Supporting Information

for

Copper-Catalyzed Photoinduced Decarboxylative Alkynylation: A Combined Experimental and Computational Study

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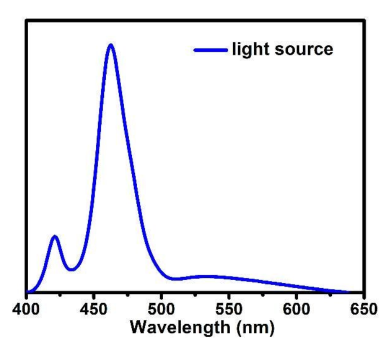
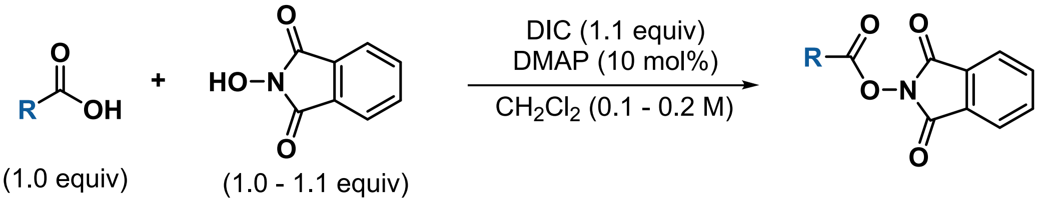
General Information

Tetrahydrofuran (THF), *N*,*N*-dimethylformamide (DMF), Acetonitrile (MeCN) and Dichloromethane (CH_2Cl_2) were obtained by passing the previously degassed solvents through an activated alumina column. Anhydrous Dimethylacetamide (DMA), Methanol (MeOH) and 1,2-Dichloroethane (DCE) were purchased from J&K Scientific. All reagents were purchased at the highest commercial quality and used without further purification unless otherwise stated. Yields refer to chromatographically and spectroscopically (^{1}HNMR) homogeneous material, unless otherwise stated. Reactions were monitored by thin layer chromatography (TLC), GC/MS, GC/FID, or LC/MS. TLC was performed on pre-coated silica gel plated, using short-wave UV light as the visualizing agent, and phosphomolybdic acid, *p*-anisaldehyde, or $KMnO_4$ and heat as developing agents. Column chromatography was performed using silica gel 60 (300-400 mesh). ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR were measured on a Bruker AVANCE III-400, 500, 600 spectrometer. Chemical shifts are reported in ppm (δ) relative to internal tetramethylsilane (TMS, δ 0.0 ppm) or with the solvent reference relative to TMS employed as the internal standard. Data are reported as follows: chemical shift (multiplicity [singlet (s), doublet (d), triplet (t), quartet (q), broad (br) and multiplet (m)], coupling constants [Hz], integration). Melting points are uncorrected. HRMS(ESI) was recorded on a Bruker miccOTOF-Q111, and HRMS(EI) was recorded on a Waters Micromass GCT Premier. The blue LEDs light was purchased from Kessil A360WE (90W MAX). The emission spectrum of the lamp (λ_{max}= 462 nm) is shown below:



Emission spectra of the lamp

Synthesis of NHPI Redox-Active Esters (Procedure A)



NHPI esters were prepared according to a previously reported procedure.[1-3] Around-bottom flask or culture tube was charged with carboxylic acid (1.0 equiv), *N*-hydroxyphthalimide (1.0-1.1 equiv) and 4-dimethylaminopyridine (0.1 equiv). CH_2Cl_2 was added (0.1-0.2 M), and the mixture was stirred vigorously. [Note: Carboxylic acid was added via syringe (if liquid)]. DIC (1.1 equiv) was then added dropwise via syringe, and the mixture was allowed to stir until the acid was consumed (determined by TLC). Typical reaction times were between 0.5 and 12 hours. The mixture was filtered (through a thin pad of Celite®, SiO2, or frit funnel) and rinsed with additional CH_2Cl_2/Et_2O. Solvents were removed under reduced pressure, and purification of the crude mixture by column chromatography afforded the desired NHPI redox-active ester. If necessary, the NHPI redox-active ester could be further recrystallized from CH_2Cl_2/MeOH. All the previously reported NHPI redox-active esters are shown below (Figure S1).

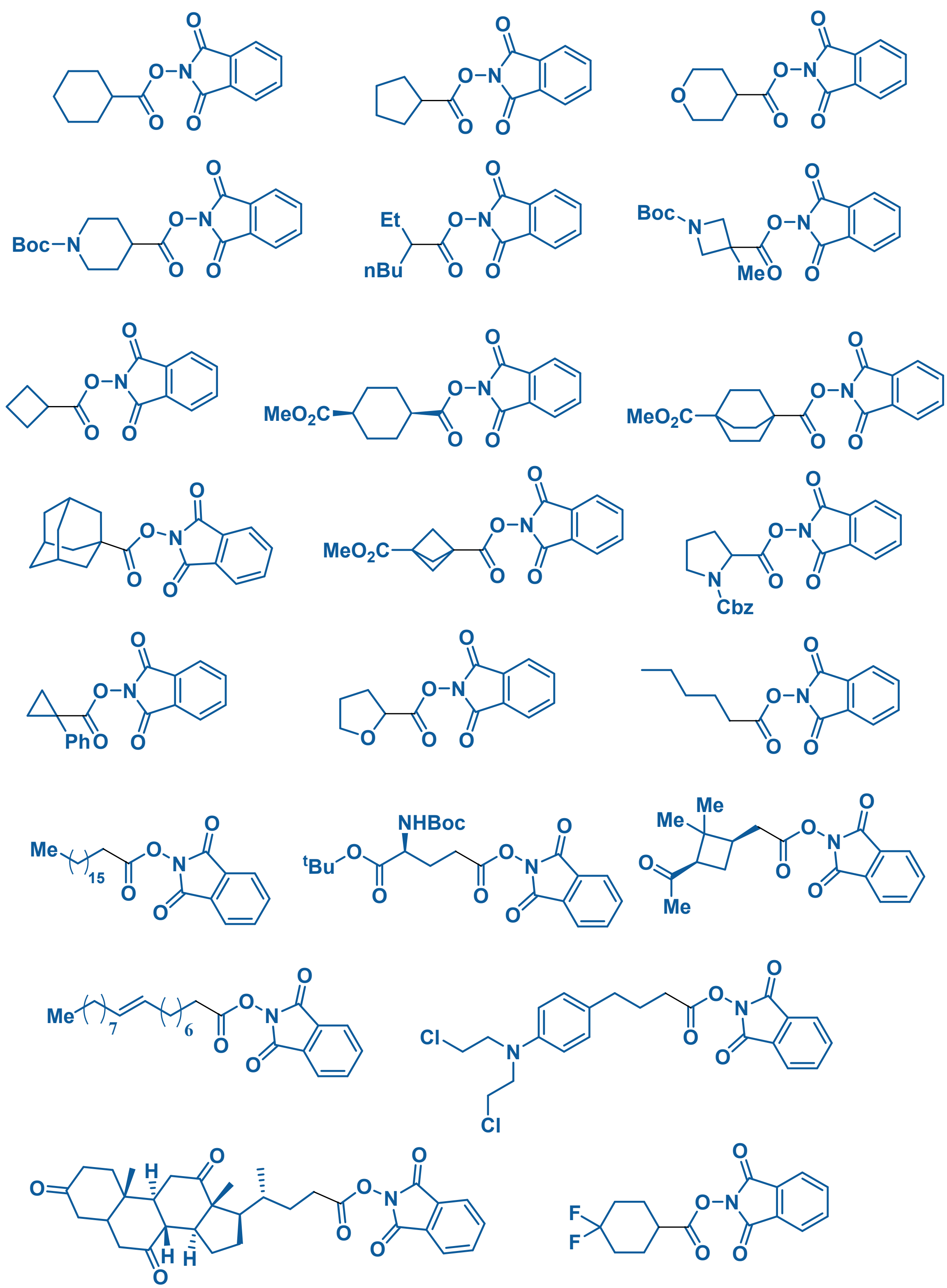
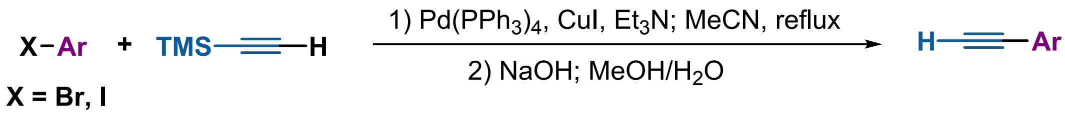


Figure S1. Previously Reported NHPI Redox-Active Esters

Synthesis of Terminal Alkyne (Procedure B)



A mixture of aryl halides (1.0 equiv), trimethylsilylacetylene (1.5 e.q.), $Pd(PPh_3)_4$ (3 mol%), CuI (5 mol%), and triethylamine (3 equiv) in acetonitrile (0.5M) was refluxed for 4 h. After cooling, water was added. After extraction with EtOAc, the organic phase was washed with brine and then was dried over $MgSO_4$. After filtration, the solvent was removed. 0.2 M NaOH (1.5 equiv) and methanol ($MeOH/H_2O$=1:1) were added. The mixture was stirred for 2 h at room temperature before filtration over Celite®. The filtrate was evaporated and the residue was purified by flash chromatography to give aryl alkynes.

Besides the commercially available terminal alkynes, the alkynes shown below have been previously reported in the literature.[4-6]

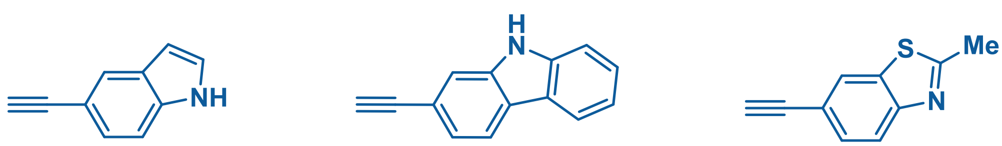
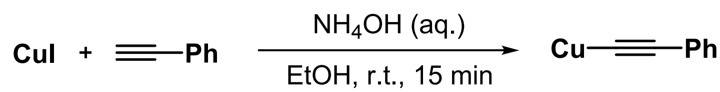


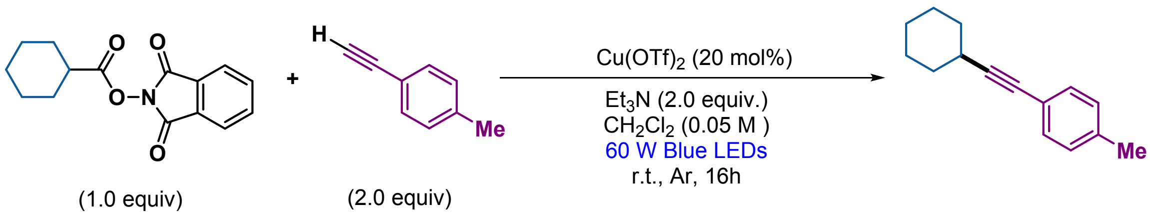
Figure S2. Previously Reported Terminal Alkyne

Synthesis of Copper (I) Phenylacetylide (Procedure C)



Cuprous iodide (1.0 g, 5.0 mmol) was dissolved in ammonium hydroxide to form a blue solution. While stirring, phenylacetylene (0.5 g, 5.1 mmol in 50 mL ethanol) was added dropwise to the solution. The mixture was allowed to stand for 15 min to form a yellow precipitate suspension. The precipitate was filtered out and washed with water, ethanol, and diethyl ether, three times each. The solid was vacuum-dried. The bright yellow solid was obtained and stored in glovebox. The spectroscopic data for the yellow solid was consistent with the literature.[7]

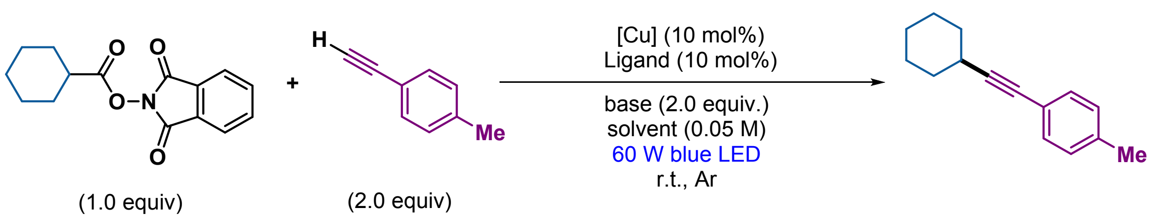
Optimization Tables



Entry	Condition	Yield[a] (%)
1	no change	23
2	in the dark	NR
3	r.t. to 80 °C & in the dark	0
4	without $Cu(OTf)_2$	NR
5	without Et_3N	NR
6	in the air	NR
7	add $Ir(ppy)_3$ (2 mol%)	13
8	add $Ru(bpy)_3(PF_6)_2$ (2 mol%)	8
9	$Cu(OTf)_2$ (20 mol% to 10 mol%)	21
10	$Cu(OTf)_2$ (20 mol% to 1.0 equiv)	42

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard.

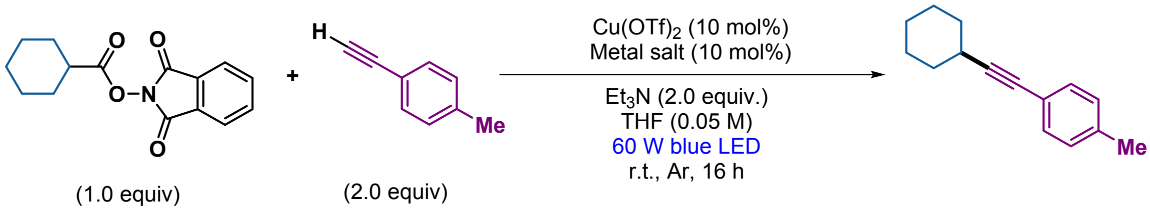
Optimization of ligand, base, solvent and reaction time



Entry	Cu salt	Ligand	Base	Solvent	Time	Yield[a] (%)
1	$Cu(OTf)_2$	none	Et_3N	CH_2Cl_2	16 h	21
2	$Cu(OTf)_2$	none	DABCO	CH_2Cl_2	16 h	0
3	$Cu(OTf)_2$	none	DMAP	CH_2Cl_2	16 h	NR
4	$Cu(OTf)_2$	none	Et_2NH	CH_2Cl_2	16 h	NR
5	$Cu(OTf)_2$	none	proton sponge[b]	CH_2Cl_2	16 h	10
6	$Cu(OTf)_2$	none	TMG	CH_2Cl_2	16 h	0
7	$Cu(OTf)_2$	none	DIPEA	CH_2Cl_2	16 h	12
8	$Cu(OTf)_2$	none	K_2CO_3	CH_2Cl_2	16 h	0
9	$Cu(OTf)_2$	none	Cs_2CO_3	CH_2Cl_2	16 h	0
10	$Cu(OTf)_2$	none	Et_3N	CH_2Cl_2	5 h	11
11	$Cu(OTf)_2$	none	Et_3N	CH_2Cl_2	8 h	15
12	$Cu(OTf)_2$	none	Et_3N	CH_2Cl_2	24 h	23
13	$Cu(OTf)_2$	PPh_3	Et_3N	CH_2Cl_2	16 h	0
14	$Cu(OTf)_2$	dppb	Et_3N	CH_2Cl_2	16 h	8
15	$Cu(OTf)_2$	phen	Et_3N	CH_2Cl_2	16 h	10
16	$Cu(OTf)_2$	bpy	Et_3N	CH_2Cl_2	16 h	3
17	$Cu(OTf)_2$	terpy	Et_3N	CH_2Cl_2	16 h	5
18	$Cu(OTf)_2$	none	Et_3N	DCE[c]	16 h	13
19	$Cu(OTf)_2$	none	Et_3N	PhCl	16 h	2
20	$Cu(OTf)_2$	none	Et_3N	MeOH	16 h	0
21	$Cu(OTf)_2$	none	Et_3N	THF	16 h	25
22	$Cu(OTf)_2$	none	Et_3N	MeCN	16 h	12
23	$Cu(OTf)_2$	none	Et_3N	DMF	16 h	14
24	$Cu(OTf)_2$	none	Et_3N	NMP	16 h	14
25	$Cu(OTf)_2$	none	Et_3N	DMA	16 h	16
26	$Cu(OTf)_2$	none	Et_3N	PhH	16 h	11

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard. [b] N^1,N^1,N^8,N^8-tetramethylnaphthalene-1,8-diamine. [c] 1,2-Dichloroethane

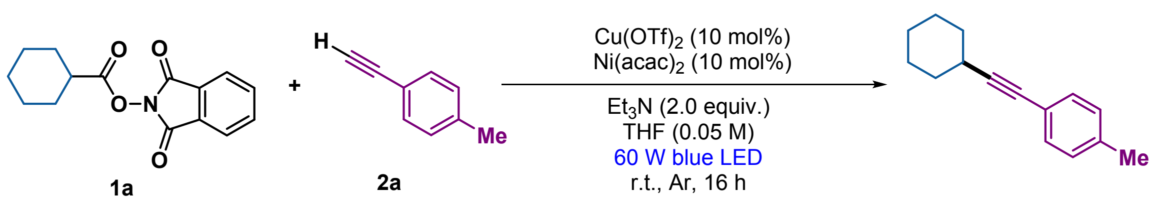
Optimization of additives



Entry	Metal salt	Yield[a] (%)
1	AgOAc	NR
2	$Fe(acac)_2$	20
3	$Ni(acac)_2$	33
4	$Mn(acac)_2$	NR
5	$Co(OAc)_2$	15
6	$Ni(OTf)_2$	15
7	$Ni(cod)_2$	< 5
8	NiI_2	12
9	$NiCl_2$•$6H_2O$	11
10	$Ni(OAc)_2$•$4H_2O$	< 5
11	$NiBr_2$•DME	14
12	$NiCl_2$•DME	11
13	$Ni(PPh_3)_2Cl_2$	0
14	$Ni(dppe)Cl_2$	0
15	$Ni(hfacac)_2$[b]	16

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard. [b] Nickel bis(hexafluoroacetylacetonate)

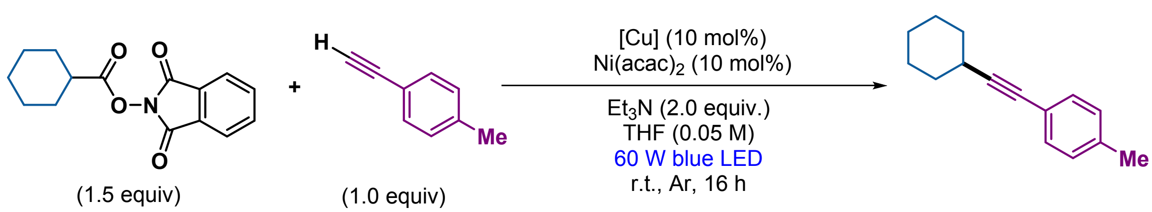
Optimization of reactant ratios



Entry	**1a** (equiv)	**2a** (equiv)	Yield[a] (%)
1	1.0	2.0	33
2	1.0	1.5	37
3	1.0	1.0	58
4	1.5	1.0	67
5	2.0	1.0	67
6	3.0	1.0	52

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard.

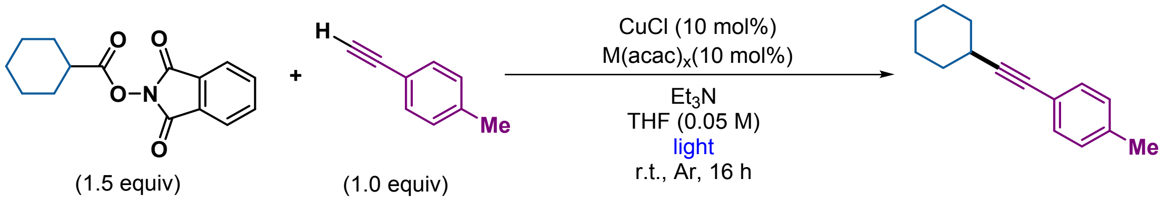
Optimization of Cu salts



Entry	[Cu]	Yield[a] (%)
1	CuOTf	58
2	$(CuOTf)_2$•PhH	41
3	$(CuOTf)_2$•$PhCH_3$	69
4	$Cu(MeCN)_4PF_6$	69
5	CuCl	72
6	CuBr	38
7	CuI	51
8	Cu_2O	NR
9	$CuSO_4$	NR
10	$Cu(OAc)_2$	NR
11	Cu powder	67

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard.

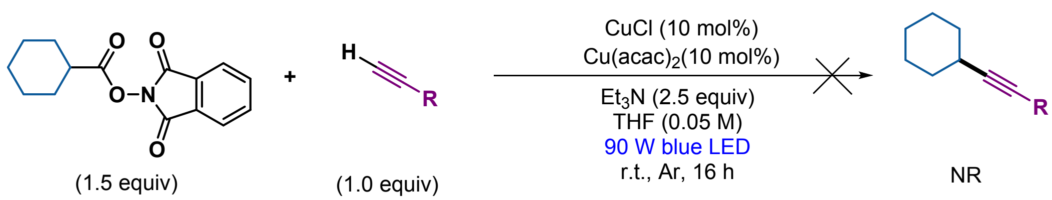
Optimization of Et_3N volume, light source and acetylacetonate



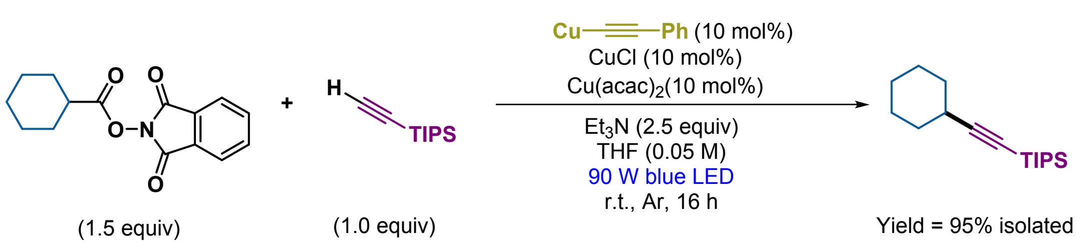
Entry	Et_3N (equiv)	Light source	$M(acac)_x$	Yield[a] (%)
1	1.0	60 W blue LED	$Ni(acac)_2$	54
2	2.5	60 W blue LED	$Ni(acac)_2$	73
3	4.0	60 W blue LED	$Ni(acac)_2$	NR
4	2.5	90 W blue LED	$Ni(acac)_2$	74
5	2.5	10 W blue LED[b]	$Ni(acac)_2$	67
6	2.5	20 W CFL	$Ni(acac)_2$	68
7	2.5	10 W UV (365 nm)	$Ni(acac)_2$	< 5
8	2.5	90 W blue LED	Li(acac)	NR
9	2.5	90 W blue LED	$Mn(acac)_2$	NR
10	2.5	90 W blue LED	$Fe(acac)_2$	12
11	2.5	90 W blue LED	$Fe(acac)_3$	13
12	2.5	90 W blue LED	$Co(acac)_2$	68
13	2.5	90 W blue LED	$Co(acac)_3$	70
14	2.5	90 W blue LED	$Cu(acac)_2$	72
15	2.5	90 W blue LED	$Zn(acac)_2$	36

[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard. [b] Light belt

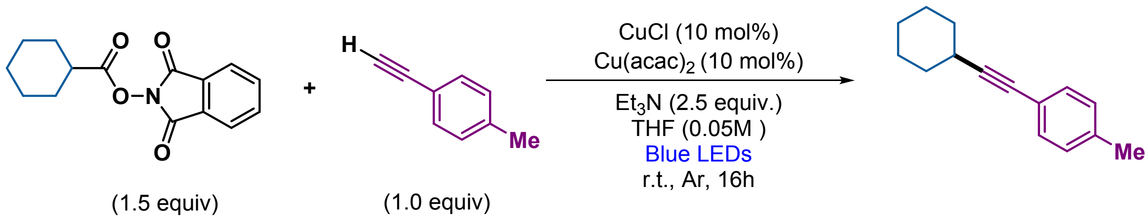
Control experiment



R = Alkyl, Silyl, Alkenyl

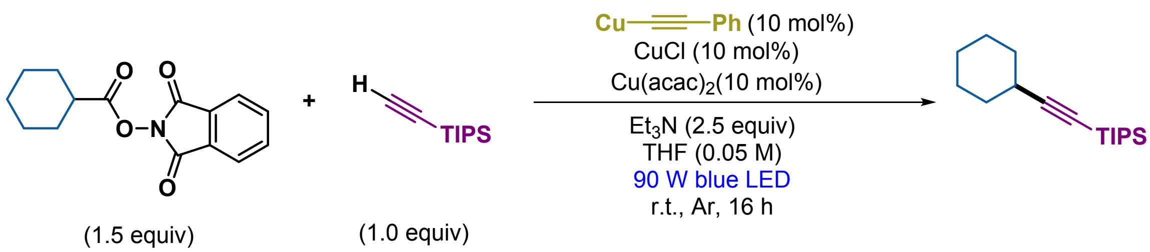


Conditional control experiment



Entry	Condition	Yield[a] (%)
1	without change	72
2	without CuCl	NR
3	without $Cu(acac)_2$	21
4	without Et_3N	NR
5	in the dark	NR
6	in the air	NR

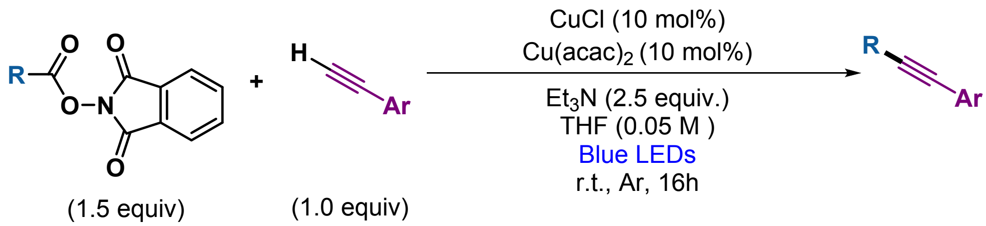
[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard.



Entry	Condition	Yield[a] (%)
1	without change	95[b]
2	without Cu—≡—Ph	NR
3	without CuCl	10
4	without $Cu(acac)_2$	5
5	without CuCl & $Cu(acac)_2$	NR
6	without Et_3N	14
7	in the dark	NR

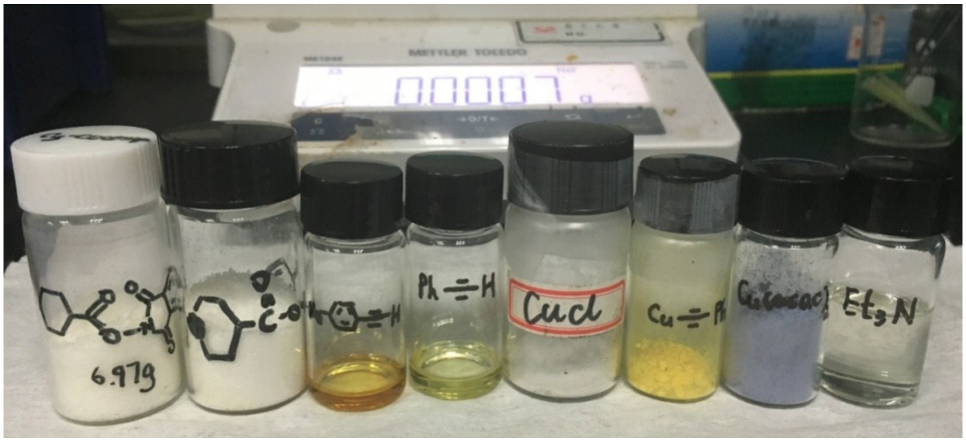
[a] Yield determined by ^{1}H NMR with Dibromomethane as an internal standard.[b] isolated yield.

Procedure for Decarboxylative Alkynylation via Aryl Alkynes (Procedure D)

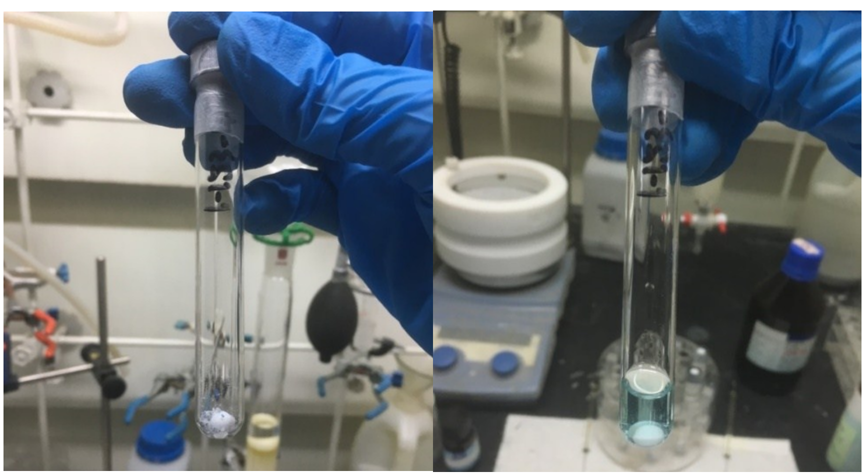


In glovebox, the redox active esters (0.1 mmol, 1.5 equiv), cuprous chloride (10 mol%), cupric acetylacetonate (10 mol%), and terminal alkyne (if solid, 0.1 mmol, 1.0 equiv) were mixed in a sealed culture tube. Then anhydrous THF (1 mL) was added. Terminal alkyne (if liquid, 0.1 mmol, 1.0 equiv), triethylamine (2.5 equiv) and anhydrous THF (1 mL) were added followed in sequence. The tube was set between two lamp (10 cm away from the lamp, 90 W each) and stirred at room temperature (with a fan to cool down the reaction) for 16 h. The solvent was removed under vacuum. The crude product was purified by column chromatography or PTLC to afford the corresponding alkyne (silica, 0 – 100% EtOAc/PE).

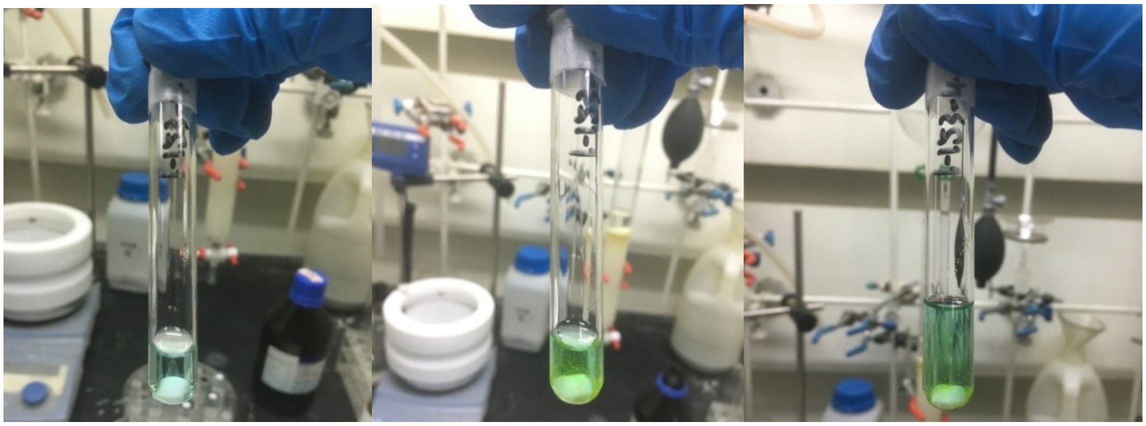
Graphical Procedure for Decarboxylative Alkynylation via Aryl Terminal Alkynes



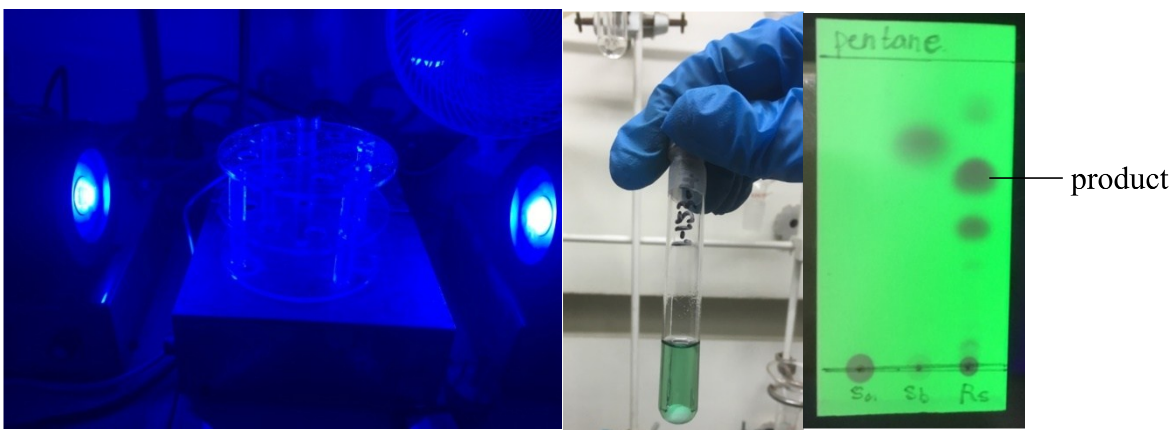
All reagents for this reaction (*From left to right*).
NHPI ester of cyclohexanecarboxylic acid (stored under air before used),
NHPI ester of tetrahydro-2H-pyran-4-carboxylic acid (stored under air before used),
4-ethynyltoluene (stored in the refrigerator, under air before used),
phenylacetylene (stored in the refrigerator, under air before used),
cuprous chloride (stored under argon before used),
copperphenylacetylide (stored under argon before used),
cupric acetylacetonate (stored under argon before used),
triethylamine (stored under air before used).



(Left) Mix cuprous chloride (1.0 mg, 0.01mmol), cupric acetylacetonate (2.6 mg, 0.01mmol), and RAEs (1,3-dioxoisoindolin-2-yl cyclohexanecarboxylate, 41.0 mg, 0.15 mmol) seal the tubein glove box and then take it out. **(Right)** After 1 mL of THF added via syringe.



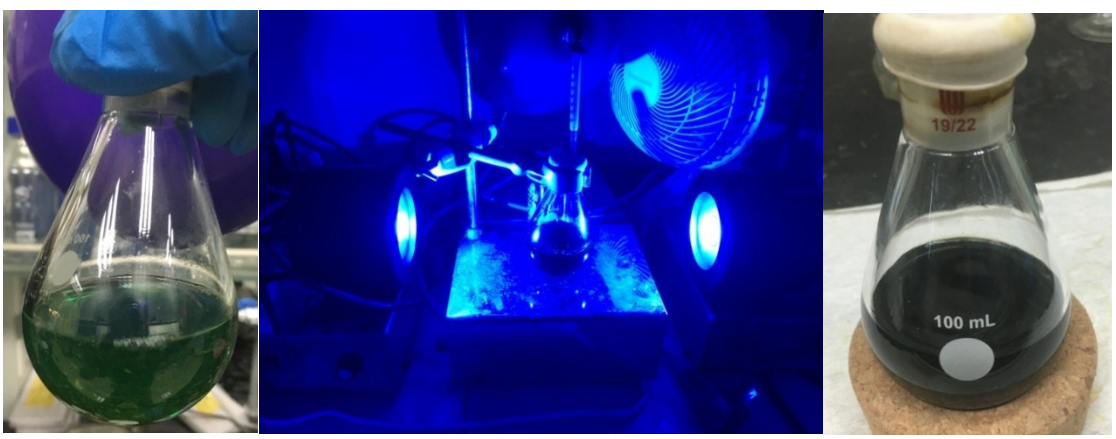
(Left) After 4-ethynyltoluene (13µL, 0.1 mmol) added via microsyringe. **(Center)** After triethylamine (35µL, 0.25 mmol) added via syringe. **(Right)** After another 1mL of THF added via syringe.



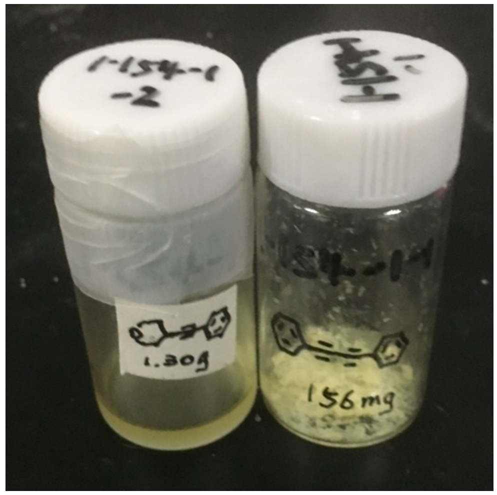
(Left) Set tube between the lamp. **(Center)** The mixture after 16 h. **(Right)** TLC result (Sa = NHPI ester, Sb = Alkynes, Rs = Reaction mixture, elute: pentane)

Graphical Supporting Information for Decarboxylative Alkynylation via Aryl Terminal Alkynes (Gram Scale)

(Left) Mix cuprous chloride (99 mg, 1 mmol), cupric acetylacetonate (260 mg, 1 mmol), and RAEs (1,3-dioxoisoindolin-2-yl tetrahydro-2H-pyran-4-carboxylate, 4.1 g, 15 mmol) seal the flaskin glove box and then take it out. **(Center)** After 50 mL of THF (0.2 M) added via syringe. **(Right)** After phenylacetylene (1.1 mL, 10 mmol) added via syringe.

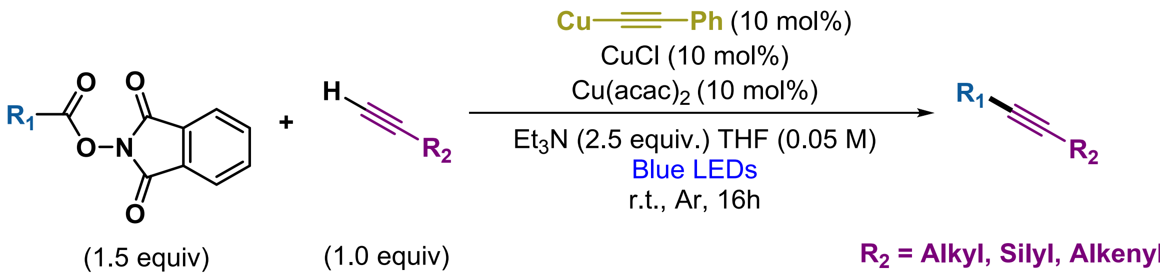


(Left) After triethylamine (3.5 mL, 25 mmol) added via syringe. **(Center)** Set the flask between the lamp **(Right)** The mixture after 16 h.



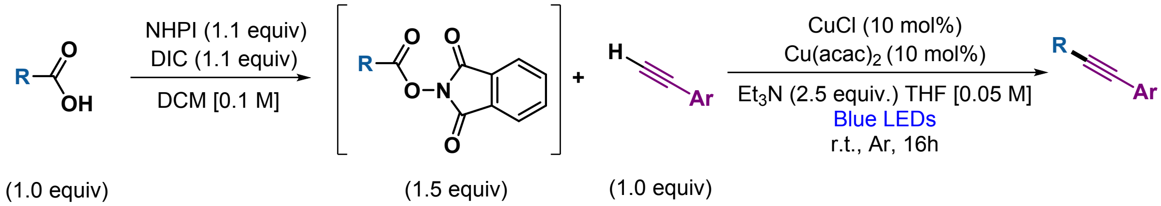
The products after purification.

Procedure for Decarboxylative Alkynylation via Non-aryl Alkynes (Procedure E)



In glovebox, the alkyl redox active esters (1.5 equiv), cuprous chloride (10 mol%), cupric acetylacetonate (10 mol%), copperphenylacetylide (10 mol%) and terminal alkyne (if solid, 1.0 equiv) were mixed in a sealed culture tube. Then anhydrous THF (1 mL) was added. Terminal alkyne (if liquid, 1.0 equiv), triethylamine (2.5 equiv) and anhydrous THF (1 mL) were added followed in sequence. The tube was set between two lamp (10 cm away from the lamp, 90 W each) and stirred at room temperature (with a fan to cool down the reaction) for 16 h. The solvent was removed under vacuum. The crude product was purified by column chromatography or PTLC to afford the corresponding alkyne.

Procedure for *in situ* Activation of Carboxylic Acids in Decarboxylative Alkynylation (Procedure F)



A culture tube was charged with carboxylic acid (0.15mmol, 1 equiv) and N-hydroxyphthalimide (0.165mmol, 1.1equiv). Dichloromethane was added (1.5 mL, 0.1M), and the mixture was stirred vigorously. Then, N,N'-Diisopropylcarbodiimide (DIC, 0.165mmol, 1.1 equiv) was added dropwise via syringe, and the mixture was allowed to stir until the acid was consumed (determined by TLC). After consumption of all starting material, the solvent was removed on a rotary evaporator at 35 °C under reduced pressure and dried on a high-vacuum line for at least 5 minutes to remove residual CH_2Cl_2. Next, the tube was moved into glovebox. Cuprous chloride (0.01 mmol, 10 mol%), cupric acetylacetonate (0.01 mmol, 10 mol%), and terminal alkyne (if solid, 0.1 mmol, 1.0 equiv) were mixed in a sealed tube. Then anhydrous THF (1 mL) was added. Terminal alkyne (if liquid, 0.1 mmol, 1.0 equiv), triethylamine (0.25 mmol, 2.5 equiv) and anhydrous THF (1 mL) were added followed in sequence. The tube was set between two lamp (10 cm away from the lamp, 90 W each) and stirred at room temperature (with a fan to cool down the reaction) for 16 h. The solvent was removed under vacuum. The crude product was purified by column chromatography or PTLC to afford the corresponding alkyne.

Characterization Data for Products

Compound 3

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 13.7 mg (69%) of the title compound **3**.

Physical State: colorless oil.

R_f = 0.71 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.30 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.8 Hz, 2H), 2.63 – 2.53 (m, 1H), 2.33 (s, 3H), 1.95 – 1.83 (m, 2H), 1.82 – 1.71 (m, 2H), 1.62 – 1.46 (m, 3H), 1.43 – 1.28 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ137.4, 131.6, 129.0, 121.2, 93.8, 80.6, 32.9, 29.8, 26.1, 25.1, 21.5 ppm.

This compound was previously reported.[8]

Compound 4

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 13.1 mg (71%) of the title compound **4**.

Physical State: colorless oil.

R_f = 0.70 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.27 (d, J = 8.1 Hz, 2H), 7.07 (d, J = 7.5 Hz, 2H), 2.81 (p, J = 7.5 Hz, 1H), 2.32 (s, 3H), 2.04 – 1.94 (m, 2H), 1.83 – 1.57 (m, 6H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ137.4, 131.5, 129.0, 121.2, 93.9, 80.2, 34.1, 30.9, 25.2, 21.5 ppm.

This compound was previously reported.[9]

Compound 5

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 10.0 mg (59%) of the title compound **5**.

Physical State: colorless oil.

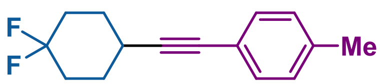
R_f = 0.70 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.29 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.8 Hz, 2H), 3.29 – 3.16 (m, 1H), 2.33 (s, 3H), 2.22 (pd, J = 9.5, 1.5 Hz, 2H), 2.02 – 1.88 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ137.6, 131.5, 129.1, 121.0, 93.3, 81.3, 30.3, 25.7, 21.6, 19.3 ppm.

HRMS (EI): calculated for $C_{13}H_{14}$ [M]:170.1096, found:170.1100.

Compound 6



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 17.3 mg (74%) of the title compound **6**.

Physical State: colorless oil.

R_f = 0.69 (pentane).

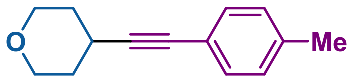
^{1}H NMR (400 MHz, CDCl$_3$): δ7.29 (d, J = 8.1 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 2.84 – 2.76 (m, 1H), 2.34 (s, 3H), 2.26 – 2.08 (m, 2H), 2.00 – 1.81 (m, 6H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ138.0, 131.6, 129.1, 123.1, 90.4, 82.0, 31.8 (t, J = 24.2 Hz), 28.7 (t, J = 5.0 Hz), 27.3, 21.6 ppm.

^{19}F NMR (471 MHz, CDCl$_3$): δ-96.4 (dd, J = 1109.3, 221.9 Hz) ppm.

HRMS (EI-TOF): calculated for $C_{15}H_{16}F_2$ [M]:234.1220, found:234.1223.

Compound 7



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 15.2 mg (76%) of the title compound **7**.

Physical State: colorless oil.

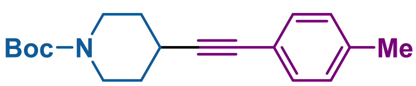
R_f = 0.45 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.30 (d, *J* = 8.1 Hz, 2H), 7.10 (d, *J* = 7.8 Hz, 2H), 3.95 (ddd, *J* = 11.6, 5.6, 3.7 Hz, 2H), 3.55 (ddd, *J* = 11.6, 8.5, 3.0 Hz, 2H), 2.84 (dt, *J* = 8.6, 4.4 Hz, 1H), 2.34 (s, 3H), 1.97 – 1.85 (m, 2H), 1.81 – 1.69 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ137.9, 131.6, 129.1, 120.6, 91.5, 81.7, 66.5, 32.5, 26.9, 21.6 ppm.

HRMS (ESI-TOF): calculated for $C_{14}H_{16}O$ $[M+H]^+$: 201.1274, found: 201.1239.

Compound 8



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 22.2mg (74%) of the title compound **8**.

Physical State: colorless oil.

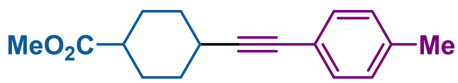
R_f = 0.25 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.28 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 7.8 Hz, 2H), 3.78 – 3.67 (m, 2H), 3.24 (ddd, *J* = 13.4, 8.3, 3.4 Hz, 2H), 2.78 (tt, *J* = 7.9, 3.9 Hz, 1H), 2.33 (s, 3H), 1.90 – 1.79 (m, 2H), 1.72 – 1.61 (m, 2H), 1.46 (s, 9H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ154.9, 137.9, 131.6, 129.1, 120.6, 91.1, 82.1, 79.6, 42.7, 42.0, 31.6, 28.6, 27.7, 21.5 ppm.

HRMS (ESI-TOF): calculated for $C_{19}H_{25}NO_2$ $[M+H]^+$:300.1958, found: 300.1957.

Compound 9



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (50:1 pentane:EtOAc) afforded 16.5 mg (64%, dr = 1 : 1.5) of the title compound **9**.

Physical State: colorless oil.

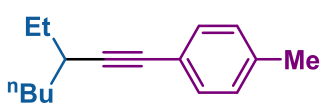
R_f = 0.38 (20:1 pentane:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ7.34 – 7.24 (2H), 7.12 – 7.04 (2H), 3.75 –3.62 (3H), 2.94 – 2.85, 2.52 – 2.42, 2.39 – 2.26, 2.15 – 1.76, 1.69 – 1.43 ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ176.2, 176.0, 137.7, 137.6, 131.6, 131.5, 129.0, 129.0, 120.9, 120.8, 92.8, 91.9, 82.1, 80.7, 51.7, 51.7, 42.3, 32.0, 30.3, 29.6, 28.2, 27.6, 25.2, 21.5 ppm.

HRMS (EI-TOF): calculated for $C_{17}H_{20}O_2$ [M]:256.1463, found:256.1465.

Compound 10



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 12.2 mg (57%) of the title compound **10**.

Physical State: colorless oil.

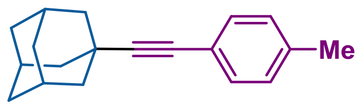
R_f = 0.69 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.29 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 2.50 – 2.41 (m, 1H), 2.33 (s, 3H), 1.64 – 1.45 (m, 5H), 1.45 – 1.28 (m, 3H), 1.05 (t, J = 7.4 Hz, 3H), 0.92 (t, J = 7.2 Hz, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ137.4, 131.6, 129.0, 121.3, 93.1, 81.9, 34.7, 34.1, 29.9, 28.4, 22.8, 21.5, 14.3, 12.1 ppm.

HRMS (EI-TOF): calculated for $C_{16}H_{22}$ [M]:214.1722, found:214.1727.

Compound 11



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 6.5 mg (26%) of the title compound **11**.

Physical State: white solid.

m.p.:85 - 88°C

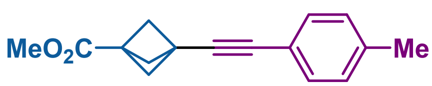
R_f= 0.72 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.27 (d, J = 8.4 Hz, 2H), 7.06 (d, J = 7.9 Hz, 2H), 2.32 (s, 3H), 2.02 – 1.97 (m, 3H), 1.95 (d, J = 2.8 Hz, 6H), 1.72 (t, J = 6.3, 2.9 Hz, 6H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ137.3, 131.5, 128.8, 121.0, 97.6, 79.3, 42.9, 36.4, 28.1, 21.4 ppm.

HRMS (ESI-TOF): calculated for $C_{19}H_{22}$ $[M+H]^+$: 251.1794, found: 251.1795.

Compound 12



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 20.2 mg (84%) of the title compound **12**.

Physical State: white solid.

m.p.:102 - 104 °C

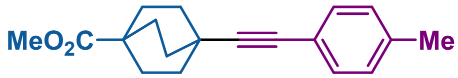
R_f= 0.35 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.30 (d, J = 8.1 Hz, 2H), 7.09 (d, J = 8.4 Hz, 2H), 3.68 (s, 3H), 2.39 (s, 6H), 2.33 (s, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ170.0, 138.4, 131.8, 129.1, 119.7, 87.0, 80.8, 56.0, 51.9, 39.9, 29.1, 21.6 ppm.

HRMS (ESI-TOF): calculated for $C_{16}H_{16}O_2$ $[M+Na]^+$: 263.1043, found: 263.1039.

Compound 13



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 14.7 mg (52%) of the title compound **13**.

Physical State: white solid.

m.p.:74 - 76 °C

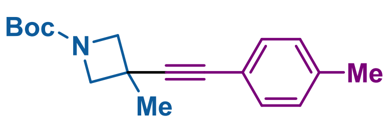
R_f= 0.37 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.25 (d, *J* = 7.7 Hz, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 3.65 (s, 3H), 2.32 (s, 3H), 1.91 – 1.77 (m, 12H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ178.2, 137.6, 131.6, 129.0, 120.8, 95.6, 80.8, 51.9, 38.2, 31.8, 28.1, 21.5 ppm.

HRMS (ESI-TOF): calculated for $C_{19}H_{22}O_2$ $[M+H]^+$: 283.1693, found: 283.1690.

Compound 14



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (10:1 pentane:EtOAc) afforded 16.3 mg (57%) of the title compound **14**.

Physical State: white solid.

m.p.:67 - 69 °C

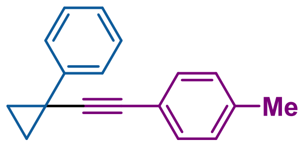
R_f= 0.41 (10:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.29 (d, *J* = 8.2 Hz, 2H), 7.10 (d, *J* = 7.7 Hz, 2H), 4.15 (d, *J* = 8.0 Hz, 2H), 3.79 (d, *J* = 8.0 Hz, 2H), 2.34 (s, 3H), 1.61 (s, 3H), 1.45 (s, 9H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ156.5, 138.3, 131.6, 129.2, 120.0, 92.3, 82.9, 79.8, 62.5, 61.8, 28.5, 26.7, 21.6 ppm.

HRMS (ESI-TOF): calculated for $C_{18}H_{23}NO_2$ $[M+H]^+$: 286.1802, found: 286.1803.

Compound 15



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 15.1 mg (65%) of the title compound **15**.

Physical State: colorless oil.

$\boldsymbol{R_f}$= 0.45 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.44 – 7.38 (m, 2H), 7.36 – 7.29 (m, 4H), 7.20 (tt, *J* = 6.6, 1.2 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 2H), 2.34 (s, 3H), 1.54 (q, *J* = 4.1, 3.6 Hz, 2H), 1.36 – 1.31 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ137.8, 135.0, 131.7, 129.1, 128.5, 126.1, 125.6, 124.2, 93.1, 78.6, 21.6, 20.7, 16.4 ppm.

HRMS (ESI-TOF): calculated for $C_{18}H_{16}$ $[M+H]^+$: 233.1325, found: 233.1323.

Compound 16

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (50:1 pentane:EtOAc) afforded 6.5 mg (35%) of the title compound **16**.

Physical State: colorless oil.

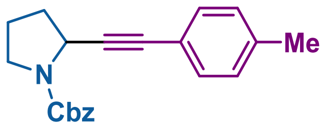
$\boldsymbol{R_f}$= 0.28 (50:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.32 (d, *J* = 8.2 Hz, 2H), 7.10 (d, *J* = 7.8 Hz, 2H), 4.80 (dd, *J* = 7.2, 5.0 Hz, 1H), 4.05 – 3.97 (m, 1H), 3.89 – 3.82 (m, 1H), 2.34 (s, 3H), 2.30 – 2.16 (m, 1H), 2.15 – 1.87 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ138.5, 131.7, 129.1, 119.8, 88.5, 84.7, 68.8, 68.1, 33.6, 25.7, 21.6 ppm.

This compound was previously reported.[10]

Compound 17



Following **Procedure D** on 0.30 mmol scale. Purification by PTLC (10:1 pentane:EtOAc) afforded 32.5 mg (34%) of the title compound **17**.

Physical State: colorless oil.

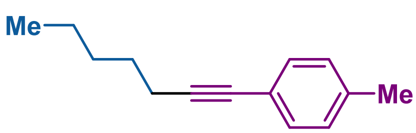
R_f= 0.31 (10:1 pentane:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ7.54 – 7.00 (m, 9H), 5.43 – 5.01 (m, 2H), 4.95 – 4.70 (m, 1H), 3.74 – 3.31 (m, 2H), 2.35 (s, 3H), 2.27 – 1.76 (m, 4H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ154.7, 138.6, 137.1, 131.8, 131.7, 129.1, 128.5, 128.1, 127.8, 127.7, 126.4, 120.0, 88.8, 88.5, 82.5, 66.9, 66.8, 49.3, 48.9, 46.3, 45.9, 34.1, 33.4, 24.7, 23.9, 21.6, 21.3 ppm.

HRMS (ESI-TOF): calculated for $C_{21}H_{21}NO_2$ $[M+H]^+$: 320.1645, found: 320.1644.

Compound 18



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 10.4 mg (56%) of the title compound **18**.

Physical State: colorless oil.

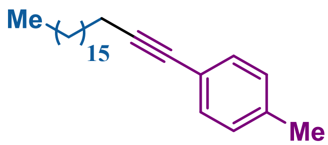
R_f= 0.71 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.28 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 2.39 (t, J = 7.1 Hz, 2H), 2.33 (s, 3H), 1.66 – 1.56 (m, 2H), 1.49 – 1.29 (m, 4H), 0.92 (t, J = 7.1 Hz, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ137.5, 131.5, 129.1, 121.1, 89.8, 80.7, 31.3, 28.7, 22.4, 21.5, 19.6, 14.2 ppm.

This compound was previously reported.[9]

Compound 19



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 16.6 mg (47%) of the title compound **19**.

Physical State: white solid.

m.p.:31 - 32 °C

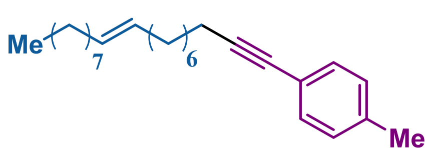
R_f= 0.71 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.28 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.8 Hz, 2H), 2.39 (t, J = 7.1 Hz, 2H), 2.33 (s, 3H), 1.65 – 1.55 (m, 2H), 1.44 (t, J = 7.5 Hz, 2H), 1.26 (s, 26H), 0.92 – 0.84 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ137.5, 131.5, 129.1, 121.1, 89.8, 80.7, 30.0 – 29.8 (m), 29.7, 29.5, 29.3, 29.1, 29.0 ppm.

HRMS (ESI-TOF): calculated for $C_{26}H_{42}$ [M+Na]$^+$: 377.3179, found: 377.3155.

Compound 20



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 16.2 mg (46%) of the title compound **20**.

Physical State: colorless oil.

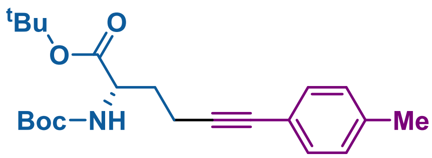
R_f= 0.68 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.28 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 5.41 – 5.30 (m, 2H), 2.39 (t, J = 7.1 Hz, 2H), 2.33 (s, 3H), 2.08 – 1.95 (m, 4H), 1.45 (dt, J = 13.5, 4.8 Hz, 2H), 1.39 – 1.21 (m, 20H), 0.88 (t, J = 6.6 Hz, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ137.5, 131.5, 130.1, 129.9, 129.1, 121.1, 89.8, 80.7, 32.1, 29.9, 29.9, 29.7, 29.5, 29.3, 29.2, 29.1, 29.0, 27.4, 27.3, 22.8, 21.5, 19.6, 14.3 ppm.

HRMS (ESI-TOF): calculated for $C_{26}H_{40}$ $[M+Na]^+$: 375.3022, found: 375.2985.

Compound 21



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 15.3 mg (41%) of the title compound **21**.

Physical State: colorless oil.

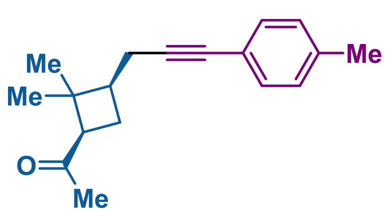
***R*$_f$**= 0.27 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.29 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 2H), 5.19 (d, *J* = 8.3 Hz, 1H), 4.28 (q, *J* = 7.3 Hz, 1H), 2.54 – 2.38 (m, 2H), 2.33 (s, 3H), 2.19 – 2.07 (m, 1H), 2.00 – 1.85 (m, 1H), 1.47 (s, 9H), 1.44 (s, 9H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ171.5, 155.5, 137.9, 131.6, 129.1, 120.6, 88.1, 82.2, 81.4, 79.9, 53.8, 32.2, 28.5, 28.2, 21.6, 16.1 ppm.

HRMS (ESI-TOF): calculated for $C_{22}H_{31}NO_4$ $[M+H]^+$: 374.2326, found: 374.2324.

Compound 22



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 8.9 mg (35%) of the title compound **22**.

Physical State: colorless oil.

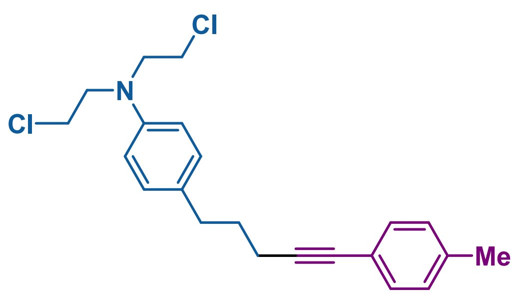
***R**$_f$*= 0.40 (20:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.25 (d, J = 7.1 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 2.86 (dd, J = 10.1, 7.5 Hz, 1H), 2.39 – 2.19 (m, 6H), 2.05 (s, 3H), 2.03 – 1.87 (m, 2H), 1.40 (s, 3H), 0.98 (s, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ207.9, 137.7, 131.4, 129.1, 120.9, 87.8, 81.2, 54.3, 43.6, 41.2, 30.8, 30.4, 23.3, 21.5, 20.4, 16.9 ppm.

HRMS (ESI-TOF): calculated for $C_{18}H_{22}O$ $[M+H]^+$: 255.1743, found: 255.1745.

Compound 23



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (40:1 pentane:EtOAc) afforded 17.9 mg (48%) of the title compound **23**.

Physical State: pale yellow oil.

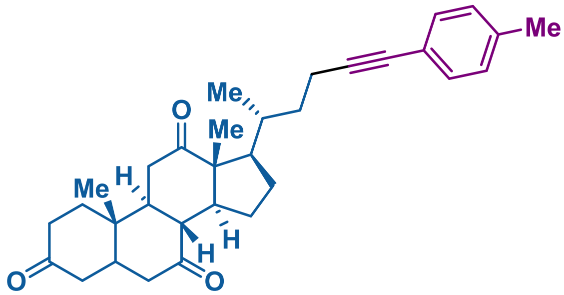
***R**$_f$*= 0.26 (40:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.30 (d, *J* = 8.1 Hz, 2H), 7.11 (t, *J* = 8.6 Hz, 4H), 6.64 (d, *J* = 8.7 Hz, 2H), 3.75 – 3.66 (m, 4H), 3.67 – 3.58 (m, 4H), 2.70 (t, *J* = 7.5 Hz, 2H), 2.41 (t, *J* = 7.0 Hz, 2H), 2.34 (s, 3H), 1.87 (p, *J* = 7.2 Hz, 2H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ144.4, 137.6, 131.5, 131.0, 129.9, 129.1, 121.0, 112.3, 89.3, 81.2, 53.8, 40.7, 33.8, 30.7, 21.6, 18.9 ppm.

HRMS (ESI-TOF): calculated for $C_{22}H_{25}Cl_2N$ $[M+H]^+$: 374.1437, found: 374.1439.

Compound 24



Following **Procedure D** on 0.20 mmol scale. Purification by PTLC (5:1 pentane:EtOAc) afforded 60.1 mg (64%) of the title compound **24**.

Physical State:white solid.

m.p.:208 - 210 °C

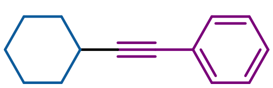
$\boldsymbol{R_f}$= 0.26 (5:1 pentane:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ7.27 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 7.9 Hz, 2H), 2.95 – 2.81 (m, 3H), 2.48 (ddd, J = 16.7, 8.5, 4.6 Hz, 1H), 2.39 – 2.18 (m, 10H), 2.18 – 2.11 (m, 2H), 2.12 – 1.99 (m, 3H), 1.97 (ddd, J = 14.6, 5.3, 3.1 Hz, 1H), 1.86 (td, J = 11.5, 7.2 Hz, 1H), 1.84 – 1.74 (m, 1H), 1.67 – 1.56 (m, 1H), 1.50 – 1.31 (m, 7H), 1.09 (s, 3H), 0.89 (d, J = 6.4 Hz, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ212.1, 209.2, 208.9, 137.6, 131.5, 129.1, 121.1, 89.8, 80.7, 57.1, 51.9, 49.2, 47.0, 45.9, 45.7, 45.1, 42.9, 38.8, 36.6, 36.2, 35.5, 35.4, 34.7, 29.8, 27.9, 25.3, 22.1, 21.5, 18.8, 17.1, 12.0 ppm.

HRMS (ESI-TOF): calculated for $C_{32}H_{40}O_3$ $[M+H]^+$: 473.3050, found: 473.3051.

Compound 25



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 11.2 mg (60%) of the title compound **25**.

Physical State: colorless oil.

$\boldsymbol{R_f}$= 0.73 (pentane).

^{1}**H NMR (400 MHz, CDCl$_3$):** δ7.42 – 7.35 (m, 2H), 7.30 – 7.20 (m, 3H), 2.58 (tt, *J* = 9.2, 3.8 Hz, 1H), 1.95 – 1.83 (m, 2H), 1.81 – 1.71 (m, 2H), 1.60 – 1.49 (m, 3H), 1.39 – 1.28 (m, 3H) ppm.

^{13}**C NMR (101 MHz, CDCl$_3$):** δ131.7, 128.3, 127.5, 124.2, 94.6, 80.6, 32.9, 29.8, 26.1, 25.1 ppm.

This compound was previously reported.[11]

Compound 26

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (50:1 pentane:EtOAc) afforded 14.5 mg (68%) of the title compound **26**.

Physical State: colorless oil.

R_f = 0.38 (50:1 pentane:EtOAc).

^{1}**H NMR (500 MHz, CDCl$_3$):** δ7.33 (d, J = 8.7 Hz, 2H), 6.80 (d, J = 8.8 Hz, 2H), 3.79 (s, 3H), 2.56 (dt, J = 9.2, 5.1 Hz, 1H), 1.95 – 1.81 (m, 2H), 1.81 – 1.67 (m, 2H), 1.61 – 1.46 (m, 3H), 1.42 – 1.31 (m, 3H) ppm.

^{13}**C NMR (126 MHz, CDCl$_3$):** δ158.9, 132.9, 116.3, 113.8, 92.9, 80.1, 55.3, 32.9, 29.7, 26.0, 25.0 ppm.

This compound was previously reported.[8]

Compound 27

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (50:1 pentane:EtOAc) afforded 17.0 mg (75%) of the title compound **27**.

Physical State: white solid.

m.p.:64 - 65 °C

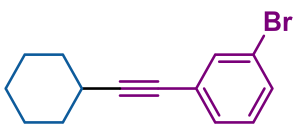
R_f = 0.32 (50:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.87 (d, J = 8.5 Hz, 2H), 7.46 (d, J = 8.5 Hz, 2H), 2.65 – 2.56 (m, 1H), 2.58 (s, 3H), 1.94 – 1.84 (m, 2H), 1.80 – 1.70 (m, 2H), 1.60 – 1.47 (m, 3H), 1.42 – 1.31 (m, 3H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ197.6, 135.7, 131.8, 129.4, 128.3, 98.5, 80.2, 32.6, 29.9, 26.7, 26.0, 25.0 ppm.

HRMS (ESI-TOF): calculated for $C_{16}H_{18}O$ $[M+H]^+$: 227.1430, found: 227.1431.

Compound 28



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 15.8 mg (60%) of the title compound **28**.

Physical State: colorless oil.

R$_f$= 0.69 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.55 (t, J = 1.8 Hz, 1H), 7.38 (dq, J = 8.0, 1.1 Hz, 1H), 7.31 (dt, J = 7.8, 1.3 Hz, 1H), 7.14 (t, J = 7.9 Hz, 1H), 2.58 (ddd, J = 12.8, 8.8, 3.6 Hz, 1H), 1.92 – 1.83 (m, 2H), 1.80 – 1.71 (m, 2H), 1.61 – 1.46 (m, 3H), 1.42 – 1.30 (m, 3H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ134.5, 130.7, 130.2, 129.7, 126.3, 122.1, 96.1, 79.3, 32.7, 29.7, 26.0, 25.0 ppm.

HRMS (EI-TOF): calculated for $C_{14}H_{15}Br$ [M]:262.0357, found:262.0362.

Compound 29

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pure pentane) afforded 12.7 mg (63%) of the title compound **29**.

Physical State: colorless oil.

R_f = 0.69 (pentane).

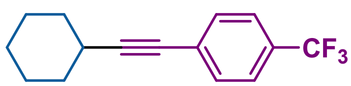
^{1}H NMR (400 MHz, CDCl$_3$): δ7.40 – 7.33 (m, 2H), 6.96 (t, *J* = 8.7 Hz, 2H), 2.56 (tt, *J* = 9.1, 3.8 Hz, 1H), 1.95 – 1.81 (m, 2H), 1.80 – 1.70 (m, 2H), 1.60 – 1.46 (m, 3H), 1.42 – 1.28 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ162.1 (d, *J* = 247.9 Hz), 133.5 (d, *J* = 8.1 Hz), 120.3 (d, *J* = 3.5 Hz), 115.5 (d, *J* = 22.0 Hz), 94.2, 79.6, 32.8, 29.9, 26.0, 25.1ppm.

^{19}F NMR (471 MHz, CDCl$_3$): δ -112.6 ppm.

This compound was previously reported.[12]

Compound 30



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 17.4 mg (69%) of the title compound **30**.

Physical State: colorless oil.

R_f = 0.65 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.53 (d, *J* = 8.3 Hz, 2H), 7.48 (d, *J* = 8.3 Hz, 2H), 2.60 (ddd, *J* = 12.8, 8.7, 3.6 Hz, 1H), 1.94 – 1.84 (m, 2H), 1.82 – 1.71 (m, 2H), 1.60 – 1.48 (m, 3H), 1.43 – 1.30 (m, 3H) ppm.

^{13}C NMR (151 MHz, CDCl$_3$): δ131.9, 129.3 (q, *J* = 32.6 Hz), 128.2, 125.2 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.1 Hz), 97.4, 79.6, 32.7, 29.8, 26.0, 25.0 ppm.

^{19}F NMR (471 MHz, CDCl$_3$): δ -62.7 ppm.

This compound was previously reported.[12]

Compound 31

Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (20:1 pentane:EtOAc) afforded 13.2 mg (63%) of the title compound **31**.

Physical State: white solid.

m.p.:48 - 50 °C

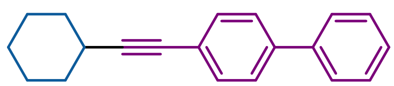
R_f= 0.37 (20:1 pentane:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ7.55 (d, J = 8.1 Hz, 2H), 7.45 (d, J = 8.1 Hz, 2H), 2.60 (dt, J = 9.3, 5.0 Hz, 1H), 1.92 – 1.83 (m, 2H), 1.79 – 1.69 (m, 2H), 1.59 – 1.47 (m, 3H), 1.41 – 1.30 (m, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ132.2, 132.0, 129.3, 118.8, 110.8, 99.7, 79.5, 32.5, 29.9, 25.9, 25.0 ppm.

HRMS (EI-TOF): calculated for $C_{15}H_{15}N$ [M]:209.1204, found:209.1196.

Compound 32



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 20.3 mg (78%) of the title compound **32**.

Physical State: colorless oil.

