63326200
C	-5.98716000	-0.44931700	-3.46896500
C	-5.54754000	0.17846900	-4.79707600
H	-5.52027900	1.27394600	-4.68087600
C	-5.12367900	-4.52420100	-1.86706000
C	-5.92970000	-3.43535400	-1.59908900
C	-5.48683400	-2.41552500	-0.72418400
C	-4.23563400	-2.54466800	-0.10651300
C	-3.42676900	-3.64632100	-0.36594500
C	-3.86049800	-4.63777500	-1.25884200

H	-5.44342000	-5.30738100	-2.54598100
H	-6.90300500	-3.34281400	-2.06638200
H	-3.89990300	-1.78049100	0.58256100
H	-2.46959900	-3.72497400	0.13476100
O	-3.14485300	-5.73928900	-1.59054700
C	-1.84971600	-5.89609800	-1.02854200
H	-1.45735600	-6.82717800	-1.43907000
H	-1.19026700	-5.06548500	-1.31136500
H	-1.89434900	-5.96882600	0.06530200
C	-6.40133600	-1.29814500	-0.53920500
O	-7.57725900	-1.20382800	-0.70595400
H	-5.71272800	-1.51314400	-3.45136800
H	-7.07850800	-0.38571300	-3.34279300
C	-4.12539900	-0.28490400	-5.17090600
H	-4.18015900	-1.24580900	-5.70194300
H	-3.56651500	-0.47684500	-4.25122300
C	-3.35387500	0.73155300	-6.02265300
H	-3.94894500	1.00405900	-6.90359000
H	-3.24775700	1.65479200	-5.43457300
C	-1.98071100	0.28322200	-6.47771000
C	-1.52685100	0.58487300	-7.76825500
C	-1.11472200	-0.40864200	-5.61991000
C	-0.24742700	0.21980800	-8.18924600
H	-2.18760500	1.11473500	-8.45086300
C	0.16552800	-0.77431000	-6.03432100
H	-1.43833000	-0.66387400	-4.61779400
C	0.60692300	-0.46144400	-7.32100200
H	0.08021300	0.46463000	-9.19634400
H	0.81823000	-1.30314600	-5.34469900
H	1.60370800	-0.74814100	-7.64527900
C	-6.54007100	-0.12155000	-5.93385300
H	-6.21220300	0.30667200	-6.89058400
H	-6.64966000	-1.20514900	-6.07044000
H	-7.53049900	0.28891700	-5.70520400

TS18^{doublet}

C	-0.26424600	-1.99798300	-1.65730900
C	-0.07779800	-0.64063100	-1.78844800
C	-1.19147100	0.22064800	-1.95391300
C	-2.50956000	-0.33621700	-1.99339900
C	-2.67237300	-1.73304700	-1.82556900
C	-1.57151800	-2.54359300	-1.66926800
H	-0.08717700	2.08266300	-2.01856200

H	0.59134200	-2.65525700	-1.53361200
H	0.91913200	-0.20881100	-1.76417900
C	-1.07122200	1.62443400	-2.07020800
H	-3.67199900	-2.13736500	-1.80378600
H	-1.71133200	-3.61352200	-1.55239400
C	-3.46651100	1.76747100	-2.29917100
C	-2.19540300	2.39511000	-2.22925500
H	-2.11639800	3.47387200	-2.27877800
C	-9.45205900	2.56274500	-2.35404900
C	-8.24783000	1.93940100	-2.11490000
C	-7.03543700	2.61179900	-2.41818400
C	-7.07827400	3.93870300	-2.94922100
C	-8.33582200	4.55121200	-3.17973200
C	-9.49909000	3.87299500	-2.89235200
H	-10.37833700	2.04426300	-2.12697400
H	-8.20407000	0.93597200	-1.70102200
C	-5.84082700	4.55984600	-3.24613500
H	-8.36308200	5.55788400	-3.58827700
H	-10.46096200	4.34254700	-3.07437500
C	-4.66323500	3.89044300	-3.01965700
C	-4.70316300	2.56826900	-2.50004200
H	-5.83469800	5.56078500	-3.66892500
H	-3.71736400	4.35183000	-3.27415700
N	-3.60864400	0.44853900	-2.19283800
N	-5.85239900	1.96732500	-2.21843800
Ni	-5.73067700	-0.21298000	-1.96921800
Cl	-5.46731900	-0.53311400	0.29923500
C	-6.43822200	-0.64222700	-4.05126300
C	-5.43770300	0.15472900	-4.91163600
H	-4.95033800	0.91301600	-4.29936600
C	-4.18800000	-4.68193800	-3.40246600
C	-4.99901000	-3.56311200	-3.52690400
C	-5.77867200	-3.12437000	-2.44824700
C	-5.73915300	-3.84119800	-1.24433400
C	-4.91095200	-4.95195700	-1.10274500
C	-4.12344800	-5.37219900	-2.18305400
H	-3.58162000	-5.03354200	-4.23066500
H	-5.02021300	-3.02606500	-4.46551400
H	-6.31535600	-3.47744500	-0.40139000
H	-4.87623100	-5.46734500	-0.15059200
O	-3.25740300	-6.42410300	-2.14333800
C	-3.17282000	-7.17073700	-0.93928200
H	-2.44190100	-7.95898300	-1.12666500

H	-2.83090200	-6.54768000	-0.10265200
H	-4.13838300	-7.62278400	-0.67904100
C	-6.56283600	-1.86260400	-2.43571400
O	-7.70785500	-1.76350500	-2.01316400
H	-6.72374000	-1.55344100	-4.58770300
H	-7.36503300	-0.08527800	-3.89134800
C	-6.22473200	0.93529400	-5.98542300
H	-6.62166800	0.25197100	-6.74893100
H	-7.09545800	1.39854600	-5.50584400
C	-5.40667900	2.05478900	-6.65807100
H	-4.61438800	1.62691300	-7.28231400
H	-4.90882900	2.63627600	-5.86892100
C	-6.27229500	2.97486100	-7.48701600
C	-7.17027900	3.84898600	-6.85730000
C	-6.22920600	2.95920900	-8.88489600
C	-7.99908200	4.68422600	-7.60347400
H	-7.22191200	3.86716300	-5.77209500
C	-7.05732000	3.79473400	-9.63777900
H	-5.53921700	2.28571900	-9.38809900
C	-7.94500100	4.66086400	-8.99939900
H	-8.68882700	5.35388500	-7.09605600
H	-7.00778500	3.76804500	-10.72300900
H	-8.58987400	5.31174100	-9.58314300
C	-4.32634800	-0.71185500	-5.50682800
H	-4.73984000	-1.49161600	-6.16056200
H	-3.63339400	-0.11162100	-6.10666500
H	-3.74387500	-1.19801500	-4.71838200

TS19^{doublet}

C	-5.31056700	0.17485200	0.67170700
C	-4.54118600	1.19092400	1.19986400
C	-3.21146100	1.38653400	0.76067900
C	-2.66998300	0.51572000	-0.23249900
C	-3.48492300	-0.50256900	-0.78048700
C	-4.77737600	-0.67001700	-0.32828100
H	-2.75353100	3.08271800	2.03338700
H	-6.32975800	0.02708600	1.01585600
H	-4.94213900	1.85234800	1.96339500
C	-2.36512100	2.40139100	1.28163200
H	-3.06891600	-1.14411500	-1.54877100
H	-5.39374600	-1.45882100	-0.74896700
C	-0.57644100	1.57930800	-0.11302600
C	-1.07214600	2.50484800	0.84267300

H	-0.42148400	3.27377300	1.24034000
C	3.98212200	-0.70364300	-3.33017000
C	2.69403100	-0.55299700	-2.85828300
C	2.39787300	0.45823700	-1.91641500
C	3.43690400	1.33135700	-1.47406600
C	4.74662000	1.14955100	-1.97388300
C	5.01682900	0.14653800	-2.88314200
H	4.20049000	-1.48222900	-4.05448800
H	1.89167100	-1.19361000	-3.20913900
C	3.09055700	2.35487500	-0.54798000
H	5.53392400	1.81711600	-1.63355000
H	6.02501900	0.01464900	-3.26422100
C	1.79709700	2.47376300	-0.11011800
C	0.81168500	1.55895000	-0.56236500
H	3.85972500	3.03874700	-0.20014000
H	1.52892500	3.25621400	0.58908000
N	-1.36575400	0.62297500	-0.63348200
N	1.11901700	0.57853500	-1.43600400
Ni	-0.41168500	-0.60368500	-1.91157000
C	-1.62692400	-0.96870200	2.63712900
C	-1.12393700	-1.65299800	1.55115100
C	0.19930400	-1.42078400	1.12071400
C	1.00430800	-0.50422900	1.83034100
C	0.48953300	0.19153600	2.91891400
C	-0.83750200	-0.01944600	3.31335500
H	-2.64911000	-1.11948000	2.96592900
H	-1.74263900	-2.35230700	1.00571700
H	2.02340300	-0.32738700	1.50563600
H	1.12059700	0.90689700	3.43199900
O	-1.45592400	0.64154000	4.32650400
C	-0.73724800	1.67192600	4.98489700
H	-0.43505900	2.45601700	4.27803100
H	-1.42138700	2.09051400	5.72439800
H	0.15291800	1.28080800	5.49368100
C	0.79683000	-1.96800500	-0.06963600
O	1.88186900	-2.26260700	-0.43766700
Cl	-0.79181100	-2.98000700	-1.31582500
H	-0.95086900	-0.36314100	-3.35592300

TS20^{doublet}

C	-2.37974400	-1.88834800	-4.67652000
C	-1.99768200	-0.56718900	-4.82565400
C	-2.65654100	0.45533600	-4.10918200

C	-3.72238300	0.10872800	-3.22153900
C	-4.08082700	-1.25134000	-3.06388000
C	-3.42112800	-2.22778300	-3.78866900
H	-1.52600300	2.12909200	-4.90577000
H	-1.87170000	-2.66779300	-5.23645800
H	-1.18956500	-0.29672100	-5.50049500
C	-2.33776900	1.83516100	-4.24597200
H	-4.87679800	-1.51058500	-2.37466200
H	-3.71144700	-3.26706500	-3.66961500
C	-4.13246200	2.37442100	-2.72830800
C	-3.06001400	2.77930800	-3.56489200
H	-2.83422000	3.83115200	-3.68885500
C	-8.97766100	3.72136300	0.58926000
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TS21^{doublet}

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12. Supplementary references

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13. NMR spectrum

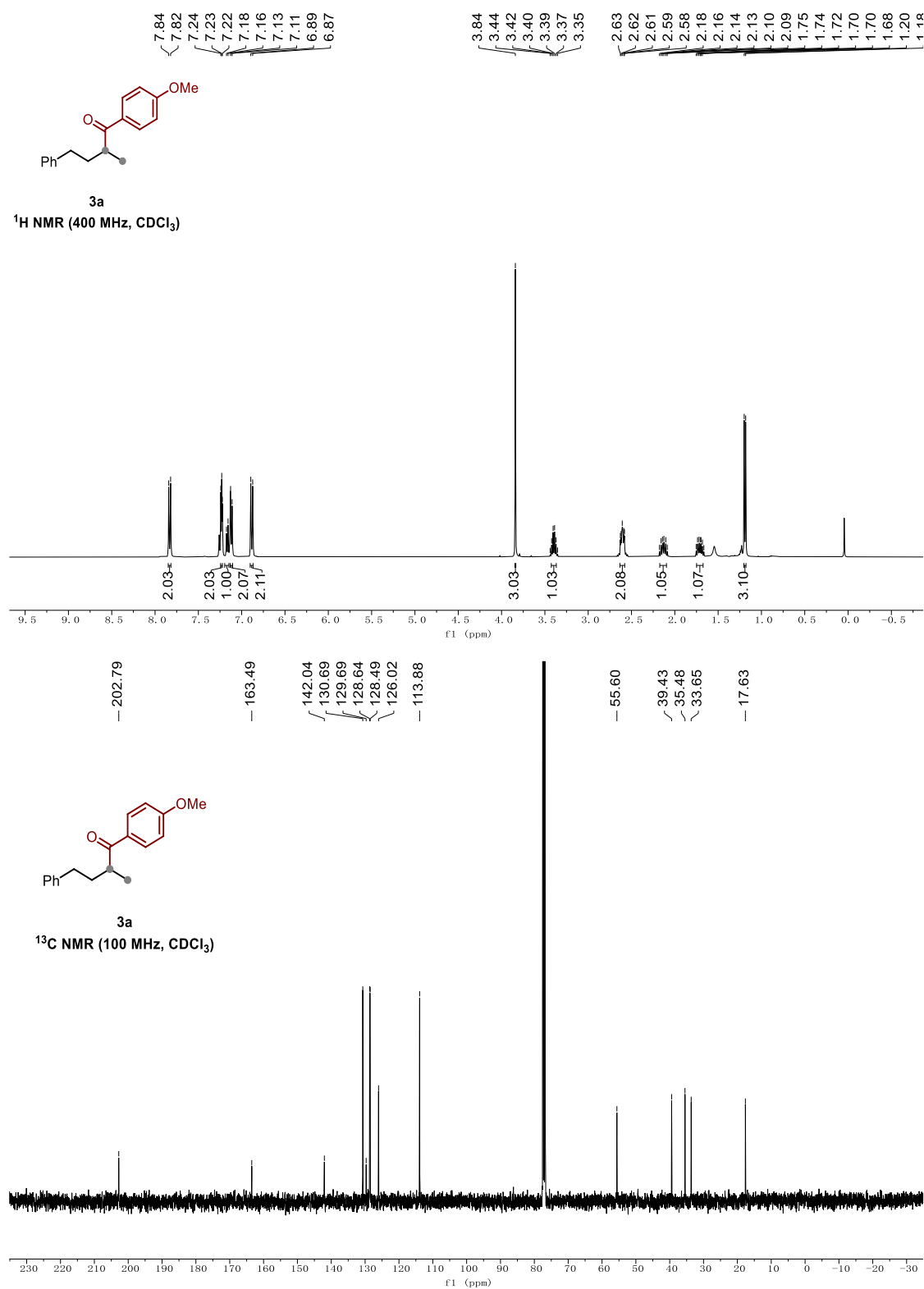


Figure S5. ¹H NMR and ¹³C NMR spectra of **3a**.

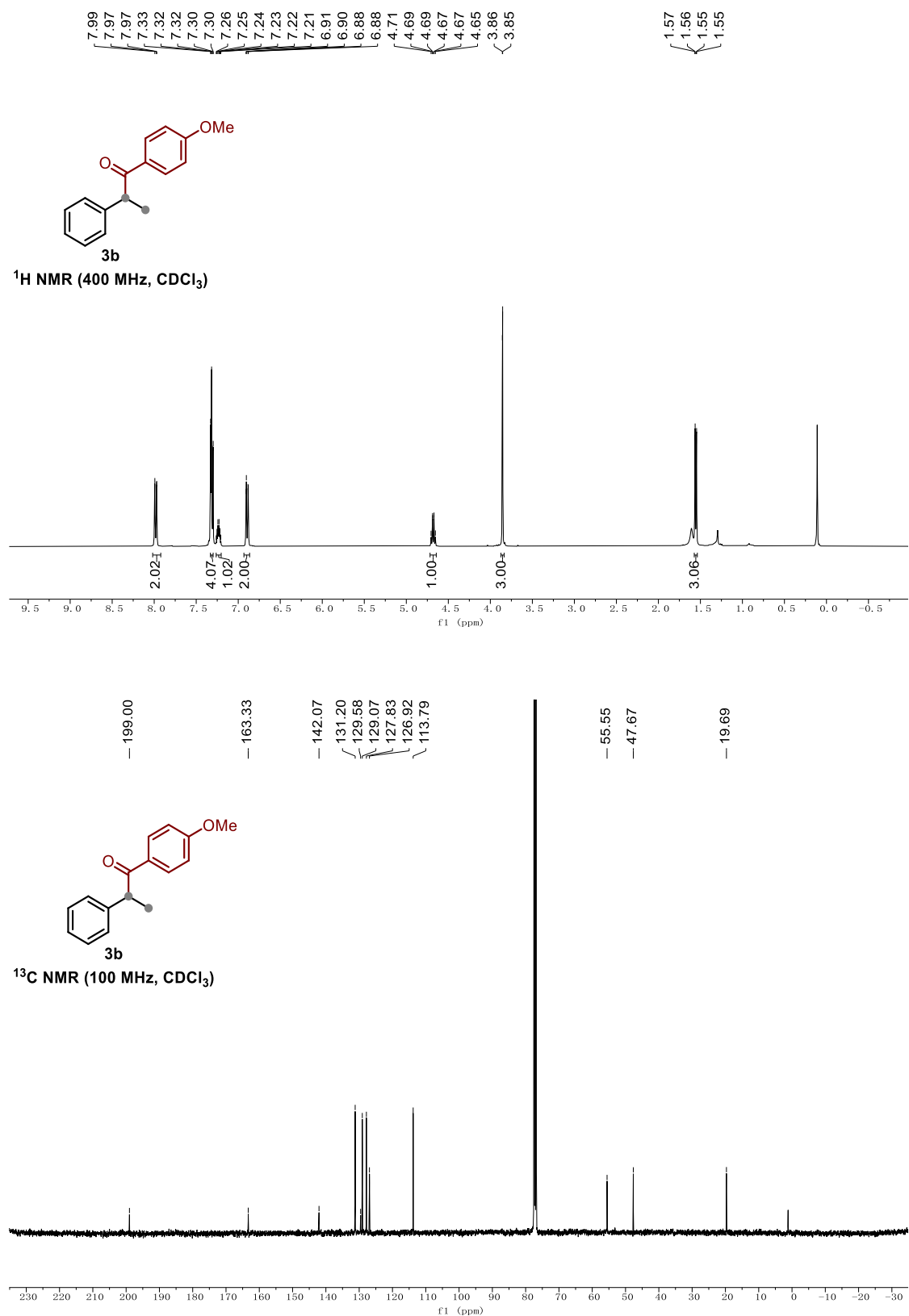


Figure S6. ^1H NMR and ^{13}C NMR spectra of **3b**.

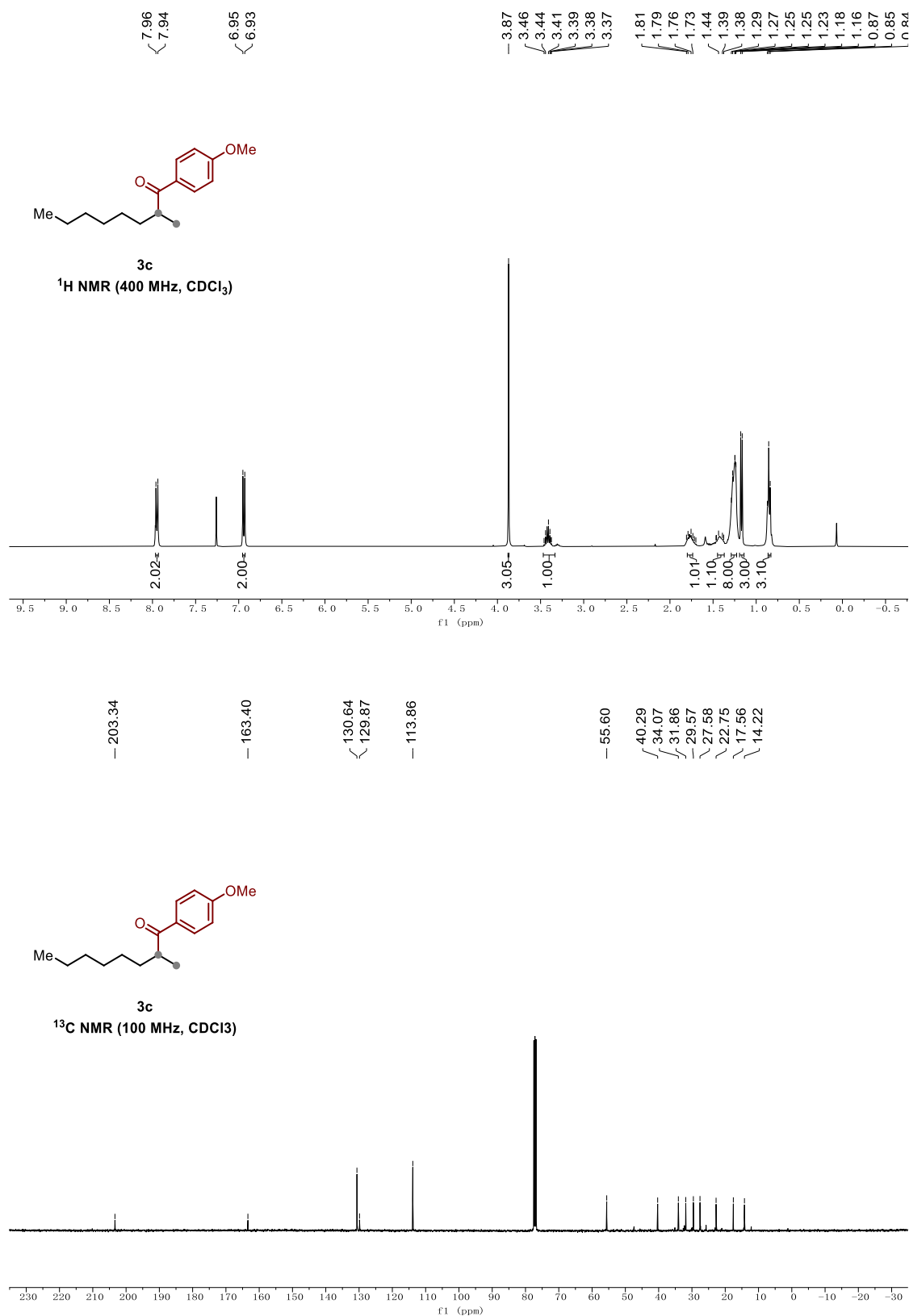


Figure S7. ¹H NMR and ¹³C NMR spectra of **3c**.

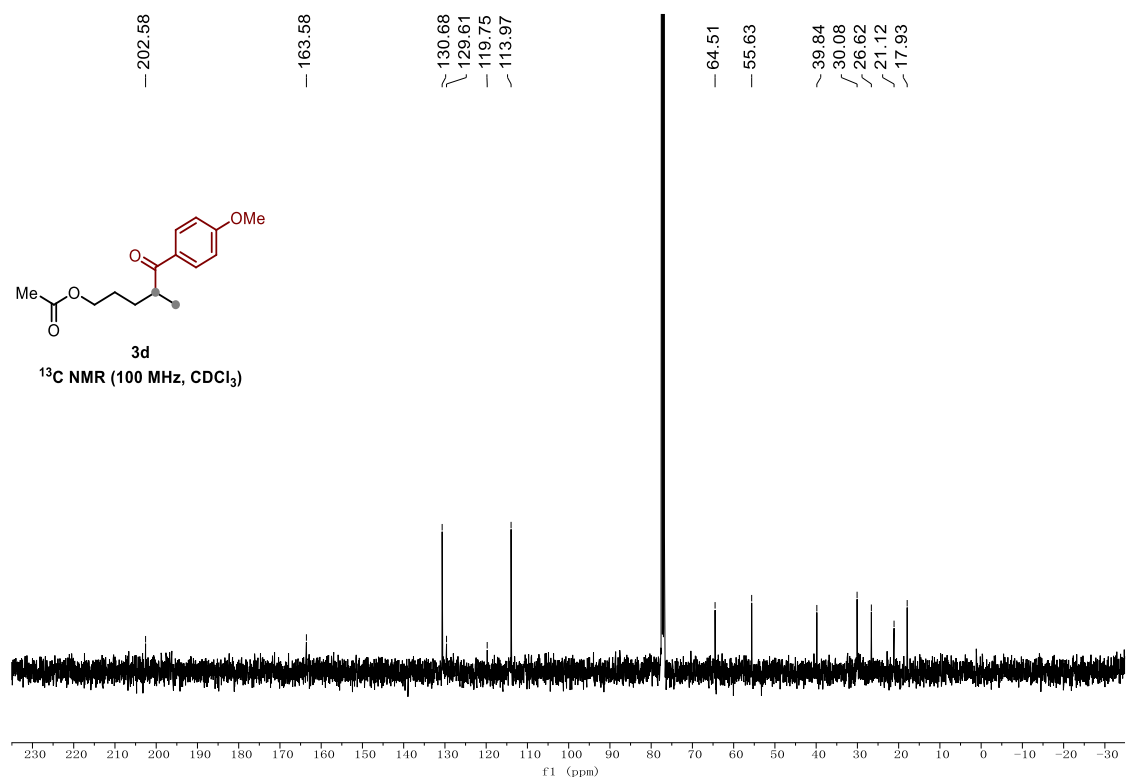
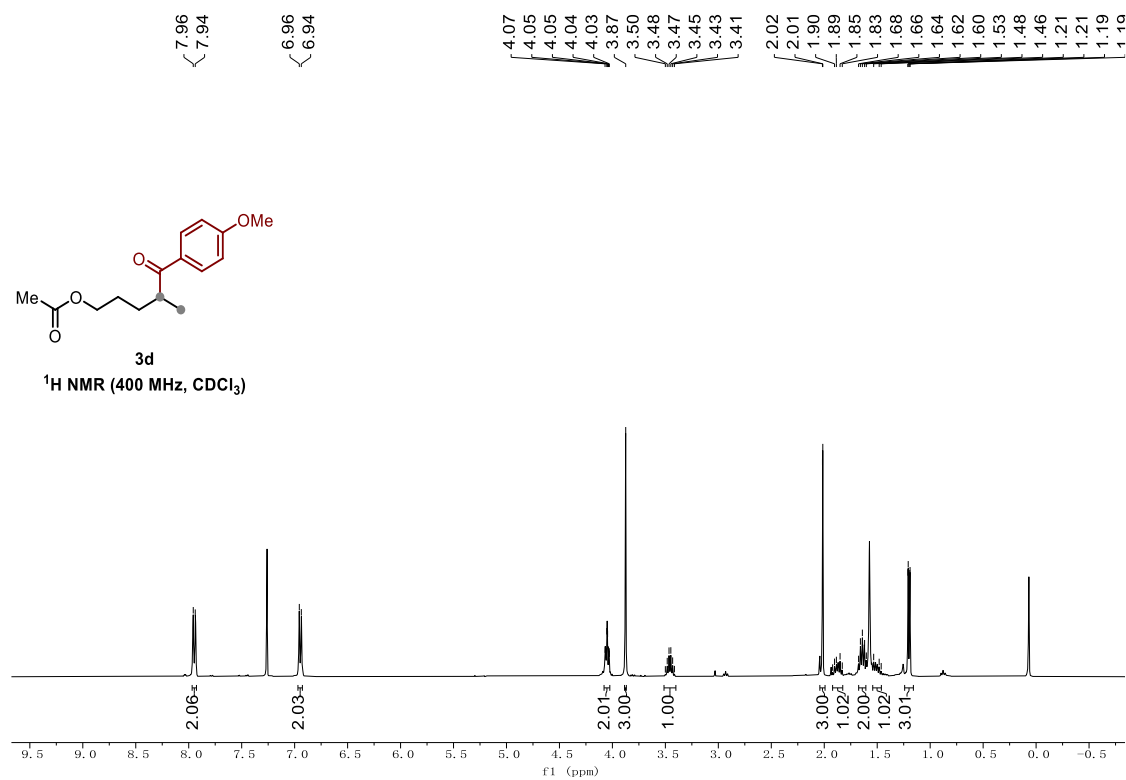


Figure S8. ^1H NMR and ^{13}C NMR spectra of **3d**.

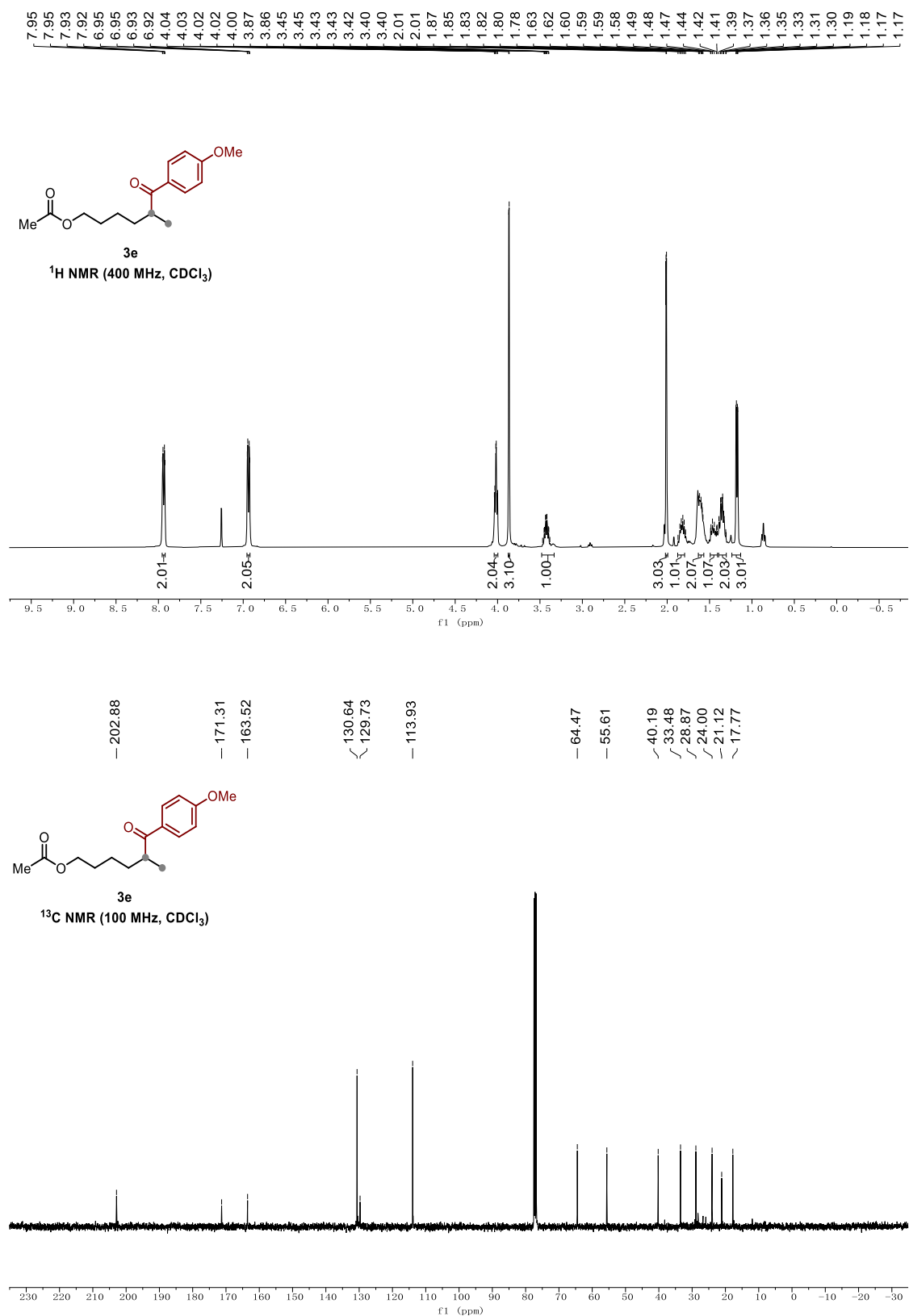


Figure S9. ¹H NMR and ¹³C NMR spectra of **3e**.

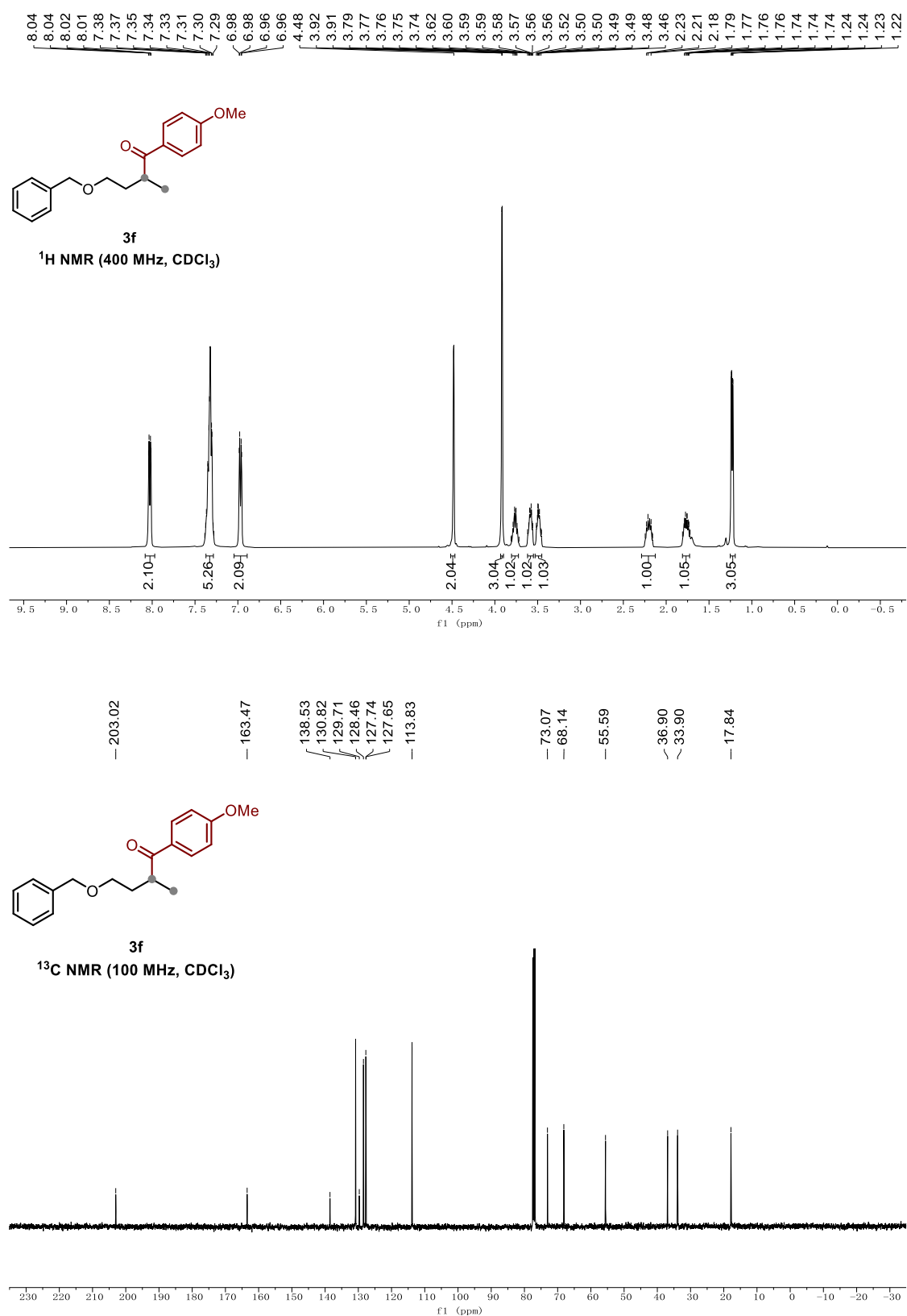


Figure S10. ¹H NMR and ¹³C NMR spectra of **3f**.

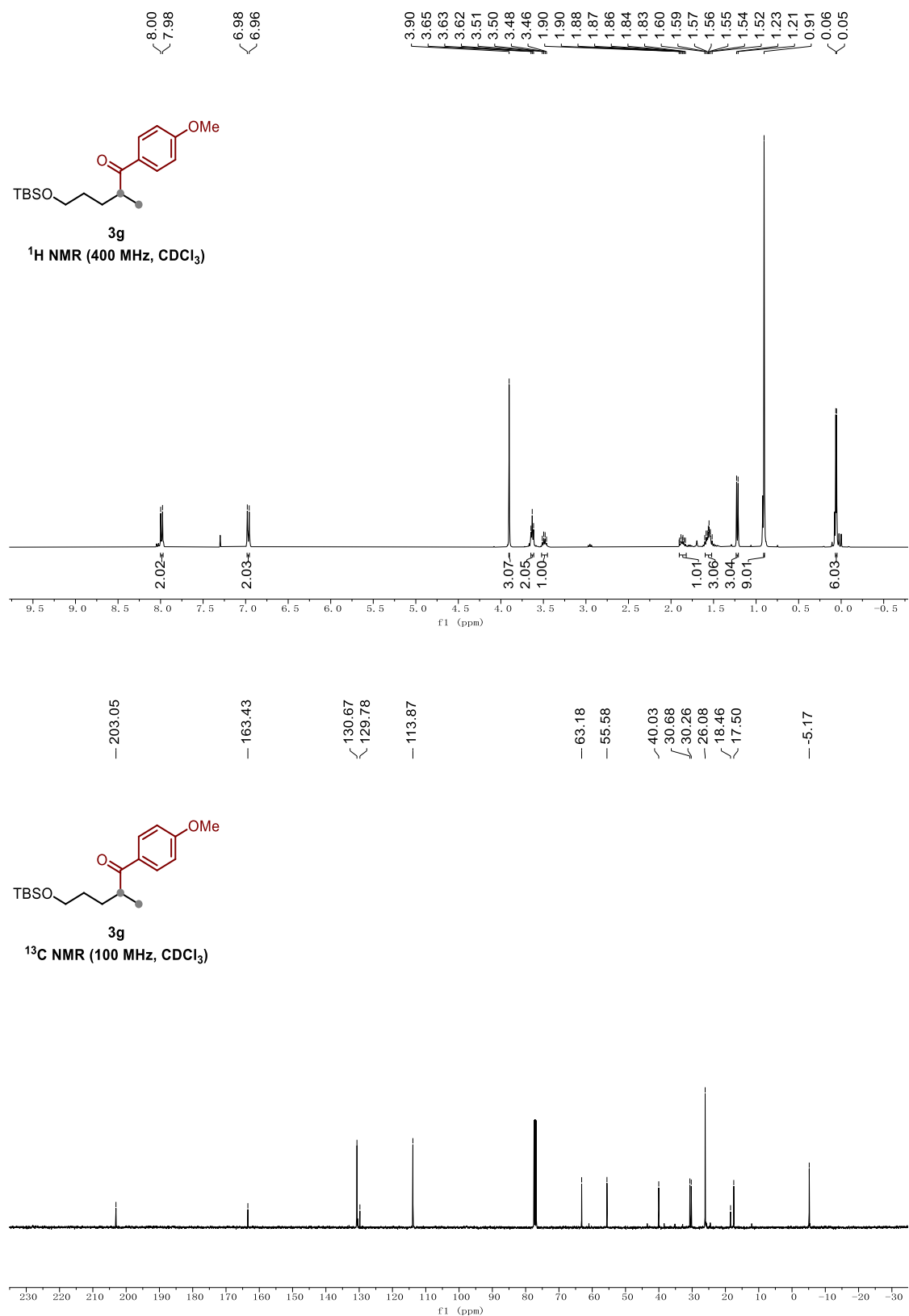


Figure S11. ¹H NMR and ¹³C NMR spectra of **3g**.

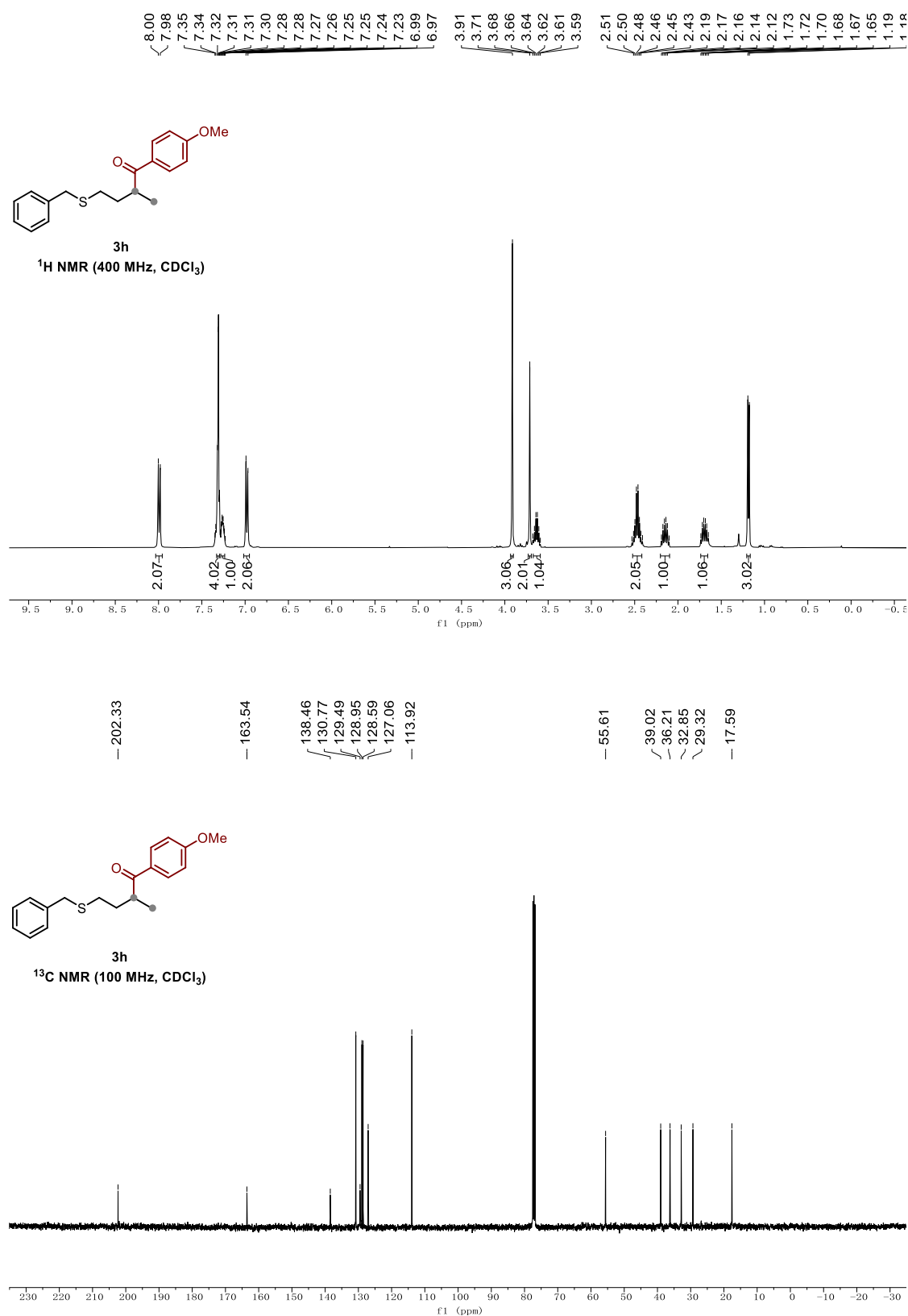


Figure S12. ¹H NMR and ¹³C NMR spectra of **3h**.

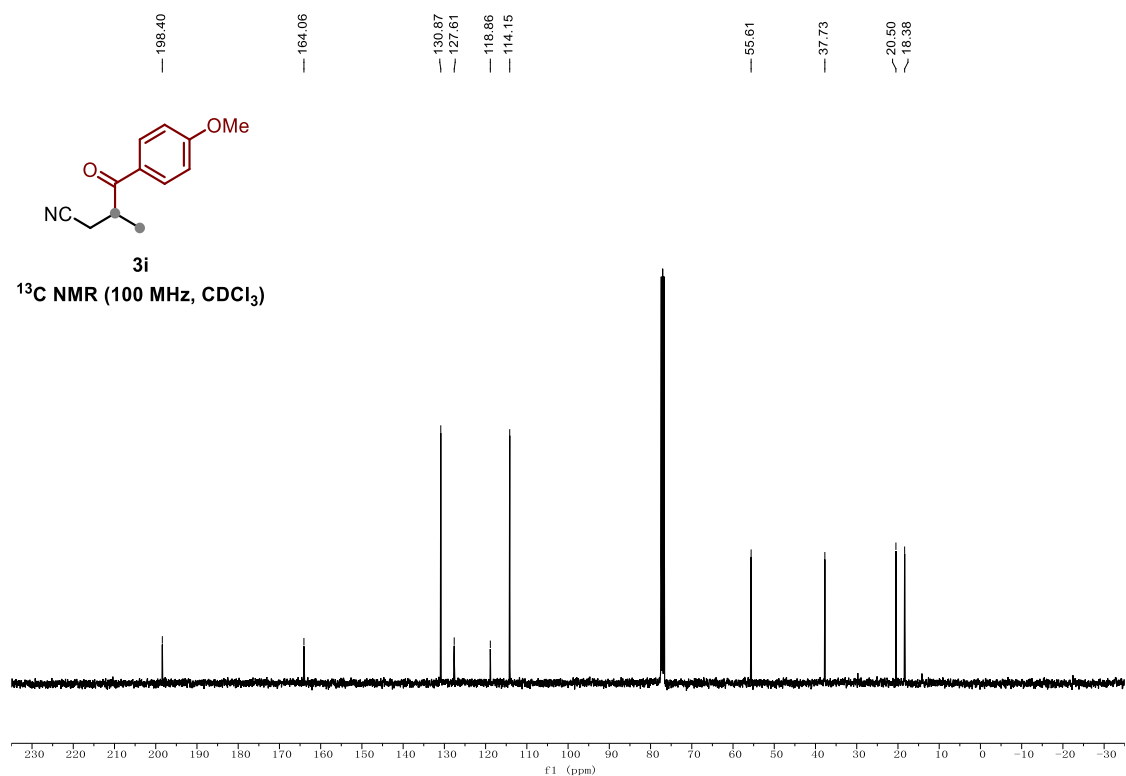
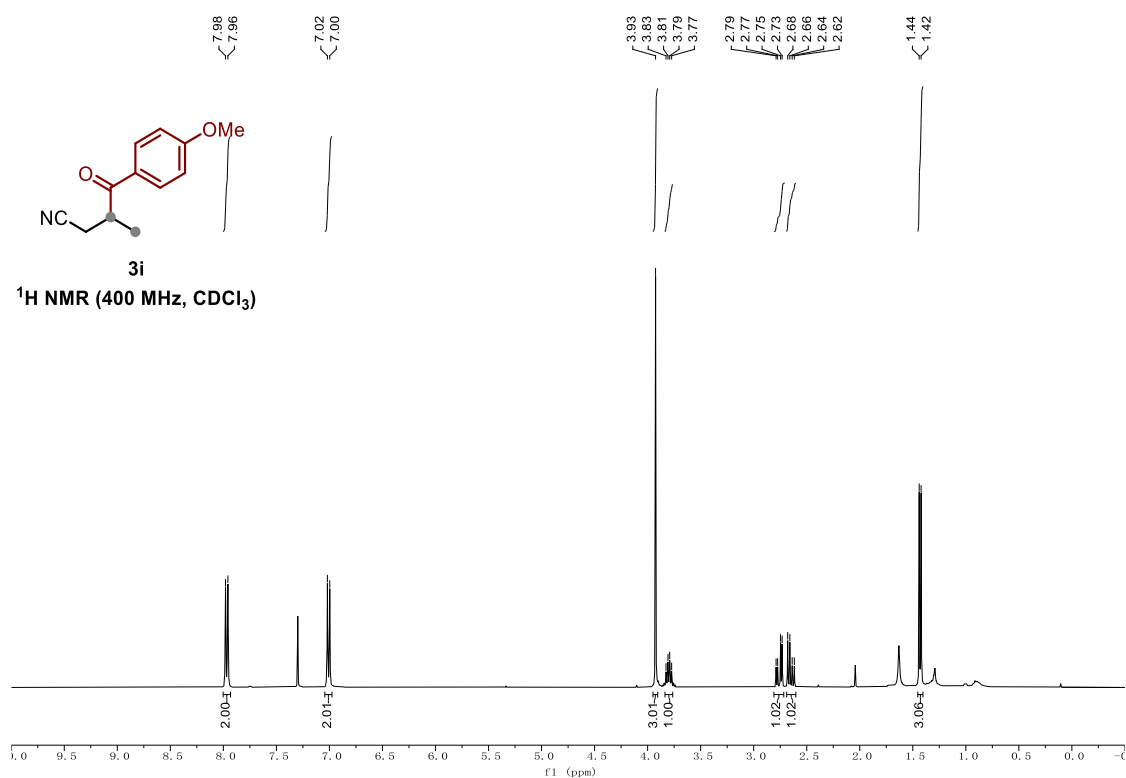


Figure S13. ^1H NMR and ^{13}C NMR spectra of **3i**.

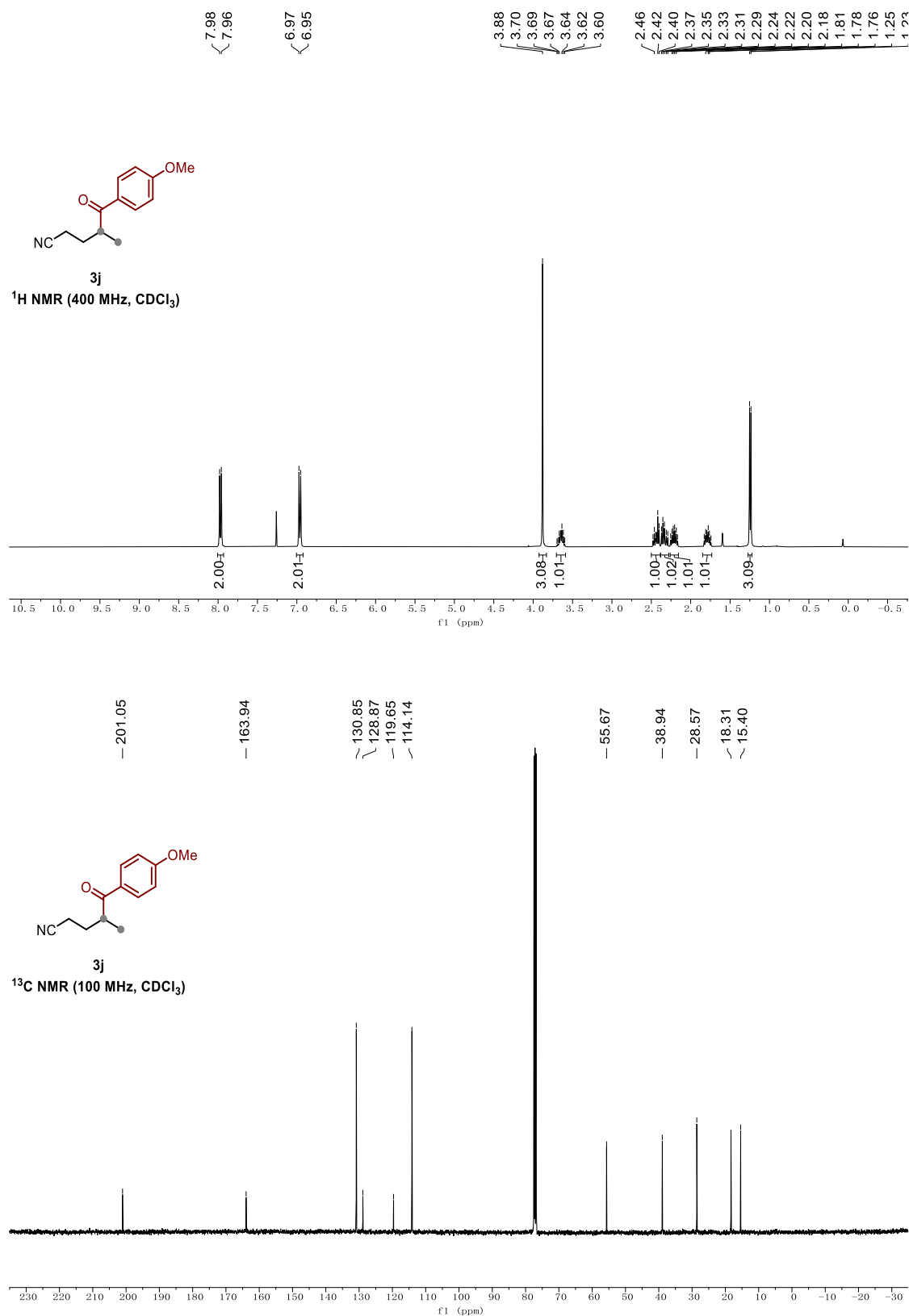


Figure S14. ¹H NMR and ¹³C NMR spectra of **3J**.

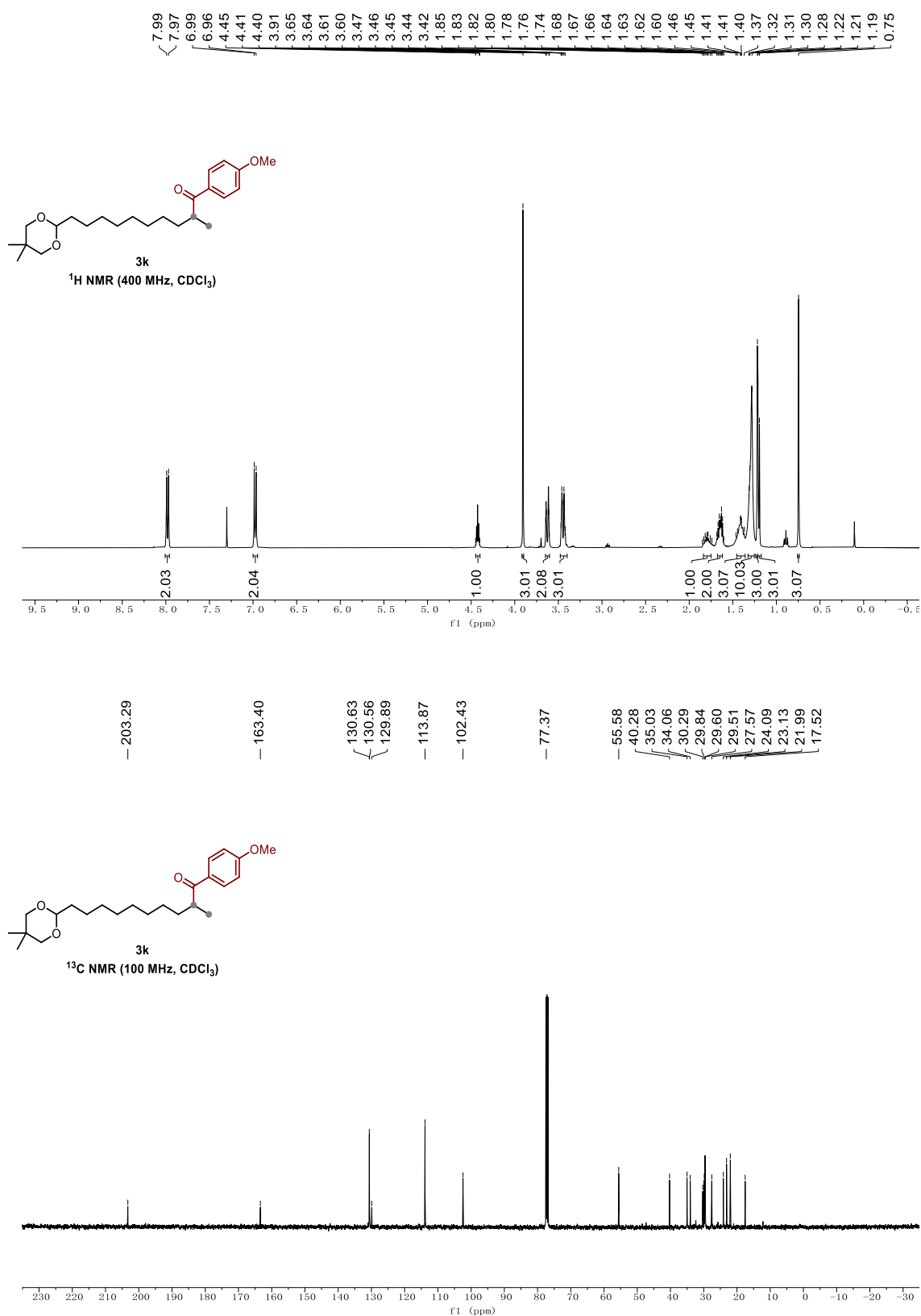


Figure S15. ¹H NMR and ¹³C NMR spectra of **3k**.

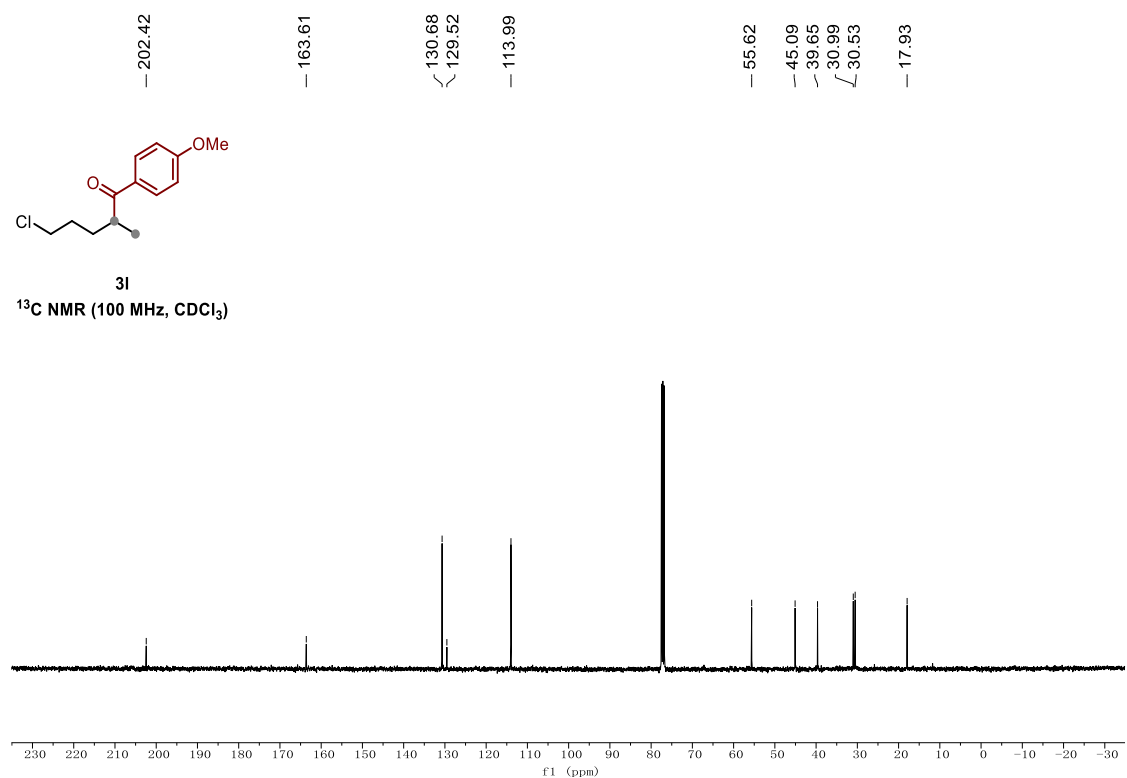
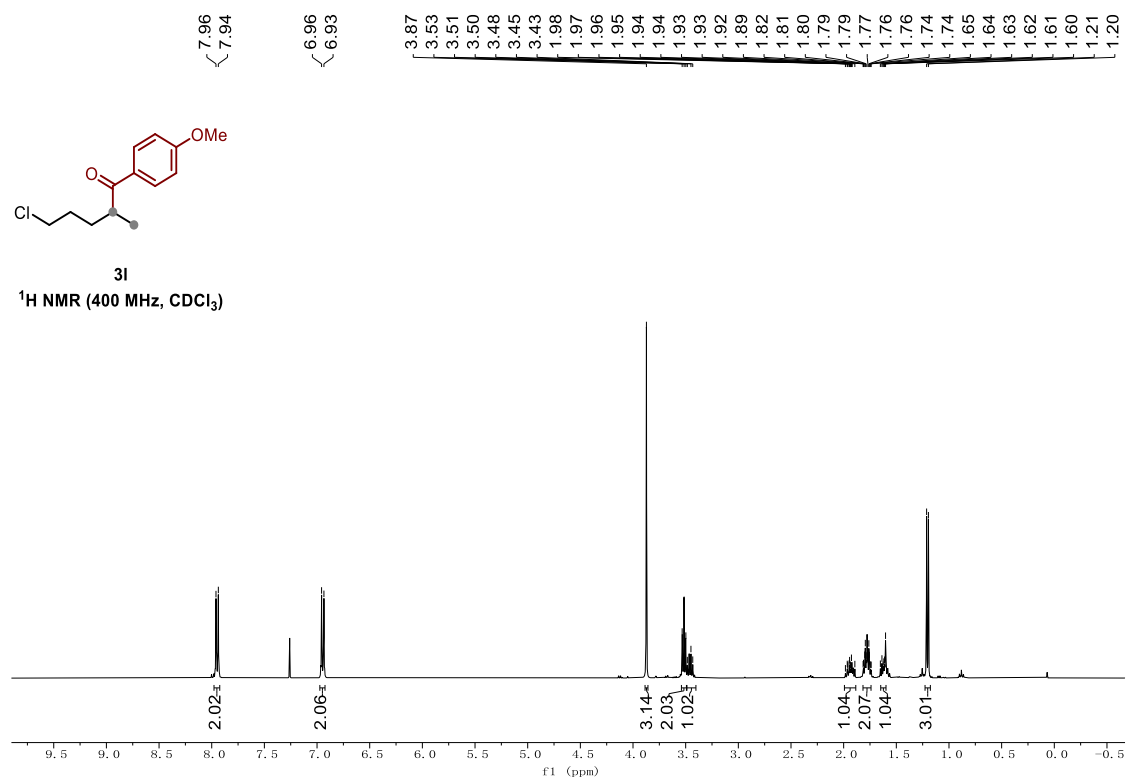


Figure S16. ¹H NMR and ¹³C NMR spectra of **3l**.

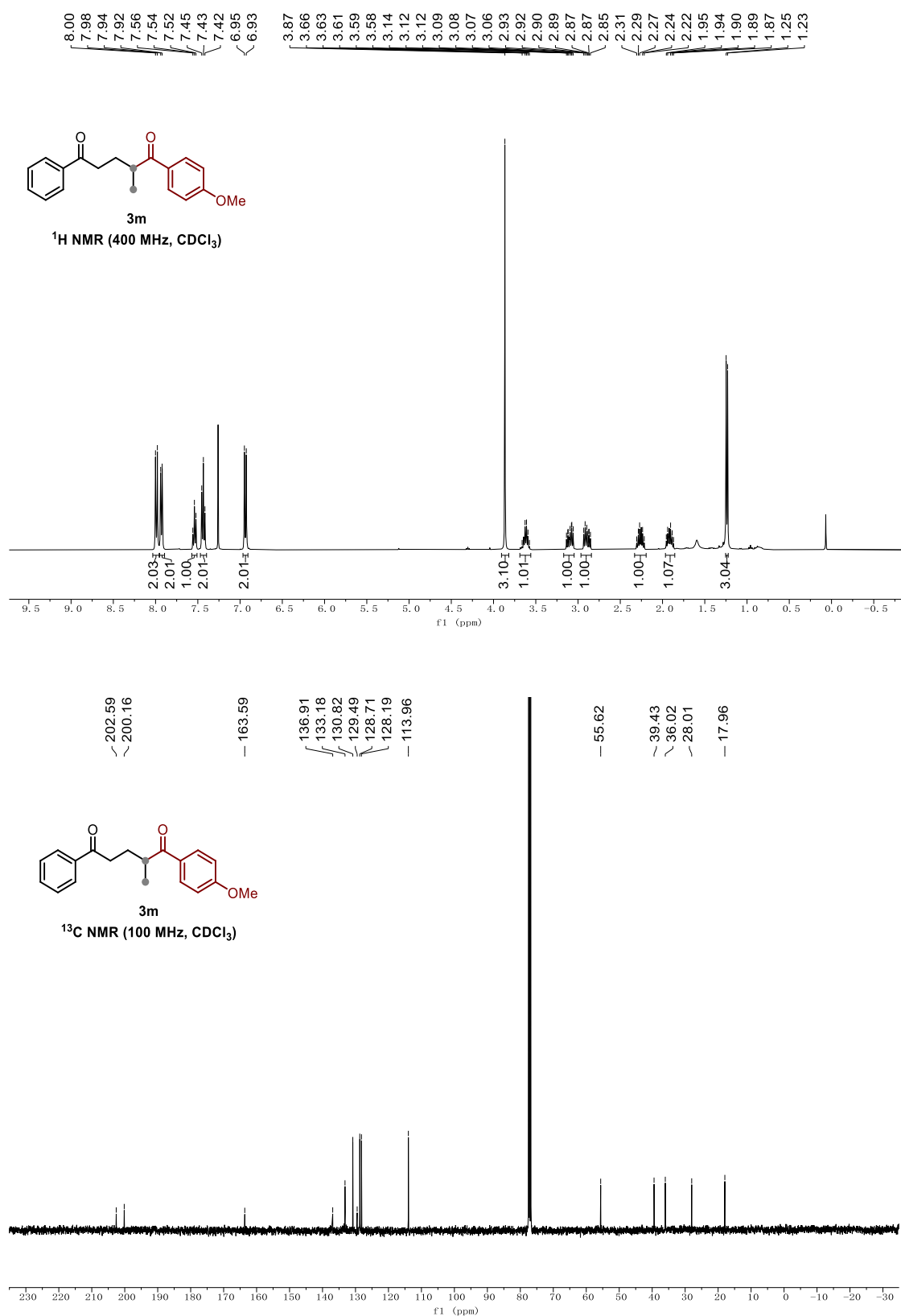


Figure S17. ¹H NMR and ¹³C NMR spectra of **3m**.

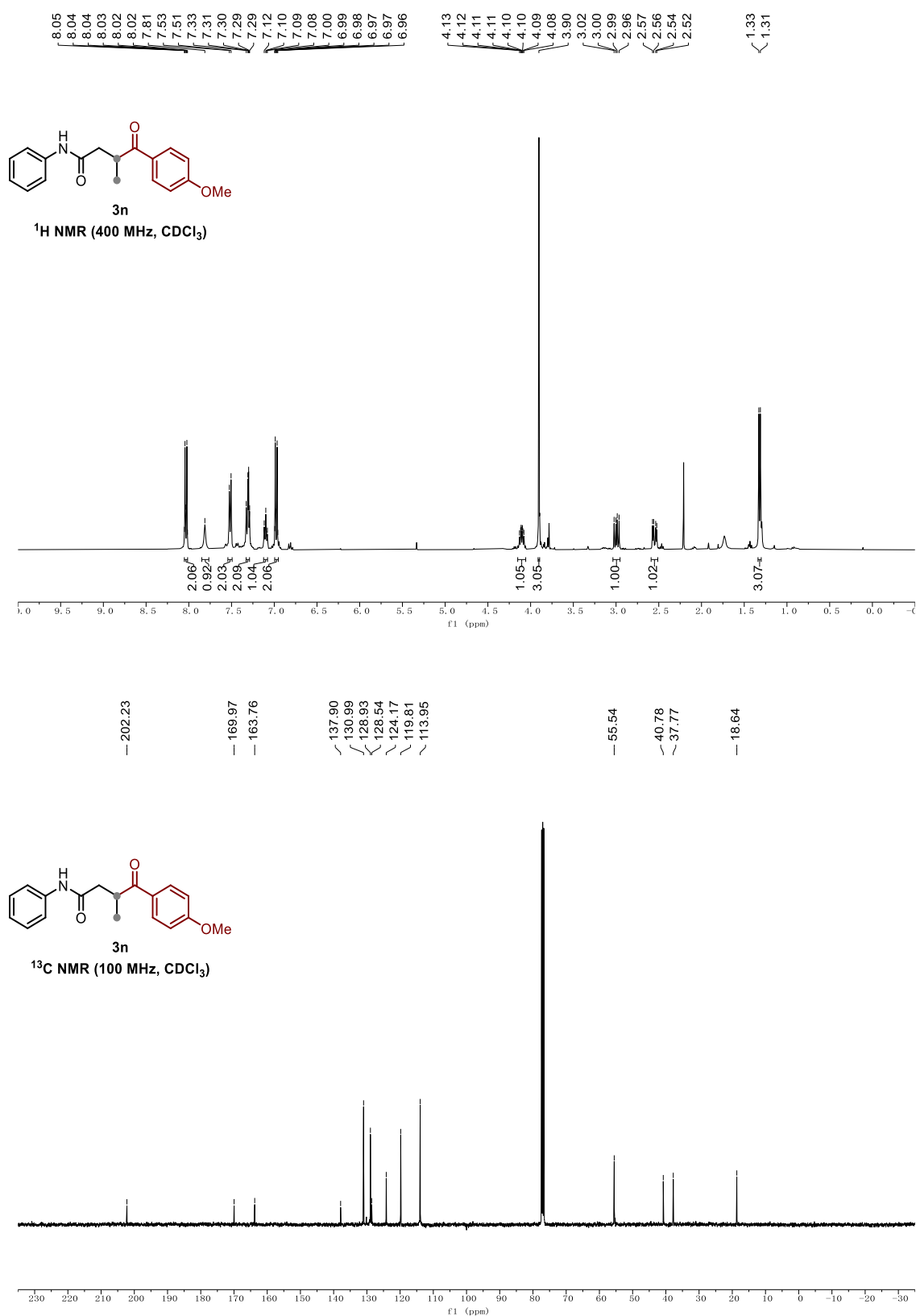


Figure S18. ¹H NMR and ¹³C NMR spectra of **3n**.

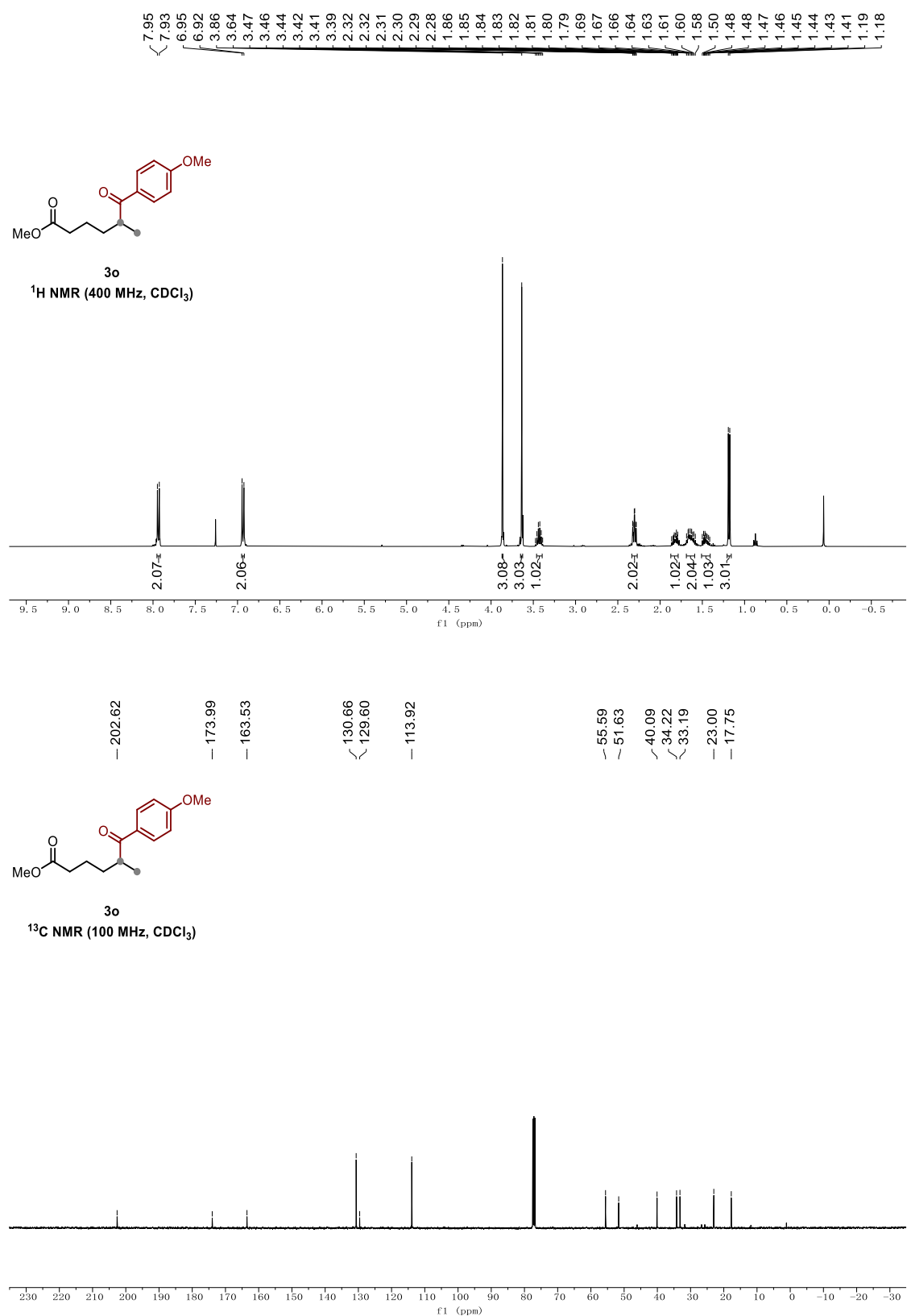


Figure S19. ¹H NMR and ¹³C NMR spectra of **3o**.

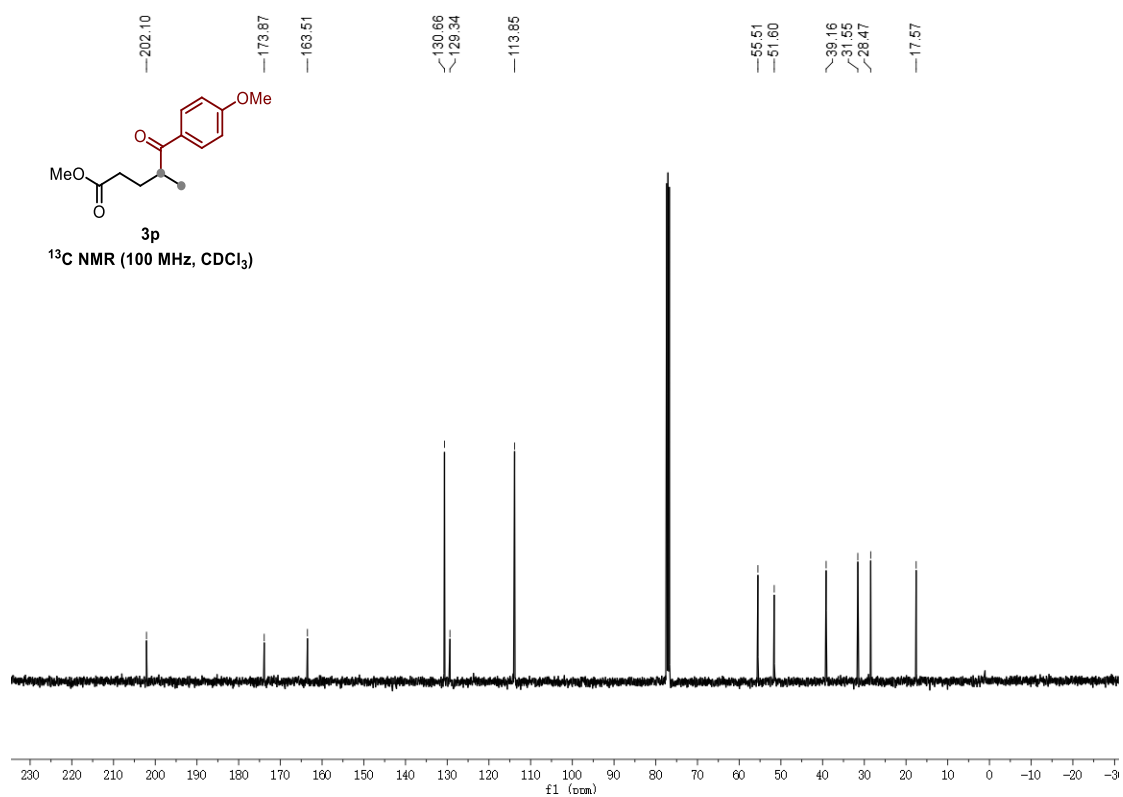
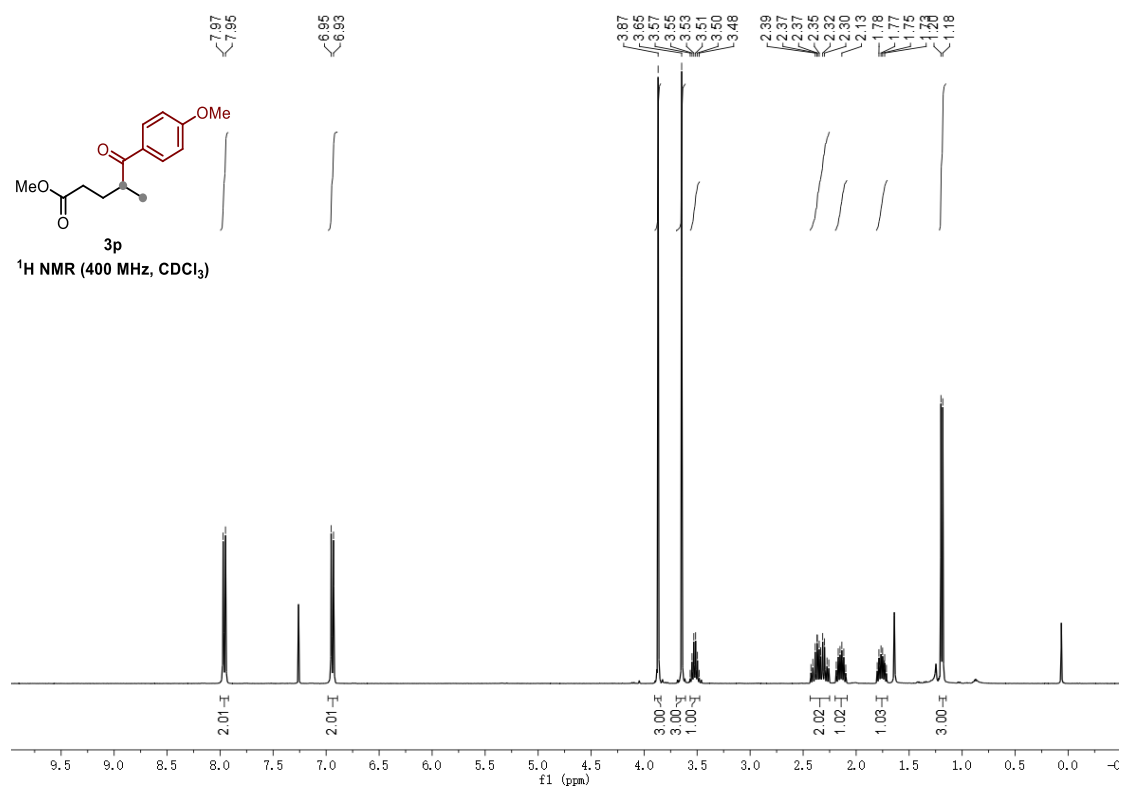


Figure S20. ^1H NMR and ^{13}C NMR spectra of **3p**.

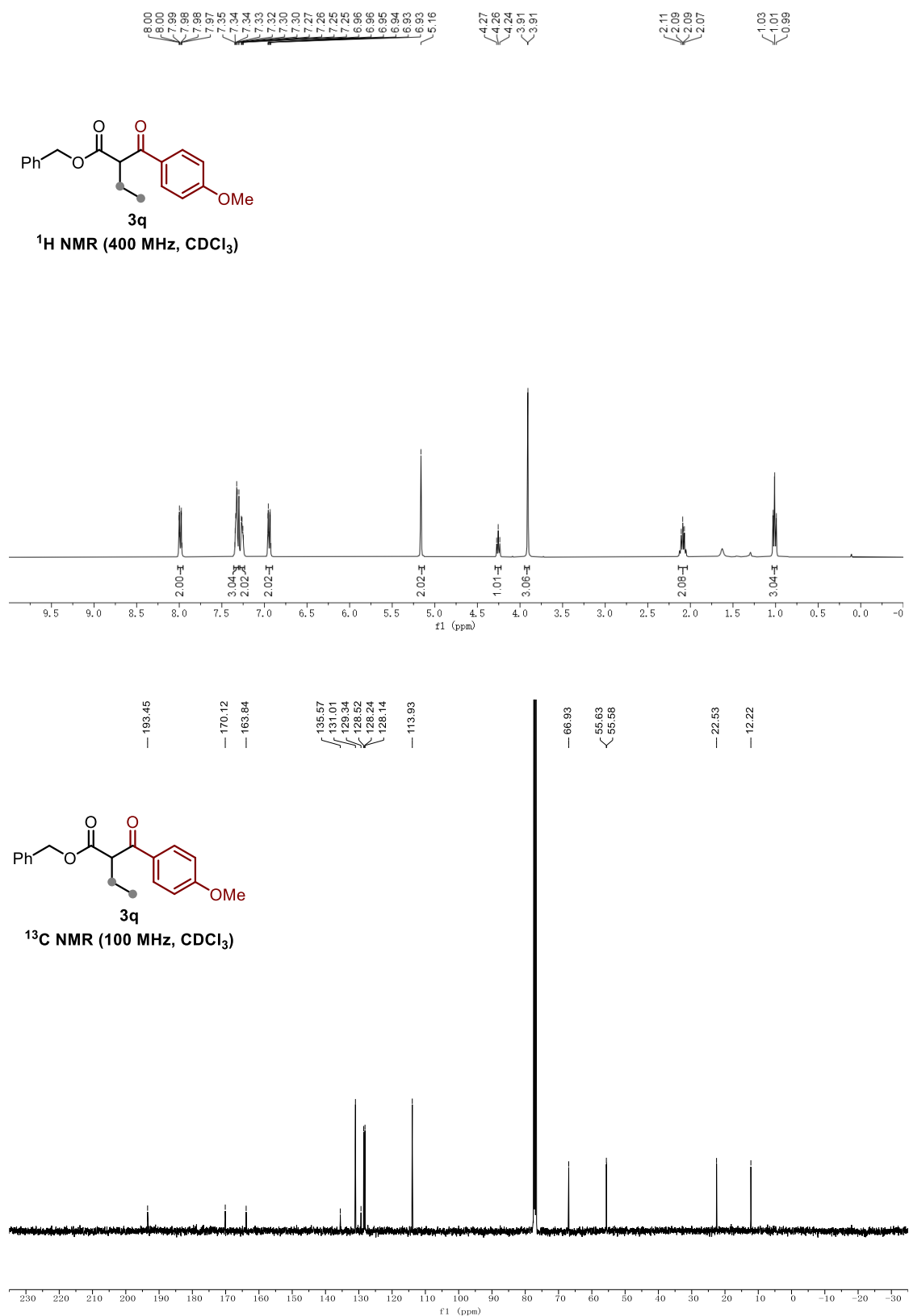


Figure S21. ^1H NMR and ^{13}C NMR spectra of **3q**.

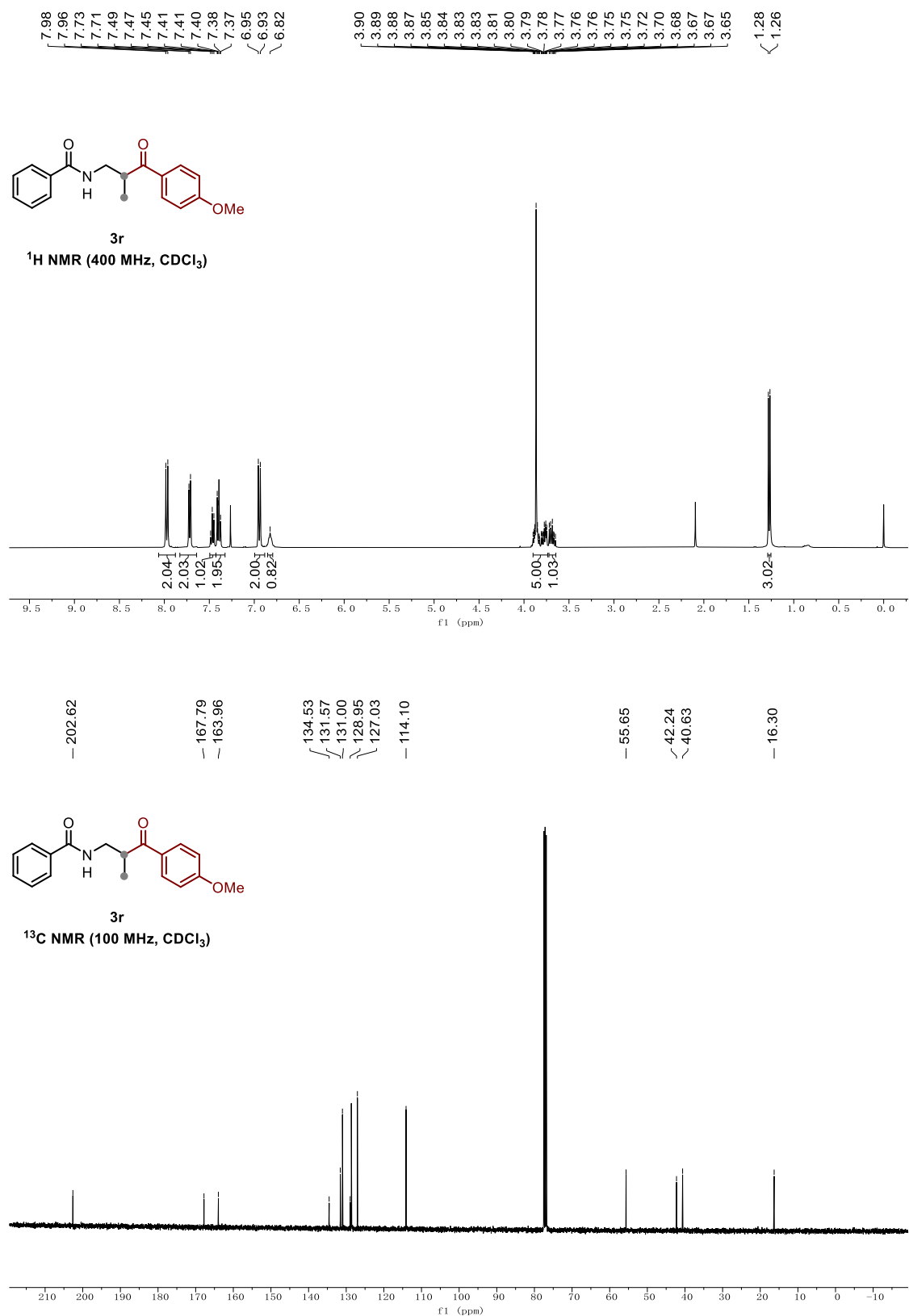


Figure S22. ¹H NMR and ¹³C NMR spectra of **3r**.

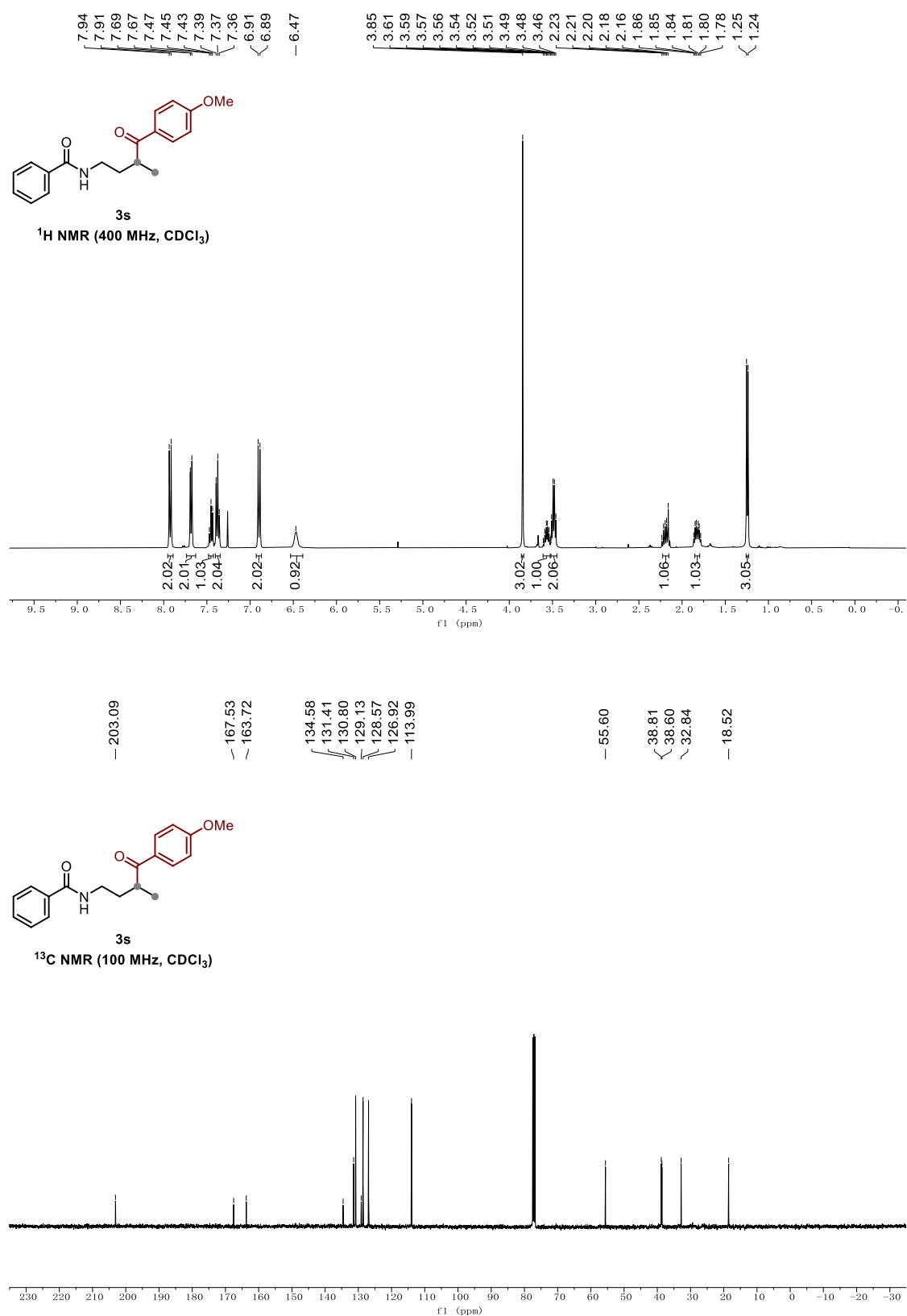


Figure S23. ¹H NMR and ¹³C NMR spectra of **3s**.