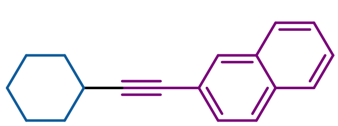
R_f= 0.70 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ7.62 – 7.56 (m, 2H), 7.56 – 7.50 (m, 2H), 7.50 – 7.41 (m, 4H), 7.38 – 7.31 (m, 1H), 2.62 (tt, J = 9.0, 3.5 Hz, 1H), 1.97 – 1.85 (m, 2H), 1.84 – 1.72 (m, 2H), 1.63 – 1.49 (m, 3H), 1.43 – 1.32 (m, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ140.7, 140.2, 132.1, 128.9, 127.6, 127.1, 127.0, 123.2, 95.3, 80.5, 32.9, 29.9, 26.1, 25.1 ppm.

This compound was previously reported.[12]

Compound 33



Following **Procedure D** on 0.10mmol scale. Purification by PTLC (pentane) afforded 12.9 mg (55%) of the title compound **33**.

Physical State: colorless oil.

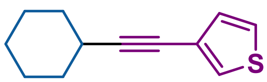
R_f= 0.69 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.94 – 7.89 (m, 1H), 7.76 (t, *J* = 8.7 Hz, 3H), 7.50 – 7.42 (m, 3H), 2.64 (tt, *J* = 9.2, 3.8 Hz, 1H), 1.99 – 1.89 (m, 2H), 1.84 – 1.75 (m, 2H), 1.64 – 1.53 (m, 3H), 1.43 – 1.34 (m, 3H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ133.2, 132.5, 131.1, 129.0, 127.9, 127.8, 127.7, 126.4, 126.3, 121.6, 95.0, 81.0, 32.9, 29.9, 26.1, 25.1 ppm.

HRMS (ESI-TOF): calculated for $C_{18}H_{18}$ $[M+H]^+$: 235.1481, found: 235.1473.

Compound 34



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (pentane) afforded 14.6 mg (77%) of the title compound **34**.

Physical State: colorless oil.

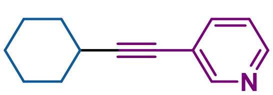
R_f= 0.67 (pentane).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.34 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.22 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.07 (dd, *J* = 5.0, 1.2 Hz, 1H), 2.55 (tt, *J* = 9.4, 3.8 Hz, 1H), 1.94 – 1.83 (m, 2H), 1.80 – 1.70 (m, 2H), 1.60 – 1.46 (m, 3H), 1.41 – 1.29 (m, 3H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ130.2, 127.5, 125.0, 123.2, 94.1, 75.5, 32.9, 29.8, 26.1, 25.1 ppm.

HRMS (ESI-TOF): calculated for $C_{12}H_{14}S$ $[M+H]^+$: 191.0889, found: 191.0852.

Compound 35



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (5:1 pentane:EtOAc) afforded 10.4 mg (56%) of the title compound **35**.

Physical State: colorless oil.

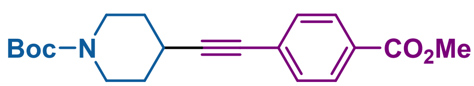
***R**$_f$*= 0.29 (5:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ8.64 (s, 1H), 8.49 (s, 1H), 7.67 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.21 (dd, *J* = 8.0, 4.8 Hz, 1H), 2.65 – 2.56 (m, 1H), 1.93 – 1.84 (m, 2H), 1.80 – 1.69 (m, 2H), 1.61 – 1.48 (m, 3H), 1.42 – 1.30 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl3): δ 152.5, 147.9, 138.6, 123.1, 121.6, 98.2, 76.9, 32.7, 29.8, 26.0, 25.0 ppm**.**

HRMS (ESI-TOF): calculated for $C_{13}H_{15}N$ $[M+H]^+$: 186.1277, found: 186.1276.

Compound 36



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (10:1 pentane:EtOAc) afforded 21.9 mg (64%) of the title compound **36**.

Physical State: colorless oil.

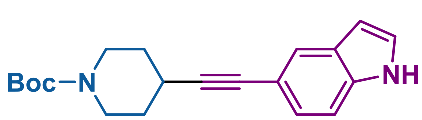
***R**$_f$*= 0.33 (10:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.95 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 3.91 (s, 3H), 3.79 – 3.68 (m, 2H), 3.28 – 3.19 (m, 2H), 2.86 – 2.76 (m, 1H), 1.92 – 1.81 (m, 2H), 1.74 – 1.60 (m, 2H), 1.46 (s, 9H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ166.7, 154.9, 132.6, 131.7, 129.5, 128.5, 95.3, 81.5, 79.7, 52.3, 42.8, 42.1, 31.4, 28.6, 27.8 ppm.

HRMS (ESI-TOF): calculated for $C_{20}H_{25}NO_4$ $[M+H]^+$: 344.1856, found: 344.1858.

Compound 37



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (5:1 pentane:EtOAc) afforded 21.6 mg (67%) of the title compound **37**.

Physical State: brown oil.

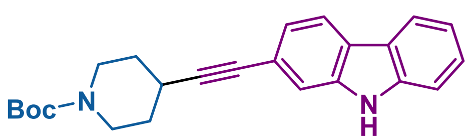
R_f= 0.25 (5:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ8.45 (s, 1H), 7.73 (dt, *J* = 1.6, 0.8 Hz, 1H), 7.30 (dt, *J* = 8.4, 0.9 Hz, 1H), 7.23 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.20 (dd, *J* = 3.2, 2.4 Hz, 1H), 6.50 (ddd, *J* = 3.1, 2.0, 0.9 Hz, 1H), 3.81 – 3.71 (m, 2H), 3.28 (ddd, *J* = 13.4, 8.2, 3.4 Hz, 2H), 2.82 (tt, *J* = 7.9, 4.0 Hz, 1H), 1.94 – 1.81 (m, 2H), 1.78 – 1.63 (m, 2H), 1.48 (s, 9H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ155.0, 135.3, 127.8, 125.7, 125.1, 124.5, 114.7, 111.1, 102.7, 89.0, 83.4, 79.6, 42.8,42.1, 31.8, 28.6, 27.7 ppm.

HRMS (ESI-TOF): calculated for $C_{20}H_{24}N_2O_2$ $[M+H]^+$: 325.1911, found: 325.1913.

Compound 38



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (5:1 pentane:EtOAc) afforded 22.7 mg (61%) of the title compound **38**.

Physical State: yellow solid.

m.p.:170 - 172 °C

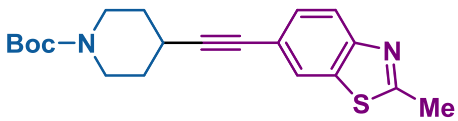
R_f= 0.31 (5:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ8.12 (s, 1H), 8.04 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.48 (s, 1H), 7.45 – 7.39 (m, 2H), 7.28 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.23 (td, *J* = 4.8, 2.3 Hz, 1H), 3.85 – 3.72 (m, 2H), 3.28 (ddd, *J* = 13.4, 8.3, 3.4 Hz, 2H), 2.85 (tt, *J* = 8.0, 4.0 Hz, 1H), 1.96 – 1.84 (m, 2H), 1.80 – 1.67 (m, 2H), 1.48 (s, 9H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ155.0, 140.1, 139.2, 126.3, 123.4, 123.2, 120.7, 120.6, 120.3, 119.8, 113.9, 110.8, 91.4, 83.1, 79.7, 42.8,42.0, 31.7, 28.6, 27.8 ppm.

HRMS (ESI-TOF): calculated for $C_{24}H_{26}N_2O_2$ $[M+H]^+$: 375.2067, found: 375.2069.

Compound 39



Following **Procedure D** on 0.10 mmol scale. Purification by PTLC (5:1 pentane:EtOAc) afforded 24.7 mg (67%) of the title compound **39**.

Physical State: colorless oil.

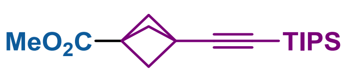
R$_f$= 0.43 (5:1 pentane:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.96 (d, *J* = 1.5 Hz, 1H), 7.72 (d, *J* = 8.3 Hz, 1H), 7.37 (dd, *J* = 8.3, 1.5 Hz, 1H), 3.84 – 3.69 (m, 2H), 3.25 (ddd, *J* = 13.4, 8.5, 3.4 Hz, 2H), 2.88 – 2.77 (m, 1H), 2.83 (s, 3H), 1.94 – 1.78 (m, 2H), 1.76 – 1.64 (m, 2H), 1.47 (s, 9H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ154.8, 134.0, 128.1, 125.4, 123.2, 121.3, 121.2, 92.0, 81.7, 79.5, 42.7,41.7, 31.4, 28.5, 27.7, 20.2 ppm.

HRMS (ESI-TOF): calculated for $C_{20}H_{24}N_2O_2S$ [M+H]$^+$: 357.1631, found: 357.1632.

Compound 40



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 18.3 mg (60%) of the title compound **40**.

Physical State: white solid.

m.p.:82-85 °C

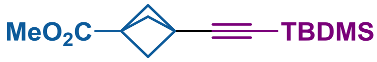
R$_f$= 0.40 (20:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, CDCl$_3$): δ3.66 (s, 3H), 2.30 (s, 6H), 1.12 – 0.90 (m, 21H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ170.1, 106.1, 81.5, 56.1, 51.8, 39.6, 29.0, 18.7, 11.3ppm.

HRMS (ESI-TOF): calculated for $C_{18}H_{30}O_2Si$ [M+H]$^+$: 307.2088, found: 307.2084.

Compound 41



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (40:1 petroleum ether:EtOAc) afforded 17.5 mg (66%) of the title compound **41**.

Physical State: white solid.

m.p.:85-86 °C

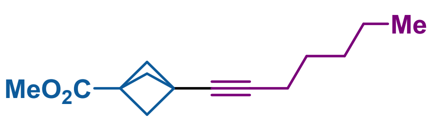
***R**$_f$*= 0.24 (40:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ3.66 (s, 3H), 2.30 (s, 6H), 0.91 (s, 9H), 0.08 (s, 6H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ170.0, 104.8, 83.6, 56.0, 51.8, 39.6, 28.9, 26.2, 16.6, -4.4ppm.

HRMS (ESI-TOF): calculated for $C_{15}H_{24}O_2Si$ [M+H]$^+$: 265.1618, found: 265.1615.

Compound 42



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 21.6 mg (98%) of the title compound **42**.

Physical State: white solid.

m.p.:75-76 °C

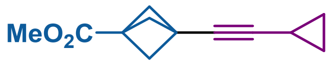
***R**$_f$*= 0.39 (20:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, CDCl$_3$): δ3.65 (s, 3H), 2.26 (s, 6H), 2.14 (t, J = 7.3 Hz, 2H), 1.47 (td, J = 9.2, 8.3, 6.2 Hz, 2H), 1.37 – 1.25 (m, 4H), 0.89 (t, J = 7.1 Hz, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ170.1, 81.5, 78.4, 55.9, 51.8, 39.5, 31.2, 28.8, 28.6, 22.3, 18.9, 14.1ppm.

HRMS (ESI-TOF): calculated for $C_{14}H_{20}O_2$ [M+H]$^+$: 221.1536, found: 221.1534.

Compound 43



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 18.2 mg (96%) of the title compound **43**.

Physical State: white solid.

m.p.:69-72 °C

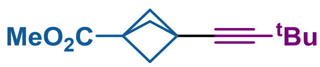
$\boldsymbol{R_f}$= 0.35 (20:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ3.65 (s, 3H), 2.25 (s, 6H), 1.21 (tt, J = 8.2, 5.0 Hz, 1H), 0.75 – 0.70 (m, 2H), 0.67 – 0.62 (m, 2H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ170.1, 84.3, 74.0, 55.9, 51.8, 39.5, 28.8, 8.3, -0.5 ppm.

HRMS (ESI-TOF): calculated for $C_{12}H_{14}O_2$ $[M+H]^+$:191.1067, found: 191.1064.

Compound 44



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 11.0 mg (53%) of the title compound **44**.

Physical State: white solid.

m.p.:75-78 °C

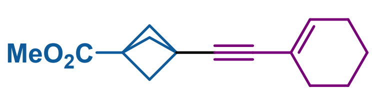
$\boldsymbol{R_f}$= 0.42 (20:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ3.66 (s, 1H), 2.25 (s, 2H), 1.18 (s, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ170.3, 89.4, 76.8, 55.9, 51.8, 39.5, 31.2, 28.8, 27.4ppm.

HRMS (ESI-TOF): calculated for $C_{13}H_{18}O_2$ $[M+H]^+$: 207.1380, found: 207.1379.

Compound 45



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography

(20:1 petroleum ether:EtOAc) afforded 11.0 mg (48%) of the title compound **45**.

Physical State: white solid.

m.p.:70-71 °C

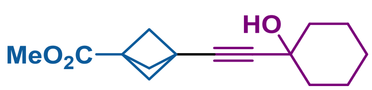
***R**f*= 0.38 (20:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ6.09 (s, 1H), 3.66 (s, 3H), 2.31 (s, 6H), 2.16 – 1.92 (m, 4H), 1.72 – 1.50 (m, 4H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ170.1, 135.5, 120.2, 85.0, 82.5, 56.0, 51.8, 39.8, 29.8, 29.3, 25.8, 22.4, 21.6ppm.

HRMS (EI-TOF): calculated for $C_{15}H_{18}O_2$ [M]:230.1307, found:230.1303.

Compound 46



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (5:1 petroleum ether:EtOAc) afforded 16.9 mg (68%) of the title compound **46**.

Physical State: white solid.

m.p.:80-83 °C

***R**f*= 0.35 (5:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ3.66 (s, 3H), 2.29 (s, 6H), 1.88 – 1.78 (m, 2H), 1.72 – 1.60 (m, 2H), 1.60 – 1.41 (m, 5H), 1.32 – 1.25 (m, 1H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ170.0, 84.2, 82.3, 68.7, 55.9, 51.9, 40.0, 39.7, 28.5, 25.3, 23.3ppm.

HRMS (ESI-TOF): calculated for $C_{15}H_{20}O_3$ $[M+H]^+$: 249.1485, found: 249.1487.

Compound 47

Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography

(pentane) afforded 25.1 mg (95%) of the title compound **47**.

Physical State: colorless oil.

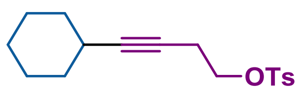
R_f= 0.92 (pentane).

^{1}H NMR (400 MHz, $CDCl_3$): δ2.46 (dt, J = 8.3, 4.6 Hz, 1H), 1.82 – 1.66 (m, 4H), 1.55 – 1.42 (m, 3H), 1.40 – 1.27 (m, 3H), 1.12 – 0.99 (m, 21H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ113.8, 79.7, 32.9, 30.0, 26.1, 24.6, 18.8, 11.4 ppm.

This compound was previously reported.[8]

Compound 48



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (10:1 petroleum ether:EtOAc) afforded 26.8 mg (88%) of the title compound **48**.

Physical State: white solid.

m.p.:58 - 61 °C

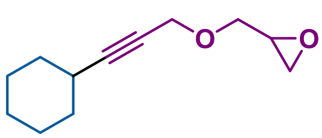
R_f= 0.33 (10:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, $CDCl_3$): δ7.80 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 4.05 (t, J = 7.3 Hz, 2H), 2.52 (td, J = 7.2, 2.2 Hz, 2H), 2.45 (s, 3H), 2.31 – 2.18 (m, 1H), 1.77 – 1.67 (m, 2H), 1.67 – 1.62 (m, 2H), 1.53 – 1.44 (m, 1H), 1.37 – 1.23 (m, 5H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ144.9, 133.1, 130.0, 128.1, 87.3, 73.8, 68.5, 32.9, 29.1, 26.0, 25.0, 21.8, 19.8 ppm.

HRMS (ESI-TOF): calculated for $C_{17}H_{22}O_3S$ $[M+Na]^+$: 329.1182, found: 329.1179.

Compound 49



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography

(20:1 petroleum ether:EtOAc) afforded 13.5 mg (69%) of the title compound **49**.

Physical State: colorless oil.

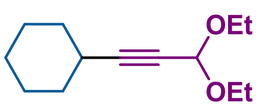
R$_f$= 0.30 (20:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ4.29 – 4.12 (m, 2H), 3.77 (dd, J = 11.3, 3.3 Hz, 1H), 3.48 (dd, J = 11.3, 5.7 Hz, 1H), 3.17 (ddt, J = 5.9, 4.1, 3.0 Hz, 1H), 2.81 (dd, J = 5.0, 4.1 Hz, 1H), 2.63 (dd, J = 5.0, 2.7 Hz, 1H), 2.40 (dddd, J = 13.2, 9.6, 3.7, 1.8 Hz, 1H), 1.79 (dq, J = 12.0, 3.4 Hz, 2H), 1.68 (tdd, J = 8.4, 4.7, 2.1 Hz, 2H), 1.57 – 1.46 (m, 1H), 1.49 – 1.35 (m, 2H), 1.37 – 1.24 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ91.8, 75.4, 70.2, 59.2, 50.7, 44.7, 32.7, 29.2, 26.0, 25.0 ppm.

HRMS (ESI-TOF): calculated for $C_{12}H_{18}O_2$ $[M+Na]^+$: 217.1199, found: 217.1194.

Compound 50



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 19.9 mg (95%) of the title compound **50**.

Physical State: colorless oil.

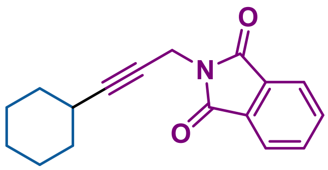
R$_f$= 0.35 (20:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, CDCl$_3$): δ5.26 (d, J = 1.5 Hz, 1H), 3.73 (dq, J = 9.5, 7.1 Hz, 2H), 3.56 (dq, J = 9.5, 7.1 Hz, 2H), 2.48 – 2.37 (m, 1H), 1.80 (dq, J = 12.5, 3.4 Hz, 2H), 1.74 – 1.63 (m, 2H), 1.55 – 1.39 (m, 3H), 1.36 – 1.23 (m, 3H), 1.22 (t, J = 7.1 Hz, 6H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ91.6, 90.5, 75.6, 60.6, 32.4, 29.0, 25.9, 25.0, 15.2 ppm.

HRMS (ESI-TOF): calculated for $C_{13}H_{22}O_2$ $[M+Na]^+$: 233.1512, found: 233.1508.

Compound 51



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (10:1 petroleum ether:EtOAc) afforded 16.6 mg (62%) of the title compound **51**.

Physical State: white solid.

m.p.:109-111 °C

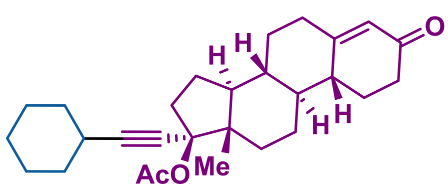
R$_f$= 0.30 (10:1 petroleum ether:EtOAc).

^{1}H NMR (500 MHz, CDCl$_3$): δ7.87 (dd, J = 5.4, 3.1 Hz, 2H), 7.72 (dd, J = 5.5, 3.0 Hz, 2H), 4.43 (d, J = 2.1 Hz, 2H), 2.36 – 2.27 (m, 1H), 1.74 (ddd, J = 14.1, 6.3, 3.3 Hz, 2H), 1.69 – 1.60 (m, 2H), 1.47 (t, J = 4.6 Hz, 1H), 1.43 – 1.32 (m, 2H), 1.30 – 1.19 (m, 3H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ167.4, 134.2, 132.3, 123.6, 87.9, 73.4, 32.6, 29.1, 27.7, 25.9, 25.0 ppm.

HRMS (ESI-TOF): calculated for $C_{17}H_{17}NO_2$ $[M+H]^+$: 268.1332, found: 268.1331.

Compound 52



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (10:1 petroleum ether:EtOAc) afforded 32.8 mg (78%) of the title compound **52**.

Physical State: white solid.

m.p.:175-176 °C

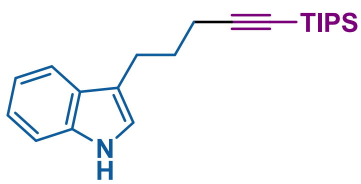
R$_f$= 0.25 (10:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ5.82 (t, J = 1.9 Hz, 1H), 2.72 – 2.58 (m, 1H), 2.51 – 2.35 (m, 3H), 2.32 – 2.19 (m, 3H), 2.13 – 2.03 (m, 1H), 2.03 – 1.96 (m, 4H), 1.94 – 1.52 (m, 12H), 1.47 – 1.22 (m, 8H), 1.14 – 1.01 (m, 1H), 0.89 (s, 3H), 0.87 – 0.79 (m, 1H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ200.1, 169.5, 166.7, 124.7, 91.5, 84.9, 79.8, 49.4, 47.8, 47.7, 42.7, 40.9, 37.6, 36.6, 35.6, 33.1, 32.7, 32.7, 30.9, 26.7, 26.4, 26.0, 24.7, 23.5, 21.7, 13.6 ppm.

HRMS (ESI-TOF): calculated for $C_{28}H_{38}O_3$ $[M+H]^+$: 423.2894, found: 423.2896.

Compound 53



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (20:1 petroleum ether:EtOAc) afforded 15.3 mg (45%) of the title compound **53**.

Physical State: colorless oil.

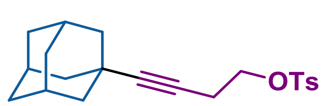
R_f= 0.27 (20:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.93 (s, 1H), 7.65 (dd, J = 7.8, 1.0 Hz, 1H), 7.36 (d, J = 8.1 Hz, 0H), 7.20 (ddd, J = 8.1, 7.0, 1.3 Hz, 1H), 7.12 (ddd, J = 8.0, 7.0, 1.1 Hz, 1H), 7.01 (d, J = 2.3 Hz, 1H), 2.93 (t, J = 7.4 Hz, 2H), 2.32 (t, J = 6.9 Hz, 2H), 1.93 (p, J = 7.1 Hz, 2H), 1.14 – 1.04 (m, 21H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ136.5, 127.7, 122.0, 121.6, 119.3, 119.1, 116.1, 111.2, 109.2, 80.7, 29.6, 24.1, 19.7, 18.8 ppm.

HRMS (ESI-TOF): calculated for $C_{22}H_{33}NSi$ $[M+H]^+$: 340.2455, found: 340.2456.

Compound 54



Following **Procedure E** on 0.10 mmol scale. Purification by column chromatography (10:1 petroleum ether:EtOAc) afforded 19.6 mg (55%) of the title compound **54**.

Physical State: white solid.

m.p.:82-85 °C

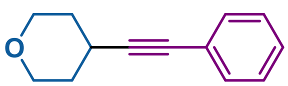
R_f= 0.33 (10:1 petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.80 (d, J = 8.2 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 4.04 (t, J = 7.3 Hz, 2H), 2.52 (t, J = 7.3 Hz, 2H), 2.45 (s, 3H), 1.95 – 1.88 (m, 3H), 1.75 (d, J = 2.9 Hz, 6H), 1.70 – 1.60 (m, 6H) ppm.

^{13}C NMR (126 MHz, CDCl$_3$): δ144.9, 133.2, 130.0, 128.1, 91.5, 72.7, 68.5, 43.1, 36.5, 29.5, 28.1, 21.8, 19.8 ppm.

HRMS (ESI-TOF): calculated for $C_{21}H_{26}O_3S$ $[M+H]^+$:359.1675, found:359.1674.

Compound 55



Following **Procedure D** on 10 mmol scale. Purification by column chromatography (50:1 to 20:1 petroleum ether:EtOAc) afforded 1.30 g (70%) of the title compound **55**.

Physical State: colorless oil.

R_f= 0.35 (20:1petroleum ether:EtOAc).

^{1}H NMR (400 MHz, CDCl$_3$): δ7.44 – 7.34 (m, 2H), 7.33 – 7.25 (m, 3H), 3.96 (ddd, J = 11.6, 5.7, 3.7 Hz, 2H), 3.55 (ddd, J = 11.6, 8.6, 3.0 Hz, 2H), 2.85 (tt, J = 8.5, 4.1 Hz, 1H), 1.95 – 1.87 (m, 2H), 1.83 – 1.70 (m, 2H) ppm.

^{13}C NMR (101 MHz, CDCl$_3$): δ131.7, 128.4, 127.9, 123.7, 92.3, 81.7, 66.5, 32.4, 26.9 ppm.

HRMS (ESI-TOF): calculated for $C_{13}H_{14}O$ $[M+H]^+$: 187.1117, found: 187.1108.

UV-vis Analysis

General Method

Spectrophotometric experiments were carried out using a Shimadzu UV-2550. Absorbance was monitored between 200 and 800 nm with a path length of 0.5 cm using a solution of THF as a background solution. Background-subtracted spectra were obtained for different solutions (see below for details).

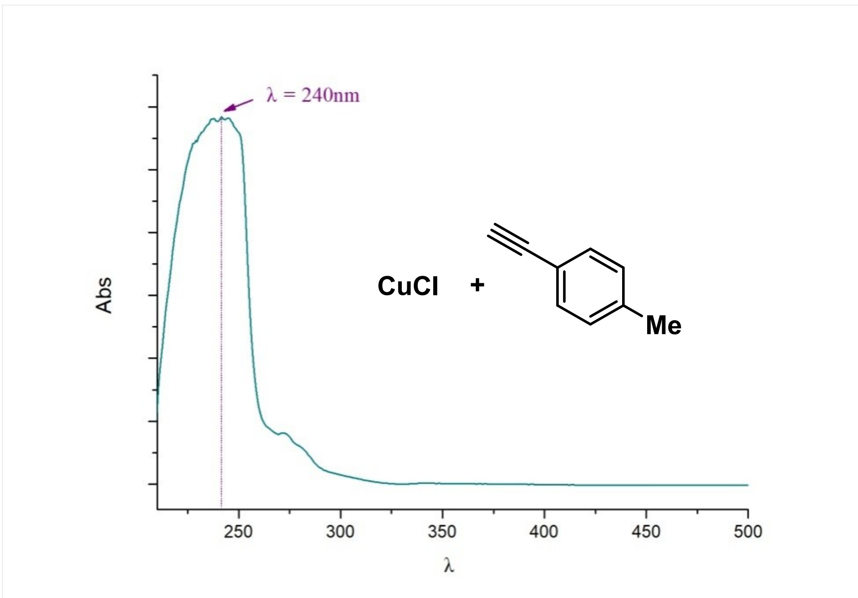


Figure S3. UV-vis Absorption Curve for Mixture of CuCl and Aryl Alkynes

Method: In glovebox, cuprous chloride (0.1 mmol) and 1-ethynyl-4-methylbenzene (0.1 mmol) were mixed in a sealed tube. 1 mL of THF was added and the tube was stirred for 15 min. Then the mixture was diluted to 5×10^{-5} M and determined for UV-vis absorption.

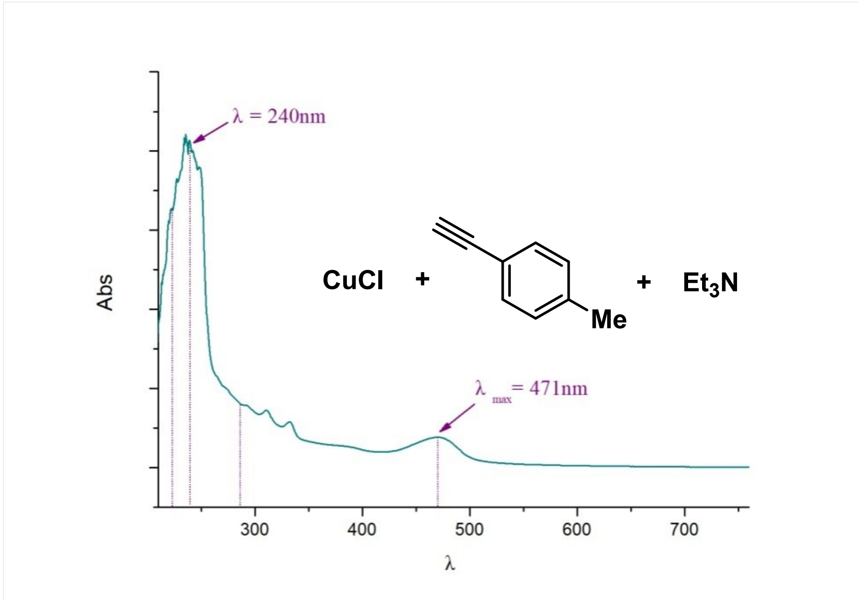


Figure S4. UV-vis Absorption Curve for Mixture of CuCl, Aryl Alkynes and Base

Method: In glovebox, cuprous chloride (0.1 mmol), 1-ethynyl-4-methylbenzene (0.1 mmol) and triethylamine (0.25 mmol) were mixed in a sealed tube. 1 mL of THF was added and the tube was stirred for 15 min. Then the mixture was diluted to 5×10^{-5} M and determined for UV-vis absorption.

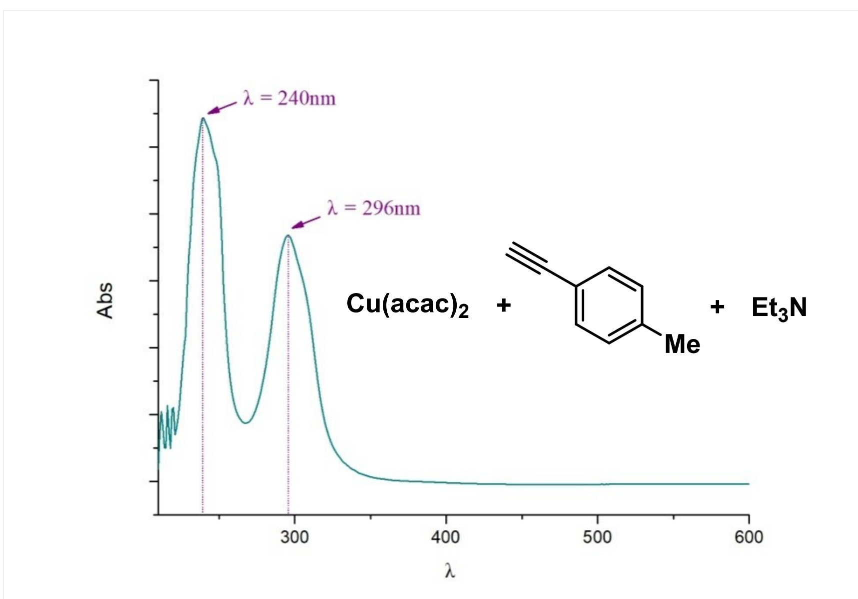


Figure S5. UV-vis Absorption Curve for Mixture of Cu(acac)$_2$, Aryl Alkynes and Base

Method: In glovebox, cupric acetylacetonate (0.1 mmol), 1-ethynyl-4-methylbenzene (0.1 mmol) and triethylamine (0.25 mmol) were mixed in a sealed tube. 1 mL of THF was added and the tube was stirred for 15 min. Then the mixture was diluted to 5×10^{-5} M and determined for UV-vis absorption.

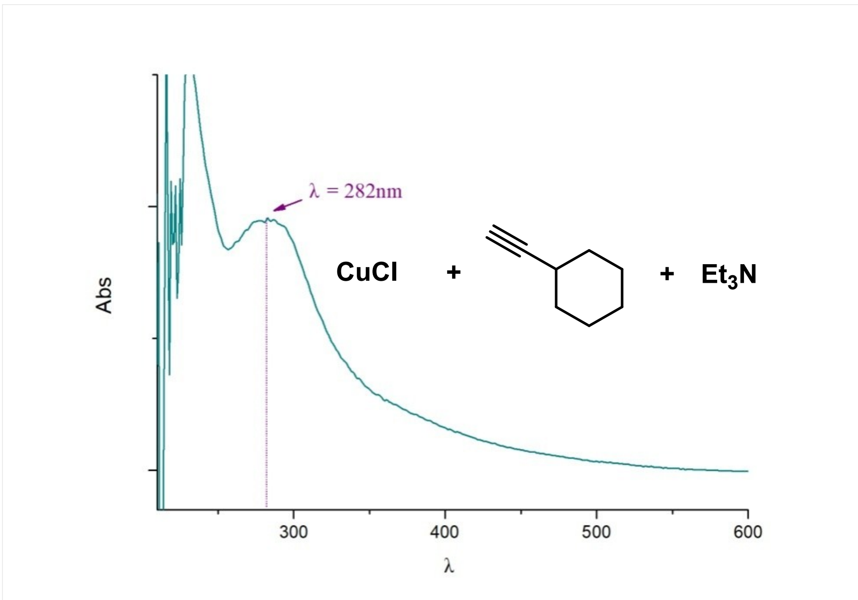


Figure S6. UV-vis Absorption Curve for Mixture of CuCl, Alkyl Alkynes and Base

Method: In glovebox, cuprous chloride (0.1 mmol), ethynylcyclohexane (0.1 mmol) and triethylamine (0.25 mmol) were mixed in a sealed tube. 1 mL of THF was added and the tube was stirred for 15 min. Then the mixture was diluted to 5×10^{-5} M and determined for UV-vis absorption.

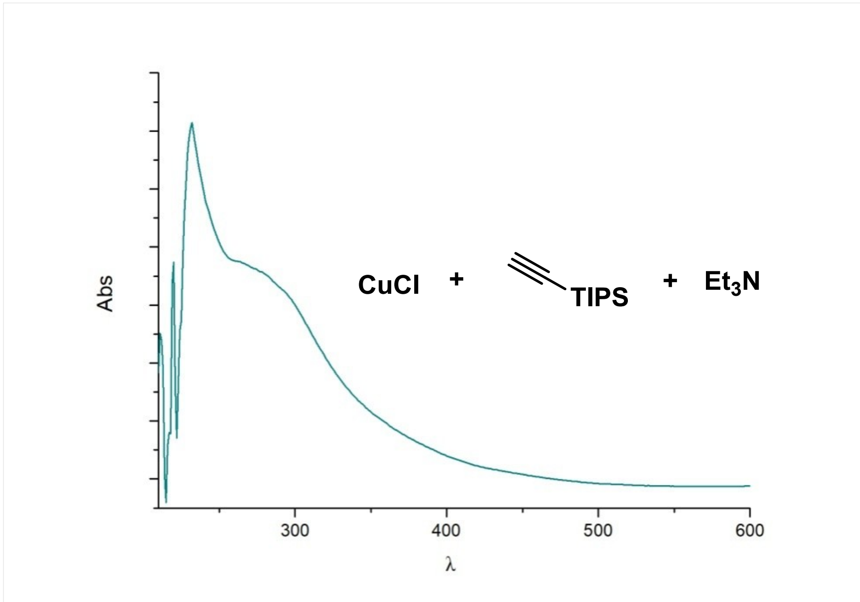


Figure S7. UV-vis Absorption Curve for Mixture of CuCl, Silyl Alkynes and Base

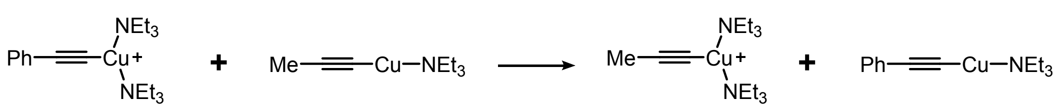
Method: In glovebox, cuprous chloride (0.1 mmol), (triisopropylsilyl)acetylene (0.1 mmol) and triethylamine (0.25 mmol) were mixed in a sealed tube. 1 mL of THF was added and the tube was stirred for 15 min. Then the mixture was diluted to 5×10^{-5} M and determined for UV-vis absorption.

Computational Details

The DFT calculations were performed with Gaussian 09[13]. Geometry optimizations of all the ground state, excitation state and transition structures were carried out at the B3LYP-D3 level of theory[14] with the 6-31G(d) basis set (SDD basis set for Cu) in tetrahydrofuran using the SMD solvation model[15]. The singlet diradical species were calculated with initial wave function guess generated by fragment guess method. Vibrational frequencies were computed at the same level to verify that optimized structures are local minimums or transition states and to evaluate zero-point vibrational energies (ZPVE) and thermal corrections at 298 K. Solvent effects in tetrahydrofuran were evaluated at the more accurate B3LYP-D3/6-311+G(d,p) level (SDD basis set for Cu) with the SMD model using the above optimized structures.

Due to the convergence difficulty when optimizing transition structure **TS3-acac**, the geometry optimization convergence criteria was changed by adding 'opt=loose' keyword in Gaussian input file. The optimization of other structures was all using Gaussian default geometry optimization convergence criteria.

After photoexcitation of Cu(I)-phenylacetylide (**Int3**, Scheme 4A), it transfers an electron to redox-active ester and is oxidized to Cu(II) acetylide cation (**Int5**). For alkyl substituted alkynes, the following exchange reaction can occur. We have calculated the thermodynamics of the exchange reaction of **Int5** with **Int3-Me**, which is summarized below:



Int5 **Int3-Me** **Int5-Me** **Int3**

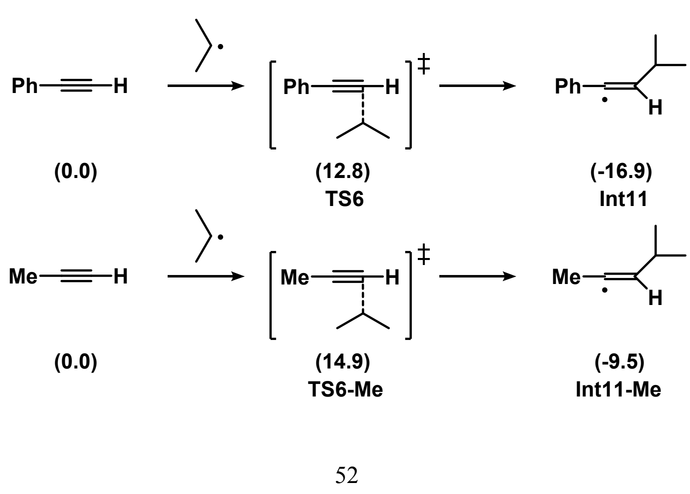
B3LYP-D3//B3LYP-D3 ΔG_{sol} = –0.3 kcal mol^{-1}

M06//B3LYP-D3 ΔG_{sol} = –0.9 kcal mol^{-1}

wB97XD//B3LYP-D3 ΔG_{sol} = –0.4 kcal mol^{-1}

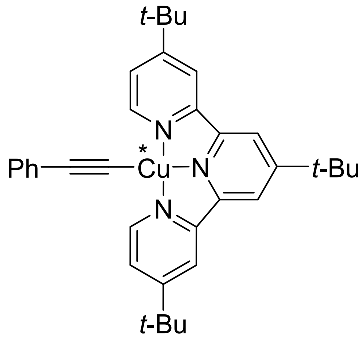
The geometries are optimized at B3LYP-D3/6-31G(d) level. To evaluate computation error caused by functional inaccuracy, the single-point energies have been computed in three different density functionals (B3LYP-D3/6-311+G(d,p), M06/6-311+G(d,p) and wB97XD/6-311+G(d,p)). All these calculations indicate that the formation of **Int5-Me** (precursor of the alkynylation for aliphatic alkynes) from **Int5** (generated from copper-phenylacetylide photocatalyst) is slightly exergonic under standard conditions. In the real reaction system, the Cu(I)-phenylacetylide catalyst load is only 10 mol%, the aliphatic alkyne substrate is much higher in concentration, which further drives this exchange reaction to generate more **Int5-Me**. We think that the aliphatic alkyne cross-coupling product is originated from **Int5-Me**, followed by a similar reaction pathway as described in the manuscript for **Int5** (Scheme 4C). The aromatic alkyne cross-coupling byproducts are also found in the reaction mixtures, which are generated from the remaining **Int5** that did not converted to **Int5-Me**.

One reviewer suggested an alternative pathway for the reaction involving the radical attack to the alkyne, which generates a phenyl stabilized vinyl radical. During the revision, we carried out the following DFT calculations. It is found that, for both aryl and alkyl substituted alkynes, the activation free energy barriers for the isopropyl radical addition to form the vinyl radicals (12.8 and 14.9 kcal mol^{-1}) are much higher than that for the radical addition to Cu(II) generating Cu(III) (6.8 kcal mol^{-1}, Scheme 4C). Therefore, this alternative pathway is not likely to work.



DFT-Computed Energies and Cartesian Coordinate

Cu(PhC≡C)(^{t}Bu$_3$-TERPY)_triplet state



G(THF)=-1719.042715 Hartree

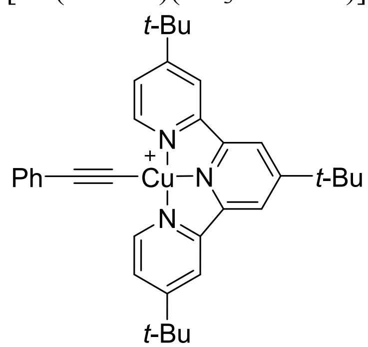
C	2.381583	-0.753591	0.002265
C	3.731262	-1.113235	0.001208
C	4.733516	-0.139582	0.002873
C	4.314647	1.204841	0.005592
C	2.960201	1.504329	0.006198
N	2.008729	0.560325	0.004539
H	3.993196	-2.165105	-0.001355
H	5.026731	2.019924	0.006953
H	2.602922	2.529458	0.007904
C	1.258915	-1.693034	0.000342
C	1.348004	-3.070939	-0.000636
N	0.043638	-1.069239	-0.000613
C	0.171613	-3.868313	-0.003829
H	2.323112	-3.542961	0.001083
C	-1.118297	-1.804564	-0.002406
C	-1.056639	-3.202075	-0.004479
H	-1.981555	-3.764244	-0.006160
C	-2.308611	-0.989296	-0.001444
C	-3.630337	-1.468538	-0.001602
N	-2.064507	0.366806	0.000586
C	-4.713785	-0.597710	0.000837
H	-3.794486	-2.540168	-0.003286
C	-3.107367	1.213192	0.002503
C	-4.424433	0.789336	0.002775
H	-2.849676	2.268158	0.003978
H	-5.211353	1.532317	0.004600
Cu	-0.061320	0.855192	0.003097

	3		
C	-0.145941	2.786095	0.003826
C	-0.199007	4.013824	0.001933
C	-0.261112	5.442137	-0.000895
C	-0.293089	6.159999	-1.214276
C	-0.291601	6.165161	1.209439
C	-0.354251	7.551839	-1.213220
H	-0.270113	5.612583	-2.151900
C	-0.352769	7.556992	1.202496
H	-0.267460	5.621770	2.149371
C	-0.384096	8.256946	-0.006840
H	-0.378436	8.088499	-2.157885
H	-0.375775	8.097694	2.144882
H	-0.431722	9.342304	-0.009130
C	0.294710	-5.394265	-0.003336
C	1.083122	-5.845168	-1.252437

C	1.052144	-5.844158	1.265135
C	-1.076470	-6.088058	-0.020341
H	0.567763	-5.540746	-2.170841
H	2.091163	-5.417363	-1.273932
H	1.184083	-6.937256	-1.263566
H	0.511910	-5.542968	2.170213
H	1.157661	-6.935836	1.277730
H	2.057142	-5.411257	1.313009
H	-0.937694	-7.174911	-0.021512
H	-1.673564	-5.830981	0.862093
H	-1.653582	-5.826013	-0.914577
C	6.207293	-0.555306	0.000183
C	6.493229	-1.409269	1.254169
C	6.491969	-1.391575	-1.266013
C	7.150977	0.657176	0.008436
H	6.291406	-0.84142	2.169689

		2	
H	5.880510	-2.316397	1.276335
H	7.546053	-1.714965	1.267088
H	6.290469	-0.810420	-2.173210
H	7.544375	-1.698512	-1.283745
H	5.877638	-2.297267	-1.300712
H	8.190123	0.310474	0.007248
H	7.009931	1.288442	-0.876080
H	7.008135	1.277586	0.900342
C	-6.144109	-1.148803	0.001457
C	-6.356202	-2.012753	-1.260191
C	-6.352470	-2.020167	1.258638
C	-7.195731	-0.028245	0.006429
H	-6.206679	-1.420322	-2.170289
H	-5.664579	-2.861258	-1.292156
H	-7.377723	-2.411516	-1.277001
H	-6.199876	-1.433179	2.171751
H	-7.374097	-2.418611	1.276304
H	-5.661172	-2.869162	1.283507
H	-8.199252	-0.468042	0.007075
H	-7.110029	0.605824	0.896034
H	-7.113365	0.610712	-0.879981

[Cu(PhC≡C)(^{t}Bu$_3$-TERPY)]$^+$



G(THF)=-1718.928757 Hartree

C	2.359283	-0.854731	-0.009447
C	3.676018	-1.291922	-0.001161
C	4.732968	-0.364057	-0.007312
C	4.384225	0.989905	-0.021144
C	3.041732	1.363865	-0.025771
N	2.054038	0.467770	-0.02015

			7
H	3.884572	-2.354545	0.011902
H	5.136556	1.767483	-0.026258
H	2.737359	2.405066	-0.033581
C	1.181675	-1.753216	-0.006125
C	1.213602	-3.147185	0.004713
N	0.011291	-1.101705	-0.012242
C	0.013889	-3.870965	0.010288
H	2.164751	-3.659698	0.010353
C	-1.162204	-1.755335	-0.008473
C	-1.190471	-3.144976	0.002177
H	-2.140510	-3.663384	0.006329
C	-2.338803	-0.855514	-0.012317
C	-3.656116	-1.291485	-0.017650
N	-2.032378	0.466451	-0.009776
C	-4.711930	-0.362740	-0.019867
H	-3.865231	-2.354188	-0.023104
C	-3.019566	1.363692	-0.010864
C	-4.362008	0.991150	-0.014926
H	-2.713940	2.404486	-0.008847
H	-5.113509	1.769584	-0.016406
Cu	0.010372	0.871574	-0.015409
C	0.007745	2.788937	-0.009963
C	0.000909	4.016320	-0.000135
C	-0.008513	5.445597	0.013189
C	1.161161	6.175008	-0.281045
C	-1.187932	6.153130	0.321954
C	1.147825	7.567860	-0.266037
H	2.073760	5.637248	-0.520687
C	-1.193257	7.545850	0.336128
H	-2.093229	5.598416	0.550493
C	-	8.25847	0.04235

	0.027370	9	8
H	2.057167	8.116318	-0.495617
H	-2.109811	8.077420	0.576857
H	-0.034600	9.344667	0.053796
C	-6.159746	-0.852921	-0.038077
C	-6.388891	-1.656470	-1.337075
C	-6.400460	-1.765298	1.184130
C	-7.163537	0.308741	0.009970
H	-6.225638	-1.029002	-2.220547
H	-5.719216	-2.520239	-1.404771
H	-7.419960	-2.026071	-1.366017
H	-6.224839	-1.223380	2.120259
H	-7.438616	-2.115423	1.182285
H	-5.751444	-2.646941	1.173080
H	-8.182381	-0.092566	0.000451
H	-7.04892	0.906474	0.921159
	9		
H	-7.060060	0.973164	-0.855121
C	-0.021318	-5.400438	0.035577
C	-0.735808	-5.856095	1.326975
C	-0.803203	-5.908794	-1.195461
C	1.386521	-6.014893	0.010268
H	-0.201314	-5.504532	2.216737
H	-1.764424	-5.484659	1.378069
H	-0.771695	-6.950586	1.360379
H	-0.327884	-5.580558	-2.126678
H	-0.822375	-7.004211	-1.189727
H	-1.840035	-5.557482	-1.198244
H	1.303334	-7.106263	0.025782
H	1.937120	-5.736783	-0.895744
H	1.979072	-5.715961	0.882315
C	6.179939	-0.856306	0.009575

C	6.410792	-1.660208	1.308026
C	6.416674	-1.769458	-1.213052
C	7.185220	0.303934	-0.040666
H	6.250874	-1.032413	2.191905
H	5.740098	-2.523075	1.377303
H	7.441366	-2.031396	1.334375
H	6.238933	-1.227758	-2.148921
H	7.454809	-2.120348	-1.213894
H	5.766954	-2.650630	-1.199914
H	8.203278	-0.098358	-0.030608
H	7.071314	0.900114	-0.952892
H	7.082607	0.969985	0.823283

2-iodopropane
G(THF)=-129.9518496 Hartree

C	1.963847	1.273803	-0.135333
C	1.364598	0.000000	0.421450
H	1.350235	-0.000000	1.510879
H	1.495394	2.166753	0.286804
H	3.031405	1.290617	0.127408
H	1.882739	1.312124	-1.226254
C	1.963848	-1.273803	-0.135334
H	1.495393	-2.166753	0.286803
H	1.882741	-1.312123	-1.226254
H	3.031404	-1.290618	0.127410
I	-0.866473	-0.000000	-0.014934

2-iodopropane radical anion
G(THF)=-130.0727597 Hartree

C	2.938451	1.294989	-0.201585
C	3.218641	-0.000168	0.483511
H	3.318595	-0.000208	1.567476
H	3.377603	2.147479	0.330869
H	3.323724	1.298515	-1.231940
H	1.852424	1.485569	-0.279640
C	2.937648	-1.29513	-0.20161

		5	7
H	3.376066	-2.147930	0.330950
H	1.851501	-1.484921	-0.279900
H	3.323139	-1.298969	-1.231891
I	-1.414934	0.000044	0.005891

Int1

G(THF)=-950.0797972 Hartree

Cu	-0.842498	0.000046	-0.000557
Cl	-3.002129	0.002743	-0.003656
N	1.144176	0.000029	0.000298
C	1.659658	1.227653	-0.686158
C	1.654613	-1.212348	-0.716321
H	2.745774	1.280965	-0.520285
H	1.497883	1.092050	-1.756566
H	2.741950	-1.103041	-0.841908
H	1.484501	-2.069615	-0.063384
C	0.984491	-1.480253	-2.058092
H	1.404193	-2.396910	-2.488057
H	-0.094926	-1.626182	-1.932500
H	1.140871	-0.673920	-2.780990
C	0.986537	2.523649	-0.250215
H	1.410394	3.355256	-0.824764
H	-0.091610	2.488135	-0.447108
H	1.134424	2.745947	0.810984
C	1.650172	-0.018290	1.410123
H	2.736913	-0.185845	1.381236
H	1.482893	0.976278	1.825907
C	0.973691	-1.045778	2.309226
H	1.378210	-0.951833	3.323497
H	-0.107665	-0.871049	2.357308
H	1.140628	-2.076204	1.981474

Int2

G(THF)=-1258.498188 Hartree

Cl	-3.18611	-1.65681	-0.09581

	7	7	8
C	-0.019179	-2.581675	-0.623548
C	0.894273	-1.762305	-0.436243
C	2.122403	-1.040169	-0.265445
C	2.777881	-0.480369	-1.377762
C	2.670856	-0.872347	1.019876
C	3.960399	0.234758	-1.201958
H	2.351046	-0.608557	-2.367521
C	3.854875	-0.157324	1.183517
H	2.160895	-1.300977	1.876818
C	4.500548	0.400398	0.076263
H	4.460588	0.664123	-2.065111
H	4.273150	-0.033317	2.178137
H	5.421647	0.960202	0.209051
Cu	-1.015691	-0.918015	-0.180707
C	-0.169564	1.295431	1.514818
H	-0.22820	2.343723	1.838568

	1		
H	0.881254	1.072593	1.313729
C	-0.118936	1.761091	-0.881077
H	-0.625584	1.516370	-1.817822
H	0.849177	1.257258	-0.901535
C	-2.269386	1.718793	0.347399
H	-2.820769	1.092127	1.049643
H	-2.188931	2.722698	0.789007
N	-0.901644	1.131829	0.225738
H	-0.498660	-3.519426	-0.835344
C	-3.043944	1.791624	-0.962580
H	-4.076580	2.084327	-0.741625
H	-2.631149	2.532049	-1.654748
H	-3.074134	0.816631	-1.456221
C	0.100247	3.272209	-0.786696
H	0.673892	3.550177	0.103078
H	0.672159	3.598052	-1.66313

			7
H	-0.840038	3.832422	-0.777848
C	-0.671344	0.388789	2.632389
H	-0.050591	0.538941	3.523238
H	-1.708594	0.600533	2.908874
H	-0.604841	-0.667824	2.346284

Int3

G(THF)=-797.6224041 Hartree

C	0.797376	0.000410	0.000516
C	2.029320	0.000531	0.000308
C	3.457856	0.000392	0.000052
C	4.180559	1.212109	0.002586
C	4.180268	-1.211503	-0.002805
C	5.573547	1.207958	0.002246
H	3.635151	2.151178	0.004813
C	5.573253	-1.207689	-0.003122
H	3.634631	-2.150438	-0.004788
C	6.276819	0.000051	-0.000604
H	6.112863	2.151445	0.004227
H	6.112341	-2.151306	-0.005369
H	7.363239	-0.000082	-0.000866
Cu	-1.044172	0.000111	0.000423
C	-3.557225	-0.534904	-1.302885
H	-4.657298	-0.561835	-1.268652
H	-3.270033	0.180646	-2.074163
C	-3.556526	1.396934	0.189322
H	-3.263780	1.708604	1.192732
H	-4.656787	1.380780	0.154783
N	-3.056223	0.000147	0.000678
C	-3.001663	-1.903489	-1.681685
H	-3.361373	-2.707218	-1.033019
H	-3.315121	-2.140434	-2.704594
H	-1.905391	-1.900800	-1.654978
C	-3.006106	2.407059	-0.812092
H	-	2.25258	-

	3.380785	2	1.827972
H	-3.305679	3.413645	-0.499536
H	-1.910293	2.371127	-0.837765
C	-3.556250	-0.861730	1.115961
H	-4.656343	-0.819487	1.122610
H	-3.268343	-1.887353	0.881767
C	-3.000453	-0.505556	2.490624
H	-3.361039	0.457351	2.863237
H	-3.311928	-1.274053	3.206916
H	-1.904149	-0.482035	2.473056

Int4
G(THF)=-797.5214788 Hartree

C	0.770811	-0.081312	0.075783
C	2.044267	-0.060328	0.059182
C	3.397418	-0.030863	0.035470
C	4.145049	1.247475	0.021620
C	4.205433	-1.271359	0.013484
C	5.506567	1.257926	-0.015841
H	3.573189	2.170486	0.040009
C	5.565867	-1.215601	-0.023603
H	3.679063	-2.221115	0.025906
C	6.259159	0.038692	-0.040089
H	6.038365	2.206453	-0.027042
H	6.142875	-2.137214	-0.040654
H	7.343173	0.064817	-0.069768
Cu	-1.048500	-0.056611	0.048774
C	-3.532924	-0.548607	-1.322840
H	-4.633345	-0.554383	-1.313550
H	-3.214322	0.130146	-2.114897
C	-3.490340	1.459839	0.063814
H	-3.275253	1.796189	1.078985
H	-4.581492	1.497616	-0.073661
N	-	0.03112	-

	3.054352	6	0.028552
C	-2.993208	-1.940874	-1.630309
H	-3.361346	-2.705810	-0.940514
H	-3.309453	-2.227321	-2.639624
H	-1.896873	-1.949249	-1.603372
C	-2.795079	2.398079	-0.916750
H	-3.052383	2.194047	-1.960201
H	-3.100303	3.427366	-0.697048
H	-1.705320	2.337270	-0.811693
C	-3.647461	-0.741368	1.107368
H	-4.738176	-0.595886	1.092487
H	-3.454466	-1.797066	0.912919
C	-3.078831	-0.389009	2.477078
H	-3.326841	0.627256	2.796546
H	-3.493092	-1.079279	3.220549
H	-1.98739	-0.49661	2.483818
	1	5	

Int5

G(THF)=-1089.800813 Hartree

C	0.846046	0.041610	-0.159547
C	2.071516	0.013076	-0.160511
C	3.500171	-0.037751	-0.154642
C	4.258665	1.113913	0.135547
C	4.174908	-1.245049	-0.425779
C	5.650223	1.055203	0.156488
H	3.744751	2.047342	0.345307
C	5.566710	-1.295298	-0.404204
H	3.596467	-2.136126	-0.651049
C	6.309106	-0.147570	-0.112667
H	6.222455	1.950251	0.384093
H	6.074039	-2.232818	-0.614146
H	7.394355	-0.190381	-0.094877
Cu	-1.061168	0.059112	0.015228
C	-0.908097	2.575880	1.404170

H	0.182120	2.563414	1.335735
H	-1.229328	3.617517	1.518864
C	-0.697728	2.724586	-1.038954
H	-0.975852	2.196813	-1.954149
H	0.364655	2.536404	-0.876147
C	-2.898454	2.201557	-0.006717
H	-3.337721	1.634746	0.817006
H	-3.169644	3.252544	0.152174
C	-0.617061	-2.775766	-0.632310
H	0.376622	-2.600222	-0.222712
H	-0.875619	-3.826674	-0.452430
C	-1.579348	-2.319639	1.588976
H	-2.317413	-1.677492	2.080319
H	-1.948961	-3.349614	1.655589
C	-2.951899	-1.940923	-0.409707
H	-3.552581	-1.281884	0.226122
H	-2.912460	-1.491283	-1.404056
N	-1.414993	2.057578	0.097034
N	-1.557330	-1.915614	0.147780
C	-0.958718	4.220044	-1.199643
H	-0.644049	4.794276	-0.323222
H	-0.376257	4.578243	-2.055587
H	-2.011435	4.441881	-1.400811
C	-3.455948	1.702090	-1.334345
H	-4.544277	1.612582	-1.257757
H	-3.233050	2.386730	-2.157330
H	-3.057575	0.717376	-1.603216
C	-1.350313	1.759969	2.611139
H	-0.865874	2.164960	3.505954
H	-2.431059	1.796408	2.777938
H	-1.040498	0.711590	2.520652

C	-3.619288	-3.312943	-0.502508
H	-4.620228	-3.178430	-0.926554
H	-3.067751	-3.991415	-1.159848
H	-3.732844	-3.788688	0.475352
C	-0.600910	-2.475071	-2.124543
H	0.211824	-3.045183	-2.586687
H	-1.531900	-2.757847	-2.624754
H	-0.406496	-1.412639	-2.310714
C	-0.238440	-2.217604	2.305172
H	-0.402587	-2.408859	3.371214
H	0.481285	-2.956867	1.943331
H	0.210174	-1.226538	2.198610

Int6-acac

G(THF)=-1142.847332 Hartree

C	-1.098973	0.354294	0.020040
C	-2.323356	0.445861	0.041839
C	-3.750452	0.523346	0.074675
C	-4.532904	-0.649712	0.104923
C	-4.408215	1.770409	0.081437
C	-5.923422	-0.574648	0.141413
H	-4.035806	-1.615400	0.100214
C	-5.799281	1.838259	0.118855
H	-3.814627	2.679432	0.058561
C	-6.563066	0.668143	0.148948
H	-6.510368	-1.488967	0.164549
H	-6.289347	2.808162	0.124713
H	-7.647633	0.724183	0.178425
C	2.161221	2.802637	-0.538329
C	3.557848	1.118358	0.621986
C	3.381372	2.361991	0.006353
H	4.228920	3.035440	-0.031043
O	1.079186	2.128621	-0.566412

O	2.656172	0.216234	0.742055
C	2.077856	4.187845	-1.137203
H	1.728141	4.117344	-2.173778
H	1.335380	4.776513	-0.585052
H	3.036569	4.711834	-1.115395
C	4.901522	0.756314	1.206640
H	4.786689	0.523910	2.272110
H	5.277609	-0.149771	0.716201
H	5.636276	1.556869	1.092079
Cu	0.831610	0.235554	0.062658
C	2.243483	-2.466761	-0.139611
H	2.758529	-2.102220	0.746484
H	2.200616	-3.563159	-0.076346
C	0.139014	-2.462576	1.105446
H	-0.916921	-2.218070	0.970873
H	0.233243	-3.556688	1.123835
C	0.093017	-2.248434	-1.334518
H	-0.898465	-1.812932	-1.205953
H	0.570784	-1.707124	-2.155381
N	0.855087	-1.930059	-0.088445
C	3.028233	-2.050051	-1.378181
H	4.077468	-2.336422	-1.244368
H	2.667197	-2.537973	-2.288606
H	2.994774	-0.966670	-1.528029
C	0.618447	-1.881775	2.430911
H	0.026837	-2.319687	3.243017
H	1.671734	-2.097426	2.631319
H	0.475615	-0.796118	2.460012
C	-0.028505	-3.730747	-1.690122
H	-0.534715	-4.302673	-0.905917
H	-0.628336	-3.819755	-2.603041
H	0.941649	-4.198651	-1.885613

Int6-Cl

G(THF)=-1257.870108 Hartree

Cl	-3.003871	-2.330421	-0.400142
C	0.671688	-0.731984	-0.372193
C	1.879952	-0.532240	-0.288927
C	3.282695	-0.279295	-0.189033
C	4.172512	-1.291023	0.224252
C	3.799240	0.997814	-0.489354
C	5.536166	-1.028749	0.334624
H	3.781839	-2.277145	0.456091
C	5.163739	1.252182	-0.374554
H	3.119991	1.782184	-0.809625
C	6.037050	0.241736	0.037537
H	6.210290	-1.818383	0.654645
H	5.546963	2.242008	-0.606850
H	7.100802	0.443271	0.126432
Cu	-1.206971	-1.003739	-0.349513
C	-1.326414	1.007584	1.704059
H	-0.236046	1.037259	1.649599
H	-1.674242	1.966847	2.105988
C	-1.134908	1.885988	-0.585573
H	-1.398298	1.640223	-1.616549
H	-0.064716	1.709758	-0.477636
C	-3.306279	1.005232	0.241952
H	-3.714695	0.157558	0.789883
H	-3.589240	1.918550	0.781983
N	-1.816781	0.884859	0.296437
C	-1.762809	-0.124512	2.626019
H	-1.300635	0.027295	3.607406
H	-2.846357	-0.161359	2.767900
H	-1.429812	-1.096907	2.244392
C	-3.883963	1.026711	-1.166556
H	-	0.95988	-

	4.974774	6	1.093648
H	-3.642288	1.946529	-1.706709
H	-3.539189	0.170177	-1.753177
C	-1.459661	3.351062	-0.293816
H	-1.160679	3.647219	0.716161
H	-0.896565	3.970778	-1.000452
H	-2.520980	3.582790	-0.423221

Int7-acac
G(THF)=-1261.316449 Hartree

C	-1.172568	-0.396110	0.134957
C	0.477201	-2.334799	0.355735
C	-0.249571	-2.997282	-0.787894
H	1.555645	-2.422923	0.223206
H	0.013663	-2.540441	-1.745334
H	0.068814	-4.052265	-0.824243
H	-1.334361	-2.971945	-0.664989
C	0.04337	-	1.74585
	4	2.724770	6
H	0.589634	-2.170754	2.515557
H	-1.029966	-2.575892	1.892868
H	0.261543	-3.795197	1.894343
C	-2.393249	-0.368323	0.049351
C	-3.812352	-0.286280	-0.081829
C	-4.663348	-0.788499	0.923576
C	-4.391416	0.303004	-1.224826
C	-6.047209	-0.702077	0.787227
H	-4.225872	-1.244694	1.806758
C	-5.775896	0.384044	-1.354305
H	-3.741987	0.691662	-2.003554
C	-6.609852	-0.116810	-0.350440
H	-6.689189	-1.093975	1.571558
H	-6.206148	0.840299	-2.241791
H	-7.68928	-0.05168	-0.45420

	1	0	4
O	2.407723	-0.444084	1.172215
C	3.517253	-0.870015	0.688560
C	3.790349	-1.147449	-0.655194
C	4.611866	-1.071513	1.713870
C	2.911997	-0.954006	-1.758515
H	4.784104	-1.516547	-0.881137
H	4.796495	-0.126619	2.239426
H	4.279845	-1.798039	2.465466
H	5.547446	-1.419682	1.268747
O	1.727820	-0.529325	-1.686826
C	3.441225	-1.269484	-3.146176
H	2.781518	-2.001151	-3.627577
H	3.414239	-0.359773	-3.758587
H	4.462500	-1.659890	-3.136958
Cu	0.666057	-0.306855	0.261133
C	2.081016	2.237526	-0.374812
H	1.989365	1.838237	-1.384469
H	2.894375	1.692343	0.105221
C	-0.355997	2.555518	-0.204837
H	-1.227689	2.170199	0.321695
H	-0.286032	3.630772	0.013846
C	0.984364	2.199936	1.803873
H	0.985062	3.292356	1.922551
H	1.965444	1.829045	2.108284
N	0.835679	1.866251	0.359482
C	2.420380	3.728995	-0.427063
H	2.567026	4.160955	0.568118
H	3.358918	3.850872	-0.980403
H	1.655007	4.315289	-0.945638
C	-0.548611	2.339199	-1.700860
H	-1.528219	2.735600	-1.991517
H	0.208503	2.854921	-2.299990
H	-	1.27546	-

	0.524443	3	1.950987
C	-0.078906	1.596850	2.715473
H	0.126138	1.909128	3.746303
H	-1.090298	1.927487	2.461926
H	-0.061860	0.503221	2.682801

Int7-Cl

G(THF)=-1376.348158 Hartree

C	0.575998	0.507996	-0.040941
C	-0.516893	2.619721	-0.737001
C	0.216799	2.543841	-2.051823
H	-1.559617	2.895079	-0.883600
H	-0.241681	1.823343	-2.736983
H	0.143099	3.535383	-2.527841
H	1.272755	2.294969	-1.931012
C	0.122034	3.420050	0.365936
H	-0.440356	3.346921	1.301759
H	1.157004	3.120710	0.546277
H	0.11734	4.47916	0.06113

	3	1	8
C	1.770179	0.252040	0.033817
C	3.151612	-0.100934	0.091509
C	3.679911	-1.056870	-0.800484
C	4.013041	0.497322	1.033006
C	5.029075	-1.398804	-0.750297
H	3.021057	-1.521080	-1.528102
C	5.360767	0.147578	1.077825
H	3.613006	1.234268	1.723005
C	5.874576	-0.799819	0.187971
H	5.422284	-2.136088	-1.444916
H	6.012924	0.616935	1.809234
H	6.926226	-1.069365	0.225265
Cu	-1.244366	0.770239	-0.056868
Cl	-3.321264	1.614901	0.320159
C	-2.302015	-1.460963	1.608888
H	-3.237208	-0.904286	1.701104
H	-2.51664	-2.51759	1.820110

	8	8	
C	-3.008130	-1.553229	-0.732016
H	-3.775246	-0.829332	-0.457196
H	-2.672298	-1.291853	-1.739438
C	-0.740956	-2.267113	-0.081621
H	0.098593	-1.962544	0.541494
H	-1.041997	-3.274256	0.239639
N	-1.858813	-1.320895	0.192931
C	-0.288071	-2.305256	-1.536345
H	0.632109	-2.896900	-1.601044
H	-1.026845	-2.770249	-2.196143
H	-0.065394	-1.301581	-1.909567
C	-3.602523	-2.963419	-0.733237
H	-4.442199	-2.984911	-1.437428
H	-2.884499	-3.725517	-1.051871
H	-3.990698	-3.247209	0.250113
C	-1.300826	-0.929802	2.628444
H	-1.724723	-1.037717	3.633381
H	-0.348785	-1.468094	2.606996
H	-1.095868	0.133790	2.459788

Int8-acac
G(THF)=-1261.381573 Hartree

C	0.413349	-2.643513	-0.809837
C	-0.052008	-2.410785	1.664968
C	0.316886	-3.138862	0.503839
H	0.574403	-4.182801	0.646292
O	0.143712	-1.463495	-1.205038
O	-0.357512	-1.187304	1.711635
C	0.910913	-3.586062	-1.890900
H	0.228548	-3.558670	-2.748395
H	1.889609	-3.237206	-2.245375
H	1.012660	-4.618393	-1.544551

C	-0.073671	-3.164342	2.987367
H	0.615763	-2.682851	3.691763
H	-1.077260	-3.098949	3.425528
H	0.200854	-4.218502	2.887939
C	0.363472	1.959784	0.425904
C	1.314570	1.181869	0.200819
C	2.645933	0.678210	-0.015499
C	2.991205	-0.648602	0.296652
C	3.627041	1.534880	-0.551879
C	4.289596	-1.103569	0.078968
H	2.236601	-1.312801	0.699701
C	4.922633	1.070366	-0.768499
H	3.361126	2.559065	-0.796252
C	5.258708	-0.249569	-0.454926
H	4.543921	-2.131159	0.324078
H	5.670693	1.740095	-1.183822
H	6.269089	-0.609910	-0.626824
Cu	-0.389840	0.151349	-0.086016
N	-2.450503	0.066213	-0.563261
C	-2.542321	0.095433	-2.048741
C	-2.935796	-1.252501	-0.058884
C	-3.204859	1.200208	0.029524
H	-2.060251	-0.819597	-2.401339
H	-3.597651	0.062603	-2.355150
H	-2.315261	-2.009485	-0.542825
H	-2.700675	-1.295620	1.004464
H	-2.728666	2.118057	-0.319109
H	-4.235512	1.206454	-0.357312
C	-4.415632	-1.569396	-0.284349
H	-4.627320	-2.559817	0.135322
H	-5.076916	-0.853515	0.215210
H	-	-	-

	4.682901	1.598255	1.345571
C	-1.868150	1.296380	-2.702495
H	-1.900421	1.171895	-3.791186
H	-2.368373	2.240049	-2.464880
H	-0.818459	1.374376	-2.400235
C	-3.224187	1.189913	1.553833
H	-3.625194	2.142720	1.917245
H	-3.855714	0.391570	1.955283
H	-2.215533	1.060943	1.959361
C	-0.262794	3.243379	0.831746
H	-1.243343	3.042270	1.274025
C	0.614685	3.923951	1.897348
H	1.609240	4.146282	1.493696
H	0.154592	4.865369	2.220018
H	0.737661	3.279643	2.774183
C	-0.466267	4.155198	-0.390584
H	-1.103747	3.679930	-1.141542
H	-0.938151	5.095130	-0.081613
H	0.496028	4.390653	-0.859858

Int8-Cl

G(THF)=-1376.422441 Hartree

Cl	3.223536	-0.382359	0.569595
C	0.809324	1.922640	-0.008966
C	-0.355217	1.483631	-0.005049
C	-1.783717	1.319584	-0.000277
C	-2.509369	1.360519	-1.205308
C	-2.469636	1.100314	1.208999
C	-3.891624	1.184334	-1.196352
H	-1.979919	1.525546	-2.138648
C	-3.852034	0.927375	1.208211
H	-1.909317	1.064130	2.138069
C	-4.566596	0.964784	0.007500
H	-4.442640	1.217111	-2.131879

H	-4.372226	0.760043	2.147029
H	-5.643598	0.824623	0.010250
Cu	0.992919	-0.082580	0.102570
C	-0.802652	-2.085163	1.253335
H	-1.185905	-3.112860	1.321691
H	-1.662603	-1.421611	1.132671
C	-0.853099	-1.942884	-1.183579
H	-0.225682	-1.700906	-2.045246
H	-1.550782	-1.113259	-1.056829
C	1.039419	-3.040730	-0.028512
H	1.721461	-2.880500	0.807086
H	0.534376	-4.004413	0.132383
N	0.027924	-1.945234	0.023132
C	1.846163	-3.086390	-1.320034
H	2.659259	-3.811323	-1.201136
H	1.246418	-3.399404	-2.180387
H	2.297999	-2.113573	-1.534170
C	-1.638421	-3.226823	-1.458636
H	-2.323822	-3.473810	-0.641684
H	-2.241332	-3.080742	-2.362330
H	-0.986133	-4.088523	-1.632026
C	-0.070980	-1.728202	2.541818
H	-0.764417	-1.822455	3.385672
H	0.782382	-2.384872	2.735558
H	0.294914	-0.695045	2.515751
C	1.921220	2.899306	-0.058497
H	2.645044	2.620534	0.715612
C	2.636488	2.827204	-1.418130
H	1.947196	3.078672	-2.232995
H	3.468912	3.539479	-1.438914
H	3.034570	1.823045	-1.590628

C	1.388740	4.312789	0.232735
H	2.216433	5.031338	0.230562
H	0.664570	4.619873	-0.530712
H	0.896553	4.356749	1.210133

Int9

G(THF)=-835.0365234 Hartree

C	-2.337784	1.331714	0.078272
C	-3.102819	0.135612	0.061772
C	-2.623524	-1.179821	-0.013439
H	-4.180039	0.250577	0.113373
O	-1.399843	-1.559995	-0.082566
O	-1.077675	1.409165	0.027341
C	-3.629840	-2.313760	-0.014918
H	-3.432634	-2.979527	0.834451
H	-4.663741	-1.963386	0.042571
H	-3.507396	-2.911793	-0.926418
C	-3.091868	2.649723	0.163992
H	-2.851636	3.263230	-0.713222
H	-4.176736	2.522844	0.219997
H	-2.753000	3.205423	1.046920
Cu	0.127766	-0.412888	-0.087744
C	2.136609	1.146471	-1.334532
H	1.472433	2.007756	-1.230683
H	3.168345	1.526180	-1.386089
C	3.094200	-0.677230	-0.006774
H	3.472633	-0.838214	-1.018052
H	3.918299	-0.239338	0.572101
N	1.986268	0.332769	-0.086969
C	2.689704	-2.027416	0.572584
H	1.939095	-2.509807	-0.062935
H	3.571293	-2.679620	0.617884
H	2.276536	-1.945117	1.580968
C	1.78003	0.39490	-

	4	8	2.610896
H	0.730628	0.077651	-2.594025
H	1.924185	1.057574	-3.472180
H	2.401903	-0.492833	-2.766303
C	2.052883	1.280644	1.069784
H	3.014996	1.814505	1.026574
H	1.253685	2.008877	0.917431
C	1.885403	0.631082	2.436514
H	2.713480	-0.038187	2.687921
H	1.851930	1.418321	3.198415
H	0.948799	0.064342	2.492334

Int10-2acac
G(THF)=-1700.95011 Hartree

C	-1.247234	-0.059600	0.254769
C	-2.198224	0.001754	1.029643
C	-3.325010	0.082502	1.893076
C	-4.632242	-0.008301	1.371518
C	-3.148393	0.262430	3.280712
C	-5.731293	0.080433	2.221119
H	-4.766997	-0.146610	0.303349
C	-4.254829	0.350433	4.120804
H	-2.142141	0.332814	3.682062
C	-5.547237	0.260174	3.595402
H	-6.734690	0.009972	1.811041
H	-4.109386	0.490620	5.188115
H	-6.407808	0.329692	4.254571
C	2.175194	0.160169	1.046533
C	3.295814	0.277764	1.913747
C	4.606277	0.236192	1.393809
C	3.110928	0.440027	3.302395
C	5.700377	0.354250	2.246148
H	4.747239	0.111519	0.324760
C	4.212511	0.557979	4.145262
H	2.102304	0.472594	3.702599
C	5.508072	0.515632	3.621591
H	6.706221	0.320887	1.837383
H	4.060779	0.683710	5.213486
H	6.36473	0.60787	4.28305

	4	6	1
C	1.233087	0.061717	0.264626
Cu	0.057700	-1.315705	-0.474323
Cu	-0.056306	1.190942	-0.672278
O	1.325280	2.306000	-1.478520
C	1.098344	3.278649	-2.280060
C	-0.165679	3.714016	-2.705452
C	2.332991	3.987253	-2.783227
C	-1.385324	3.150711	-2.301837
H	-0.202413	4.552554	-3.389874
H	2.977232	3.269024	-3.304155
H	2.093624	4.811425	-3.459297
H	2.903145	4.374302	-1.930432
O	-1.524926	2.159886	-1.502054
C	-2.677774	3.729553	-2.825593
H	-3.285950	4.081352	-1.983615
H	-2.512835	4.557485	-3.519211
H	-3.249708	2.943002	-3.331701
O	-1.307342	-2.564378	-1.082891
C	-1.066829	-3.689408	-1.645836
C	0.203471	-4.194561	-1.959733
C	-2.291935	-4.505391	-1.981334
C	1.413703	-3.532580	-1.705210
H	0.252882	-5.164833	-2.438243
H	-2.946504	-3.924758	-2.642025
H	-2.041466	-5.452615	-2.464797
H	-2.855962	-4.707624	-1.062988
O	1.537597	-2.385620	-1.148585
C	2.714376	-4.187759	-2.103237
H	3.340608	-4.321002	-1.213046
H	2.562662	-5.157195	-2.583799
H	3.260308	-3.52739	-2.78722

1 6

Int10-2Cl

G(THF)=-2515.735232 Hartree

C	1.073328	0.311044	-0.465455
C	1.840250	1.231541	-0.742691
C	2.796511	2.229153	-1.069616
C	3.962228	1.890303	-1.788920
C	2.601713	3.566705	-0.665703
C	4.905747	2.867815	-2.092010
H	4.109248	0.861895	-2.103648
C	3.551718	4.535895	-0.975178
H	1.705951	3.827451	-0.110339
C	4.704749	4.190810	-1.686879
H	5.799927	2.598115	-2.646679
H	3.394150	5.563292	-0.659588
H	5.443769	4.950381	-1.924924
C	-1.721367	1.358021	0.779428
C	-2.591888	2.418496	1.147253
C	-3.805428	2.146853	1.814115
C	-2.258672	3.755126	0.842961
C	-4.658454	3.188973	2.166273
H	-4.060250	1.118792	2.051700
C	-3.118933	4.789298	1.200884
H	-1.326320	3.964320	0.327432
C	-4.319062	4.510769	1.862099
H	-5.589663	2.970632	2.681226
H	-2.853945	5.815641	0.963516
H	-4.987016	5.321082	2.139647
C	-1.022487	0.395996	0.468143
Cu	-0.531229	-0.592094	-1.173003
Cu	0.499651	-0.665483	1.154187
Cl	-0.759440	-1.555910	2.848518

Cl	0.554135	-1.295461	-3.060218
N	2.359427	-1.707220	1.417289
C	2.408805	-2.398107	2.739037
C	2.404283	-2.709038	0.308446
C	3.500203	-0.751750	1.267477
H	1.490868	-2.974506	2.833936
H	3.250581	-3.104581	2.731020
H	2.463671	-2.140984	-0.623421
H	3.322048	-3.303565	0.400286
H	3.425187	-0.334717	0.265558
H	3.331761	0.069898	1.967856
N	-2.491475	-1.357094	-1.486346
C	-2.544904	-2.317385	-2.631139
C	-2.940305	-2.003639	-0.211466
C	-3.359827	-0.178018	-1.783956
H	-3.598931	-2.484815	-2.891156
H	-2.066430	-1.829851	-3.478793
H	-2.851912	-1.249245	0.568730
H	-2.216021	-2.784037	0.029381
H	-3.466219	0.379971	-0.852303
H	-4.356112	-0.537061	-2.070175
C	1.203577	-3.645039	0.252225
H	1.287551	-4.270428	-0.642730
H	1.139821	-4.304934	1.122036
H	0.264537	-3.085457	0.183650
C	2.527468	-1.454000	3.928780
H	2.377216	-2.029762	4.848752
H	3.508921	-0.974874	3.992639
H	1.756318	-0.679478	3.893985
C	4.903292	-1.328418	1.466163
H	5.131511	-2.122433	0.748611

H	5.626994	-0.521510	1.303857
H	5.065583	-1.719634	2.474822
C	-4.352718	-2.587932	-0.211691
H	-4.487792	-3.371450	-0.963693
H	-4.536553	-3.036523	0.771164
H	-5.117610	-1.821712	-0.371906
C	-1.860019	-3.652927	-2.371640
H	-2.400122	-4.270784	-1.647943
H	-1.816000	-4.208676	-3.315024
H	-0.834180	-3.512052	-2.024120
C	-2.818469	0.745705	-2.867967
H	-2.734525	0.250960	-3.839977
H	-3.501474	1.595231	-2.980843
H	-1.832276	1.141128	-2.598419

Int10-Cl-acac
G(THF)=-2108.342083 Hartree

C	0.645694	0.590137	-0.391503
C	1.145821	1.639153	-0.790069
C	1.794146	2.829091	-1.218610
C	3.149988	2.799795	-1.607363
C	1.095210	4.053515	-1.249505
C	3.785625	3.968615	-2.016317
H	3.687365	1.856769	-1.586685
C	1.741411	5.216469	-1.659190
H	0.051871	4.075758	-0.950261
C	3.085264	5.178378	-2.043190
H	4.829319	3.936799	-2.315558
H	1.195906	6.155468	-1.679730
H	3.585060	6.088228	-2.362815
C	2.872461	-1.179393	0.871434
H	2.767347	-0.559736	-0.017745
H	2.33464	-	0.66971

	4	2.108355	8
C	2.717913	0.890550	2.168497
H	3.720083	0.796353	2.605619
H	2.831986	1.329906	1.175843
C	2.219161	-1.243343	3.251737
H	1.553691	-0.752602	3.959602
H	3.242570	-1.167378	3.643999
N	2.143319	-0.472881	1.974387
C	-2.641771	0.463564	0.157486
C	-3.922739	1.076709	0.100803
C	-5.080435	0.360232	0.468622
C	-4.048255	2.417146	-0.321183
C	-6.328804	0.973854	0.414007
H	-4.982868	-0.670262	0.795266
C	-5.301578	3.020663	-0.371171
H	-3.156821	2.969008	-0.603710
C	-6.44402	2.302793	-0.00485
	1		0
H	-7.215078	0.414840	0.700400
H	-5.388337	4.053526	-0.696412
H	-7.420226	2.777500	-0.044910
C	-1.543486	-0.079742	0.241356
Cu	-0.307208	-0.986865	-0.972569
Cu	0.111881	-0.209628	1.349160
Cl	-1.031872	-0.773796	3.239694
O	1.113852	-1.601377	-2.144885
C	1.122338	-2.744885	-2.724319
C	0.100675	-3.703540	-2.664358
C	2.363822	-3.034836	-3.532182
C	-1.110315	-3.547137	-1.971298
H	0.248634	-4.627229	-3.210150
H	3.243108	-2.973065	-2.879917
H	2.333416	-4.020269	-4.002701

H	2.481031	-2.268890	-4.307985
O	-1.444923	-2.528118	-1.271641
C	-2.143954	-4.645276	-2.027995
H	-3.068316	-4.250273	-2.466261
H	-1.807959	-5.503953	-2.613893
H	-2.383302	-4.972392	-1.009437
C	4.351360	-1.475858	1.121053
H	4.514357	-2.128811	1.983755
H	4.752055	-1.987582	0.238339
H	4.936458	-0.562299	1.265789
C	1.821579	-2.708689	3.124008
H	2.562618	-3.300241	2.577853
H	1.732321	-3.134816	4.129426
H	0.850006	-2.816057	2.634152
C	1.863895	1.810637	3.031947
H	1.759164	1.447149	4.058259
H	2.335284	2.799148	3.070728
H	0.860225	1.931084	2.607877

CCP

G(THF)=-426.3547738 Hartree

C	1.627100	-0.307986	-0.000390
C	0.417697	-0.201892	-0.000556
C	-1.006541	-0.083429	-0.000248
C	-1.820974	-1.232866	-0.000815
C	-1.617879	1.185711	0.000635
C	-3.208744	-1.111597	-0.000561
H	-1.354482	-2.213183	-0.001471
C	-3.006425	1.297699	0.000877
H	-0.994243	2.074391	0.001093
C	-3.806324	0.151734	0.000276
H	-3.825669	-2.005897	-0.001016
H	-3.465469	2.282380	0.001540
H	-4.88879	0.242668	0.000482

2

C	3.091489	-0.400690	-0.000420
H	3.362538	-1.465771	-0.001700
C	3.680335	0.242279	-1.270893
H	4.770561	0.130644	-1.275883
H	3.279929	-0.228151	-2.174930
H	3.443002	1.311586	-1.306995
C	3.680204	0.239180	1.271677
H	3.279699	-0.233447	2.174522
H	4.770430	0.127528	1.276509
H	3.442872	1.308398	1.310358

HCP

G(THF)=-615.6846805 Hartree

C	0.679272	0.000040	-0.000255
C	1.900963	0.000021	-0.000161
C	3.321347	0.000006	-0.000054
C	4.033904	-1.217192	-0.000004
C	4.033930	1.217189	-0.000004
C	5.425701	-1.210525	0.000096
H	3.485411	-2.153687	-0.000045
C	5.425726	1.210494	0.000096
H	3.485456	2.153696	-0.000045
C	6.124946	-0.000023	0.000147
H	5.967102	-2.152099	0.000134
H	5.967147	2.152056	0.000134
H	7.211127	-0.000034	0.000225
C	-0.679273	0.000037	-0.000170
C	-1.900963	0.000032	-0.000098
C	-3.321347	0.000011	-0.000024
C	-4.033934	1.217192	0.000011
C	-4.033899	-1.217190	0.000011
C	-5.425731	1.210491	0.000082
H	-3.485464	2.153700	-0.000017
C	-5.42569	-1.21052	0.000082

	6	9	
H	-3.485402	-2.153682	-0.000017
C	-6.124946	-0.000029	0.000118
H	-5.967155	2.152051	0.000109
H	-5.967094	-2.152104	0.000109
H	-7.211127	-0.000045	0.000173

Cu(acac)$_2$(NEt$_3$)
G(THF)=-1180.27898 Hartree

C	2.686588	1.480557	0.101592
C	3.353016	0.475775	-0.617235
C	2.710818	-0.433734	-1.471011
H	4.432951	0.431950	-0.547338
O	1.447893	-0.520610	-1.647613
O	1.424594	1.675453	0.101650
C	3.539679	-1.419075	-2.260372
H	3.294719	-1.333629	-3.325283
H	4.612933	-1.265301	-2.123891
H	3.283048	-2.439352	-1.950102
C	3.485034	2.442102	0.949266
H	3.154150	2.363649	1.991916
H	4.559605	2.250366	0.899126
H	3.286701	3.470140	0.624246
O	-1.271626	1.774189	-0.046398
O	-1.246209	-0.485319	-1.745380
C	-2.532926	1.668231	-0.209172
C	-2.510489	-0.312273	-1.707557
C	-3.177855	0.681569	-0.973233
C	-3.361706	2.718570	0.492541
C	-3.316900	-1.286596	-2.533580
H	-4.259029	0.712857	-1.030579
H	-3.071475	3.713034	0.133203
H	-4.433802	2.579863	0.333565
H	-3.149514	2.689646	1.567898
H	-3.139968	-2.304280	-2.164681

H	-4.388655	-1.076231	-2.500641
H	-2.974944	-1.256116	-3.574572
Cu	0.071581	0.494046	-0.680014
N	-0.273222	-0.972355	1.436046
C	-1.278625	-1.982845	1.039145
C	-0.819246	-0.125449	2.516899
C	1.019869	-1.563897	1.841169
H	-2.171525	-1.428307	0.735167
H	-0.909030	-2.486528	0.143363
H	-1.771986	0.272295	2.154020
H	-1.042319	-0.738846	3.406425
H	1.747961	-0.748812	1.871990
H	0.956467	-1.971693	2.865983
C	1.537727	-2.649789	0.900681
H	2.590862	-2.851360	1.127747
H	0.990135	-3.591153	1.011198
H	1.466094	-2.333263	-0.141281
C	0.075602	1.034387	2.942820
H	-0.472644	1.658260	3.659388
H	0.986547	0.689394	3.444327
H	0.359243	1.648686	2.087122
C	-1.673690	-3.028499	2.091036
H	-2.167678	-2.579941	2.959035
H	-2.378357	-3.739250	1.642772
H	-0.812387	-3.600830	2.451945

Cu(acac)Cl(NEt_3)
G(THF)=-1295.304948 Hartree

C	-2.237366	1.264839	-0.528833
C	-3.097688	0.314907	0.037714
C	-2.713380	-0.973434	0.448920
H	-4.139789	0.586764	0.150330
O	-1.531025	-1.454895	0.377712
O	-	1.10656	-

	0.980952	3	0.724617
C	-3.754342	-1.909624	1.013303
H	-3.442441	-2.246417	2.008807
H	-4.740053	-1.443774	1.082606
H	-3.821694	-2.799931	0.376708
C	-2.782613	2.606860	-0.950990
H	-2.569423	2.769968	-2.013891
H	-3.858838	2.690566	-0.783502
H	-2.268083	3.397669	-0.391773
Cl	0.977615	-2.221898	-1.369595
Cu	0.053165	-0.473259	-0.220044
C	2.272233	-0.055611	1.669905
H	1.439304	-0.148239	2.369561
H	2.999658	0.639521	2.115621
N	1.728907	0.598874	0.433272
C	2.919669	-1.422697	1.491114
H	3.846333	-1.378944	0.912017
H	3.171035	-1.805681	2.486897
H	2.245483	-2.133479	1.007822
C	2.337209	1.327554	-1.917072
H	3.120515	1.184714	-2.669565
H	1.415675	0.883395	-2.307111
H	2.182638	2.403788	-1.799429
C	2.777632	0.644553	-0.628082
H	3.044649	-0.386671	-0.852904
H	3.663371	1.147590	-0.211795
C	0.336551	2.095100	1.954677
H	-0.065860	3.113789	1.981033
H	-0.509259	1.409680	1.841050
H	0.810091	1.902581	2.921286
C	1.313770	1.993417	0.787094
H	0.852799	2.424692	-0.097988
H	2.226063	2.564543	1.014440

TS1
G(THF)=-1550.854666 Hartree

Cl	2.315451	1.808055	-1.229775
C	-0.566444	-0.723724	-0.461119
C	-1.716947	-1.160957	-0.352077
C	-3.065178	-1.605736	-0.209236
C	-3.641205	-2.505698	-1.132072
C	-3.867283	-1.142425	0.857522
C	-4.963528	-2.920316	-0.992012
H	-3.036933	-2.870882	-1.957272
C	-5.189349	-1.560948	0.990427
H	-3.437821	-0.452813	1.578869
C	-5.745776	-2.451229	0.067627
H	-5.386525	-3.613572	-1.714395
H	-5.788259	-1.191561	1.818930
H	-6.776739	-2.776906	0.173439
Cu	1.197886	-0.110609	-0.565428
C	3.715808	-0.545322	1.048322
H	4.017368	0.351240	0.501012
H	3.050020	-0.210505	1.848670
C	2.377494	-2.595319	0.721100
H	1.704853	-3.053556	-0.007035
H	3.198847	-3.309497	0.897246
C	3.692352	-1.670198	-1.112281
H	4.143471	-0.729934	-1.442425
H	4.511277	-2.365551	-0.869093
N	2.905218	-1.354770	0.103559
H	-0.235933	1.792364	-0.229257
C	-0.924464	1.924703	1.697523
H	-1.560855	2.605494	2.264588
H	-1.412576	0.952405	1.620995
C	-2.20432	2.339589	-0.40702

	5		8
H	-2.489899	1.291815	-0.317916
H	-2.021896	2.542097	-1.462847
N	-0.862127	2.446510	0.281085
C	1.606243	-2.369698	2.017123
H	1.144464	-3.314720	2.325327
H	2.248776	-2.032901	2.836916
H	0.806539	-1.636135	1.872846
C	2.861596	-2.249526	-2.253923
H	3.488951	-2.335090	-3.148814
H	2.470279	-3.246107	-2.026702
H	2.013878	-1.595577	-2.490862
C	4.943373	-1.227129	1.659931
H	5.671476	-1.527527	0.899429
H	5.443200	-0.522690	2.335287
H	4.677350	-2.114017	2.245251
C	-3.270837	3.262464	0.158351
H	-3.000271	4.319175	0.071810
H	-4.188020	3.105558	-0.418709
H	-3.499605	3.042198	1.205018
C	0.446379	1.773752	2.338507
H	1.114807	1.189368	1.697832
H	0.920043	2.734345	2.558180
H	0.323434	1.234502	3.283610
C	-0.236730	3.817533	0.203532
H	-0.780567	4.450572	0.907945
H	0.786533	3.694186	0.554968
C	-0.232740	4.399749	-1.200163
H	-1.234764	4.658504	-1.553226
H	0.364024	5.317790	-1.183080
H	0.237459	3.709071	-1.905782

TS2

G(THF)=-819.7561742 Hartree

C	1.940524	0.658232	0.121284

C	1.702729	-0.742385	0.162872
C	2.691177	-1.621344	-0.326330
C	3.843602	-1.075937	-0.885414
C	4.050433	0.319143	-0.961217
C	3.081486	1.197496	-0.451038
C	0.775605	1.315000	0.744604
C	0.447190	-1.009910	0.836160
H	2.544758	-2.696841	-0.282190
H	4.606530	-1.741945	-1.283261
H	4.965435	0.707193	-1.399163
H	3.225388	2.274598	-0.484504
O	0.496361	2.500416	0.810997
O	-0.141947	-2.089590	1.046236
N	0.011083	0.251471	1.330590
O	-1.590717	0.527538	1.138390
C	-1.981893	0.378875	-0.128853
O	-	0.43225	-

	1.254716	2	1.106753
C	-3.473620	0.047841	-0.194582
H	-3.956302	0.482614	0.687794
C	-4.106263	0.614615	-1.465555
H	-4.032099	1.707885	-1.496358
H	-3.601675	0.218624	-2.352614
H	-5.167165	0.343232	-1.518615
C	-3.607326	-1.484516	-0.116688
H	-3.089400	-1.877285	0.763528
H	-4.663658	-1.774558	-0.067667
H	-3.163112	-1.951410	-1.003502

TS3-acac
G(THF)=-1261.302017 Hartree

C	1.285582	-0.068600	0.215633
C	-2.225639	-2.608254	-2.208844
C	-3.350013	-3.541082	-1.908734
H	-	-	-

	2.278454	1.996561	3.107052
H	-4.302467	-3.189613	-2.321800
H	-3.171822	-4.549875	-2.326988
H	-3.475360	-3.677749	-0.825482
C	-0.911714	-2.764046	-1.522614
H	-0.234842	-1.926598	-1.719940
H	-1.035232	-2.847729	-0.434298
H	-0.386494	-3.684190	-1.842714
C	2.476313	-0.354014	0.127523
C	3.869472	-0.654516	0.020446
C	4.329000	-1.987154	0.052582
C	4.818409	0.380245	-0.115139
C	5.689326	-2.271205	-0.047594
H	3.606591	-2.791102	0.158098
C	6.177171	0.089164	-0.213073
H	4.475411	1.410422	-0.139457
C	6.619412	-1.236366	-0.180195
H	6.025234	-3.304349	-0.020498
H	6.893988	0.899636	-0.315335
H	7.679662	-1.460777	-0.256583
O	-0.923710	-1.004607	1.826435
C	-2.001562	-1.663369	2.003688
C	-3.187327	-1.504426	1.263728
C	-1.953318	-2.703736	3.098744
C	-3.365653	-0.557233	0.247237
H	-4.024530	-2.147182	1.506864
H	-1.211989	-3.468622	2.836450
H	-1.620690	-2.237943	4.033296
H	-2.920491	-3.186264	3.259706
O	-2.486083	0.288531	-0.140425
C	-4.696712	-0.462837	-0.458484

H	-5.142714	0.520563	-0.264051
H	-4.539134	-0.540916	-1.539584
H	-5.395271	-1.239404	-0.138422
Cu	-0.593507	0.335119	0.376622
C	-1.572472	3.067292	0.568559
H	-1.264422	2.904371	1.605013
H	-2.518882	2.542832	0.428966
C	0.777872	2.980846	-0.202433
H	1.455020	2.337678	-0.762865
H	0.763500	3.962341	-0.696606
C	-1.039677	2.390021	-1.724735
H	-0.929140	3.407243	-2.123789
H	-2.103221	2.146706	-1.711272
N	-0.578712	2.373830	-0.306260
C	-1.762873	4.563760	0.314350
H	-2.522109	4.941422	1.008661
H	-0.845708	5.136712	0.483089
H	-2.113711	4.767231	-0.702265
C	-0.313206	1.401531	-2.629326
H	-0.721945	1.484642	-3.643125
H	0.762356	1.592086	-2.686507
H	-0.459989	0.371322	-2.290042
C	1.296113	3.125328	1.222611
H	2.348814	3.427130	1.183634
H	0.754346	3.886479	1.792472
H	1.243729	2.175322	1.762530

TS3-Cl

G(THF)=-1376.322897 Hartree

C	-0.525675	-0.154359	0.094554
C	-1.183745	3.896943	-0.585681
C	-2.006337	3.381558	0.546878
H	-0.887808	4.943278	-0.593387
H	-1.97664	4.048679	1.415564

	0		
H	-3.067885	3.257339	0.262255
H	-1.666652	2.384853	0.864602
C	-1.025839	3.095301	-1.832807
H	-0.213655	3.472180	-2.465366
H	-0.827331	2.038004	-1.605509
H	-1.946292	3.102947	-2.447426
C	-1.703395	-0.498596	0.104448
C	-3.091037	-0.835025	0.100966
C	-3.981311	-0.198942	0.990218
C	-3.598954	-1.791802	-0.800580
C	-5.338327	-0.511860	0.972929
H	-3.596010	0.540397	1.685571
C	-4.957564	-2.099454	-0.810413
H	-2.918226	-2.283708	-1.488890
C	-5.831914	-1.461719	0.074106
H	-6.013341	-0.012012	1.662168
H	-5.336079	-2.837774	-1.511934
H	-6.891154	-1.702404	0.062357
Cl	2.579535	2.342848	0.130048
Cu	1.224426	0.579634	0.083429
C	3.069628	-1.066546	1.522892
H	3.668015	-1.978320	1.640554
H	3.745906	-0.210182	1.576819
C	1.729686	-2.330289	-0.105621
H	2.390343	-3.171797	0.140198
H	0.897532	-2.346060	0.596485
N	2.486027	-1.064853	0.145297
C	2.039393	-0.978595	2.642396
H	1.353352	-1.830015	2.652297
H	2.568327	-0.962394	3.601602
H	1.447529	-0.058412	2.570211

C	1.197809	-2.478002	-1.524376
H	1.993270	-2.633896	-2.258738
H	0.539596	-3.353233	-1.555920
H	0.605889	-1.607578	-1.820955
C	3.553474	-0.828771	-0.879710
H	3.052162	-0.668641	-1.836821
H	4.037746	0.110081	-0.609405
C	4.596276	-1.939207	-1.010783
H	4.158274	-2.893040	-1.319319
H	5.316555	-1.639934	-1.780108
H	5.150918	-2.095983	-0.080716

TS4-acac

G(THF)=-1261.316226 Hartree

C	1.108446	-0.492369	-0.166313
C	-0.190768	-2.236092	-0.526799
C	0.372907	-3.038474	0.622833
H	-1.281344	-2.279548	-0.500520
H	0.041272	-2.636684	1.583614
H	-0.010958	-4.067373	0.539892
H	1.464872	-3.076693	0.606582
C	0.320920	-2.579684	-1.905874
H	-0.090396	-1.913264	-2.670309
H	1.412322	-2.544687	-1.957399
H	-0.002795	-3.603126	-2.150928
C	2.329479	-0.432360	-0.076443
C	3.743638	-0.319782	0.051609
C	4.564969	-0.205971	-1.089631
C	4.350785	-0.316706	1.325135
C	5.946904	-0.094314	-0.957100
H	4.105241	-0.206981	-2.073534
C	5.733515	-0.205302	1.447946
H	3.72428	-	2.20803

	6	0.401187	6
C	6.537648	-0.093702	0.309851
H	6.565821	-0.007799	-1.846061
H	6.185854	-0.204655	2.435960
H	7.615842	-0.006340	0.409570
O	-2.425447	-0.343546	-1.276205
C	-3.520625	-0.859395	-0.864981
C	-3.806985	-1.282638	0.442713
C	-4.594914	-1.007176	-1.923337
C	-2.961045	-1.173325	1.577857
H	-4.790953	-1.706445	0.608839
H	-4.811741	0.024601	-2.360039
H	-4.223116	-1.644252	-2.735232
H	-5.521574	-1.434534	-1.531330
O	-1.787661	-0.706055	1.585294
C	-3.50704	-1.64553	2.914263
	3	1	
H	-2.827715	-2.393908	3.339545
H	-3.532515	-0.800408	3.613372
H	-4.510439	-2.073878	2.841104
Cu	-0.694571	-0.214341	-0.253124
C	-2.102059	2.221415	0.596402
H	-2.027194	1.713060	1.557607
H	-2.909419	1.732923	0.047504
C	0.348151	2.521399	0.494198
H	1.218763	2.173485	-0.061431
H	0.309411	3.615934	0.394794
C	-0.973222	2.415033	-1.557785
H	-0.983517	3.514124	-1.558008
H	-1.944541	2.069677	-1.919290
N	-0.848267	1.925750	-0.156840
C	-2.435669	3.699863	0.806830
H	-2.57284	4.237225	-0.13705

	7		1
H	-3.376835	3.768114	1.364884
H	-1.669510	4.221651	1.389570
C	0.514399	2.133170	1.958318
H	1.501397	2.462176	2.302669
H	-0.236525	2.599402	2.603981
H	0.455236	1.048627	2.084496
C	0.113925	1.923941	-2.507968
H	-0.086017	2.326774	-3.507829
H	1.114491	2.252031	-2.211204
H	0.120286	0.831606	-2.576411

TS4-Cl

G(THF)=-1376.347613 Hartree

C	0.567263	0.541783	-0.059269
C	-0.398111	2.587760	-0.720571
C	0.350250	2.552801	-2.029780
H	-1.445253	2.842783	-0.879014
H	-0.079412	1.827951	-2.728404
H	0.251819	3.548296	-2.491850
H	1.412244	2.334125	-1.901372
C	0.205839	3.397016	0.396526
H	-0.363416	3.298704	1.325650
H	1.247154	3.125298	0.584939
H	0.173930	4.457629	0.100335
C	1.756639	0.264518	0.024465
C	3.131051	-0.108962	0.090970
C	3.684857	-0.963019	-0.885262
C	3.961183	0.368099	1.125556
C	5.028562	-1.323960	-0.825665
H	3.049940	-1.333986	-1.684168
C	5.303580	0.000050	1.178325
H	3.541162	1.026457	1.880098
C	5.842983	-0.845564	0.204870
H	5.441820	-1.982074	-1.585107
H	5.931665	0.375394	1.981540
H	6.890456	-1.129864	0.249014

		3	
Cu	-1.252081	0.760252	-0.059117
Cl	-3.318695	1.663126	0.301322
C	-2.328737	-1.447434	1.599747
H	-3.259798	-0.883047	1.688093
H	-2.552363	-2.502186	1.811135
C	-3.027077	-1.536197	-0.743232
H	-3.788114	-0.803717	-0.473075
H	-2.685122	-1.280791	-1.750066
C	-0.763070	-2.260135	-0.084427
H	0.076071	-1.954379	0.539241
H	-1.064786	-3.266409	0.239099
N	-1.879473	-1.311486	0.185421
C	-0.307241	-2.301582	-1.538146
H	0.614191	-2.891526	-1.599658
H	-1.044303	-2.769133	-2.198048
H	-0.085816	-1.298277	-1.913458
C	-3.633257	-2.941211	-0.742777
H	-4.467507	-2.959708	-1.453470
H	-2.918372	-3.710149	-1.052204
H	-4.031227	-3.217594	0.238757
C	-1.326908	-0.923310	2.622272
H	-1.754971	-1.027053	3.625879
H	-0.379118	-1.469268	2.604674
H	-1.113232	0.138558	2.453804

TS5-2acac
G(THF)=-1700.941096 Hartree

C	0.938496	0.553940	-0.059458
C	1.863599	1.373178	-0.074461
C	2.931584	2.303877	-0.085640
C	4.270689	1.857801	-0.066979
C	2.664599	3.690086	-0.110905

C	5.312149	2.780258	-0.072166
H	4.472536	0.791543	-0.048030
C	3.715516	4.601967	-0.116366
H	1.634503	4.032311	-0.125555
C	5.039118	4.151533	-0.096768
H	6.340113	2.430113	-0.056938
H	3.503004	5.666940	-0.135493
H	5.856004	4.867413	-0.100613
C	-1.869780	1.365490	0.070019
C	-2.940766	2.292741	0.080502
C	-4.278511	1.842652	0.061622
C	-2.677957	3.679754	0.105895
C	-5.322727	2.762004	0.066790
H	-4.477187	0.775800	0.042623
C	-3.731587	4.588490	0.111391
H	-1.648886	4.025046	0.120757
C	-5.053829	4.134091	0.091624
H	-6.349639	2.408790	0.051441
H	-3.522239	5.654087	0.130724
H	-5.872862	4.847512	0.095549
C	-0.941349	0.550017	0.056614
Cu	-0.066866	-0.603724	-1.262246
Cu	0.069776	-0.597217	1.265567
O	-1.333023	-1.464145	2.319997
C	-1.095705	-2.351691	3.210788
C	0.172701	-2.836341	3.574762
C	-2.318148	-2.900574	3.909175
C	1.399357	-2.425747	3.025113
H	0.207704	-3.594274	4.348171
H	-2.998468	-3.332924	3.165784
H	-2.07044	-3.66114	4.653605

	8	1	
H	-2.855495	-2.080034	4.399847
O	1.555020	-1.547011	2.107347
C	2.676617	-3.053164	3.533214
H	3.337137	-2.269594	3.923504
H	2.498126	-3.793720	4.316677
H	3.202469	-3.532899	2.698973
O	1.339019	-1.468415	-2.314260
C	1.104391	-2.355234	-3.206503
C	-0.162683	-2.841813	-3.572517
C	2.328634	-2.900698	-3.904386
C	-1.390629	-2.434490	-3.023371
H	-0.195458	-3.598595	-4.347147
H	3.009070	-3.332736	-3.160923
H	2.083200	-3.660694	-4.650147
H	2.864821	-2.078384	-4.393357
O	-1.548803	-1.557462	-2.104377
C	-2.666229	-3.063518	-3.533586
H	-3.328193	-2.280474	-3.922476
H	-2.485682	-3.801913	-4.318609
H	-3.191533	-3.546263	-2.700735

TS5-2Cl
G(THF)=-2515.734471 Hartree

C	0.931772	0.467625	-0.390102
C	1.780599	1.308114	-0.698635
C	2.824819	2.198382	-1.053069
C	3.890714	1.756494	-1.866477
C	2.823371	3.527434	-0.578428
C	4.926952	2.626672	-2.191254
H	3.887220	0.735243	-2.233861
C	3.866582	4.387294	-0.909162
H	2.003688	3.866310	0.047759
C	4.91953	3.94097	-

	0	9	1.713748
H	5.743501	2.279605	-2.817798
H	3.860001	5.408094	-0.538150
H	5.732076	4.615436	-1.967873
C	-1.639485	1.502841	0.629935
C	-2.555425	2.525953	0.981892
C	-3.816001	2.200833	1.527718
C	-2.218562	3.882207	0.782983
C	-4.712247	3.211048	1.863738
H	-4.072049	1.157823	1.684632
C	-3.122966	4.883103	1.124932
H	-1.249406	4.131459	0.361788
C	-4.369863	4.552029	1.664350
H	-5.679772	2.952989	2.284521
H	-2.856157	5.924565	0.970056
H	-5.072165	5.337056	1.929229
C	-0.878967	0.578274	0.333937
Cu	-0.520601	-0.627728	-1.187595
Cu	0.472025	-0.614432	1.204376
Cl	-0.875513	-1.411726	2.877904
Cl	0.703624	-1.546644	-2.890415
N	2.283479	-1.704083	1.452308
C	2.388609	-2.186002	2.858341
C	2.204376	-2.854653	0.503240
C	3.445712	-0.841380	1.081128
H	1.470459	-2.727383	3.079467
H	3.225094	-2.895077	2.931125
H	2.222576	-2.429516	-0.503972
H	3.098392	-3.481229	0.619784
H	3.317227	-0.586869	0.029812
H	3.356495	0.090940	1.643581
N	-	-	-

	2.486561	1.362117	1.474485
C	-2.528568	-2.438129	-2.509403
C	-2.994563	-1.842212	-0.151350
C	-3.296092	-0.194668	-1.929971
H	-3.575666	-2.604476	-2.798689
H	-1.998715	-2.060170	-3.382971
H	-2.900691	-1.004611	0.539389
H	-2.304832	-2.609656	0.203554
H	-3.371493	0.487562	-1.080266
H	-4.311246	-0.534132	-2.172439
C	0.961859	-3.721849	0.656506
H	0.957027	-4.468423	-0.145061
H	0.931469	-4.254150	1.611435
H	0.044997	-3.129757	0.575245
C	2.554783	-1.064744	3.876340
H	2.461472	-1.484668	4.883932
H	3.529411	-0.571744	3.809297
H	1.769834	-0.310857	3.757111
C	4.837303	-1.440777	1.291087
H	4.988393	-2.358028	0.713706
H	5.578117	-0.710140	0.946719
H	5.050395	-1.657074	2.342447
C	-4.425866	-2.378546	-0.128326
H	-4.566244	-3.235801	-0.794437
H	-4.651172	-2.711061	0.891367
H	-5.161385	-1.612932	-0.394622
C	-1.894678	-3.754041	-2.079387
H	-2.466104	-4.263714	-1.297787
H	-1.854151	-4.419937	-2.948831
H	-0.870570	-3.603420	-1.731065
C	-2.707130	0.545617	-3.124410

H	-2.677910	-0.069716	-4.028343
H	-3.326230	1.424457	-3.337453
H	-1.688864	0.893928	-2.915478

TS5-Cl-acac
G(THF)=-2108.337682 Hartree

C	0.240685	0.741821	-0.616402
C	0.781063	1.809187	-0.914059
C	1.432192	3.035009	-1.209496
C	2.761495	3.047325	-1.681572
C	0.760145	4.258643	-1.005374
C	3.399585	4.257186	-1.938203
H	3.275494	2.105251	-1.843972
C	1.409848	5.462078	-1.263709
H	-0.262805	4.248016	-0.642368
C	2.728204	5.465661	-1.729181
H	4.422943	4.258612	-2.301970
H	0.887187	6.400186	-1.101132
H	3.230726	6.407522	-1.929343
C	2.646590	-1.348978	0.398169
H	2.472500	-0.750235	-0.496149
H	1.948631	-2.188253	0.356004
C	3.055666	0.765164	1.543440
H	4.094788	0.539650	1.817577
H	3.059152	1.115954	0.508655
C	2.454028	-1.210296	2.859285
H	2.048791	-0.566920	3.639796
H	3.530770	-1.328214	3.045222
N	2.257984	-0.496207	1.565285
C	-2.579986	0.524425	0.127698
C	-3.944788	0.886217	0.027060
C	-4.943264	-0.108861	-0.054203
C	-4.320009	2.246984	-0.002867
C	-	0.25526	-

	6.281095	0	0.166914
H	-4.652013	-1.154095	-0.025789
C	-5.662096	2.596918	-0.112830
H	-3.551303	3.010693	0.062021
C	-6.644552	1.605389	-0.196194
H	-7.043967	-0.515310	-0.229951
H	-5.943807	3.645641	-0.134189
H	-7.690813	1.883953	-0.282603
C	-1.395492	0.194562	0.250672
Cu	-0.381065	-1.020436	-0.943125
Cu	0.220950	0.011109	1.348869
Cl	-0.658426	0.050243	3.468140
O	0.799999	-1.597415	-2.392166
C	1.026240	-2.832177	-2.643521
C	0.377168	-3.925769	-2.045523
C	2.088858	-3.088618	-3.685907
C	-0.671281	-3.846358	-1.112774
H	0.681359	-4.915553	-2.363458
H	3.025466	-2.610167	-3.375906
H	2.266083	-4.154305	-3.849855
H	1.788541	-2.625833	-4.633747
O	-1.156582	-2.767369	-0.622226
C	-1.319453	-5.119525	-0.625040
H	-2.385179	-5.106422	-0.883545
H	-0.859577	-6.013897	-1.052159
H	-1.253591	-5.165817	0.468393
C	4.080614	-1.879136	0.389563
H	4.293342	-2.526609	1.245815
H	4.222652	-2.475596	-0.519064
H	4.821030	-1.073238	0.374808
C	1.760393	-2.565682	2.920872
H	2.23793	-	2.27820

	6	3.311982	0
H	1.800643	-2.938277	3.950326
H	0.705714	-2.482391	2.639770
C	2.517358	1.872398	2.441309
H	2.516158	1.593524	3.498767
H	3.152098	2.758567	2.326498
H	1.495699	2.150664	2.160730

CO_2
G(THF)=-188.6589785 Hartree

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169352
O	0.000000	0.000000	-1.169352

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isobutyryloxy radical
G(THF)=-307.0888539 Hartree

O	-1.512846	-1.047710	-0.096687
C	-0.817984	-0.004199	0.071300
O	-1.541204	1.027784	-0.043128
C	0.650543	0.008802	0.389013
H	0.700052	0.027133	1.488593
C	1.324702	-1.273829	-0.111361
H	1.298429	-1.327566	-1.205458
H	2.371873	-1.287257	0.207277
H	0.836602	-2.168260	0.288591
C	1.307031	1.286025	-0.149993
H	0.805910	2.184715	0.223231
H	2.353833	1.323855	0.167800
H	1.279948	1.305988	-1.245260

----

isopropyl radical
G(THF)=-118.4654905 Hartree

C	0.012726	-0.198057	1.296280
H	0.754607	-1.010043	1.298716
H	-0.963380	-0.677699	1.500106
H	0.225733	0.461354	2.145900
C	0.012726	0.539552	-0.000000
H	-0.262994	1.592151	-0.000000
C	0.012726	-0.198057	-1.296280
H	-0.96338	-0.67769	-1.50010

	0	9	6
H	0.225733	0.461354	-2.145900
H	0.754607	-1.010043	-1.298716

N-(isobutyric)phthalimide
G(THF)=-819.6733951 Hartree

C	0.571403	1.183198	-0.350612
C	0.571713	-1.183554	-0.350432
C	1.962982	0.701223	-0.134412
C	1.963152	-0.701175	-0.134226
C	3.130302	1.424409	0.055608
C	3.130638	-1.424030	0.056027
C	4.314609	0.700185	0.251651
H	3.125164	2.509526	0.056259
C	4.314774	-0.699469	0.251859
H	3.125760	-2.509148	0.056956
H	5.247137	1.233533	0.408490
H	5.247429	-1.232552	0.408841
N	-0.156509	-0.000293	-0.596125
O	0.106421	-2.301569	-0.336974
O	0.105864	2.301116	-0.337622
O	-1.529935	-0.000466	-0.646844
C	-2.122236	-0.000381	0.624455
O	-1.466295	-0.000342	1.631216
C	-3.625565	-0.000140	0.482963
H	-4.002298	-0.000765	1.510245
C	-4.103934	1.275068	-0.232032
H	-3.760210	1.297115	-1.270785
H	-5.198693	1.301975	-0.231089
H	-3.737963	2.176528	0.271248
C	-4.104520	-1.274066	-0.233855
H	-3.738767	-2.176423	0.267976
H	-5.199289	-1.300587	-0.232710
H	-3.761054	-1.294679	-1.272720

N-(isobutyric)phthalimide radical anion
G(THF)=-819.7785558 Hartree

C	0.593866	1.205109	-0.343899
C	0.593078	-1.204186	-0.344274
C	1.939488	0.721497	-0.141733
C	1.939002	-0.721544	-0.141854
C	3.141450	1.423258	0.055424
C	3.140481	-1.424154	0.055237
C	4.316200	0.712508	0.249731
H	3.140863	2.511038	0.057667
C	4.315713	-0.714232	0.249641
H	3.139158	-2.511933	0.057279
H	5.251757	1.244201	0.405650
H	5.250909	-1.246582	0.405480
N	-0.133435	0.000727	-0.552945
O	0.087654	-2.338223	-0.364780
O	0.089309	2.339523	-0.364332
O	-1.515452	0.001056	-0.604632
C	-2.118763	0.000394	0.634434
O	-1.510570	0.000249	1.675005
C	-3.626022	-0.000284	0.467154
H	-4.023017	-0.000384	1.487303
C	-4.095275	1.271960	-0.256812
H	-3.728162	1.293506	-1.287629
H	-5.190432	1.303224	-0.279971
H	-3.737018	2.174492	0.250773
C	-4.093805	-1.273281	-0.256466
H	-3.734361	-2.175248	0.251282
H	-5.188925	-1.305902	-0.279505
H	-3.726745	-1.294608	-1.287306

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phenylacetylene
G(THF)=-308.4315702 Hartree

C	1.511884	-1.209708	-0.000008
C	0.11902	-	0.00000

	1	1.214951	0
C	-0.592307	-0.000002	0.000001
C	0.119019	1.214950	-0.000007
C	1.511880	1.209710	-0.000015
C	2.211594	0.000001	-0.000015
H	2.052661	-2.151740	-0.000008
H	-0.429008	-2.151900	0.000005
H	-0.429013	2.151897	-0.000007
H	2.052658	2.151742	-0.000021
H	3.297868	0.000003	-0.000021
C	-2.021959	-0.000002	0.000003
C	-3.233009	-0.000001	0.000024
H	-4.301917	0.000010	0.000156

----

phthalimide

G(THF)=-513.2047614 Hartree

C	1.241900	1.168942	0.000260
C	1.241897	-1.168945	0.000119
C	-0.175210	0.699367	0.000058
C	-0.175211	-0.699362	-0.000004
C	-1.357544	1.424124	-0.000043
C	-1.357544	-1.424119	-0.000160
C	-2.557867	0.700284	-0.000177
H	-1.352248	2.509465	0.000005
C	-2.557867	-0.700278	-0.000234
H	-1.352250	-2.509459	-0.000212
H	-3.503980	1.233029	-0.000238
H	-3.503981	-1.233023	-0.000342
N	2.011482	-0.000004	-0.000058
O	1.674476	-2.305382	0.000028
O	1.674493	2.305374	0.000231
H	3.025014	-0.000001	0.000215

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phthalimide anion

G(THF)=-512.7240905 Hartree

C	1.317859	-1.114879	-0.000241
C	1.317859	1.114880	0.000000
C	-0.142708	-0.696057	-0.000039
C	-0.142708	0.696057	0.000039
C	-1.325822	-1.419932	0.000036
C	-1.325822	1.419932	0.000158
C	-2.532080	-0.700189	0.000168
H	-1.319340	-2.506999	-0.000028
C	-2.532081	0.700189	0.000223
H	-1.319340	2.506998	0.000220
H	-3.479467	-1.233684	0.000219
H	-3.479467	1.233684	0.000326
N	2.116922	0.000000	-0.000151
O	1.685761	2.295391	-0.000055
O	1.685762	-2.295391	-0.000163

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triethylamine

G(THF)=-292.3649642 Hartree

N	0.000050	-0.000300	0.009476
C	-1.379258	-0.252893	0.444240
H	-1.929431	0.691416	0.391324
H	-1.410472	-0.570976	1.504375
C	0.908879	-1.068275	0.444145
H	0.366925	-2.017308	0.390952
H	1.199815	-0.936451	1.504367
C	0.470704	1.320776	0.444118
H	1.563585	1.325688	0.391199
H	0.210822	1.506893	1.504262
C	-0.058185	2.453142	-0.434058
H	-1.151481	2.522068	-0.407365
H	0.341787	3.416780	-0.096230
H	0.244092	2.297462	-1.475872
C	-2.096223	-1.276703	-0.433778
H	-1.61115	-2.25890	-0.40584

	3	7	3
H	-3.131316	-1.410046	-0.096894
H	-2.110797	-0.937804	-1.475851
C	2.154105	-1.175976	-0.433945
H	2.760336	-0.263580	-0.406589
H	2.788636	-2.004392	-0.096602
H	1.868168	-1.359171	-1.475900

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triethylamine hydrochloride
G(THF)=-753.2474939 Hartree

H	-0.683532	-0.132437	-0.191112
C	1.101706	-0.469907	-1.146380
H	0.867303	-1.533309	-1.085059
H	0.675213	-0.094592	-2.079323
C	0.720649	-0.220539	1.339391
H	1.701207	0.216150	1.544700
H	-0.005554	0.236529	2.011937
C	0.296478	1.697352	-0.208883
H	0.047325	1.875647	-1.257480
H	1.307615	2.067230	-0.024546
N	0.319559	0.200694	-0.047283
Cl	-2.505987	-0.787178	-0.560419
C	2.602201	-0.232922	-1.088753
H	3.062298	-0.748380	-1.938182
H	2.859710	0.827544	-1.166382
H	3.048729	-0.636898	-0.175071
C	-0.722095	2.377787	0.695189
H	-0.429985	2.357710	1.748697
H	-0.802196	3.427377	0.393602
H	-1.708069	1.914590	0.589261
C	0.715844	-1.730220	1.526698
H	1.515832	-2.225323	0.969330
H	0.865753	-1.946143	2.589565
H	-	-	1.22460

	0.245481	2.157833	1

Int3-Me
G(THF)=-605.8604742 Hartree

C	-2.367133	0.001241	-0.002068
C	-3.596154	0.000122	-0.001583
Cu	-0.522146	0.002656	-0.002033
C	1.987587	-0.170873	1.401027
H	3.086974	-0.223388	1.375125
H	1.714897	0.730881	1.950744
C	1.995037	1.296048	-0.548149
H	1.732934	1.319328	-1.606604
H	3.093780	1.298028	-0.478876
N	1.489204	0.000352	0.001327
C	1.413284	-1.377880	2.134907
H	1.752605	-2.332270	1.721985
H	1.732781	-1.339374	3.182434
H	0.317139	-1.361291	2.112512
C	1.416387	2.537645	0.121599
H	1.736823	2.652713	1.161040
H	1.752987	3.424340	-0.427381
H	0.320249	2.518177	0.097783
C	-5.060332	-0.002633	0.000107
H	-5.462387	-1.021500	-0.077653
H	-5.463931	0.437932	0.921406
H	-5.466430	0.573407	-0.841942
C	1.994188	-1.125228	-0.844302
H	3.093254	-1.070002	-0.876639
H	1.727096	-2.052529	-0.336061
C	1.420736	-1.166177	-2.256801
H	1.741635	-0.323169	-2.875455
H	1.761150	-2.084355	-2.748762
H	0.324645	-1.179994	-2.232429

Int4-Me
G(THF)=-605.7408834 Hartree

C	-1.970423	0.047012	-0.319081
C	-3.080006	-0.274439	0.093890
Cu	-0.363984	0.699841	-1.196702
C	0.680755	-1.111940	1.007850
H	1.444146	-1.313446	1.772823
H	-0.230970	-0.806542	1.519415
C	2.281537	-0.275030	-0.698297
H	2.486594	0.631789	-1.275720
H	1.946574	-1.031904	-1.411111
C	1.440643	1.224251	1.045775
H	1.901477	1.971275	0.392223
H	2.190807	0.925355	1.789849
N	1.123797	0.048551	0.187016
C	0.399800	-2.373179	0.202104
H	1.307521	-2.815580	-0.219647
H	-0.055654	-3.117490	0.864547
H	-0.306157	-2.171405	-0.609473
C	0.237472	1.841618	1.747372
H	-0.242422	1.151704	2.447003
H	0.575900	2.714001	2.317966
H	-0.512740	2.175001	1.022885
C	3.549786	-0.751401	0.011557
H	4.316494	-0.952414	-0.745001
H	3.949104	0.002134	0.697175
H	3.385697	-1.677088	0.572388
C	-4.401609	-0.662441	0.589507
H	-4.860537	-1.428897	-0.048534
H	-4.346448	-1.072230	1.606718
H	-5.088156	0.193780	0.617665

Int5-Me
G(THF) = -898.0394388 Hartree

C	-0.218213	1.893762	-0.336706
C	-0.377271	3.098430	-0.479491
Cu	-0.01173	0.010129	-0.07454

	0		2
C	-2.360709	-0.142157	1.570147
H	-2.488868	0.941771	1.519017
H	-3.333533	-0.588166	1.807486
C	-2.832256	0.055913	-0.832321
H	-2.399431	-0.165291	-1.810408
H	-2.739494	1.132308	-0.681871
C	-1.947259	-2.075723	0.099481
H	-1.210806	-2.443891	0.818614
H	-2.924077	-2.457961	0.421256
C	2.752262	0.501055	-0.879867
H	2.524259	1.544321	-0.662995
H	3.824027	0.346118	-0.703264
C	2.425995	-0.021406	1.507791
H	1.841218	-0.678762	2.158486
H	3.477793	-0.314895	1.603812
C	2.079167	-1.788045	-0.151355
H	1.502829	-2.280218	0.638776
H	1.575327	-1.990339	-1.099966
N	-1.952391	-0.581649	0.199076
N	1.983518	-0.314202	0.105942
C	-4.299576	-0.365038	-0.802224
H	-4.784634	-0.113293	0.145630
H	-4.827280	0.173866	-1.596726
H	-4.432092	-1.435870	-0.986115
C	-1.608258	-2.593053	-1.291758
H	-1.437803	-3.673232	-1.238972
H	-2.413105	-2.415415	-2.009998
H	-0.693495	-2.130220	-1.684625
C	-1.355827	-0.482559	2.664498
H	-1.711841	-0.063711	3.611625
H	-	-	2.80720

	1.229276	1.560022	0
H	-0.374825	-0.034702	2.458080
C	3.488881	-2.379437	-0.198559
H	3.402334	-3.455461	-0.384031
H	4.085640	-1.949474	-1.008157
H	4.028838	-2.246124	0.742913
C	2.399566	0.203794	-2.330011
H	2.913046	0.928766	-2.970309
H	2.710124	-0.796558	-2.645620
H	1.323779	0.310997	-2.510287
C	2.262319	1.424864	1.955709
H	2.510251	1.481139	3.021406
H	2.935447	2.103089	1.423846
H	1.238816	1.782550	1.817592
C	-0.563353	4.540455	-0.645483
H	-0.666634	4.808990	-1.704279
H	-1.465669	4.888842	-0.127357
H	0.288595	5.102944	-0.243255

TS6

G(THF) = -426.8766067 Hartree

C	-1.565653	-0.441471	-1.510106
C	-3.113193	-0.396953	0.387644
C	2.651980	1.371197	0.198483
C	1.391359	1.196941	-0.364887
C	0.881410	-0.102025	-0.582622
C	1.673874	-1.214337	-0.223057
C	2.932784	-1.026991	0.339855
C	3.428143	0.263299	0.553437
H	3.031393	2.376060	0.362088
H	0.786995	2.055803	-0.640029
H	1.287507	-2.215278	-0.388481
H	3.531010	-1.891548	0.614025
H	4.411398	0.404287	0.992873
C	-0.403929	-0.285742	-1.156098
H	-	-	-

	2.399603	0.573914	2.167082
H	-3.578187	-1.343335	0.115040
C	-3.867562	0.851083	0.060161
H	-4.368064	0.787728	-0.913526
H	-4.651973	1.058926	0.810771
H	-3.204598	1.726337	0.048345
C	-2.182179	-0.409040	1.554356
H	-1.571467	-1.318272	1.580056
H	-1.504151	0.453871	1.532187
H	-2.732471	-0.356429	2.510737

Int11

G(THF) = -426.9240401 Hartree

C	3.036241	-1.213231	-0.169551
C	1.682237	-1.227664	0.119183
C	0.955396	-0.000125	0.272117
C	1.682159	1.227522	0.119632
C	3.036163	1.213286	-0.169104
C	3.727912	0.000075	-0.316860
H	3.567531	-2.154559	-0.283543
H	1.149248	-2.166655	0.232380
H	1.149105	2.166433	0.233176
H	3.567393	2.154690	-0.282746
H	4.789909	0.000152	-0.542976
C	-0.386577	-0.000192	0.565121
C	-1.676595	-0.000238	0.746421
H	-2.088261	-0.000362	1.763700
C	-2.725867	-0.000074	-0.360374
H	-2.203676	-0.000451	-1.324530
C	-3.587518	1.267296	-0.266140
H	-2.975492	2.170833	-0.366451
H	-4.347791	1.278870	-1.056636
H	-4.106189	1.316131	0.699943
C	-	-	-

	3.588400	1.266855	0.265629
H	-2.976968	-2.170804	-0.365751
H	-4.106937	-1.314968	0.700555
H	-4.348784	-1.278102	-1.056009

TS6-Me
G(THF) = -235.1126128 Hartree

C	0.658248	0.007171	0.948922
C	-1.173098	-0.001542	-0.463395
C	1.767990	0.003653	0.420722
H	0.002823	0.012570	1.798068
H	-0.628302	-0.002735	-1.405965
C	-1.839189	1.286094	-0.087564
H	-1.201706	2.152036	-0.300249
H	-2.784779	1.431500	-0.640425
H	-2.097689	1.308108	0.980436
C	-1.832448	-1.290542	-0.080406
H	-1.190343	-2.154275	-0.288088
H	-	-	0.98765
	2.091015	1.307887	8
H	-2.777149	-1.444065	-0.632601
C	2.925350	-0.002164	-0.466866
H	3.552449	0.884138	-0.308128
H	3.553185	-0.885601	-0.295547
H	2.621405	-0.009810	-1.523644

Int11-Me
G(THF) = -235.1511528 Hartree

C	1.608207	-0.000904	0.621329
C	0.308287	-0.001192	0.825965
H	-0.081685	-0.002320	1.849077
C	-0.765233	0.000038	-0.258534
H	-0.268654	0.000212	-1.236864
C	-1.627006	1.266544	-0.150093
H	-1.018222	2.171143	-0.260613
H	-2.402799	1.278951	-0.925953
H	-	1.31526	0.82544

	2.127962	9	8
C	-1.628763	-1.265387	-0.151400
H	-1.021219	-2.170691	-0.262899
H	-2.129732	-1.314392	0.824115
H	-2.404589	-1.275844	-0.927239
C	2.586958	0.000238	-0.478349
H	2.085818	0.000851	-1.461162
H	3.236910	0.884274	-0.438027
H	3.237438	-0.883472	-0.439394

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M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,; Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09, revision D.01*; Gaussian Inc., Wallingford, CT, 2013.