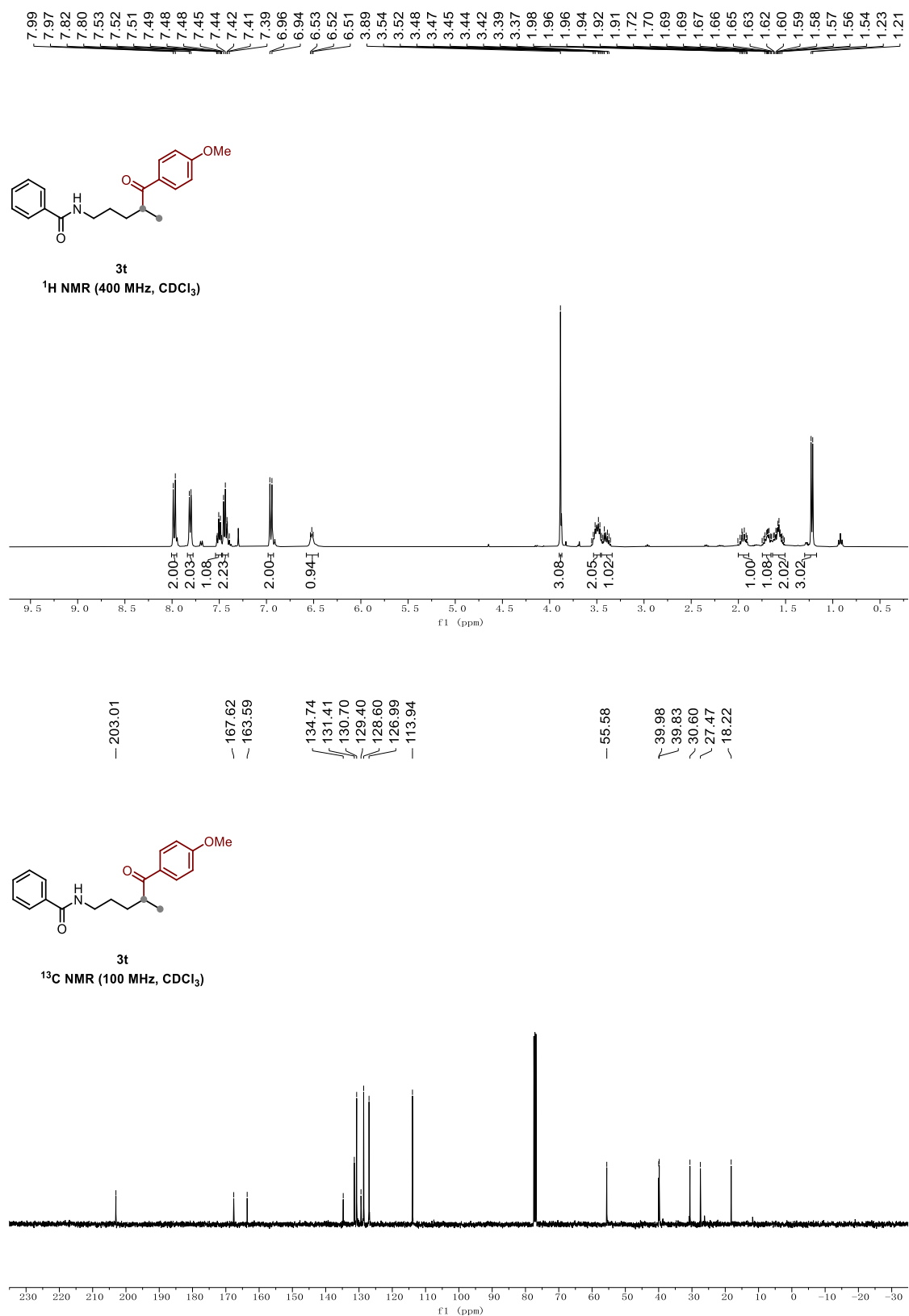


Figure S24. ¹H NMR and ¹³C NMR spectra of **3t**.

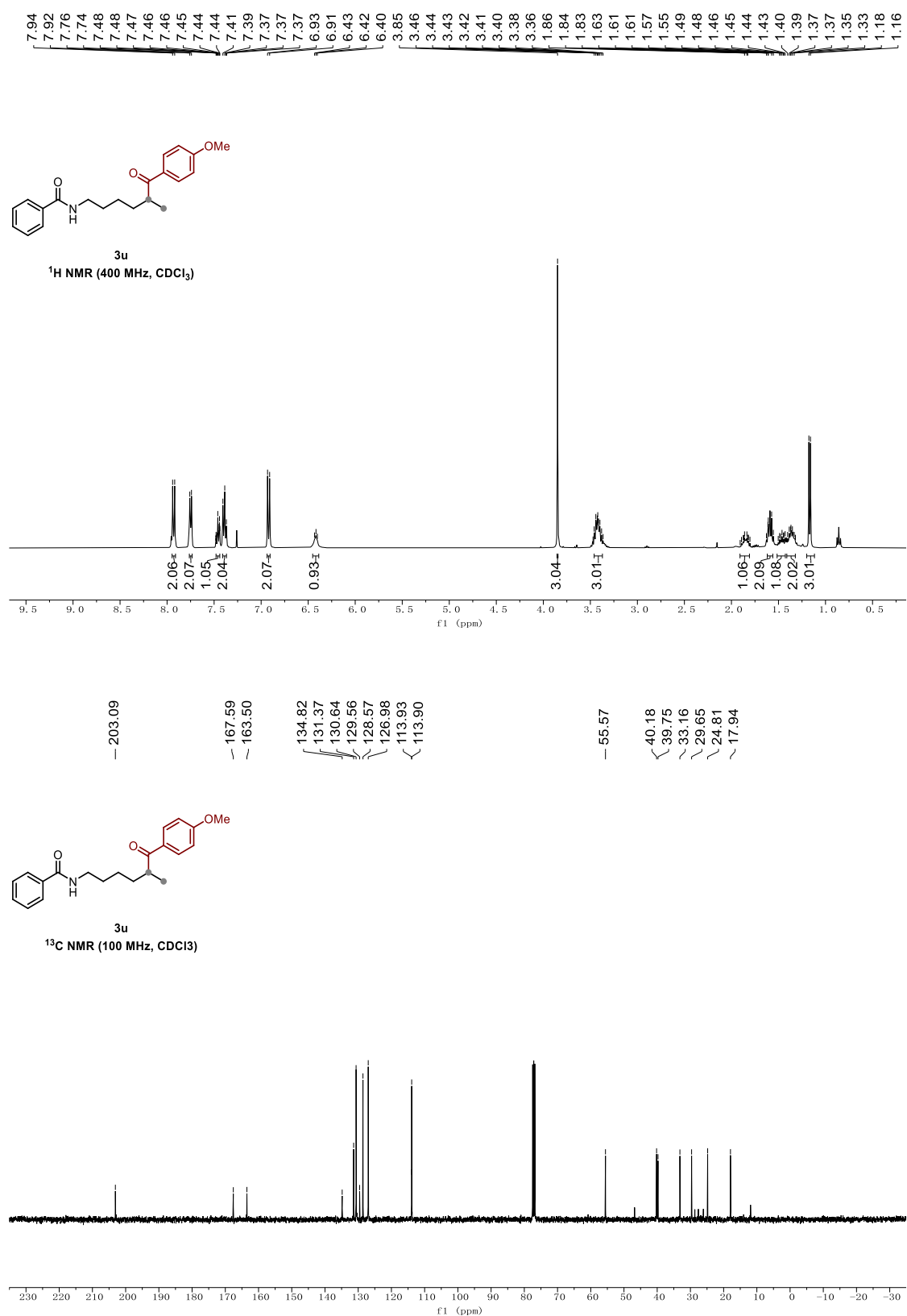


Figure S25. ¹H NMR and ¹³C NMR spectra of **3u**.

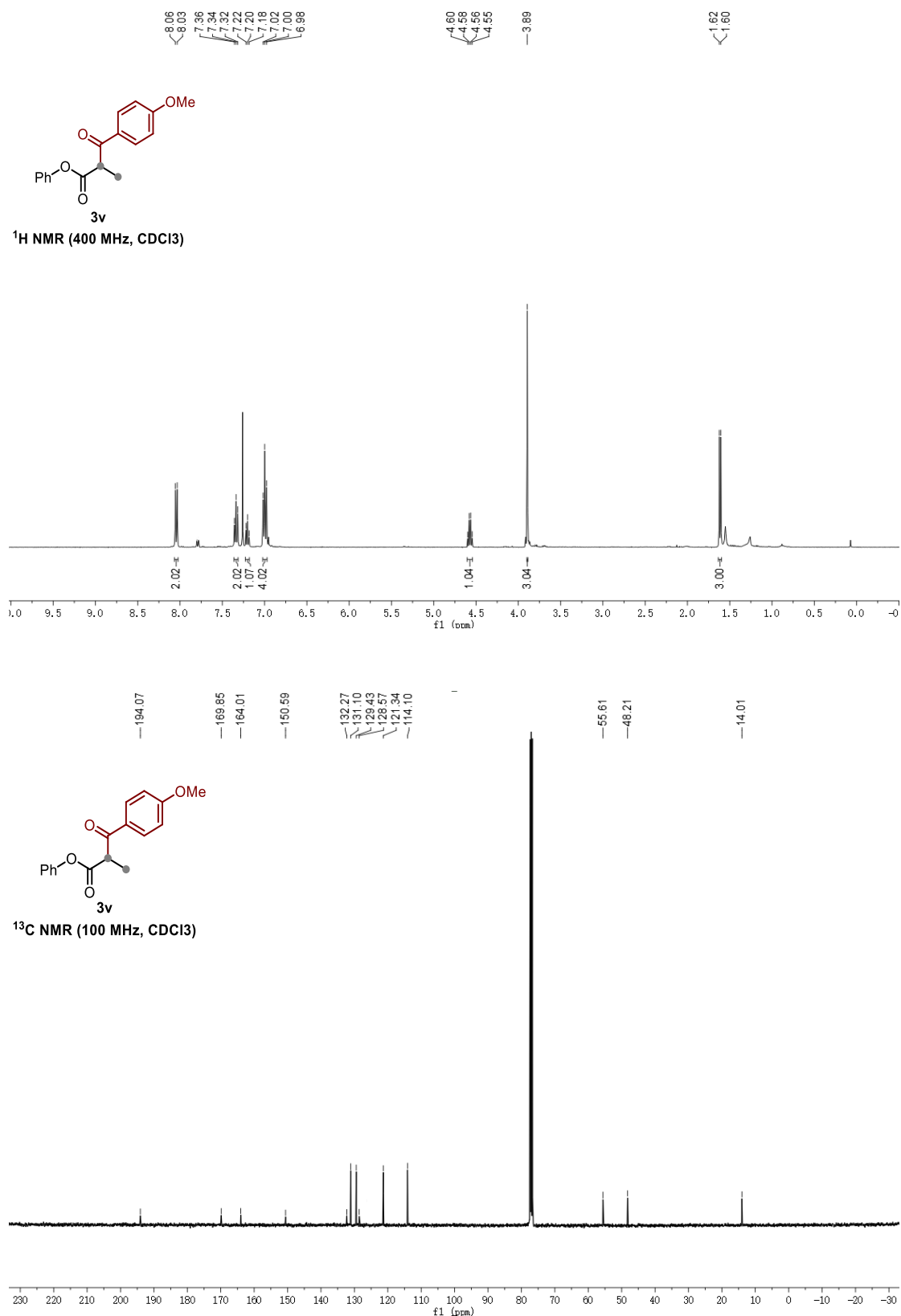


Figure S26. ¹H NMR and ¹³C NMR spectra of **3v**.

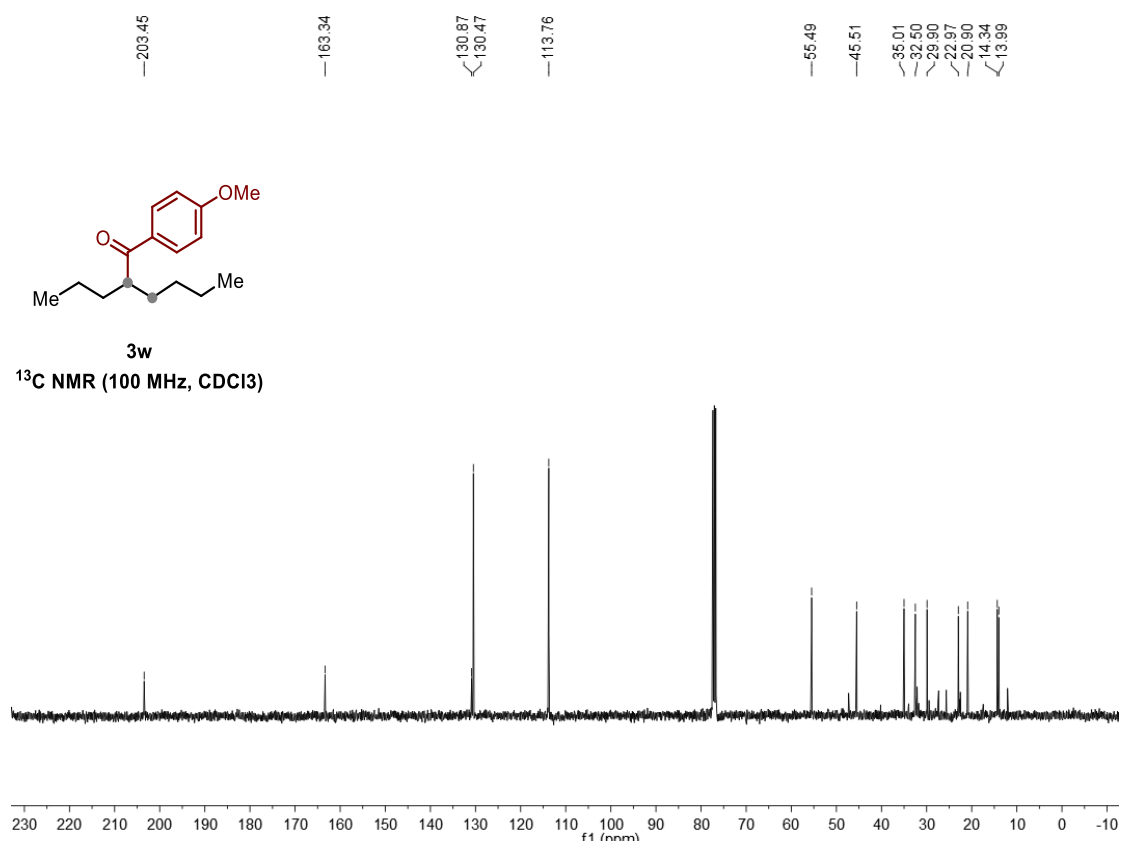
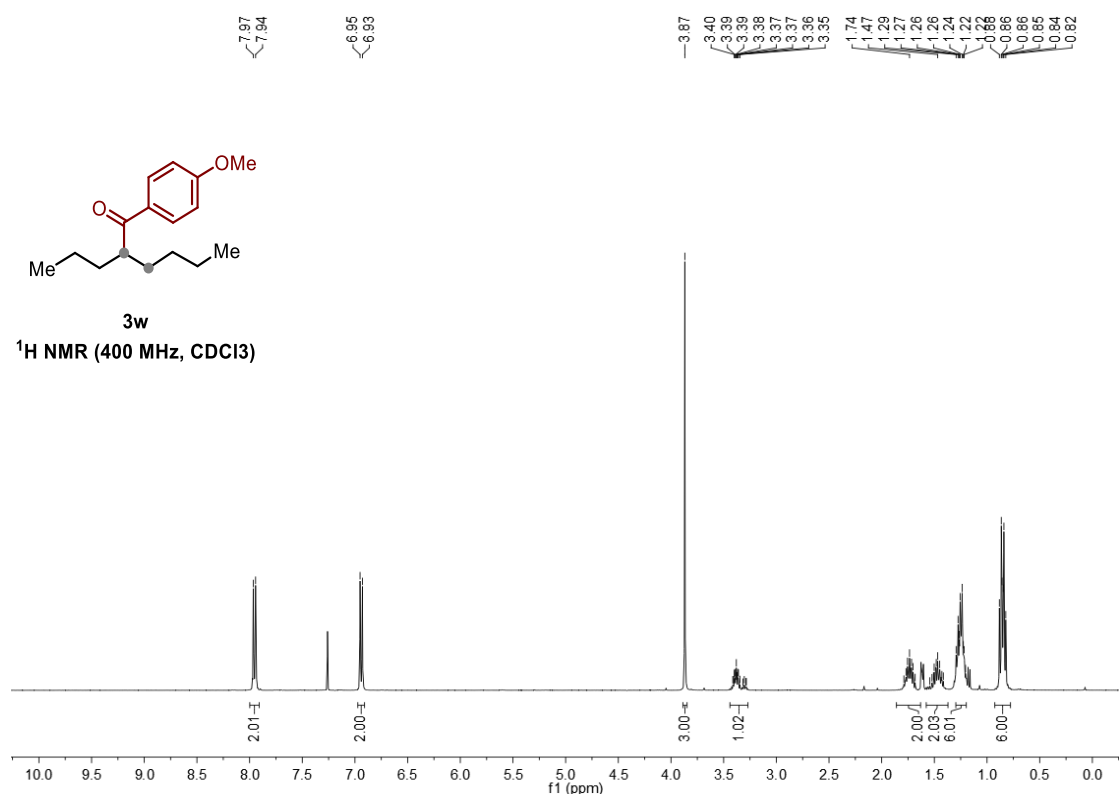


Figure S27. ^1H NMR and ^{13}C NMR spectra of **3w**.

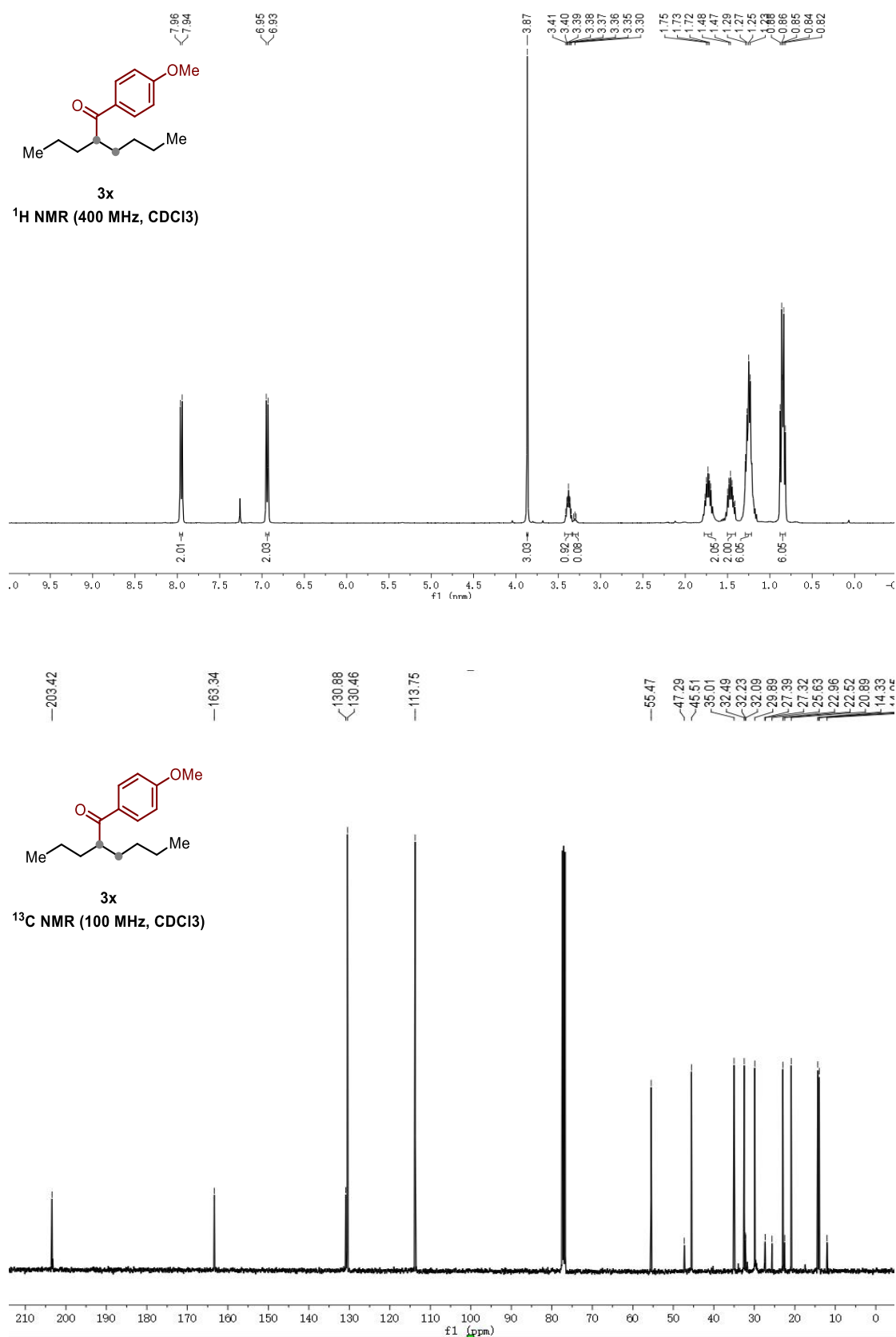


Figure S28. ¹H NMR and ¹³C NMR spectra of **3x**.

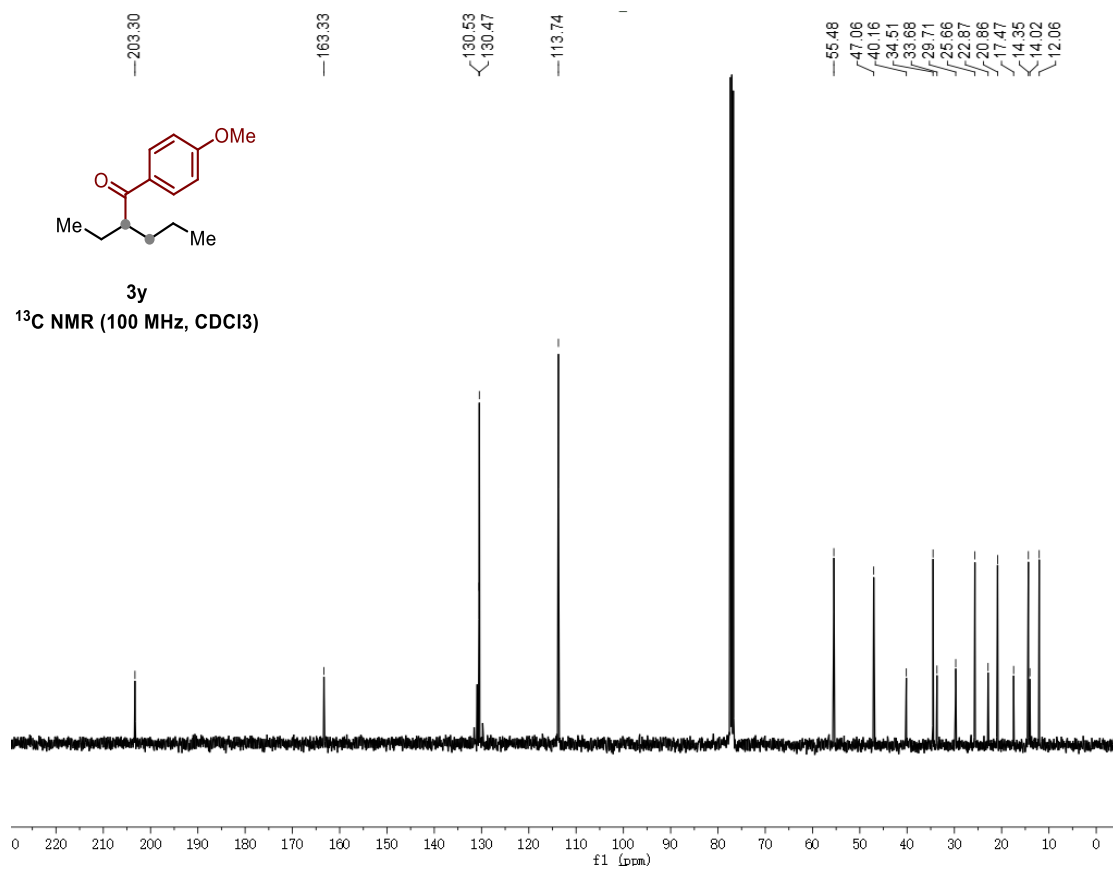
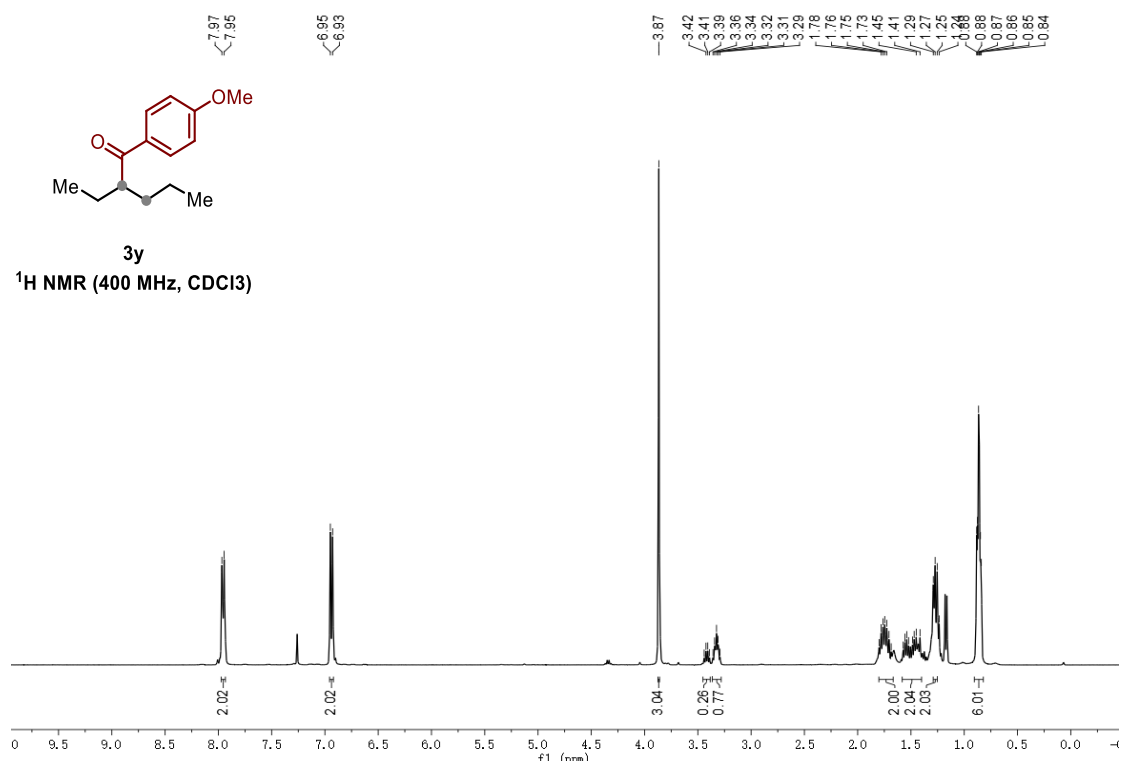


Figure S29. ^1H NMR and ^{13}C NMR spectra of **3y**

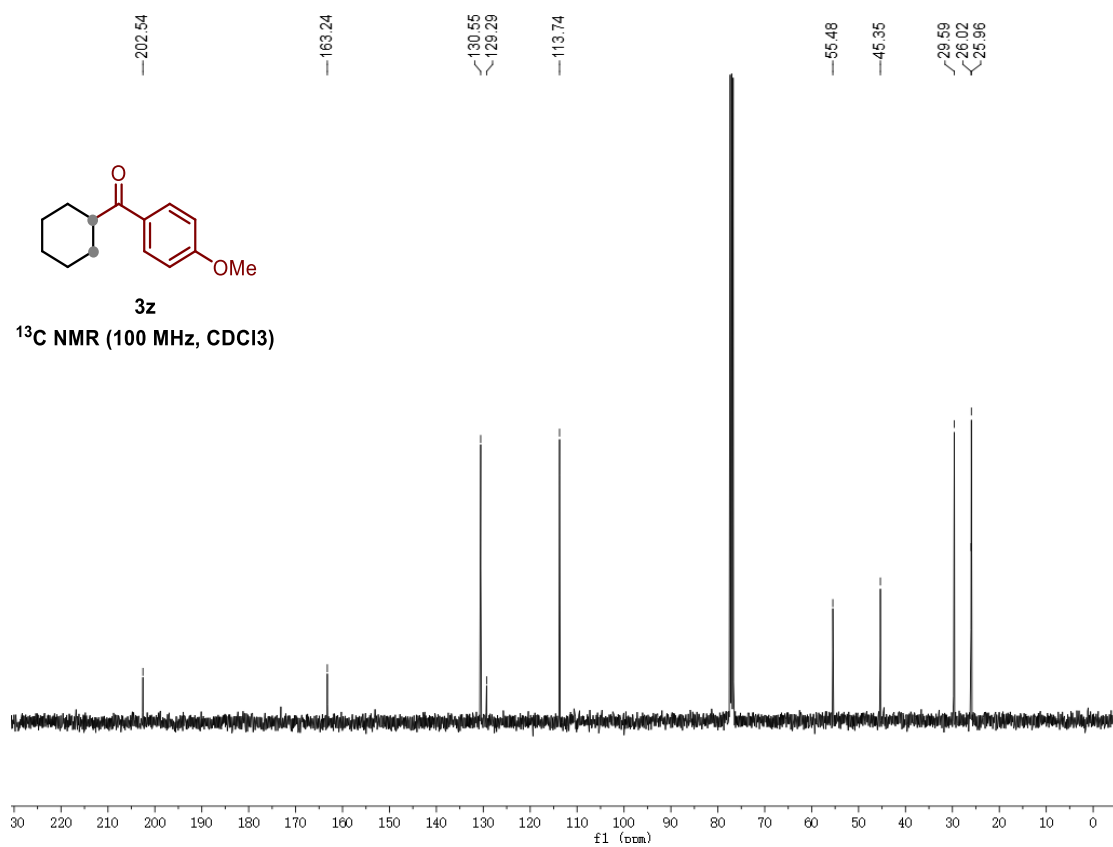
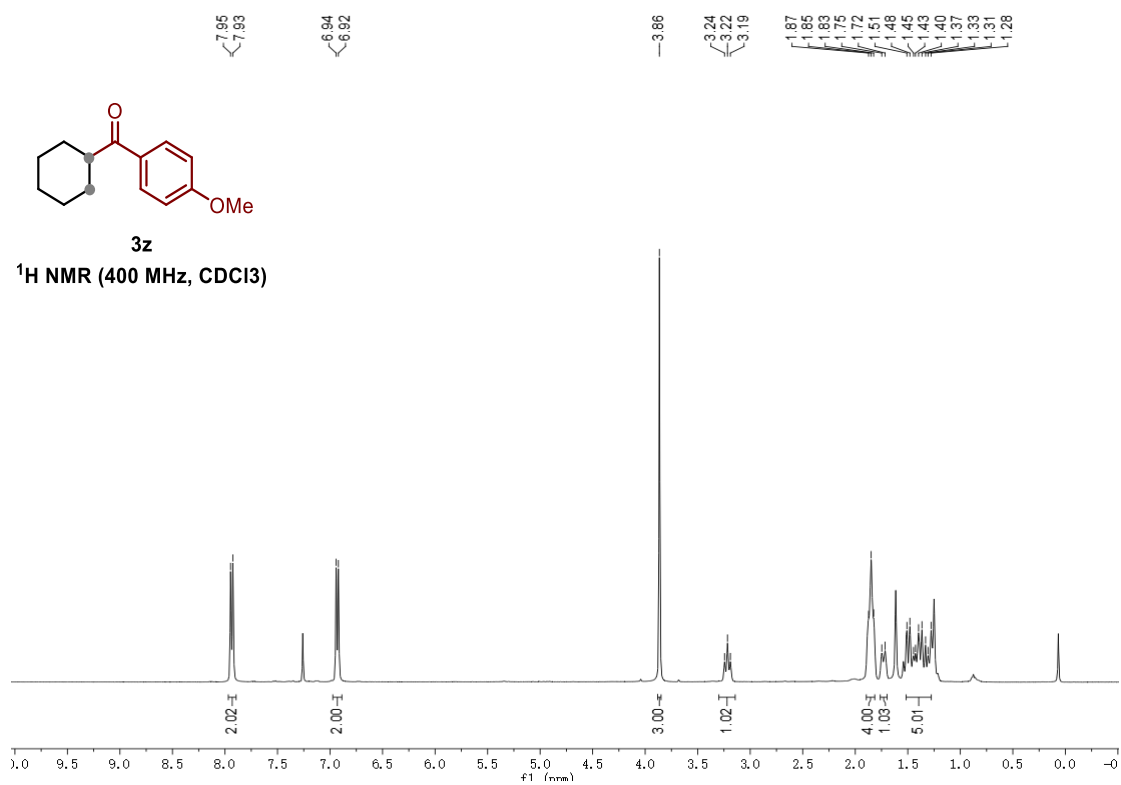


Figure S30. ^1H NMR and ^{13}C NMR spectra of **3z**.

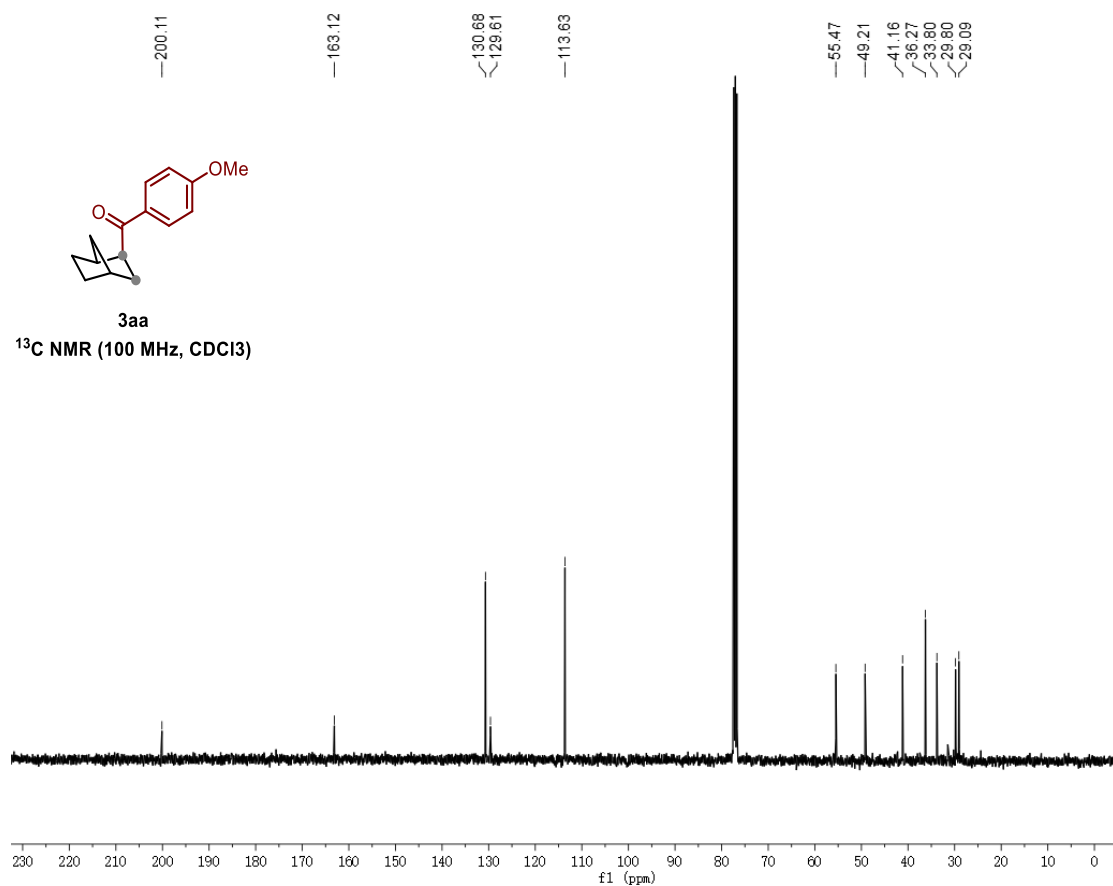
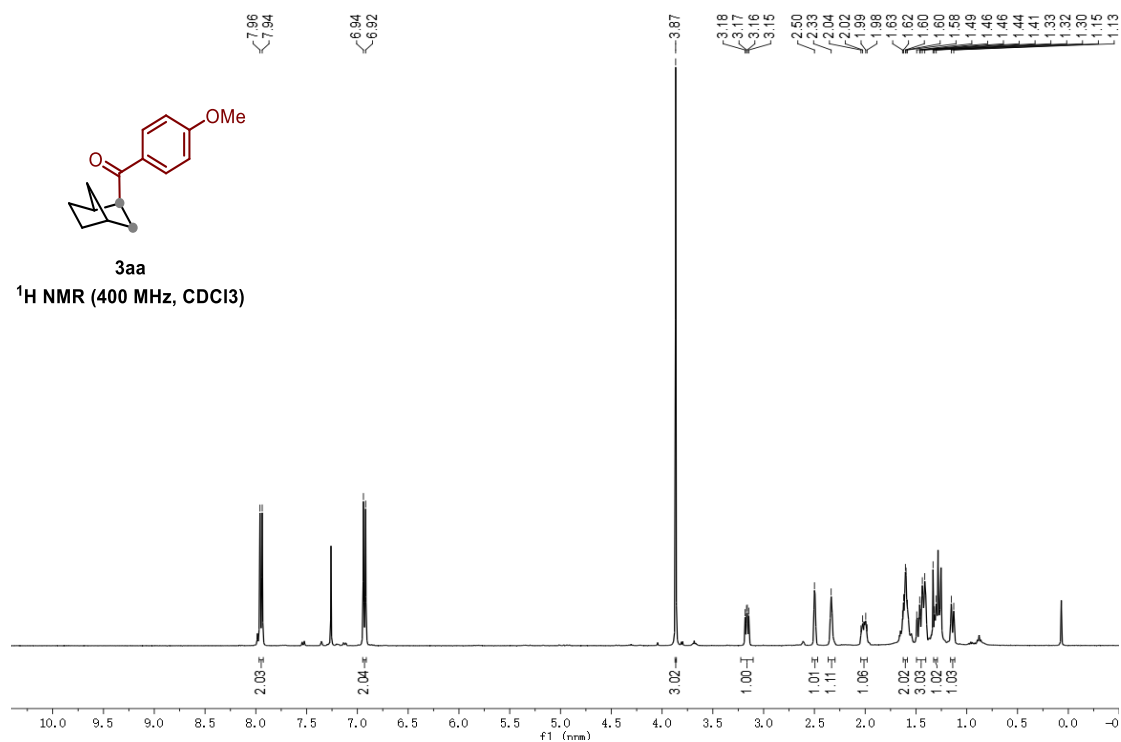


Figure S31. ¹H NMR and ¹³C NMR spectra of **3aa**.

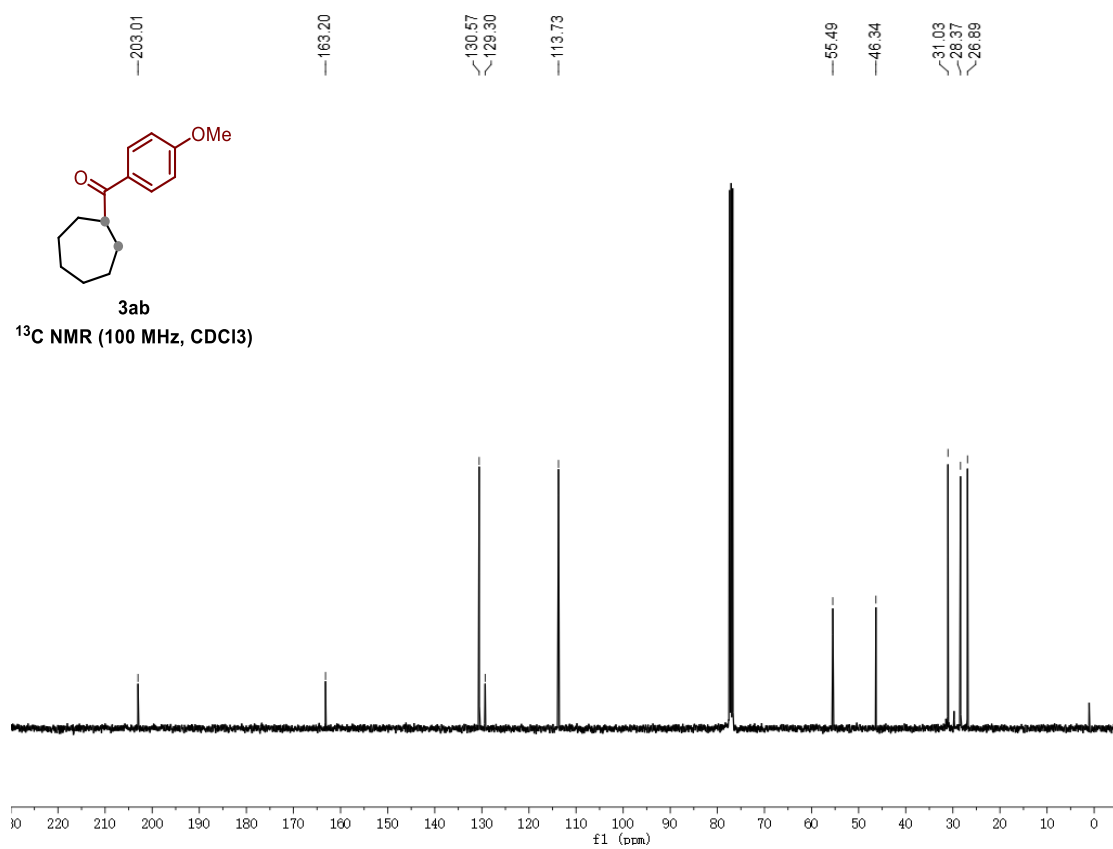
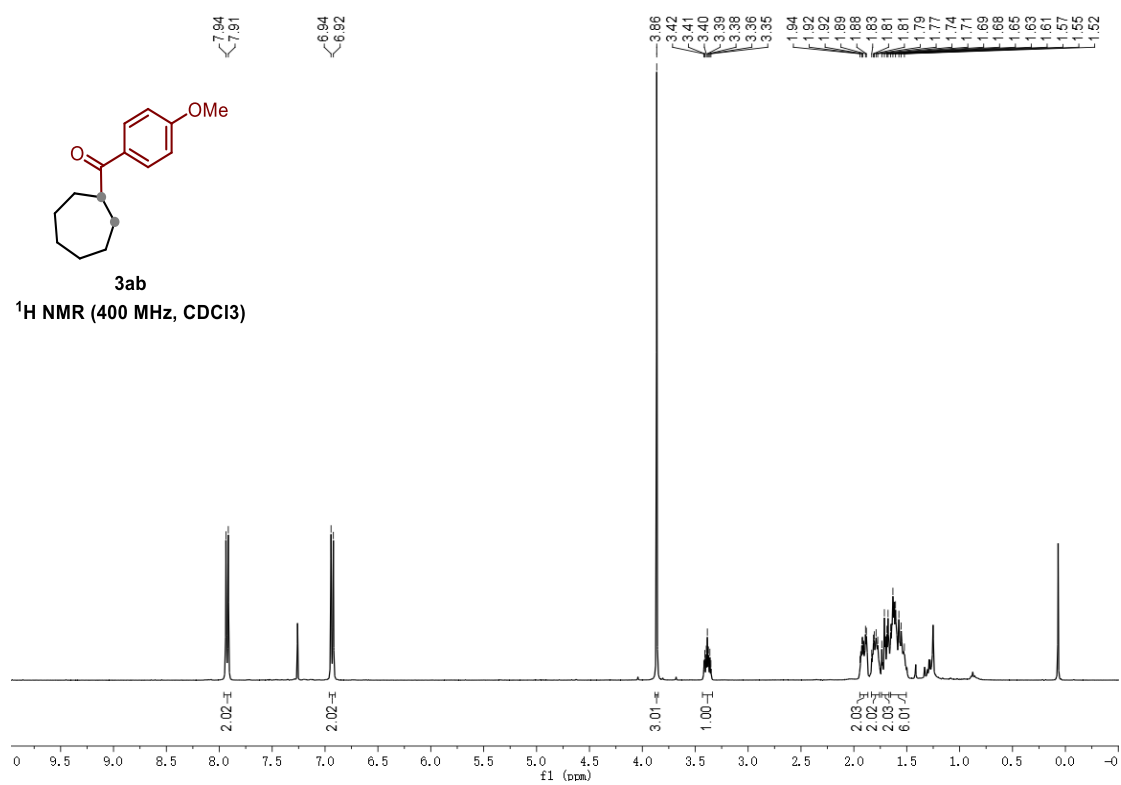


Figure S32. ¹H NMR and ¹³C NMR spectra of **3ab**.

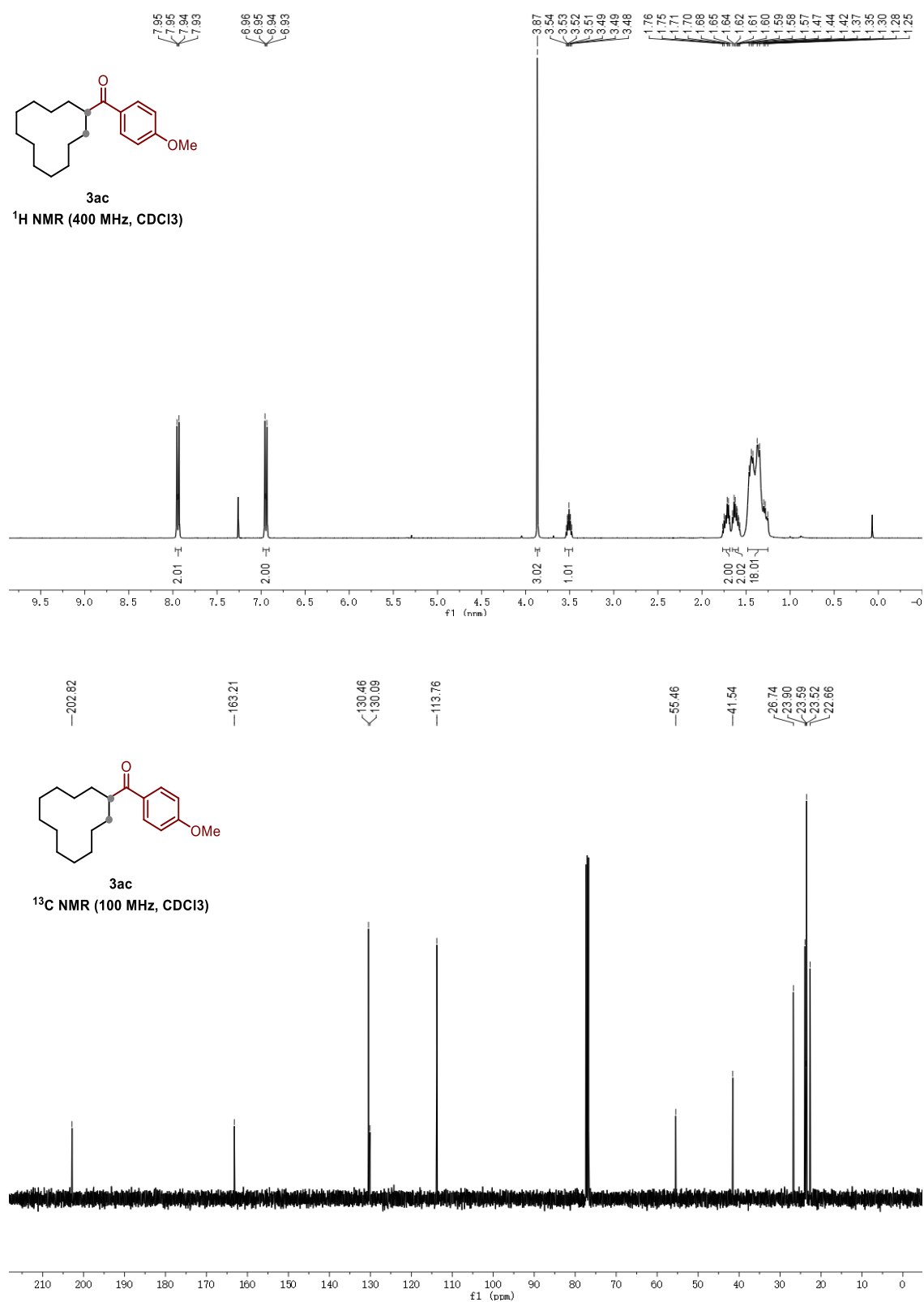


Figure S33. ¹H NMR and ¹³C NMR spectra of **3ac**.