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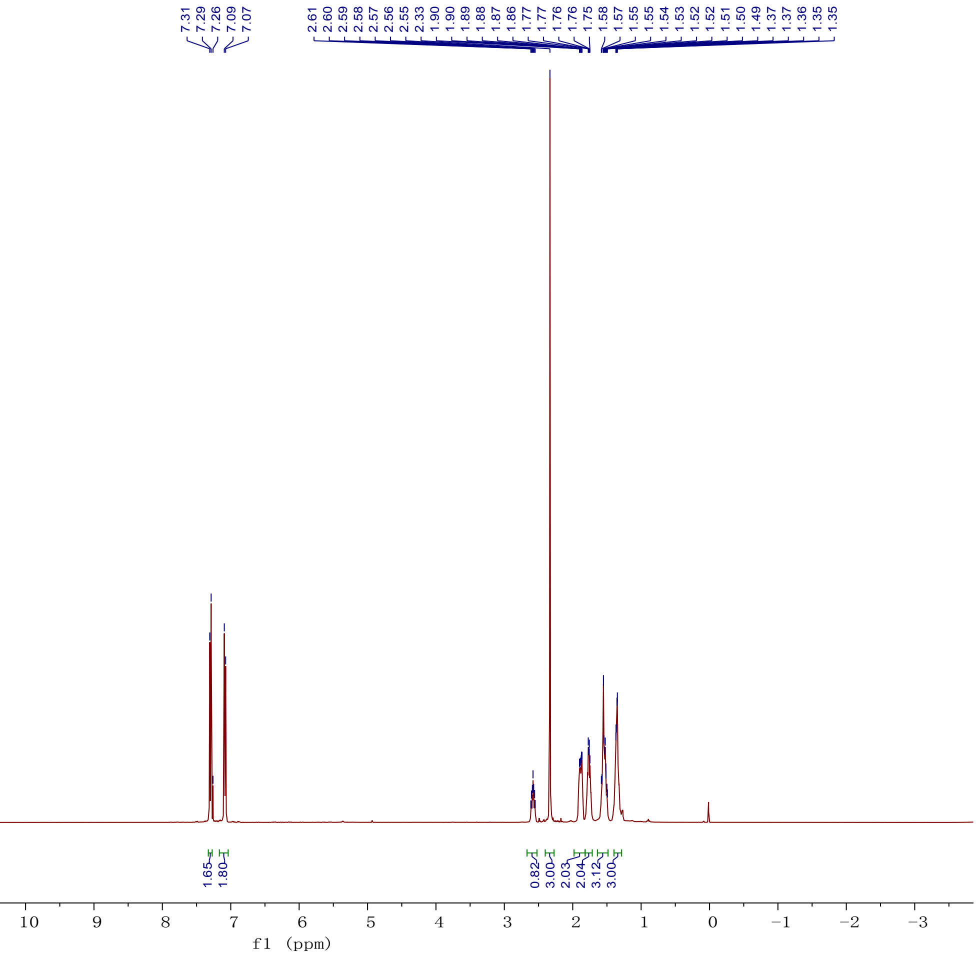
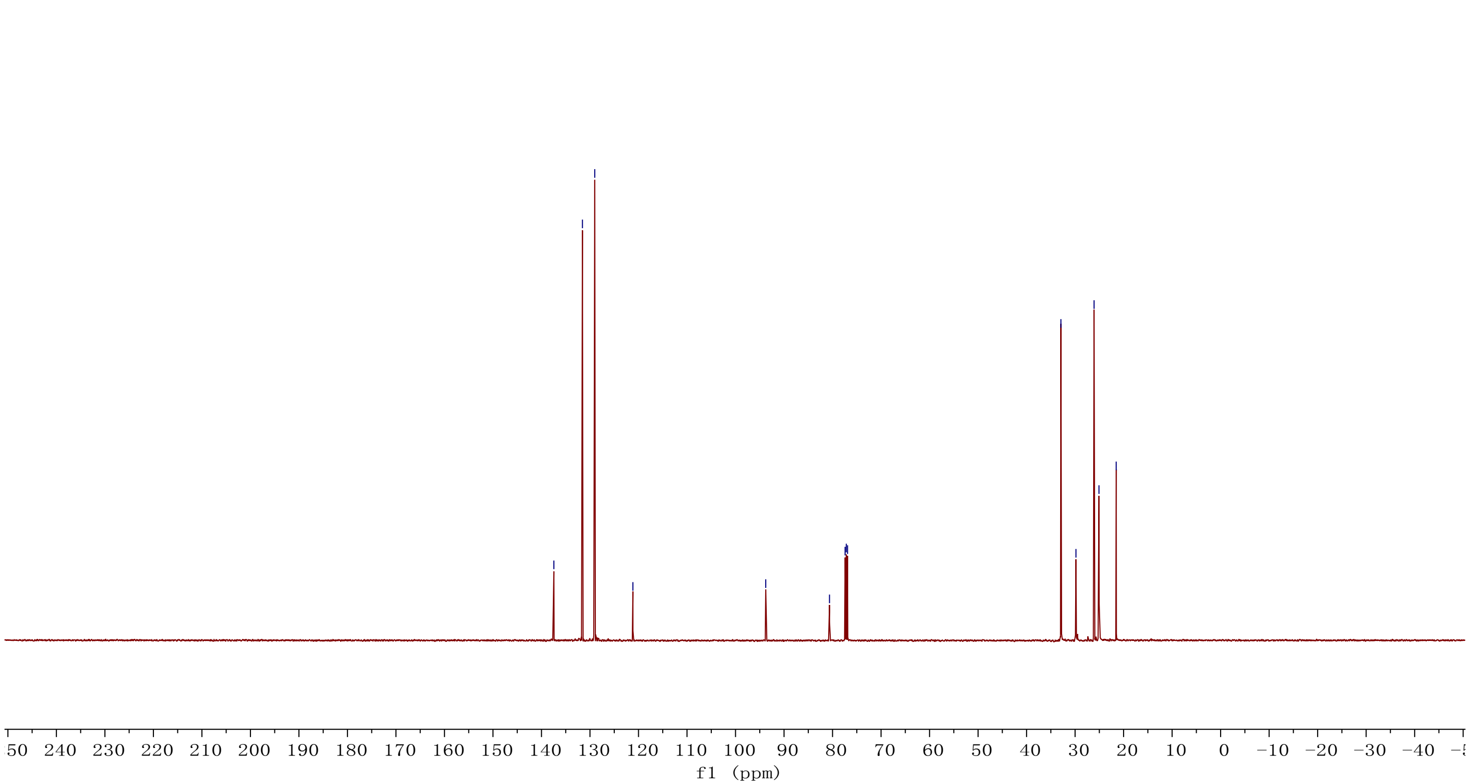
NMR Spectra

Compound 3 ¹H NMR



Compound 3 ^{13}C NMR



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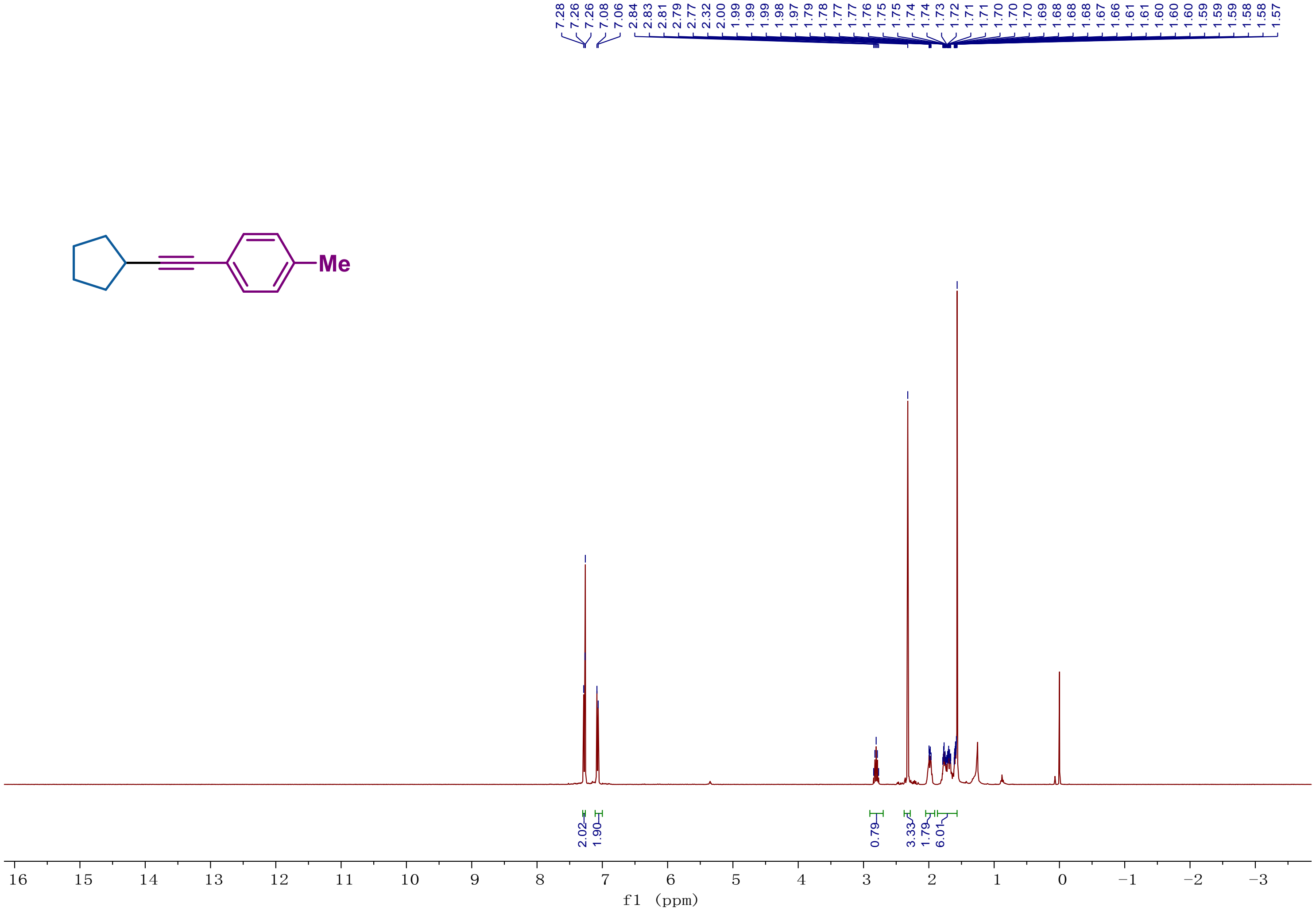

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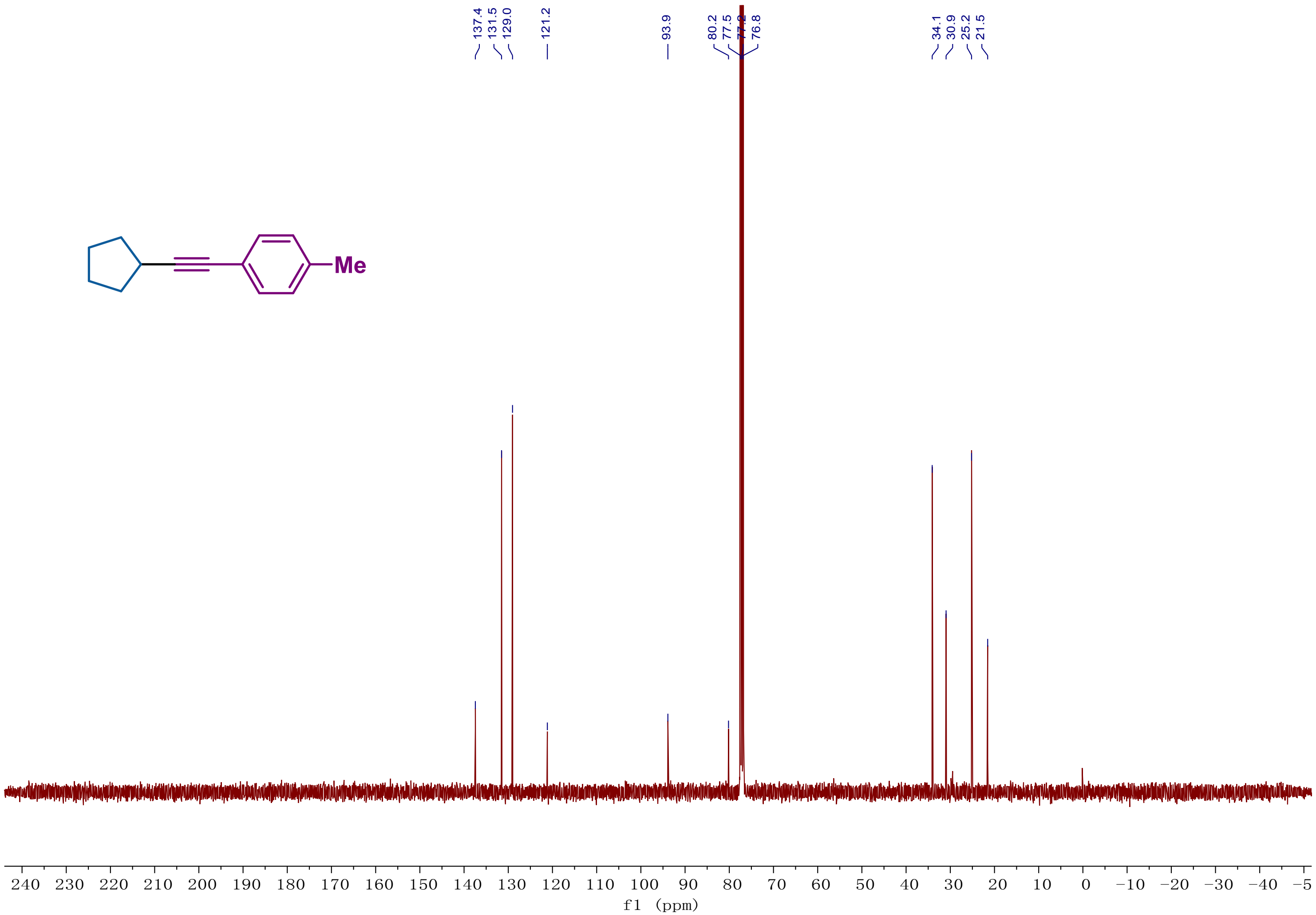

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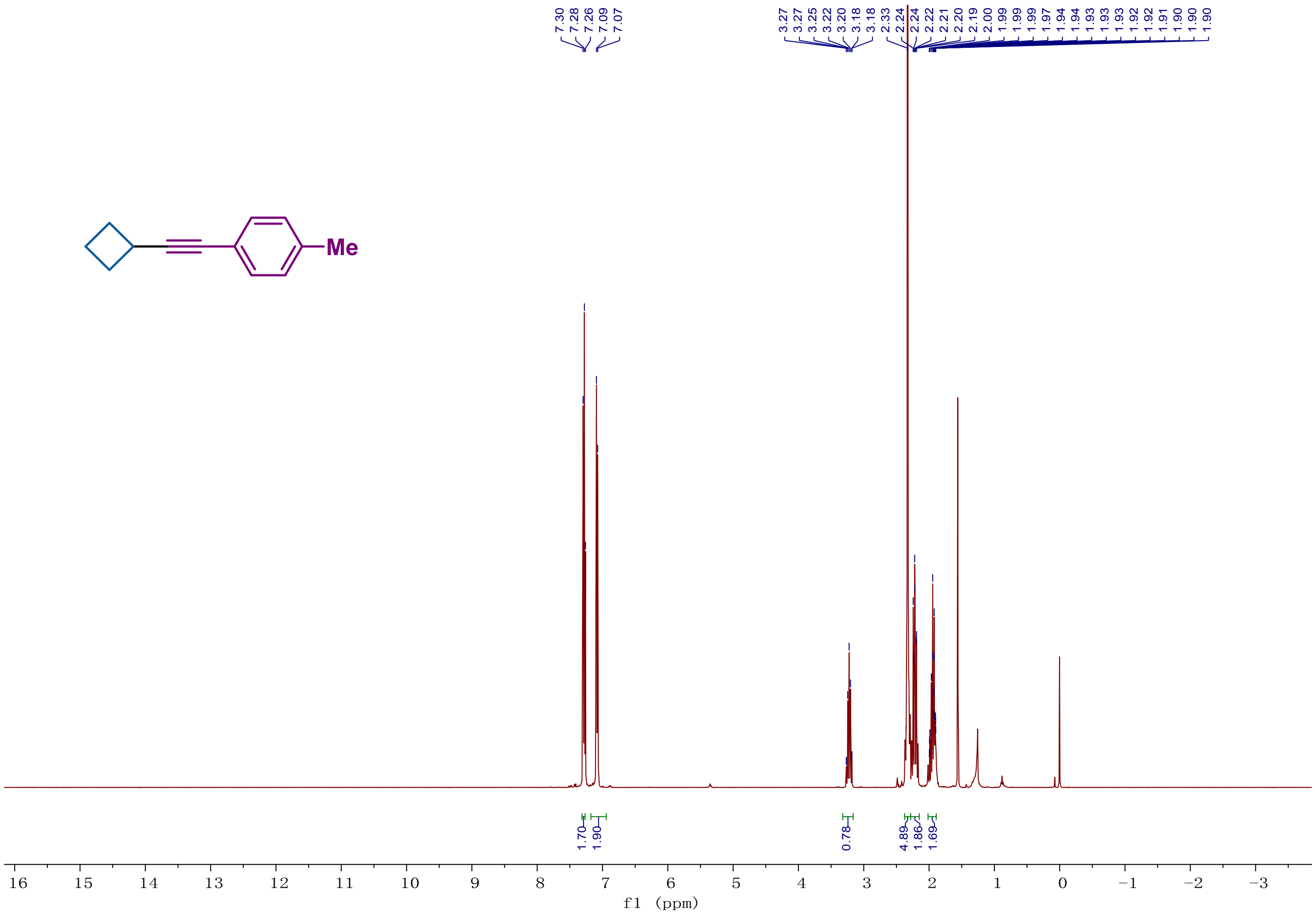
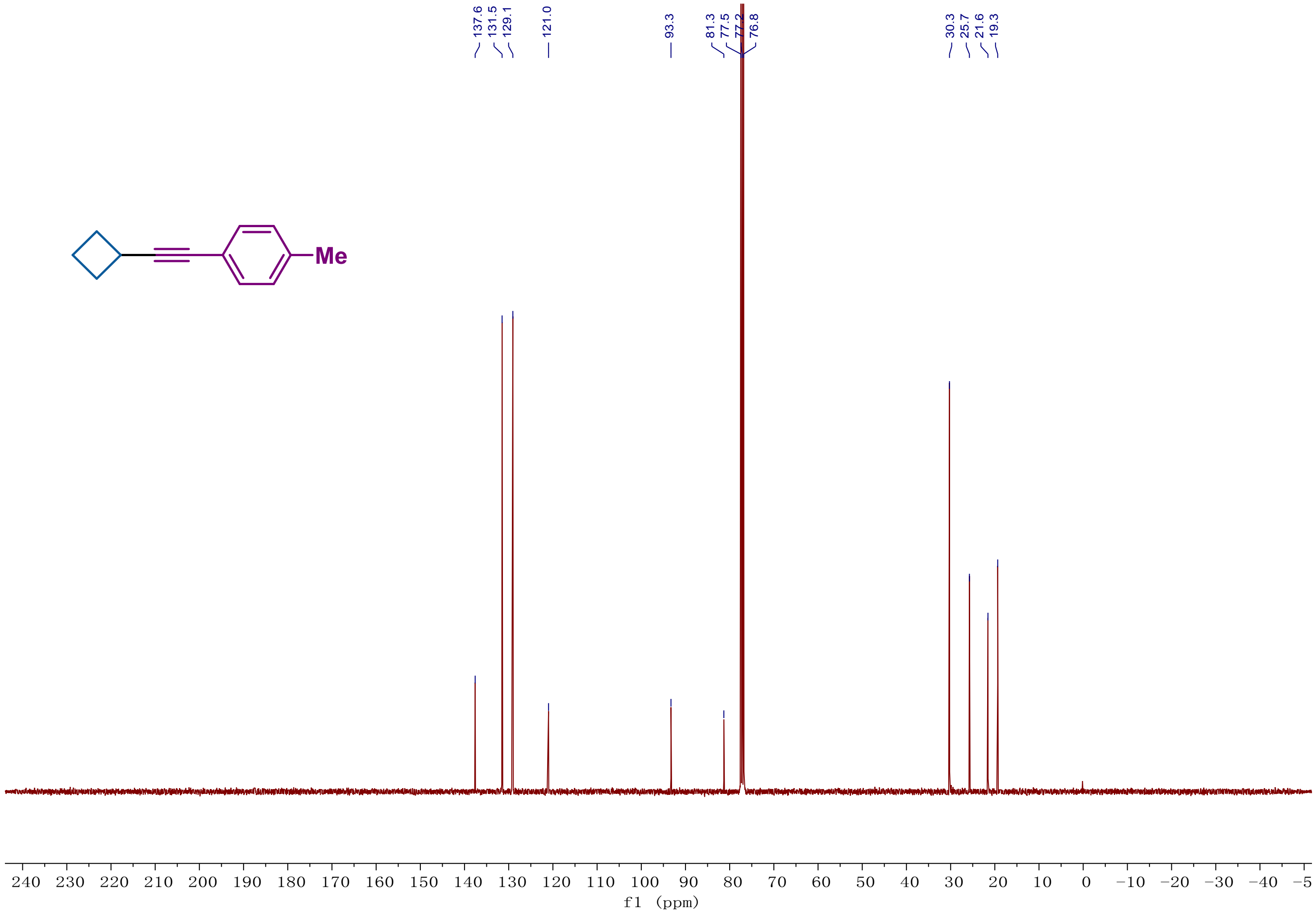


Compound 5 ^{13}C NMR



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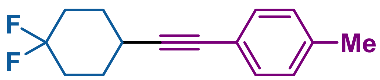

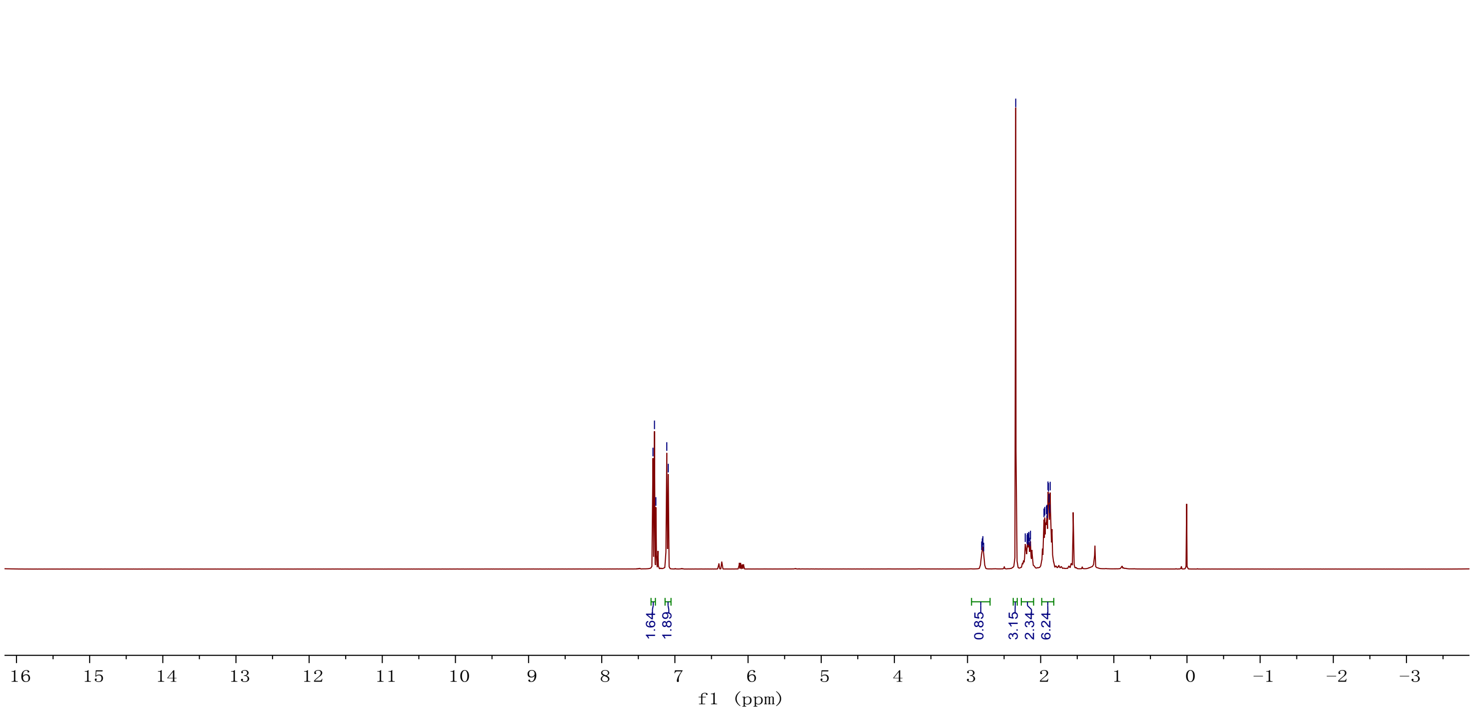

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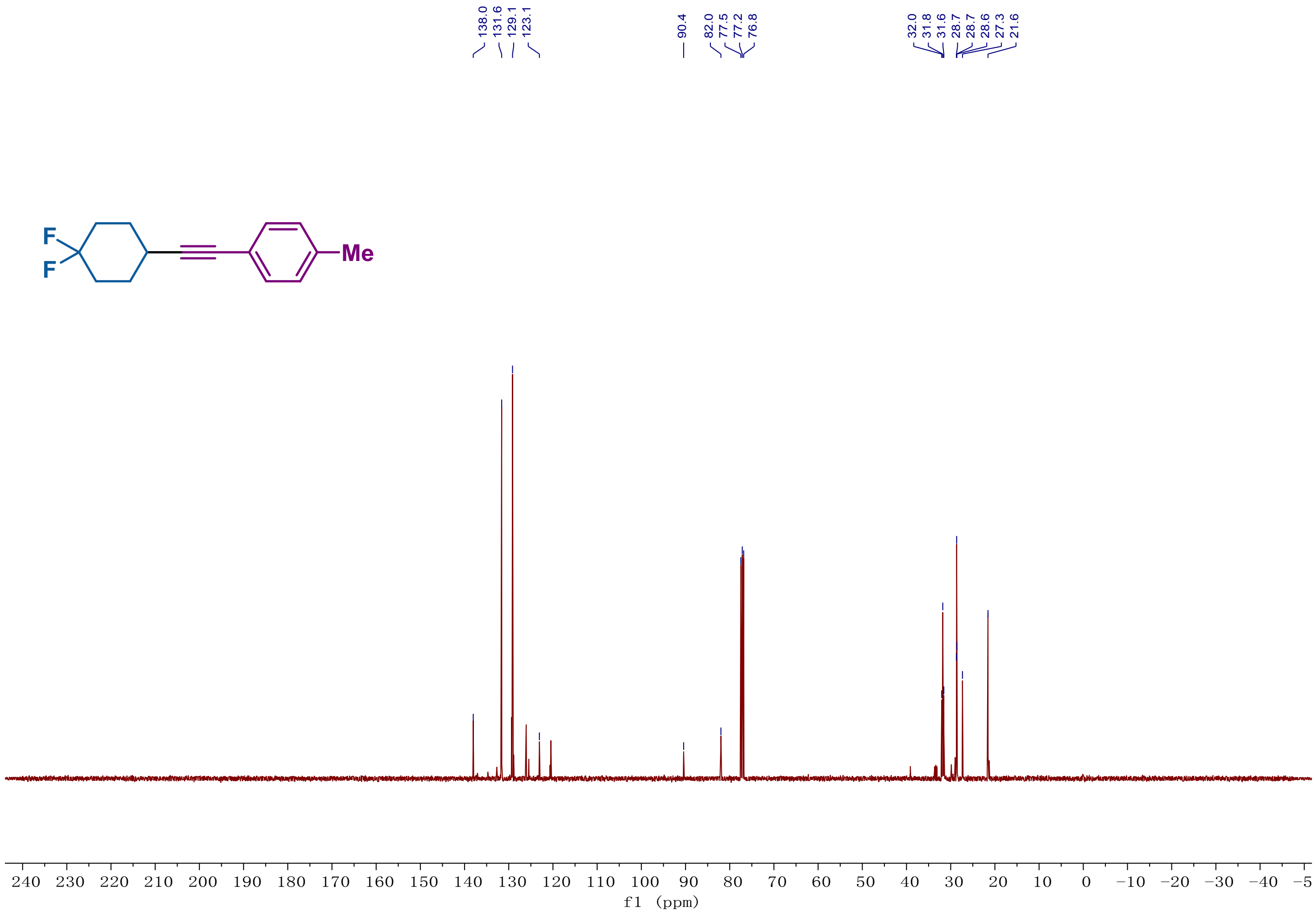
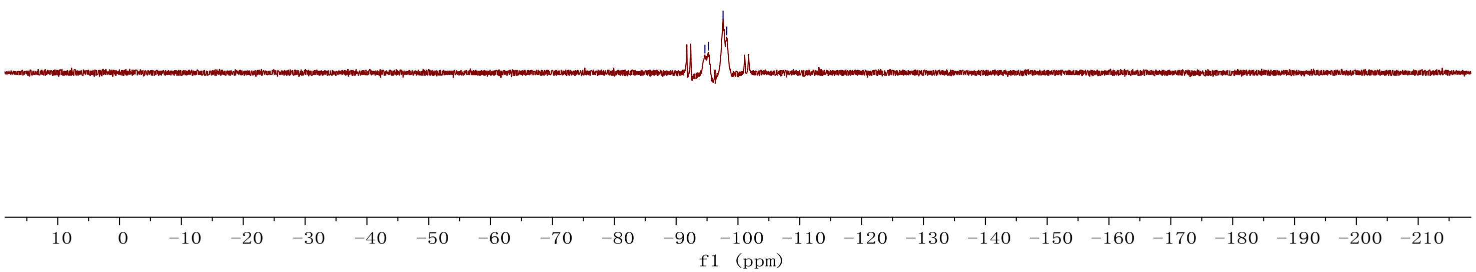


Compound 6 ^{19}F NMR



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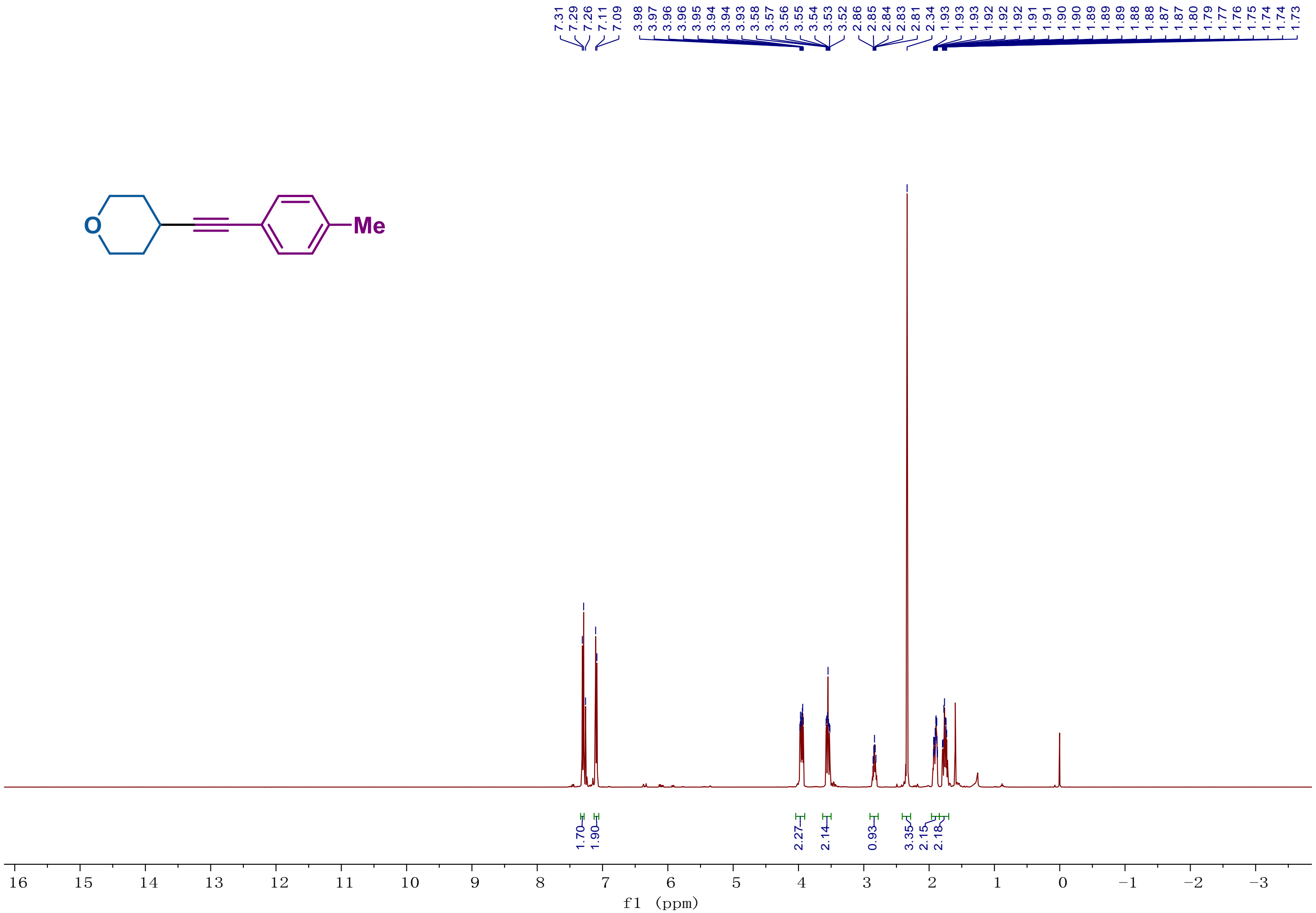

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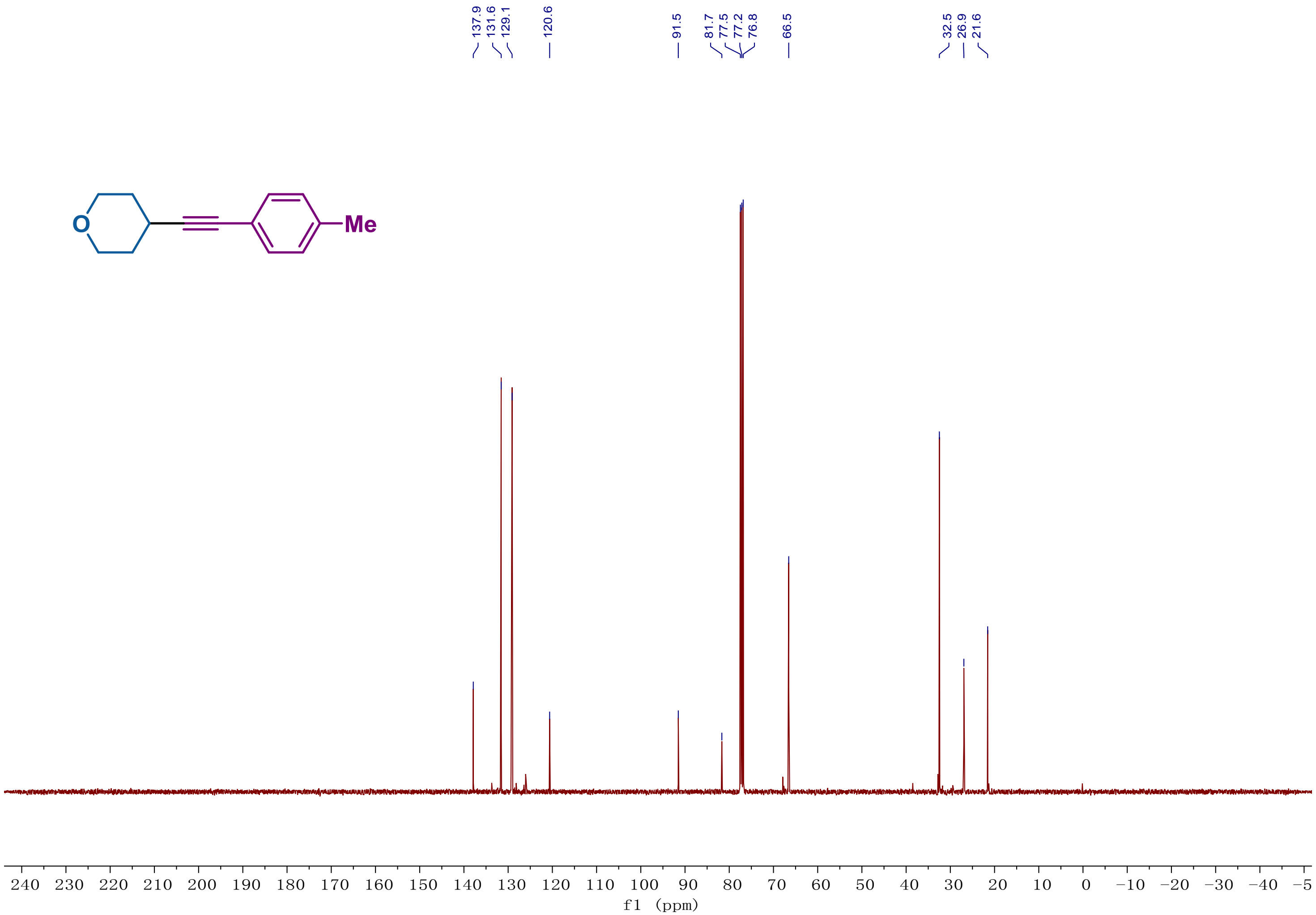

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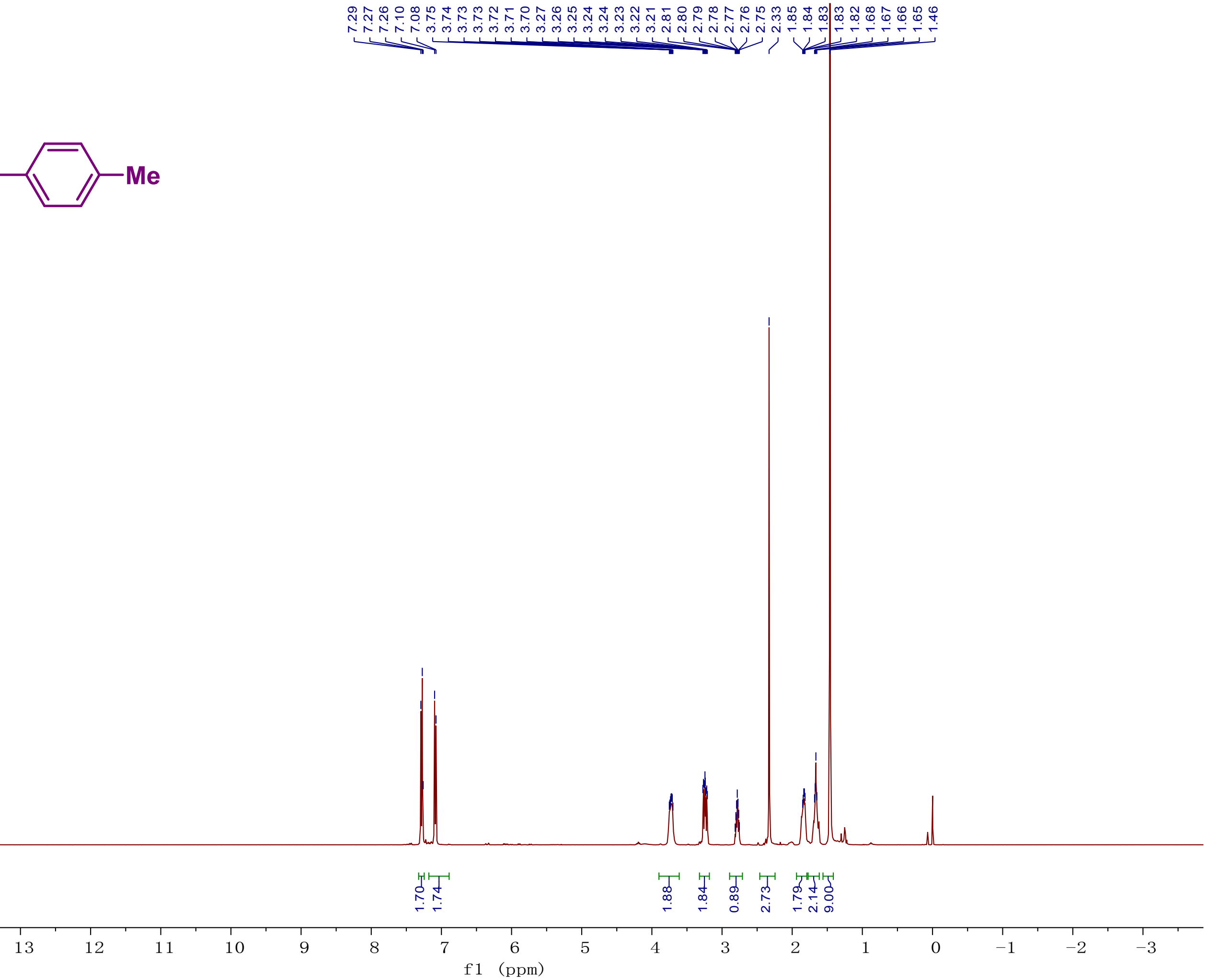

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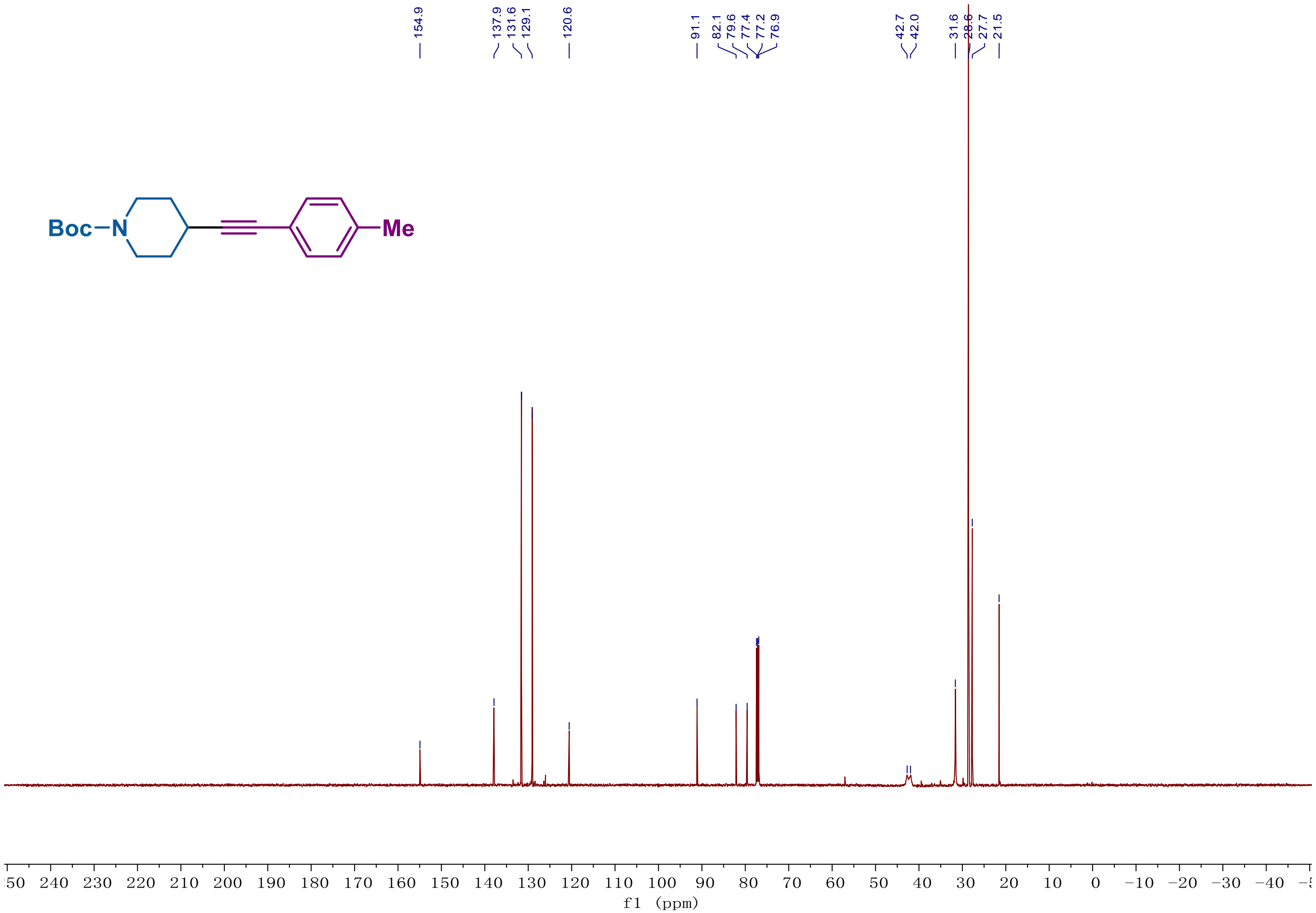

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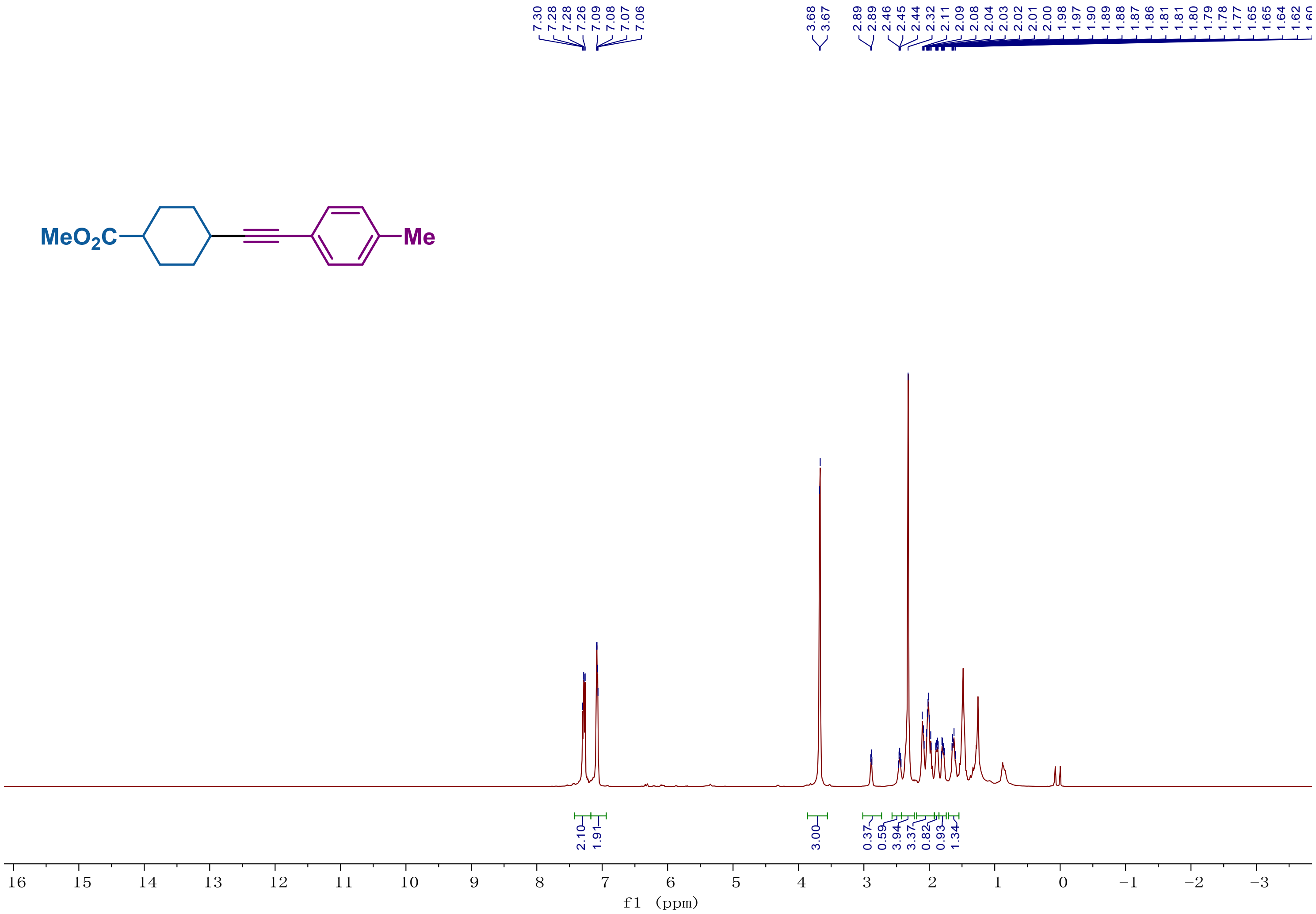
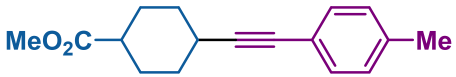
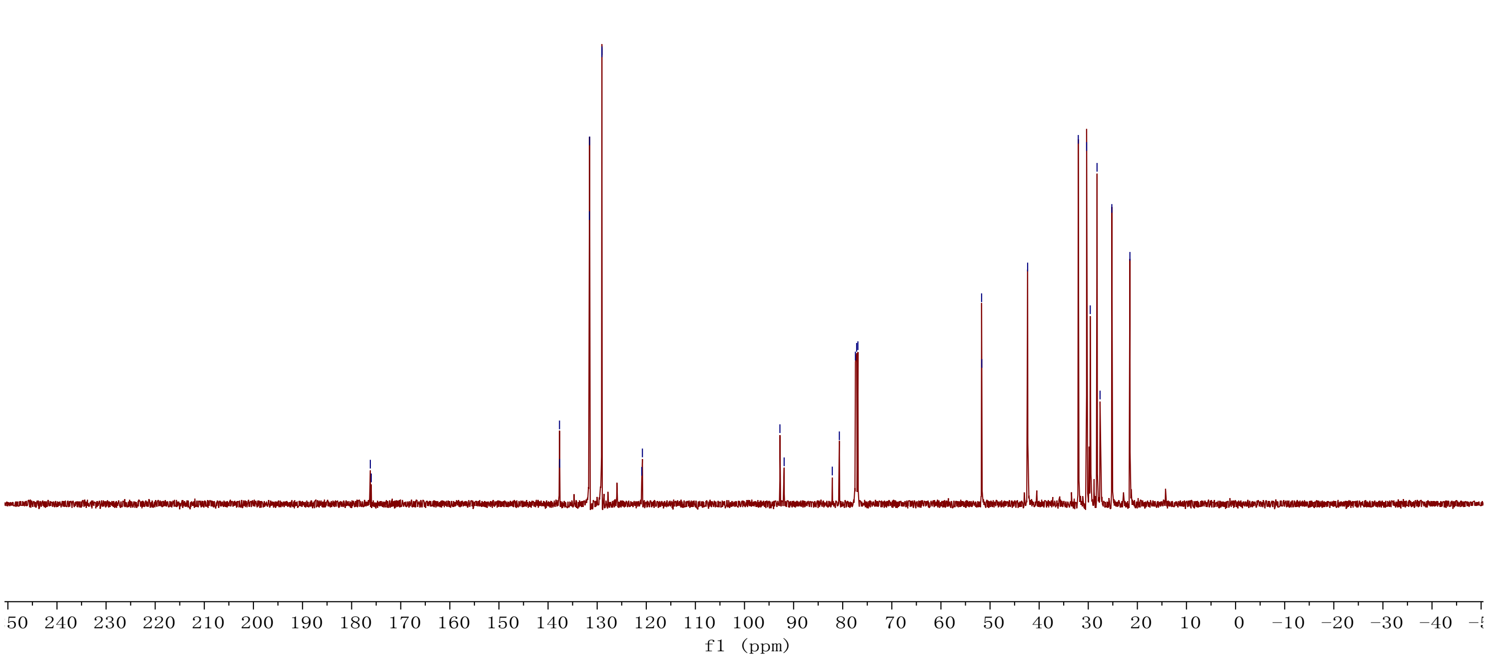


Compound 9 ^{13}C NMR





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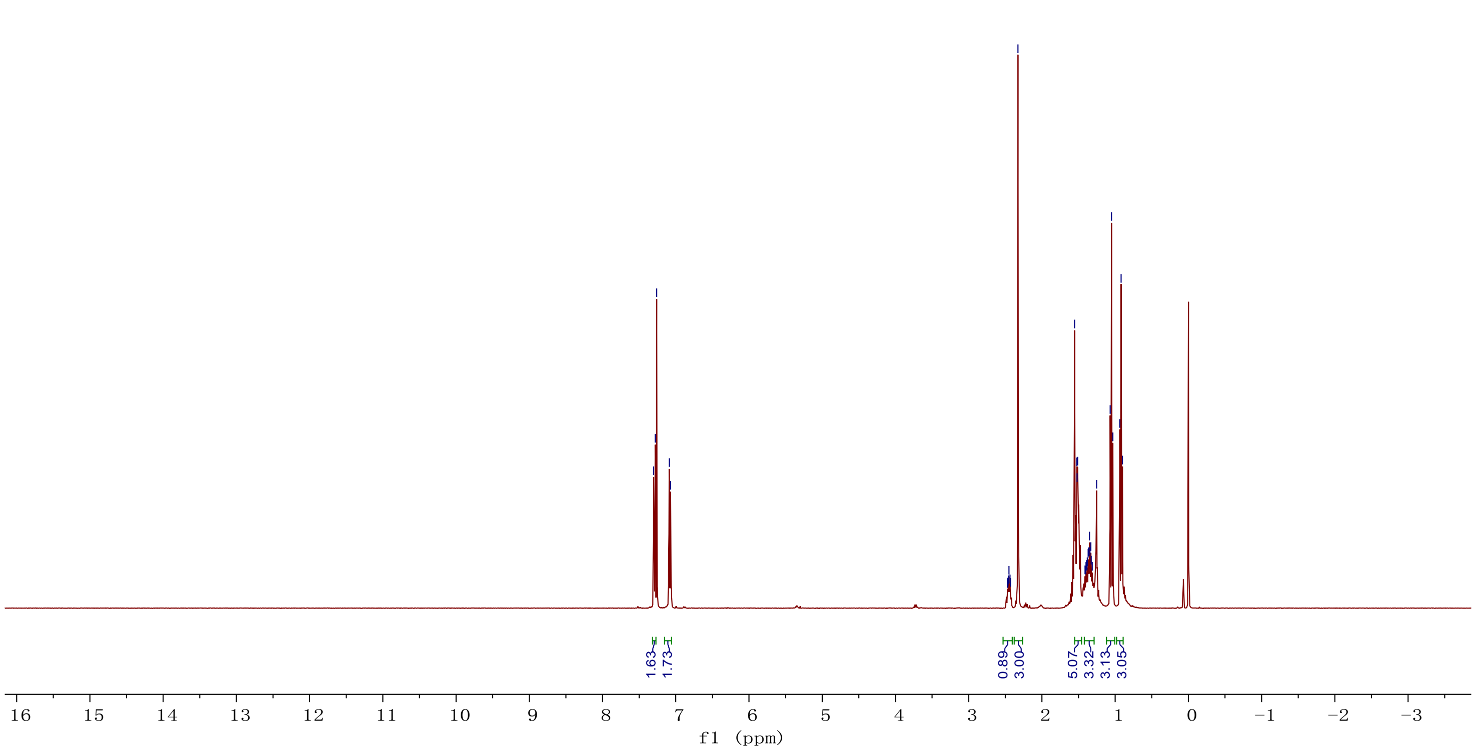

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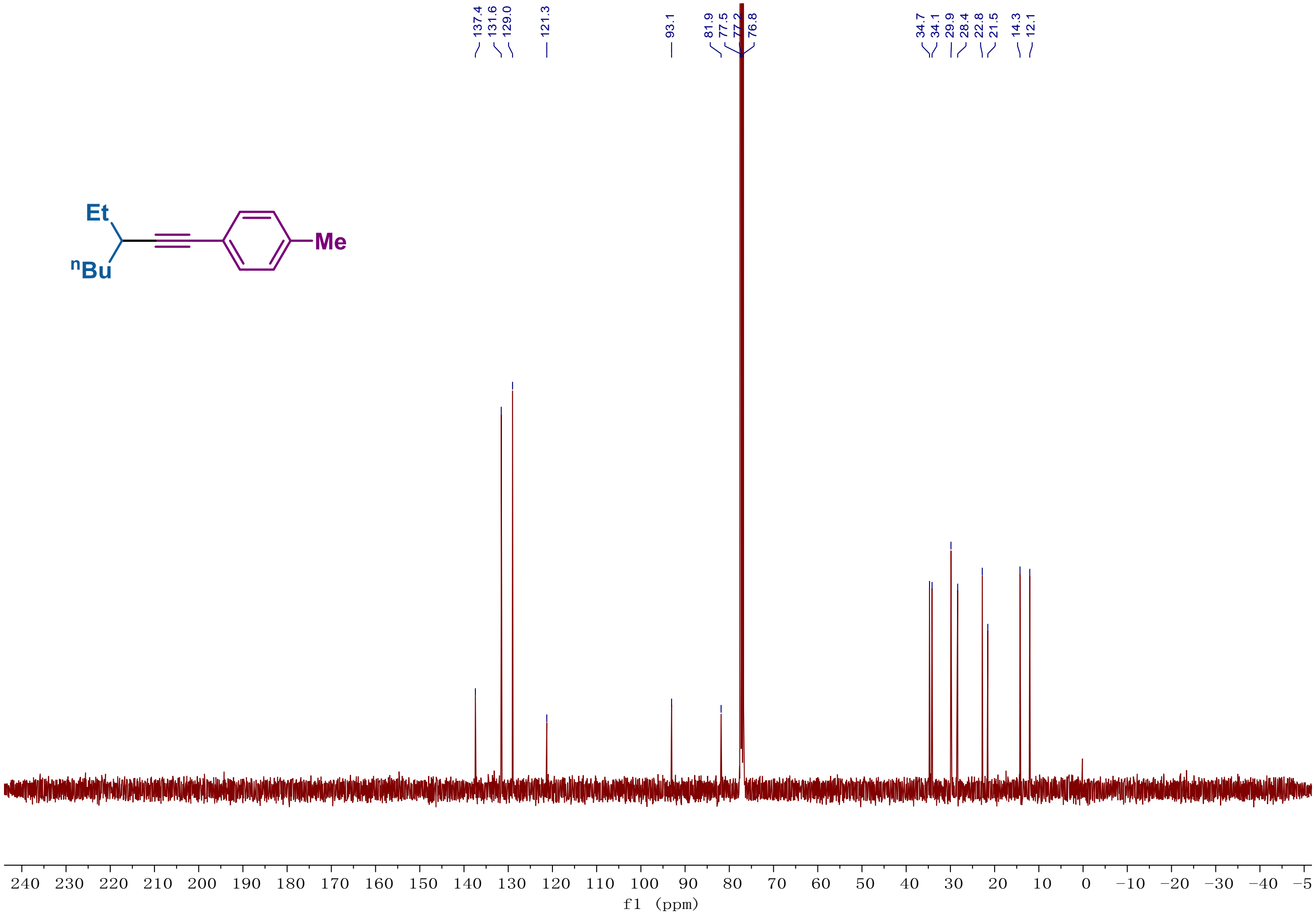

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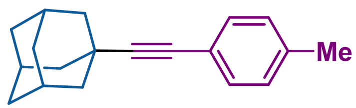

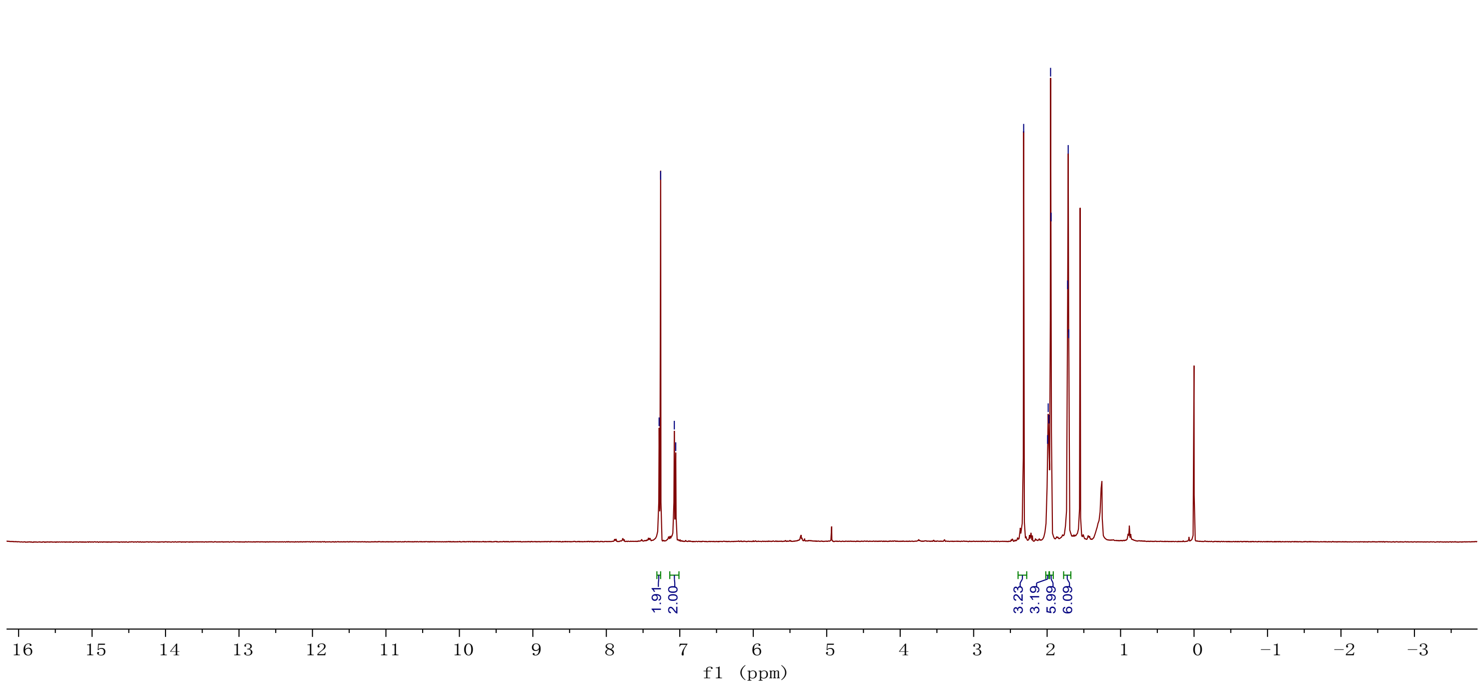

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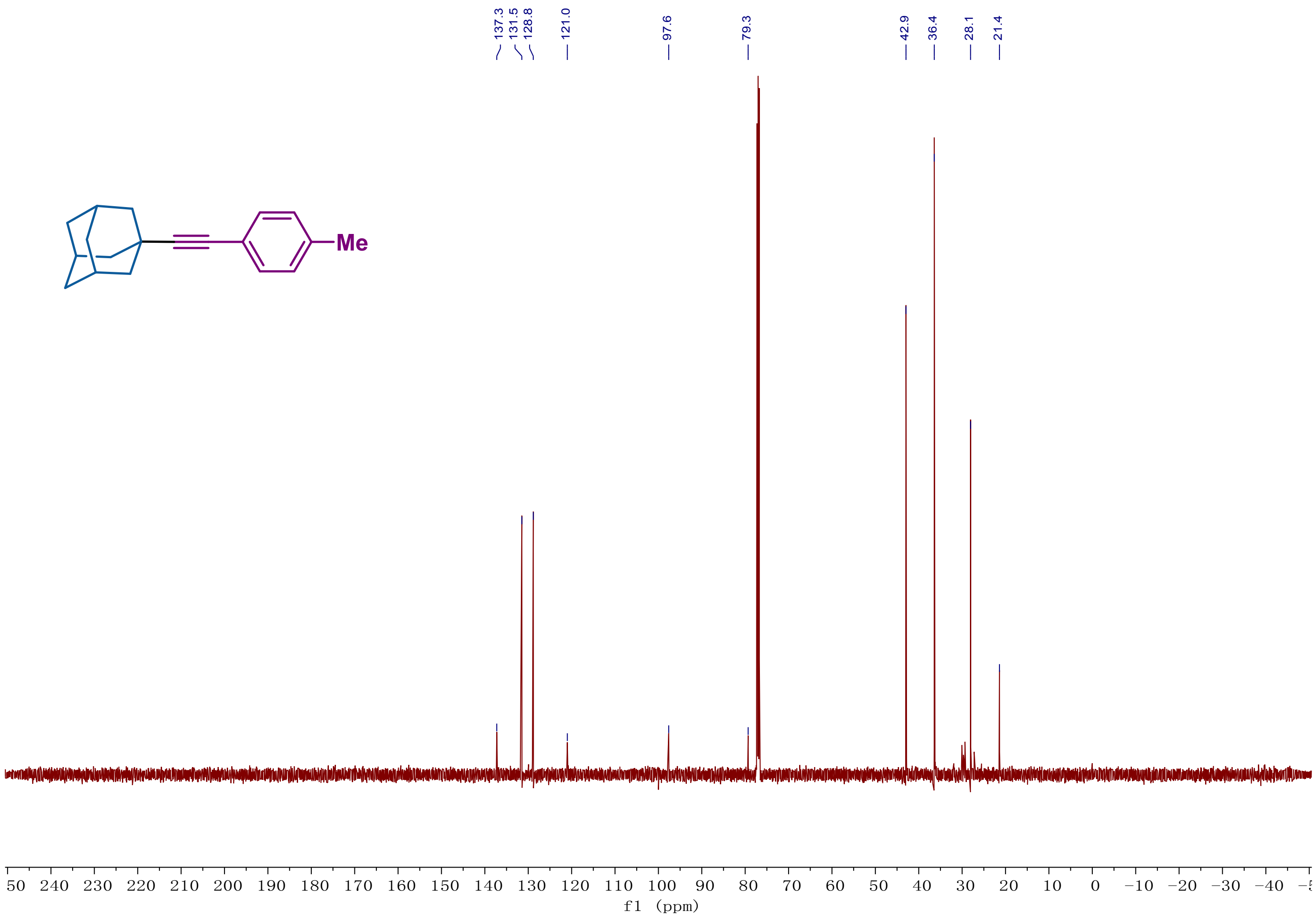

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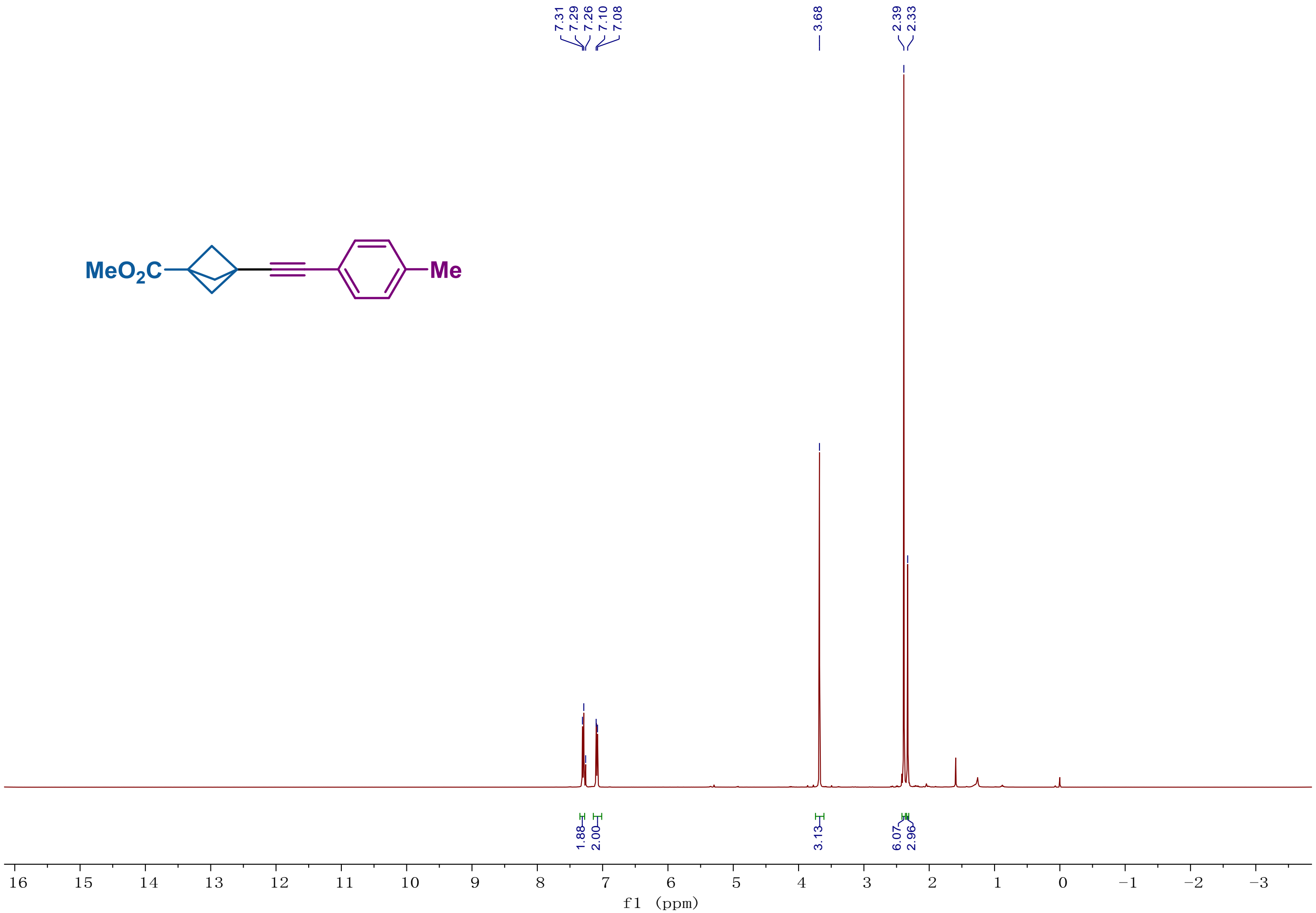

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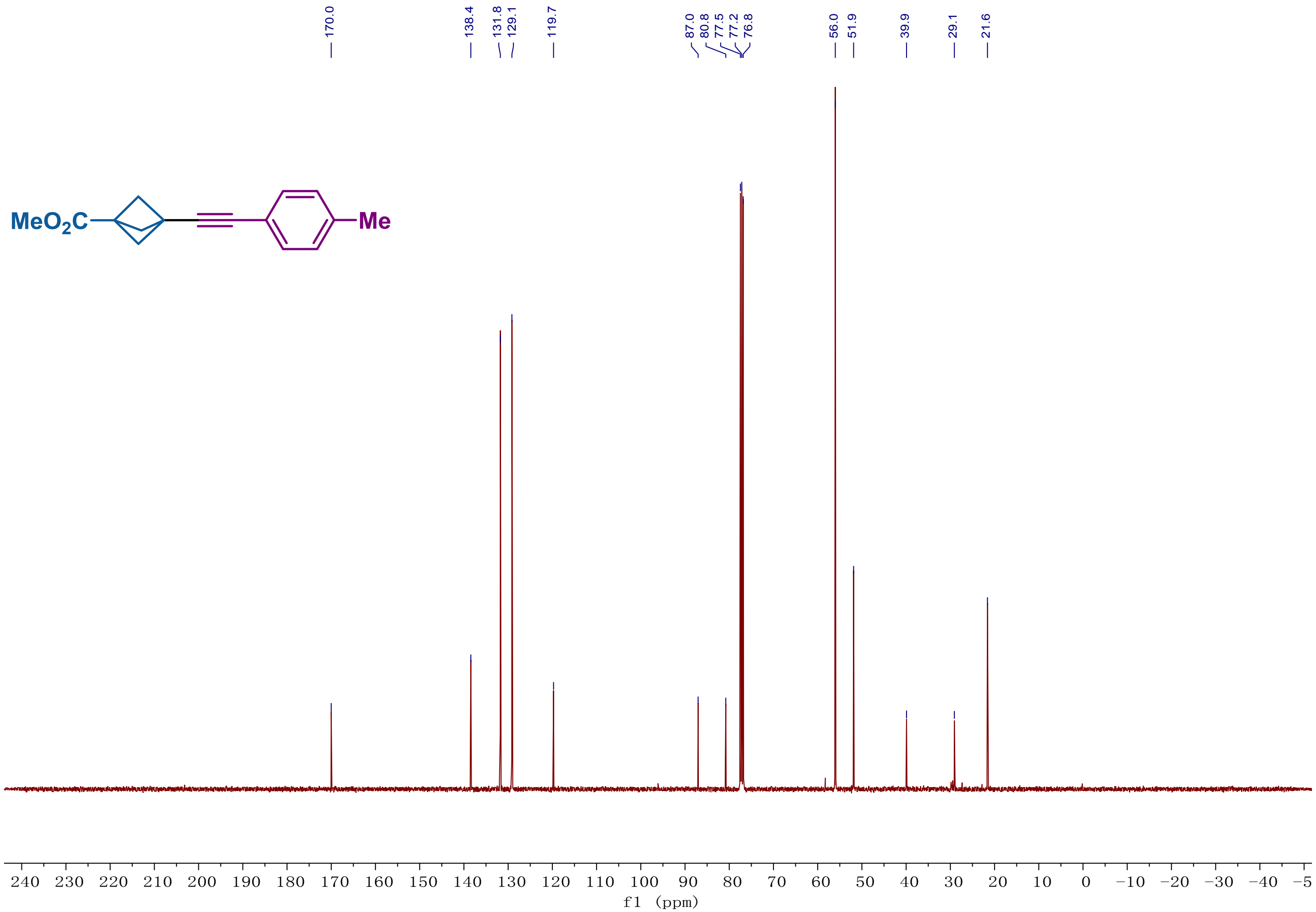

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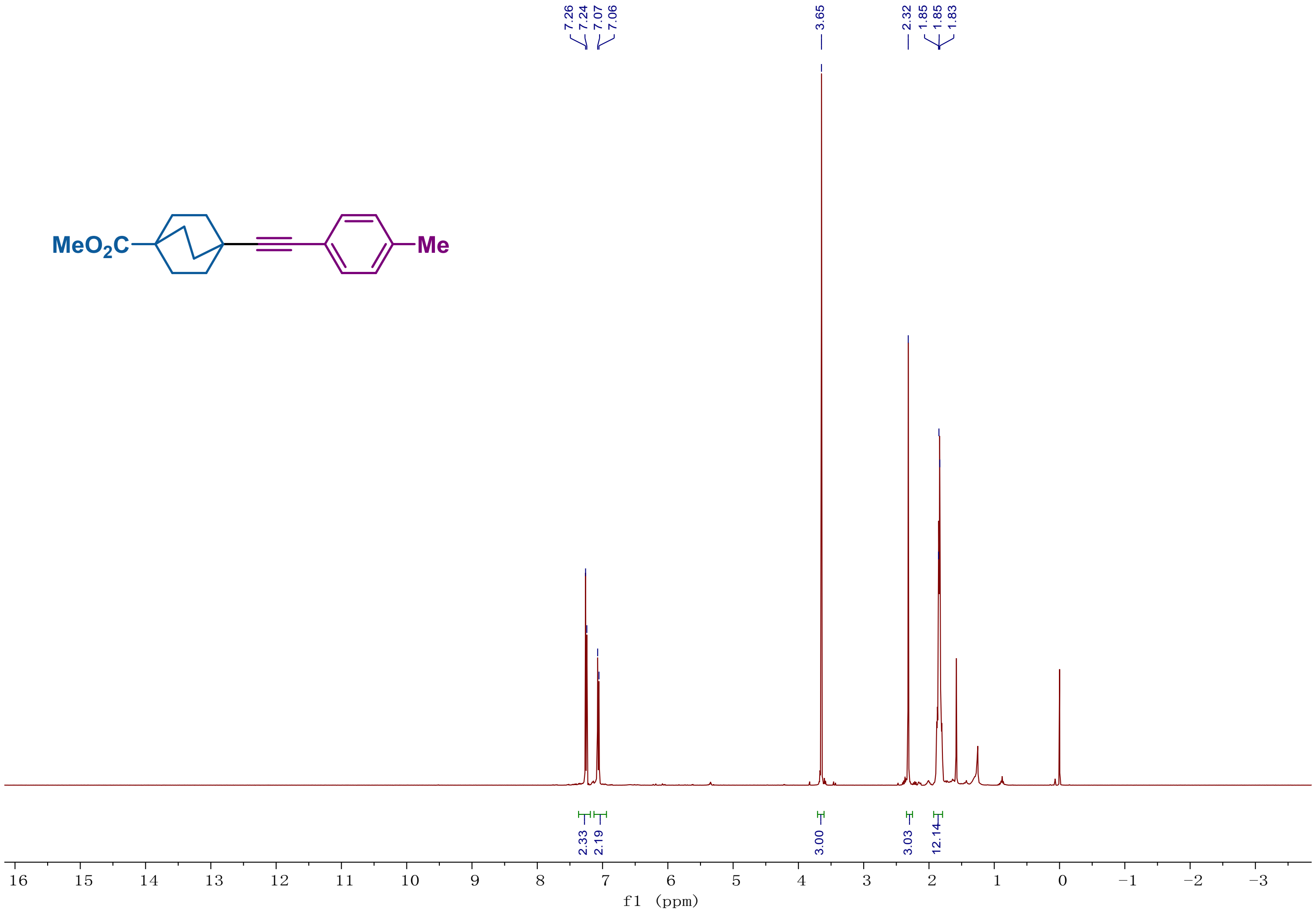

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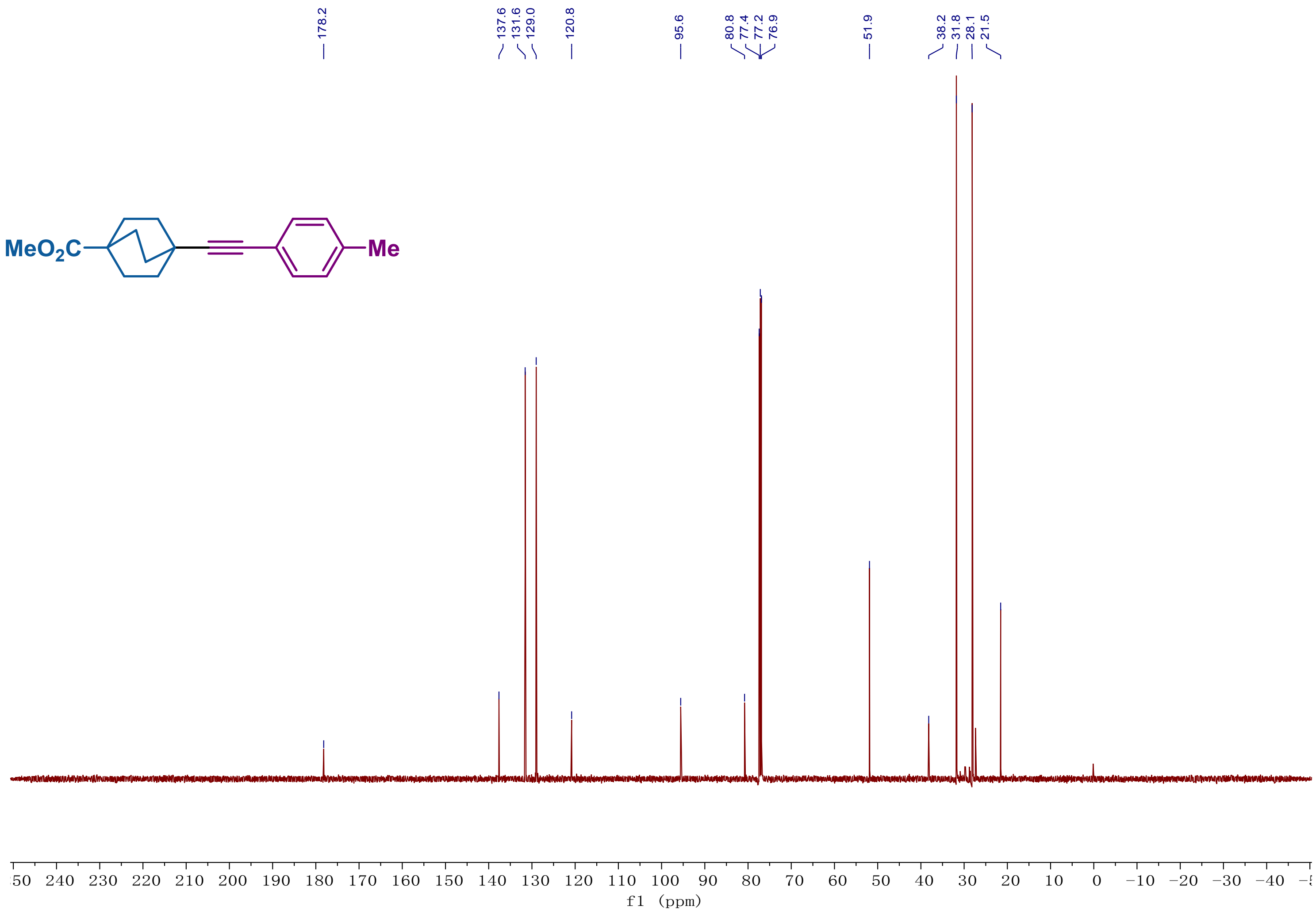

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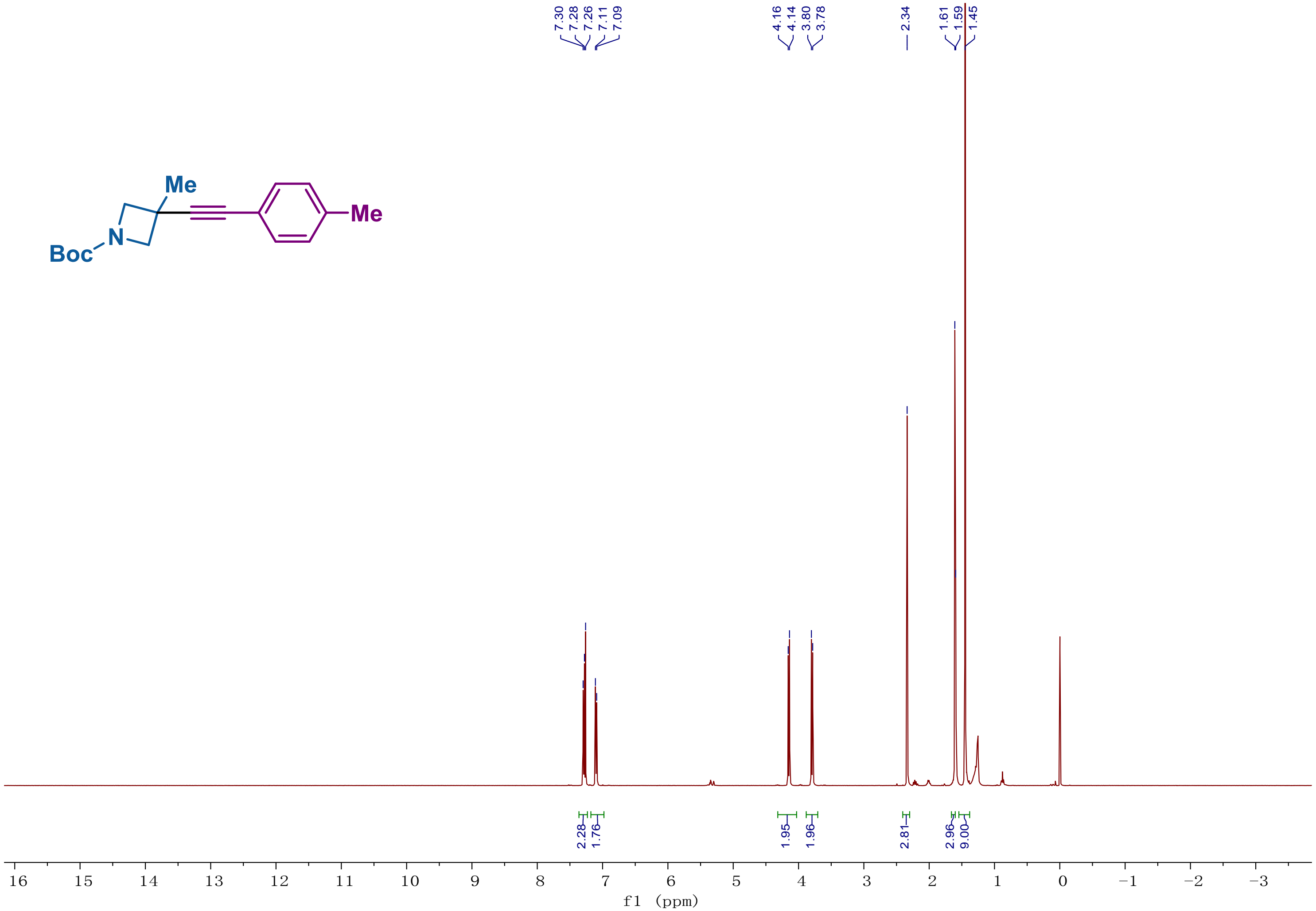

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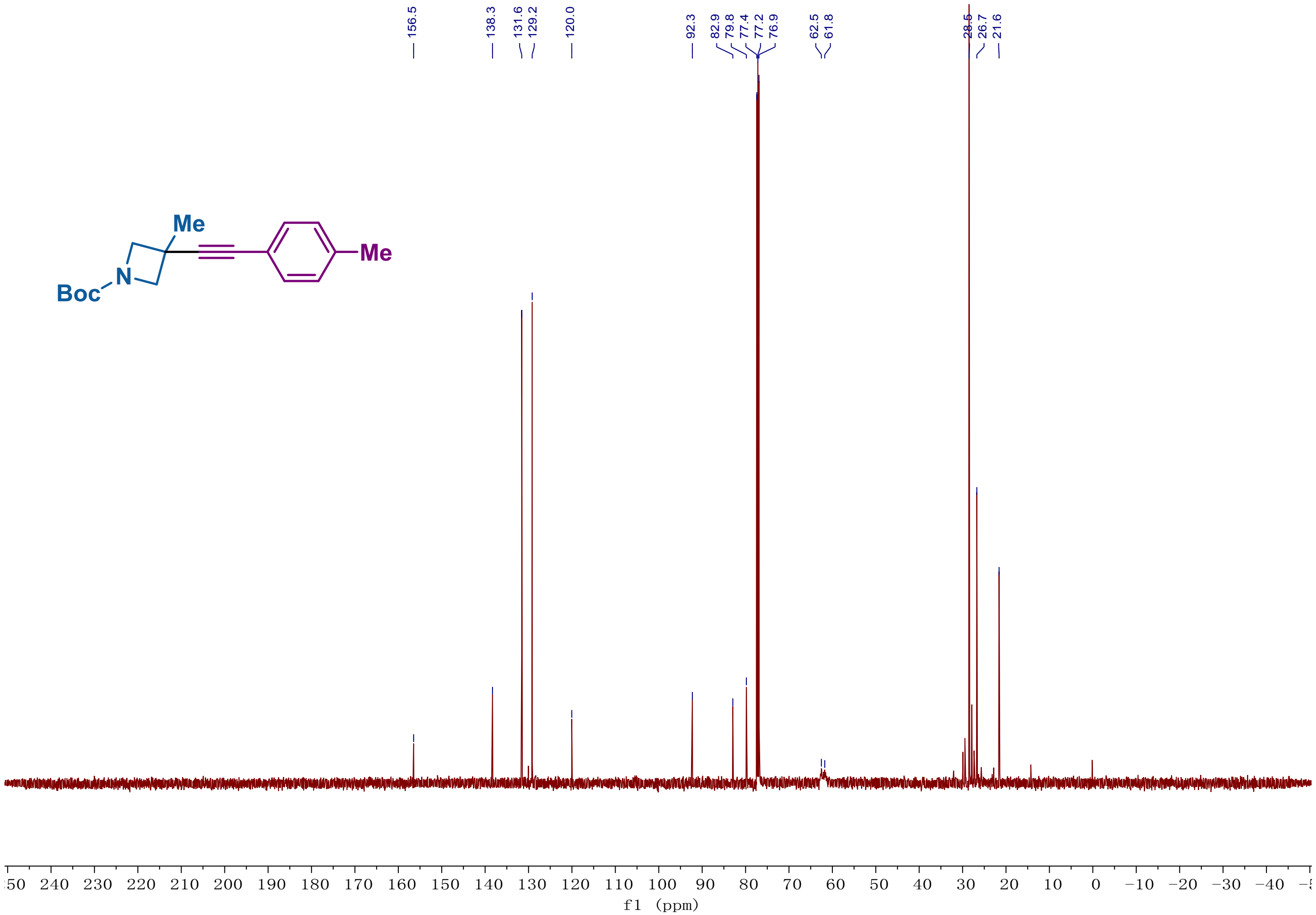

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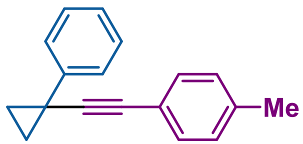

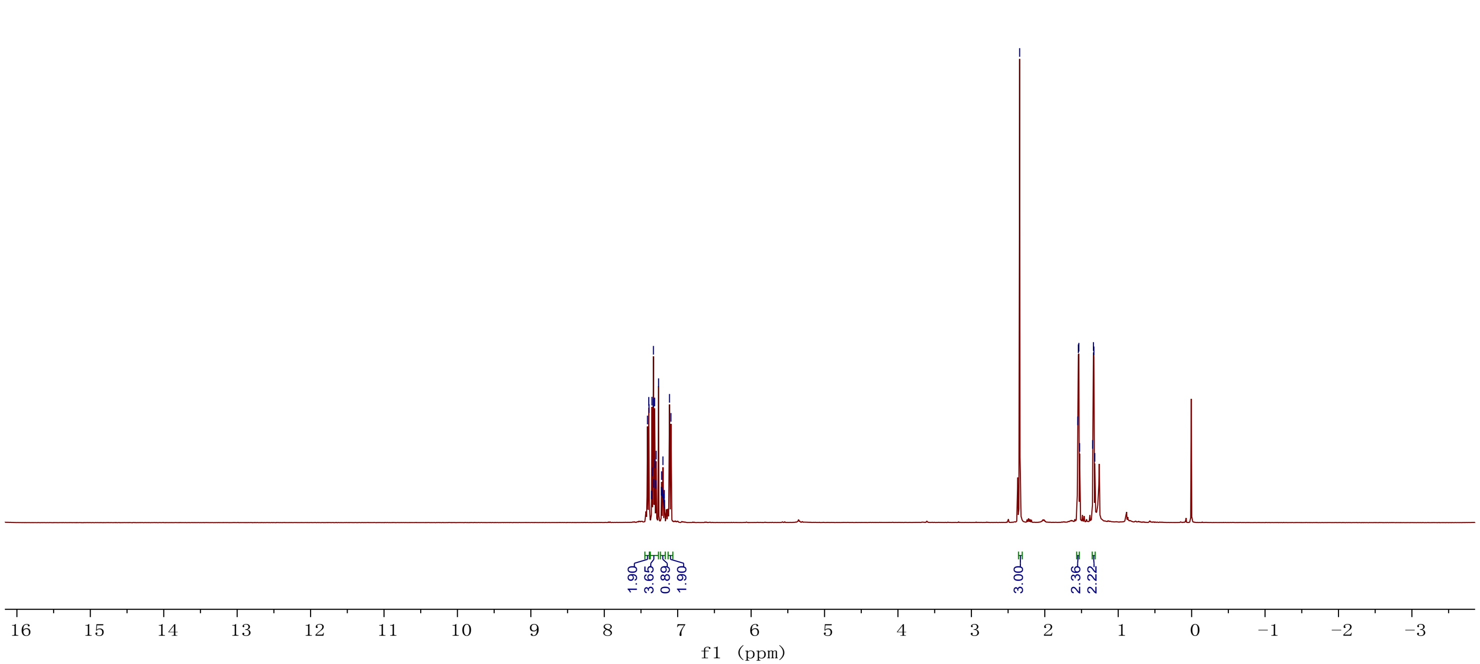

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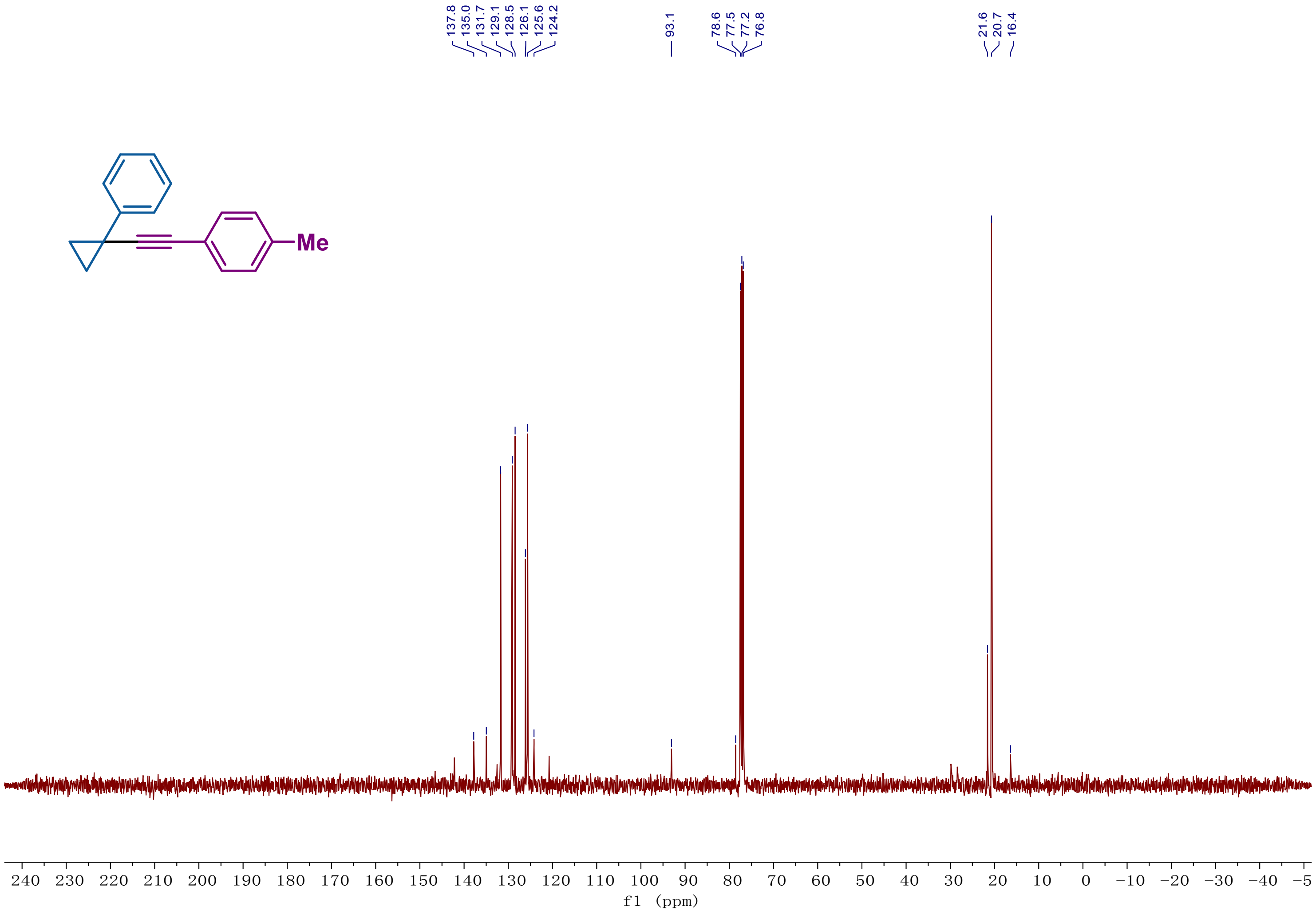

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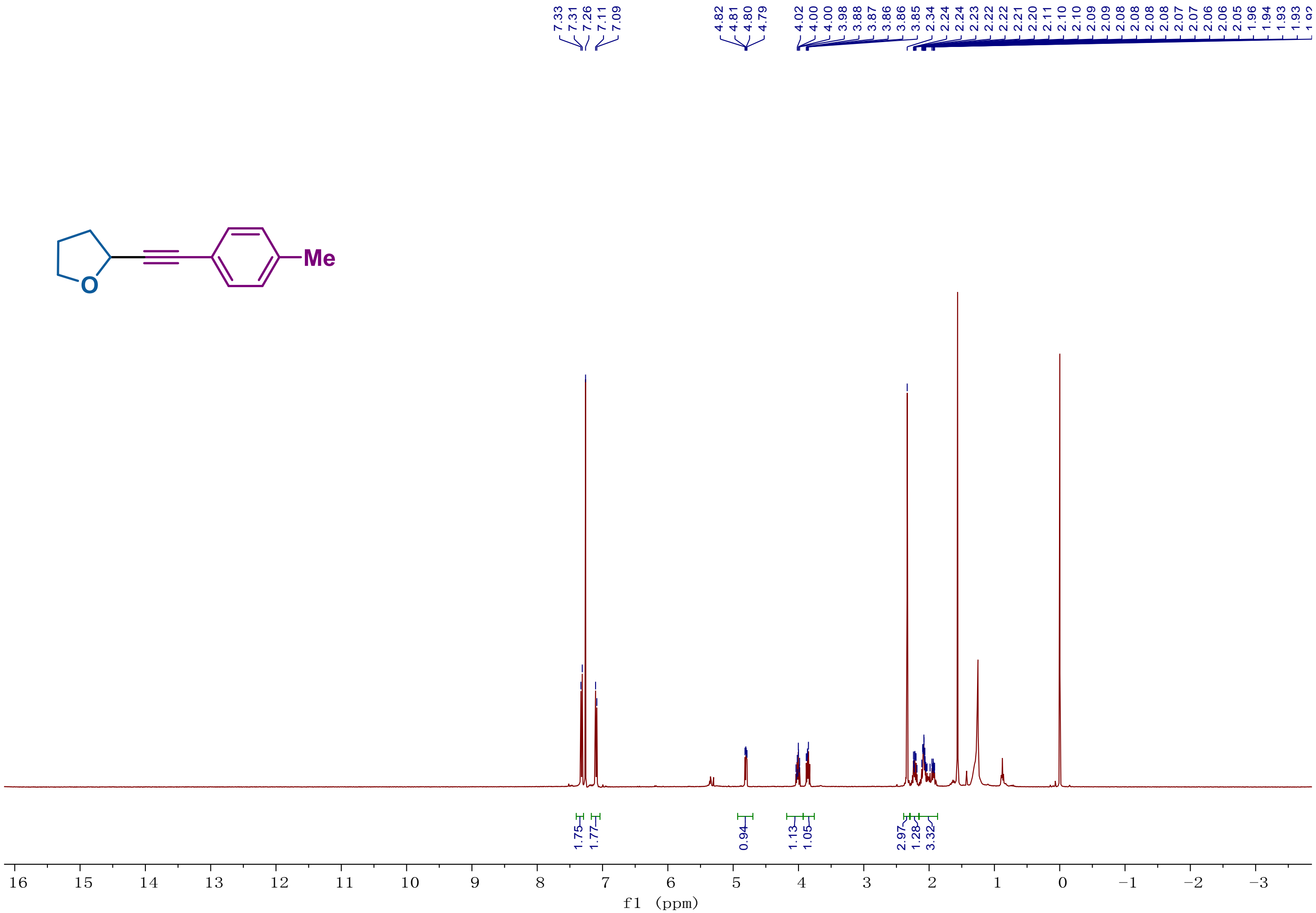

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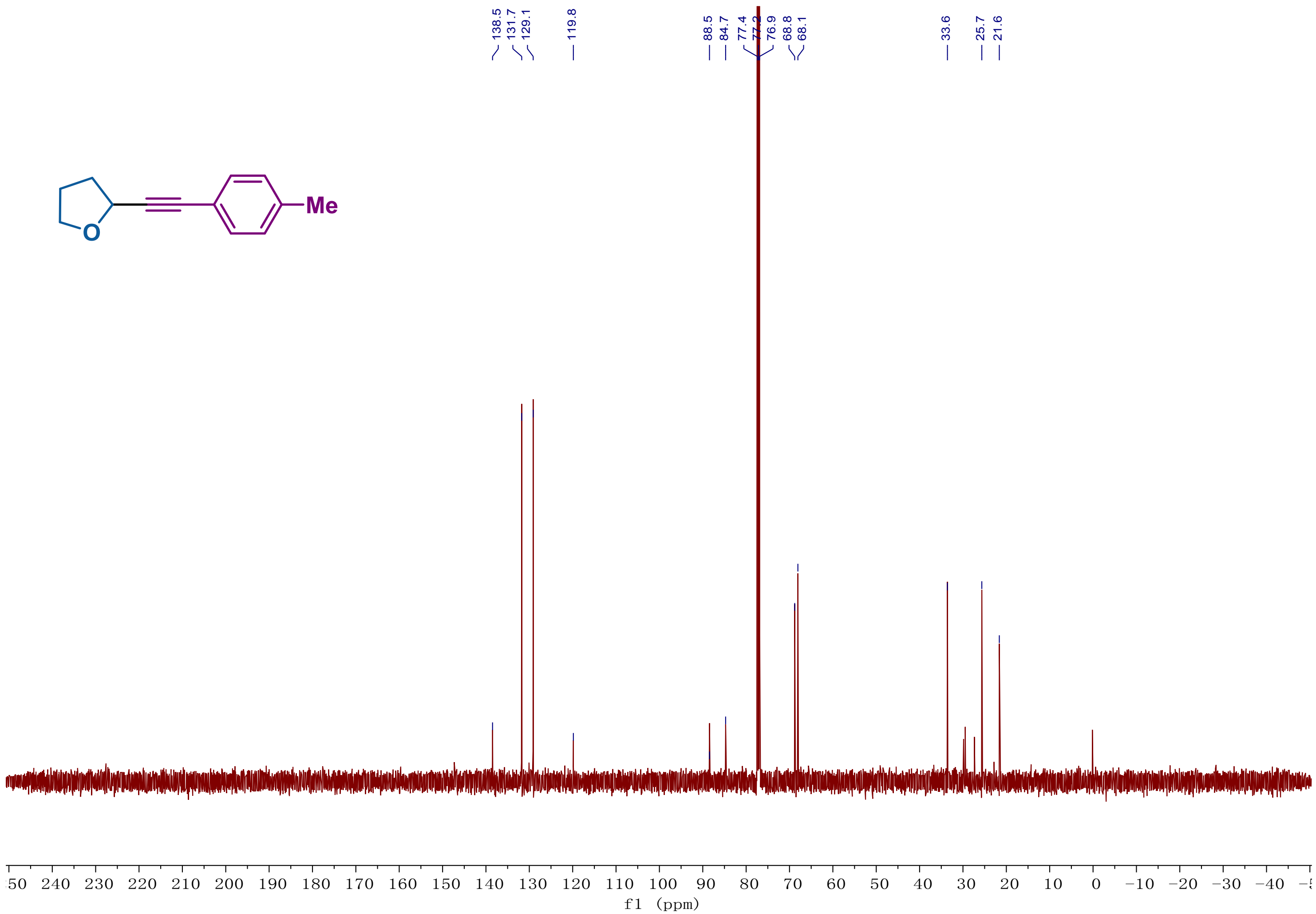

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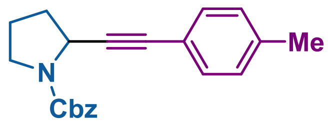

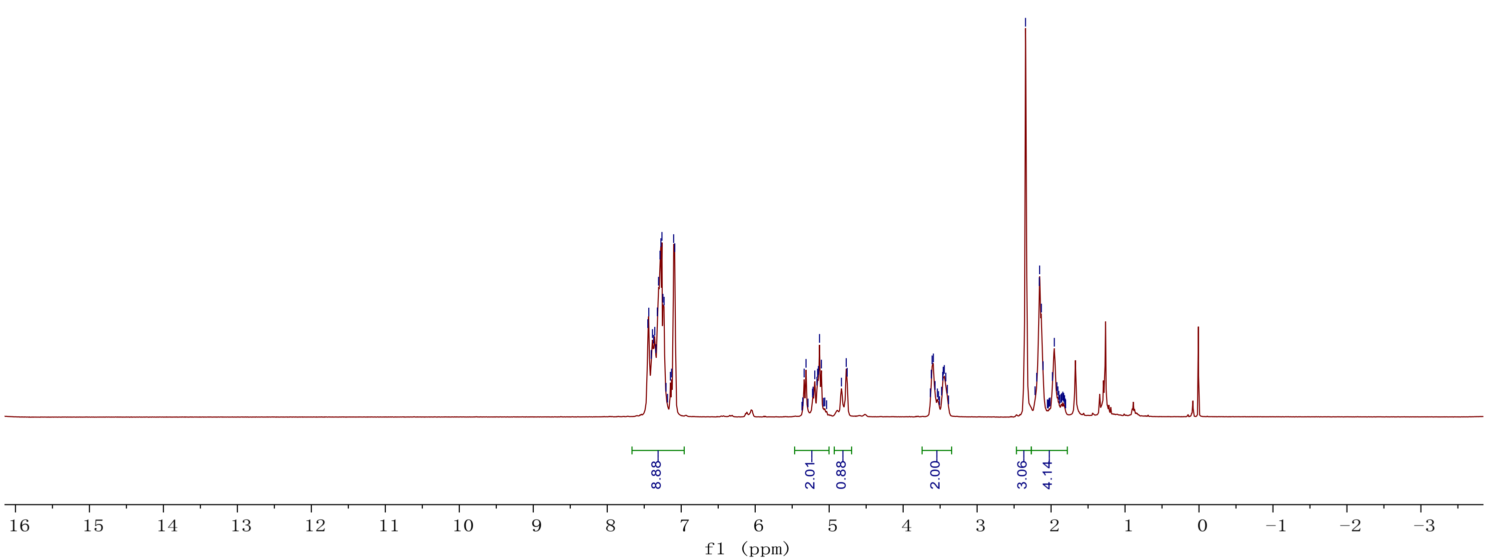

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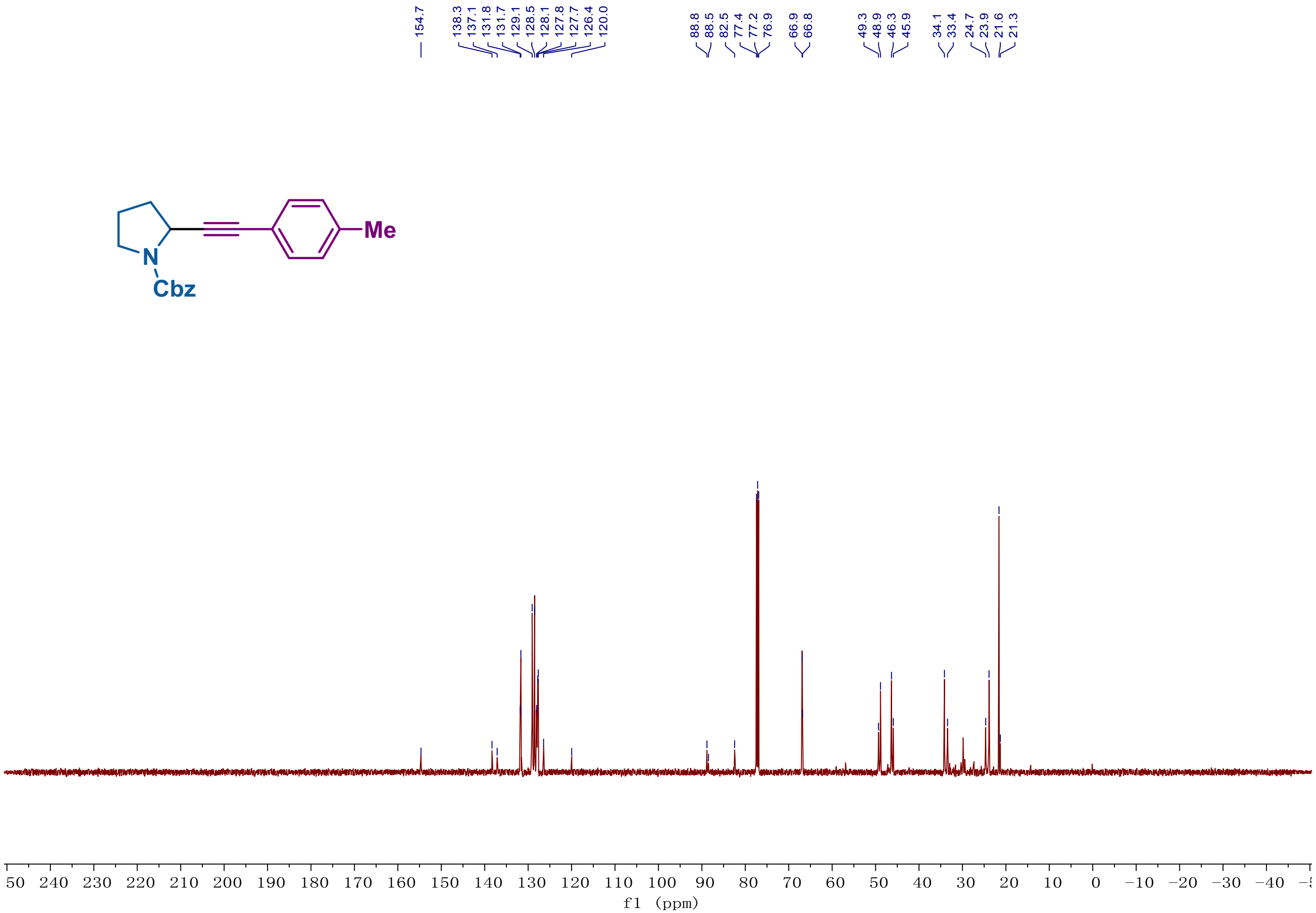

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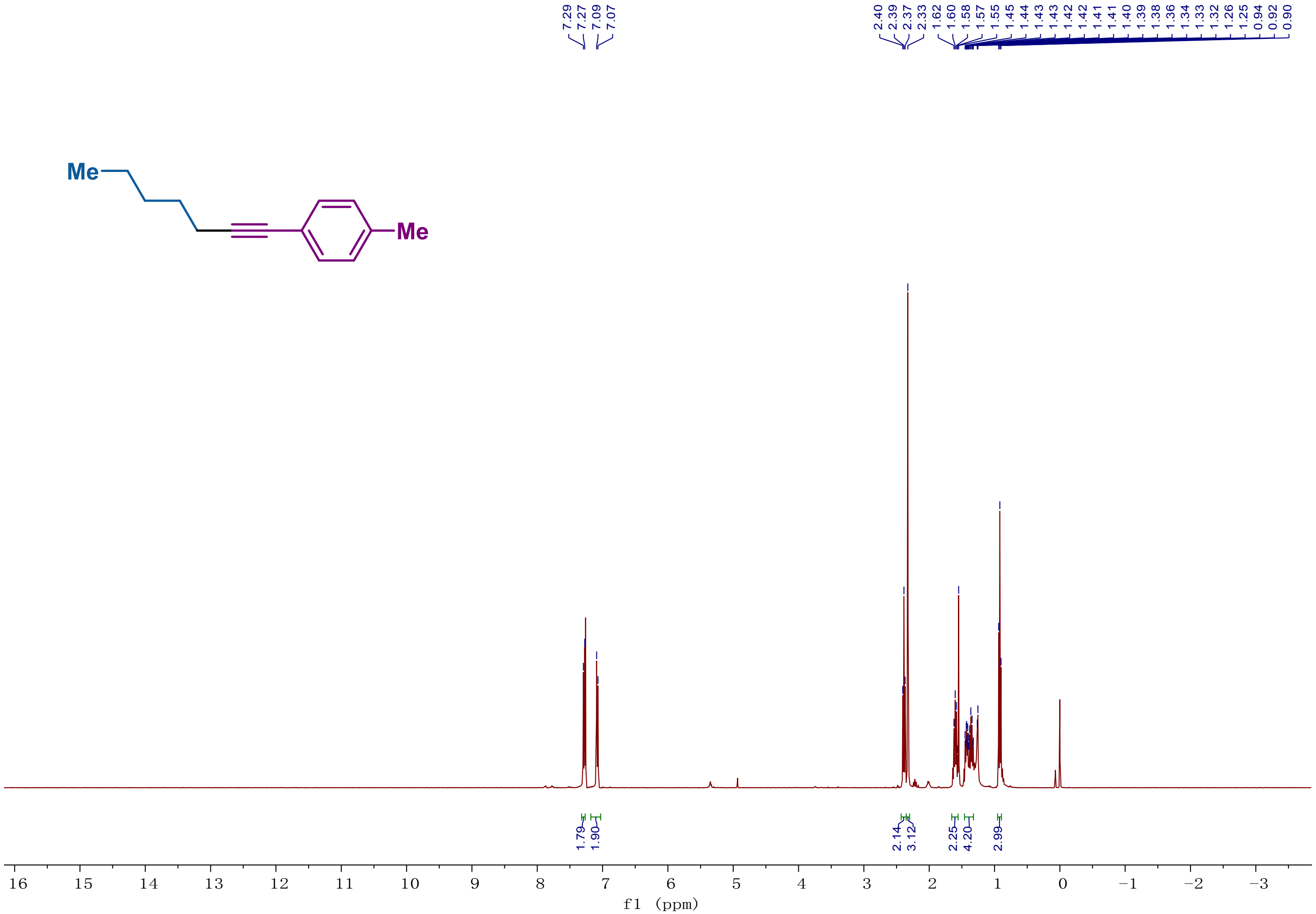

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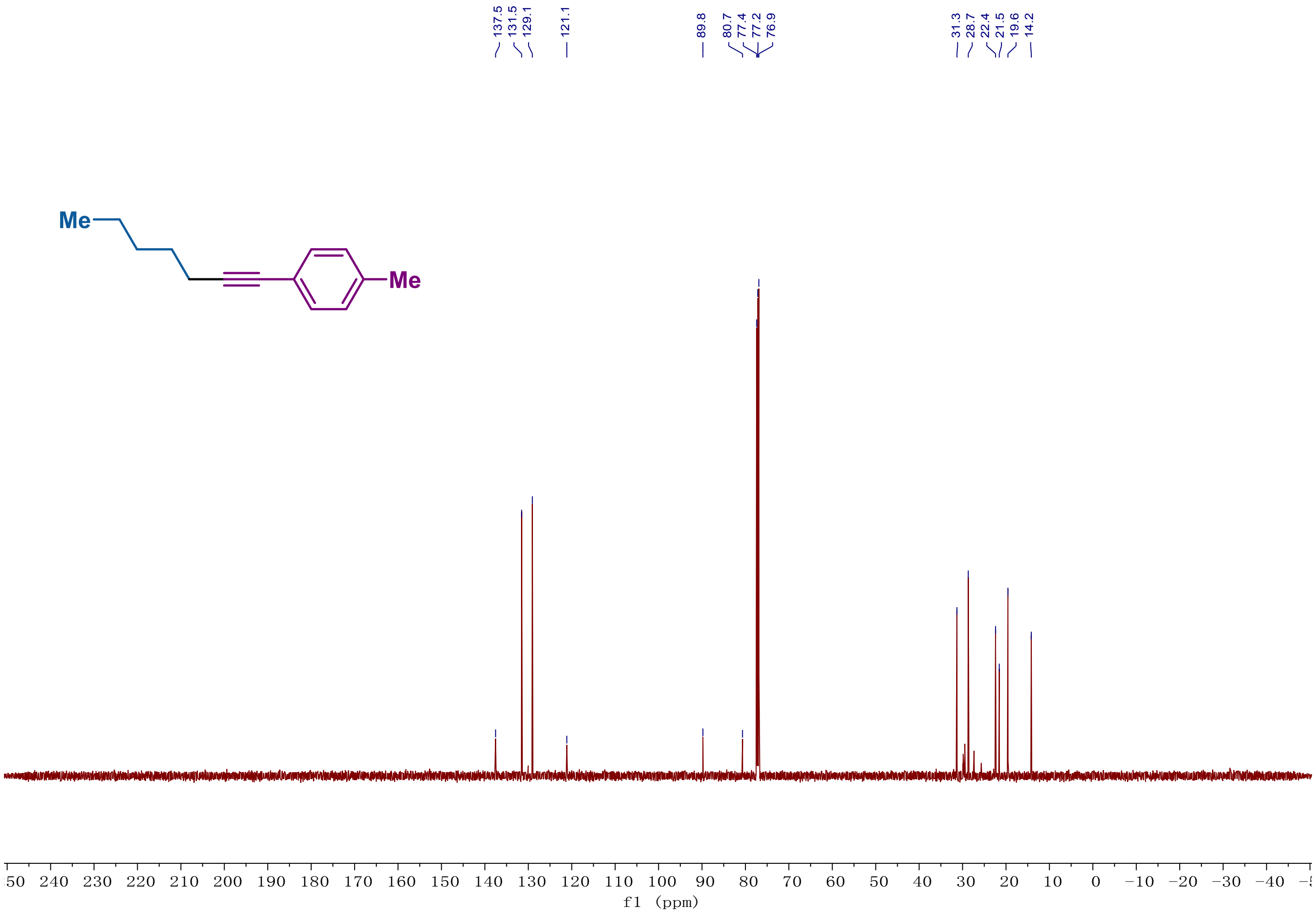

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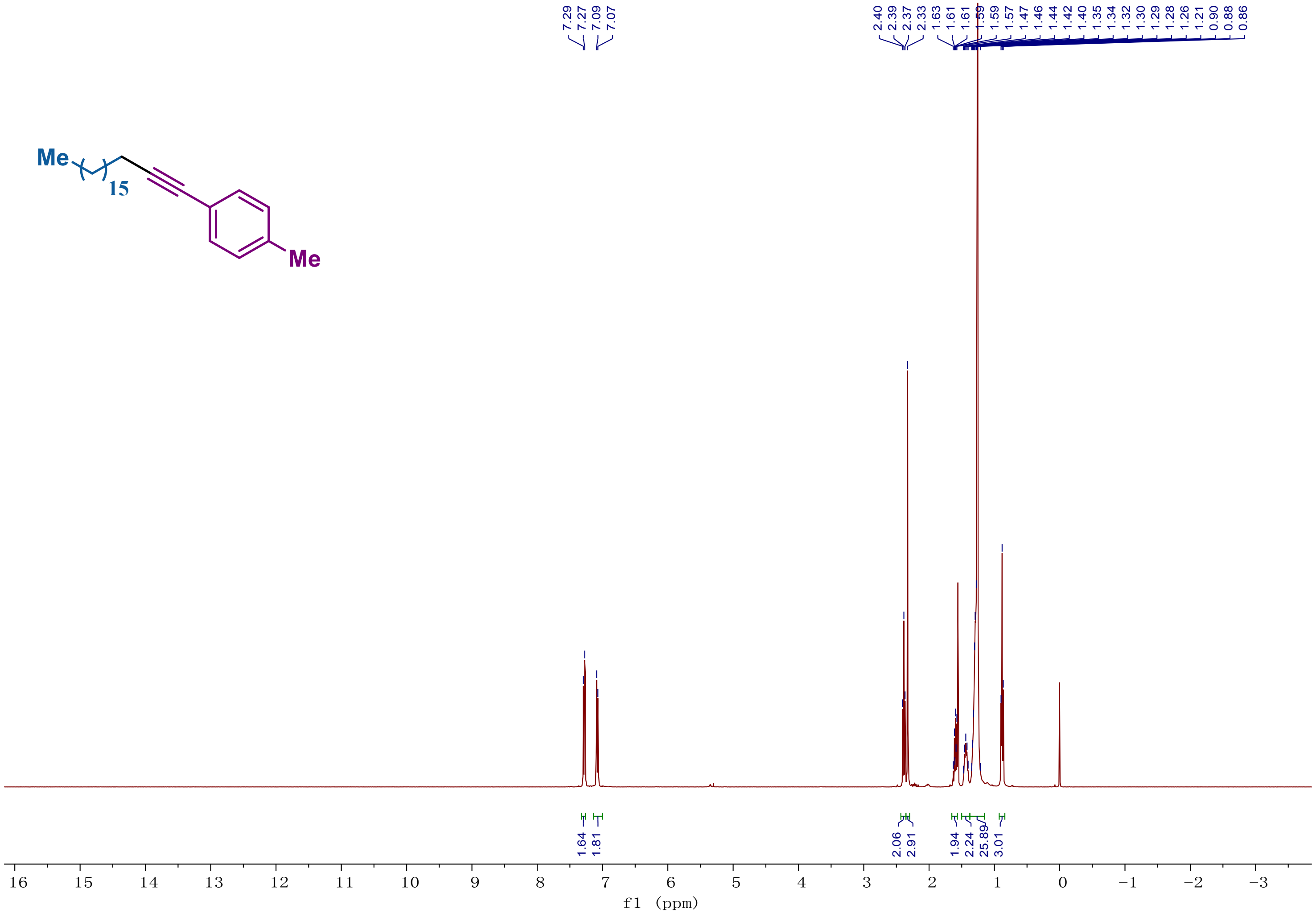

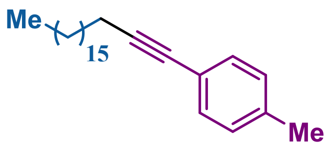

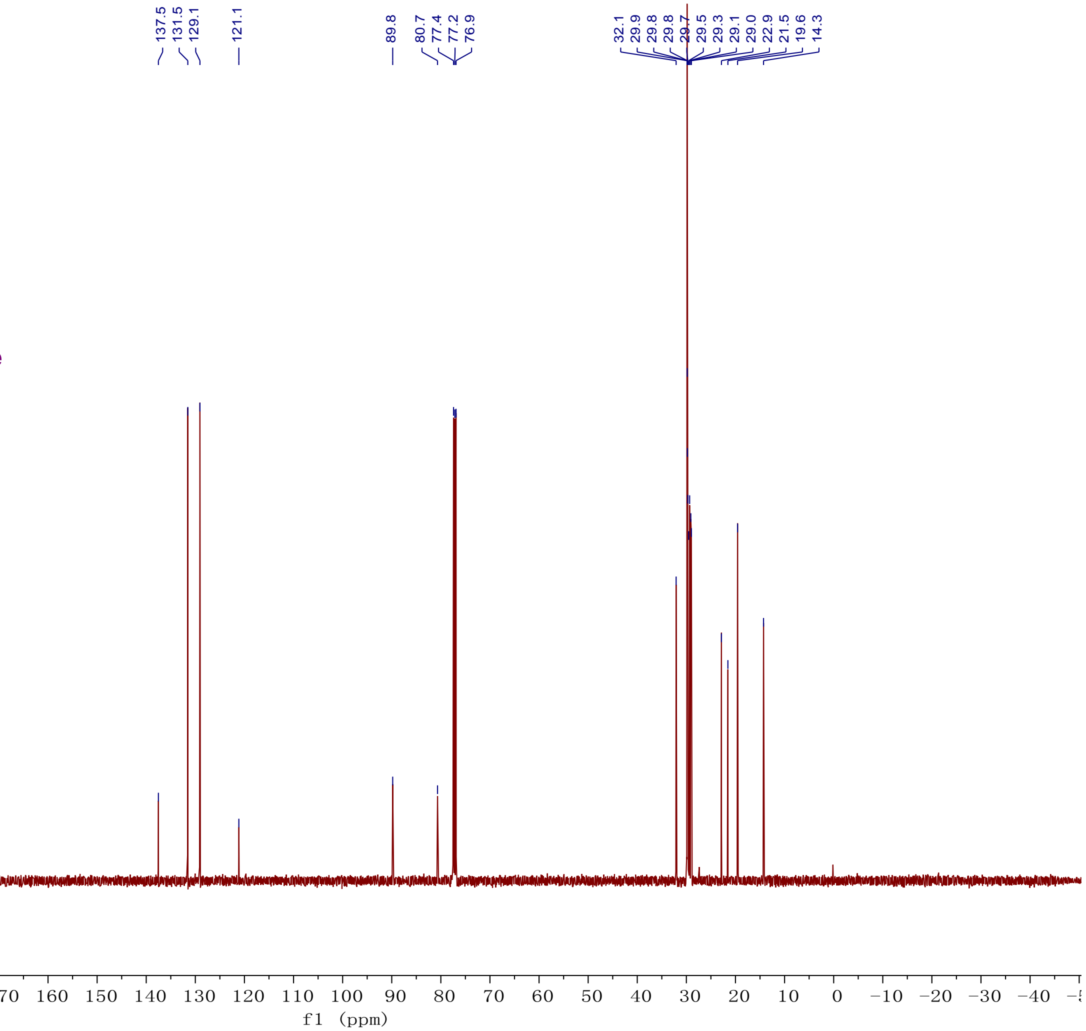
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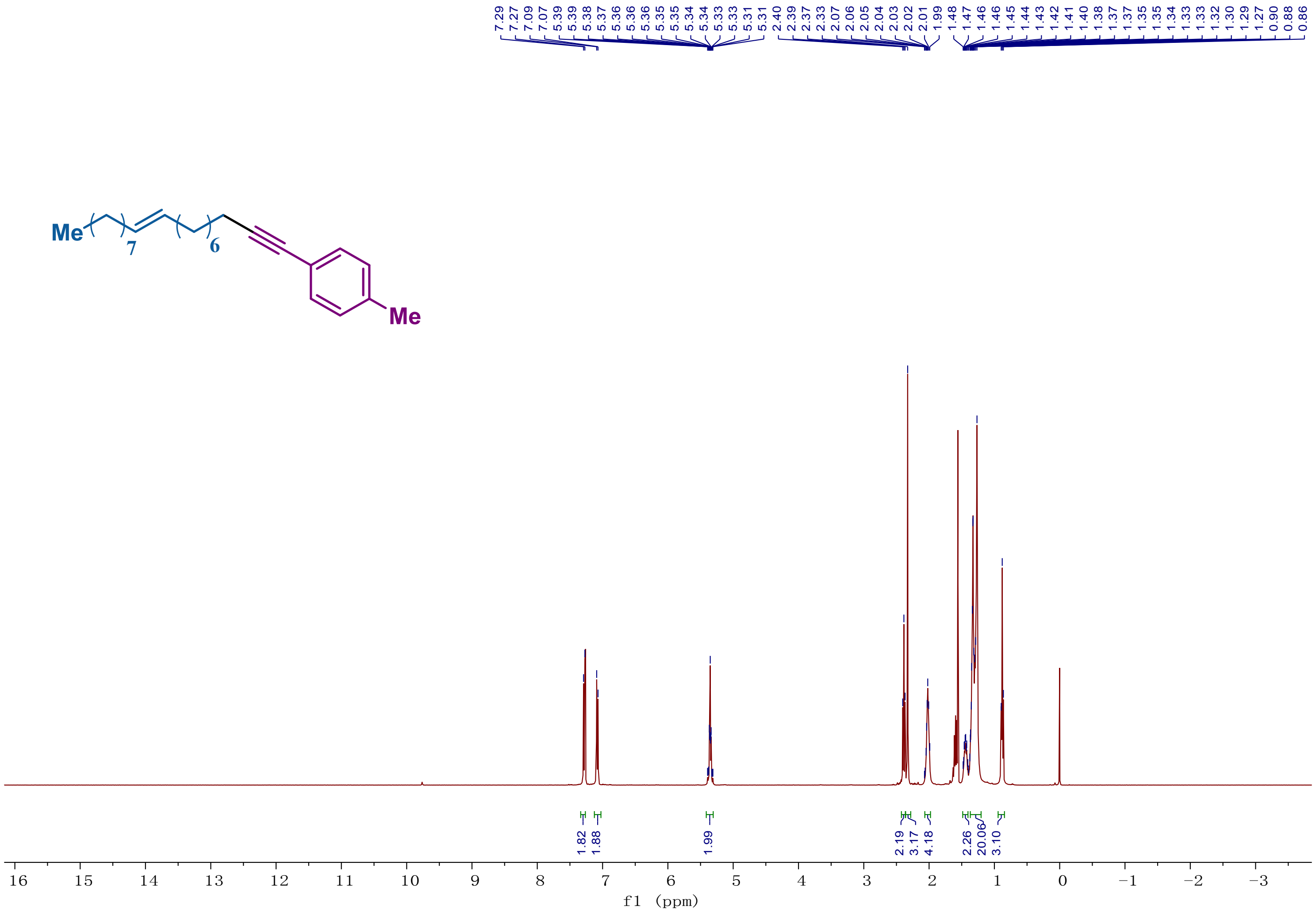
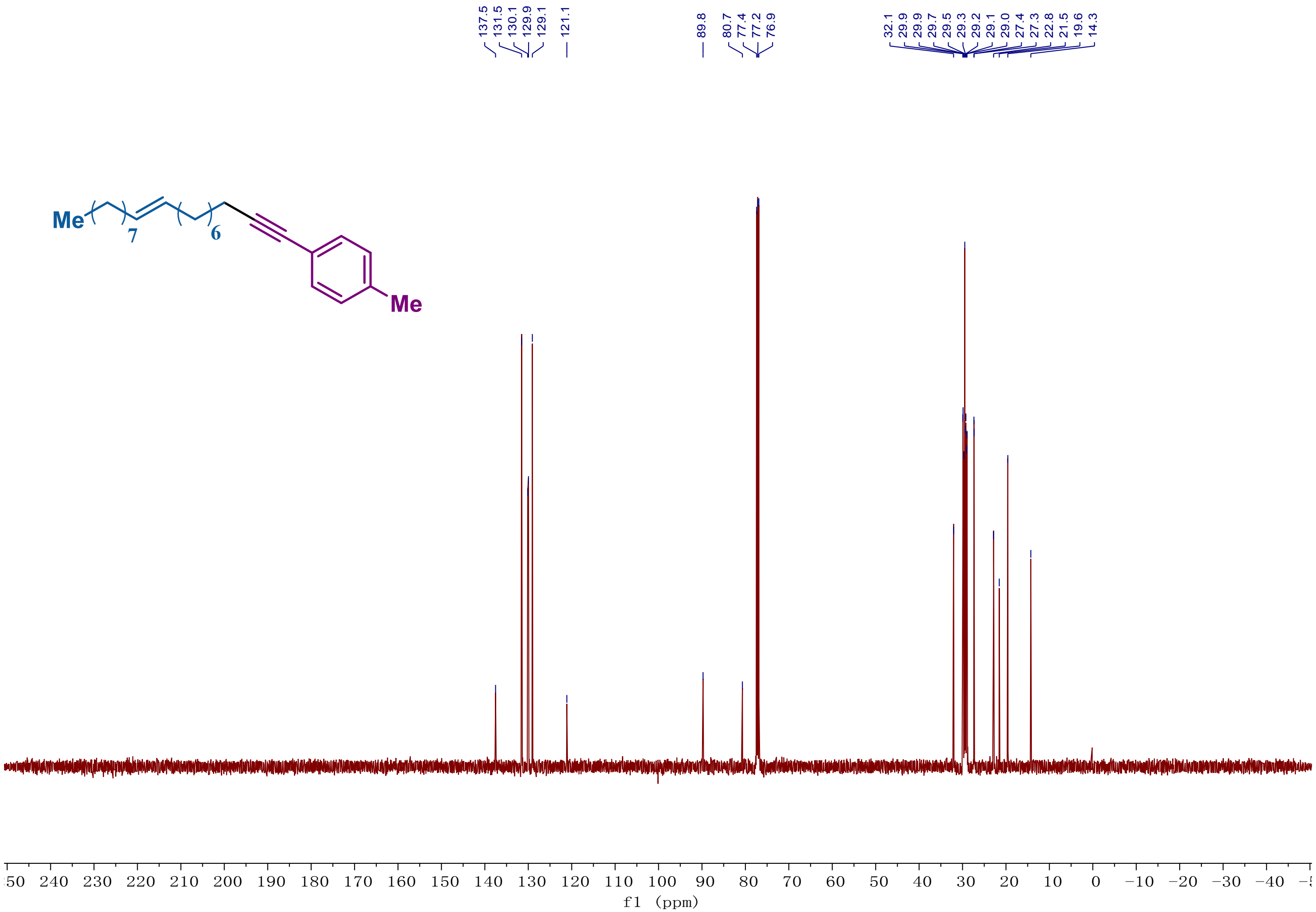
129.1
121.1
89.8
80.7
77.4
77.2
76.9
32.1
29.9
29.8
29.8
29.7
29.5
29.3
29.1
29.0
22.9
21.5
19.6
14.3
f1 (ppm)

Compound 20 ¹H NMR



Compound 20 ^{13}C NMR



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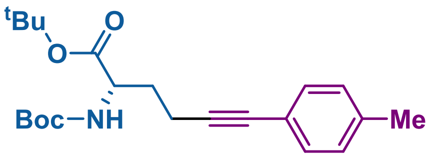

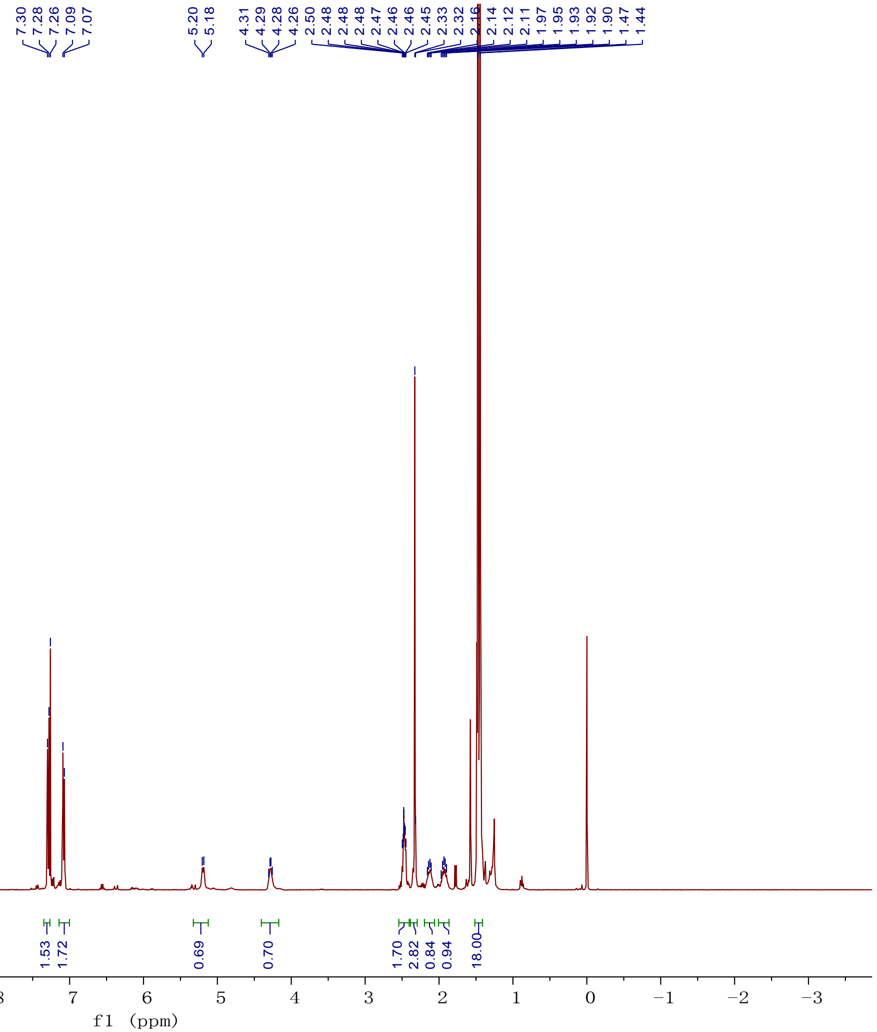

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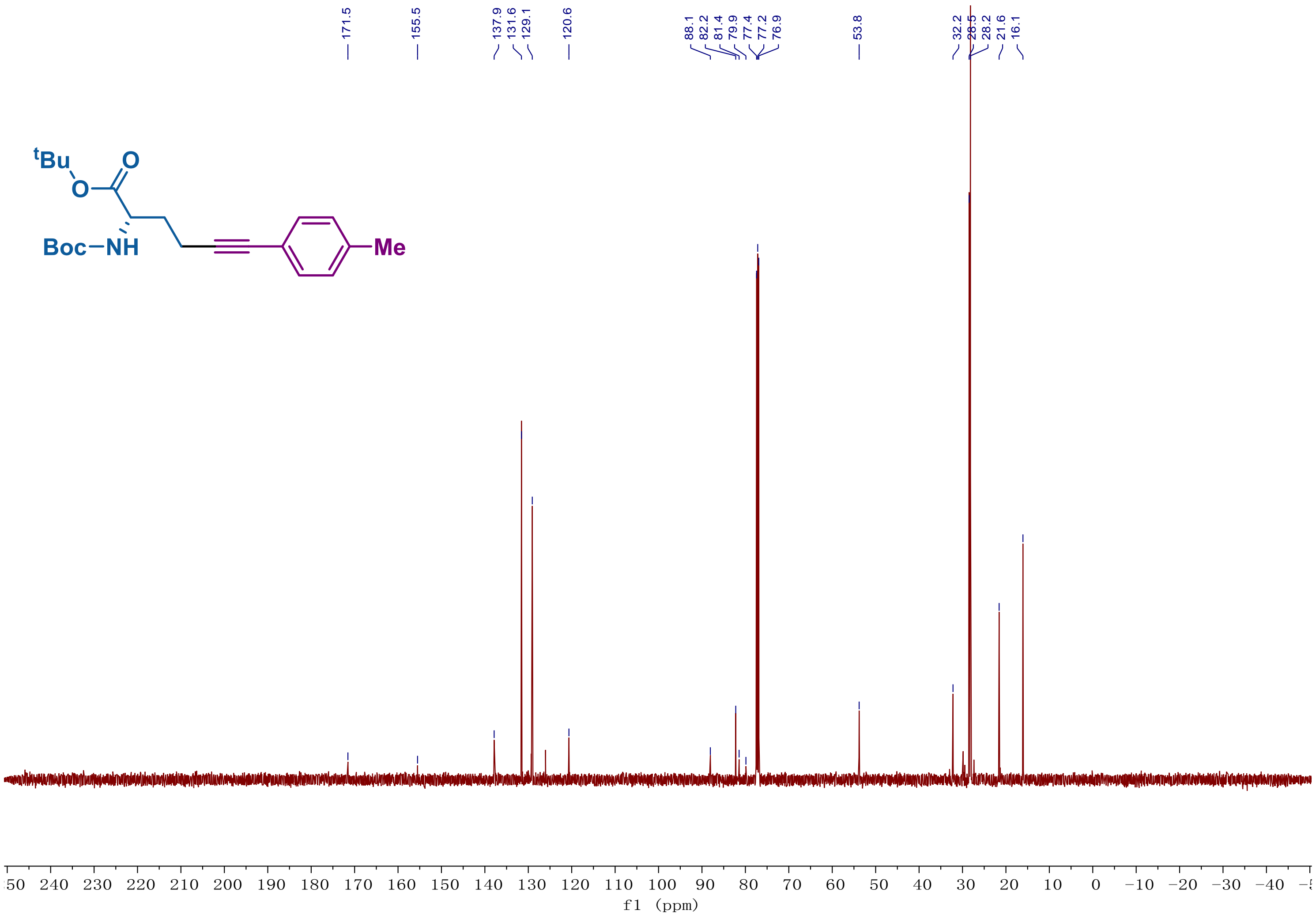

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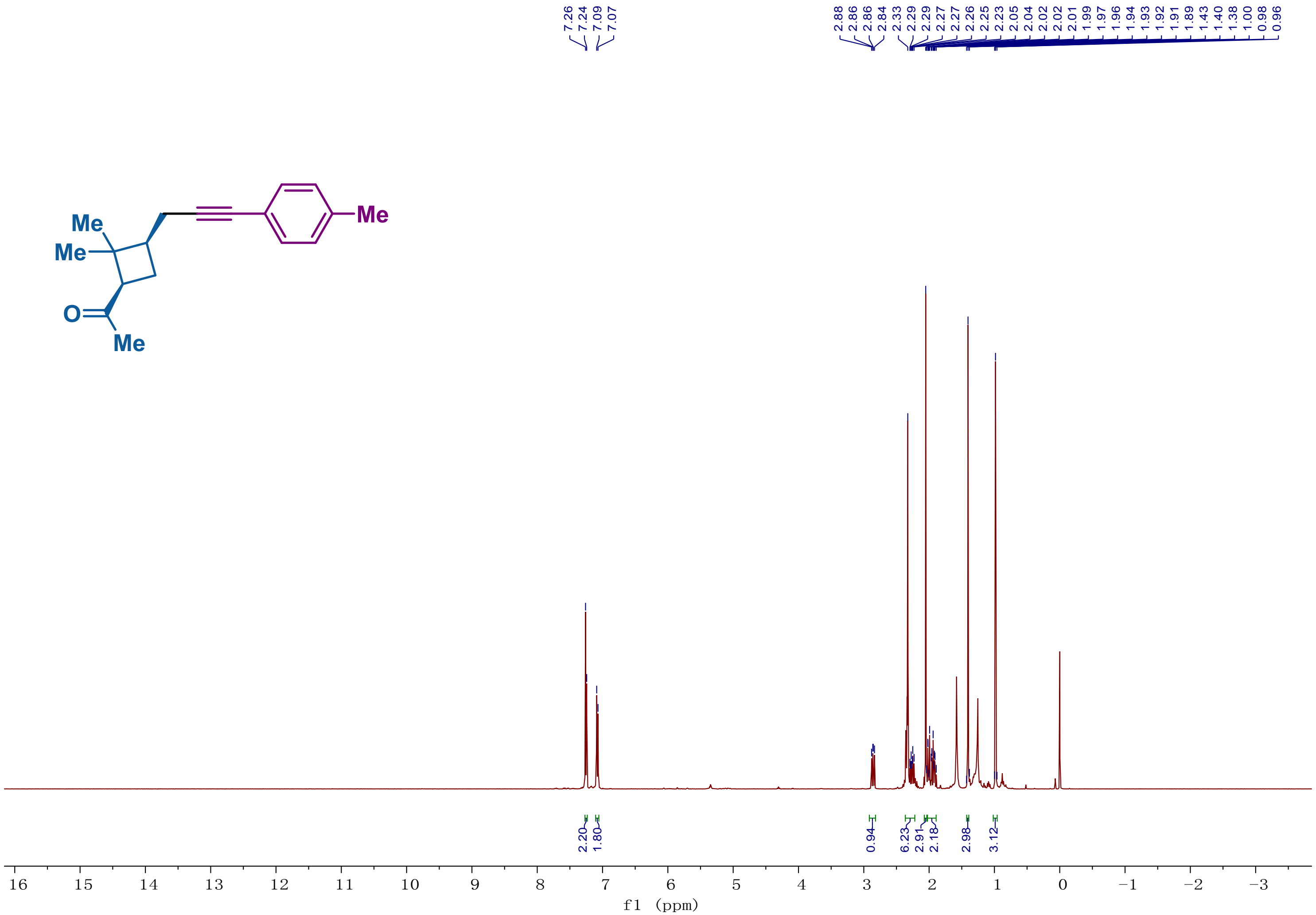

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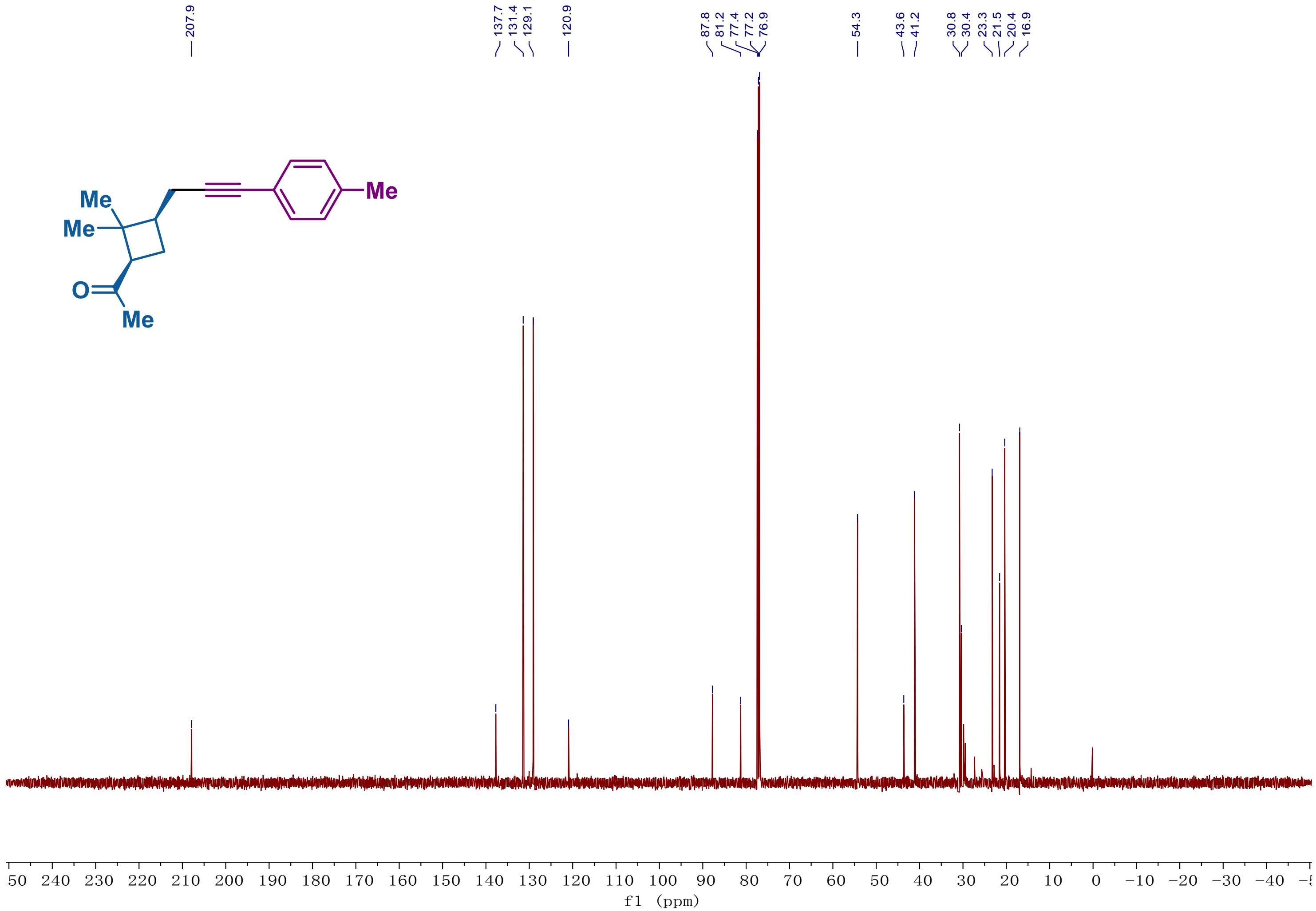