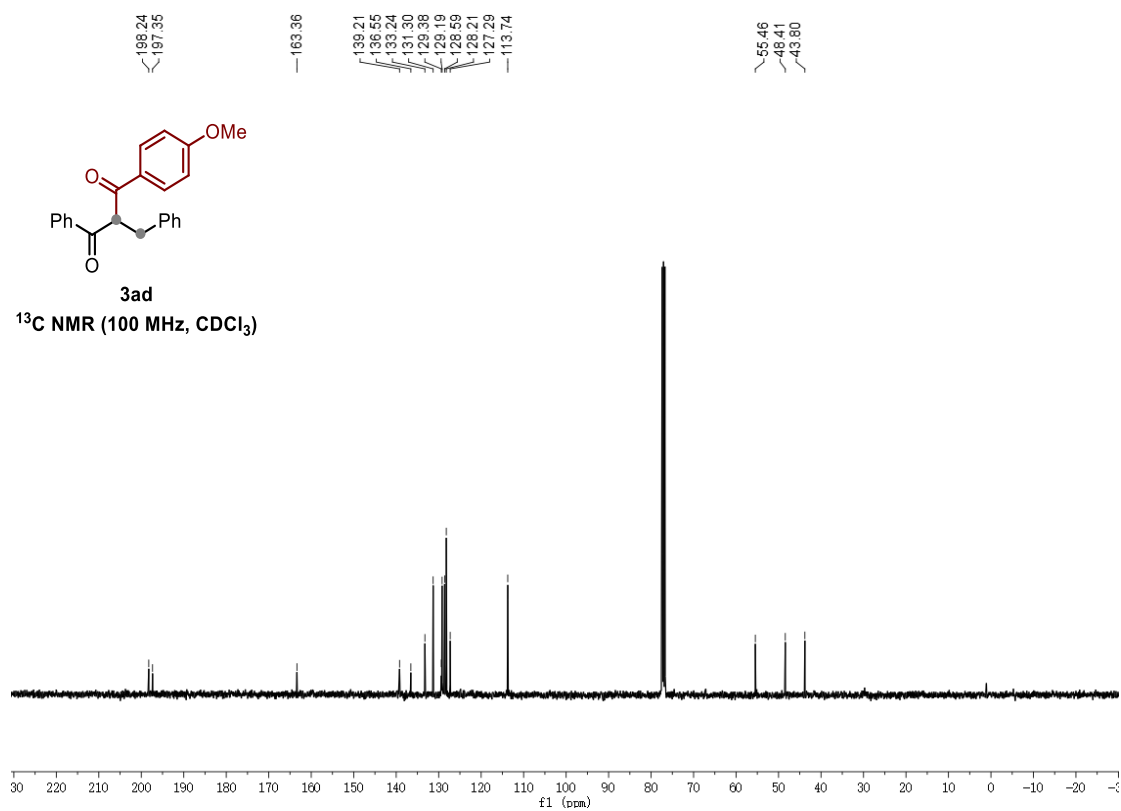
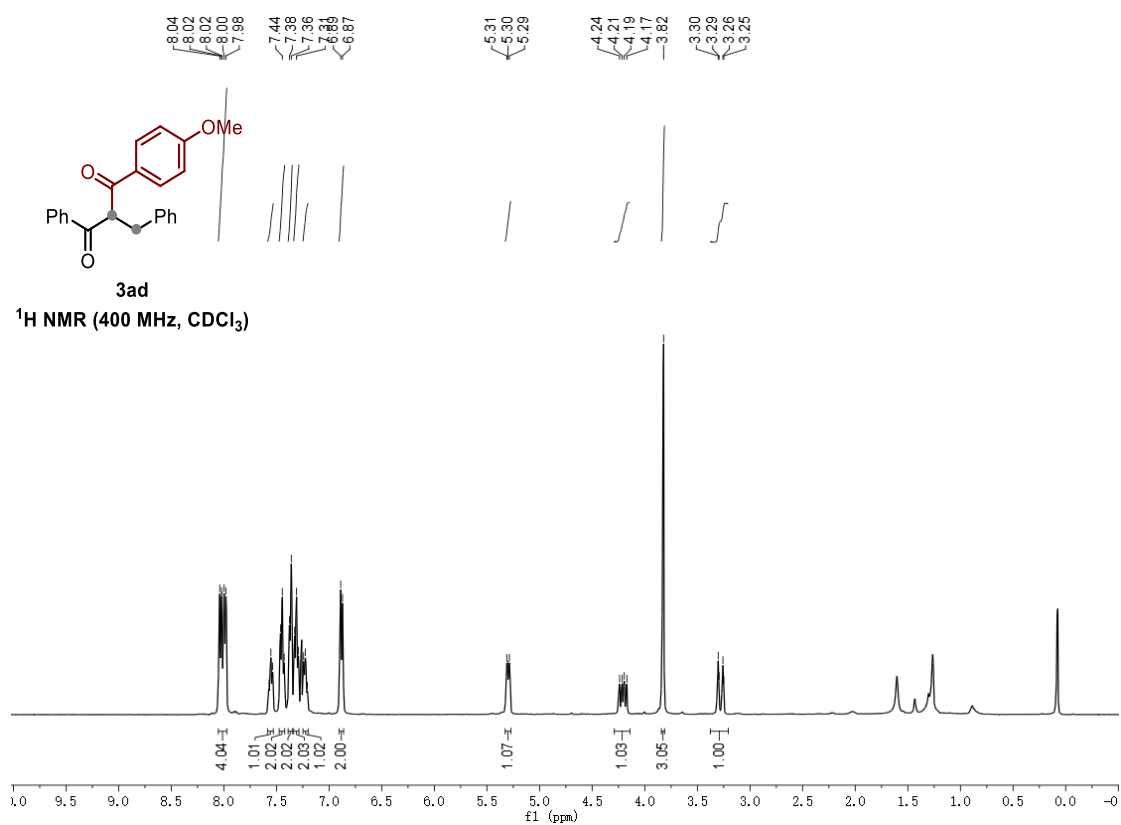


Figure S34. ^1H NMR and ^{13}C NMR spectra of **3ad**.

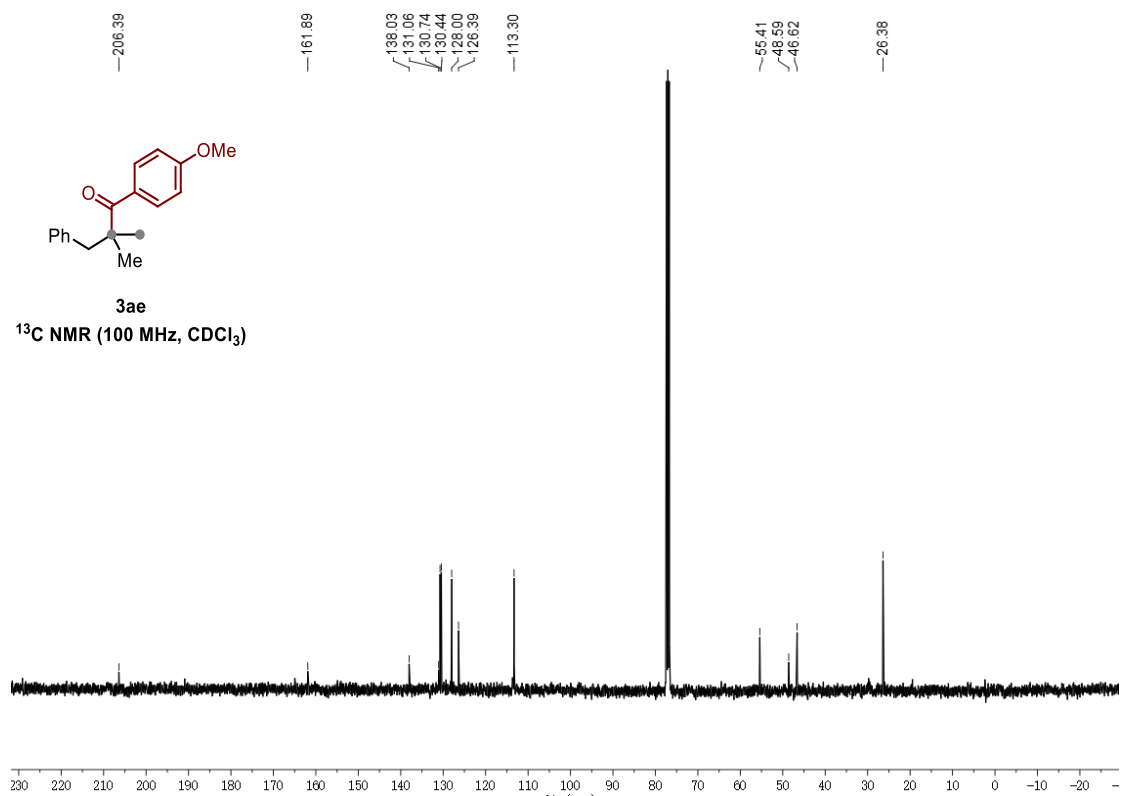
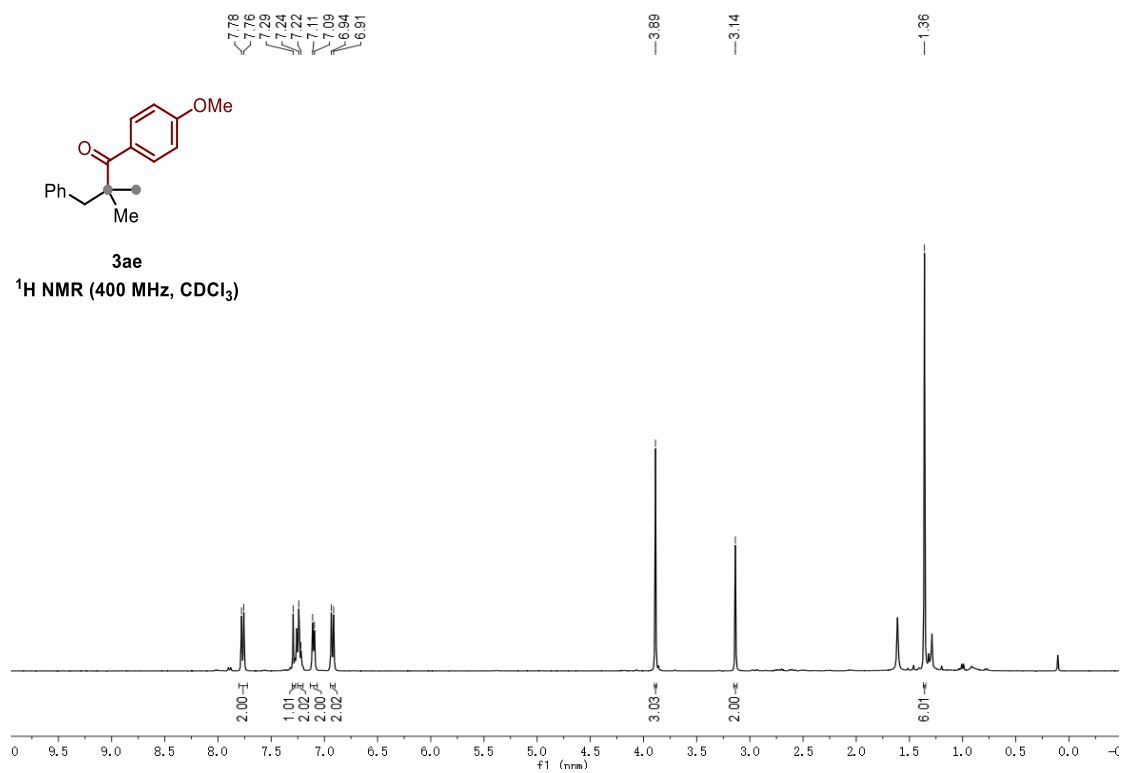


Figure S35. ^1H NMR and ^{13}C NMR spectra of **3ae**.

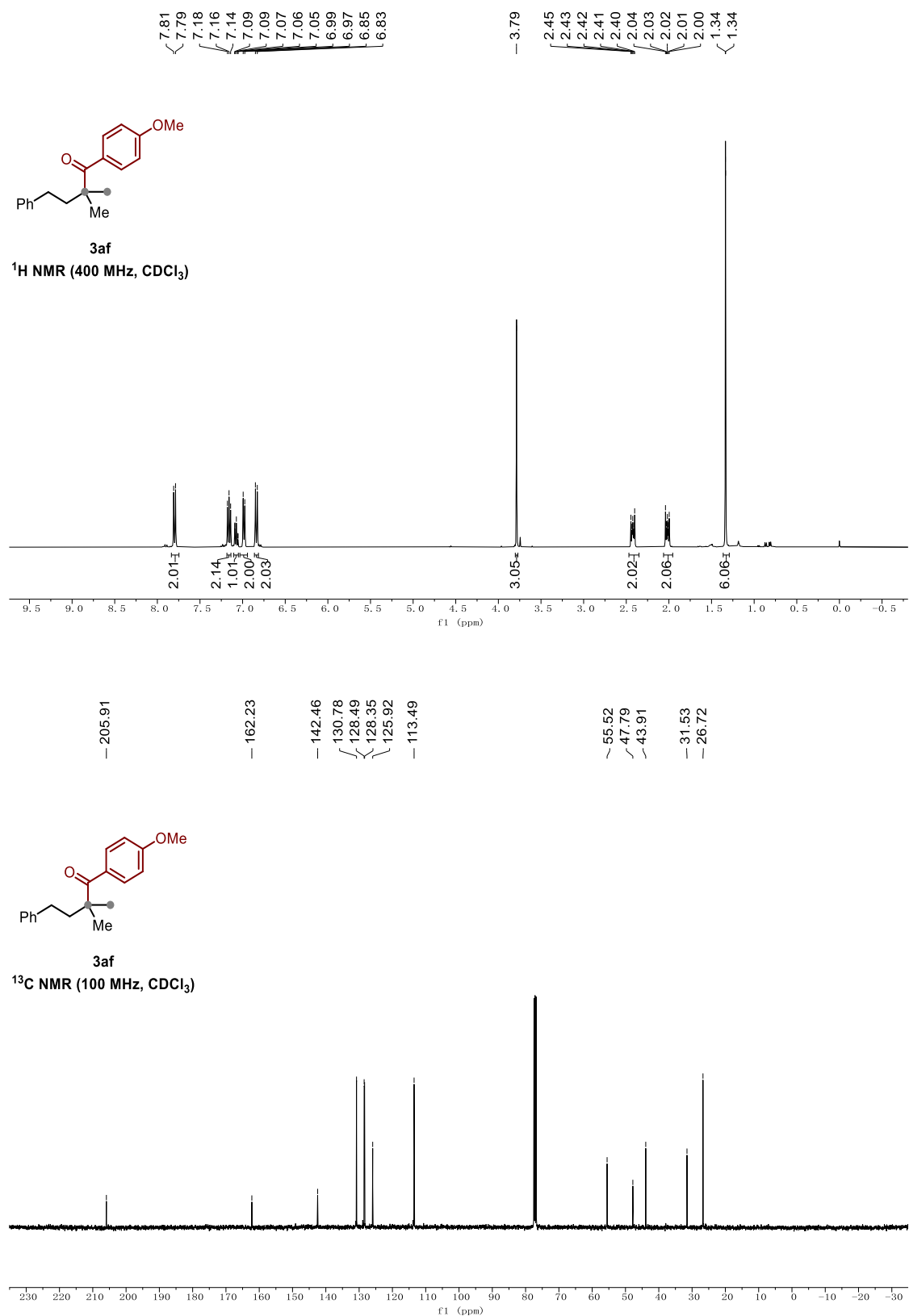


Figure S36. ¹H NMR and ¹³C NMR spectra of **3af**.

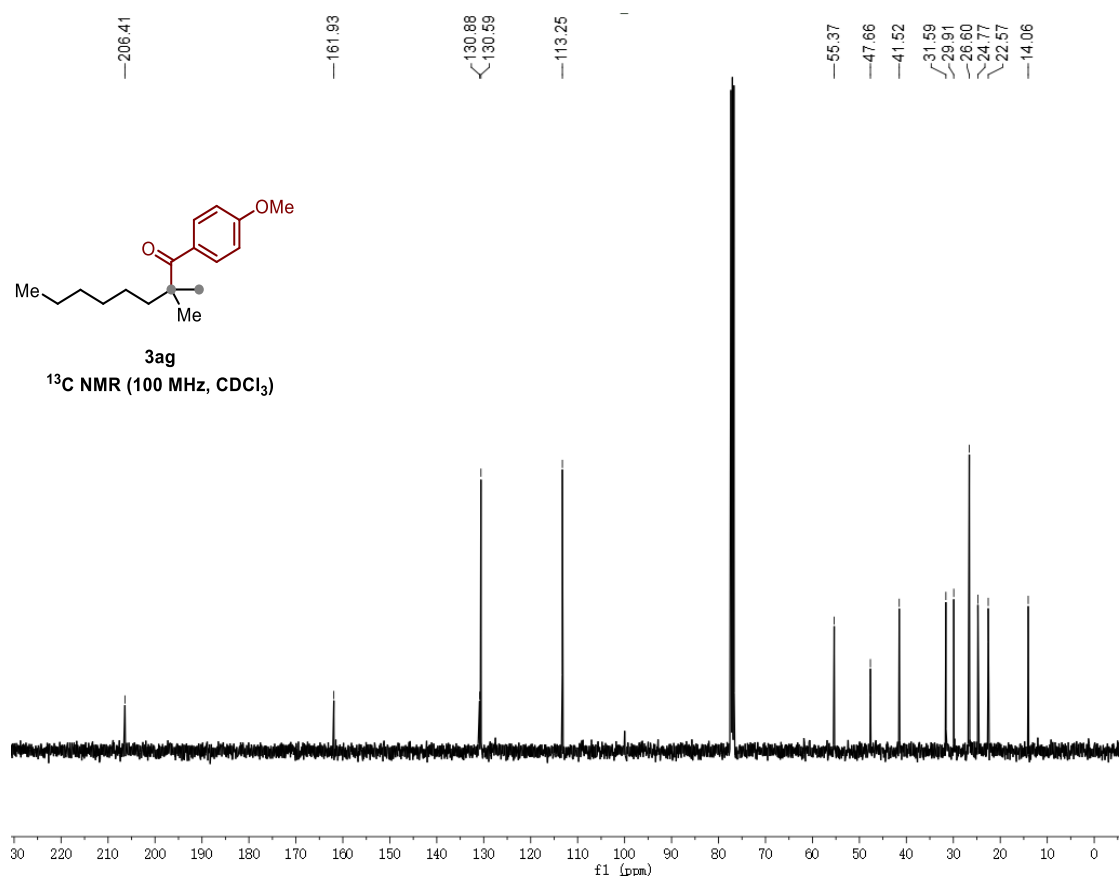
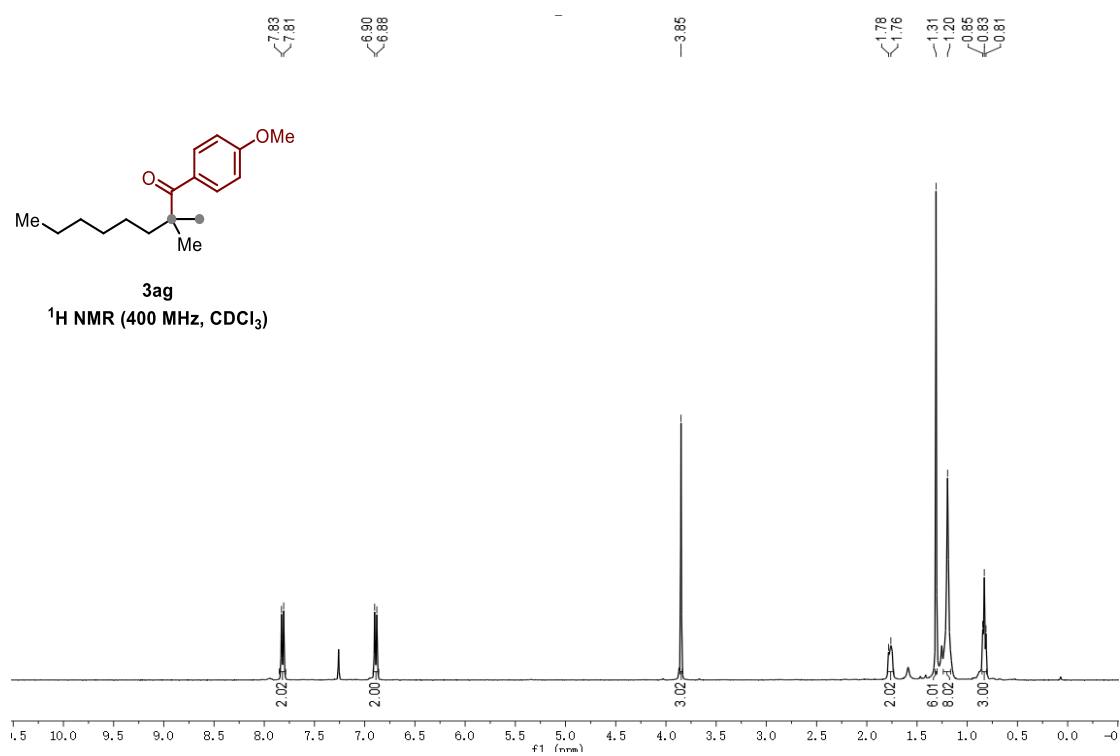


Figure S37. ^1H NMR and ^{13}C NMR spectra of **3ag**.

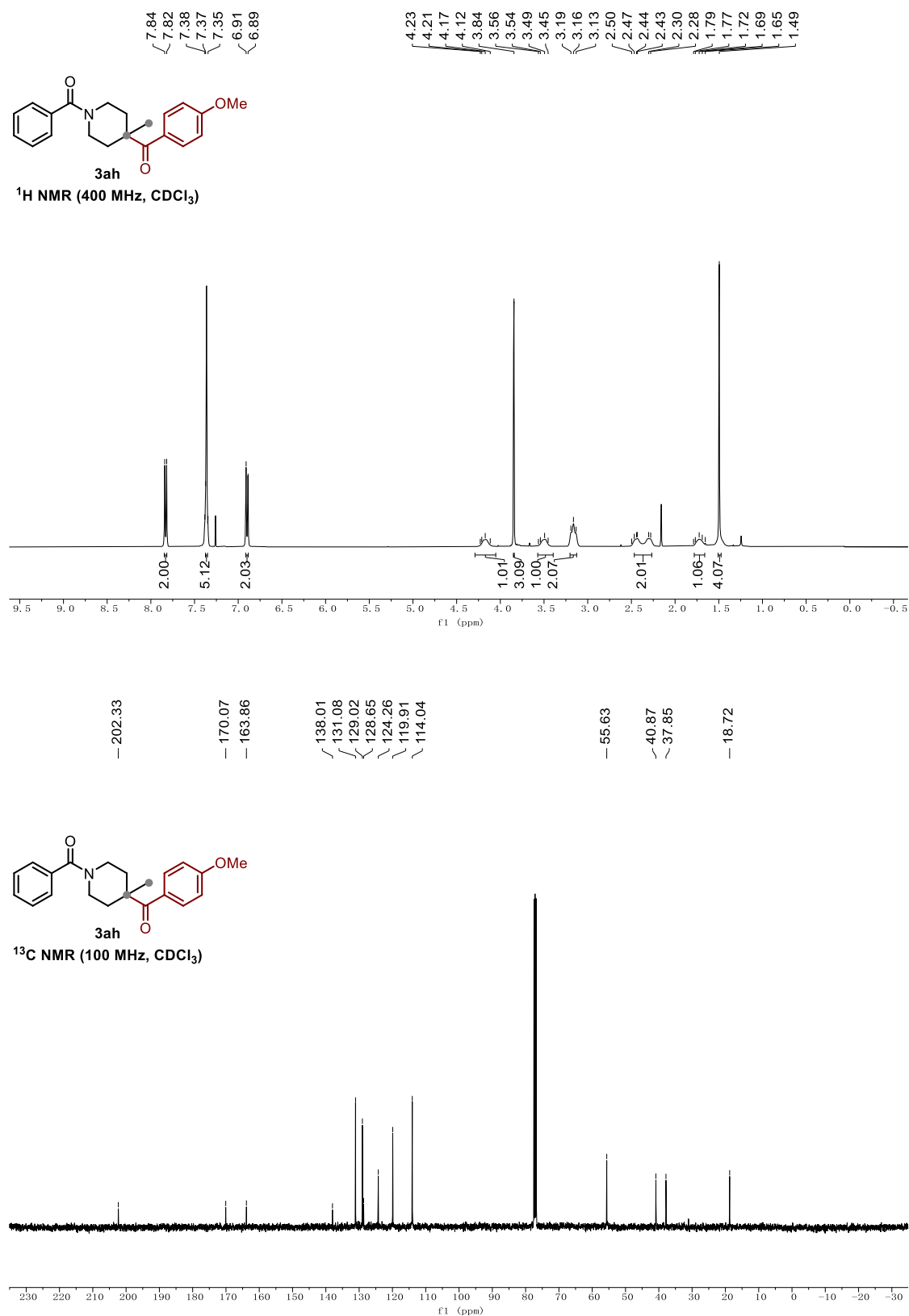


Figure S38. ¹H NMR and ¹³C NMR spectra of **3ah**.

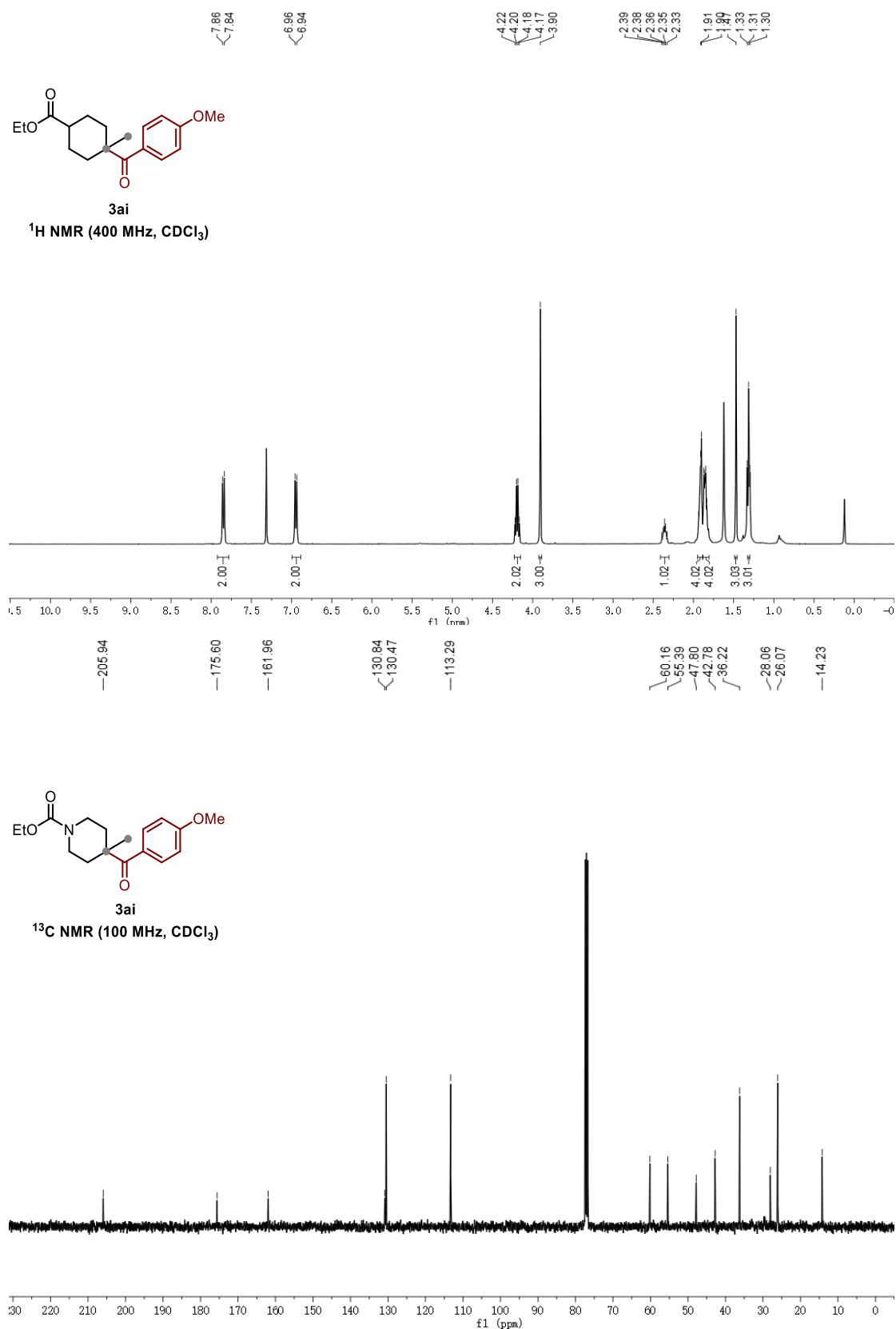


Figure S39. ^1H NMR and ^{13}C NMR spectra of **3ai**.

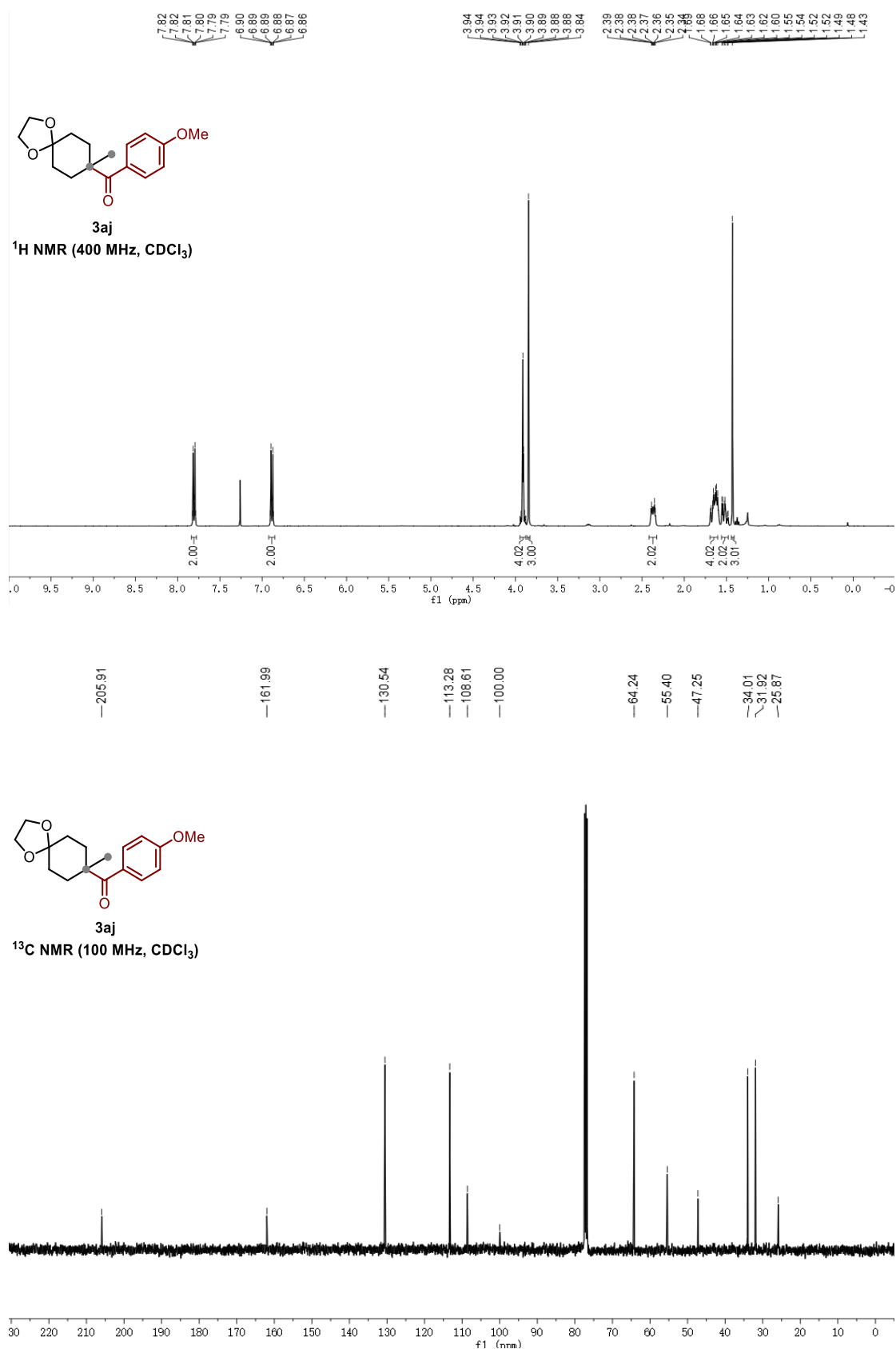


Figure S40. ¹H NMR and ¹³C NMR spectra of **3aj**.

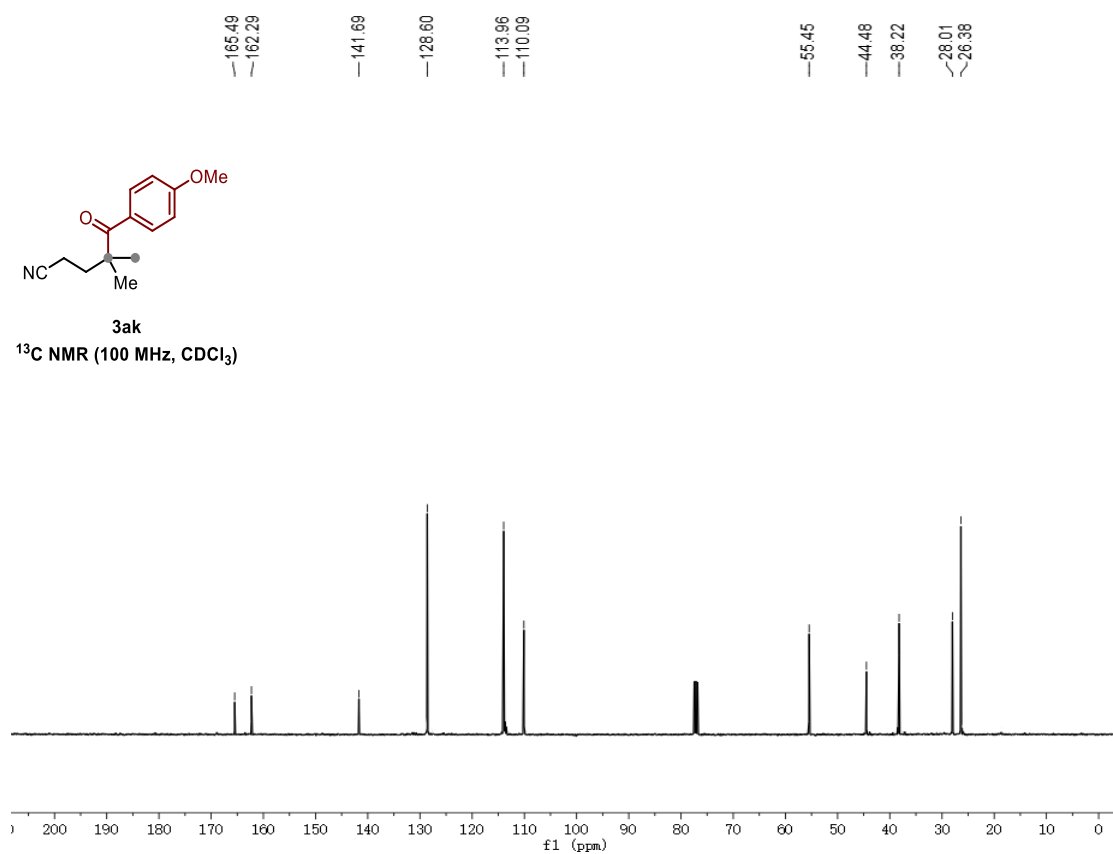
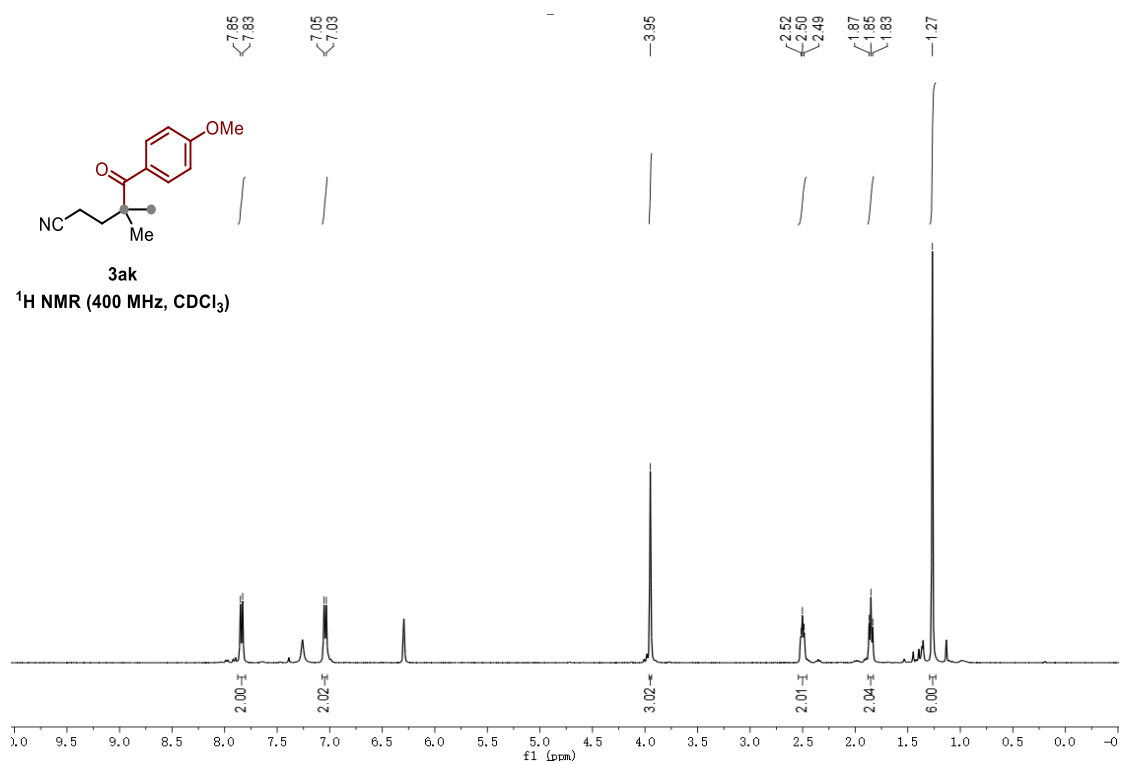


Figure S41. ¹H NMR and ¹³C NMR spectra of **3ak**.

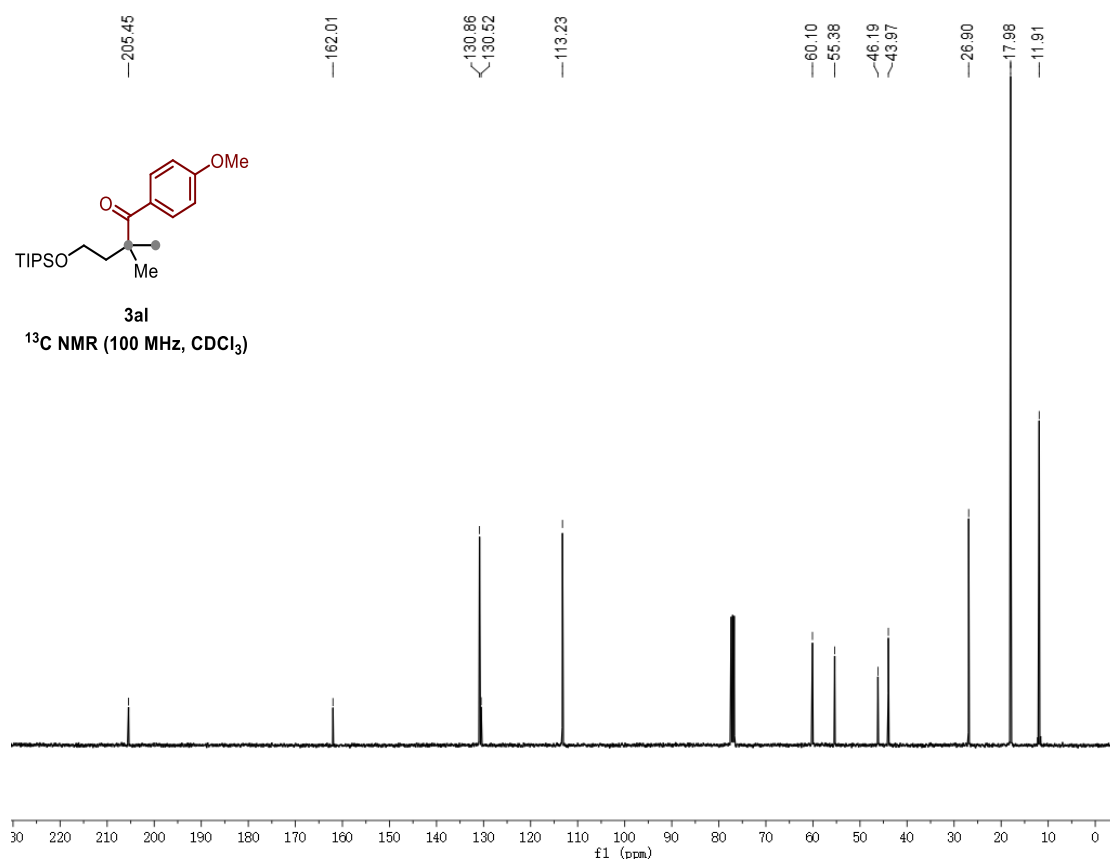
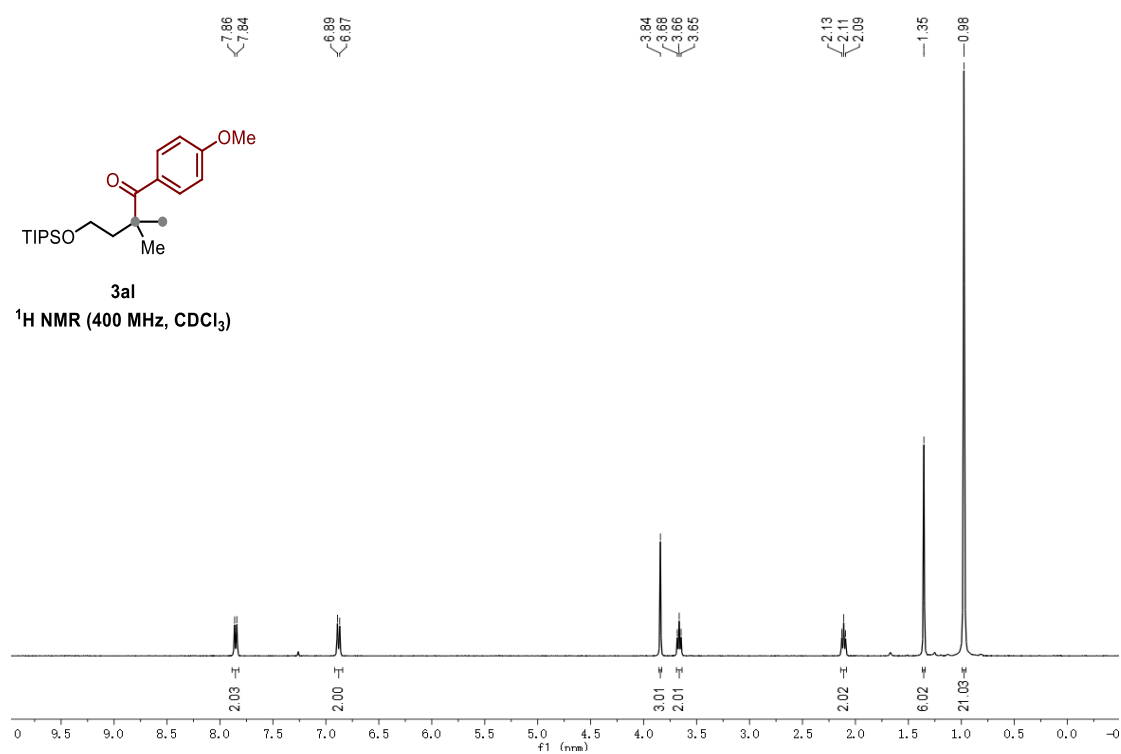


Figure S42. ^1H NMR and ^{13}C NMR spectra of **3al**.