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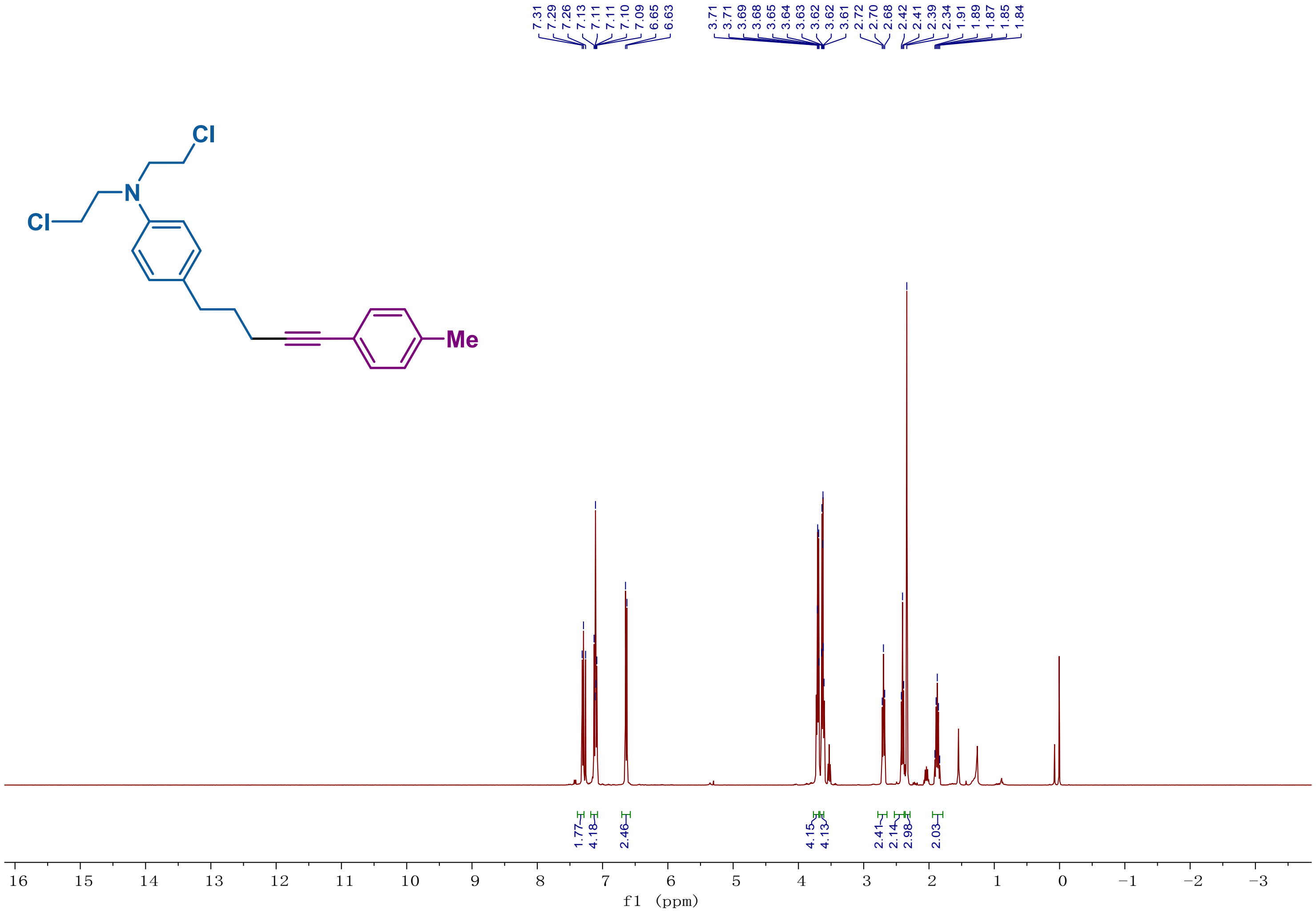

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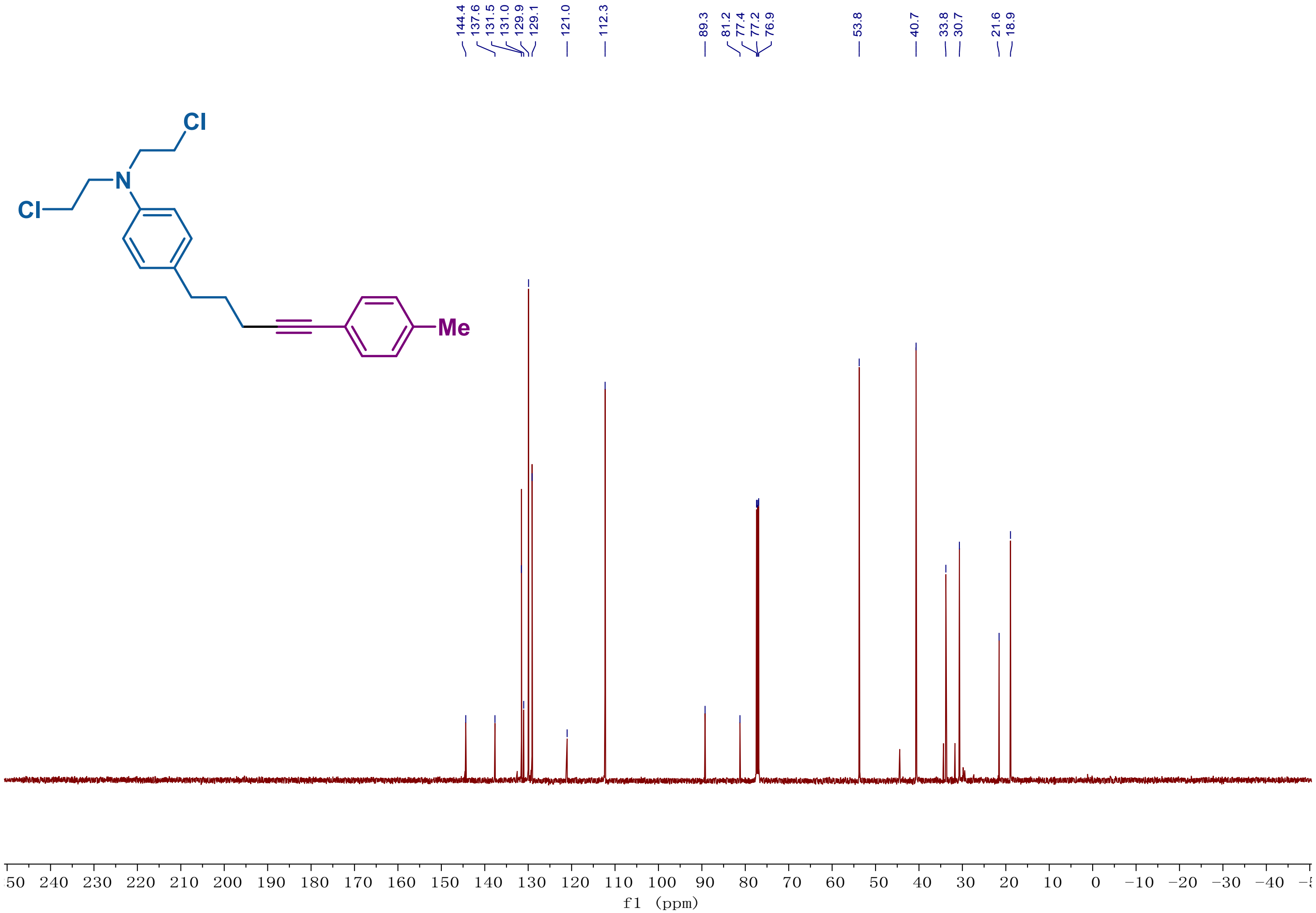

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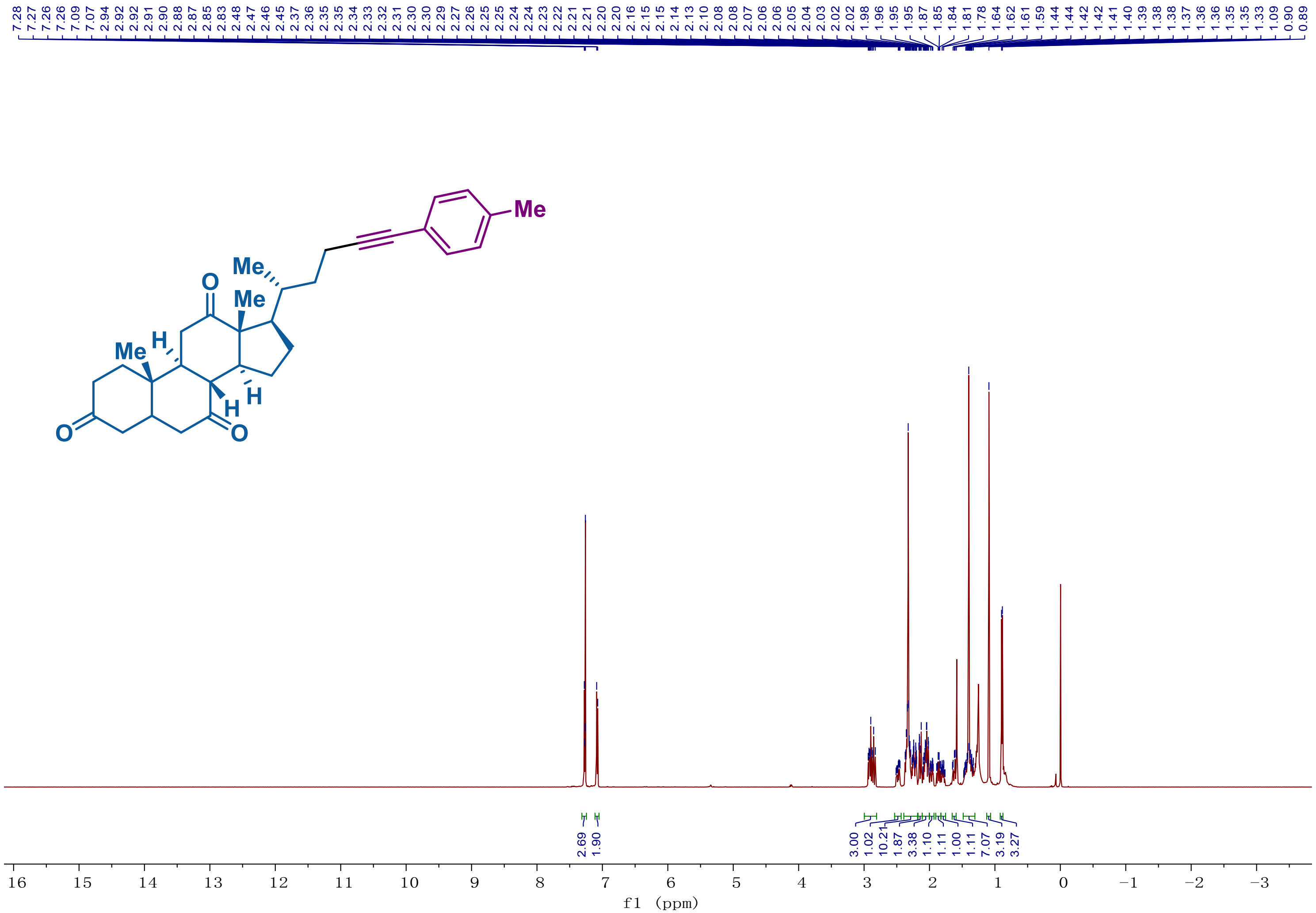
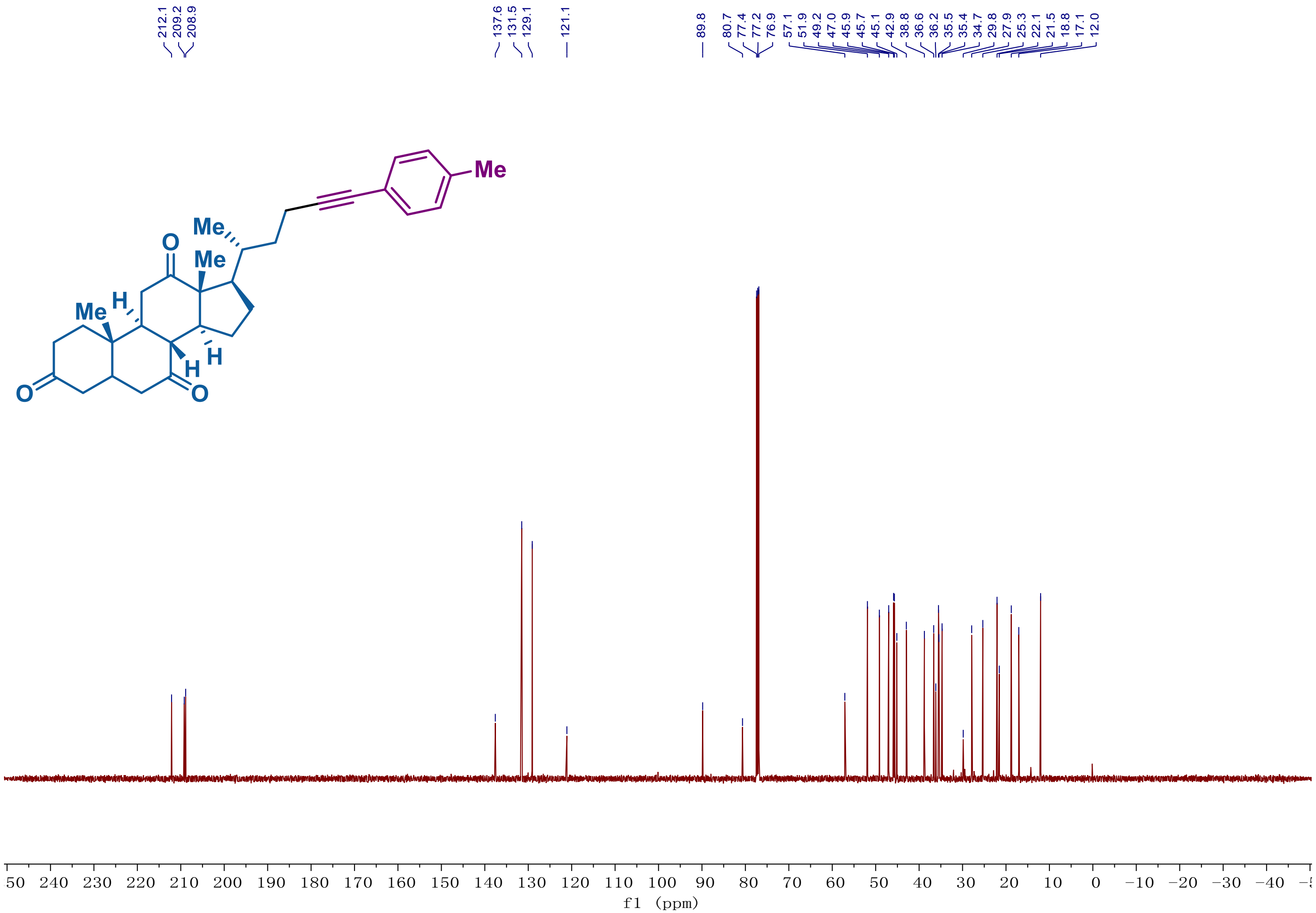
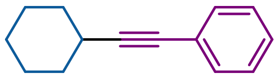
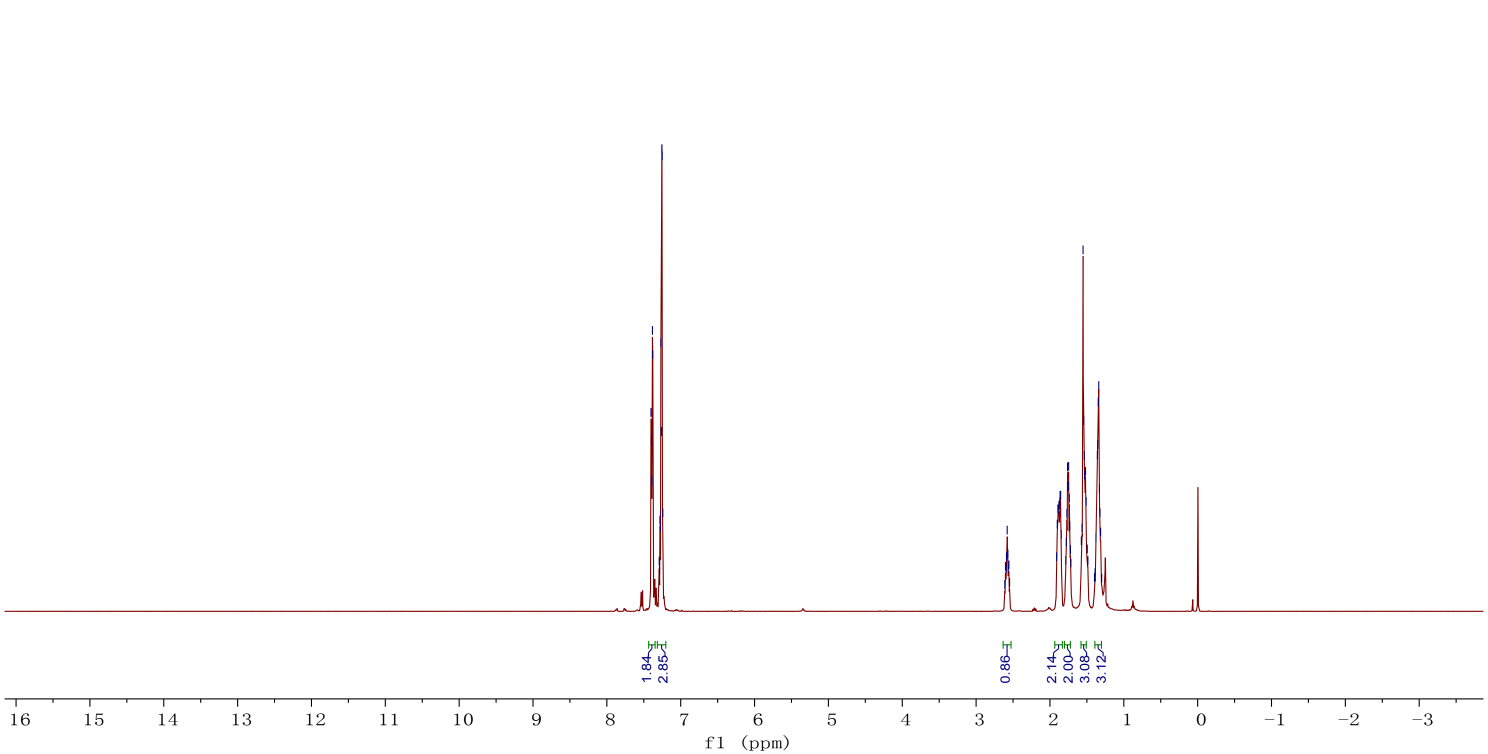


Compound 24 ^{13}C NMR

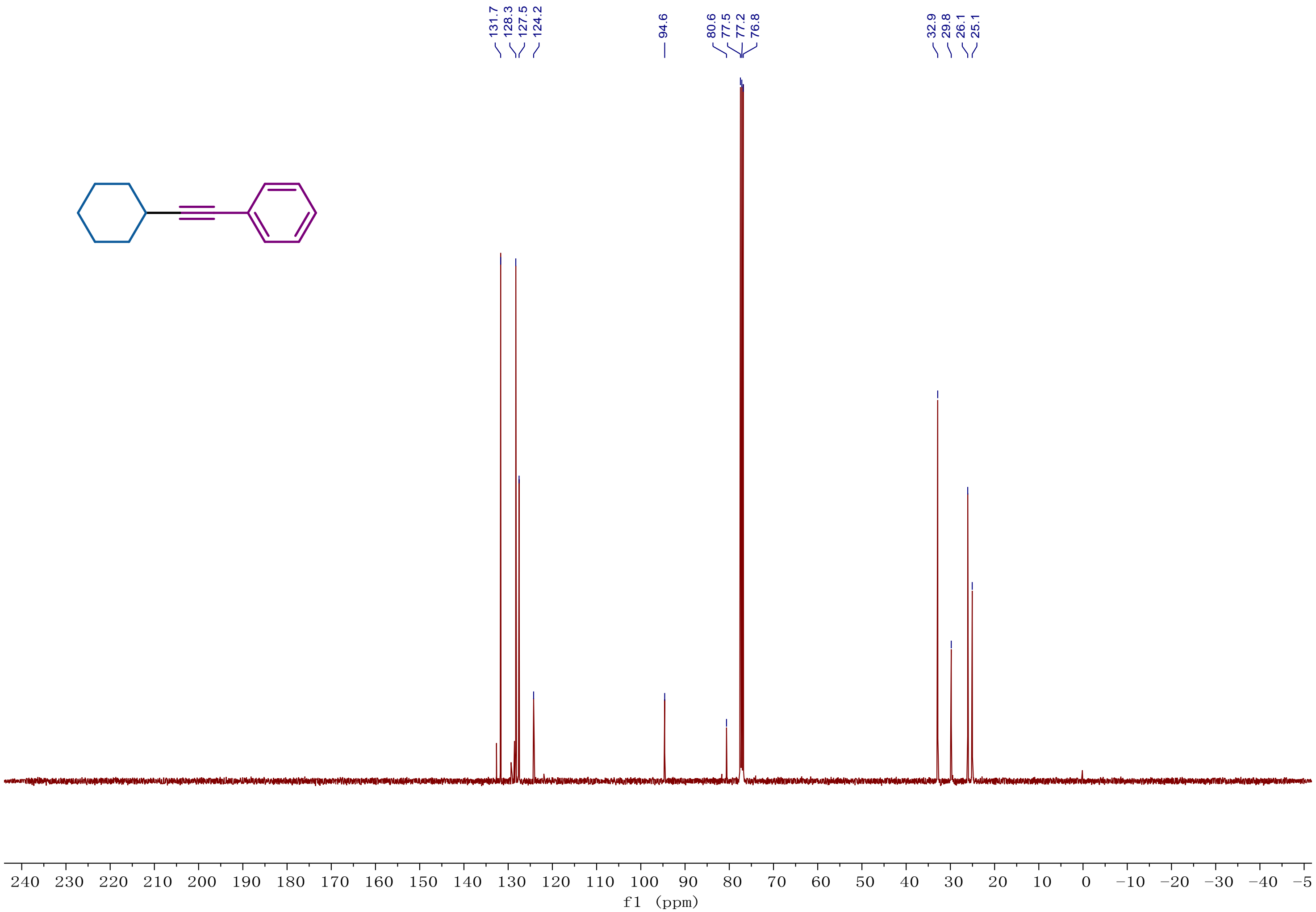


Compound 25 ^{1}H NMR

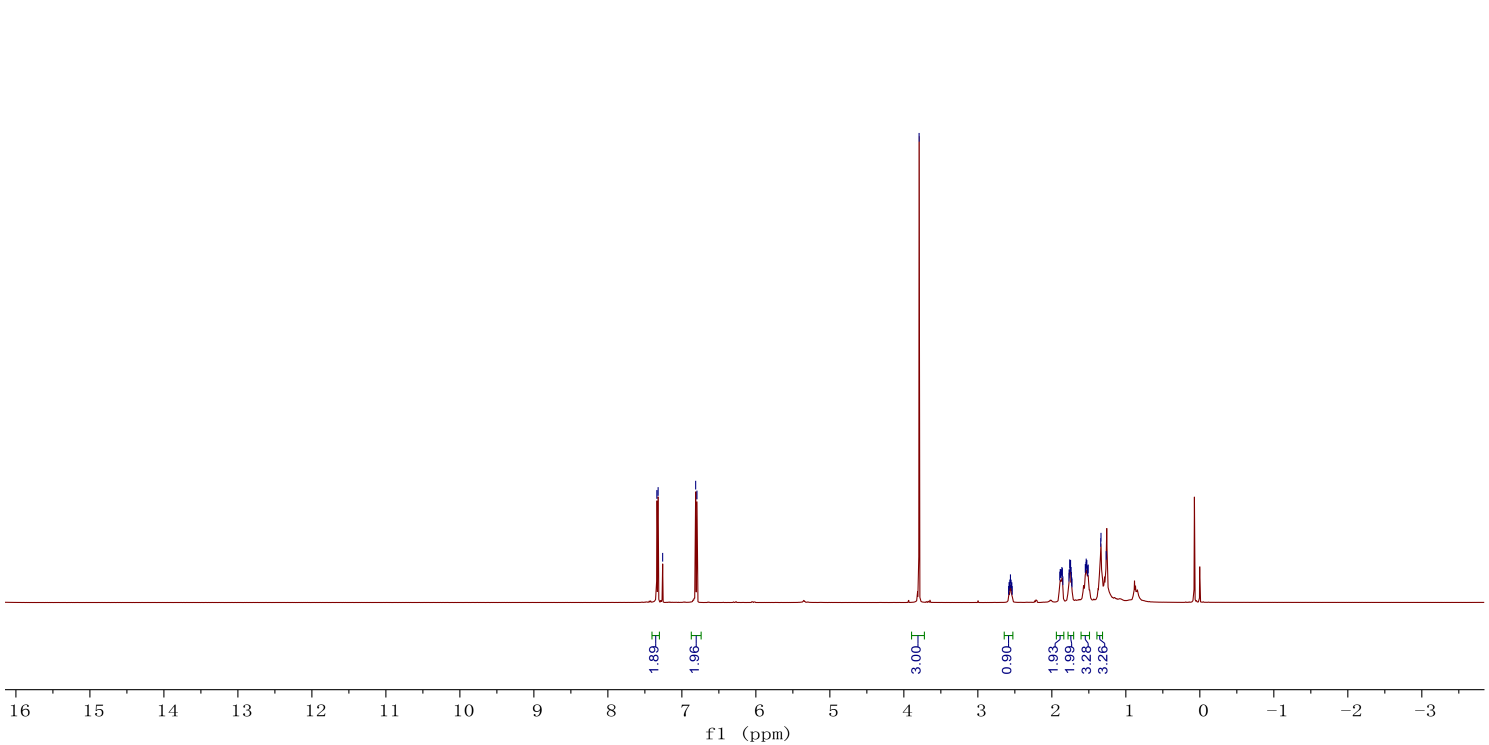




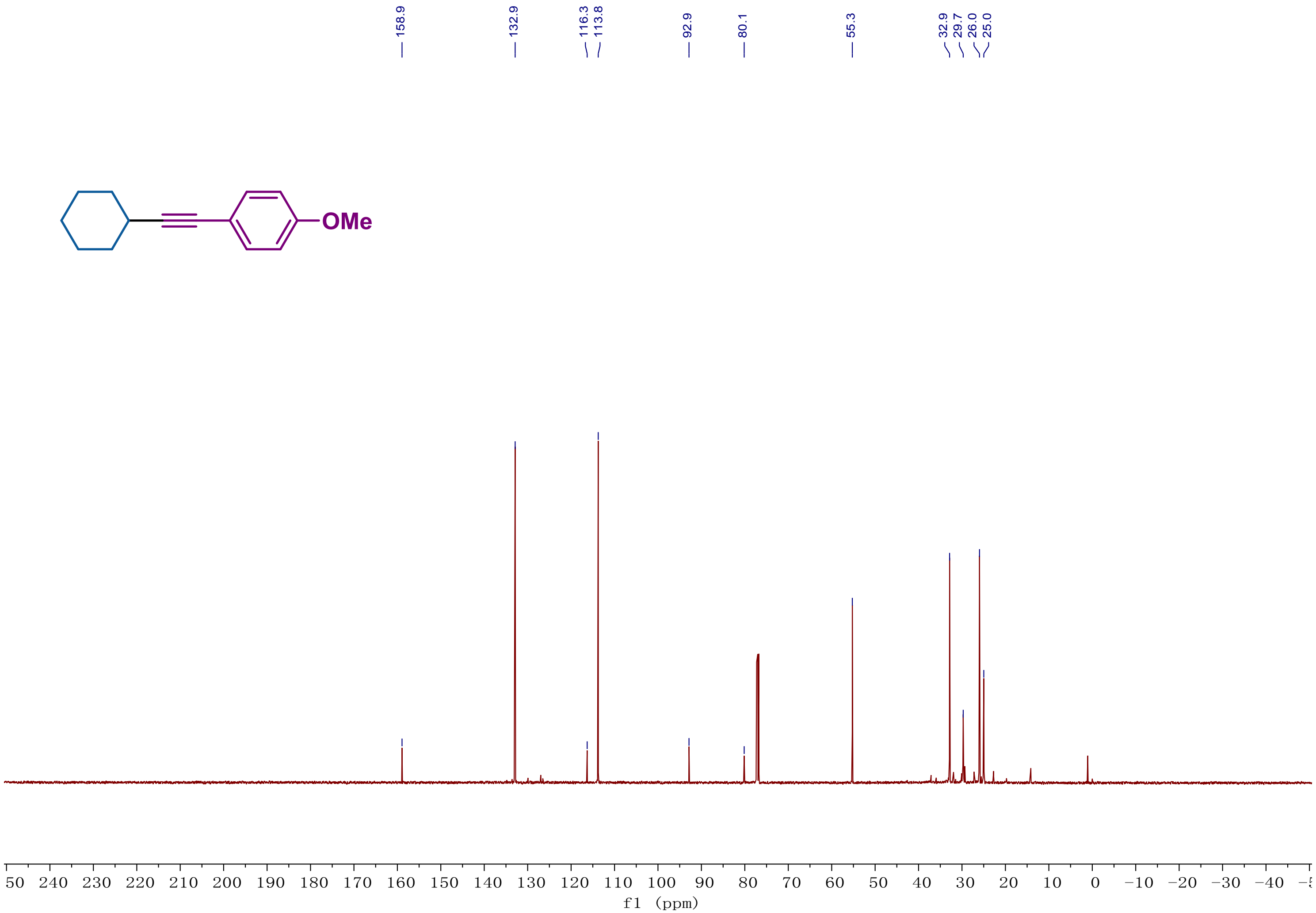
Compound 25 ^{13}C NMR



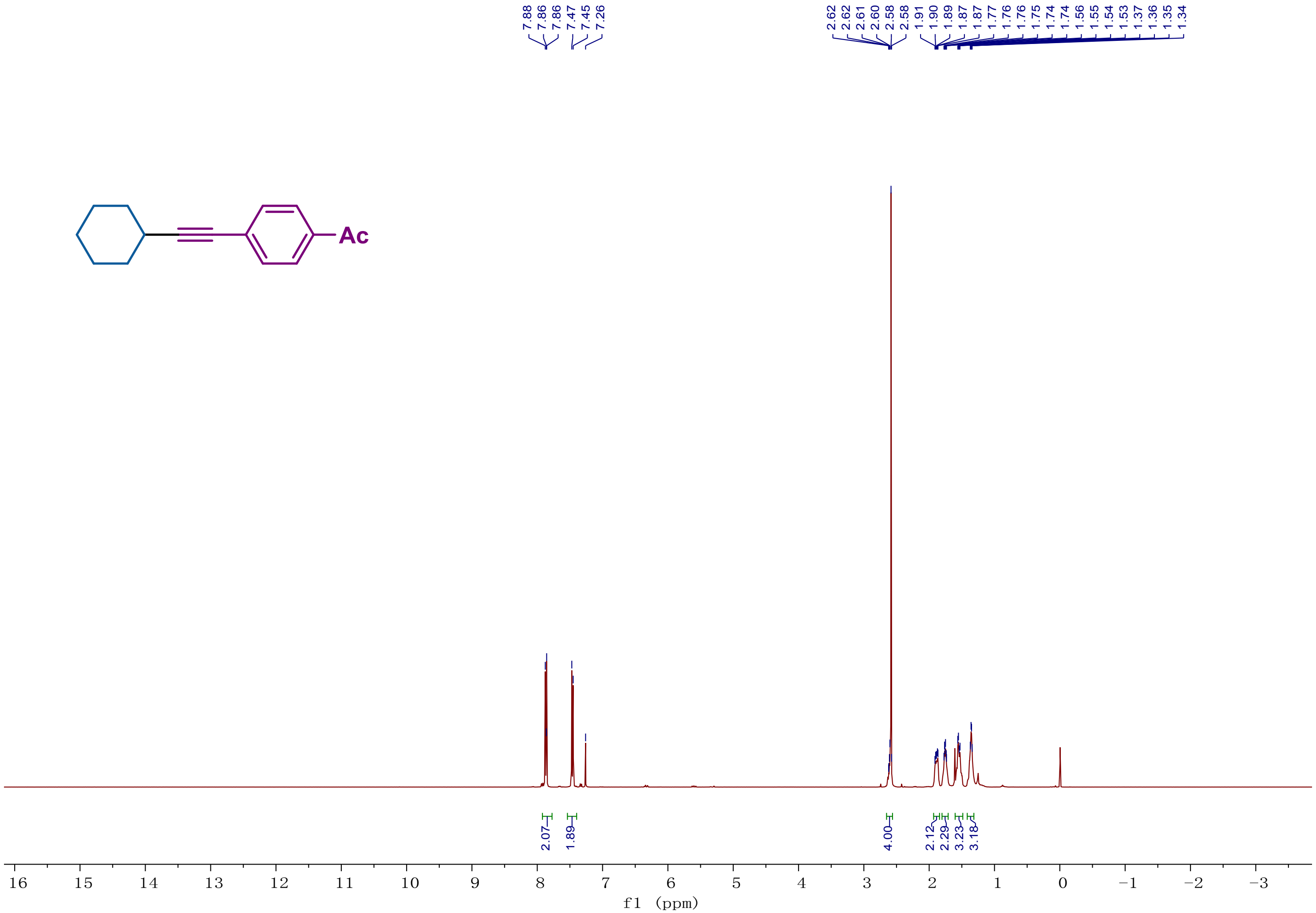
Compound 26 ¹H NMR



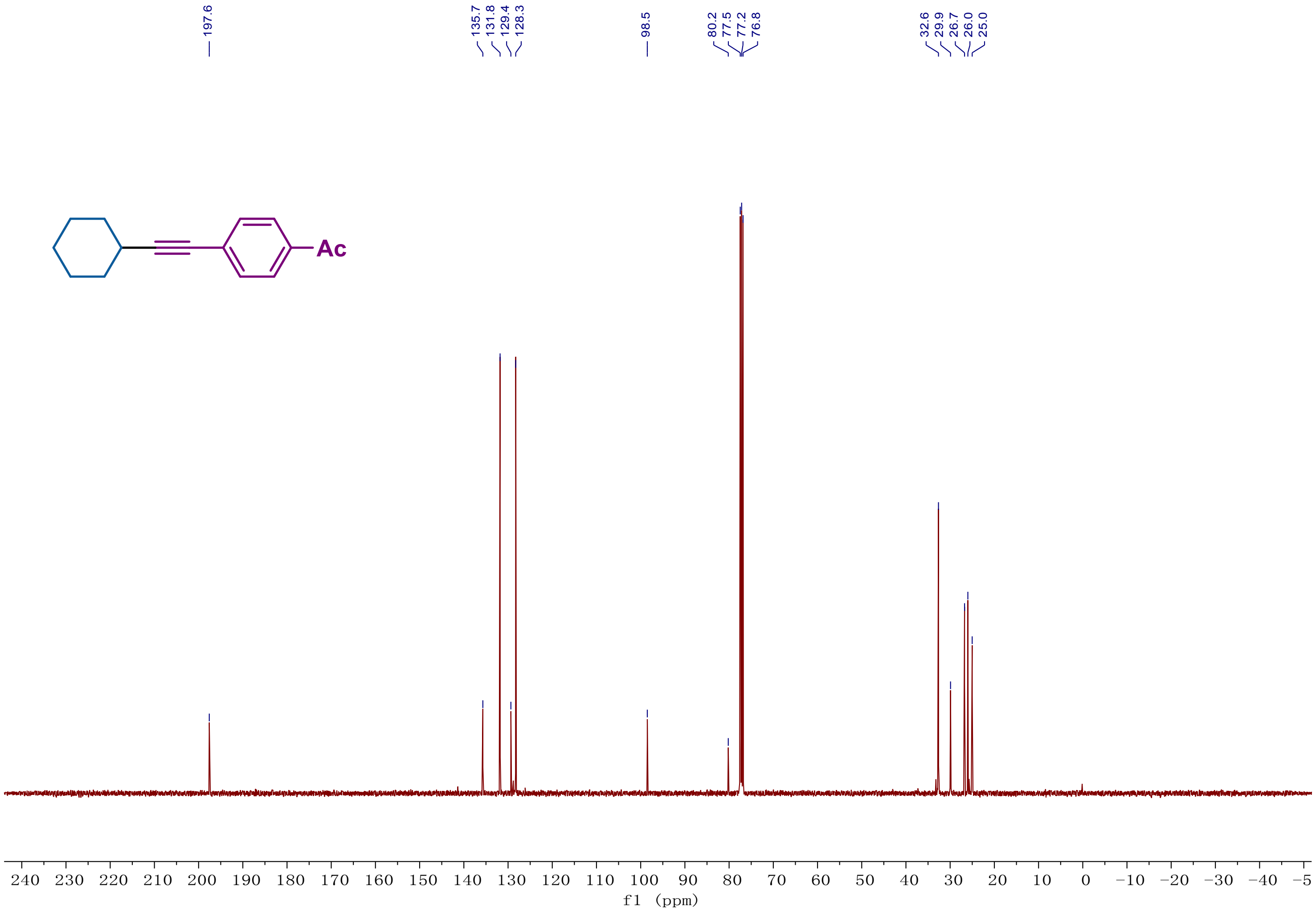
Compound 26 ^{13}C NMR



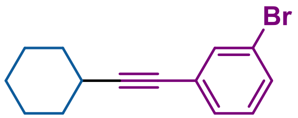
Compound 27 ^{1}H NMR

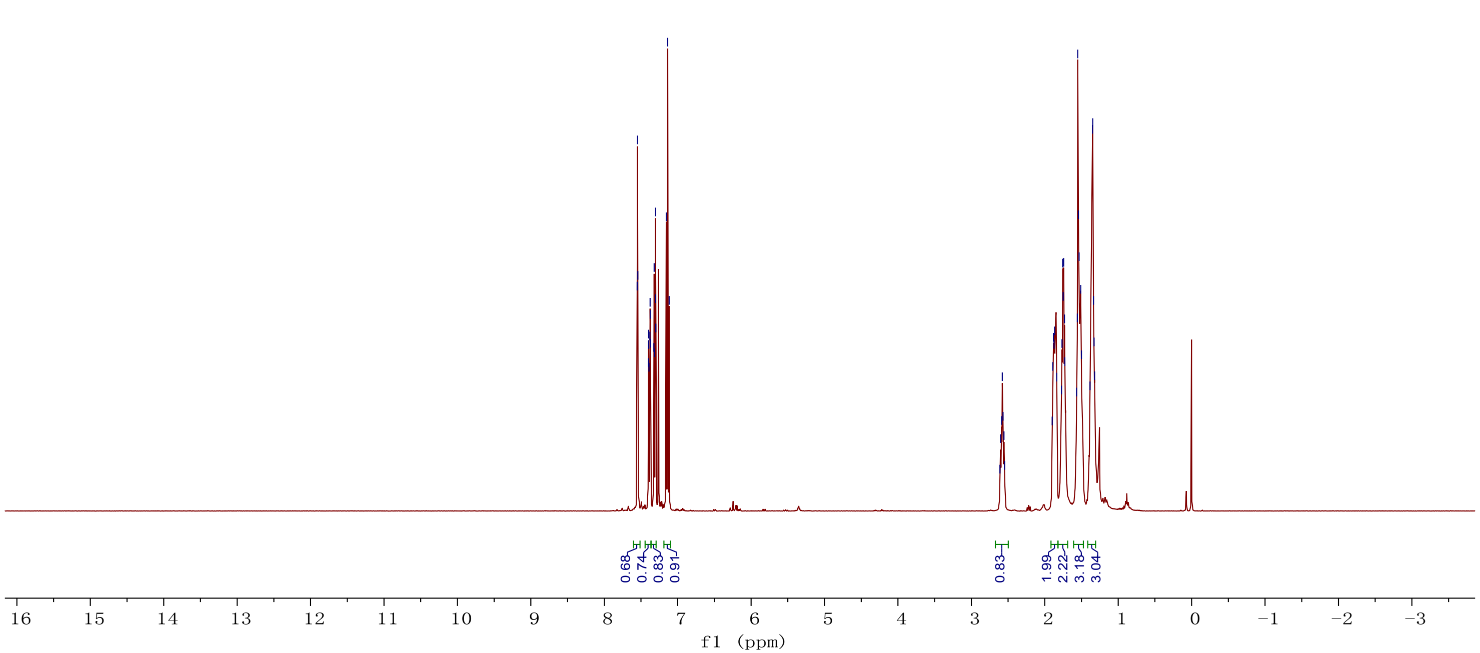


Compound 27 ^{13}C NMR

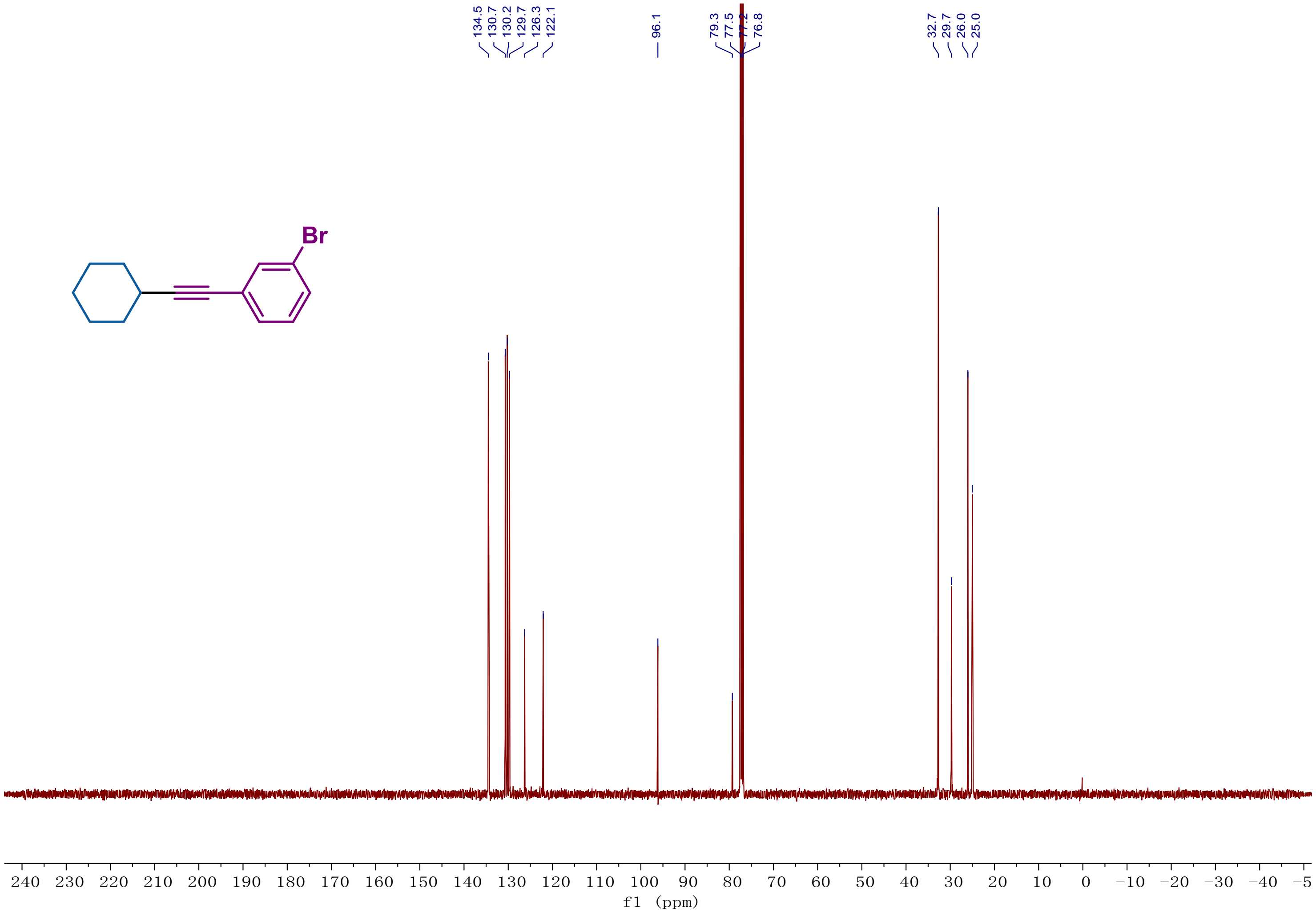


Compound 28 ^{1}H NMR





Compound 28 ¹³C NMR



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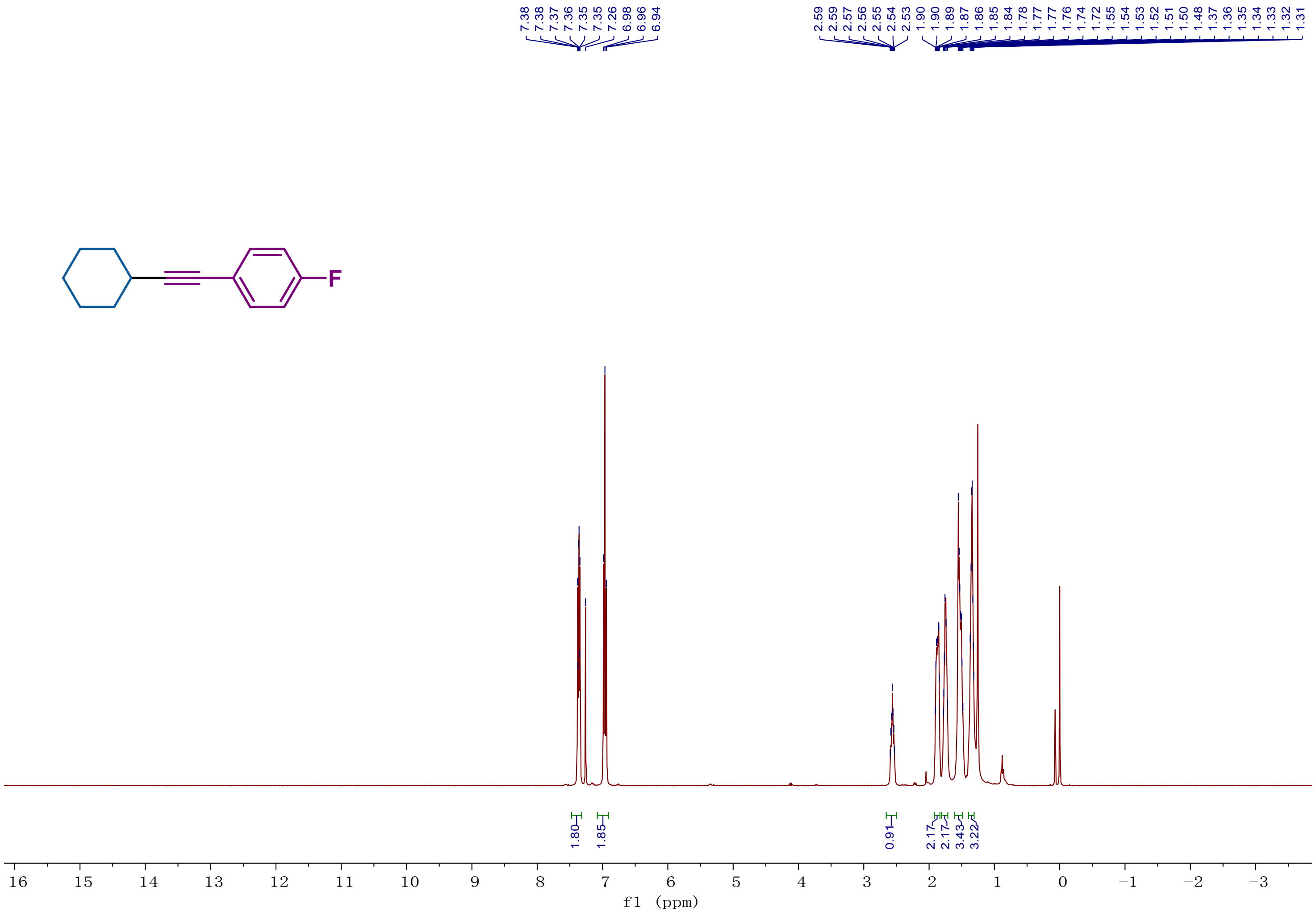

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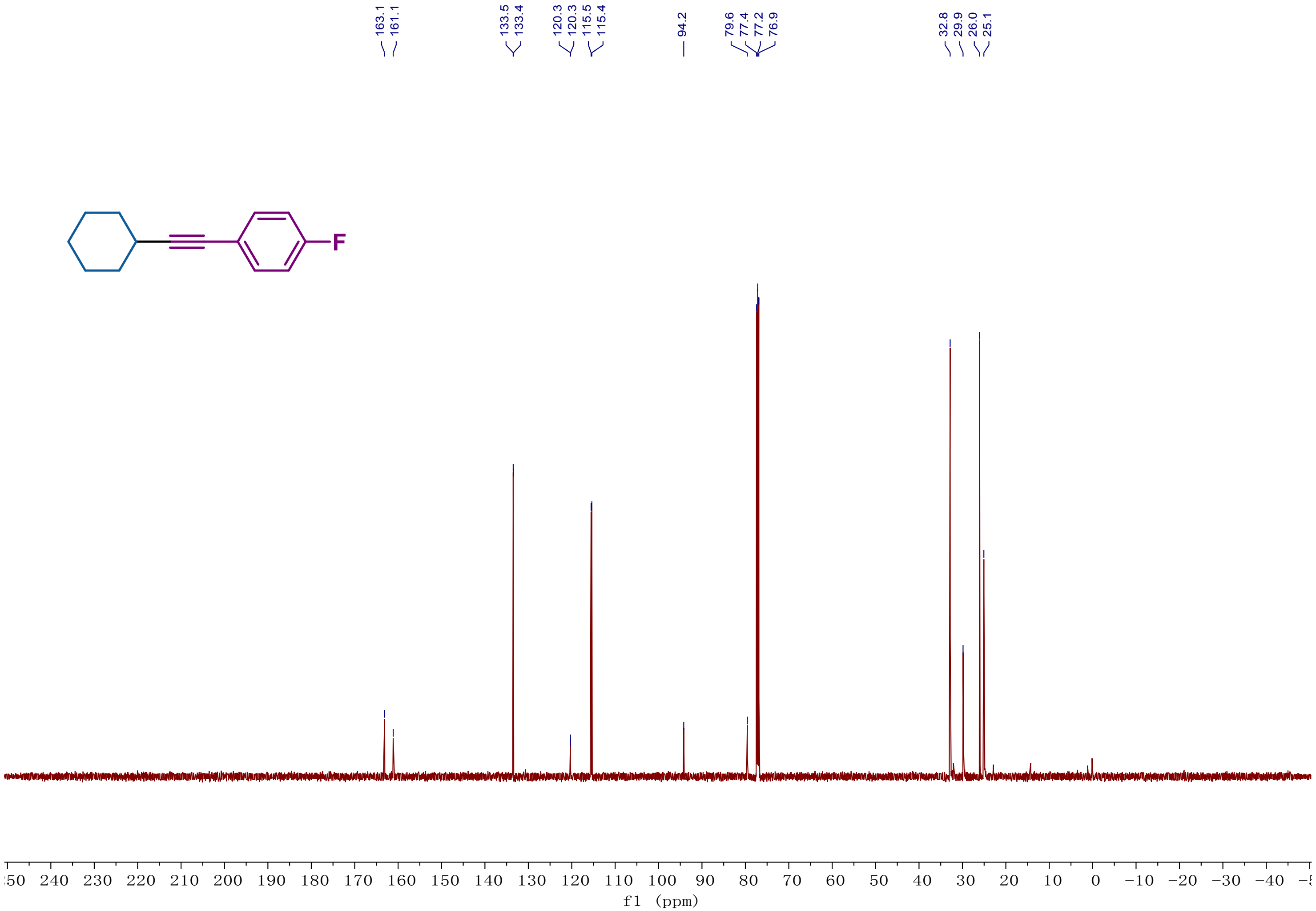
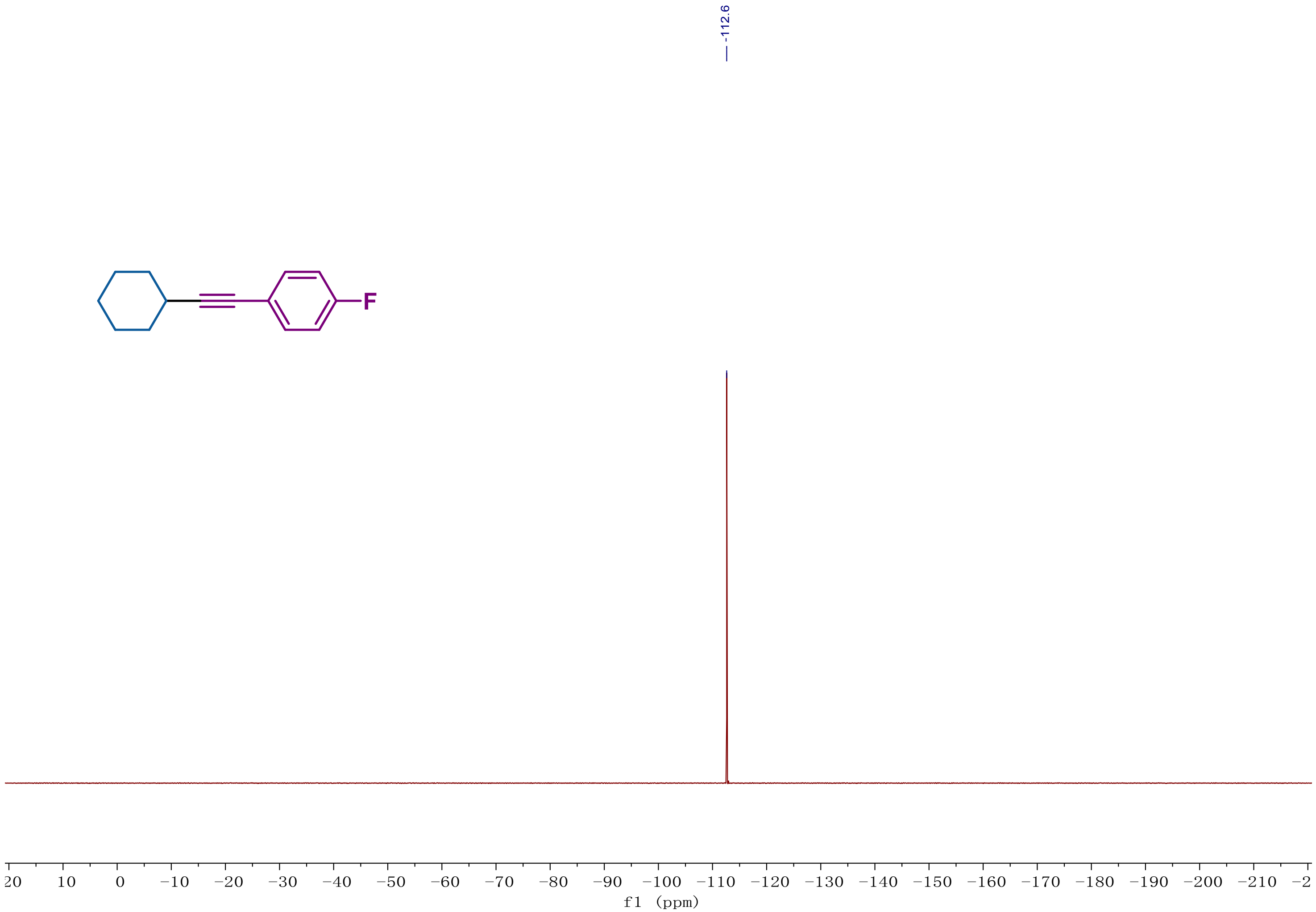
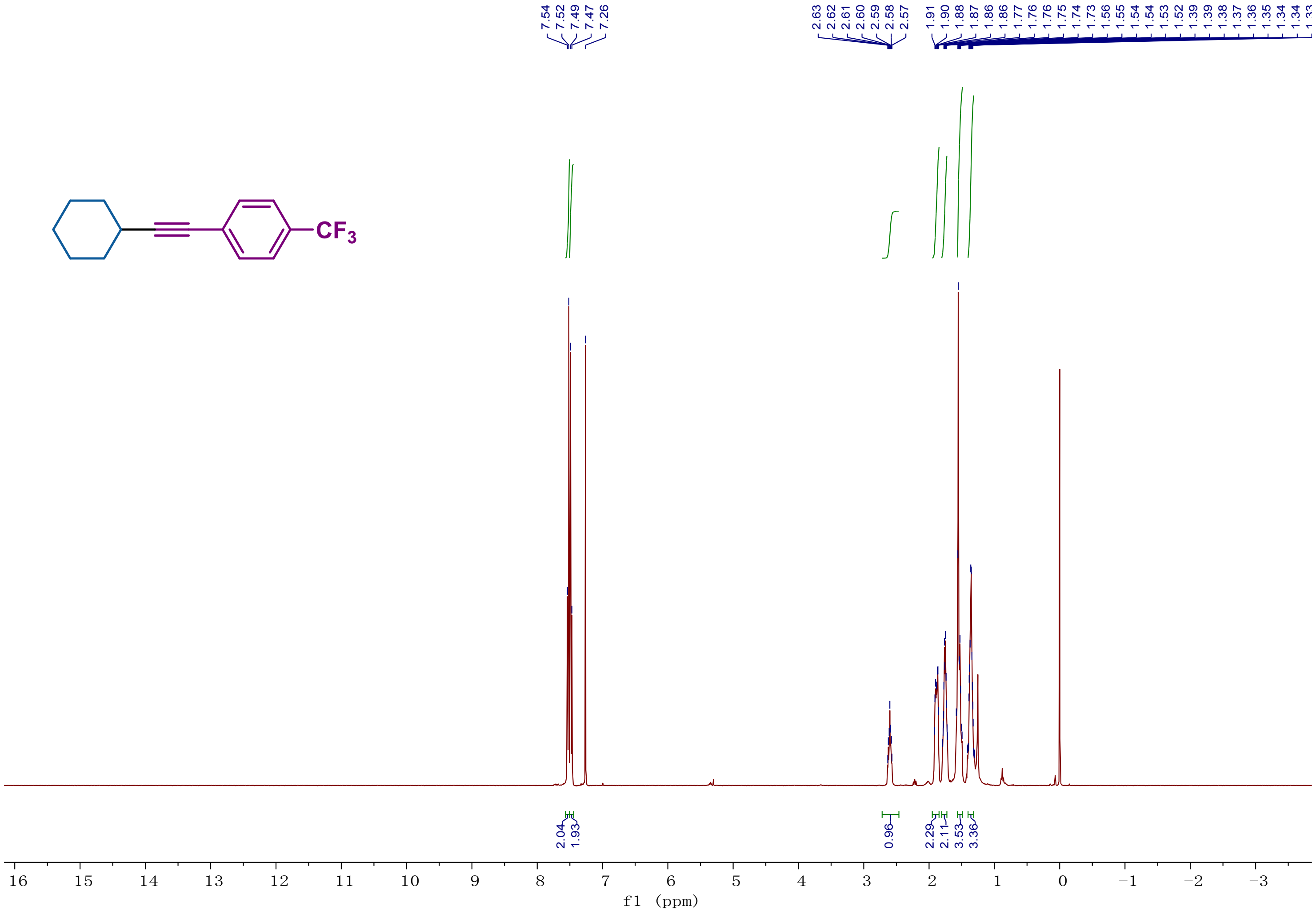