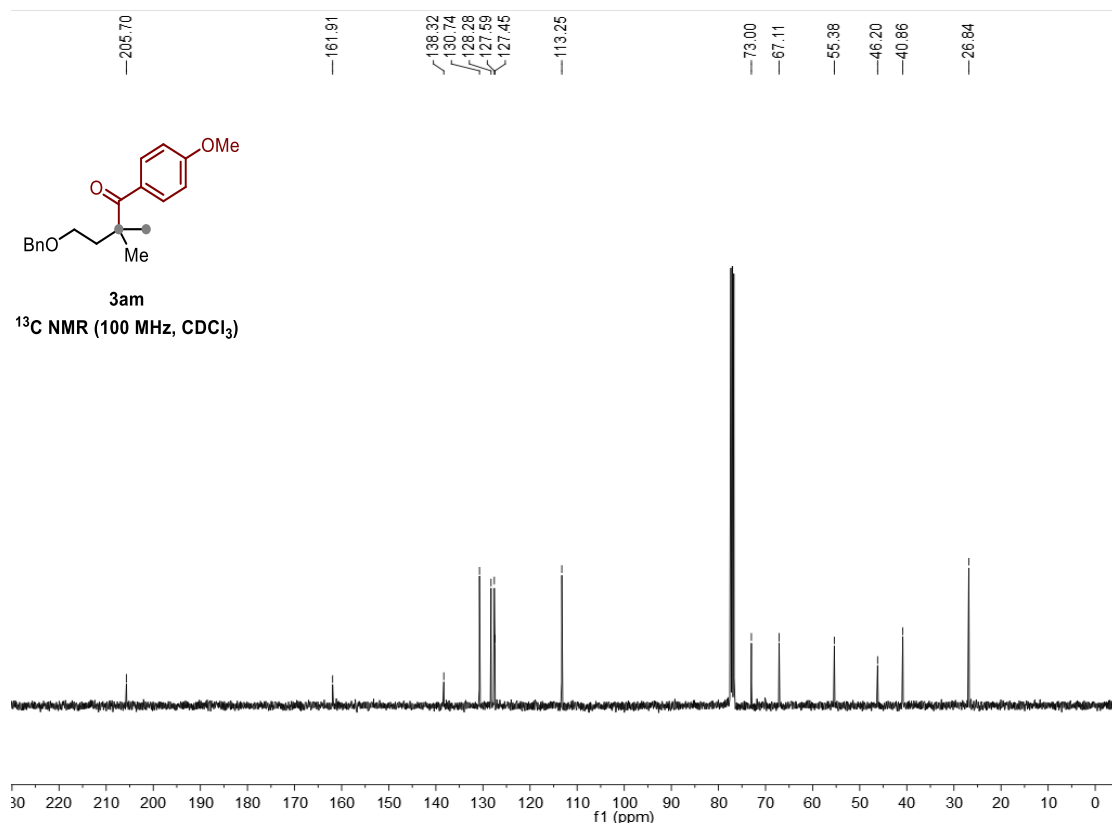
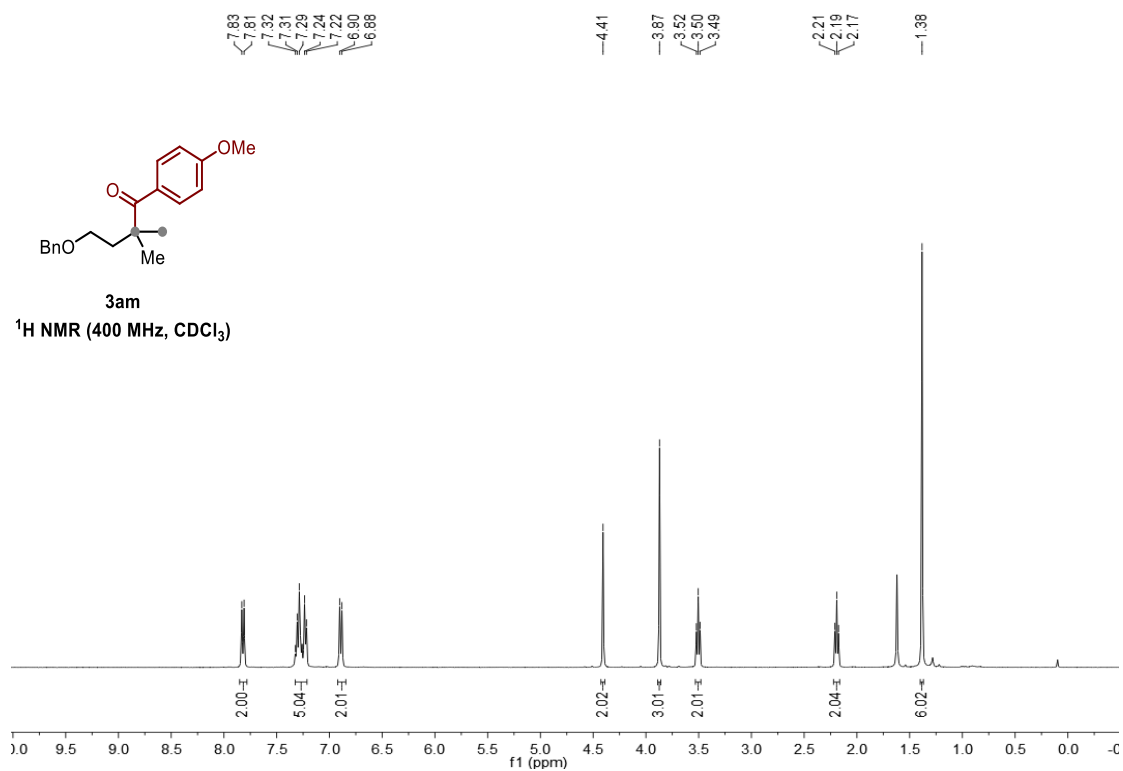


Figure S43. ^1H NMR and ^{13}C NMR spectra of **3am**.

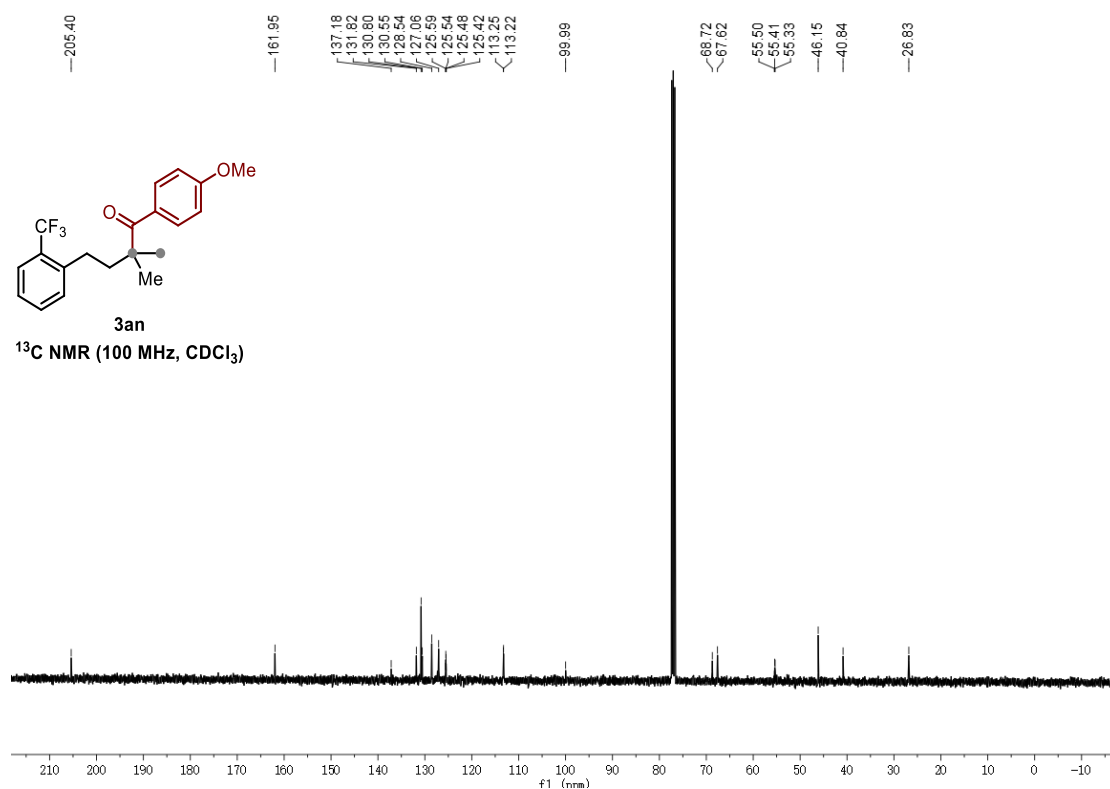
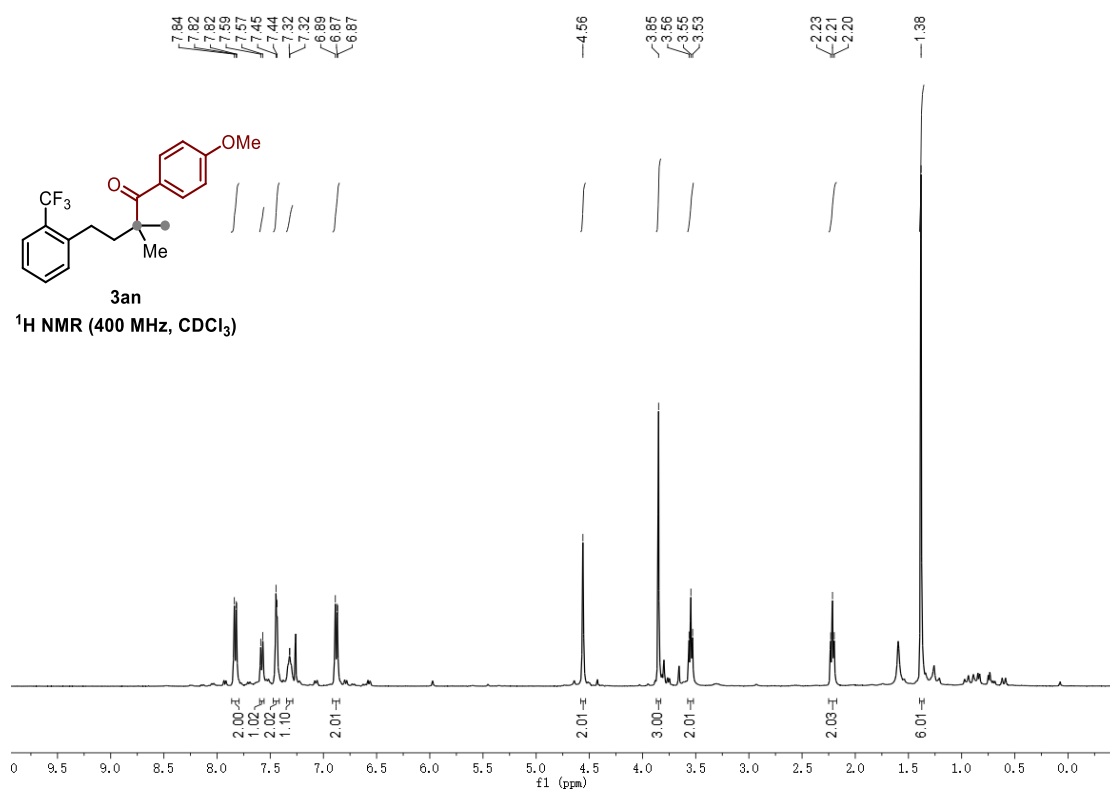


Figure S44. ^1H NMR and ^{13}C NMR spectra of **3an**.

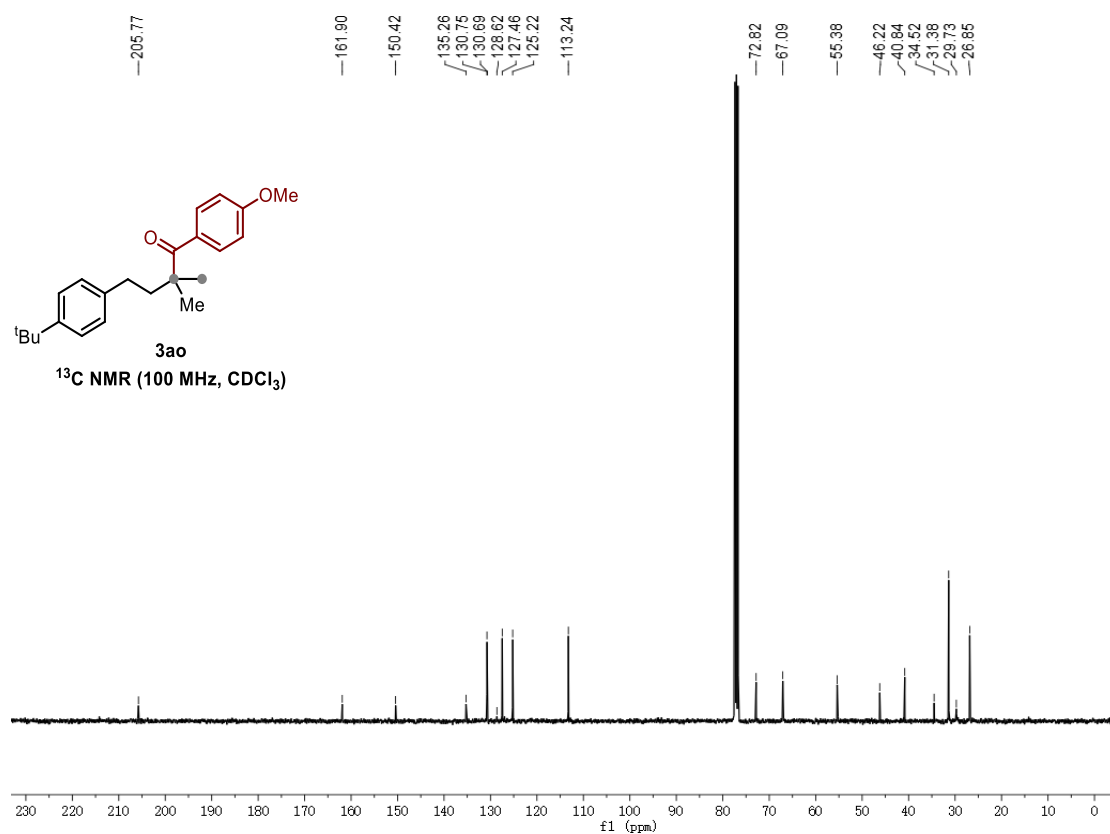
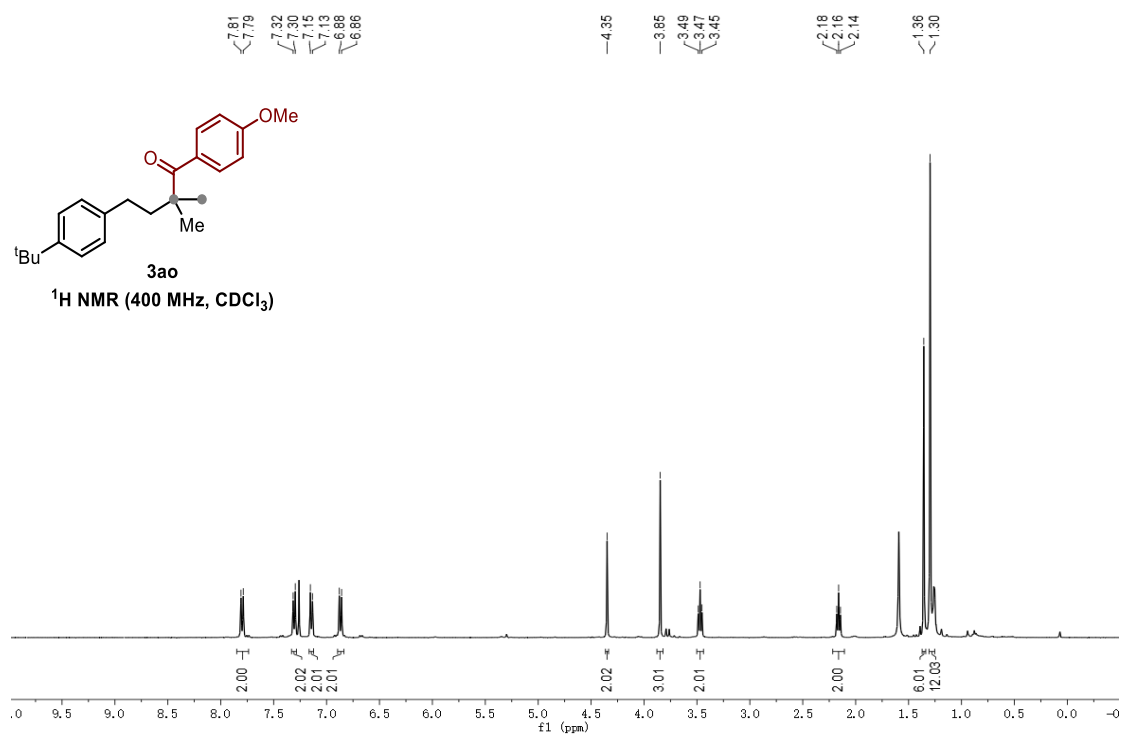


Figure S45. ^1H NMR and ^{13}C NMR spectra of **3ao**.

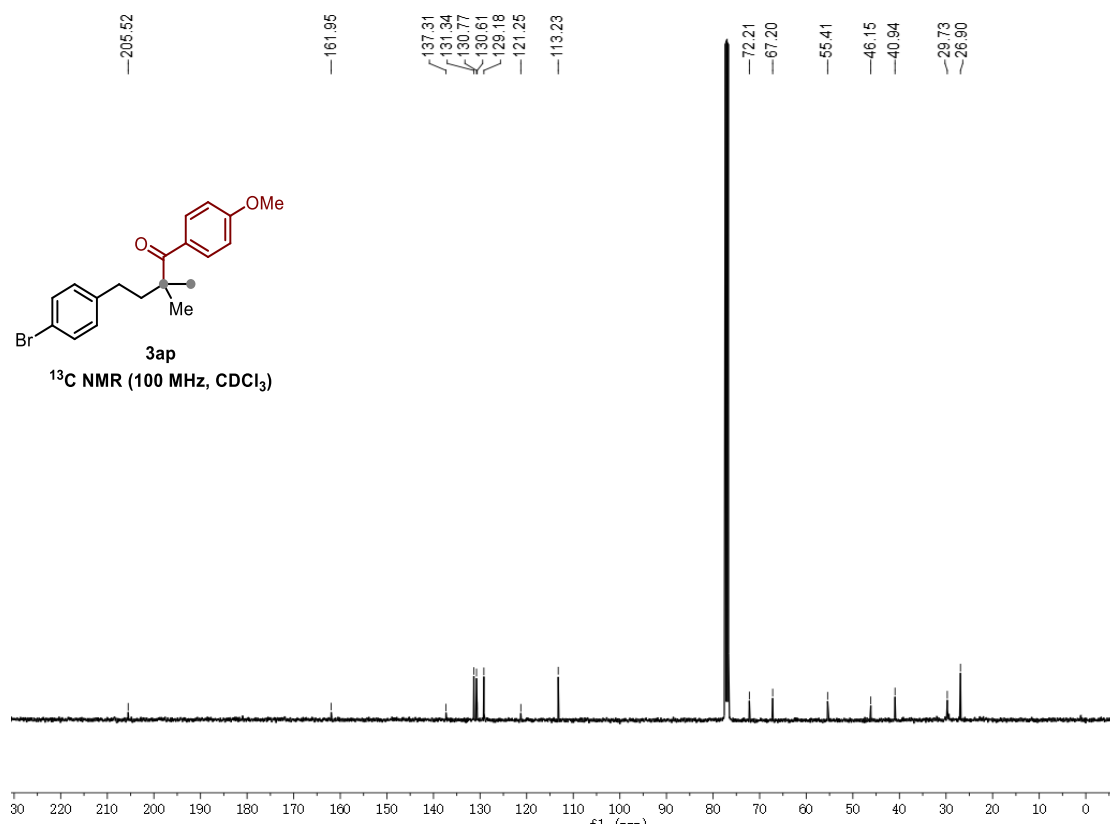
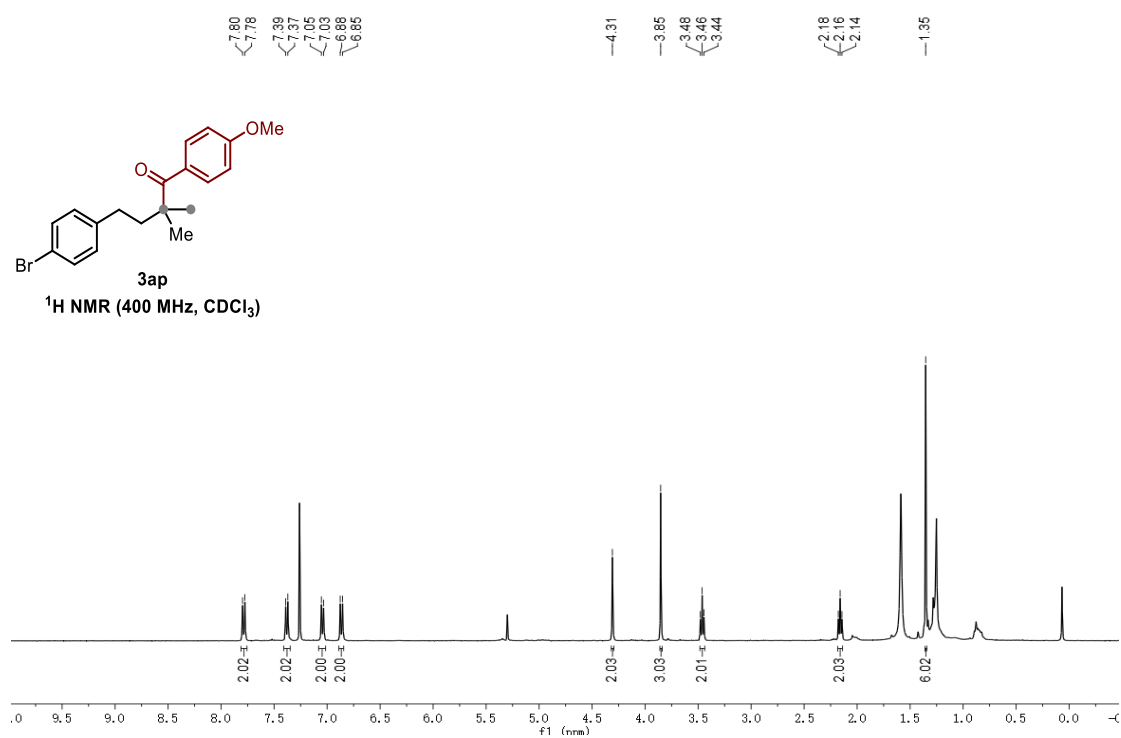


Figure S46. ^1H NMR and ^{13}C NMR spectra of **3ap**.

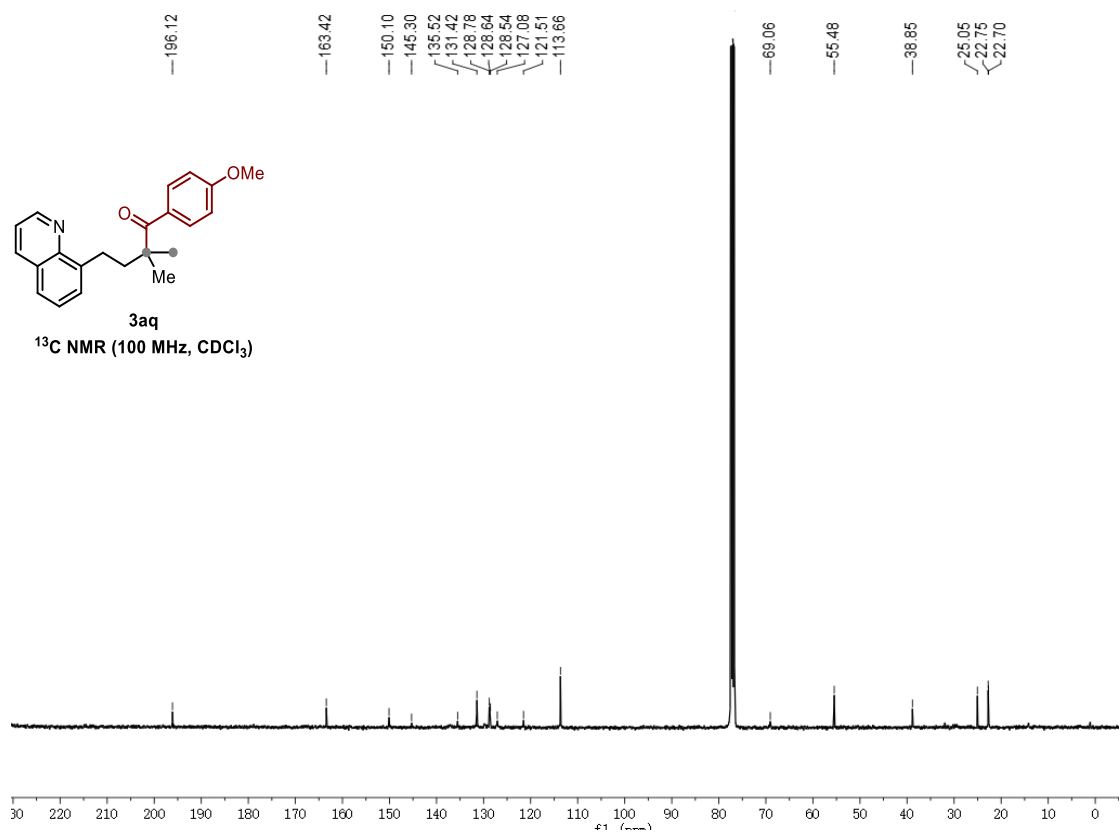
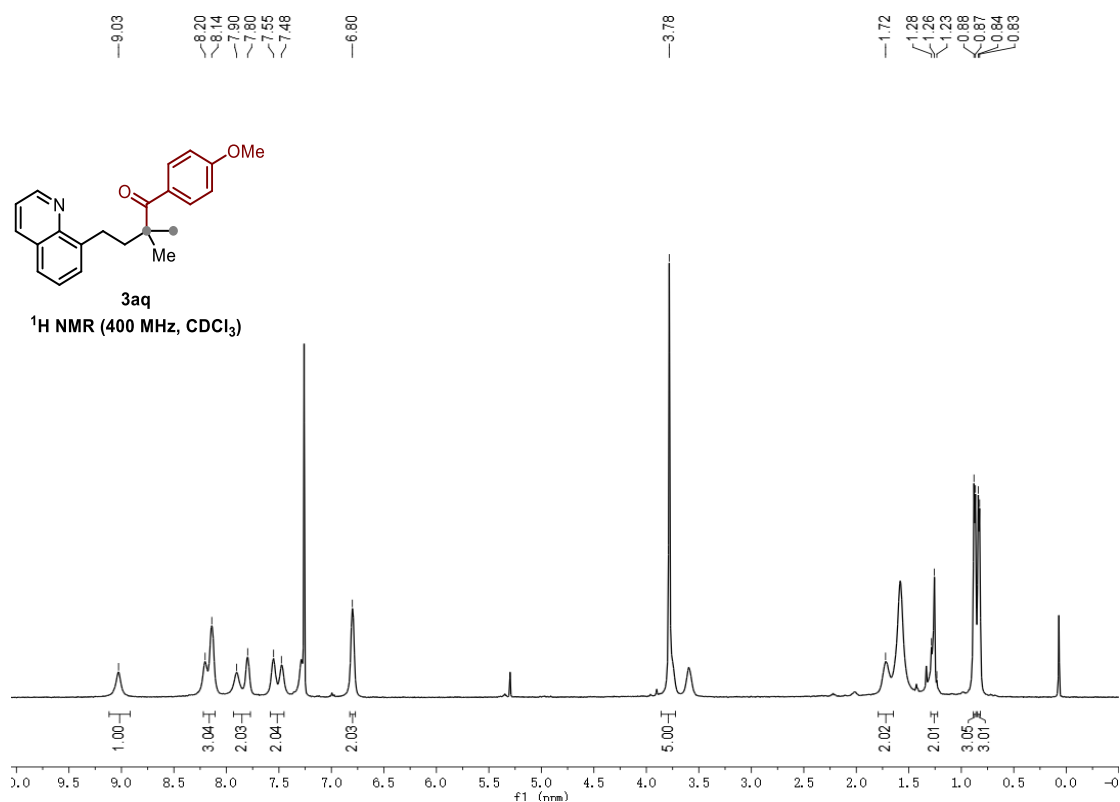


Figure S47. ^1H NMR and ^{13}C NMR spectra of **3aq**.

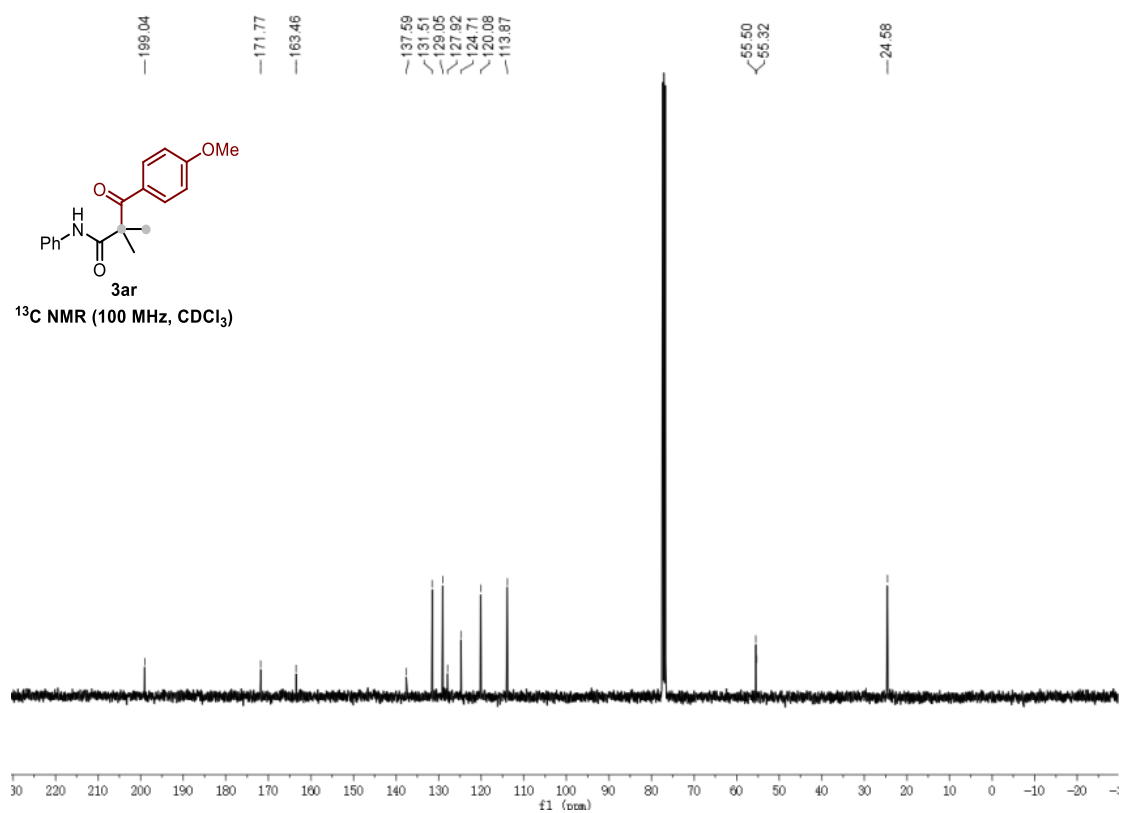
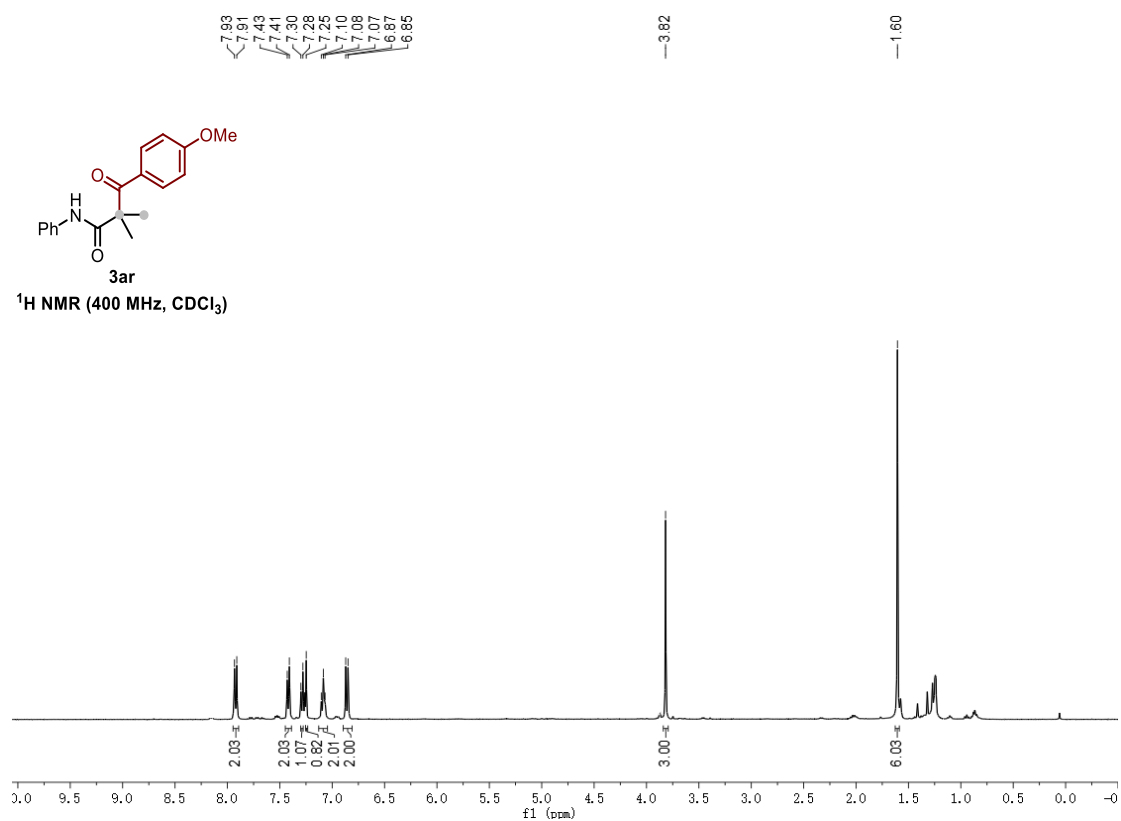


Figure S48. ^1H NMR and ^{13}C NMR spectra of **3ar**.

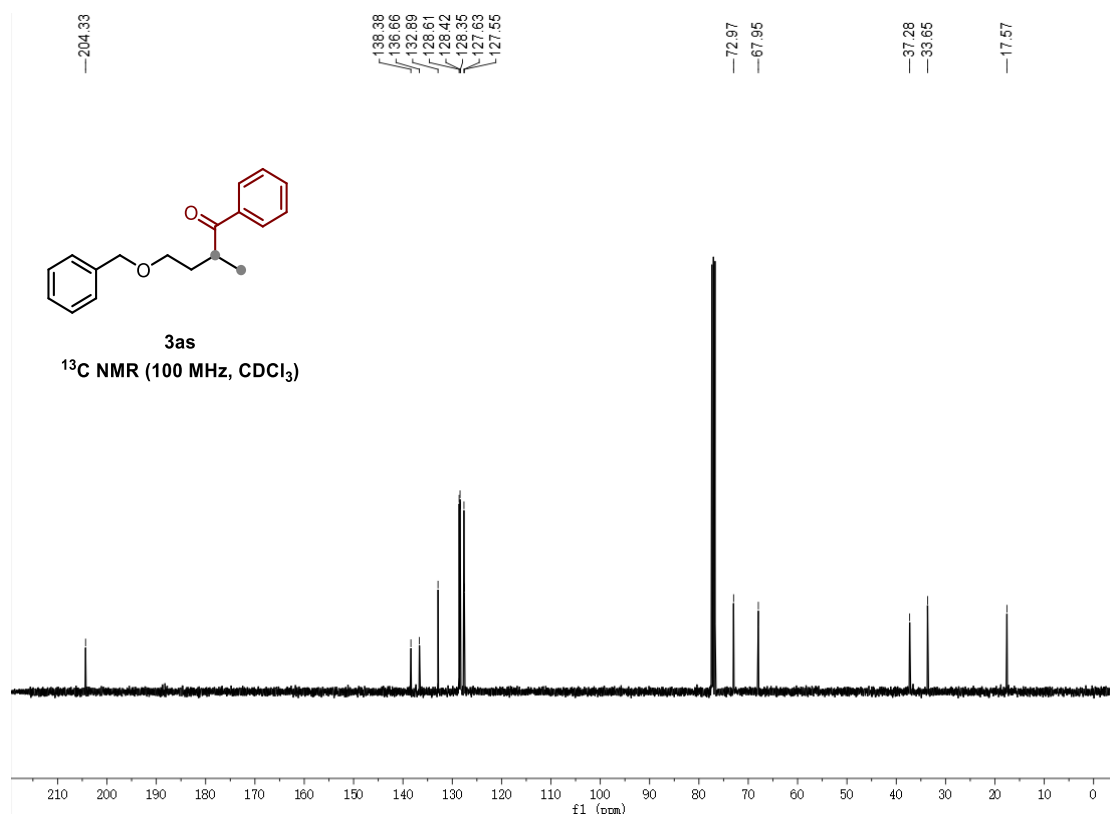
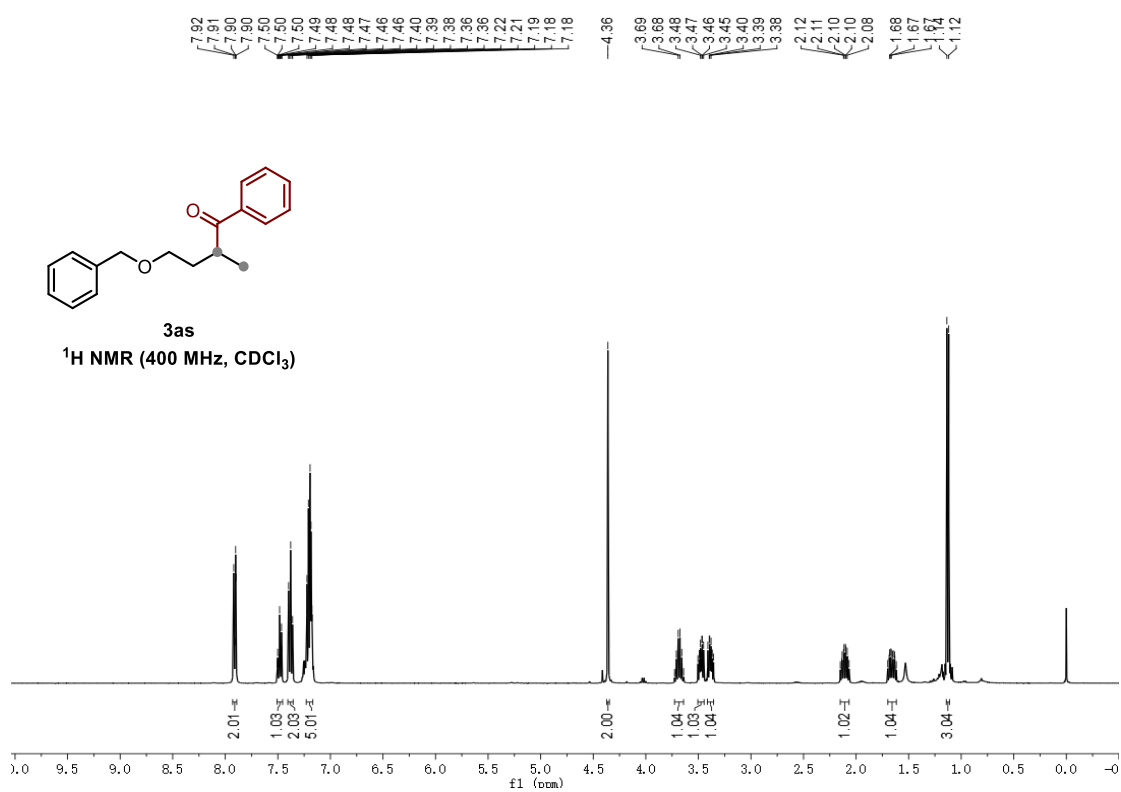


Figure S49. ^1H NMR and ^{13}C NMR spectra of **3as**.

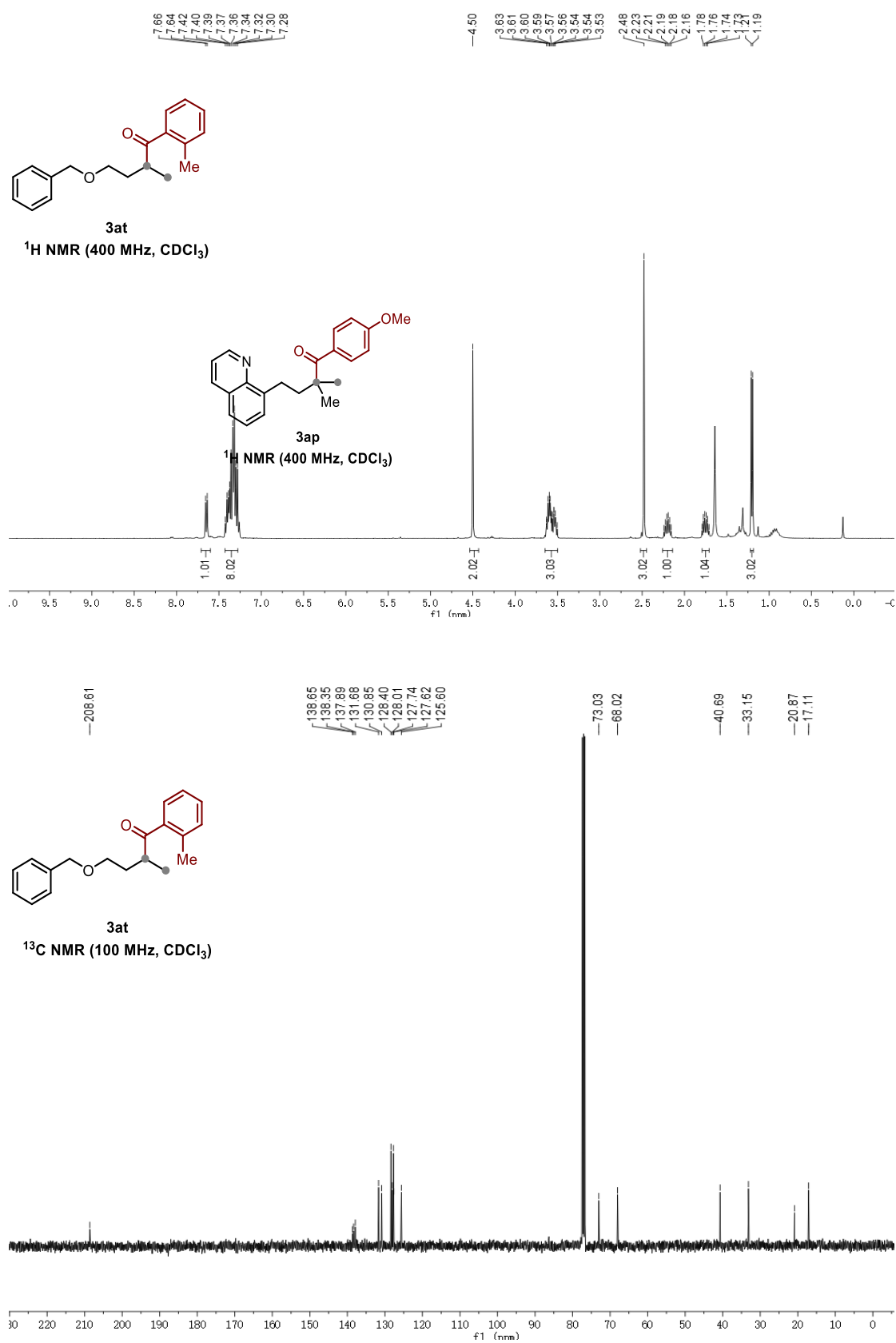


Figure S50. ¹H NMR and ¹³C NMR spectra of **3at**.

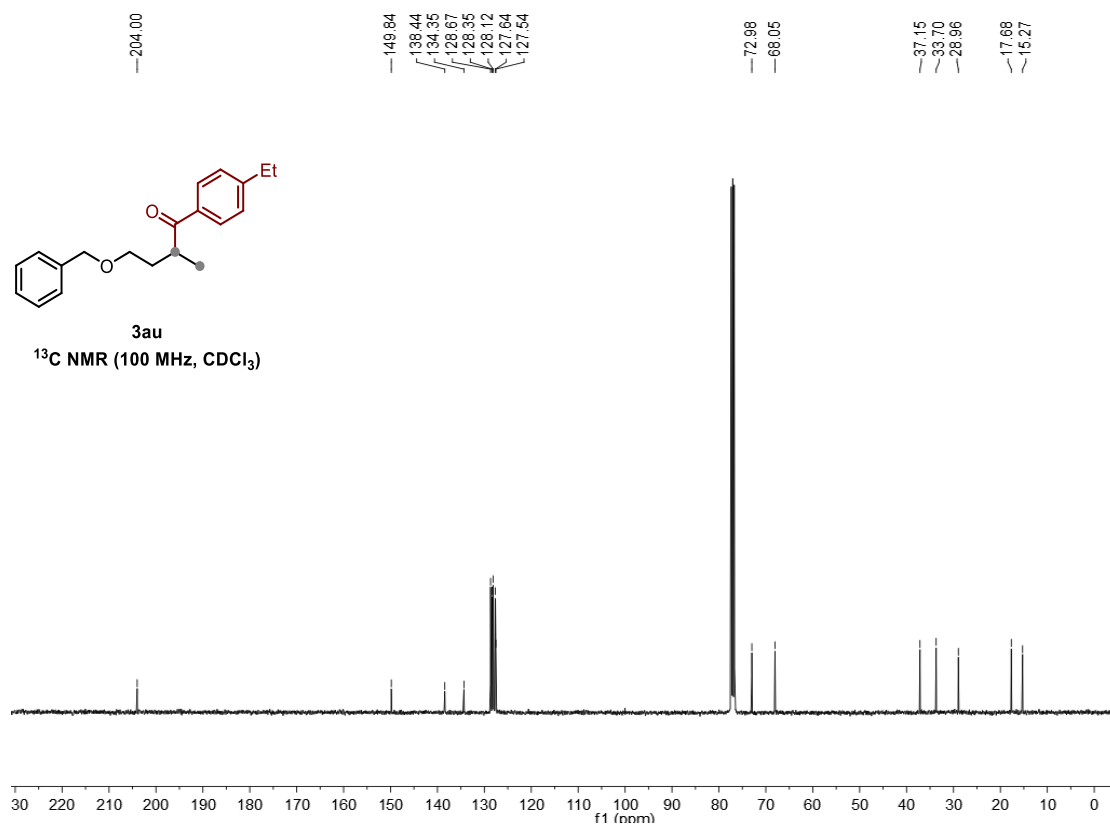
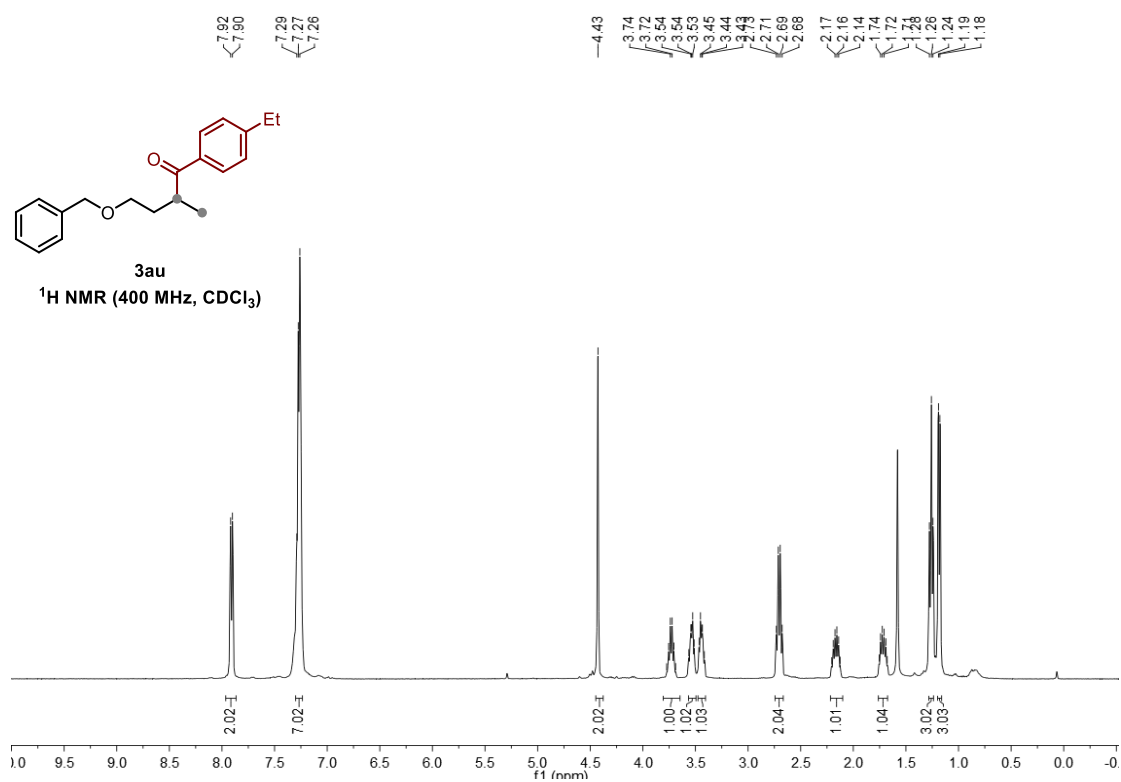


Figure S51. ^1H NMR and ^{13}C NMR spectra of **3au**.

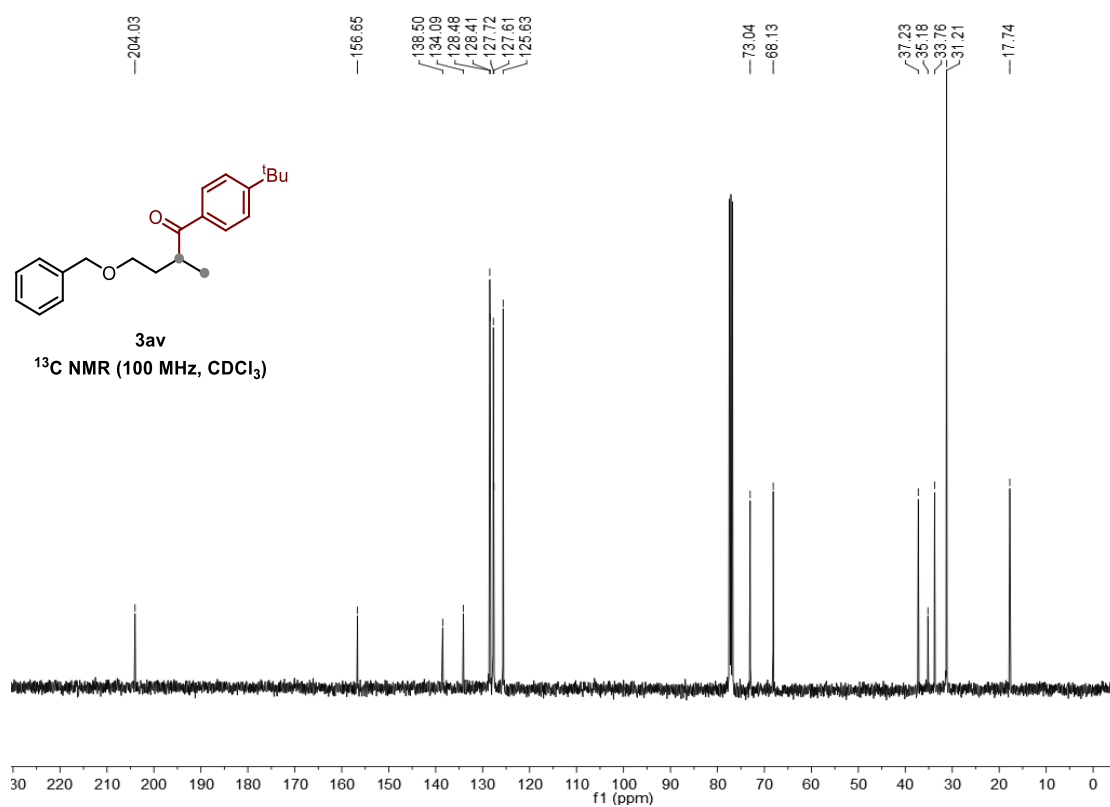
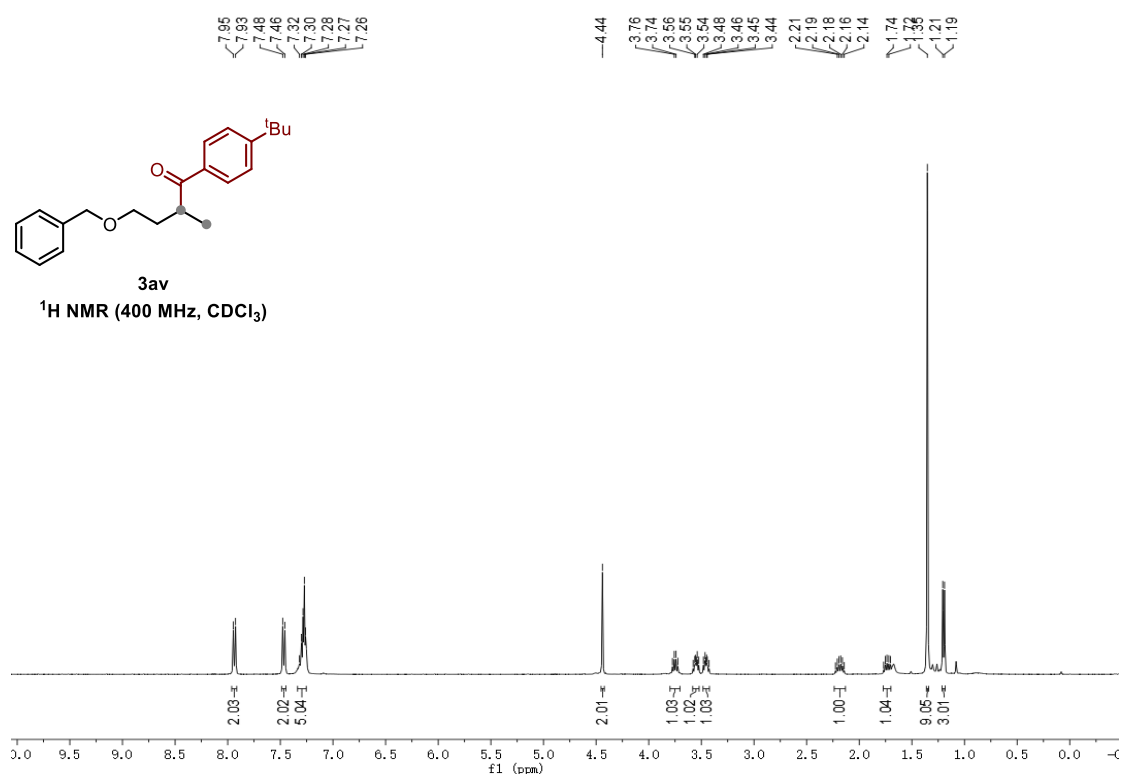


Figure S52. ^1H NMR and ^{13}C NMR spectra of **3av**.

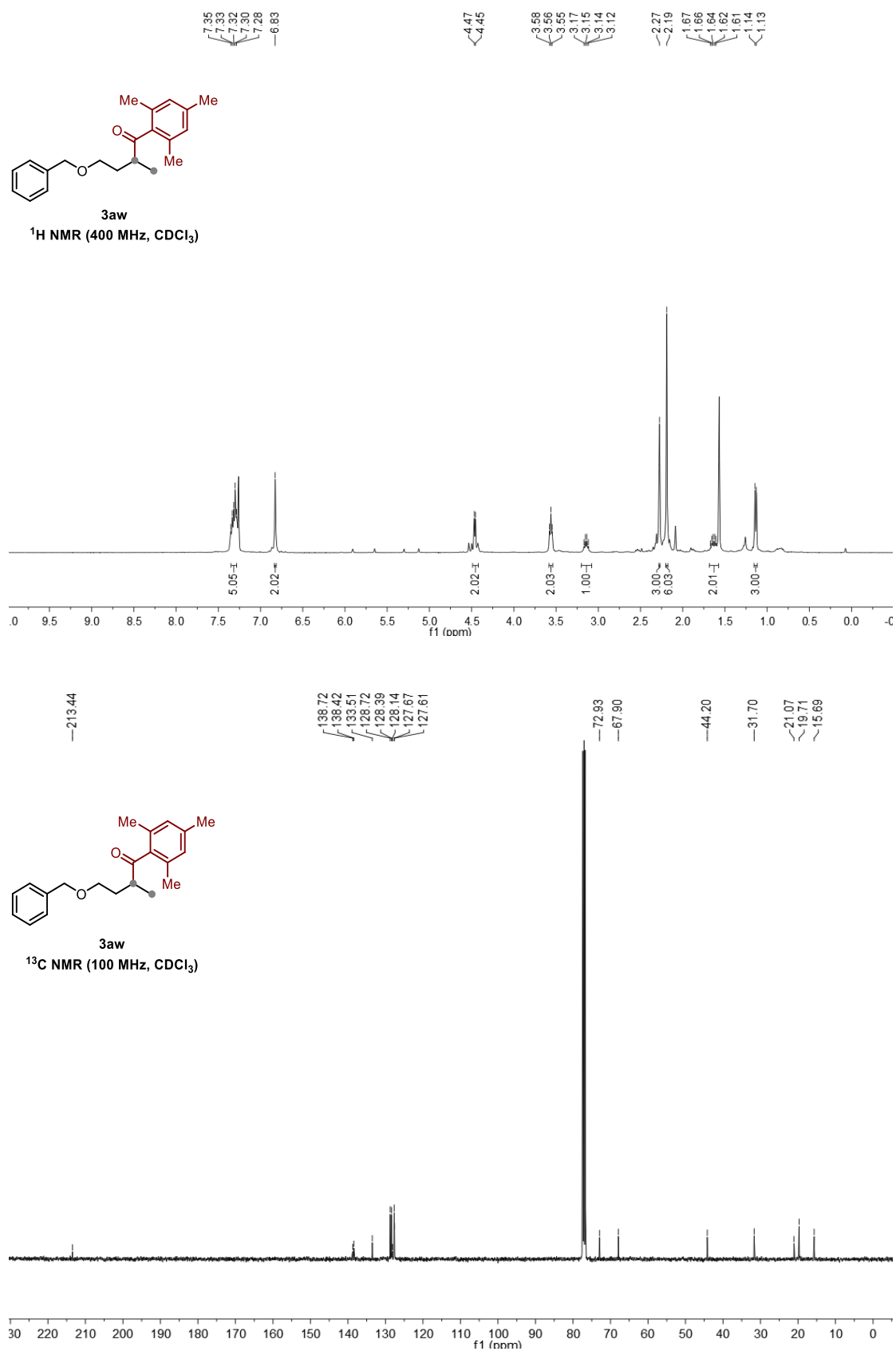


Figure S53. ^1H NMR and ^{13}C NMR spectra of **3aw**.

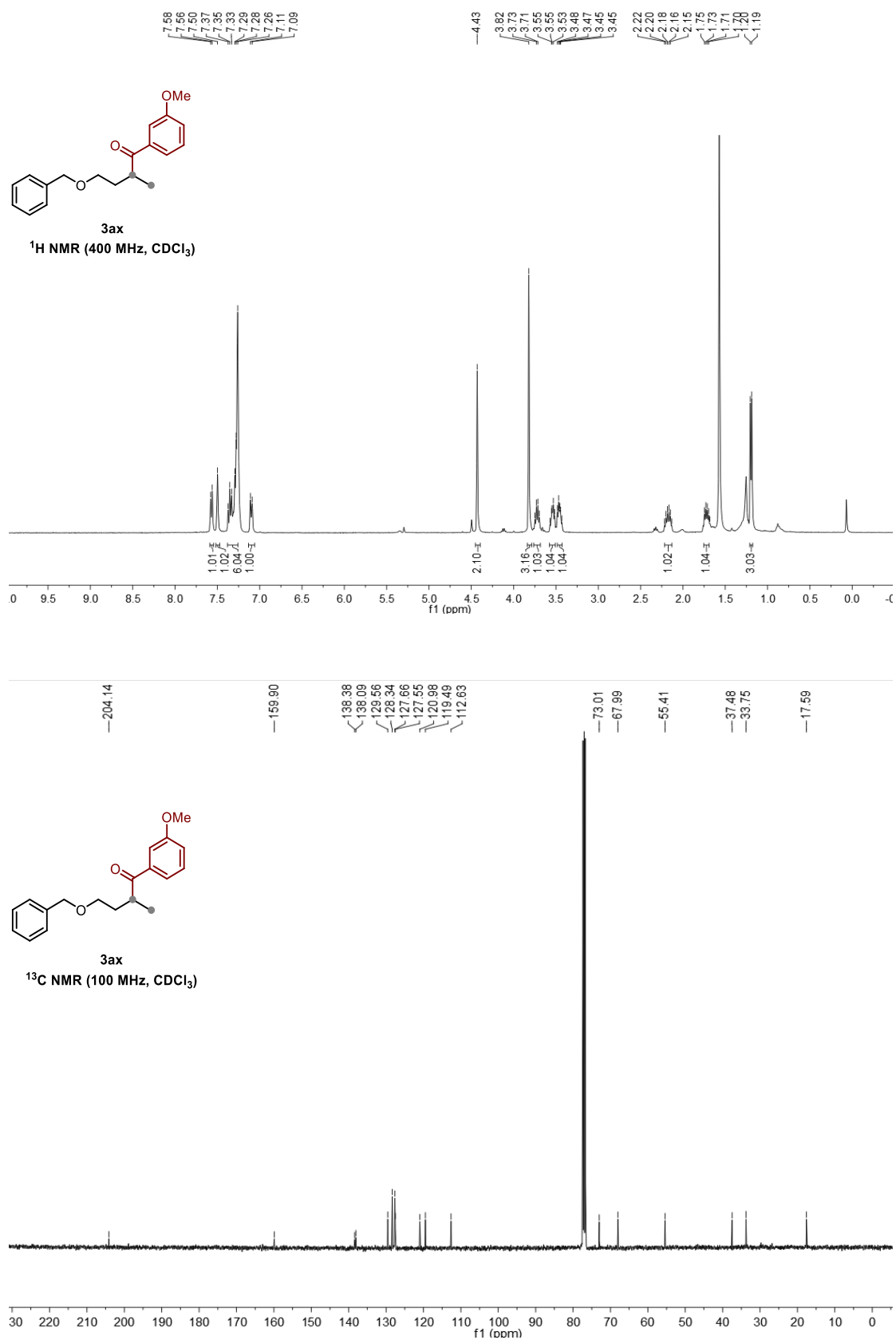
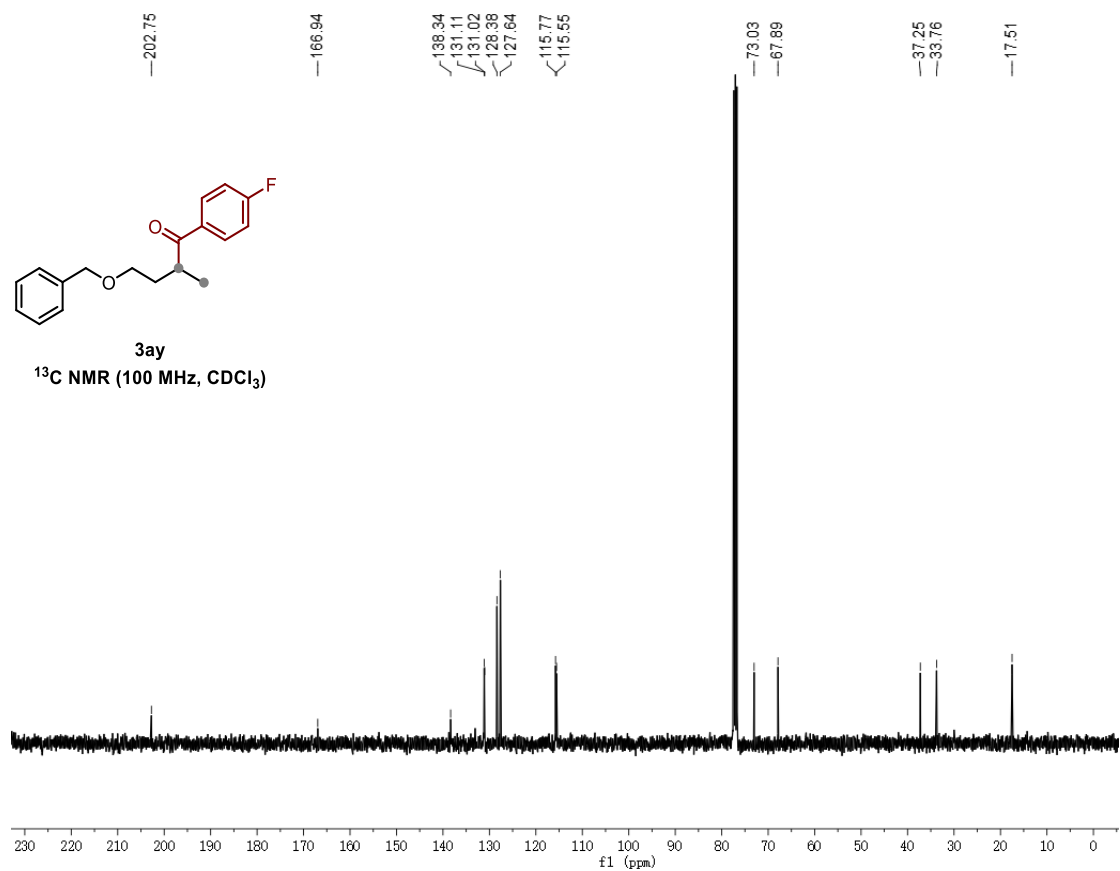
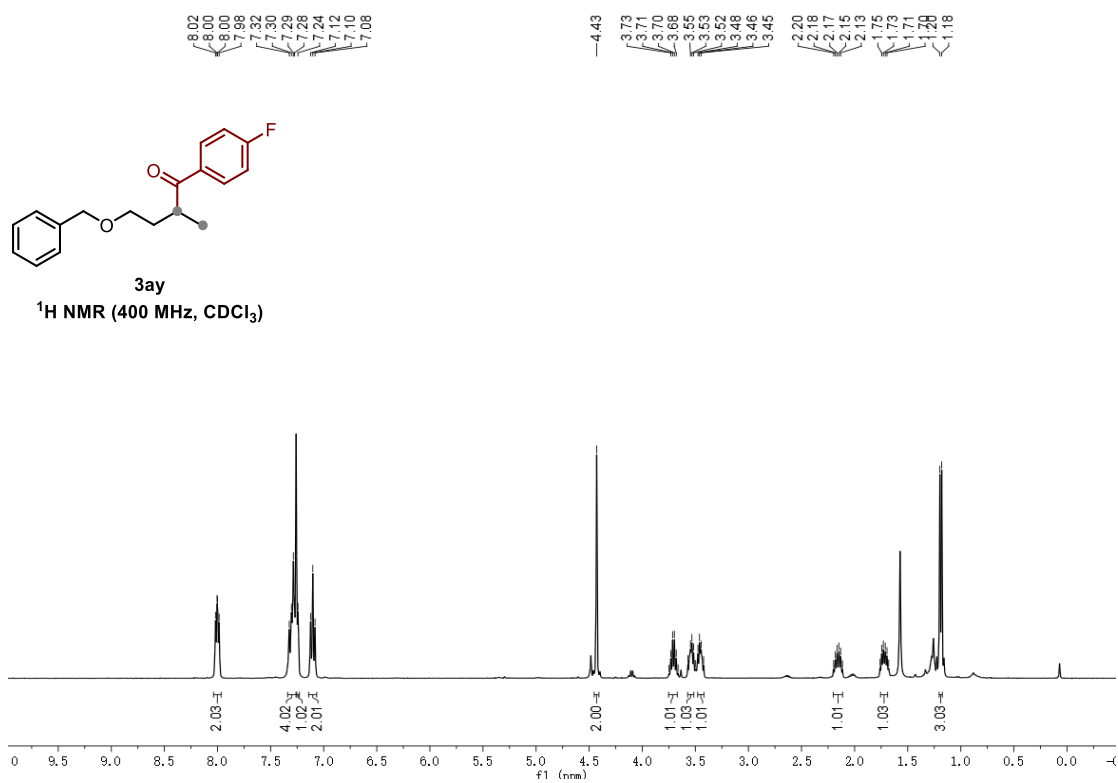


Figure S54. ¹H NMR and ¹³C NMR spectra of **3ax**.



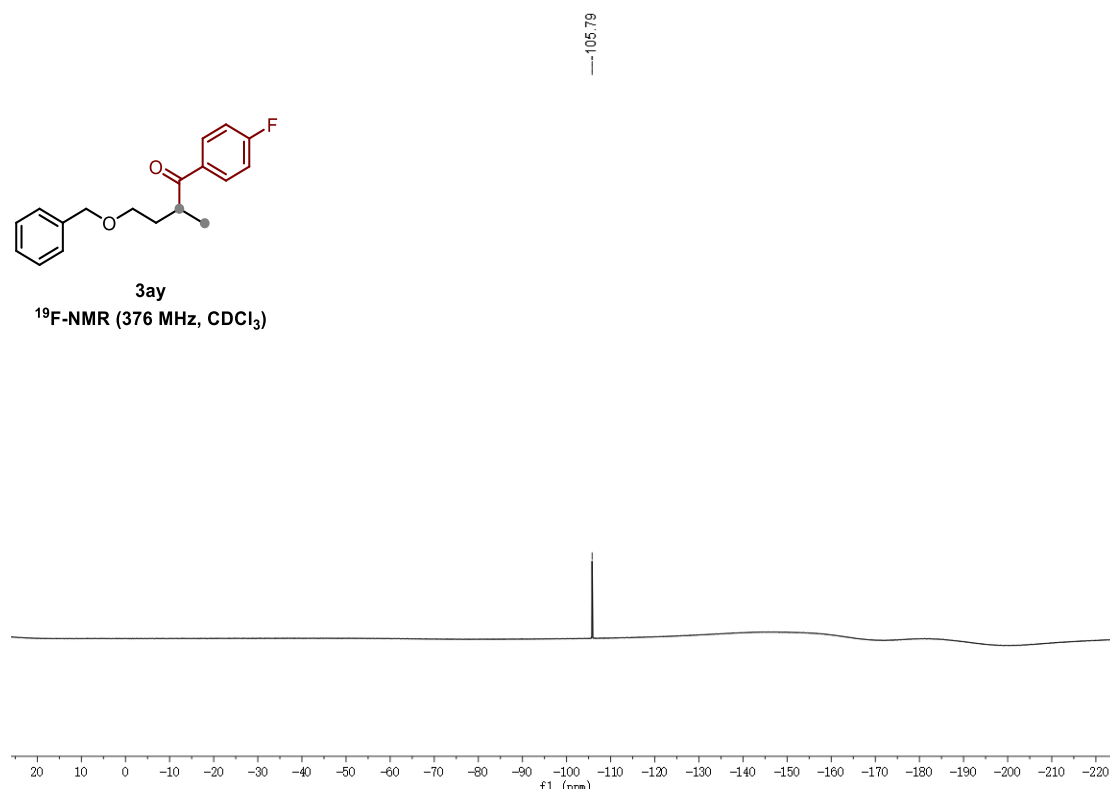


Figure S55. ¹H NMR, ¹³C NMR and ¹⁹F NMR spectra of **3ay**.

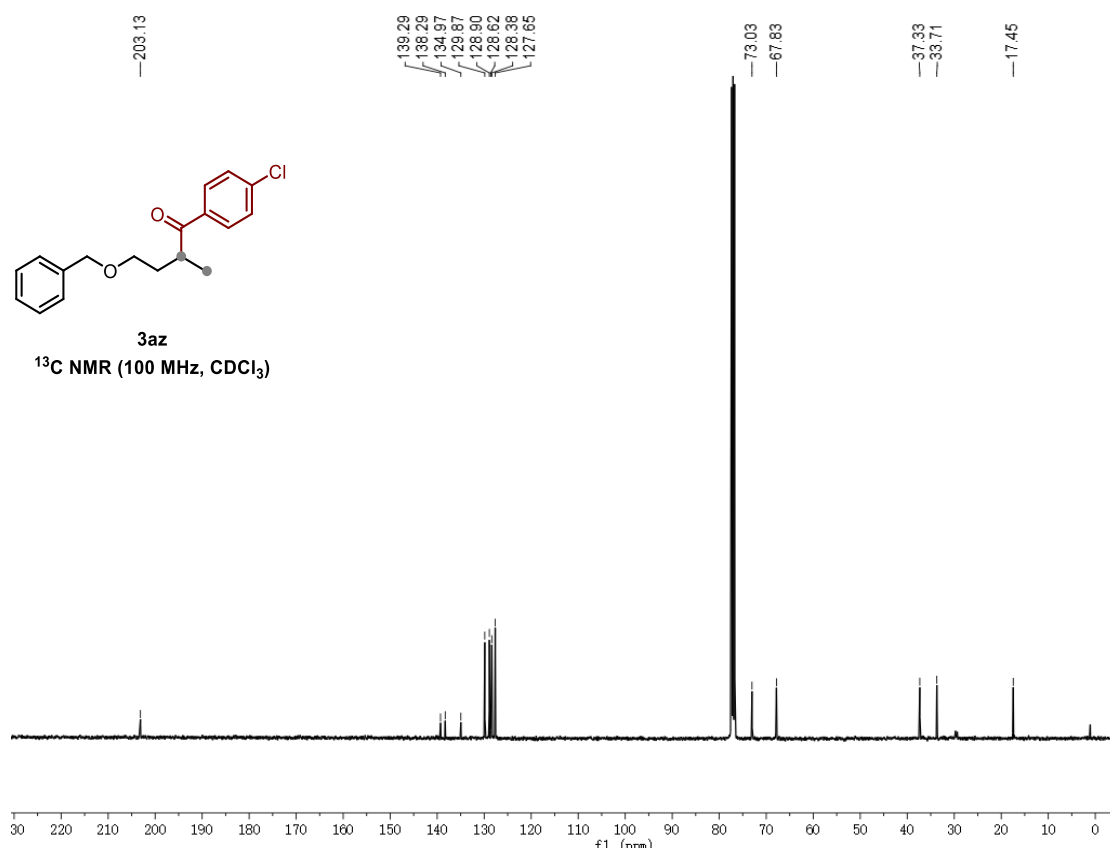
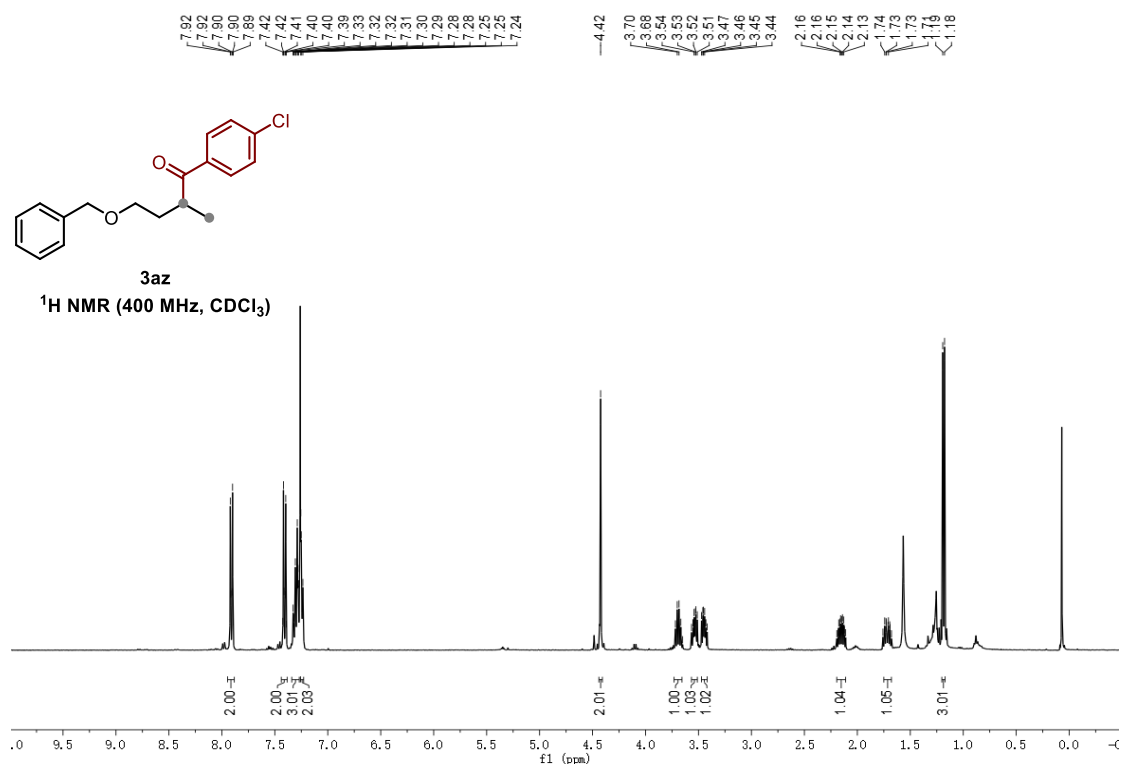


Figure S56. ^1H NMR and ^{13}C NMR spectra of **3az**.

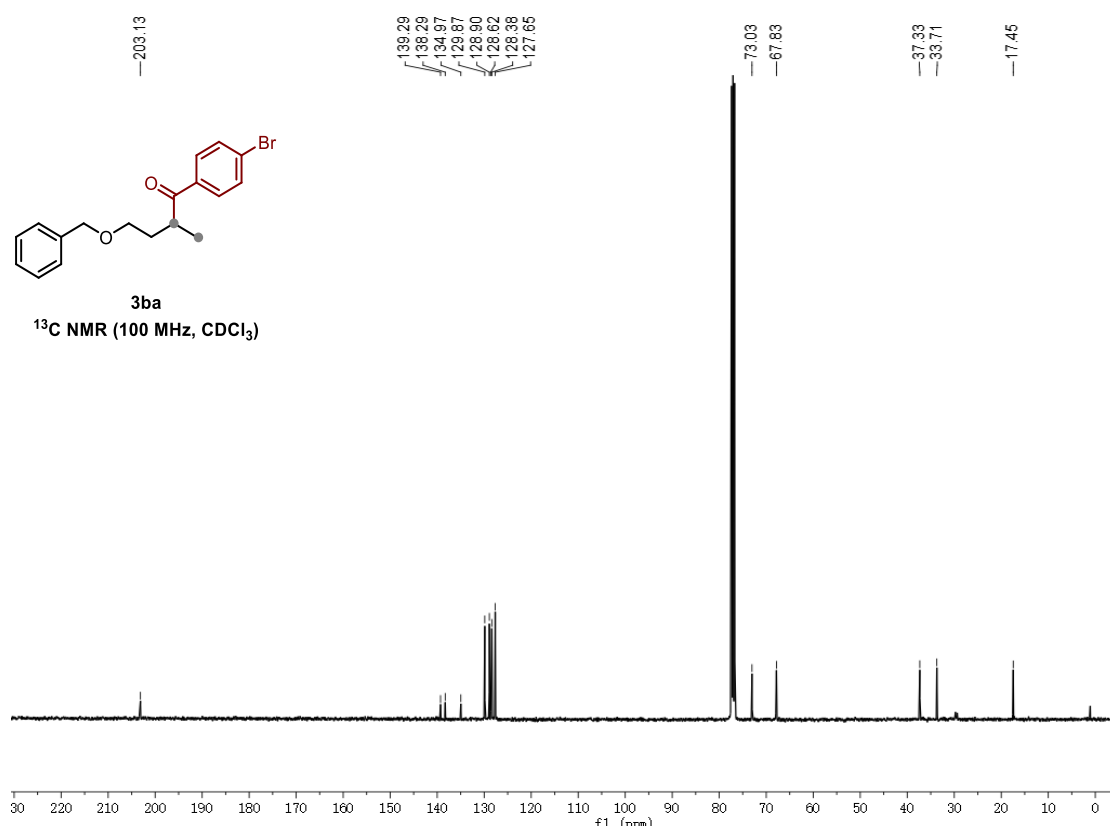
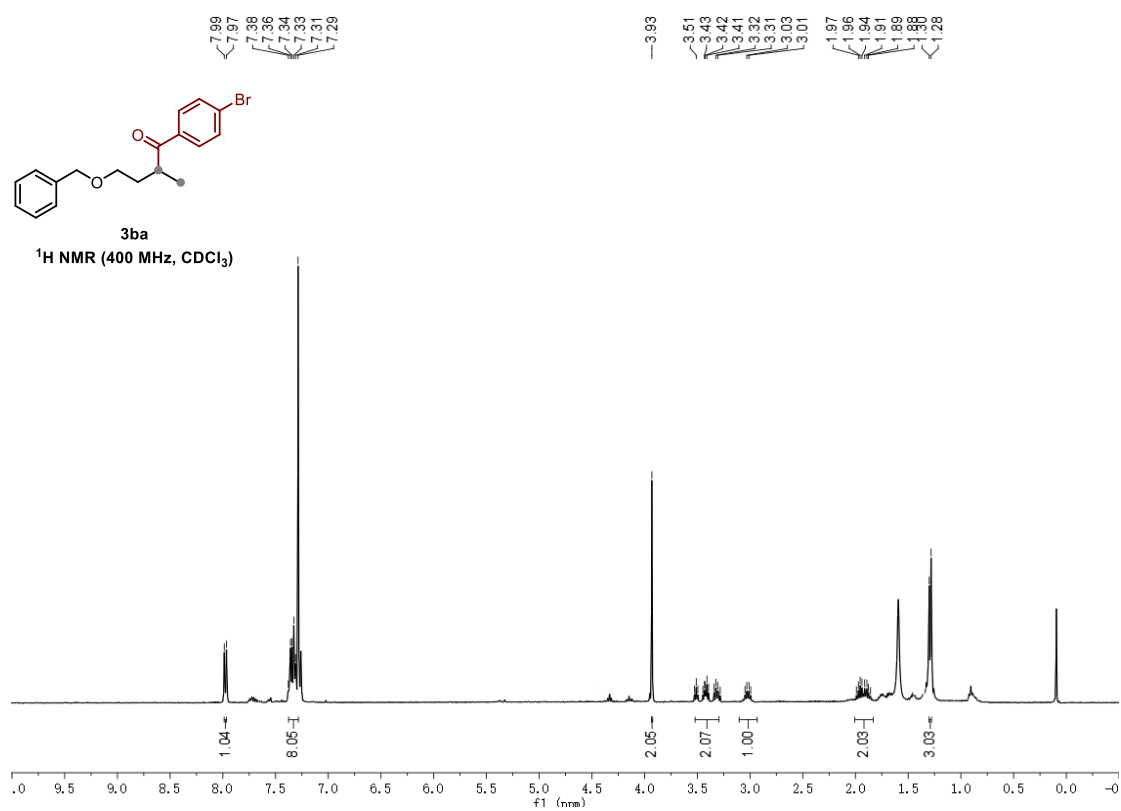


Figure S57. ^1H NMR and ^{13}C NMR spectra of **3ba**.

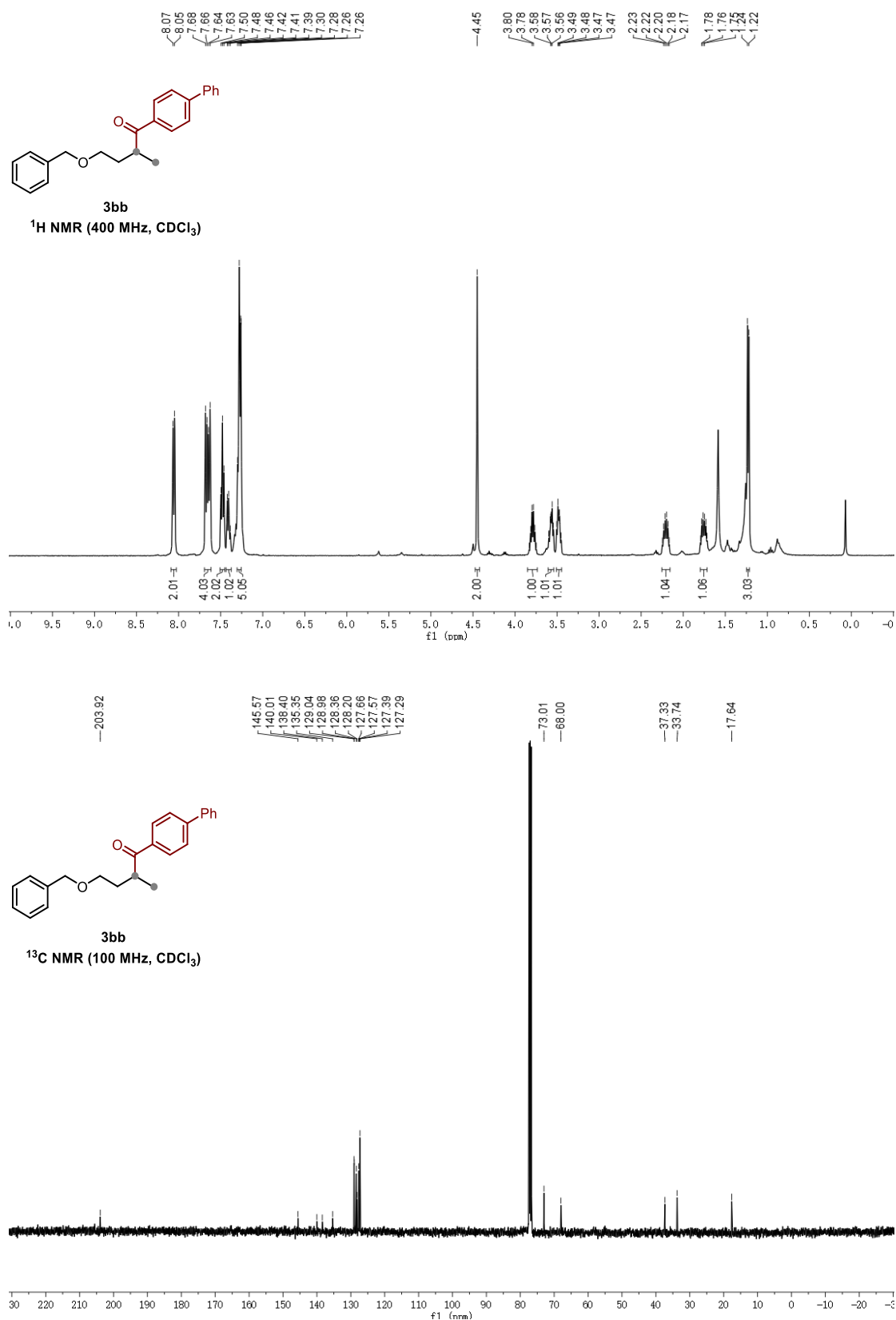


Figure S58. ¹H NMR and ¹³C NMR spectra of **3bb**.

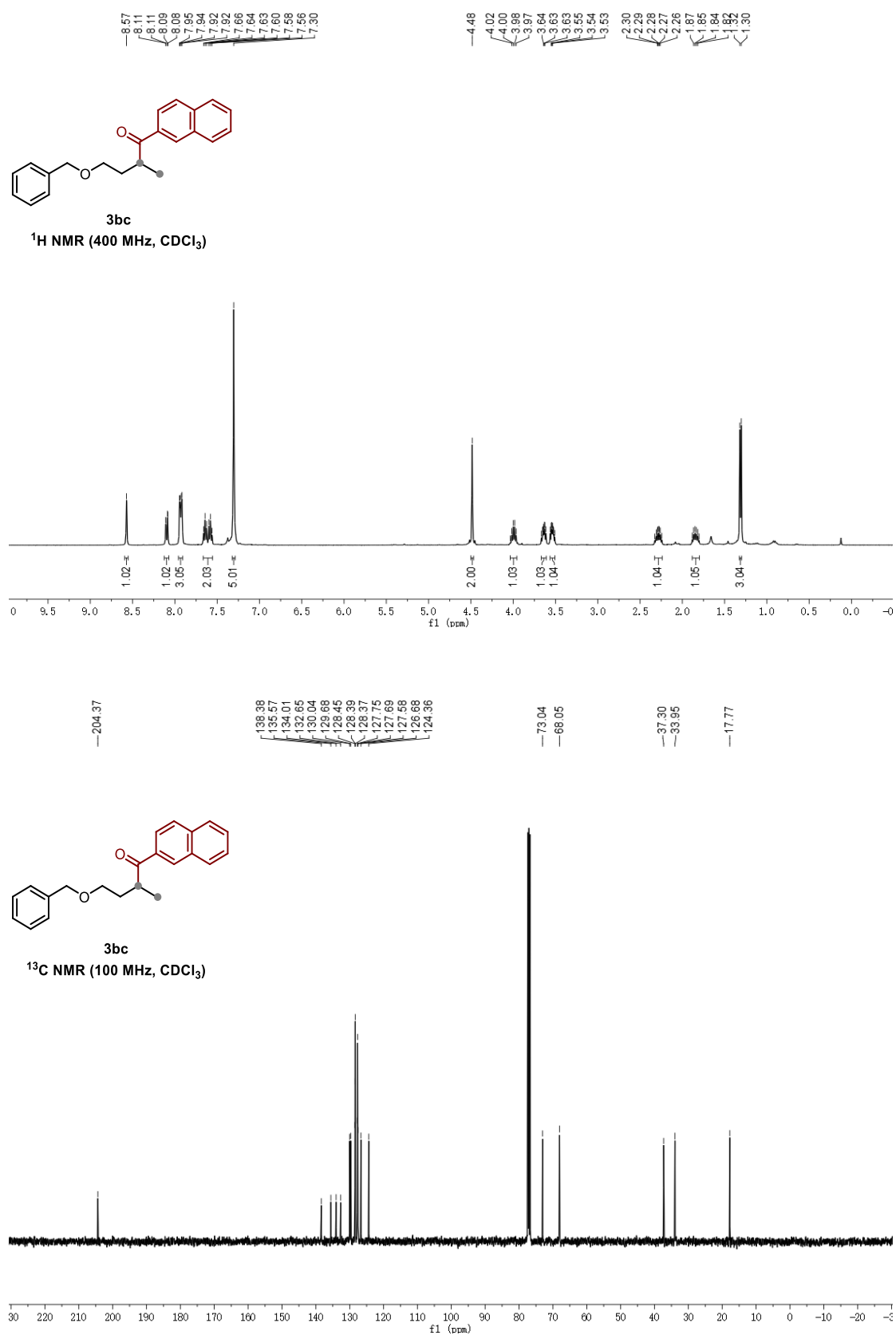


Figure S59. ¹H NMR and ¹³C NMR spectra of **3bc**.