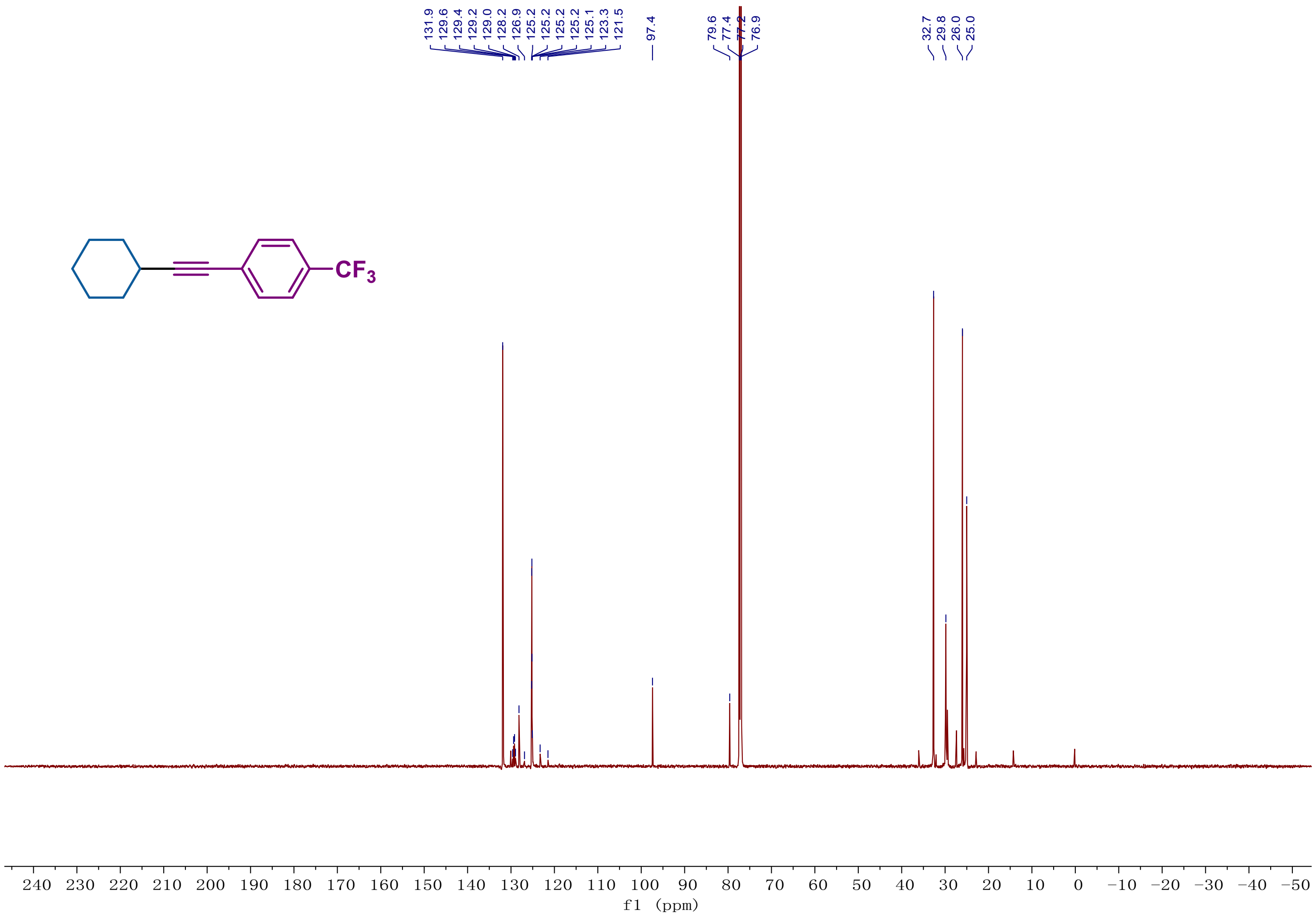
Compound 29 ^{19}F NMR



Compound 30 ^{1}H NMR

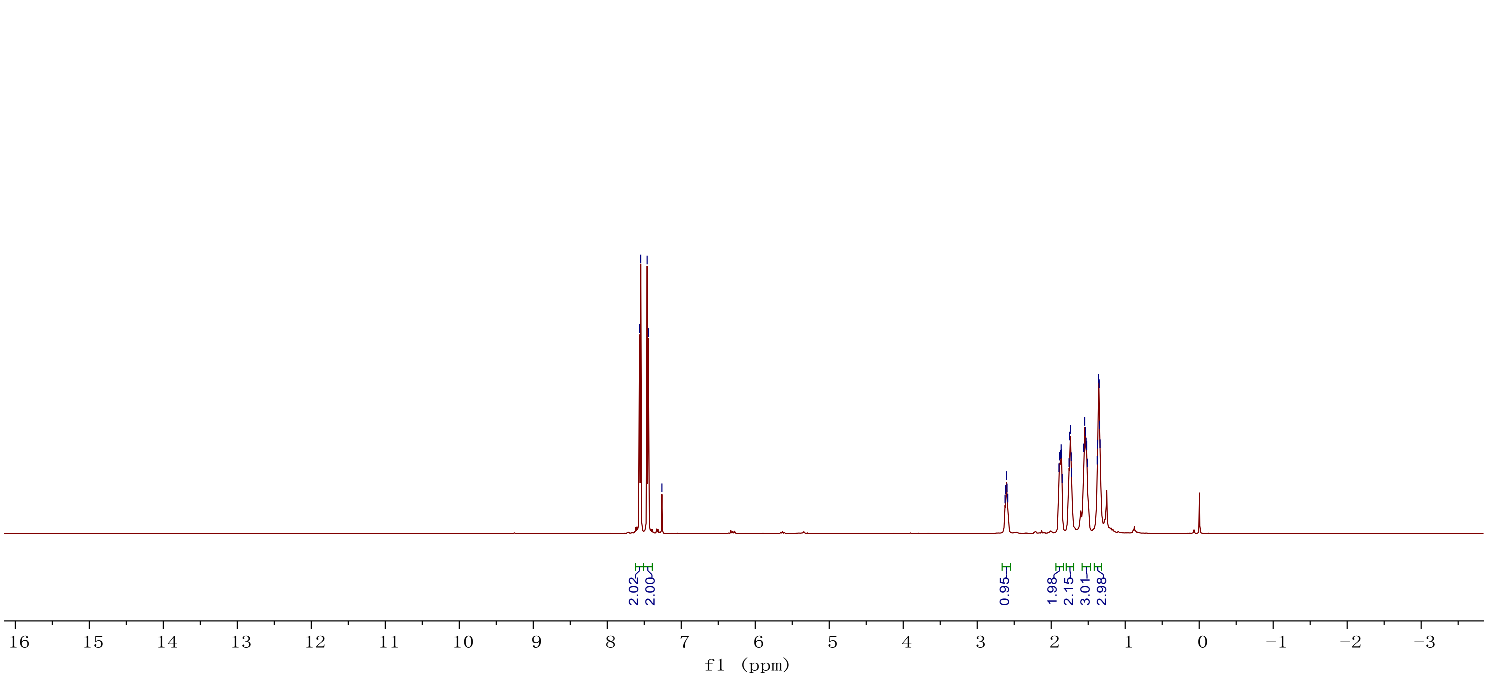


Compound 30 ^{13}C NMR

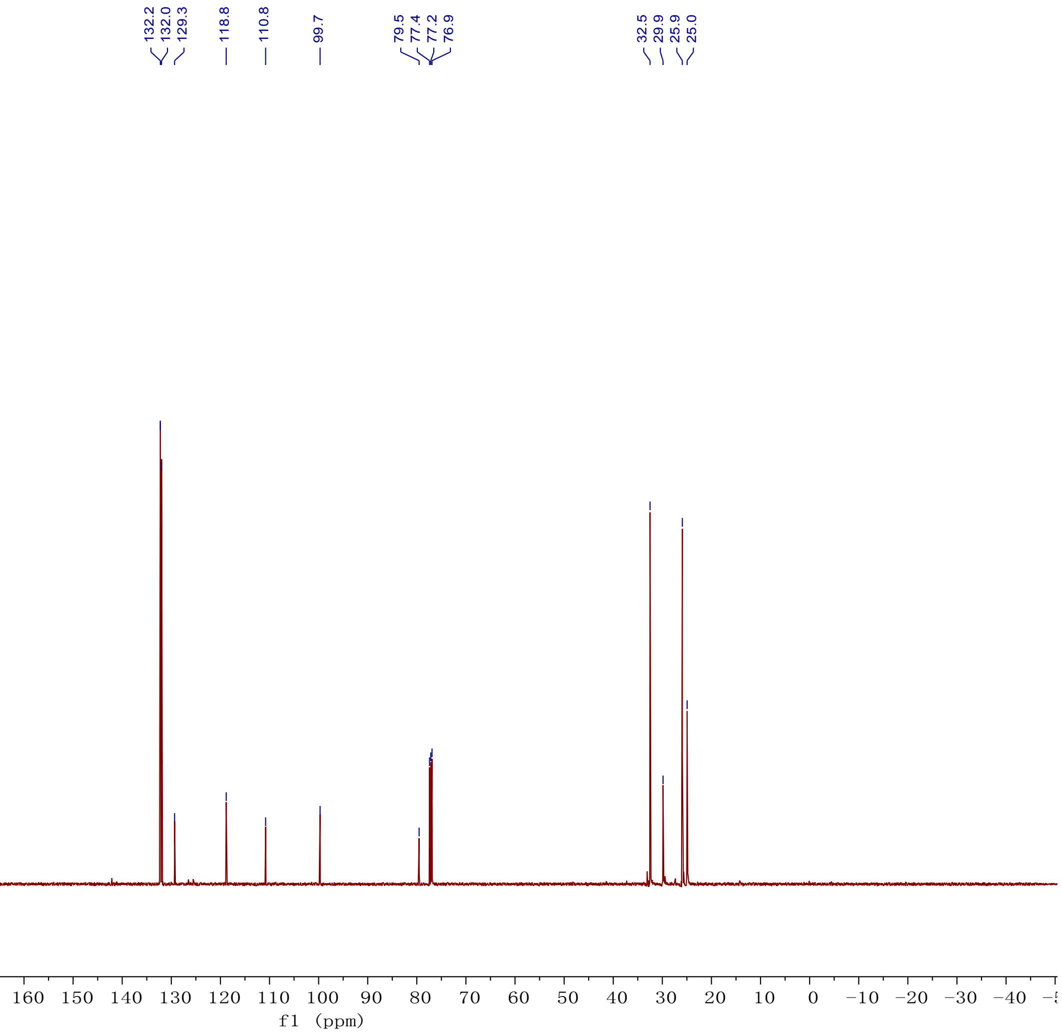


Compound 30 ^{19}F NMR

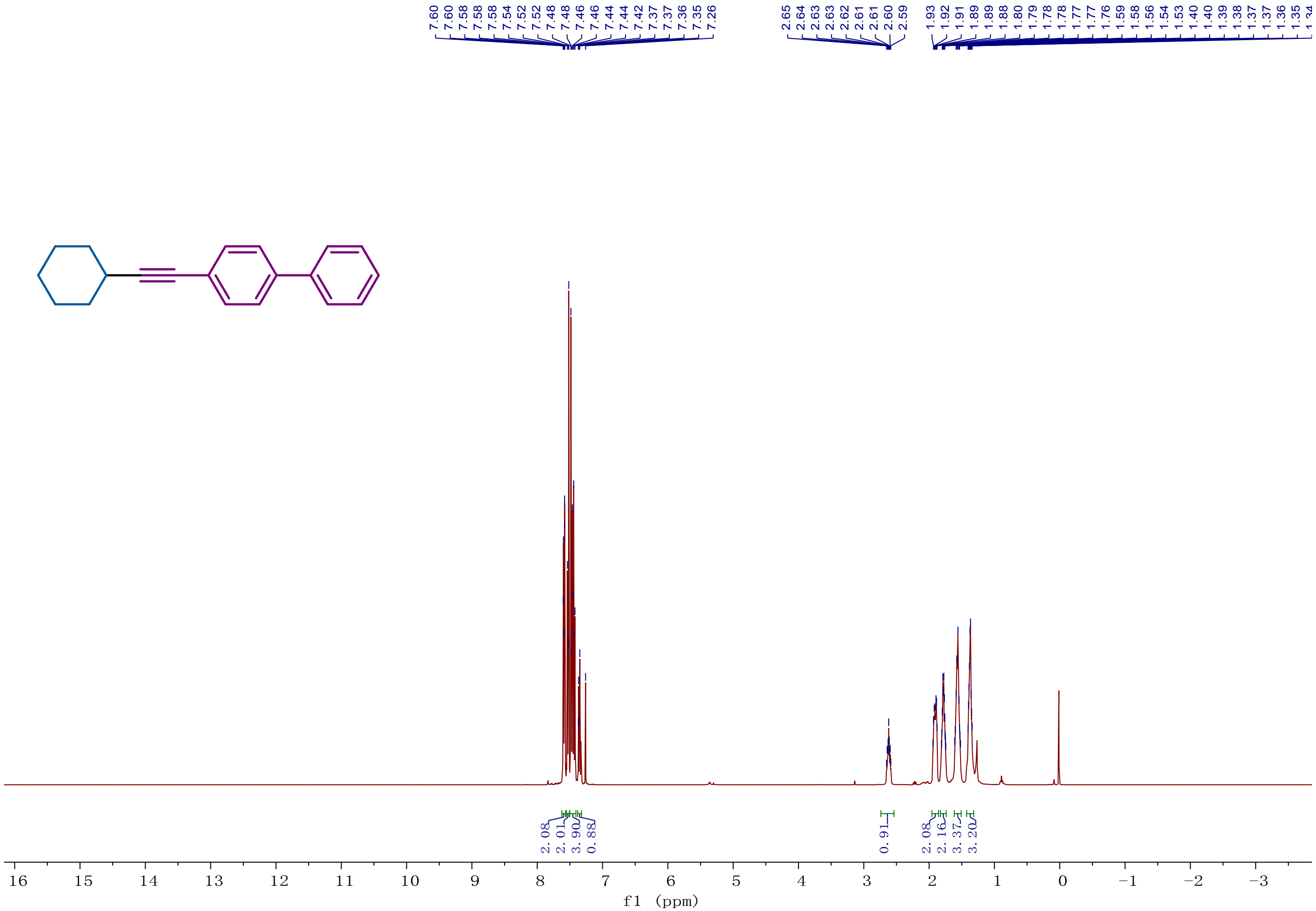
Compound 31 ¹H NMR



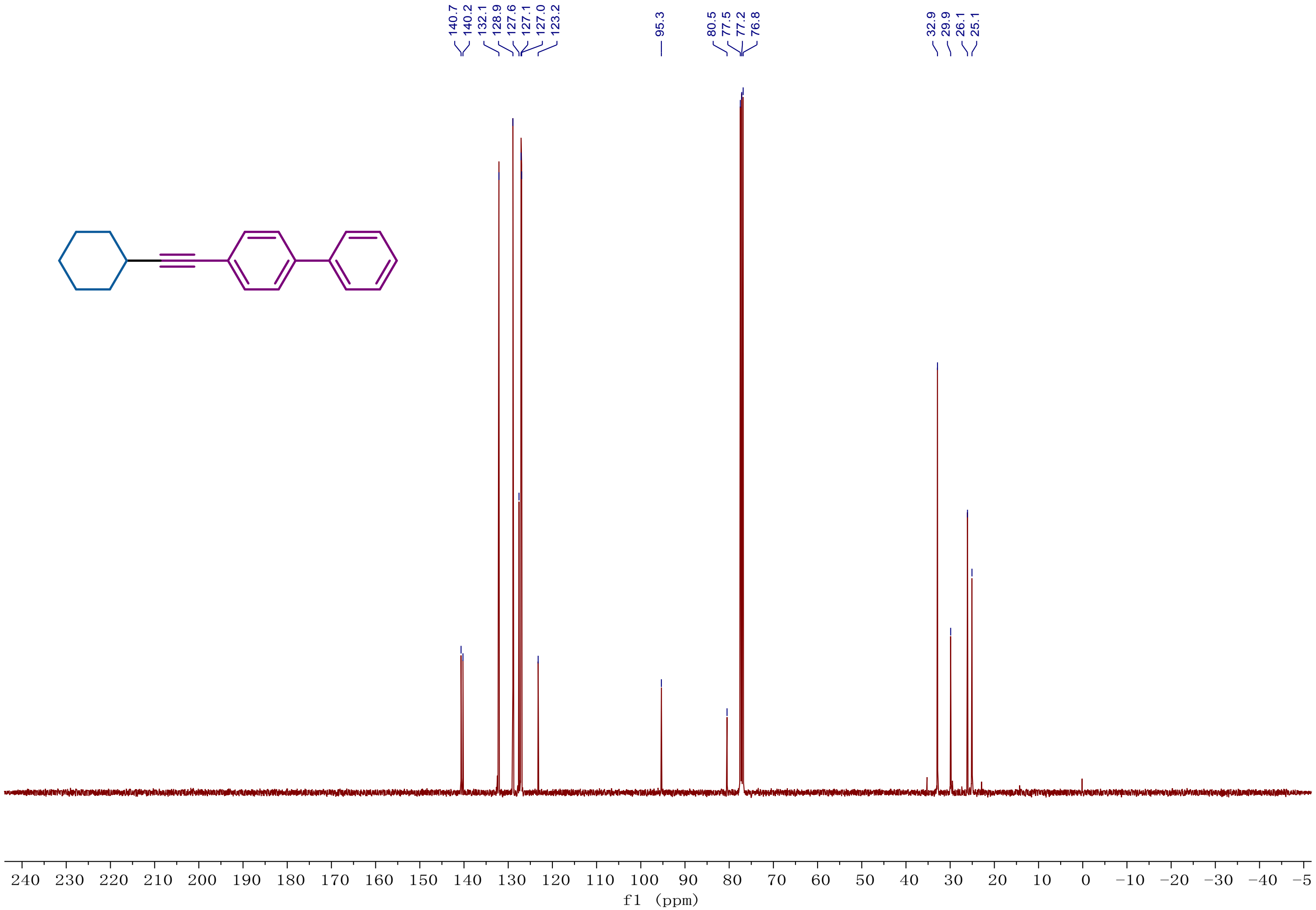
Compound 31 ^{13}C NMR



Compound 32 ^{1}H NMR



Compound 32 ^{13}C NMR



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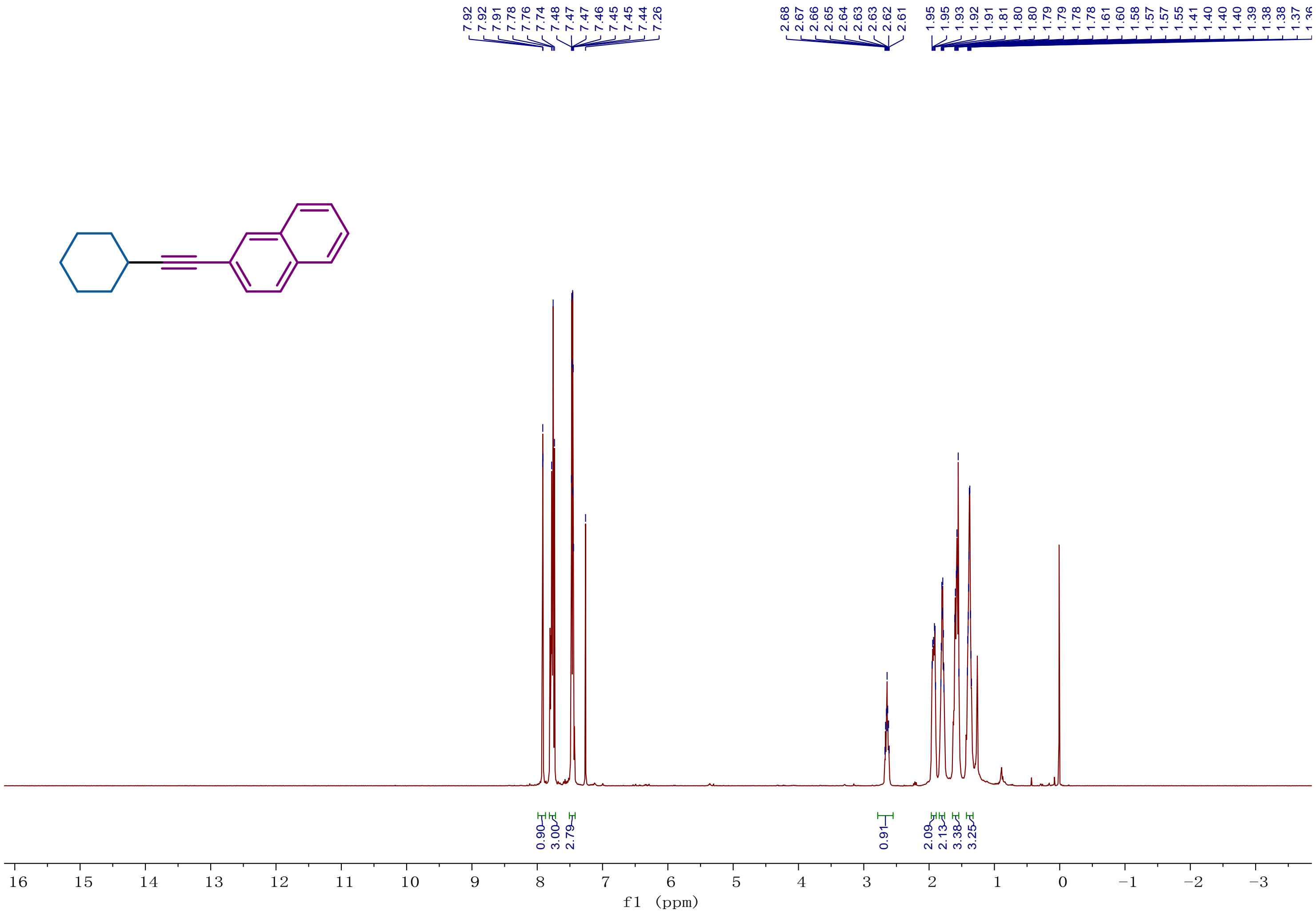
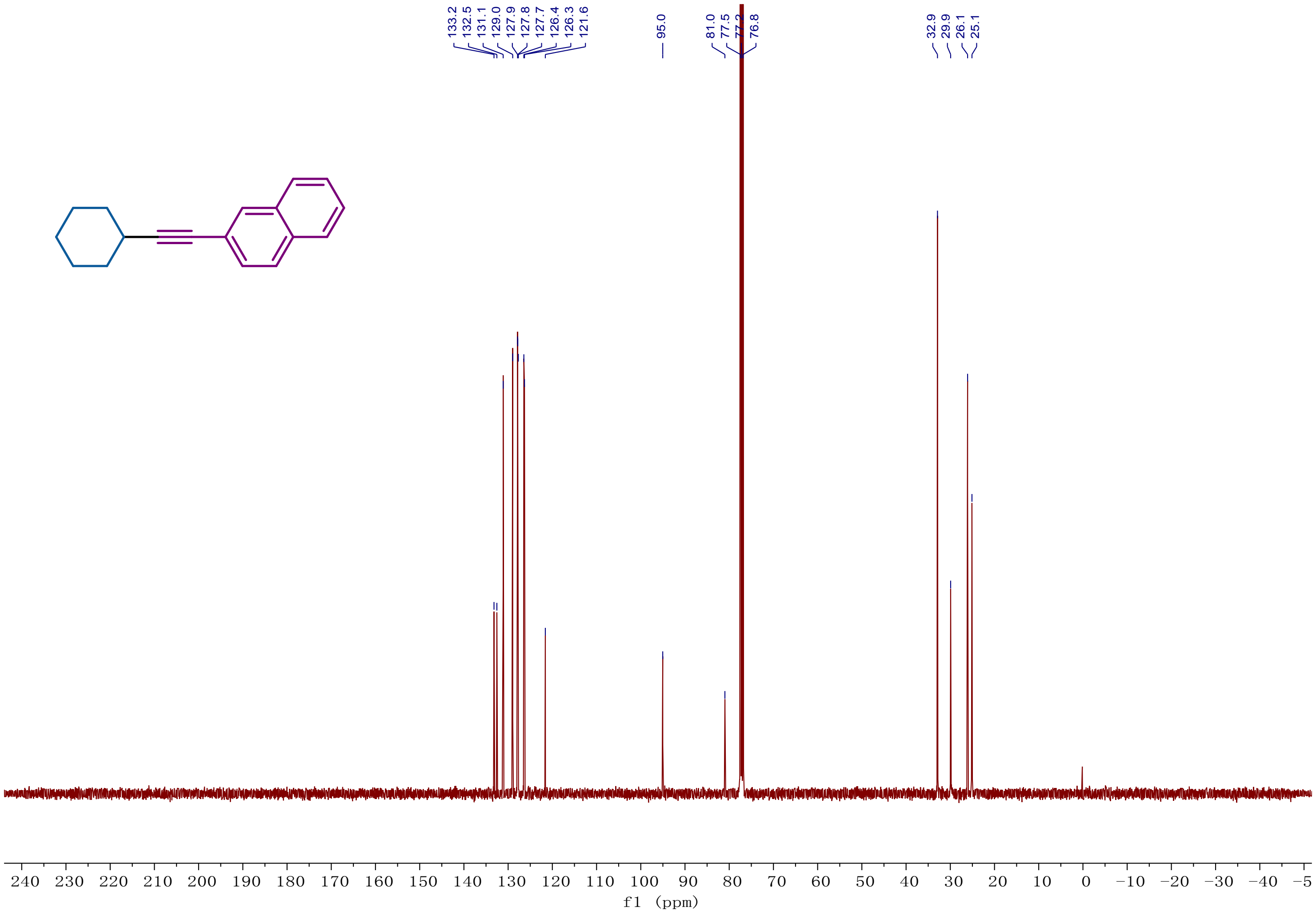
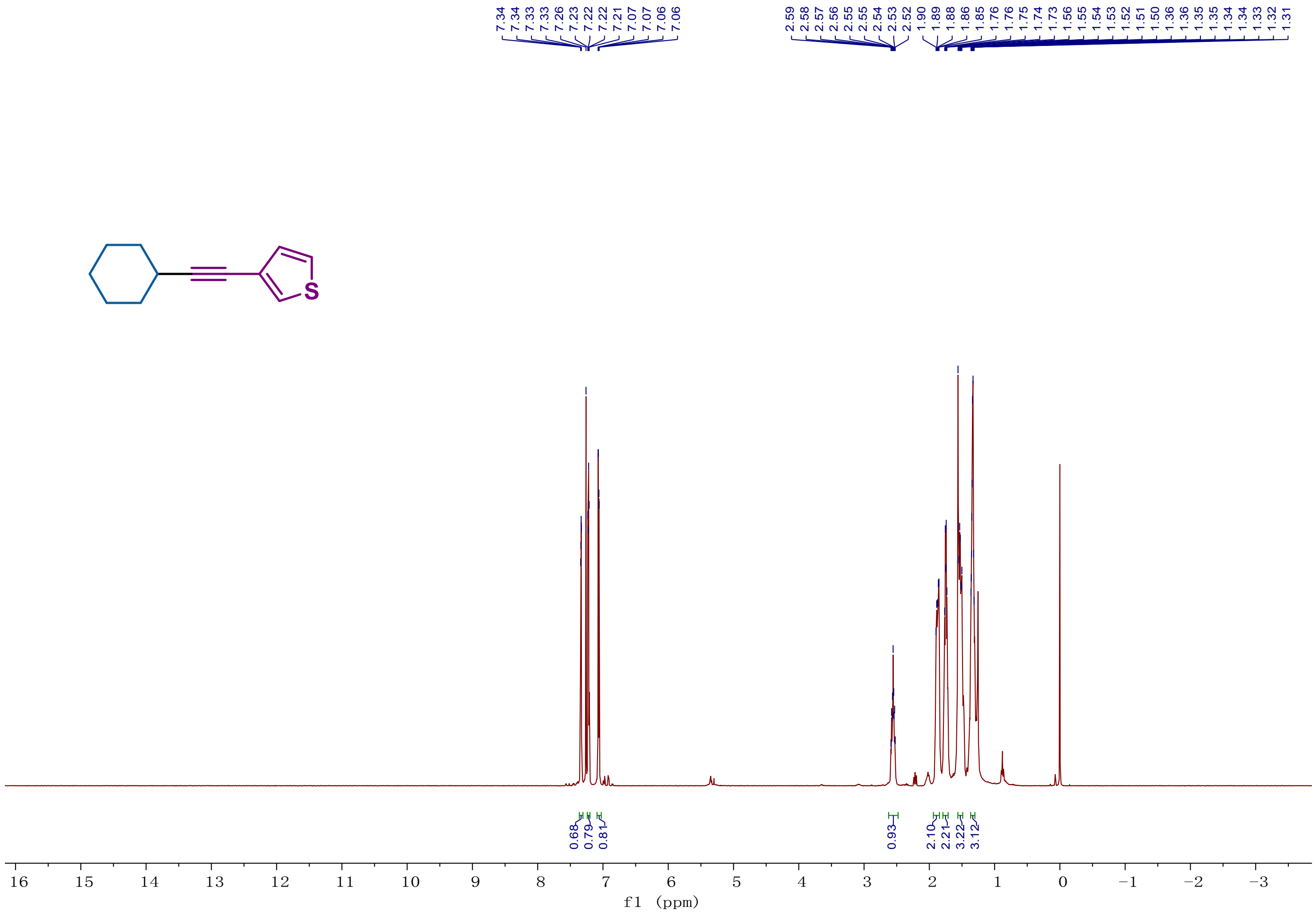


Compound 33 ^{13}C NMR



Compound 34 ^{1}H NMR



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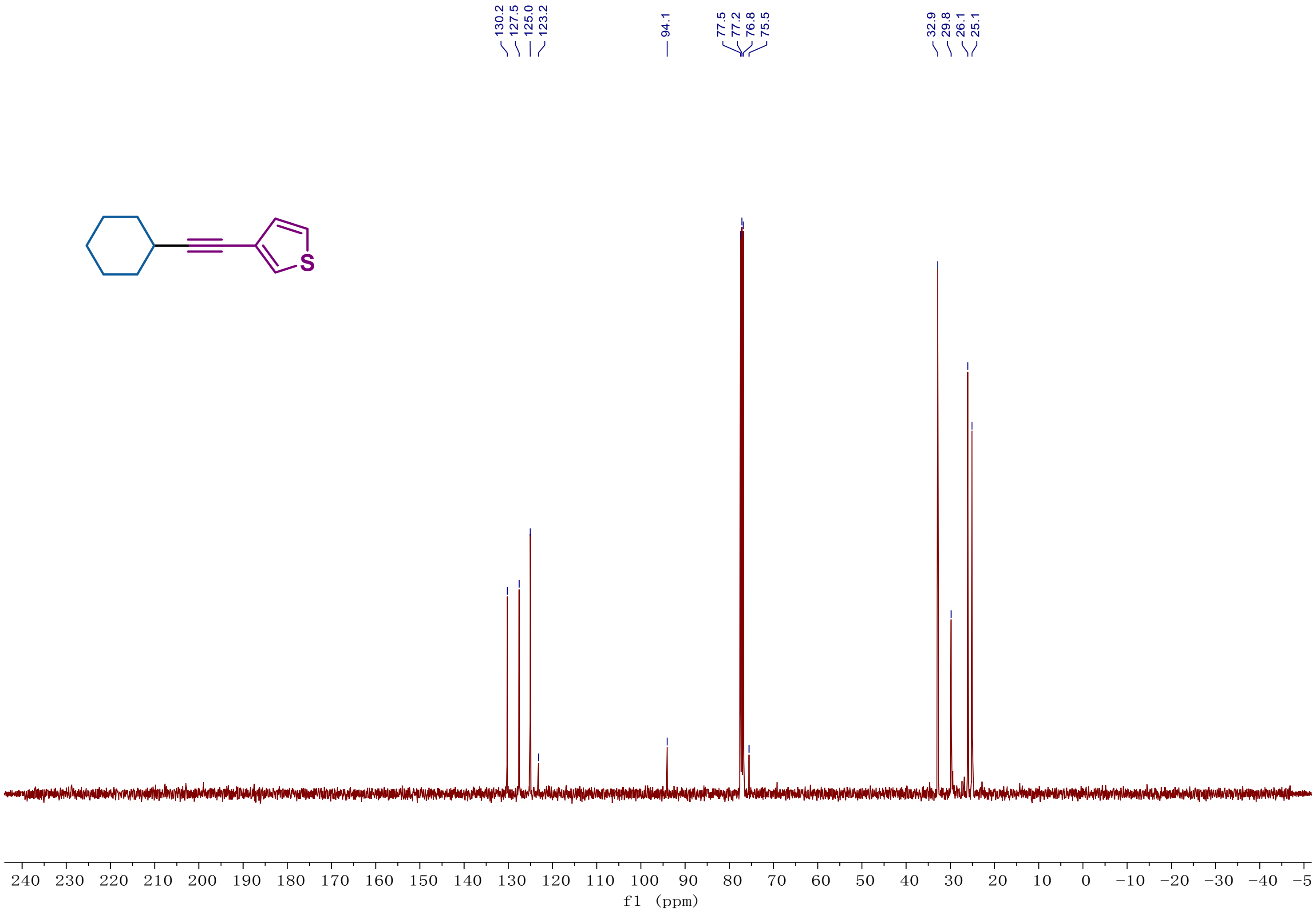

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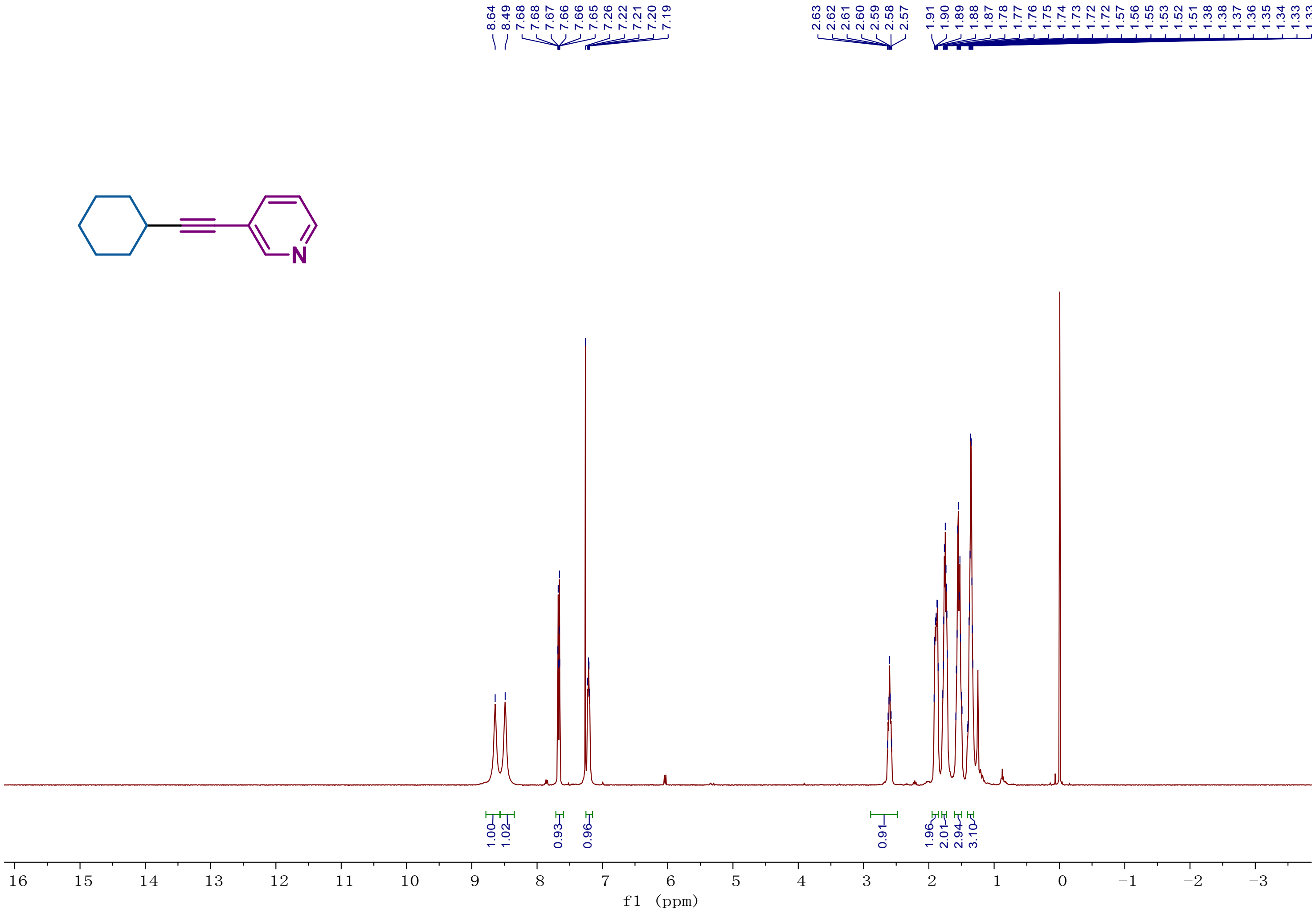

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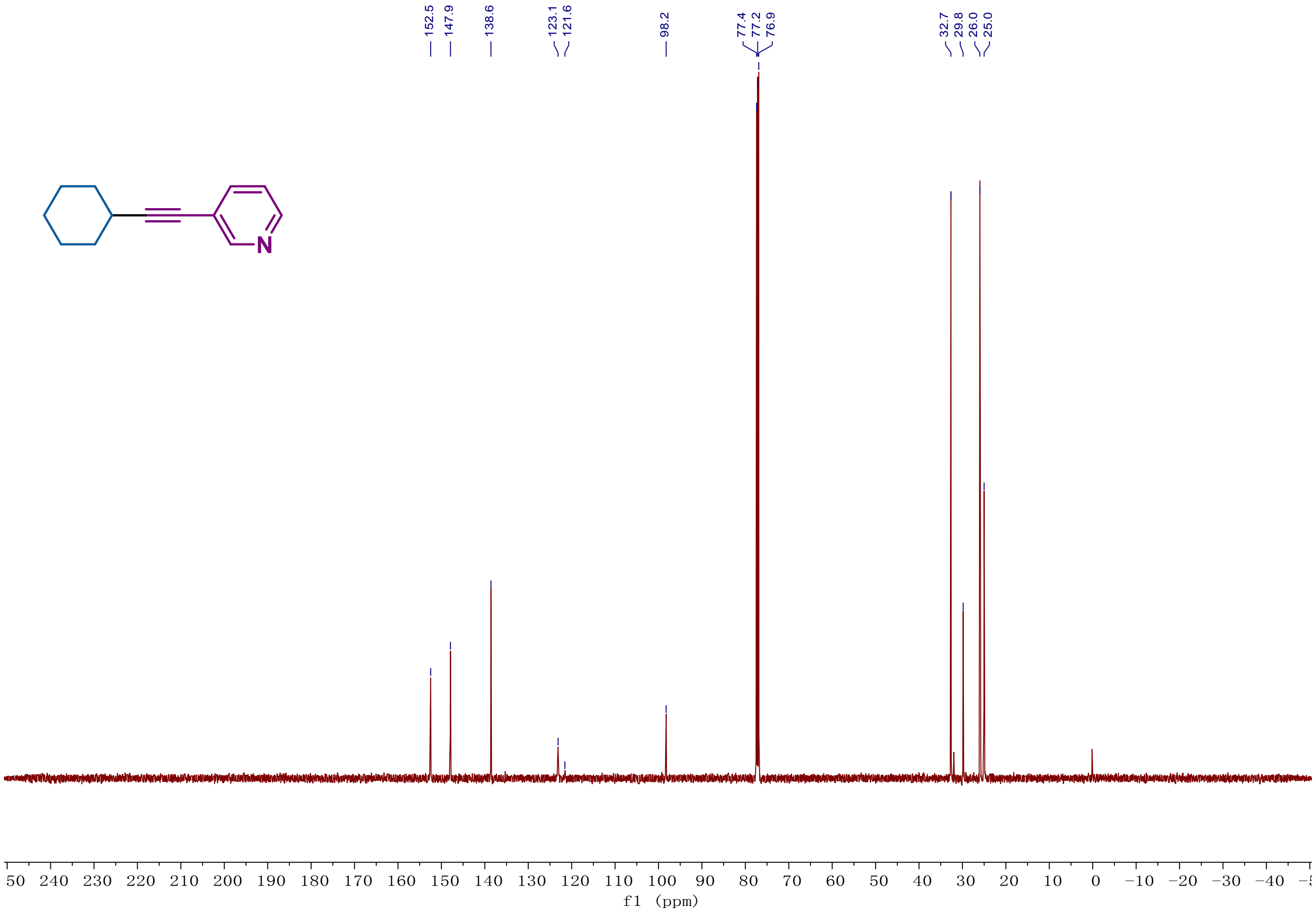

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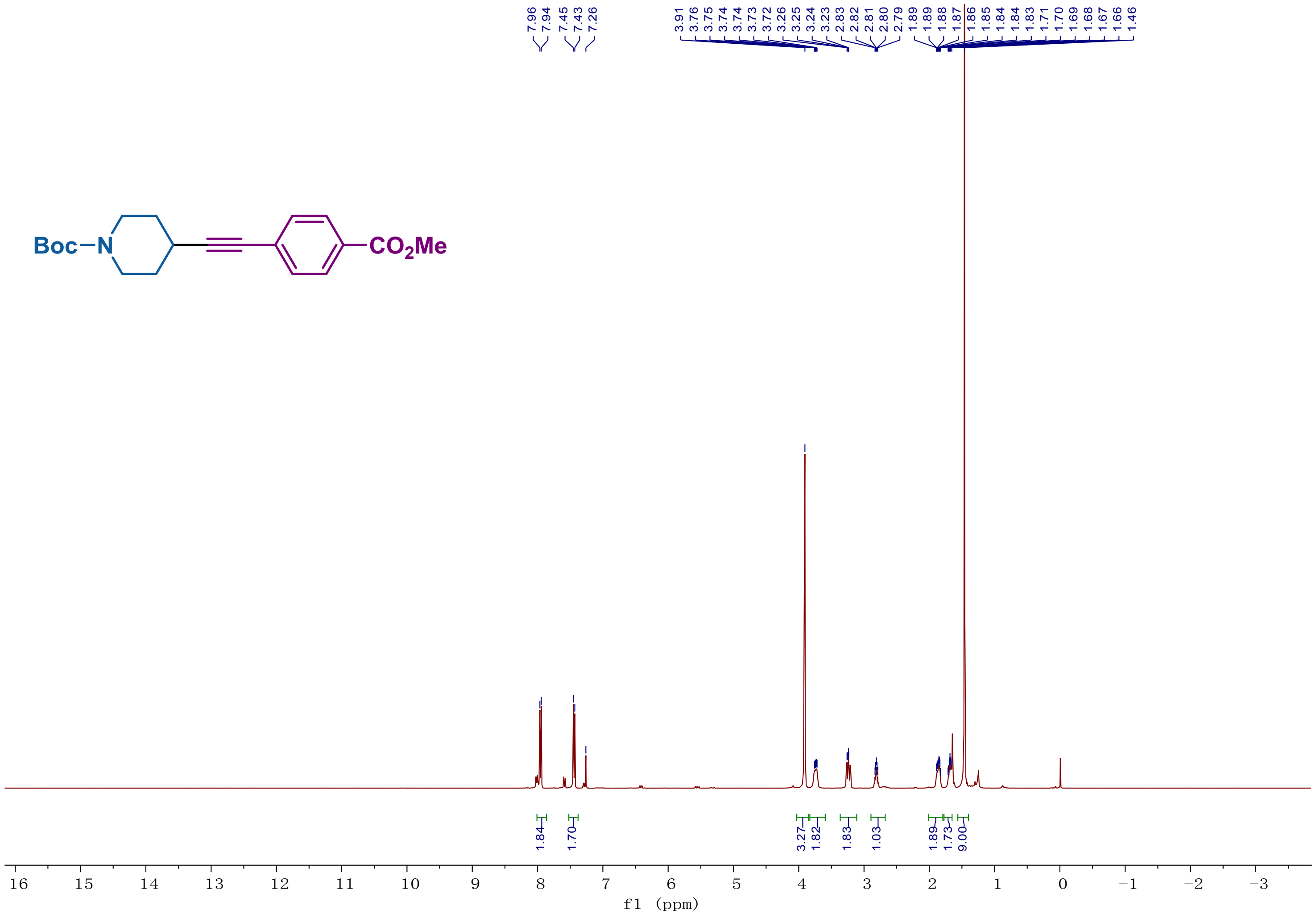

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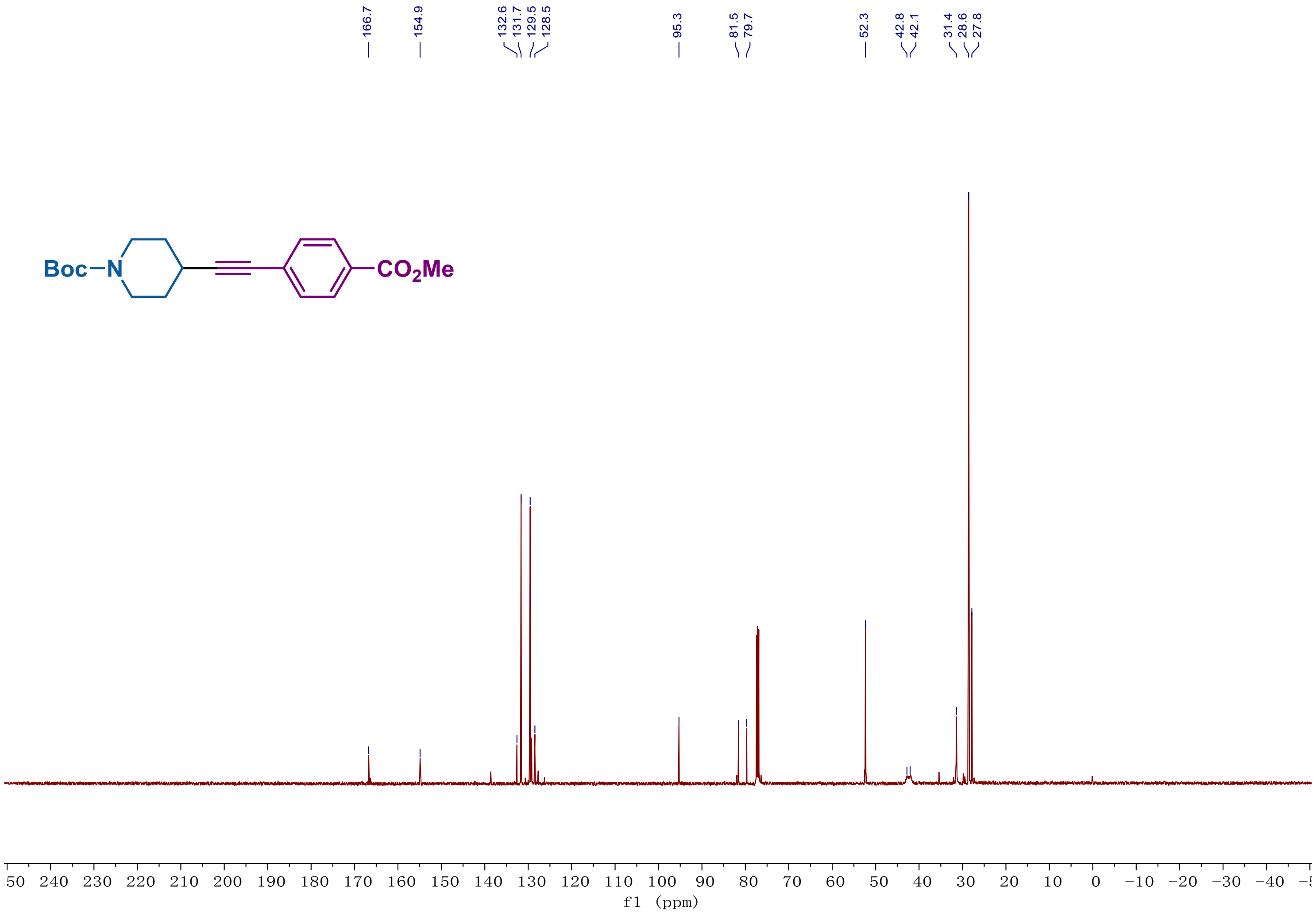

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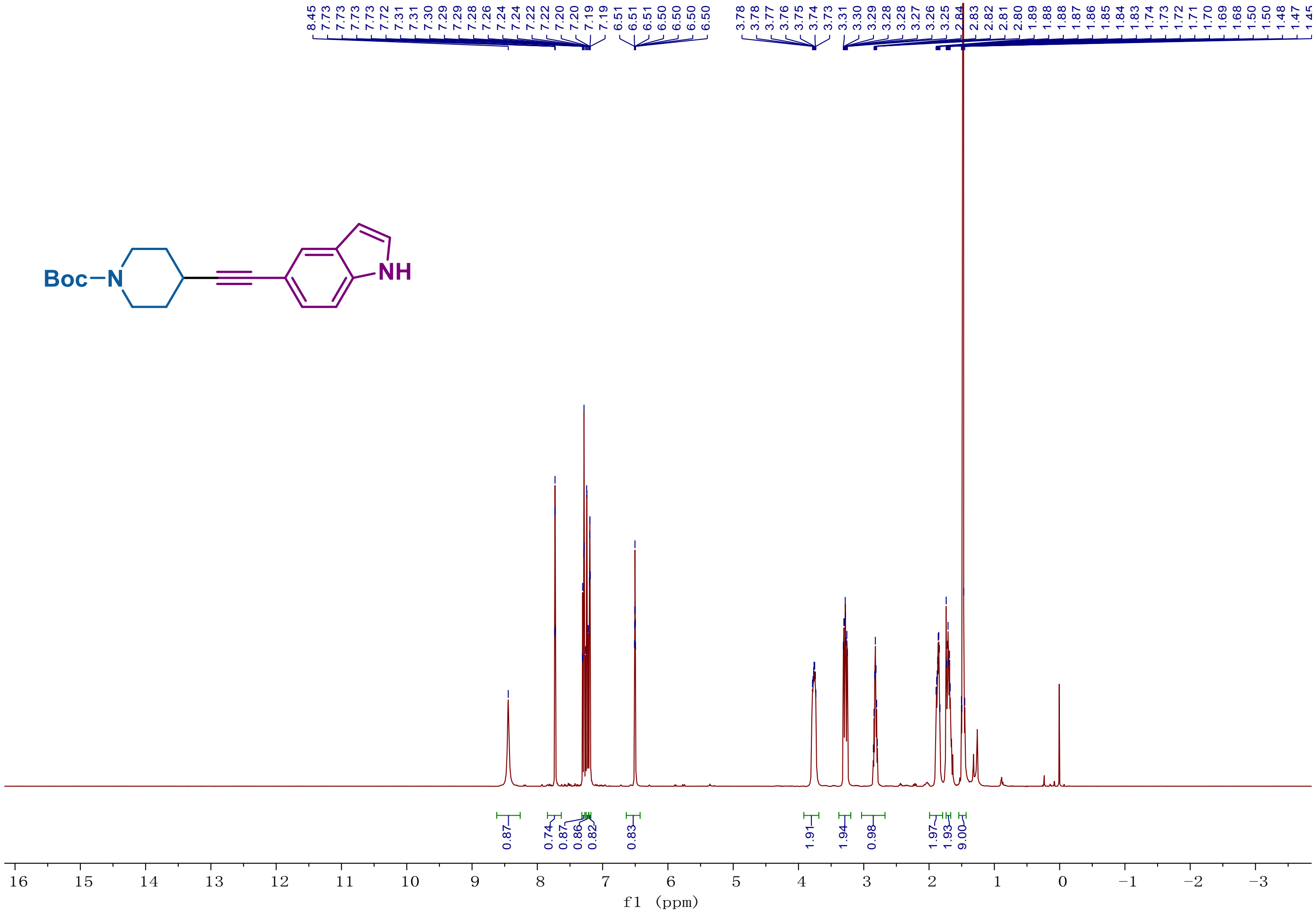

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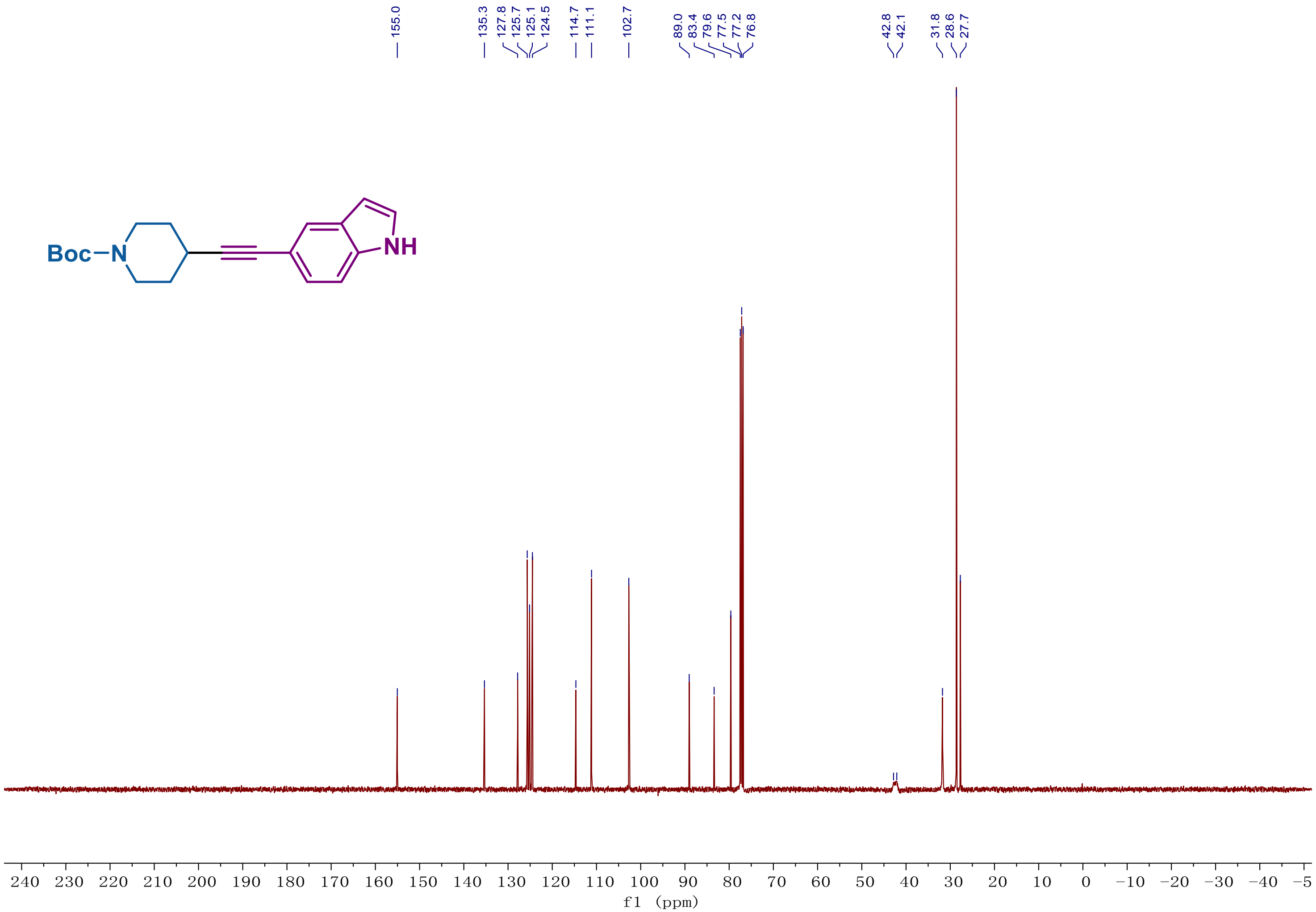

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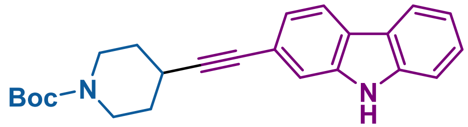

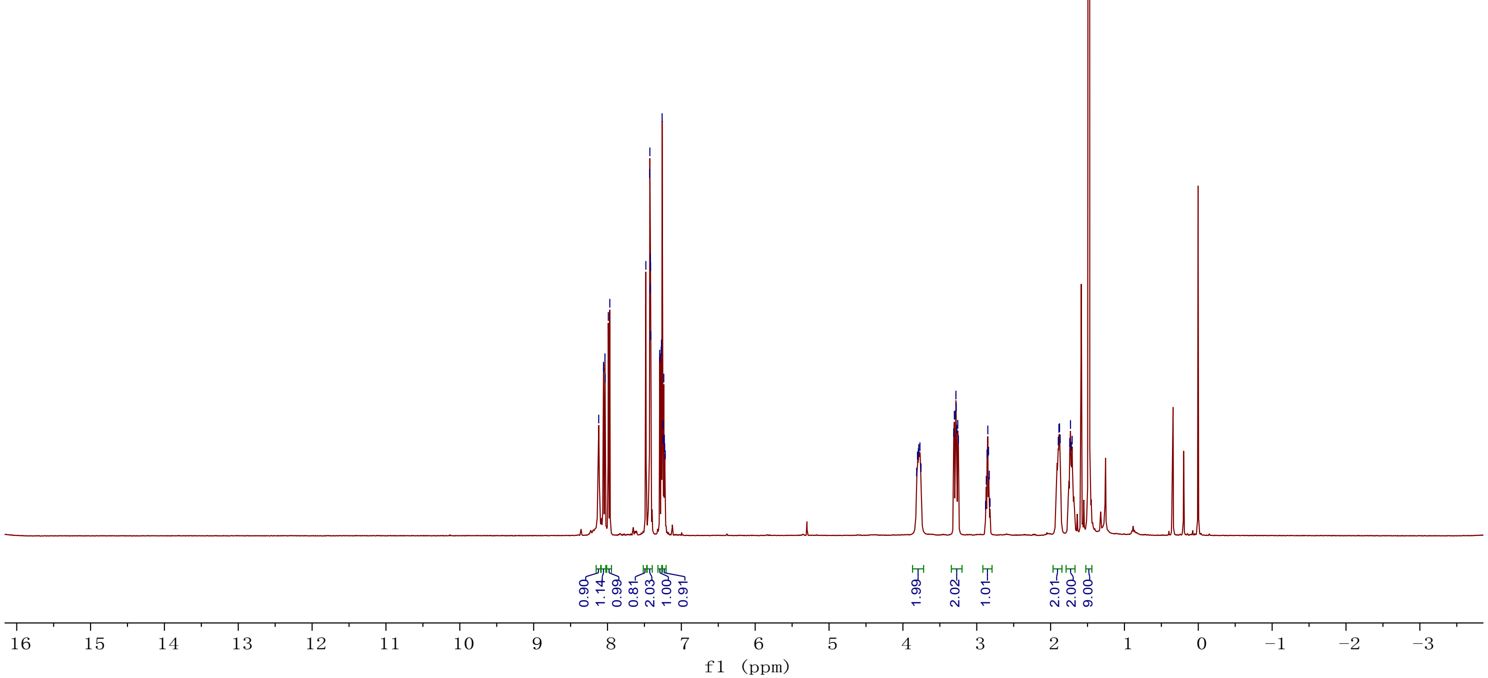

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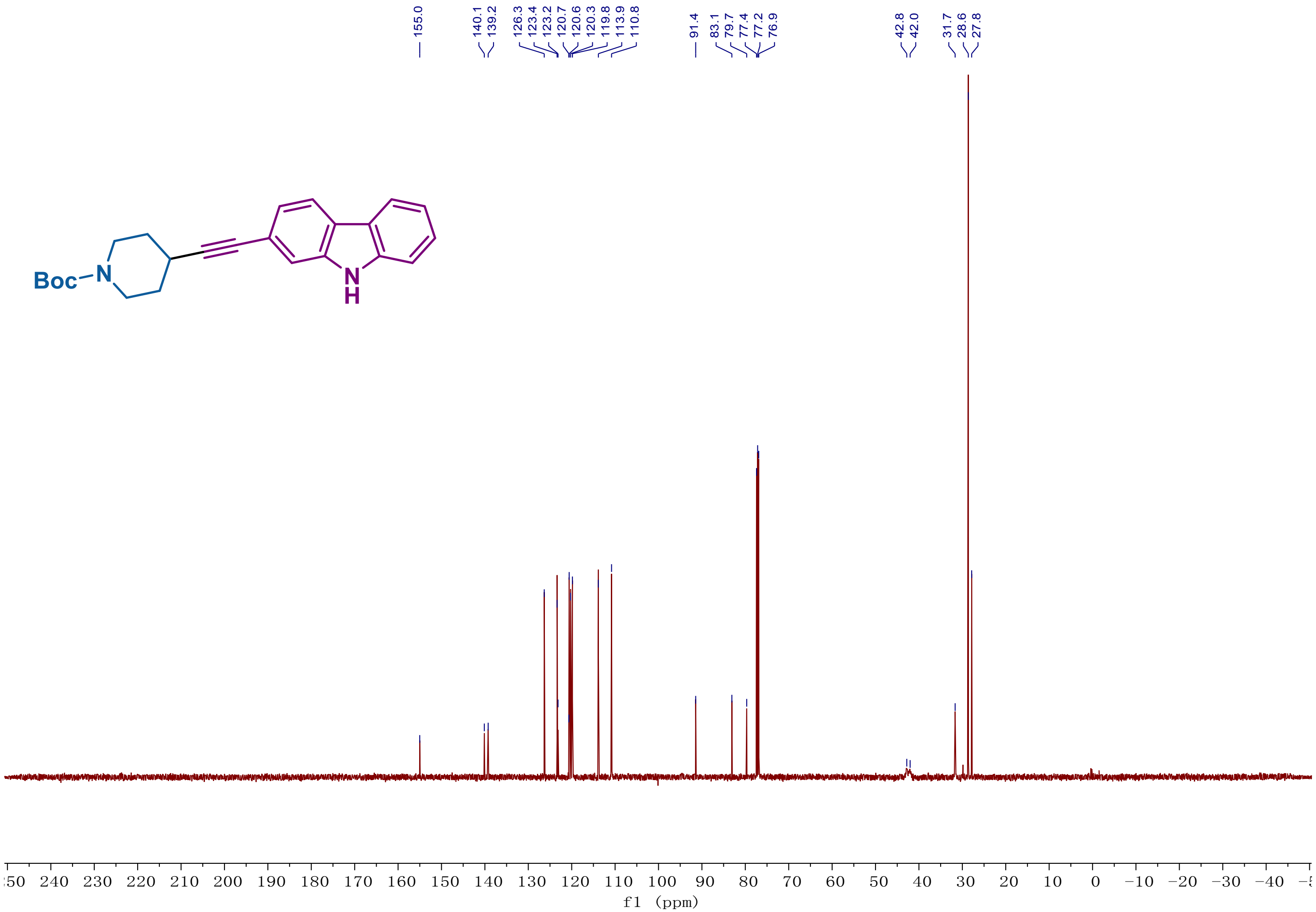

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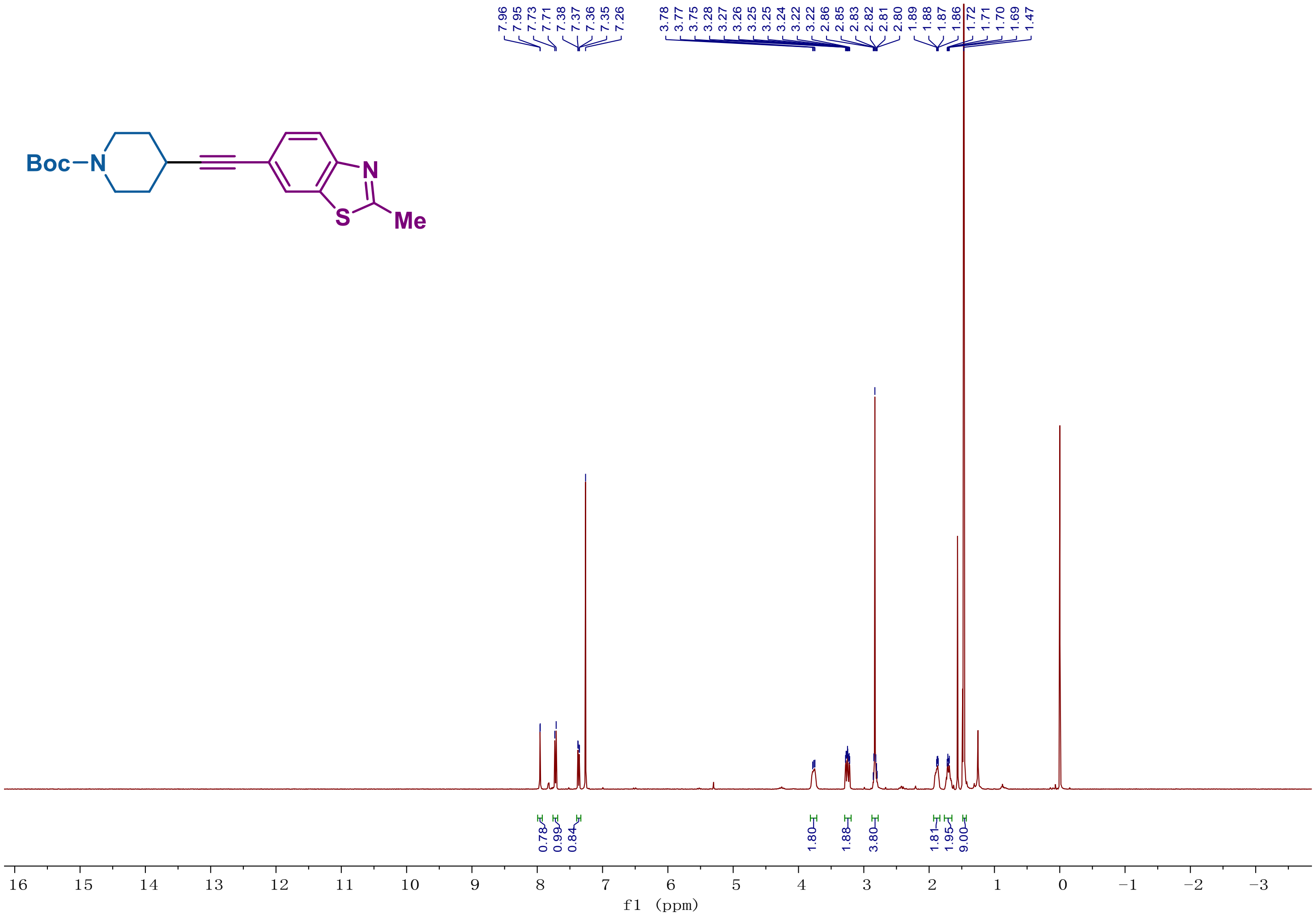

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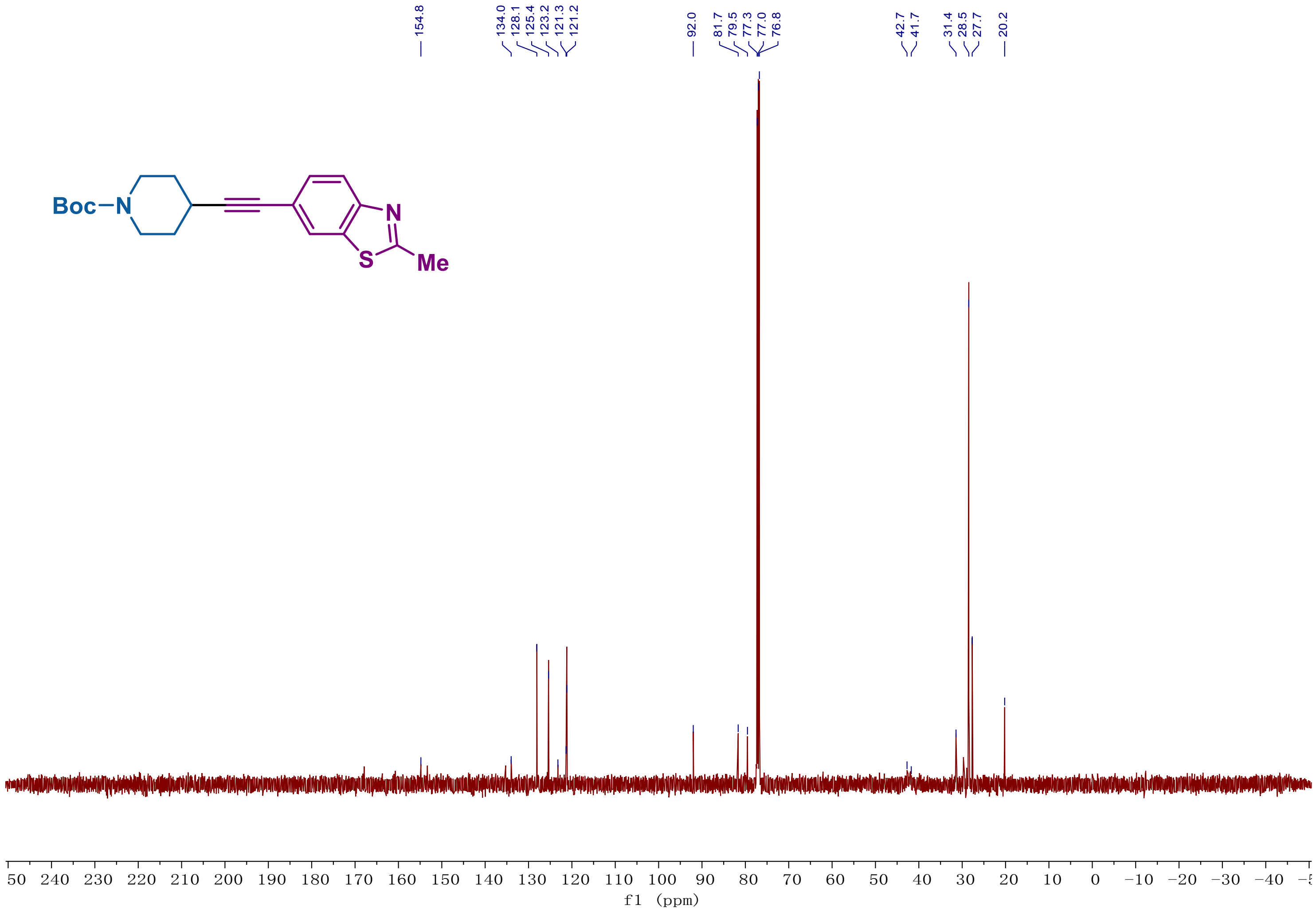

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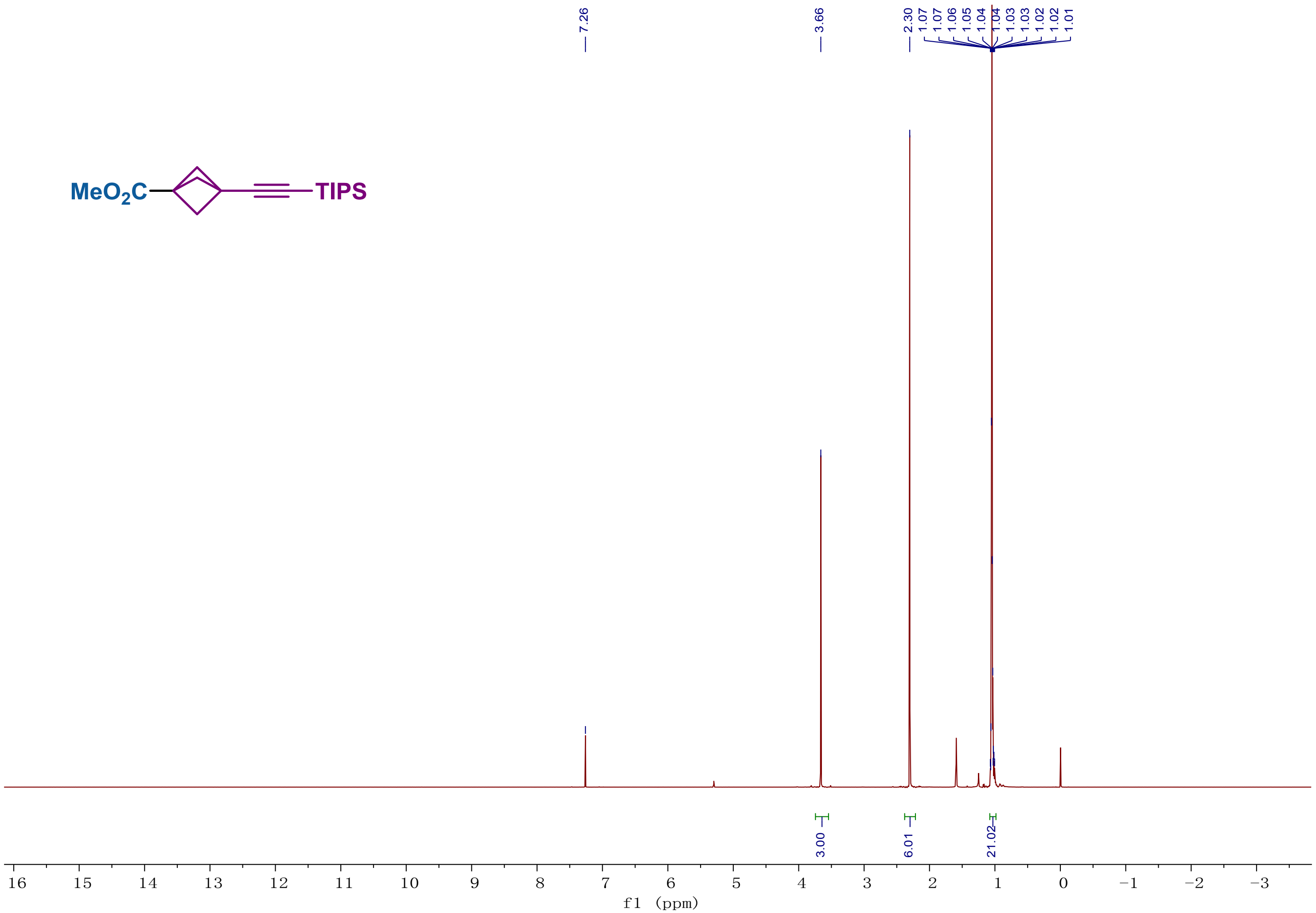
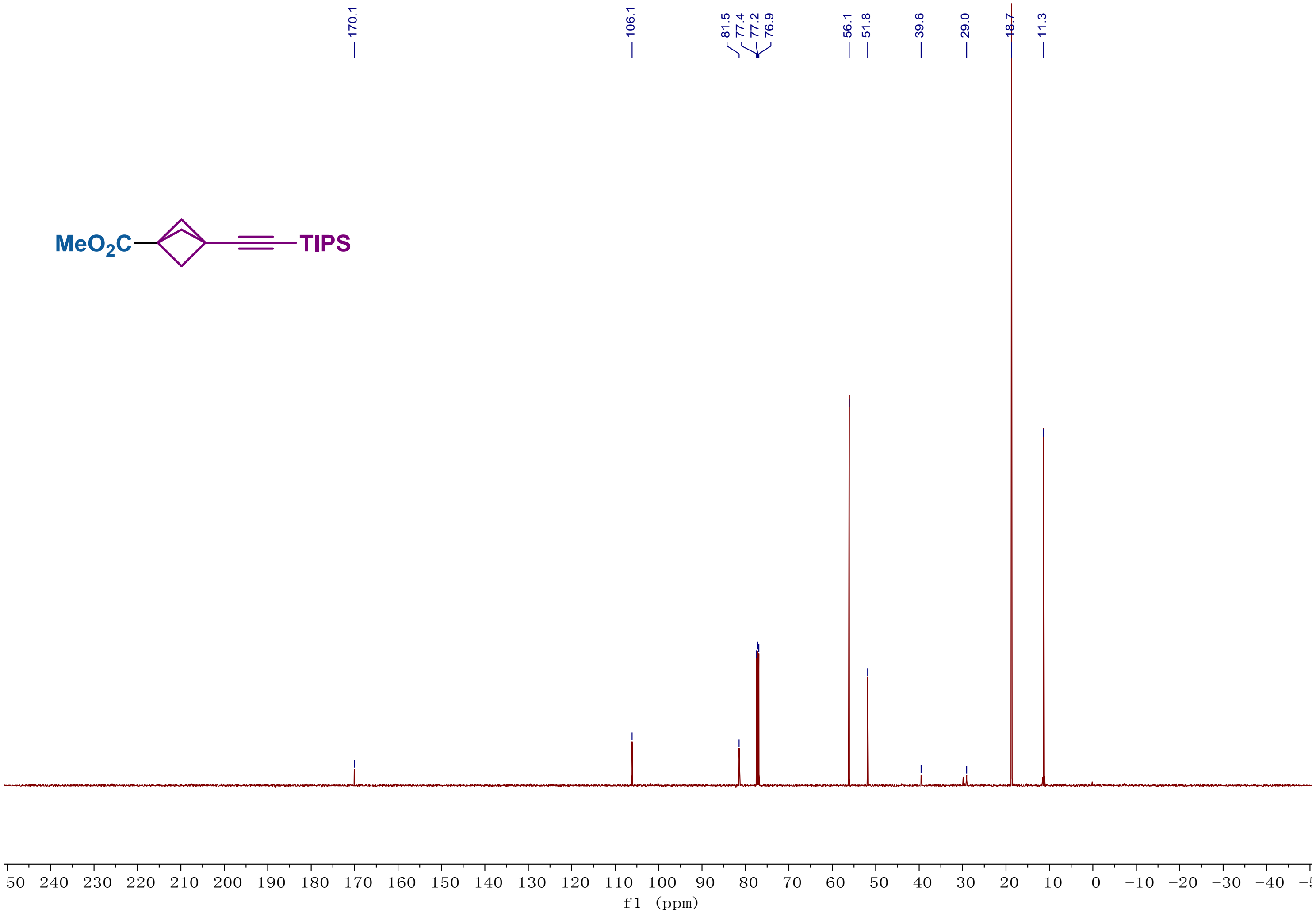