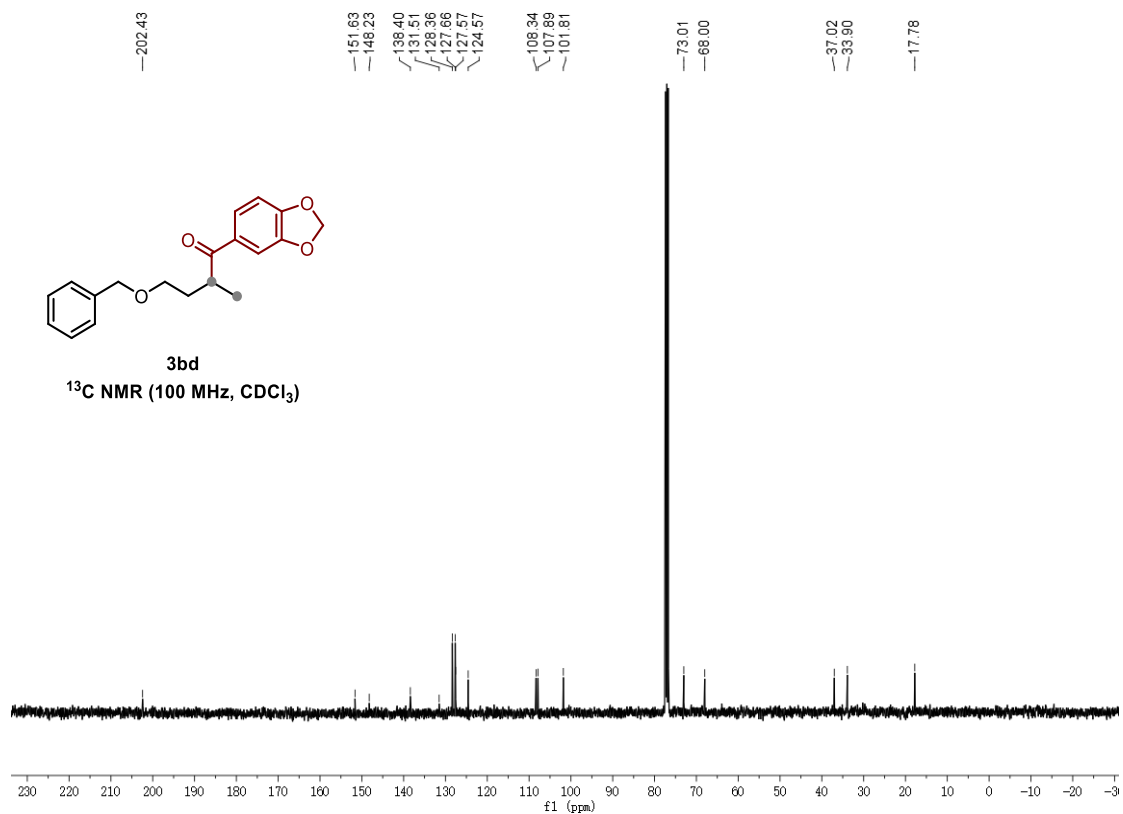
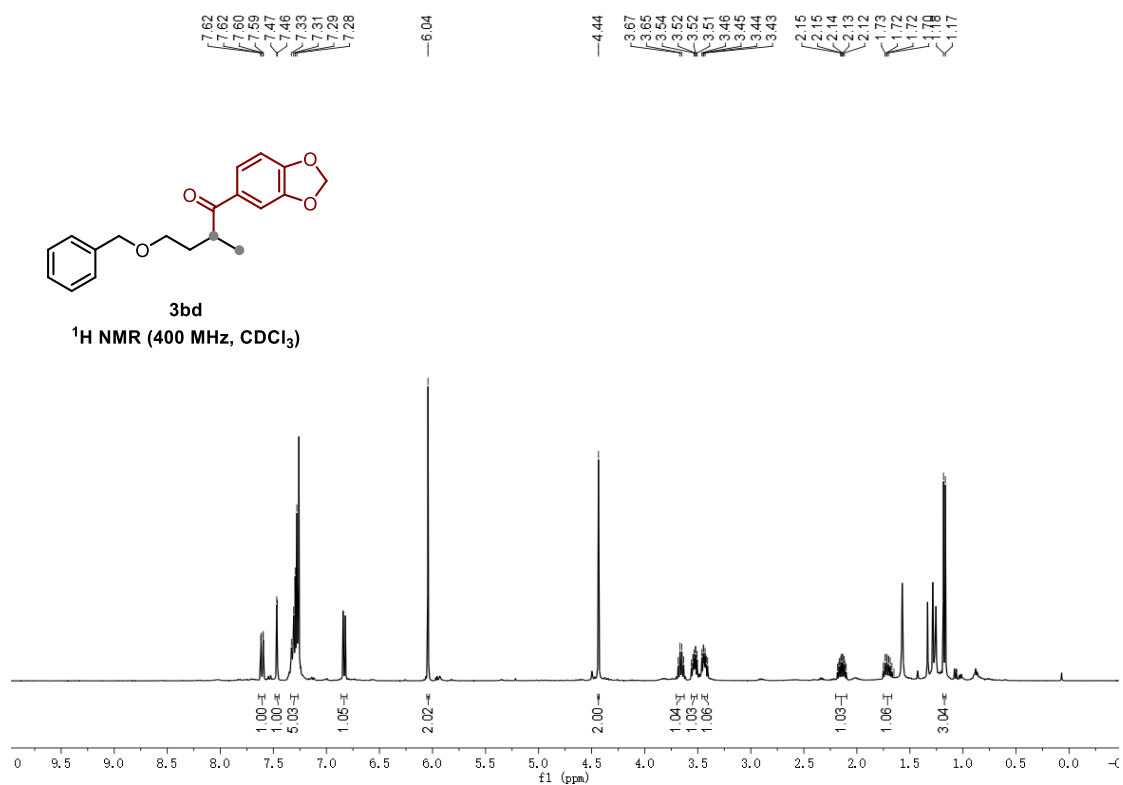


Figure S60. ^1H NMR and ^{13}C NMR spectra of **3bd**.

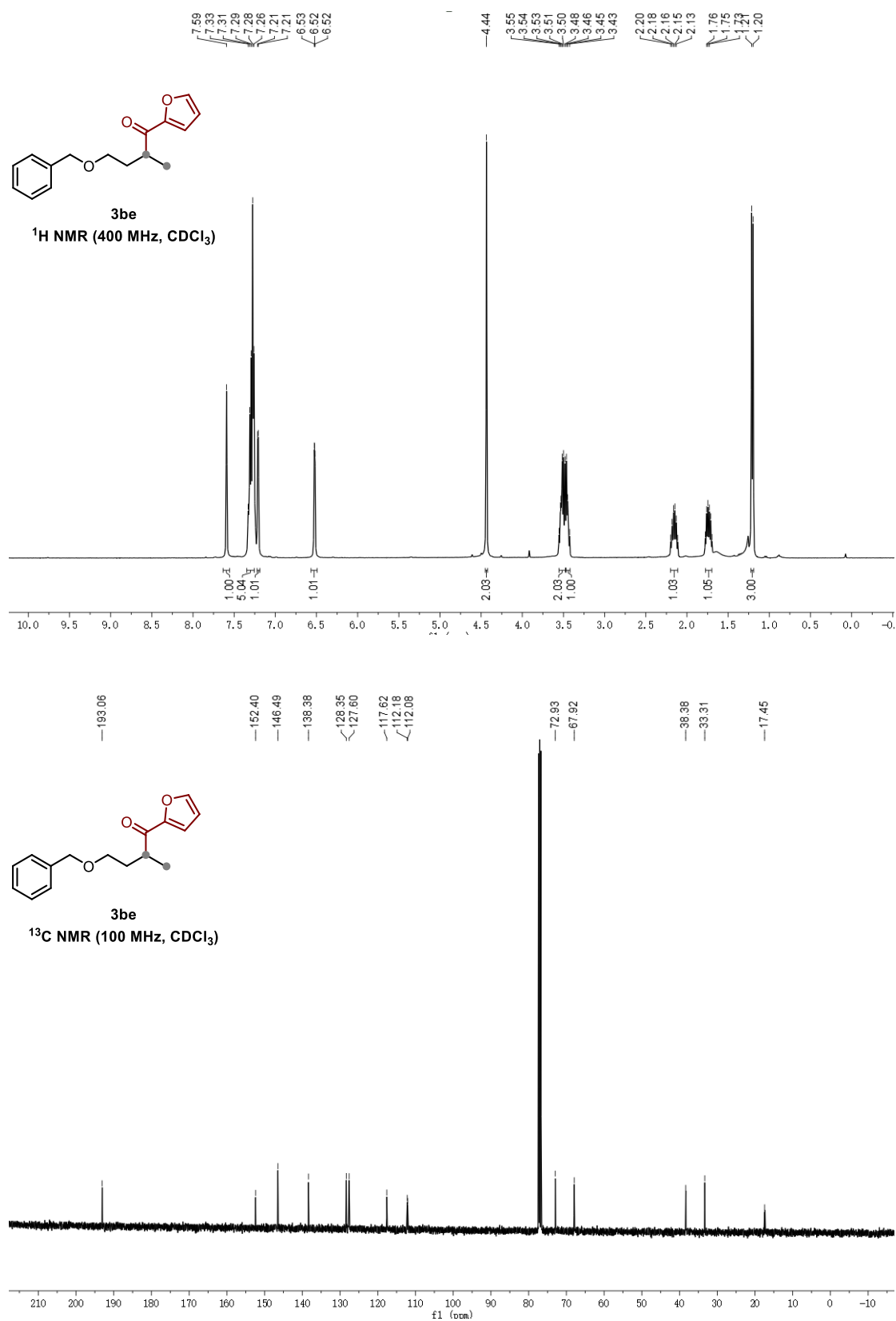


Figure S61. ¹H NMR and ¹³C NMR spectra of **3be**.

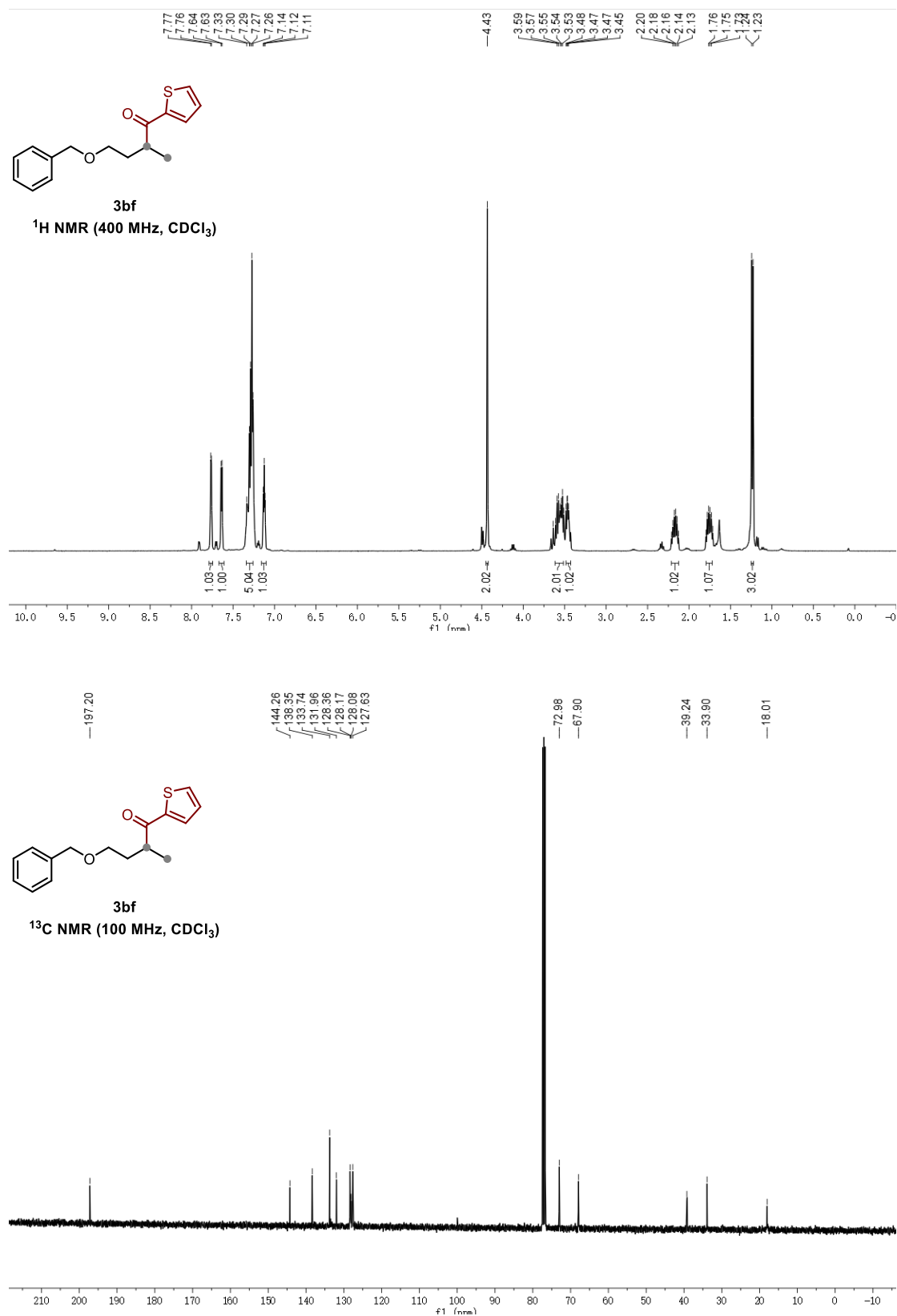


Figure S62. ¹H NMR and ¹³C NMR spectra of **3bf**.

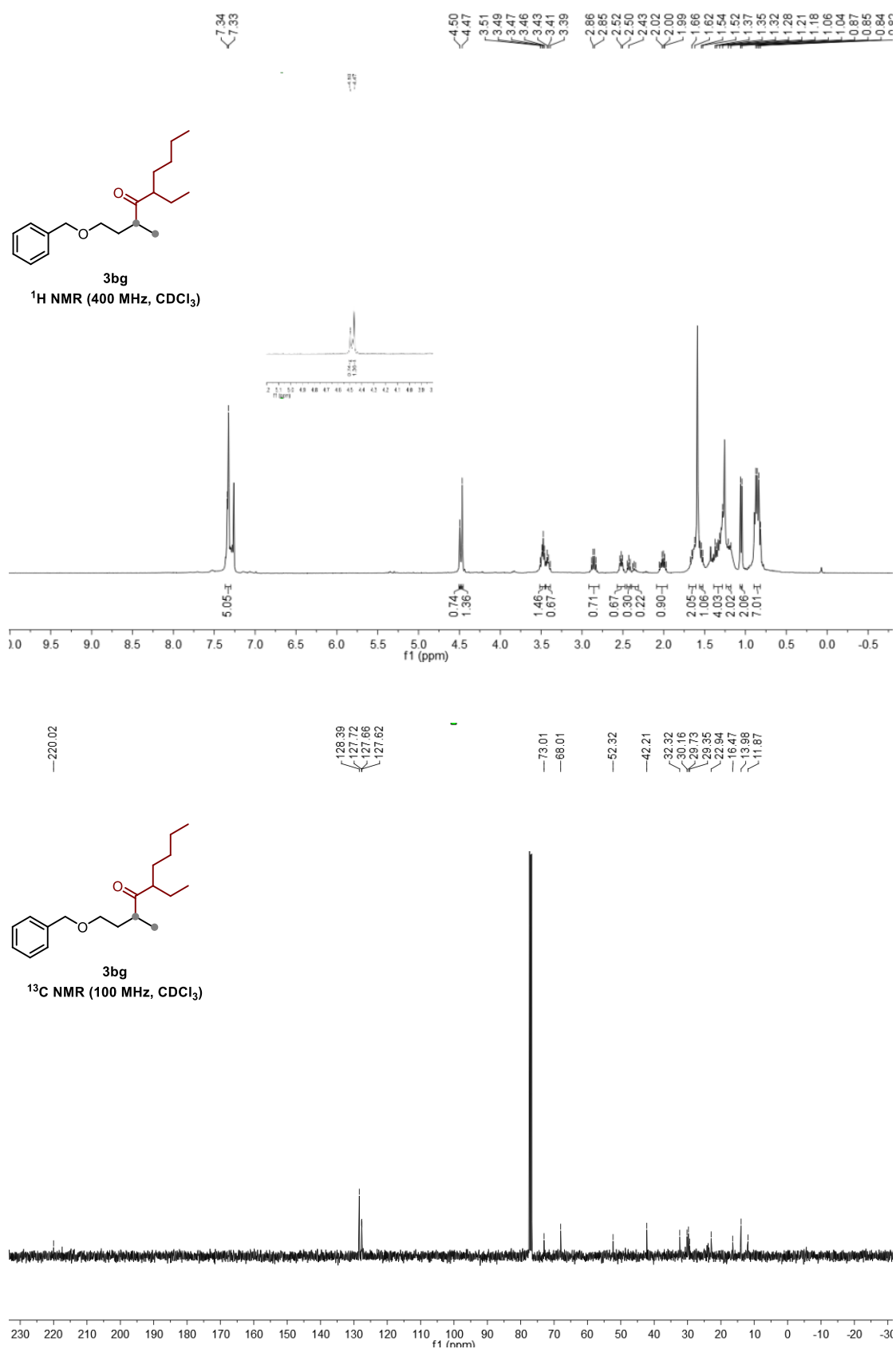


Figure S63. ¹H NMR and ¹³C NMR spectra of **3bg**.

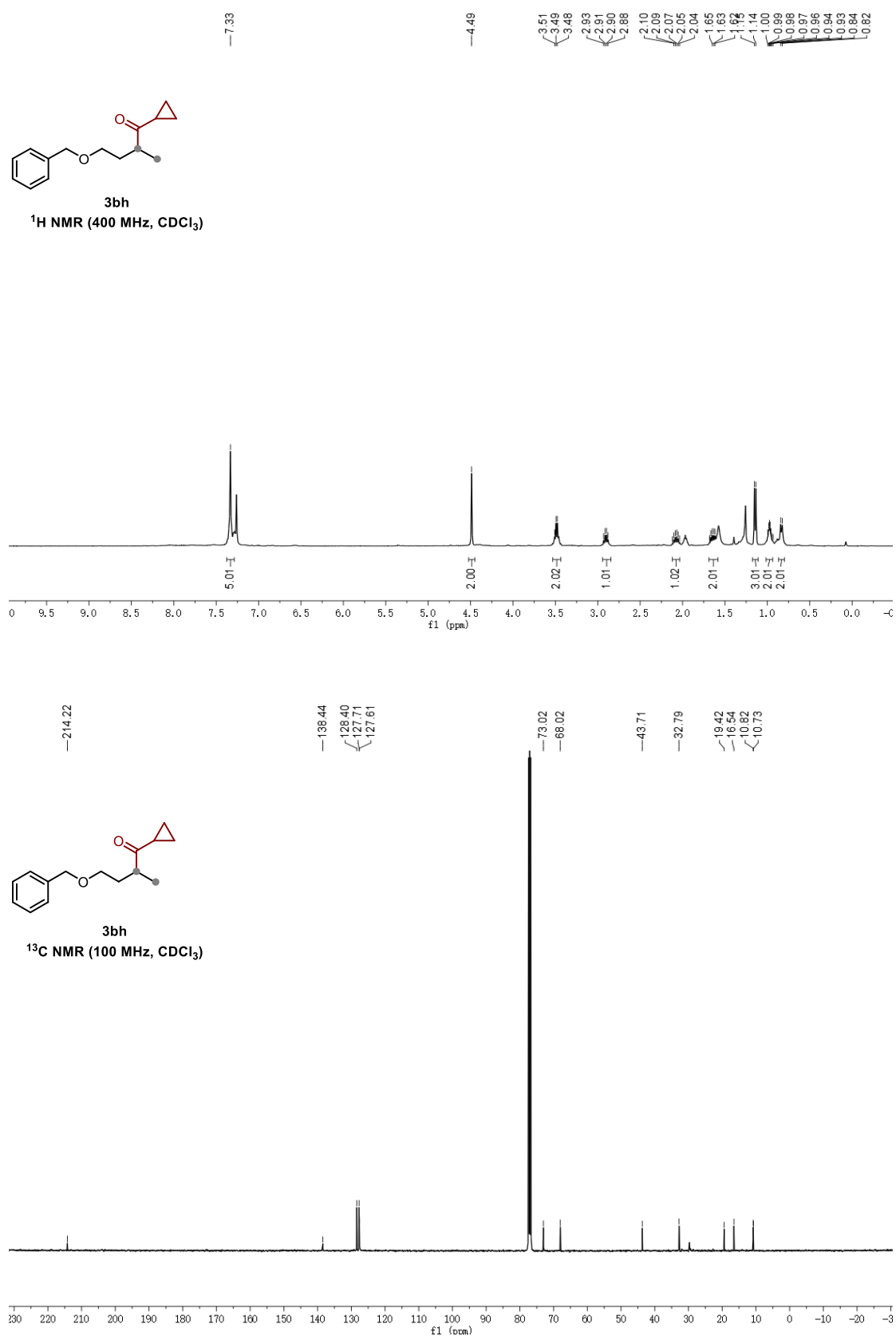


Figure S64. ¹H NMR and ¹³C NMR spectra of **3bh**.

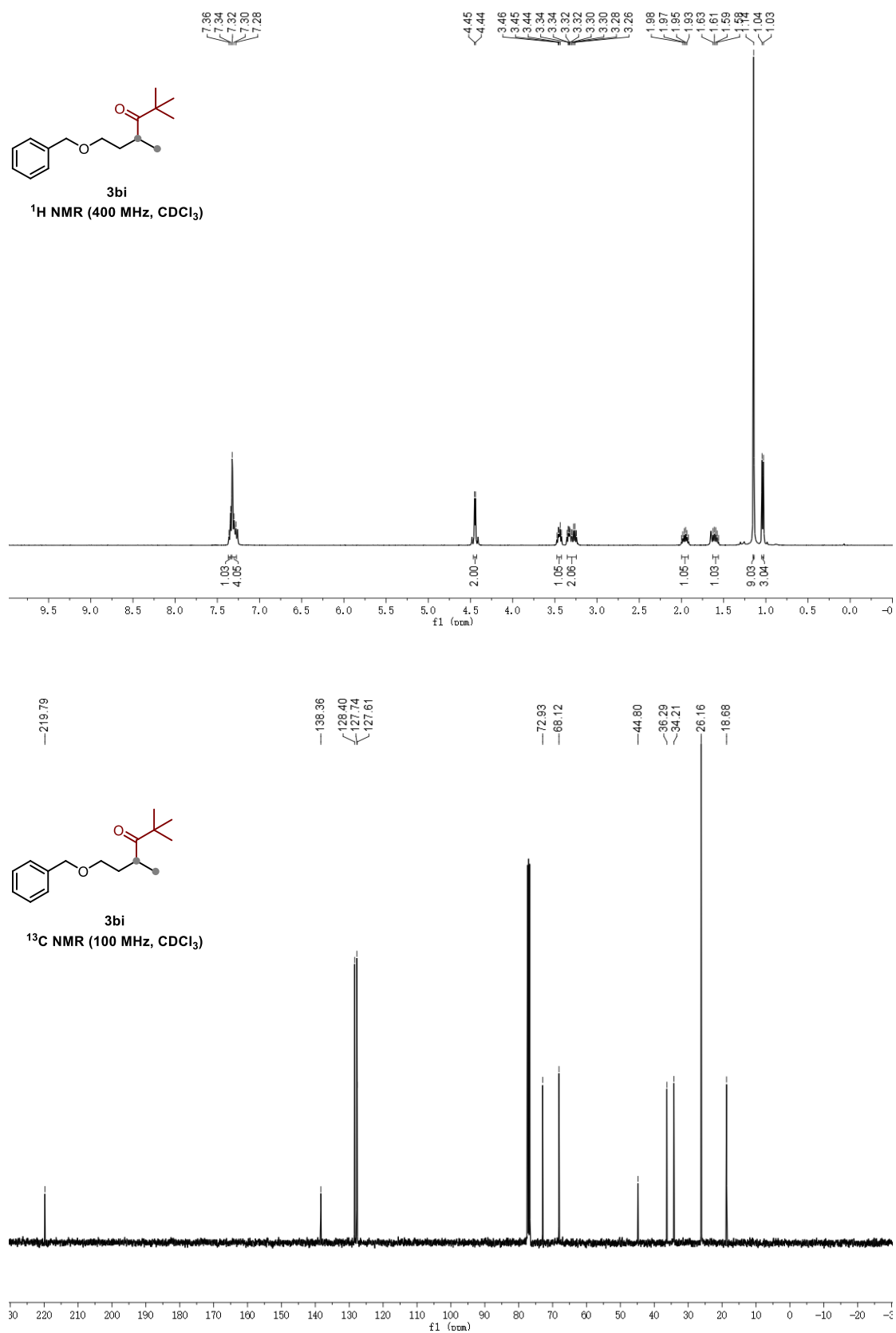


Figure S65. ¹H NMR and ¹³C NMR spectra of **3bi**.

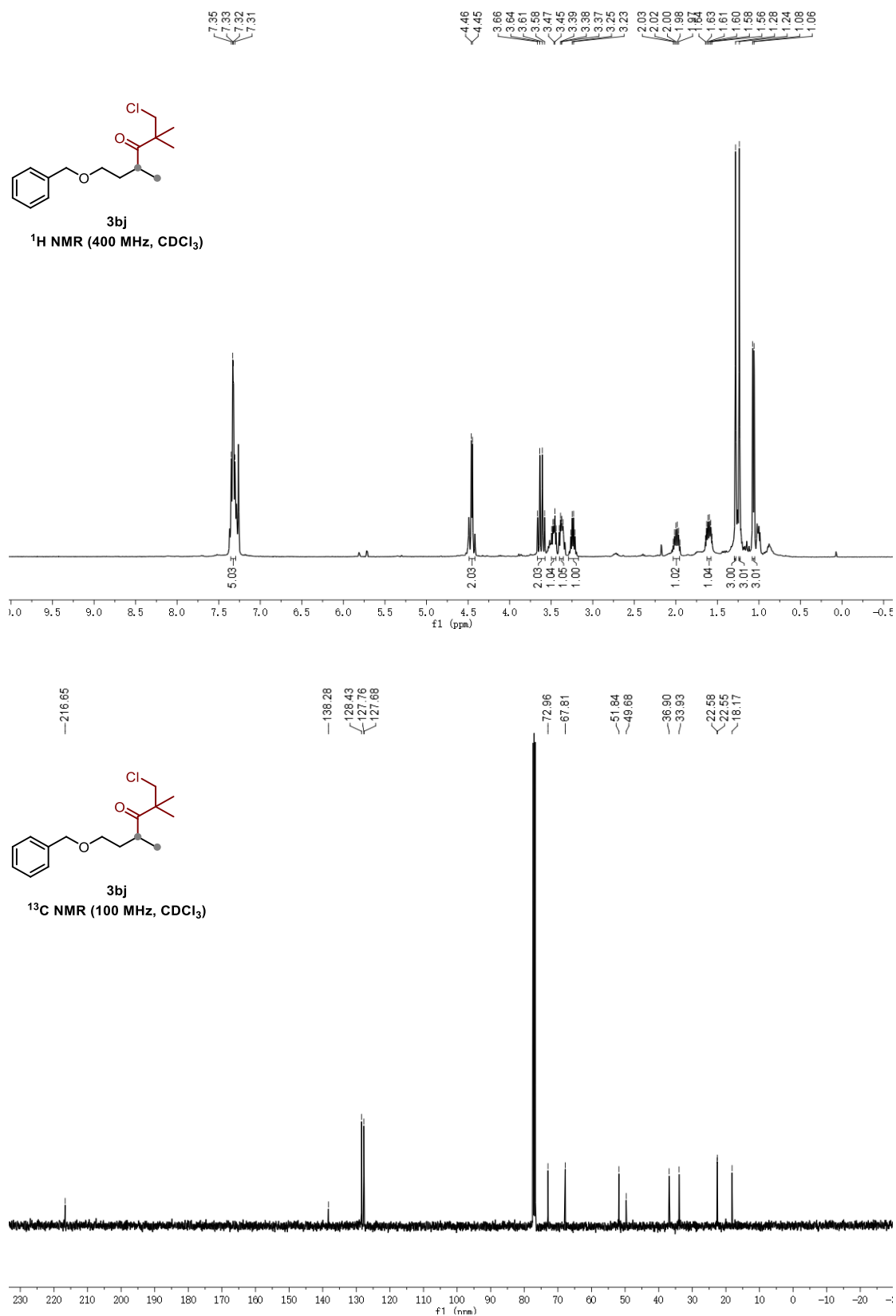


Figure S66. ¹H NMR and ¹³C NMR spectra of **3bj**.

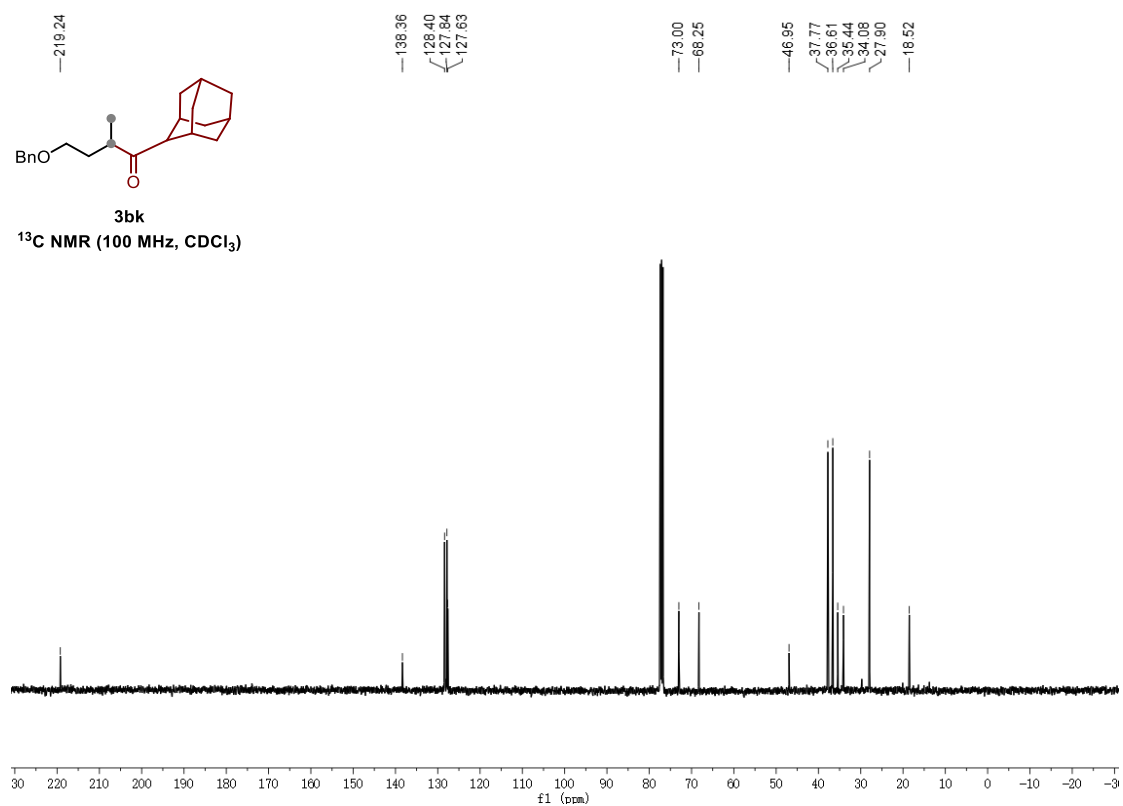
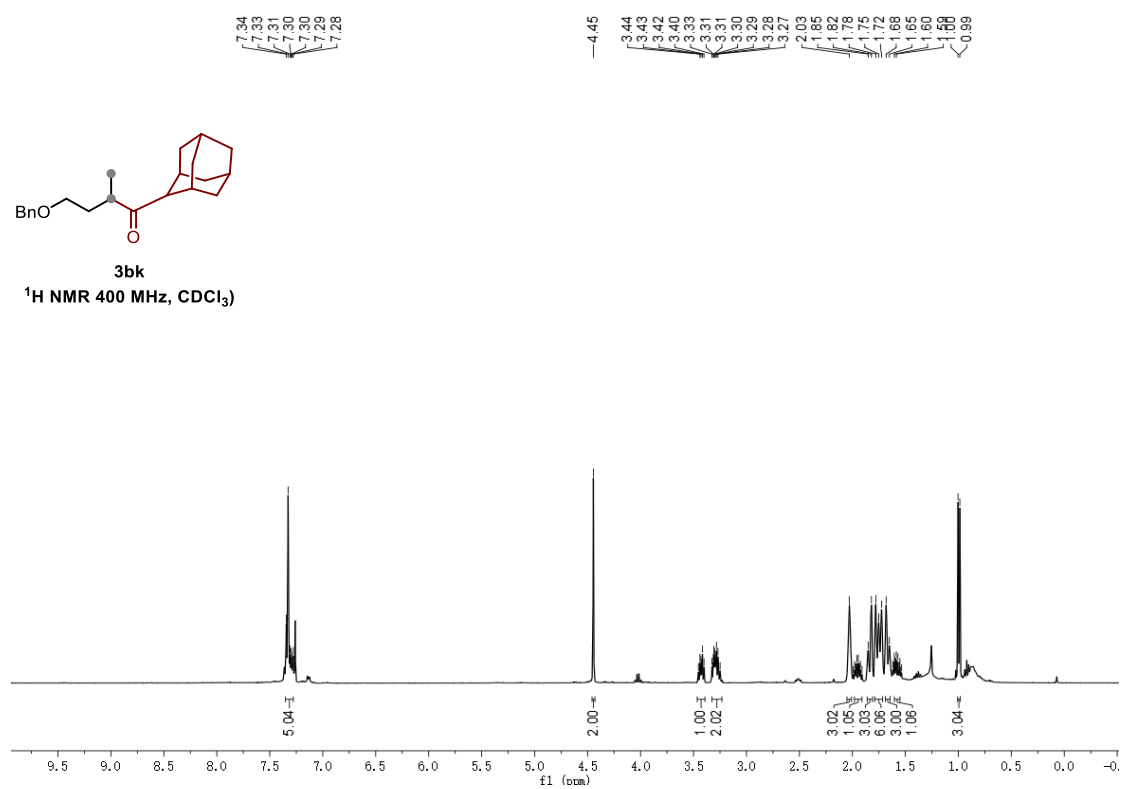


Figure S67. ^1H NMR and ^{13}C NMR spectra of **3bk**.

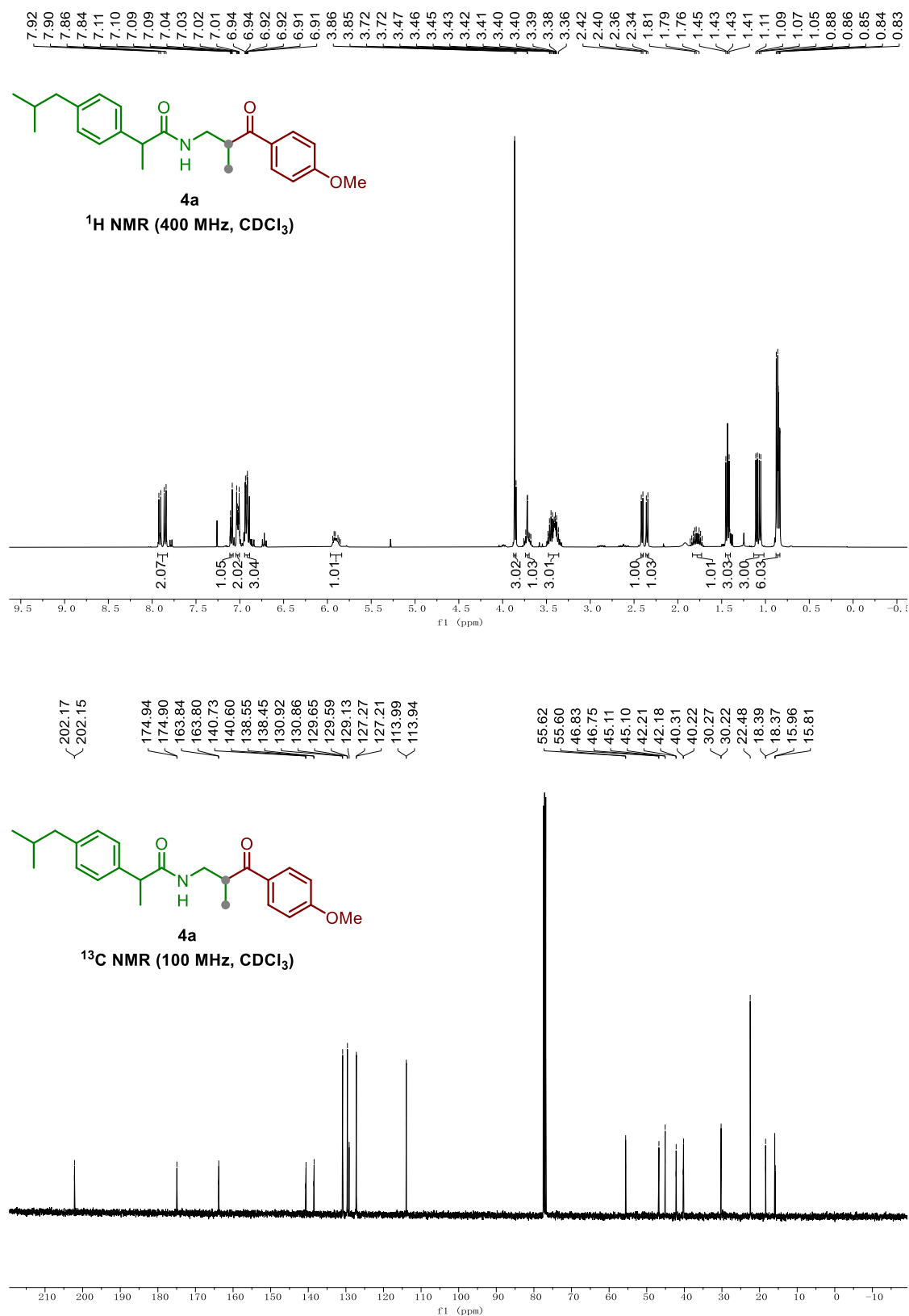


Figure S68. ¹H NMR and ¹³C NMR spectra of **4a**.

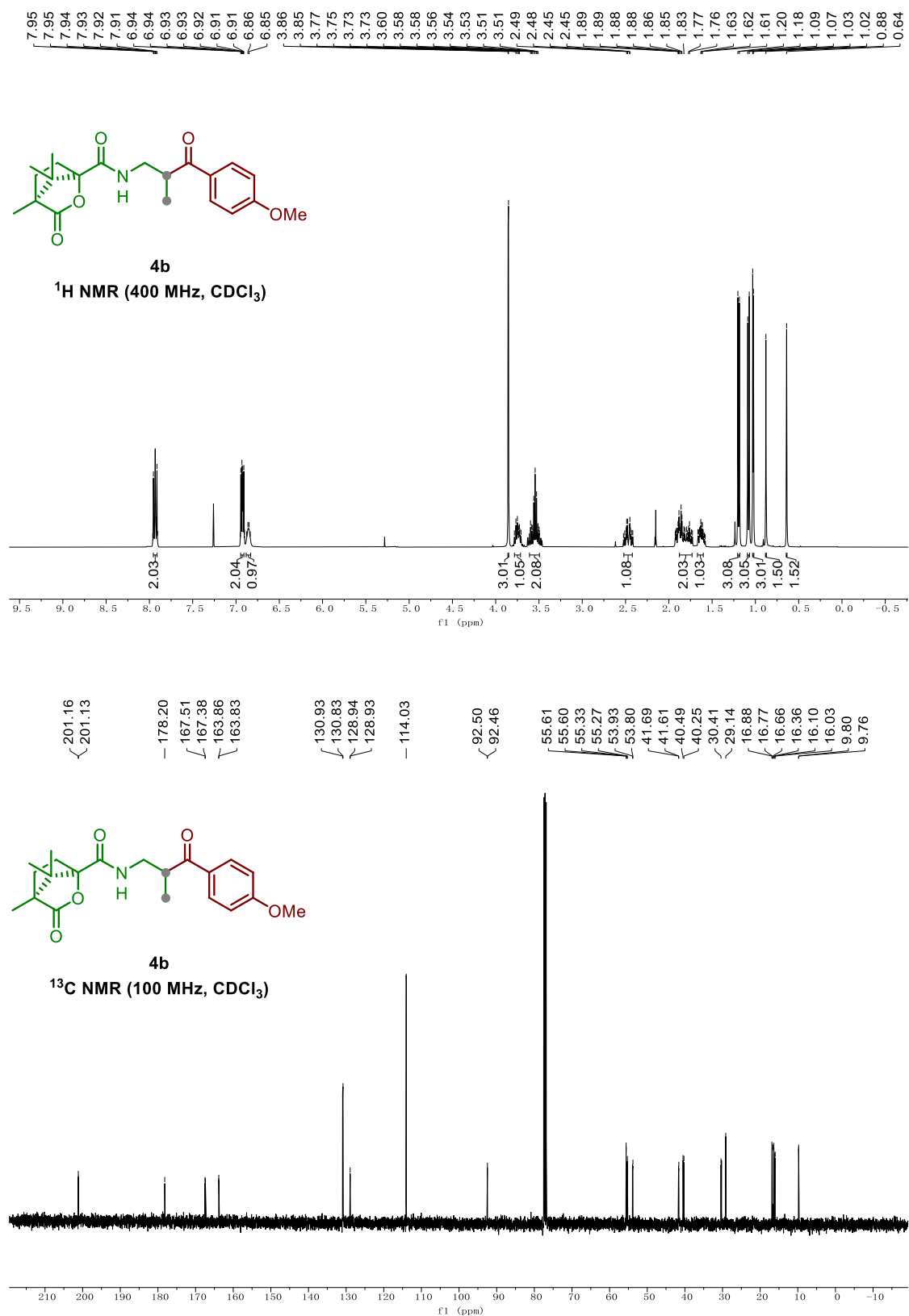


Figure S69. ¹H NMR and ¹³C NMR spectra of **4b**.

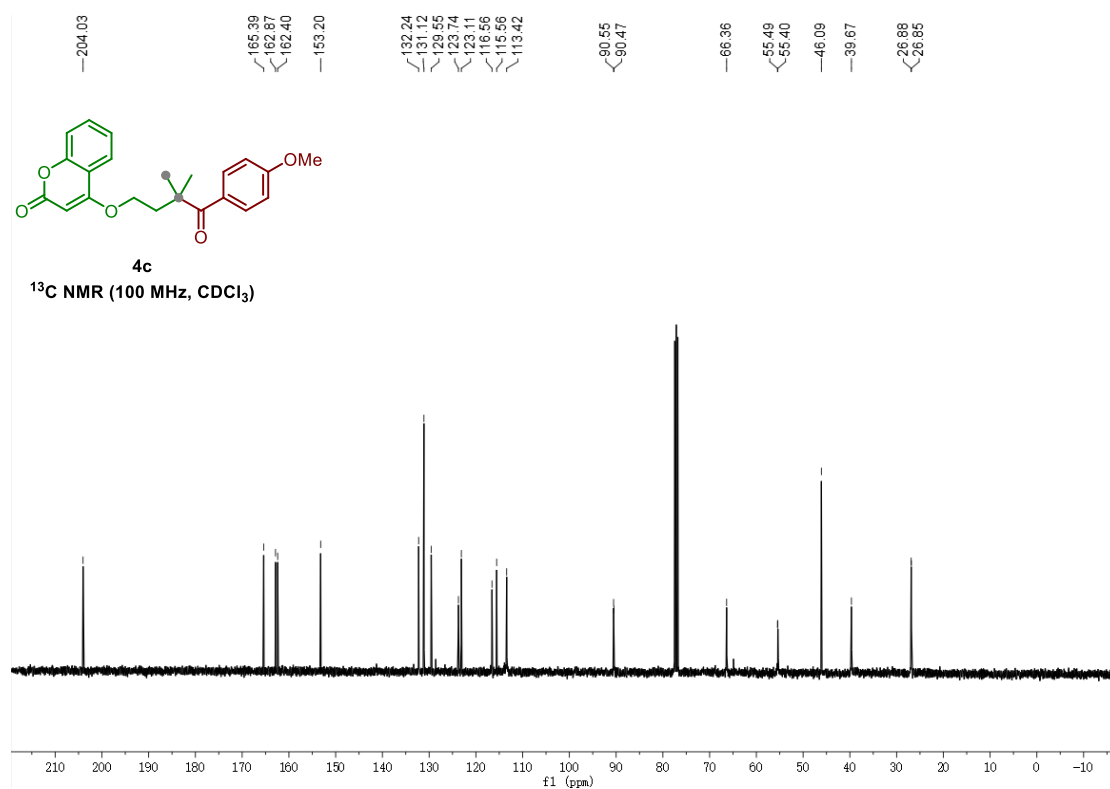
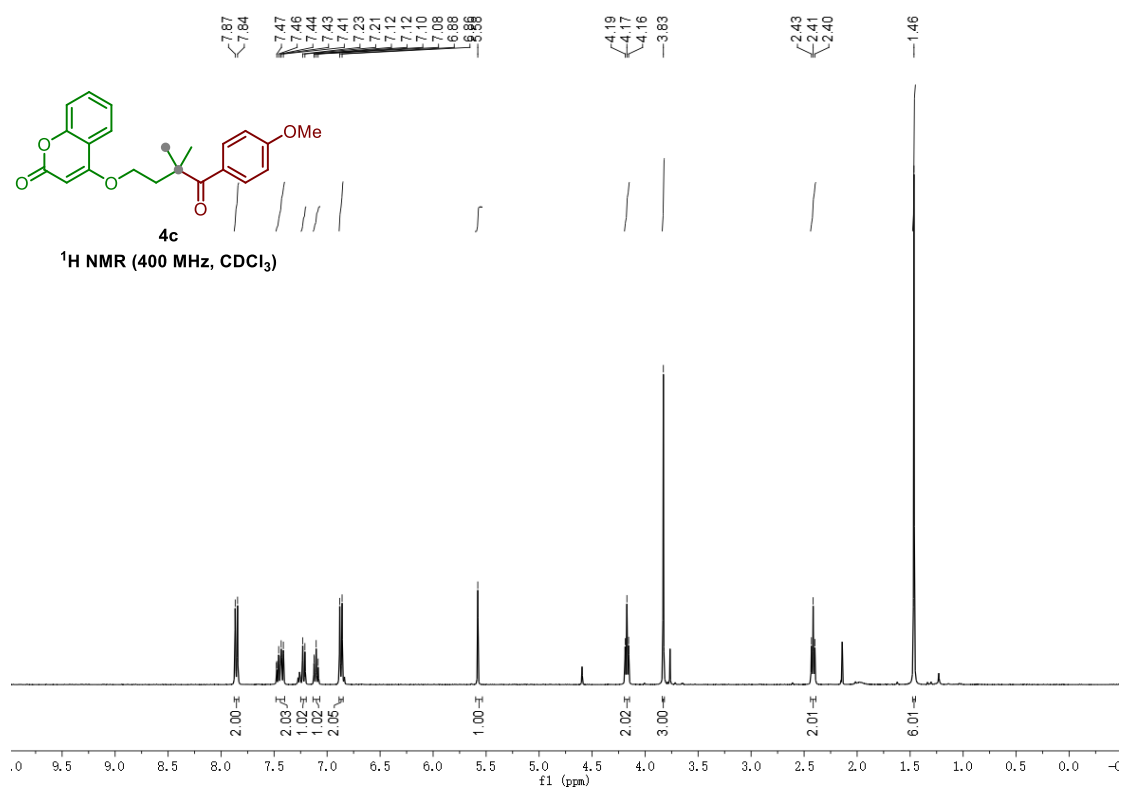


Figure S70. ^1H NMR and ^{13}C NMR spectra of **4c**.

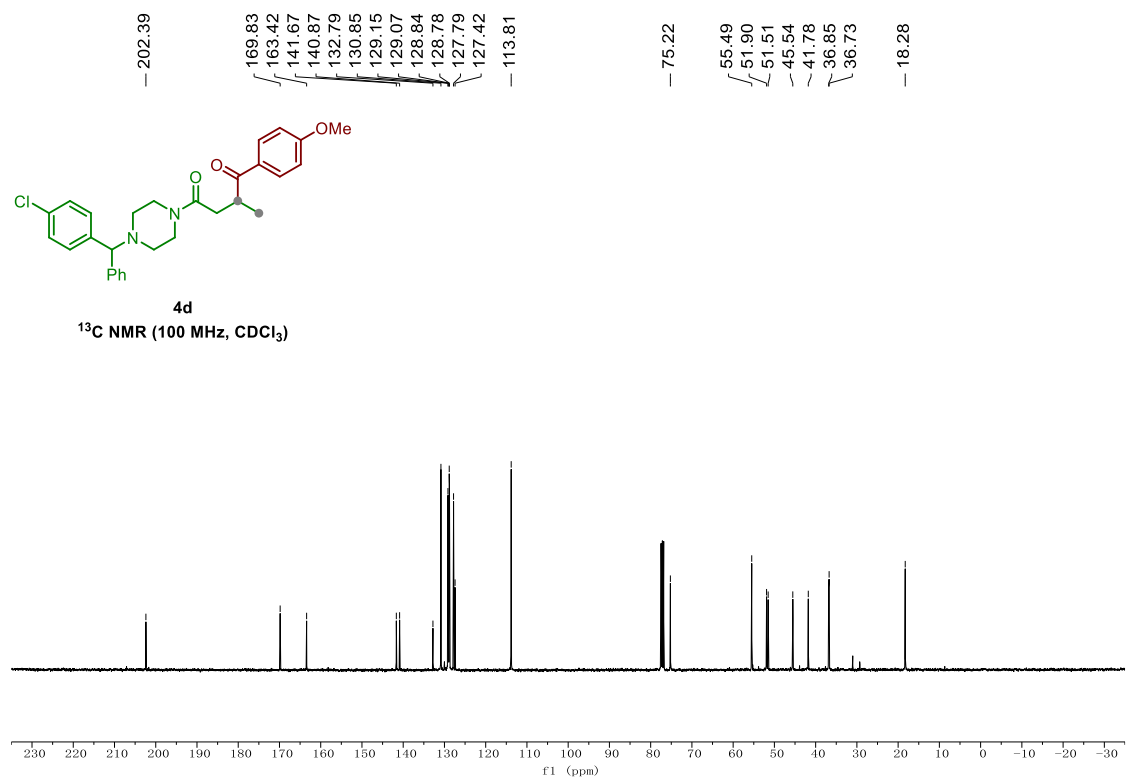
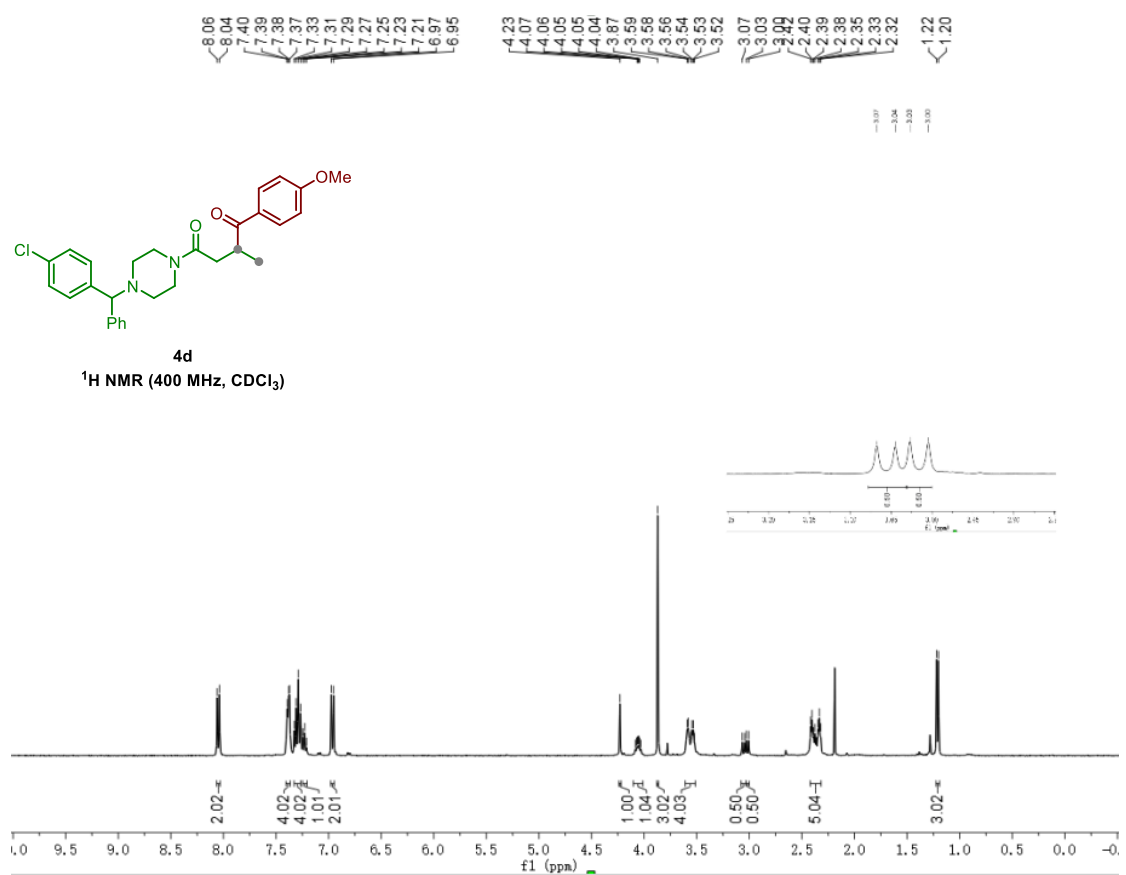


Figure S71. ^1H NMR and ^{13}C NMR spectra of **4d**.

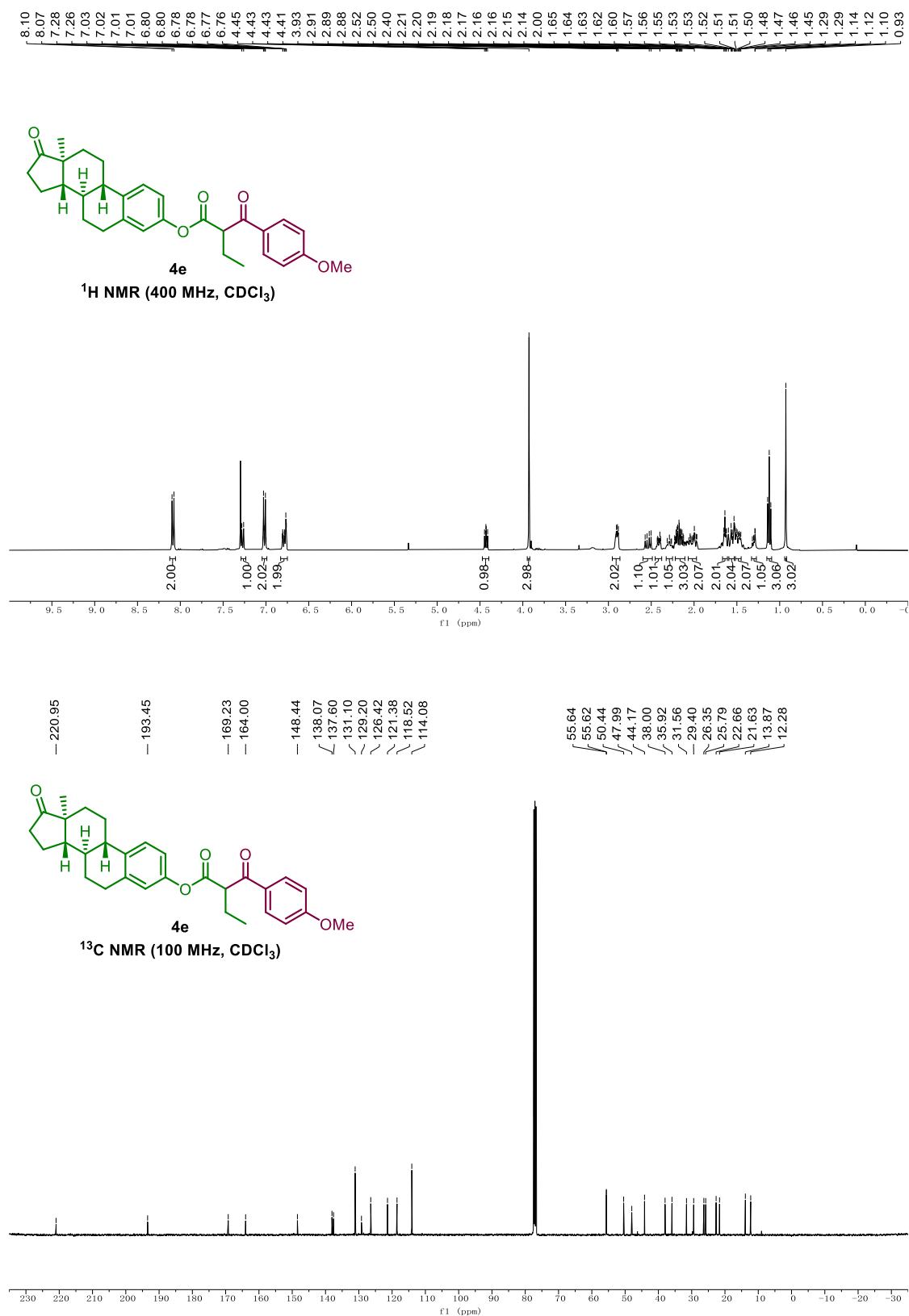


Figure S72. ¹H NMR and ¹³C NMR spectra of **4e**.

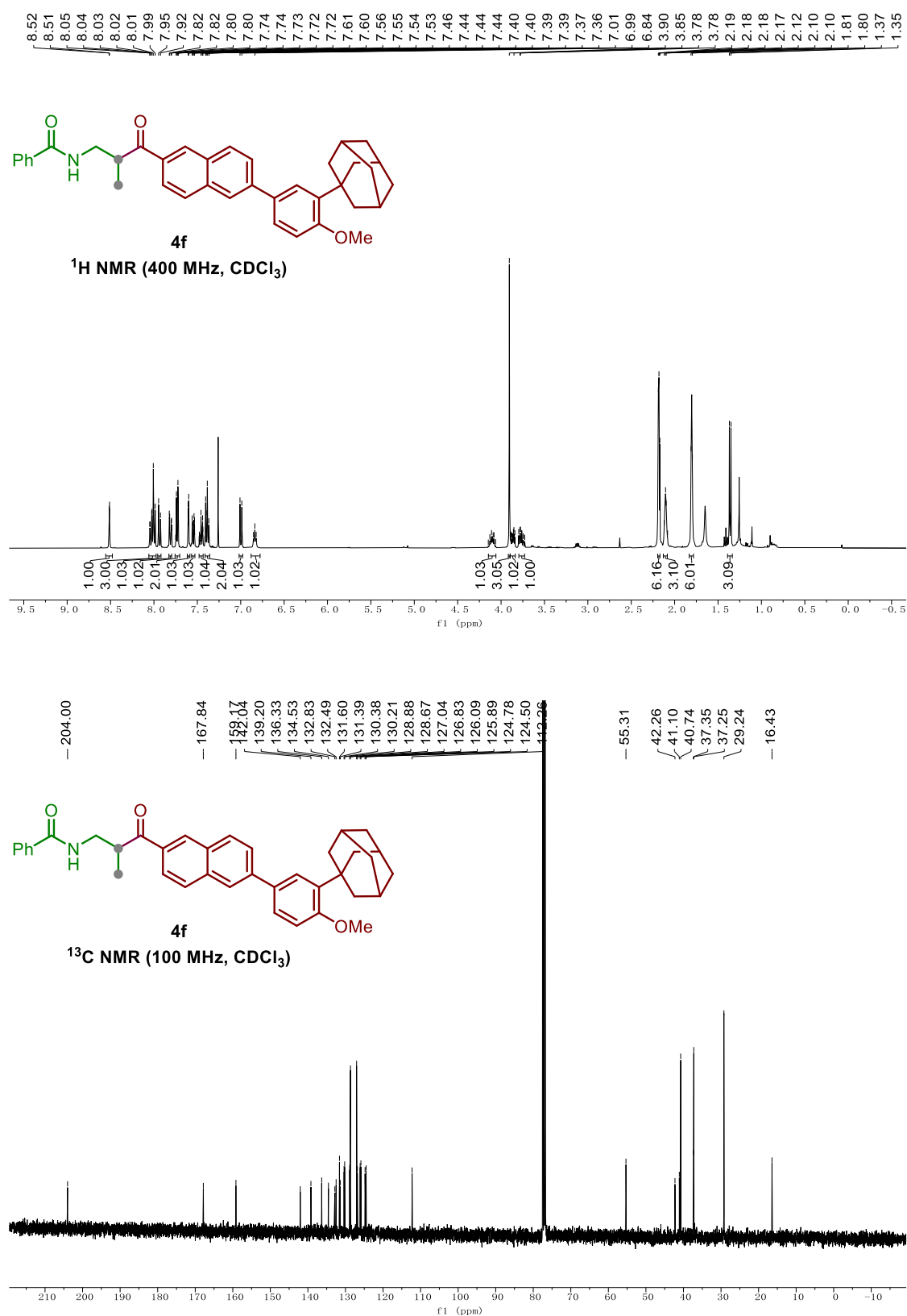


Figure S73. ¹H NMR and ¹³C NMR spectra of **4f**.

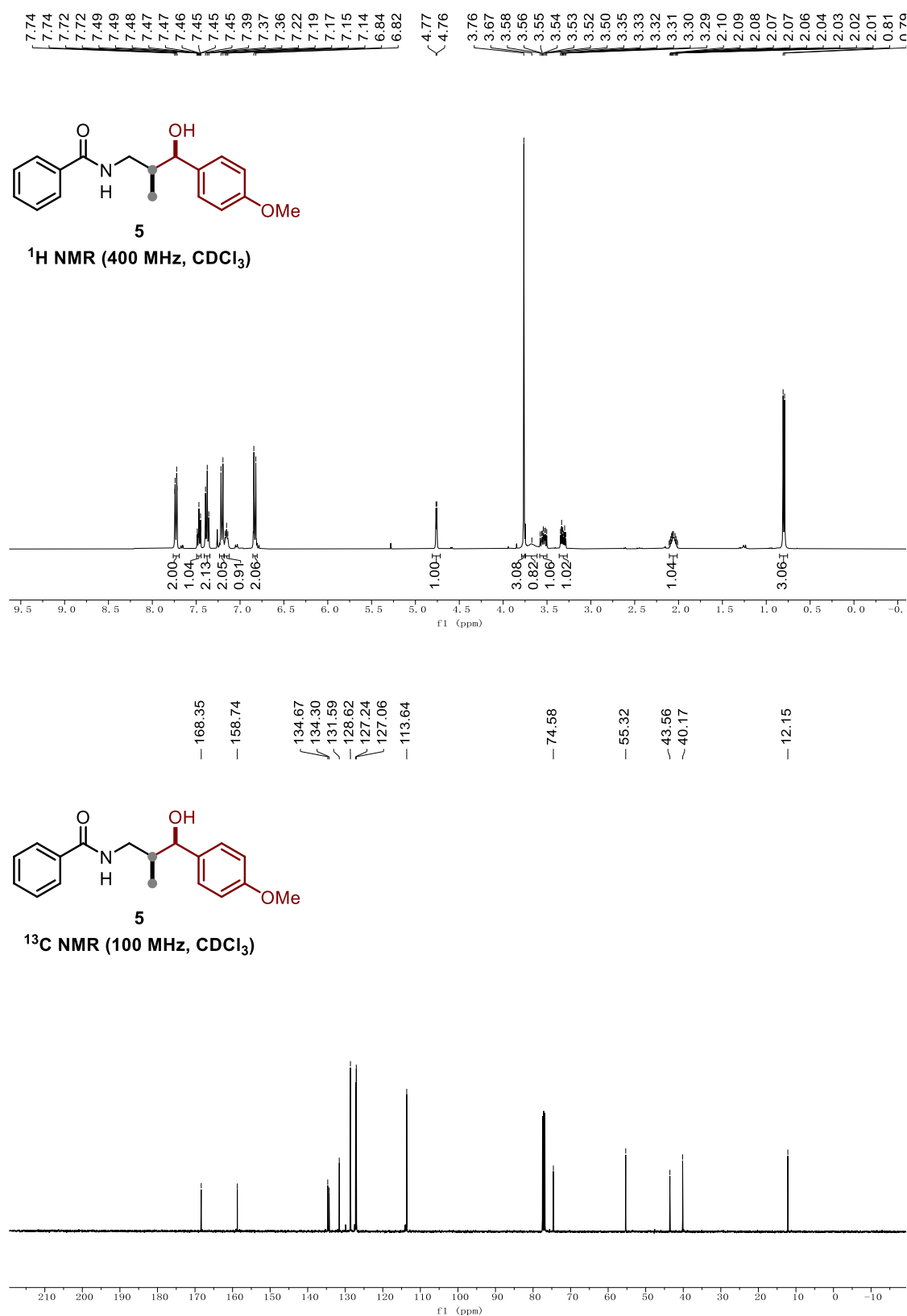


Figure S74. ¹H NMR and ¹³C NMR spectra of **5**.

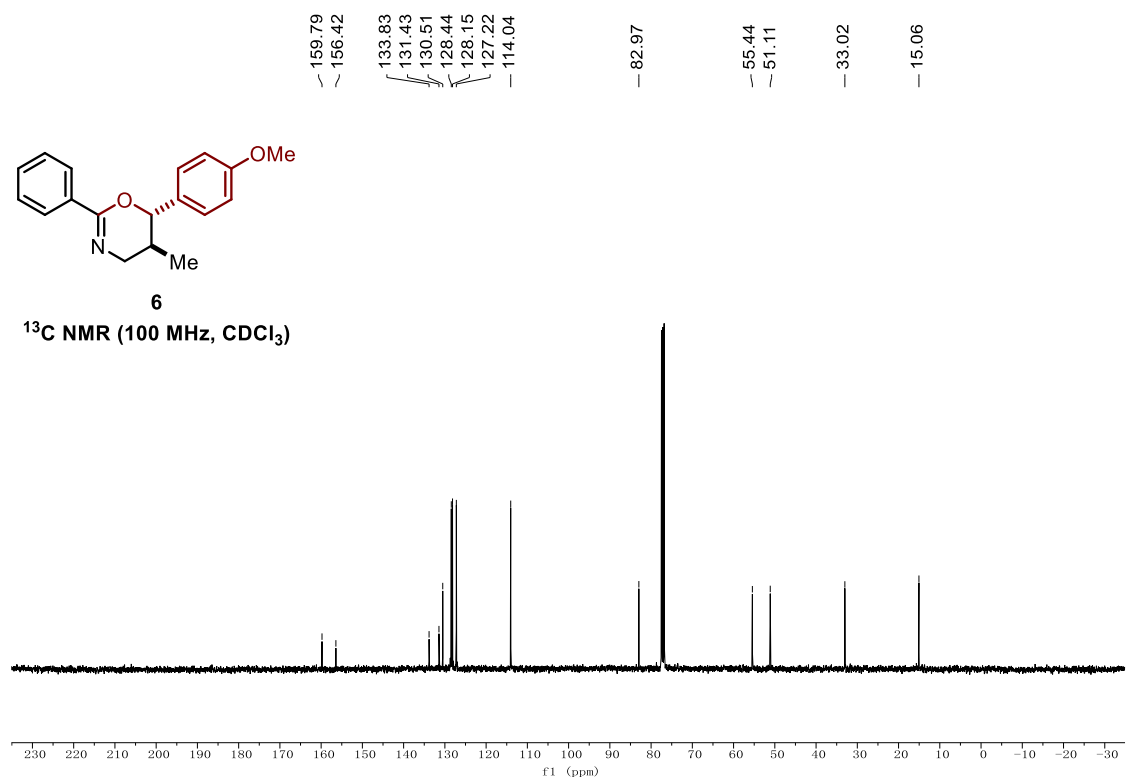
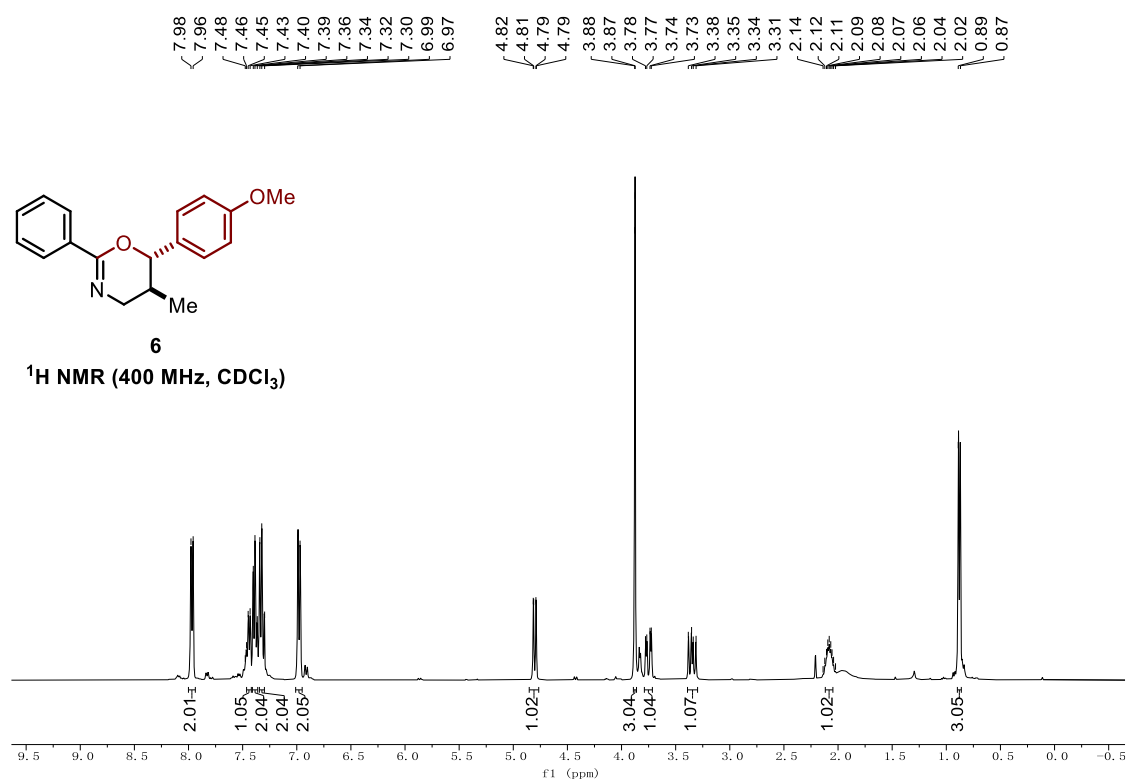


Figure S75. ^1H NMR and ^{13}C NMR spectra of **6**.

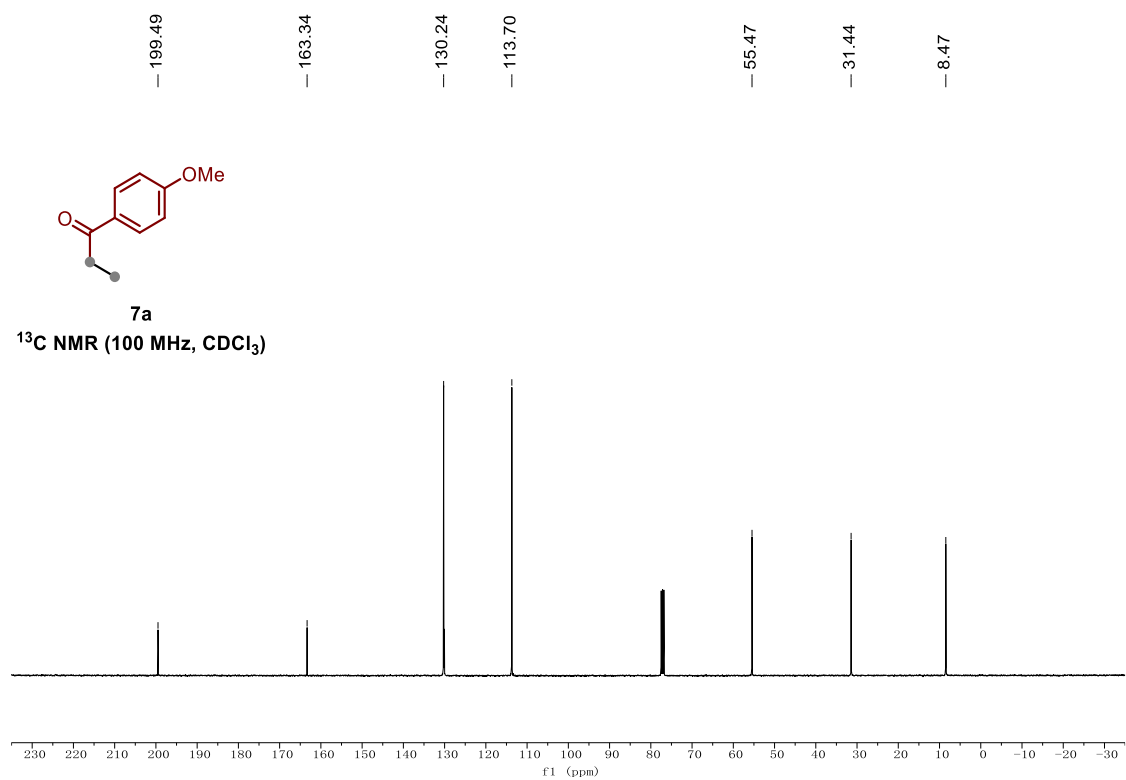
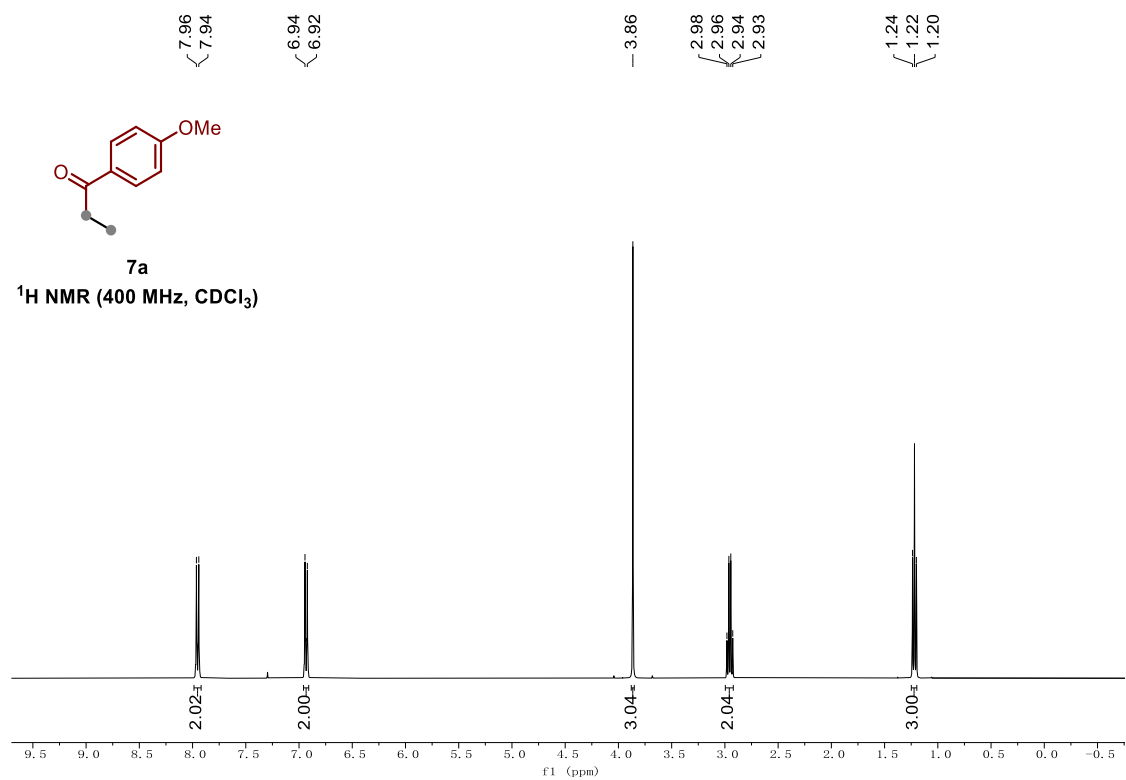


Figure S76. ^1H NMR and ^{13}C NMR spectra of **7a**.

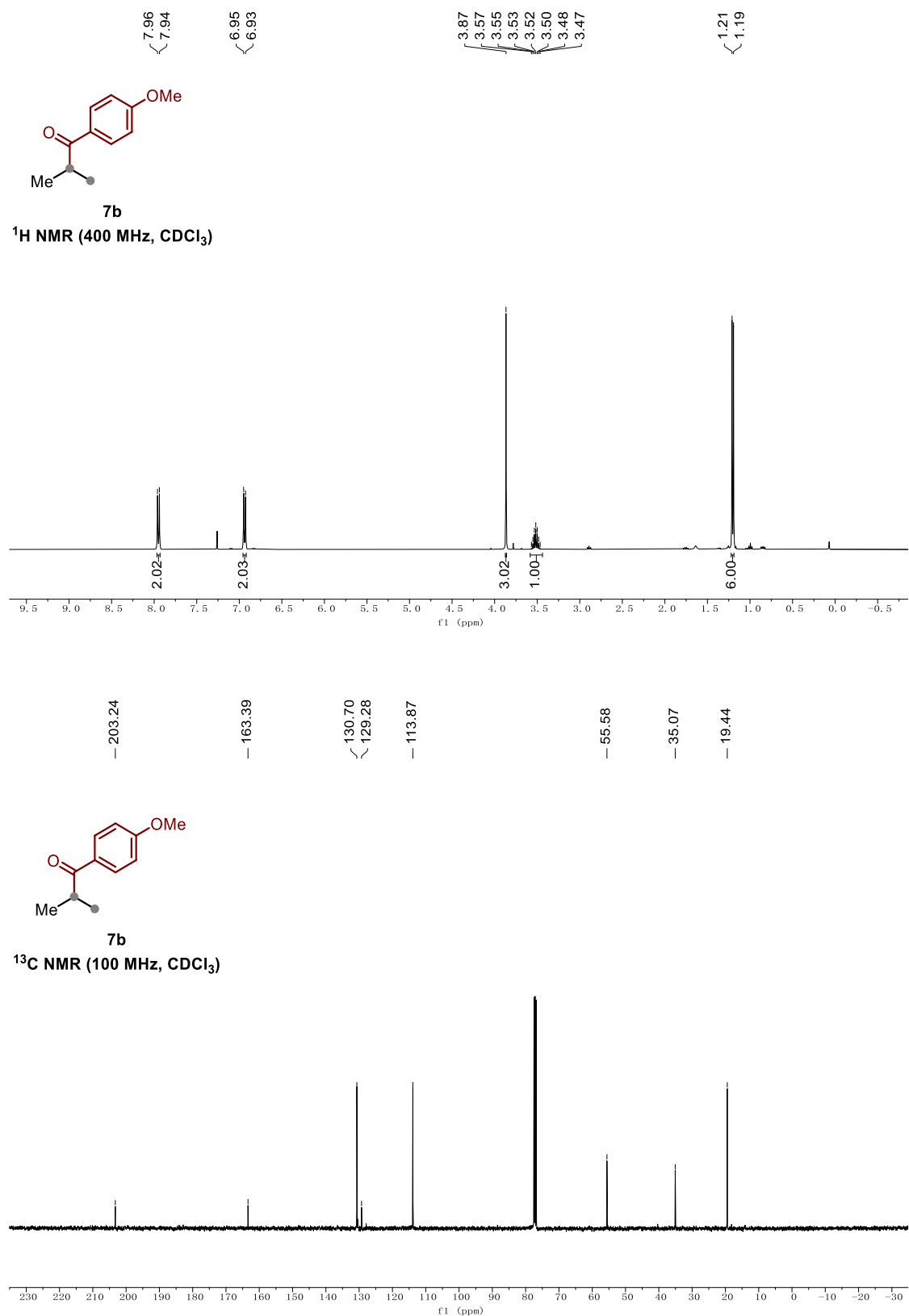


Figure S77. ¹H NMR and ¹³C NMR spectra of **7b**.

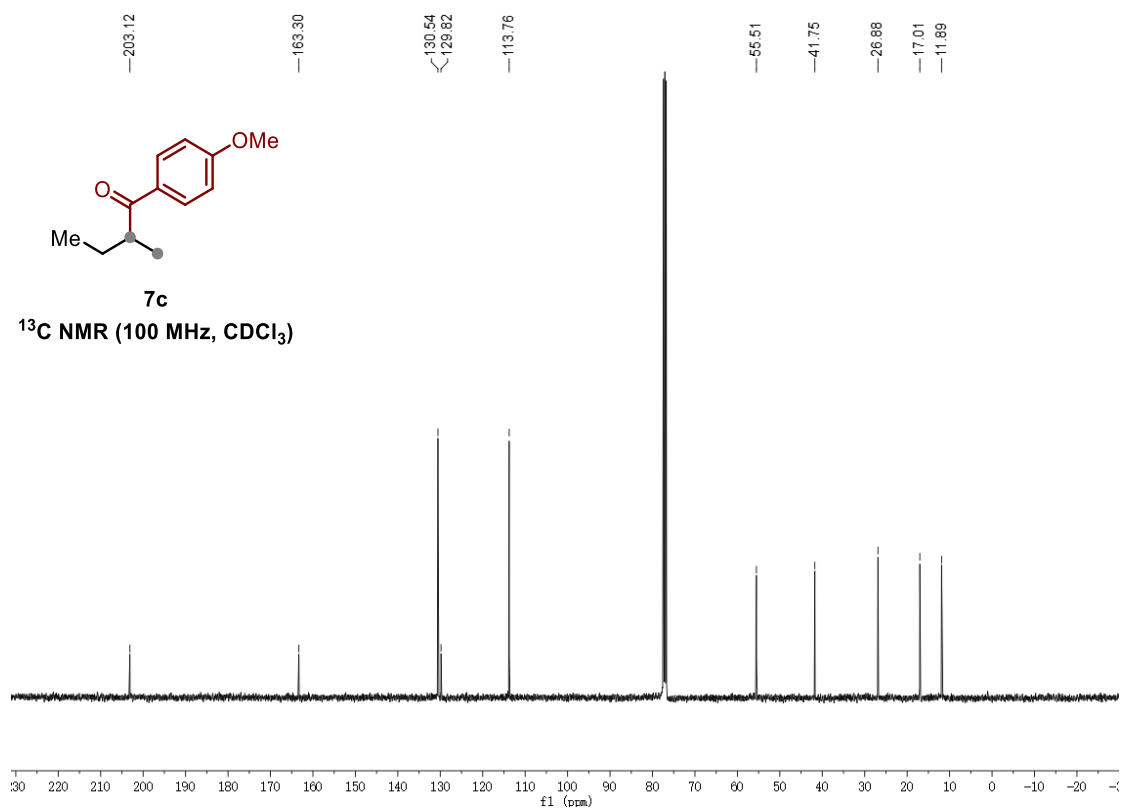
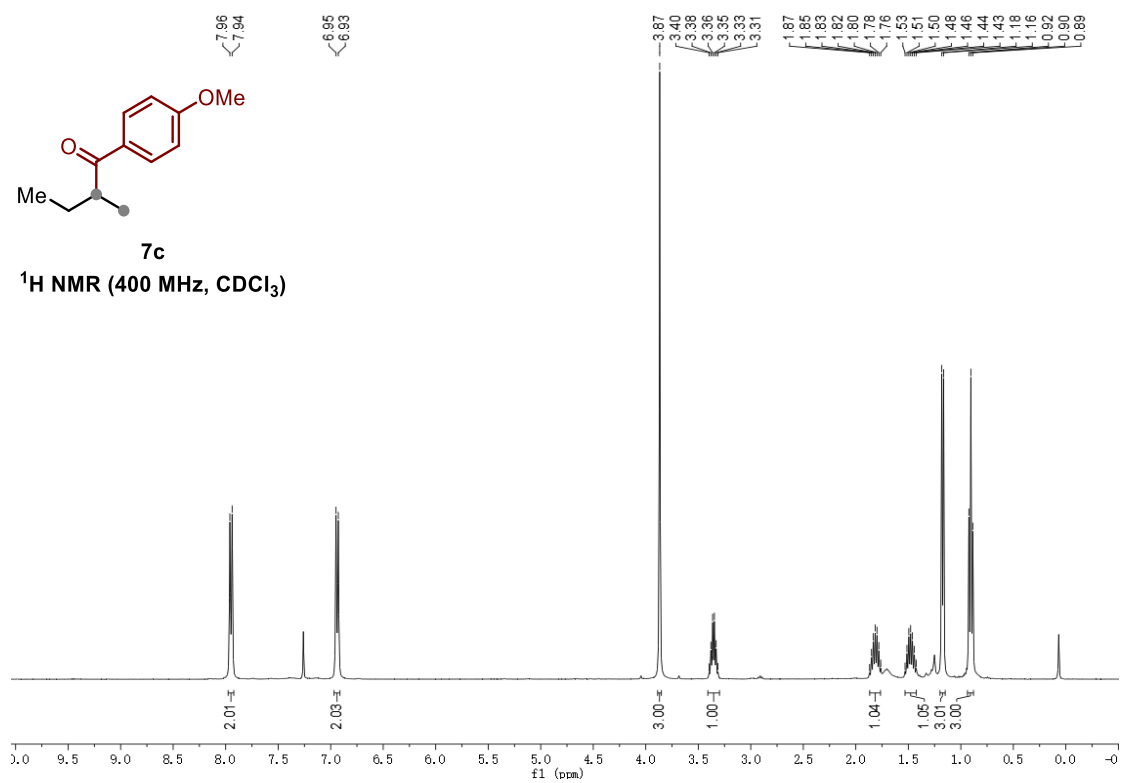


Figure S78. ¹H NMR and ¹³C NMR spectra of **7c**.

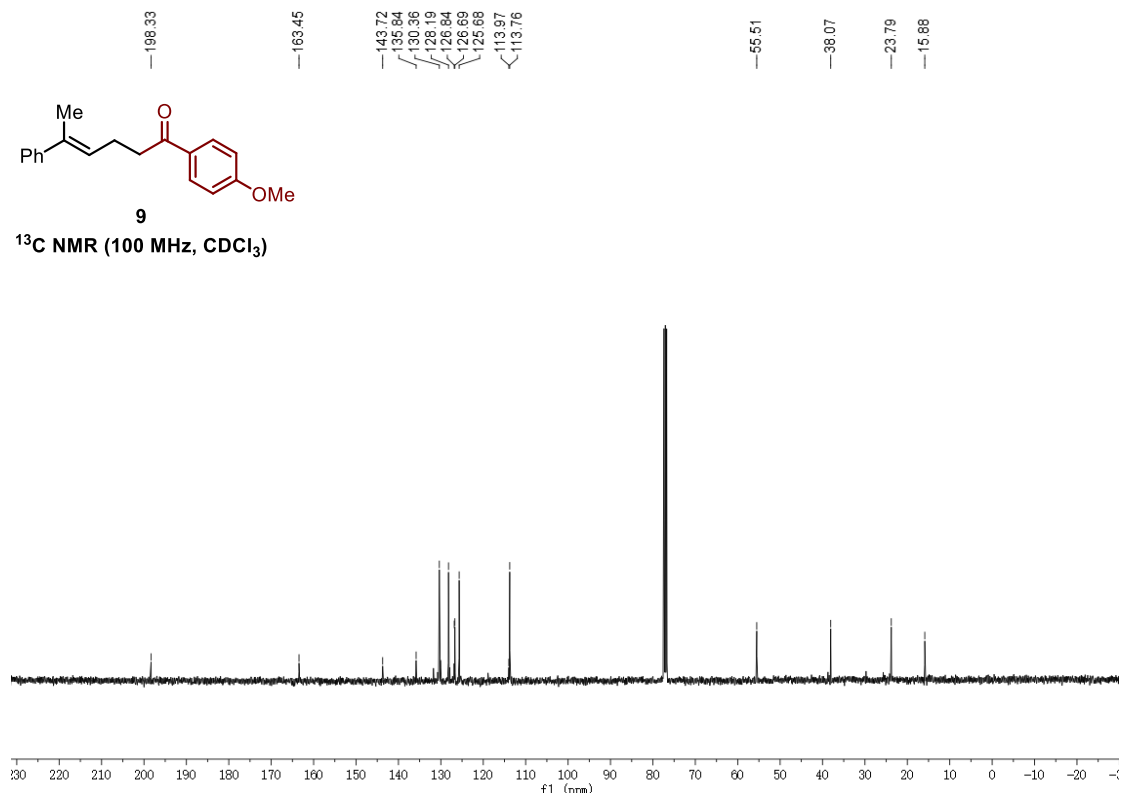
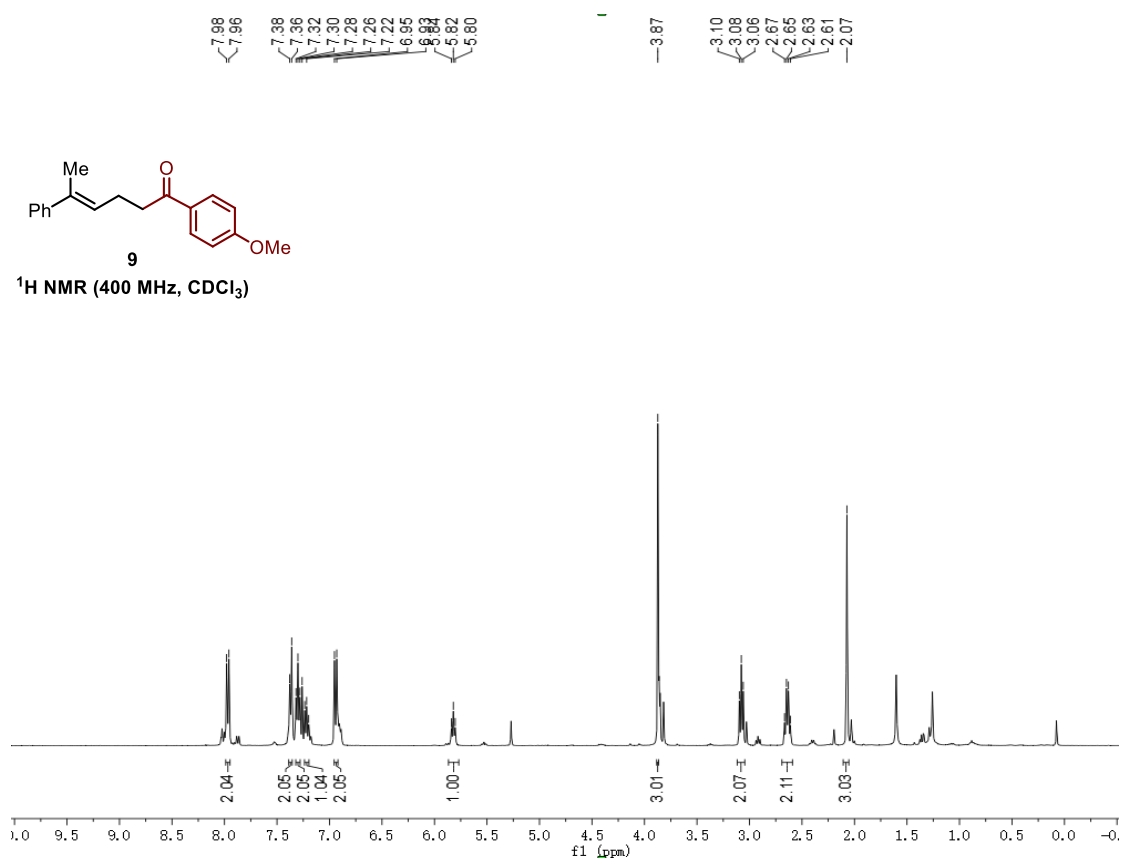


Figure S79. ^1H NMR and ^{13}C NMR spectra of **9**.