Compound 40 ^{13}C NMR



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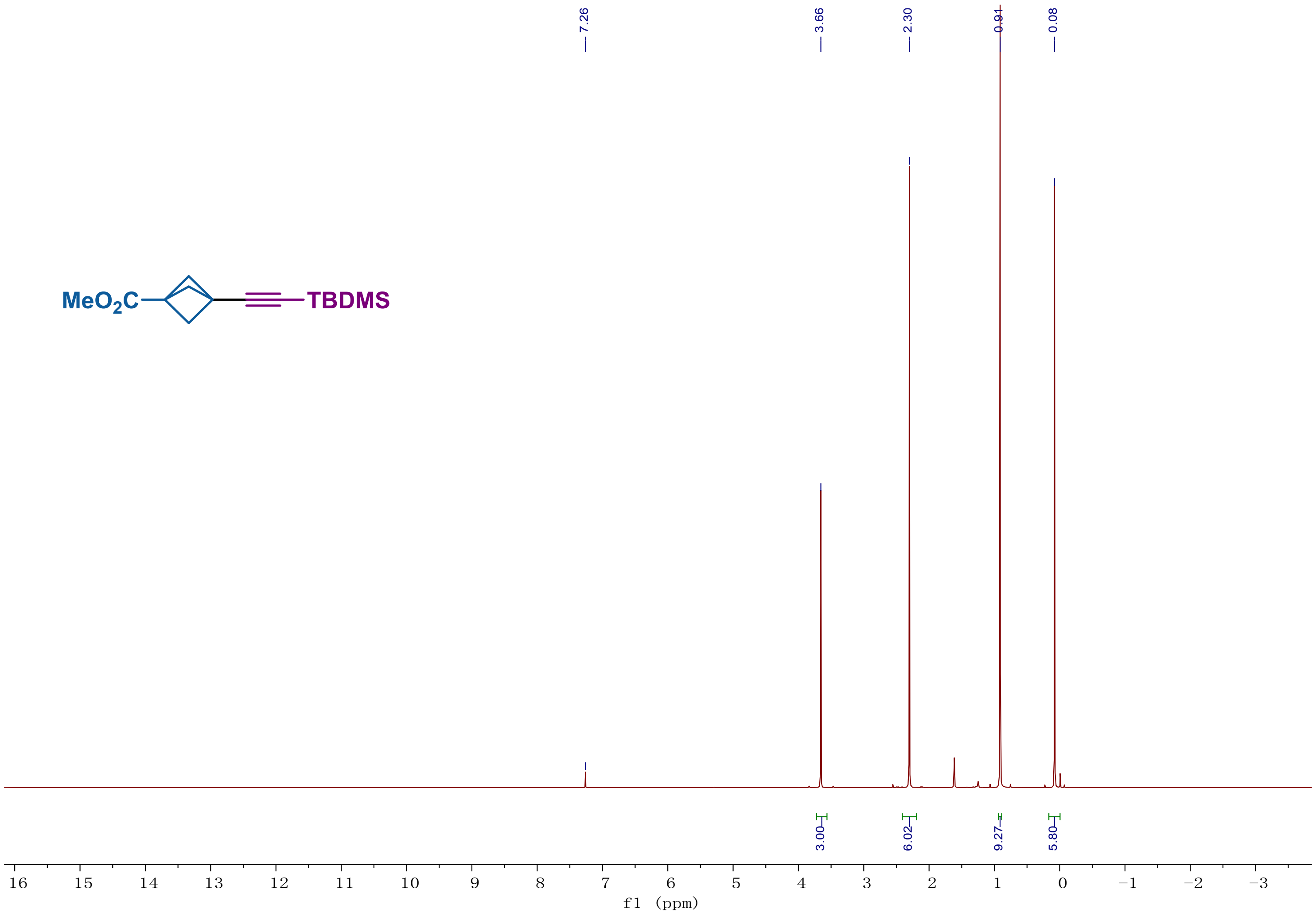
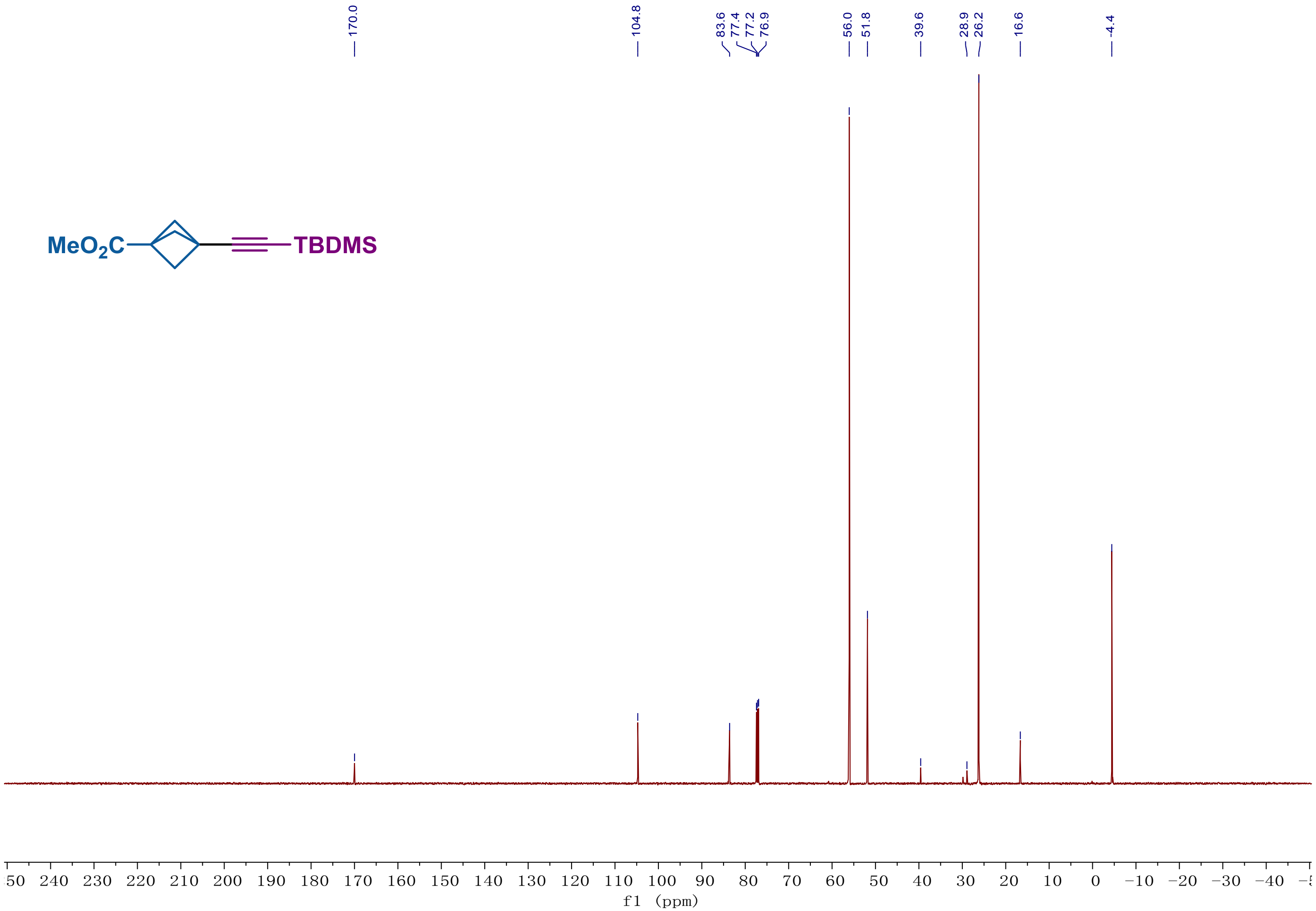


Compound 41 ^{13}C NMR



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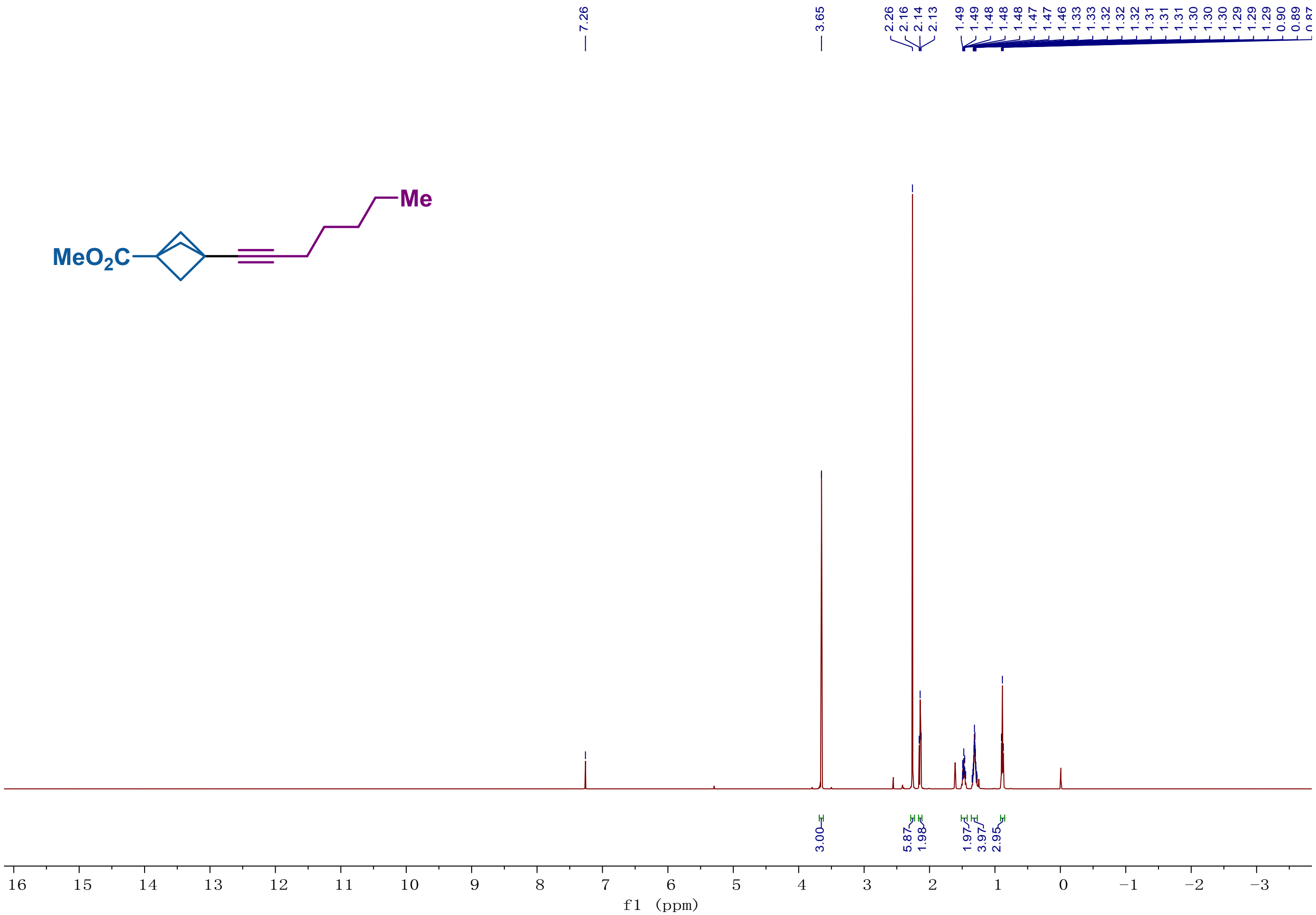

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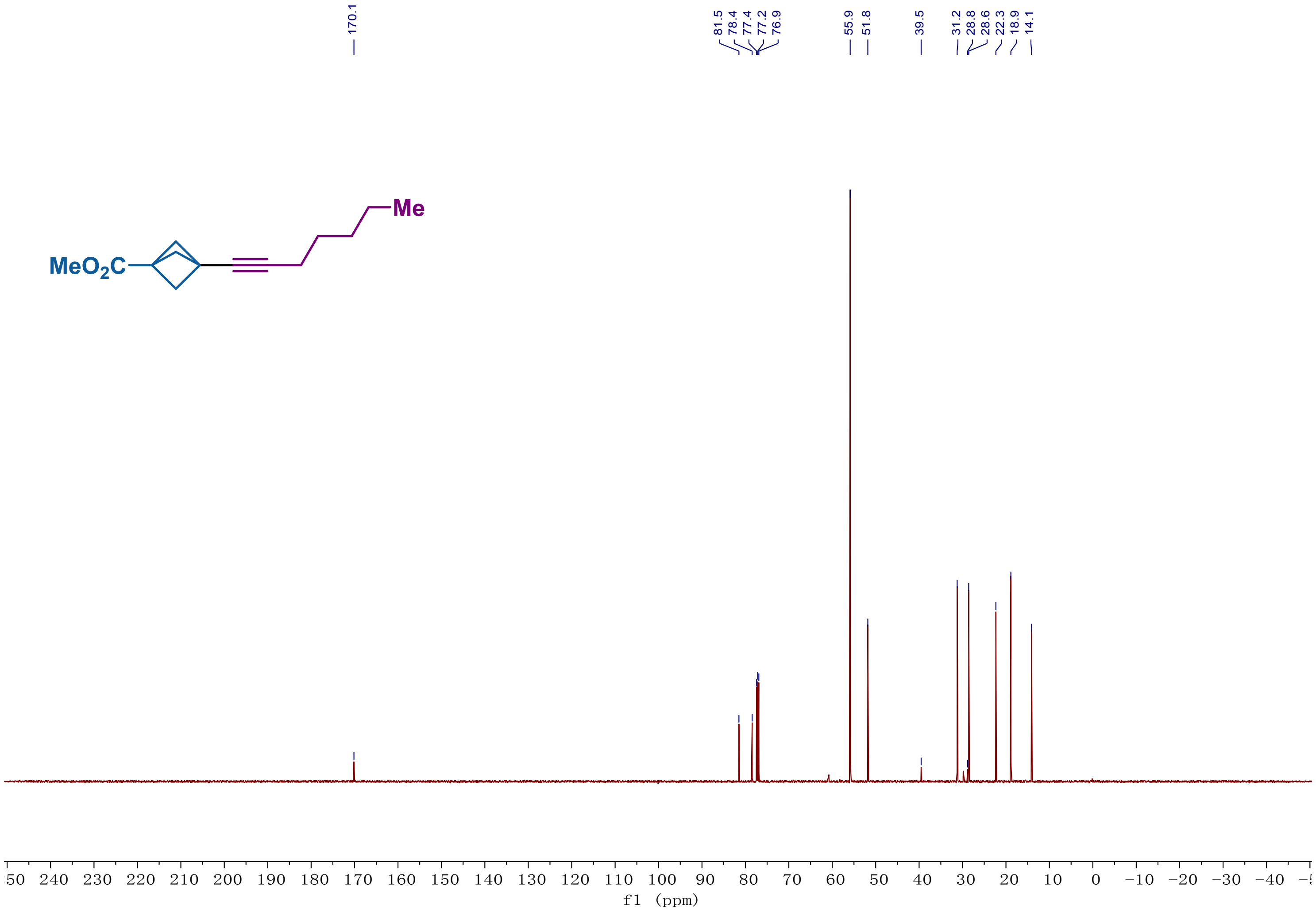

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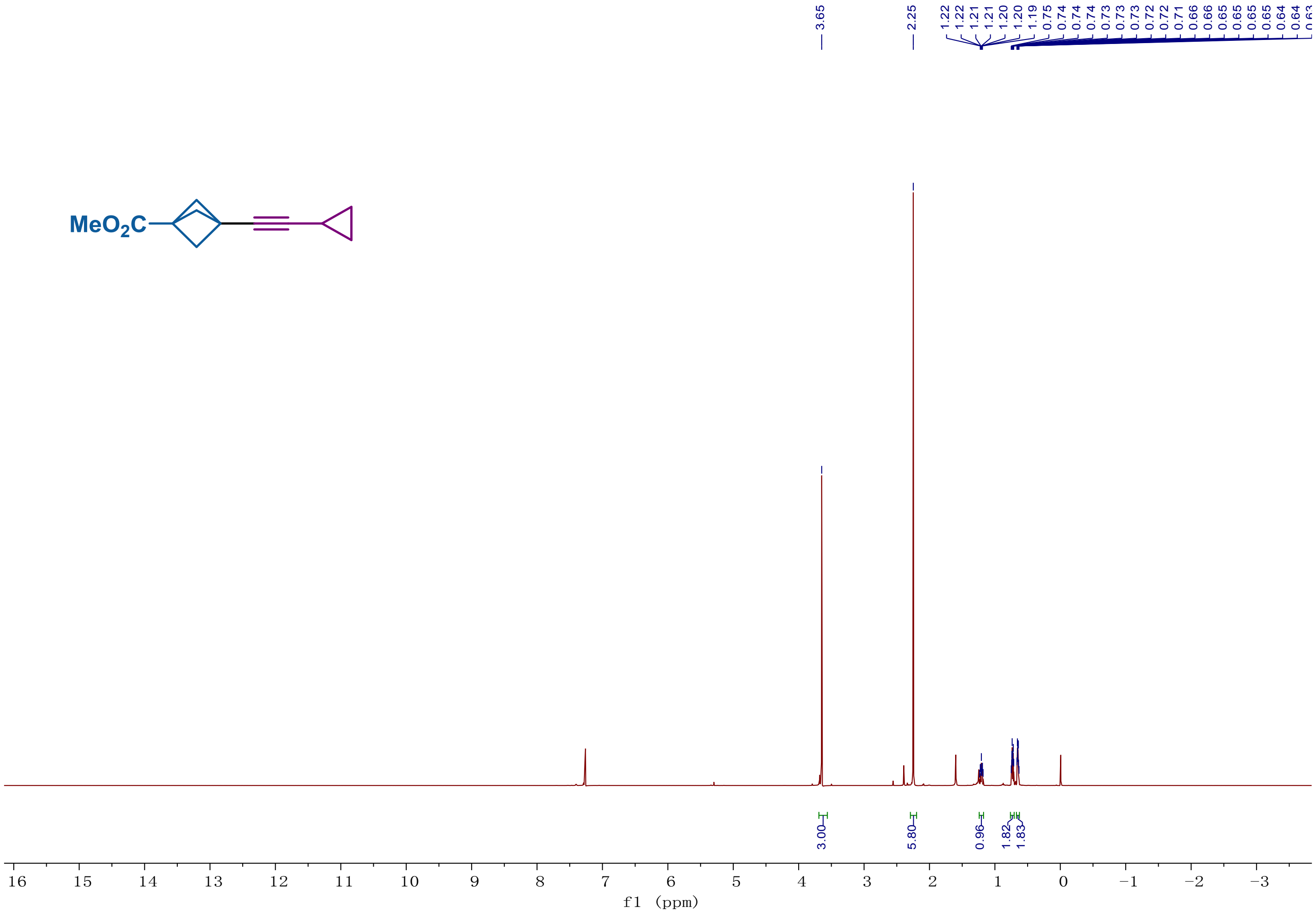

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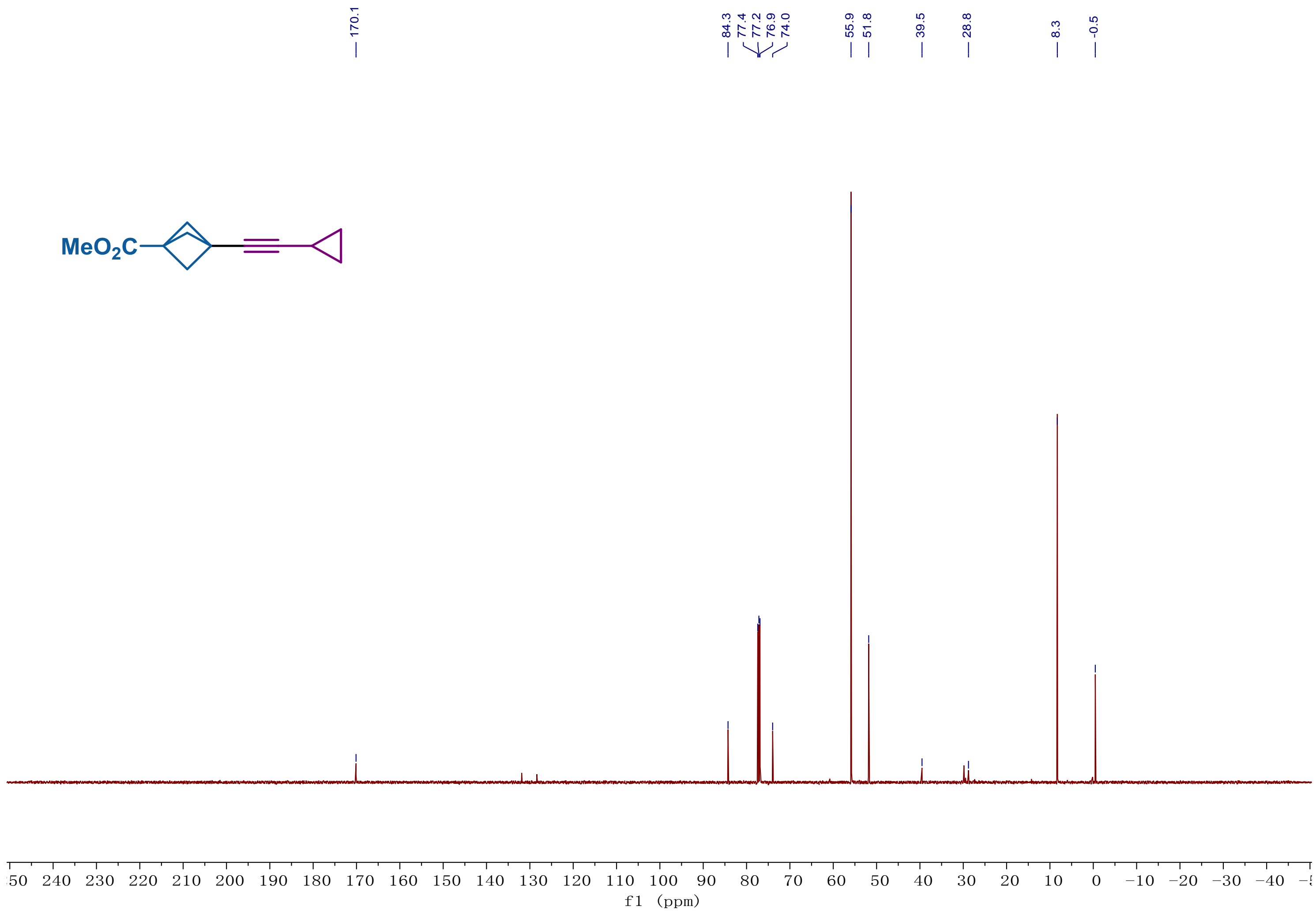

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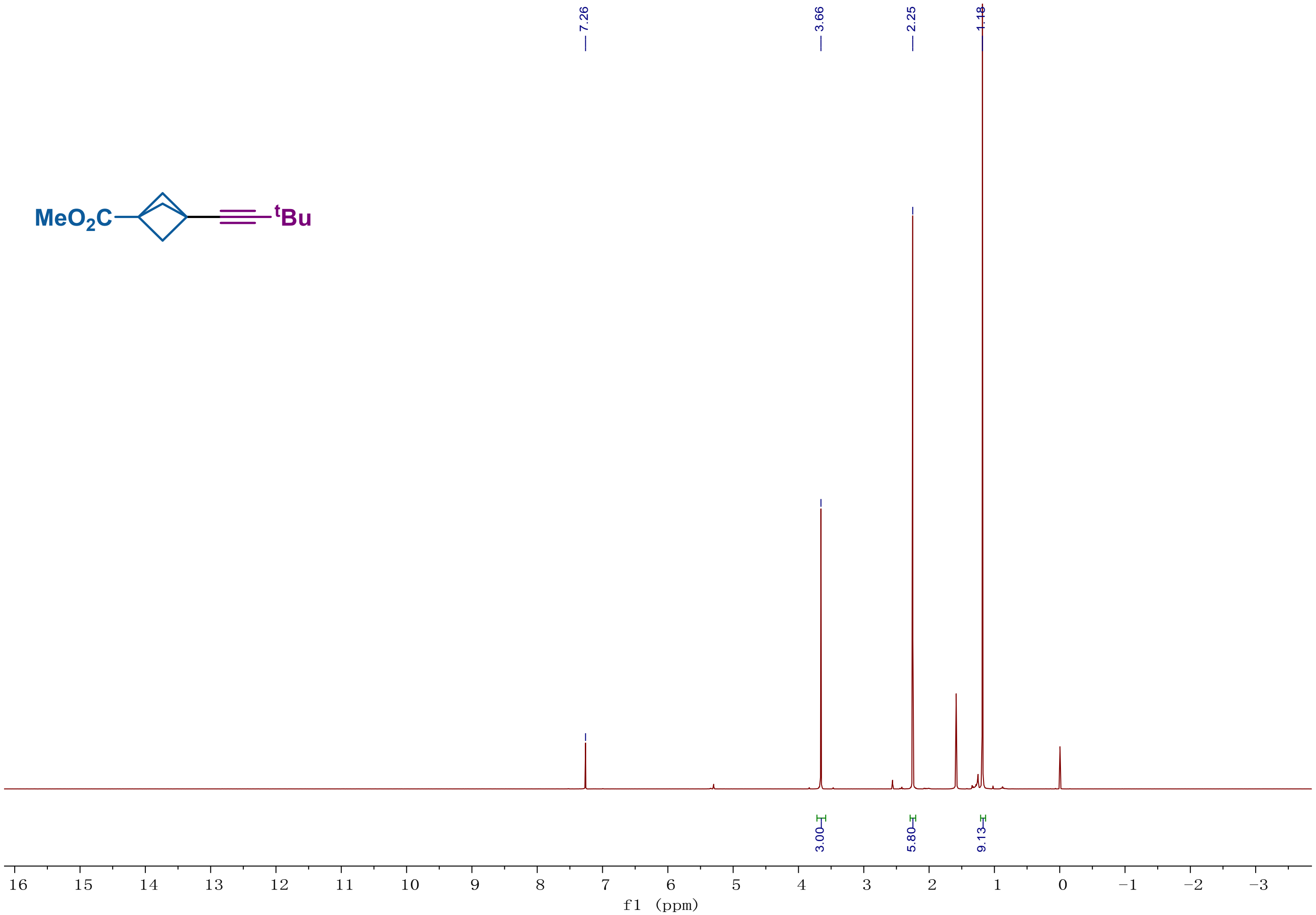
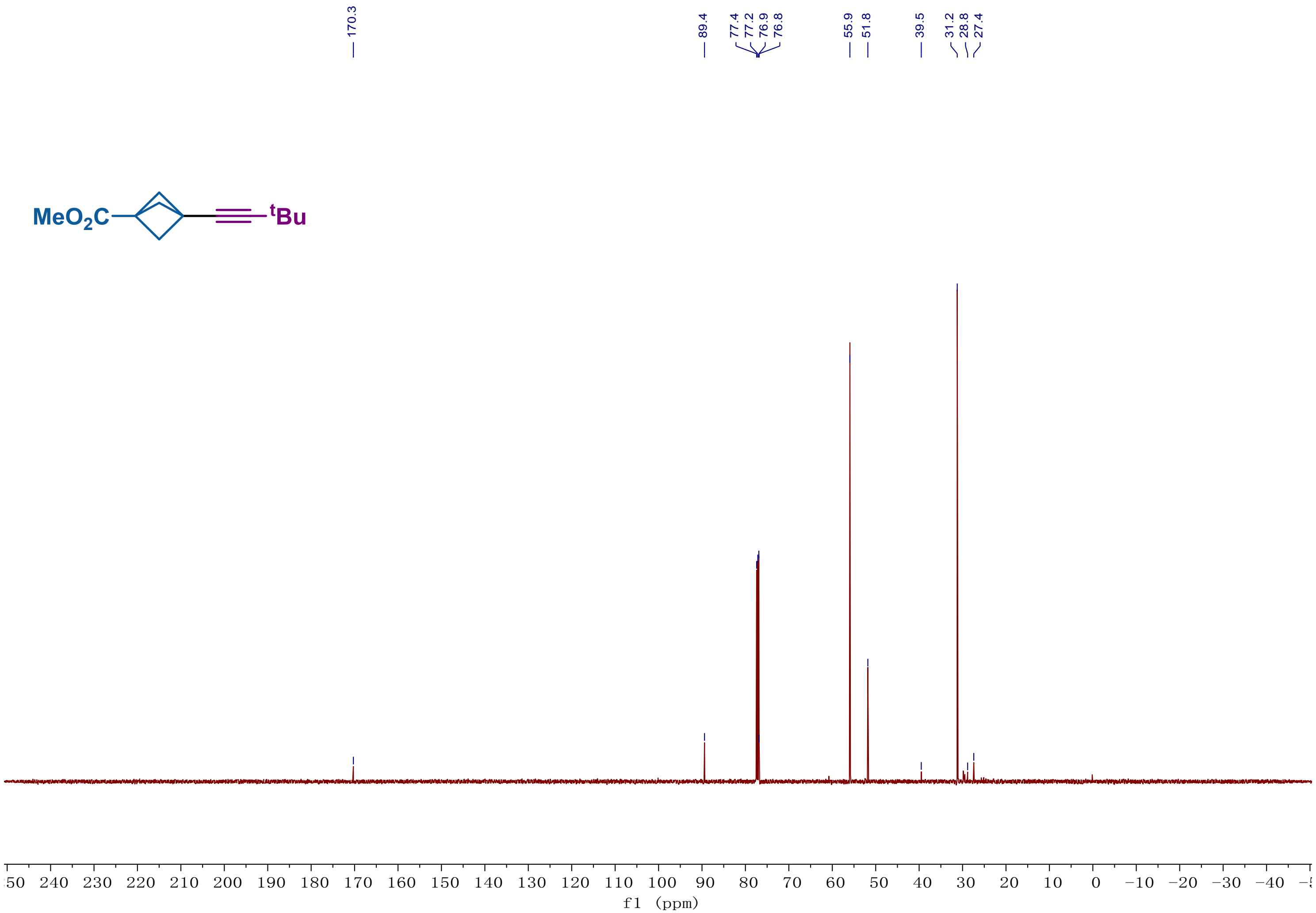


Compound 44 ^{13}C NMR



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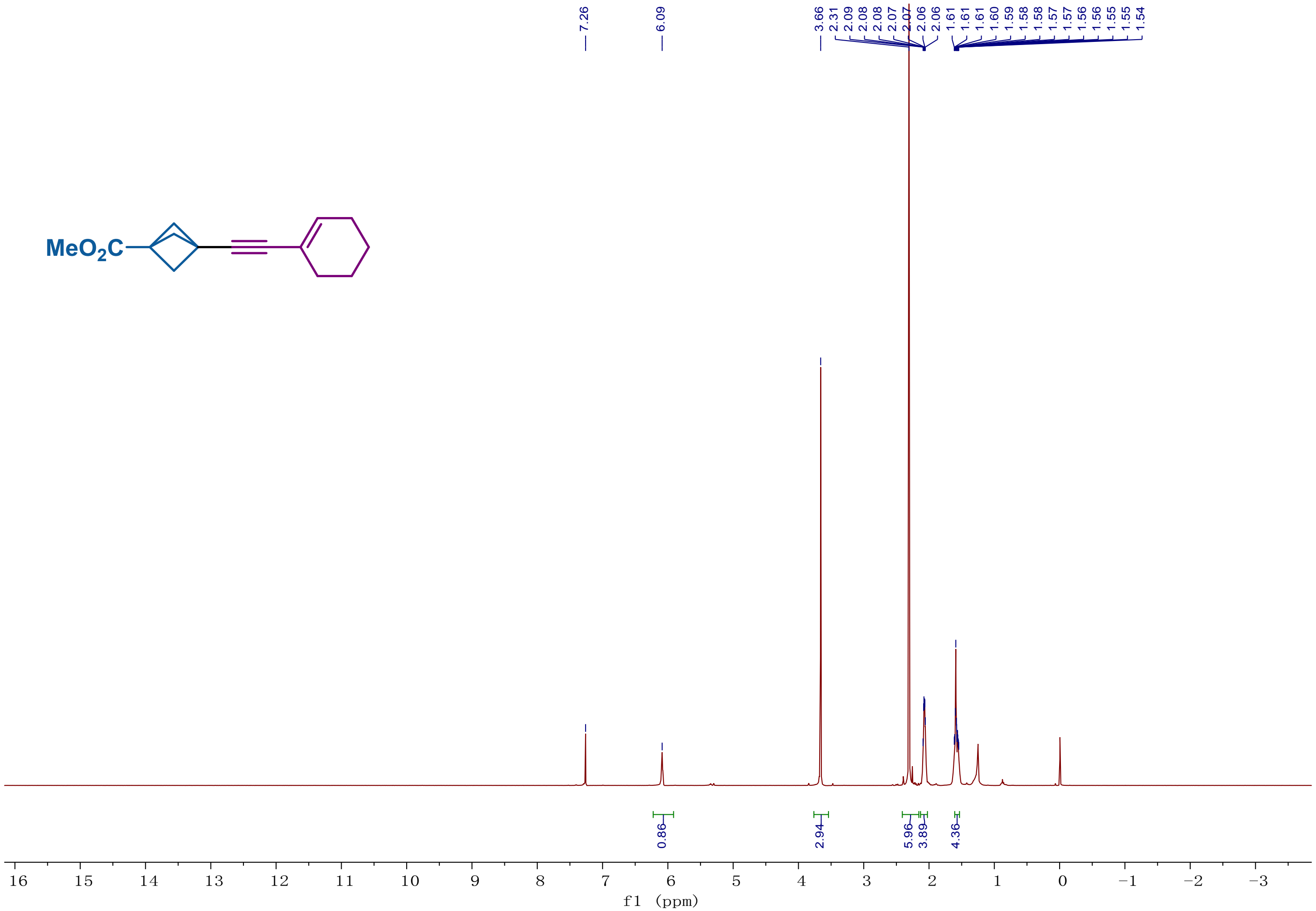
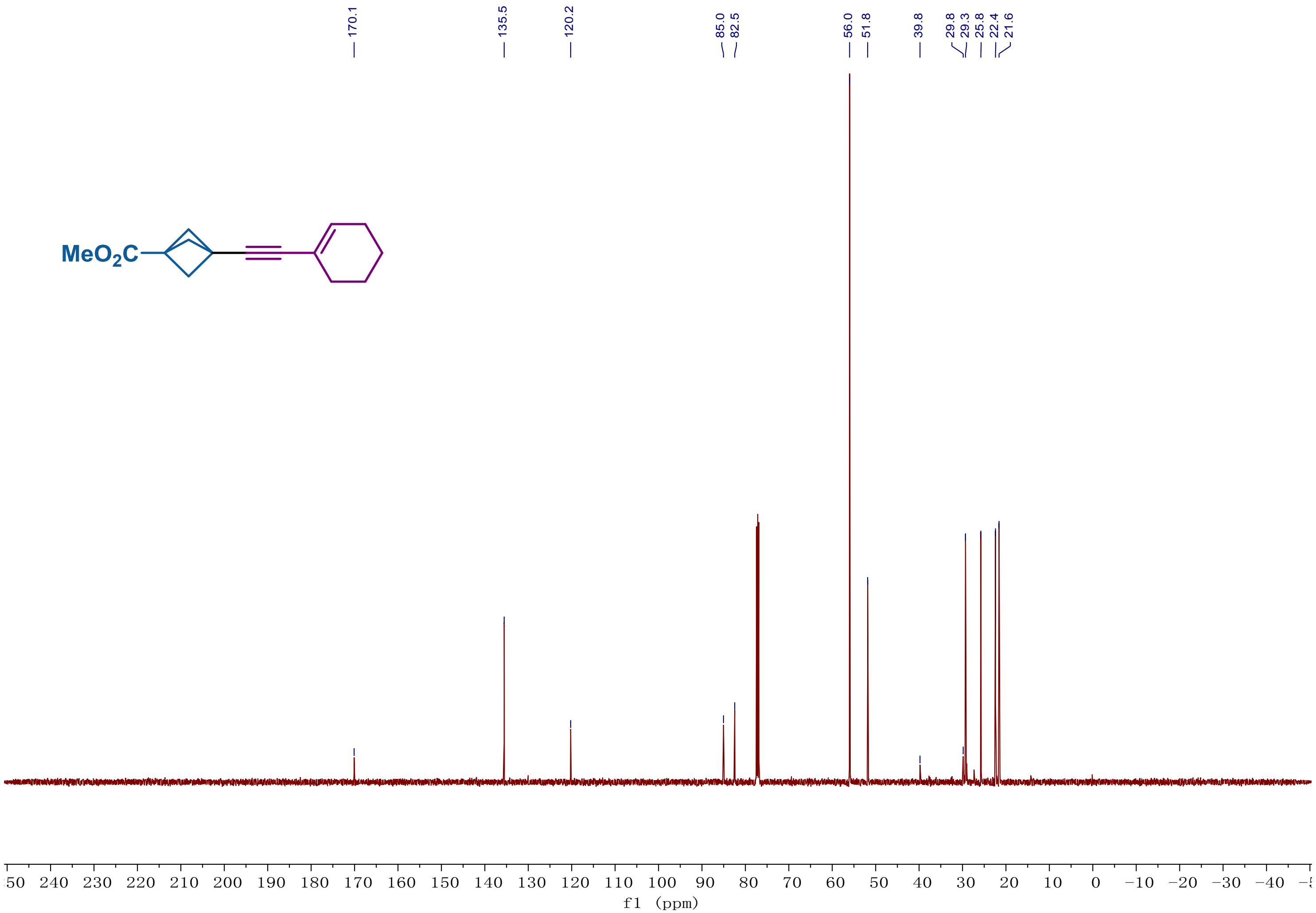
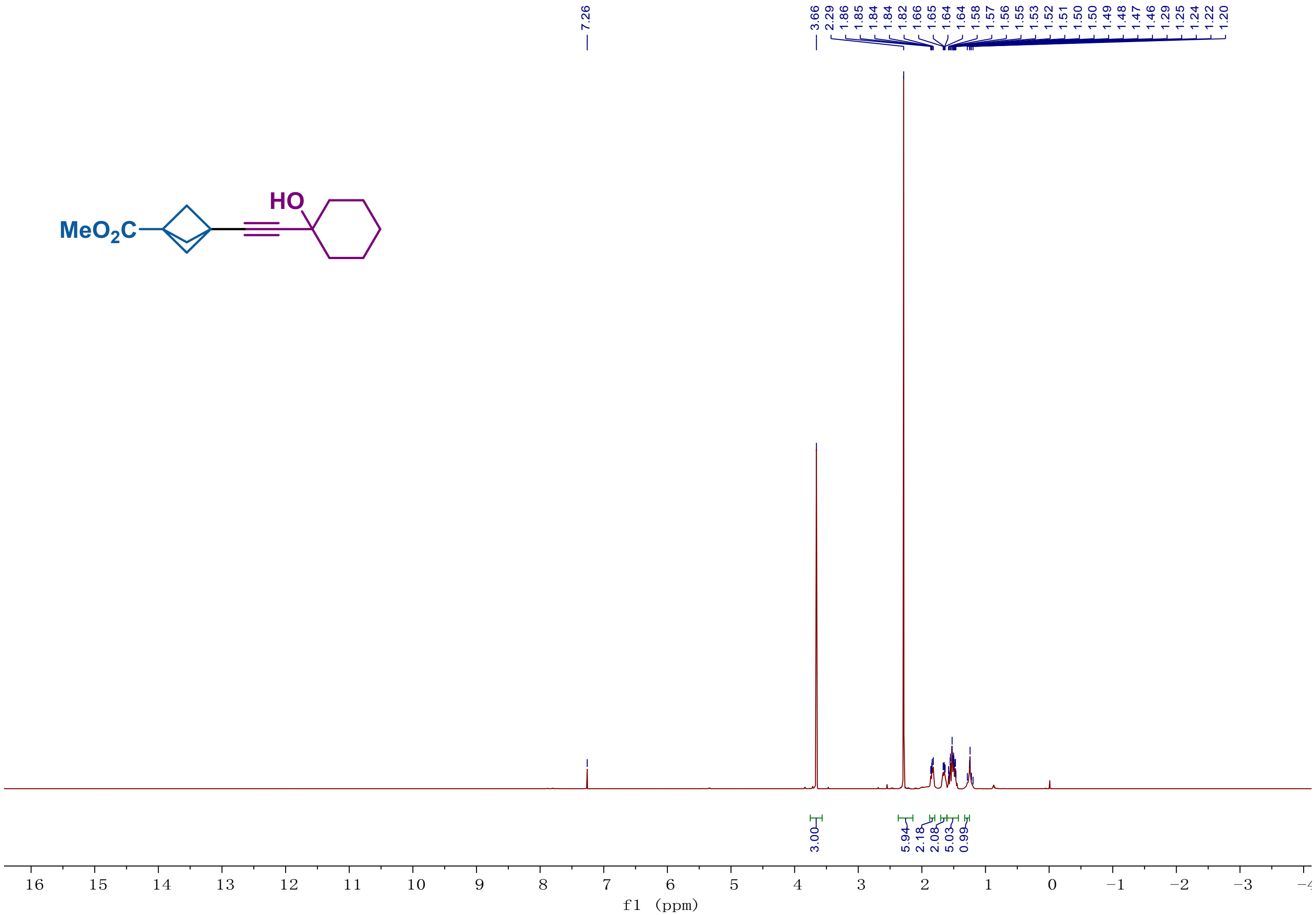


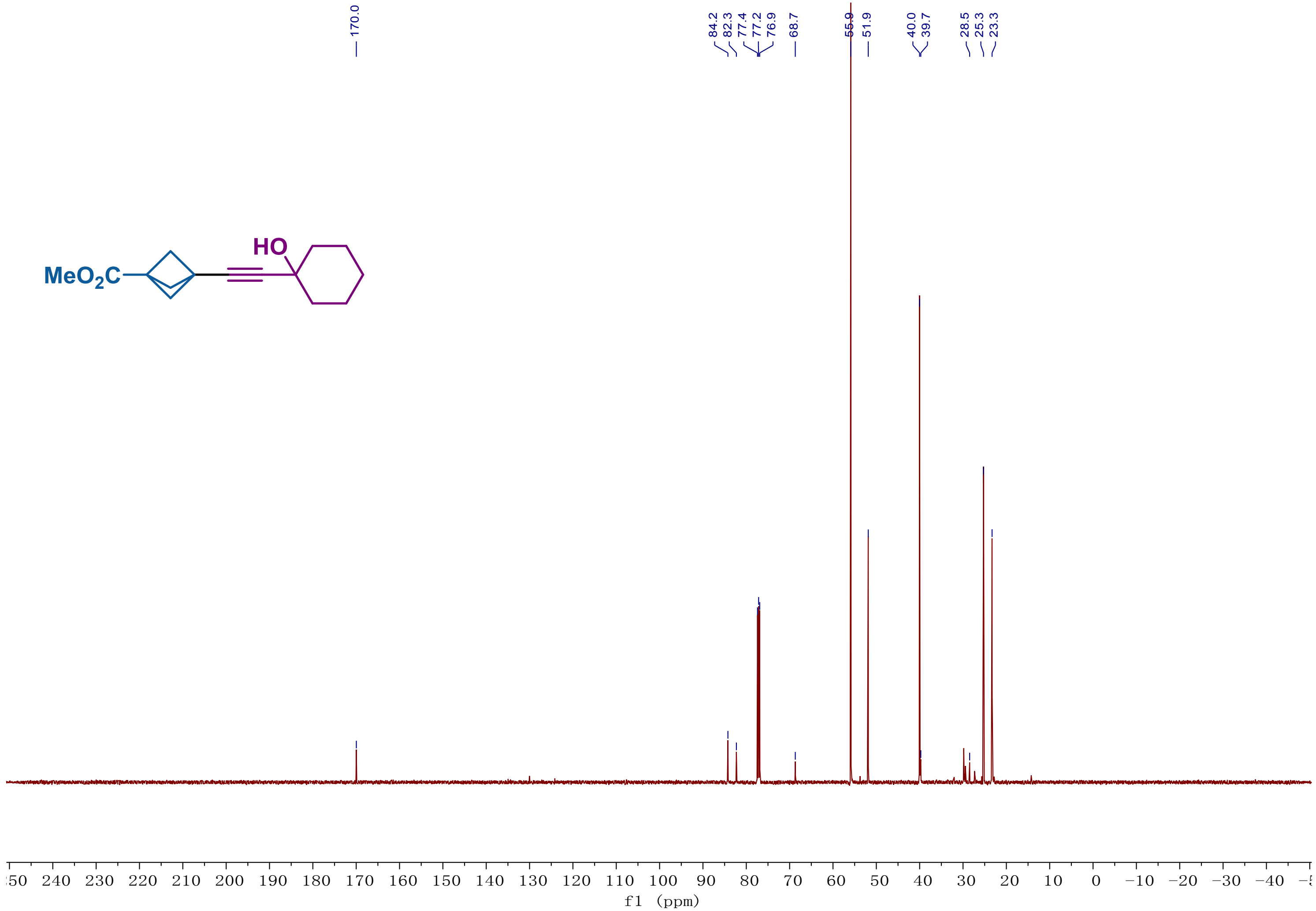
Compound 45 ^{13}C NMR



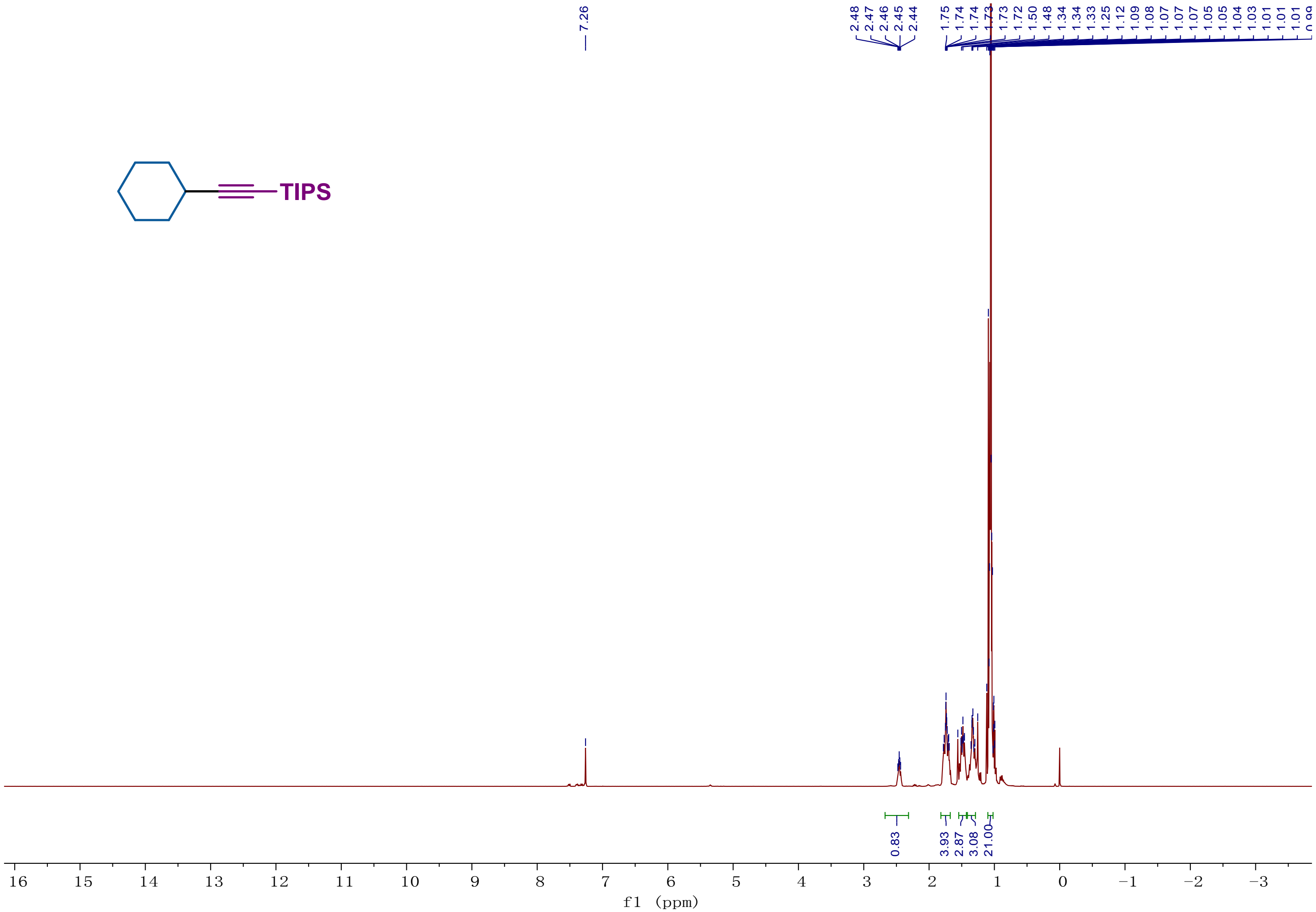
Compound 46 ^{1}H NMR



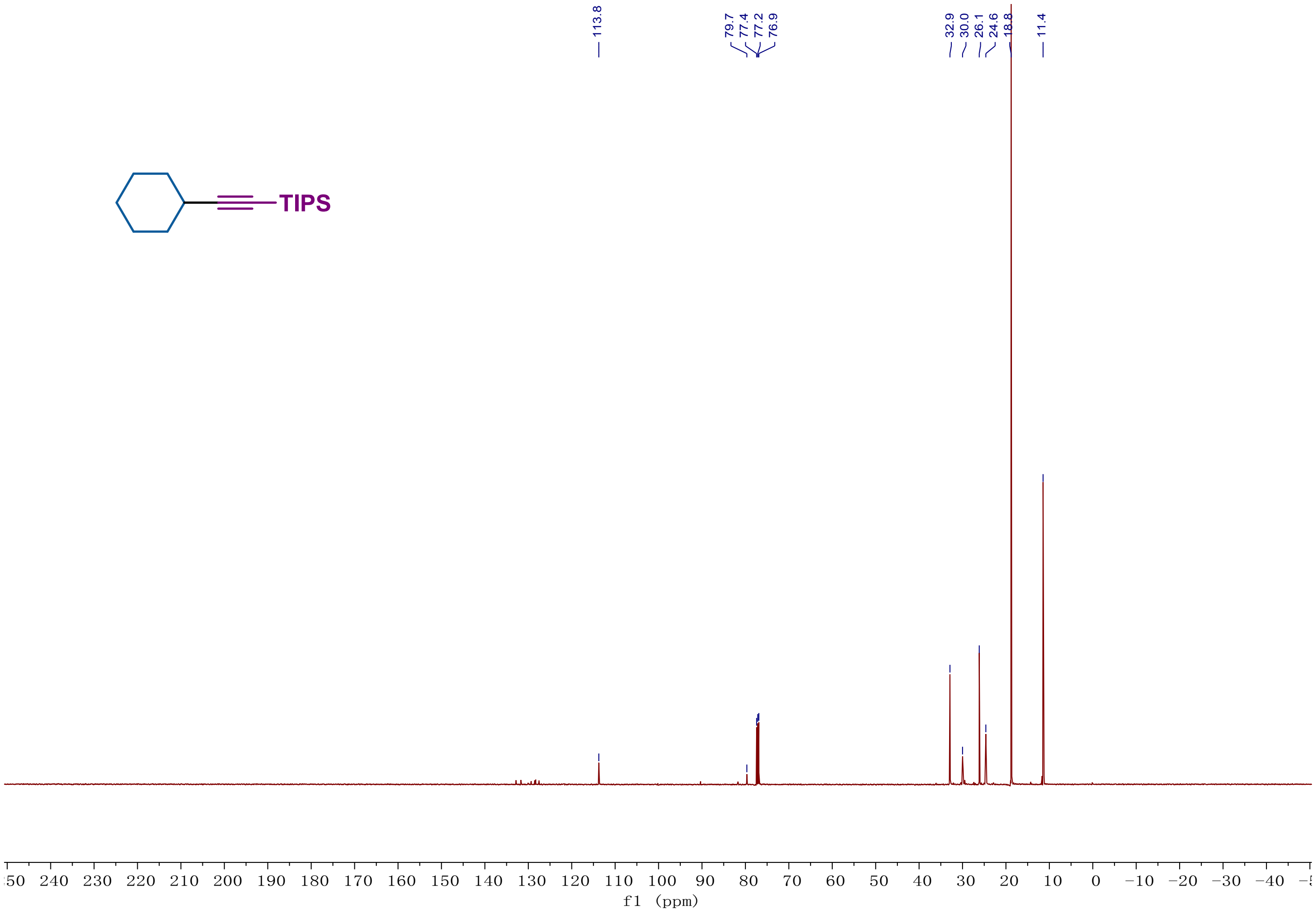
Compound 46 ^{13}C NMR



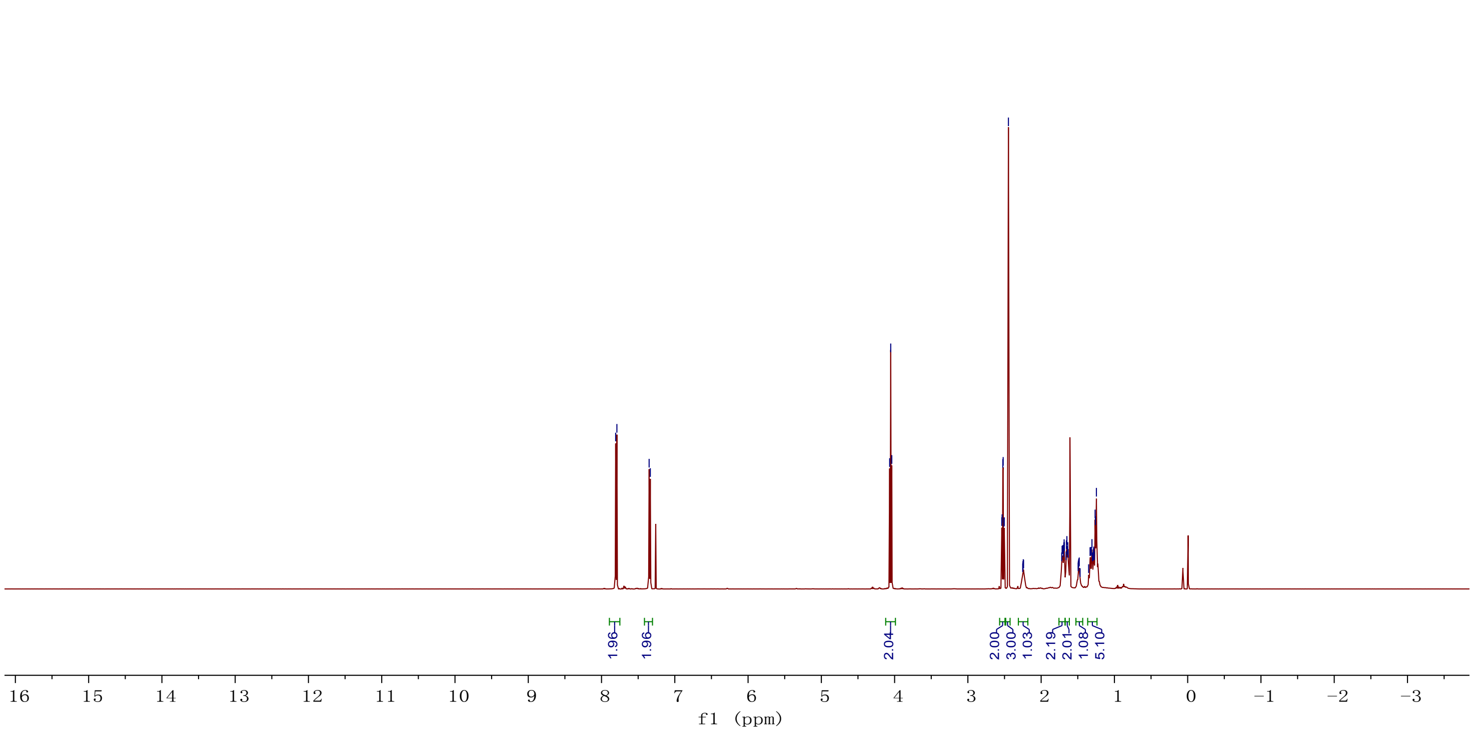
Compound 47 ^{1}H NMR



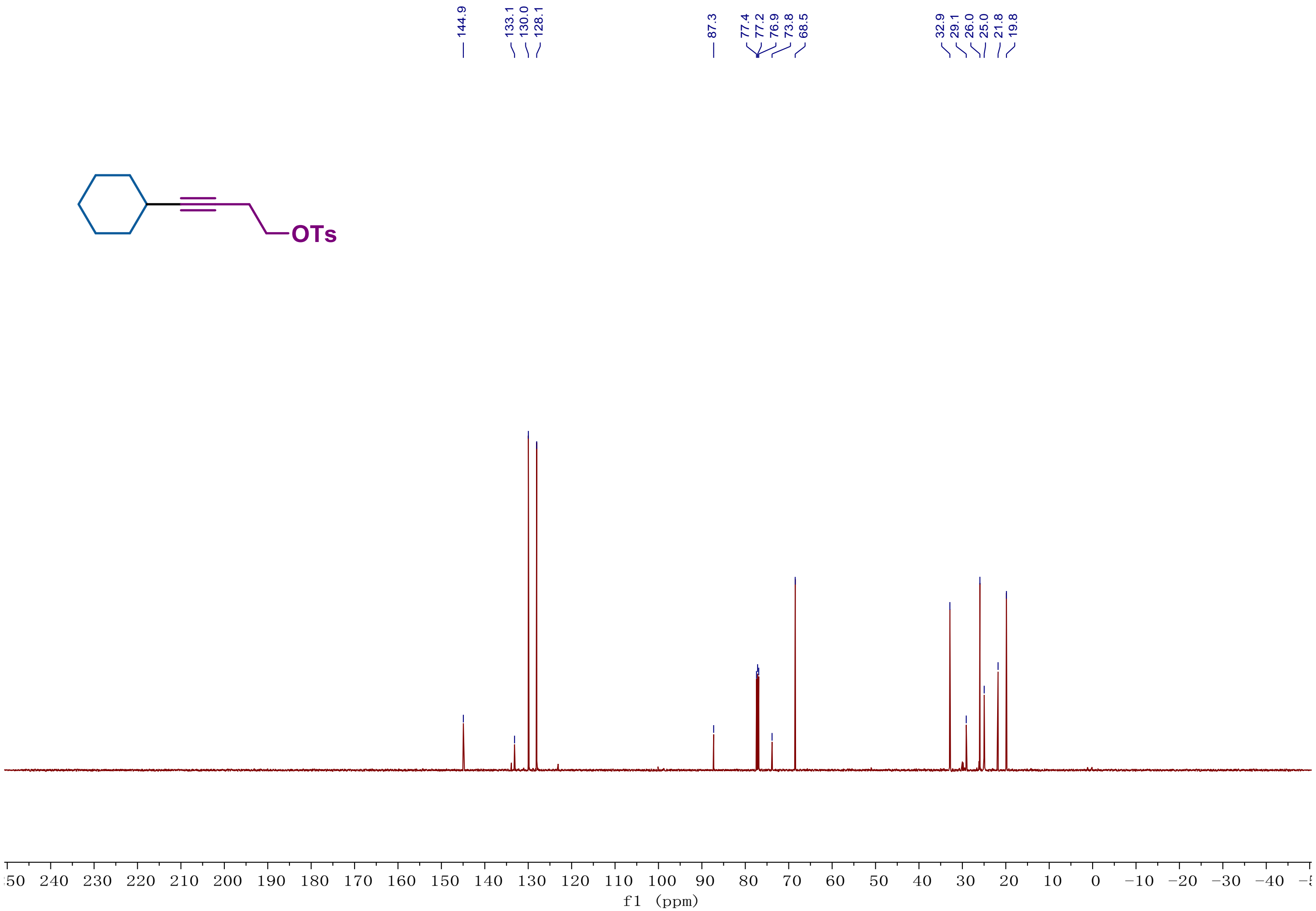
Compound 47 ^{13}C NMR



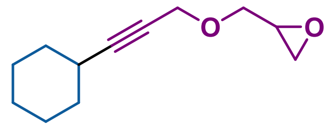
Compound 48 ¹H NMR

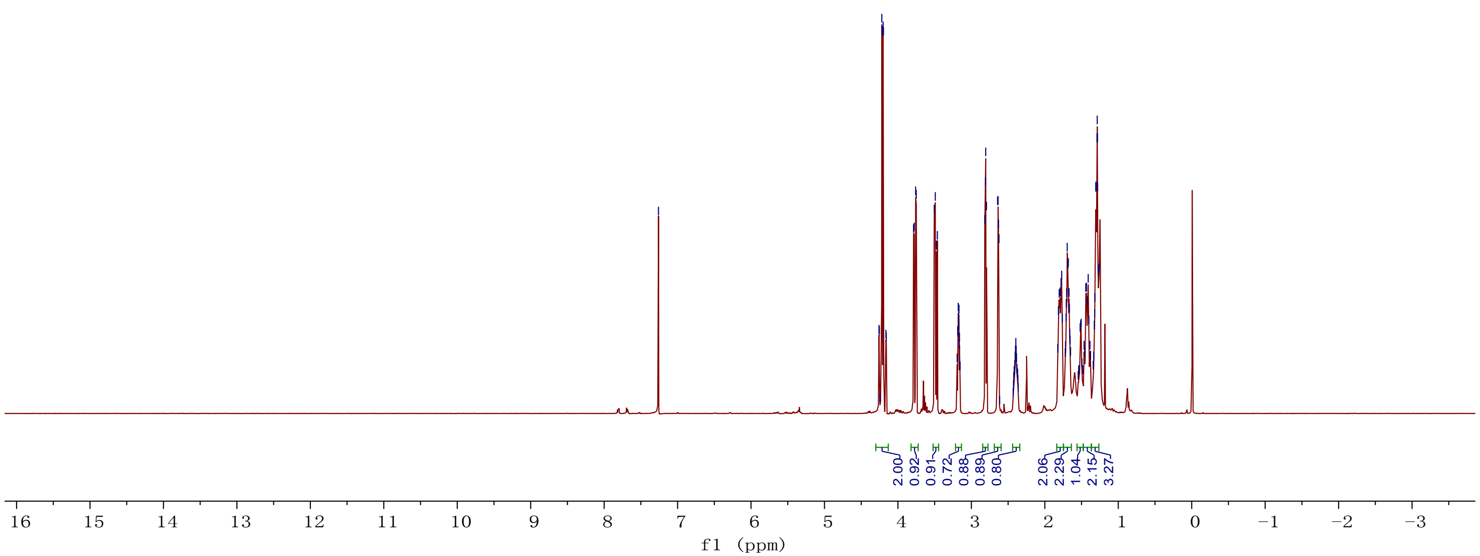


Compound 48 ^{13}C NMR



Compound 49 ^{1}H NMR





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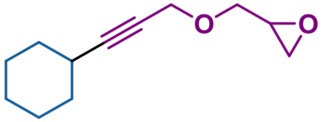
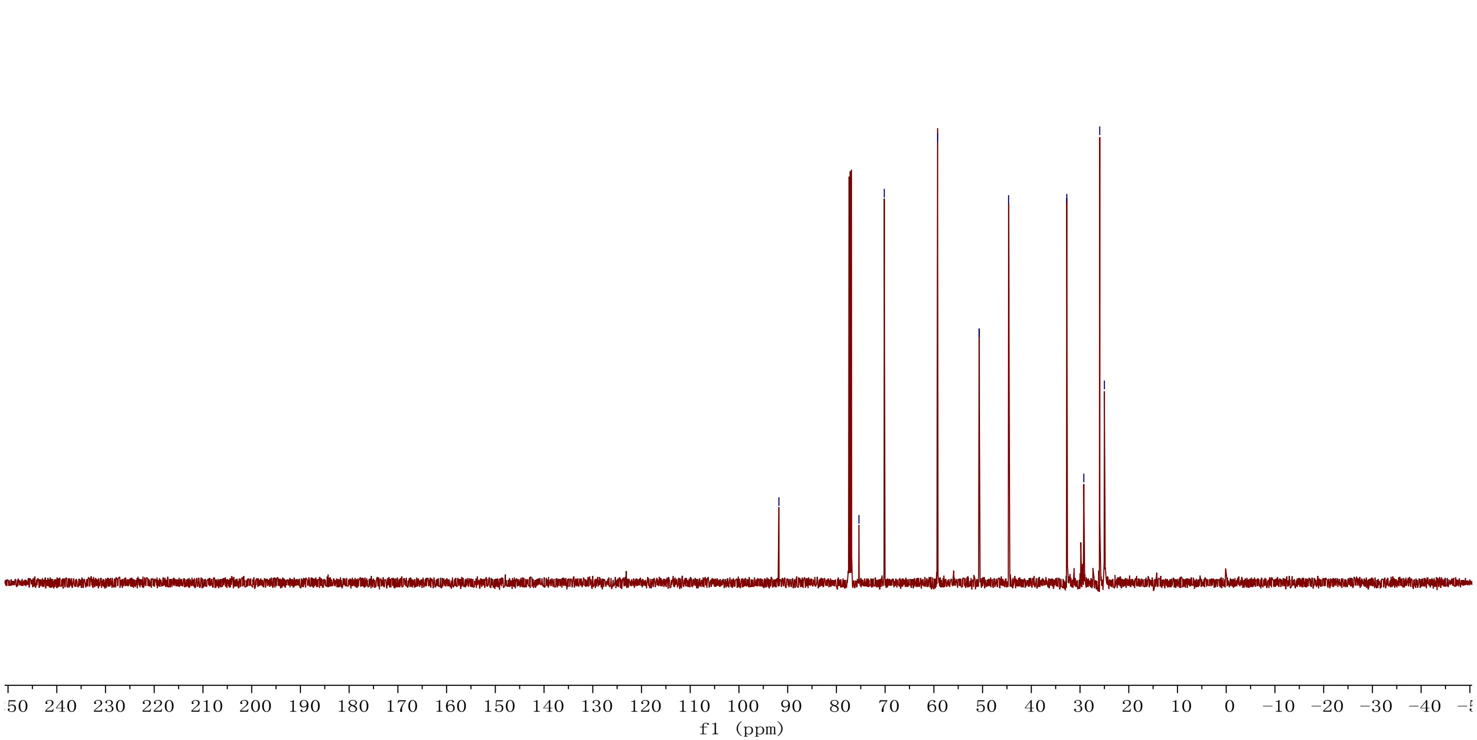
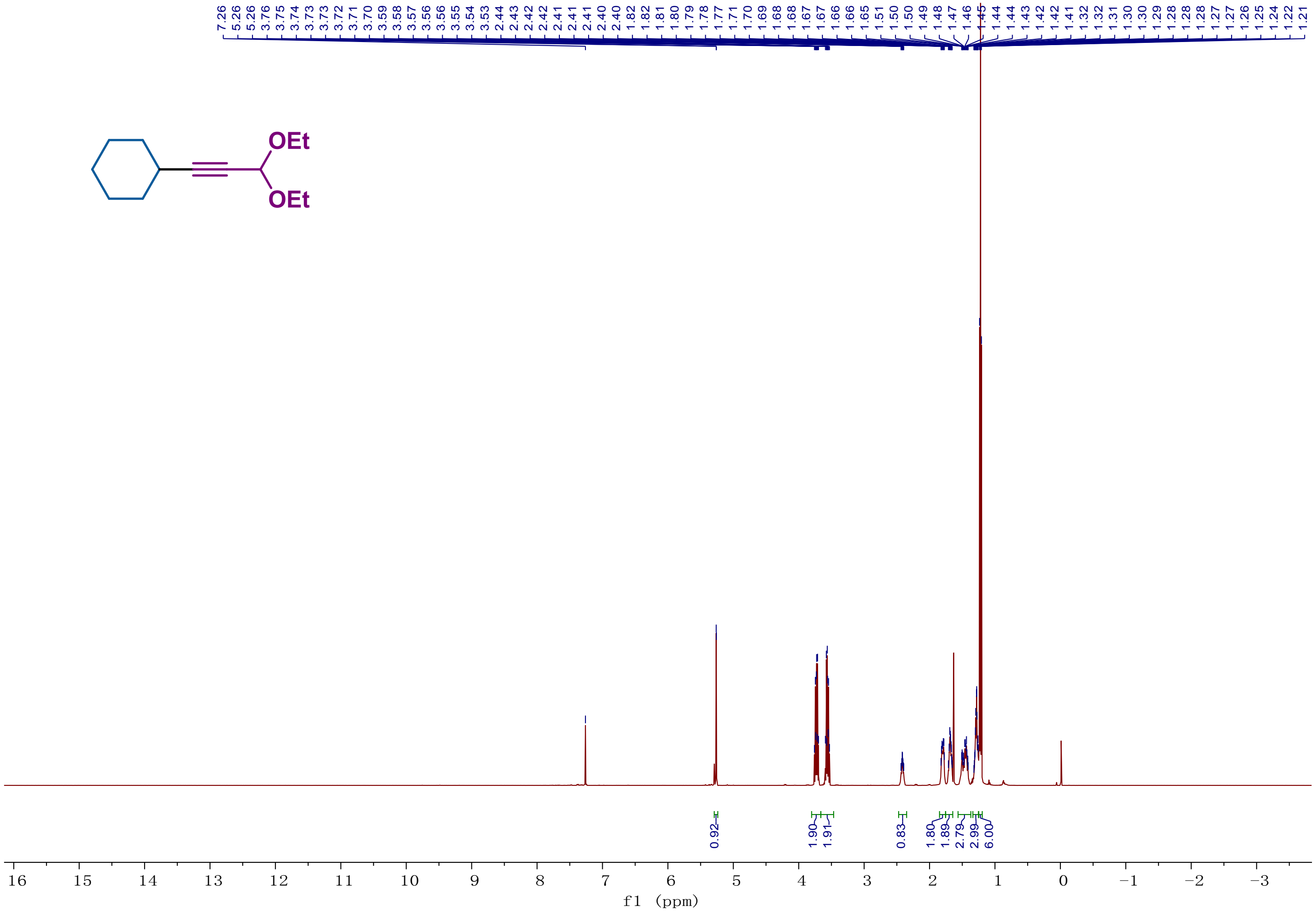
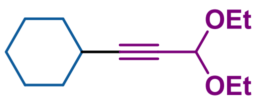


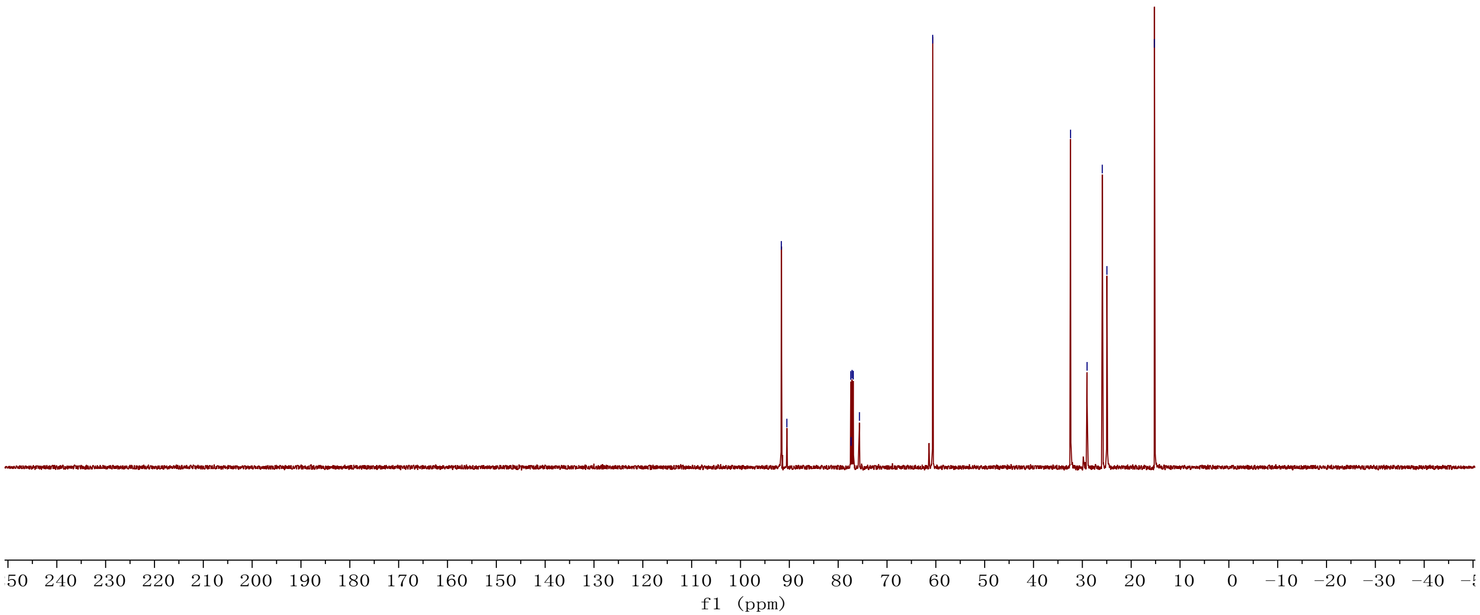


Compound 50 ^{1}H NMR

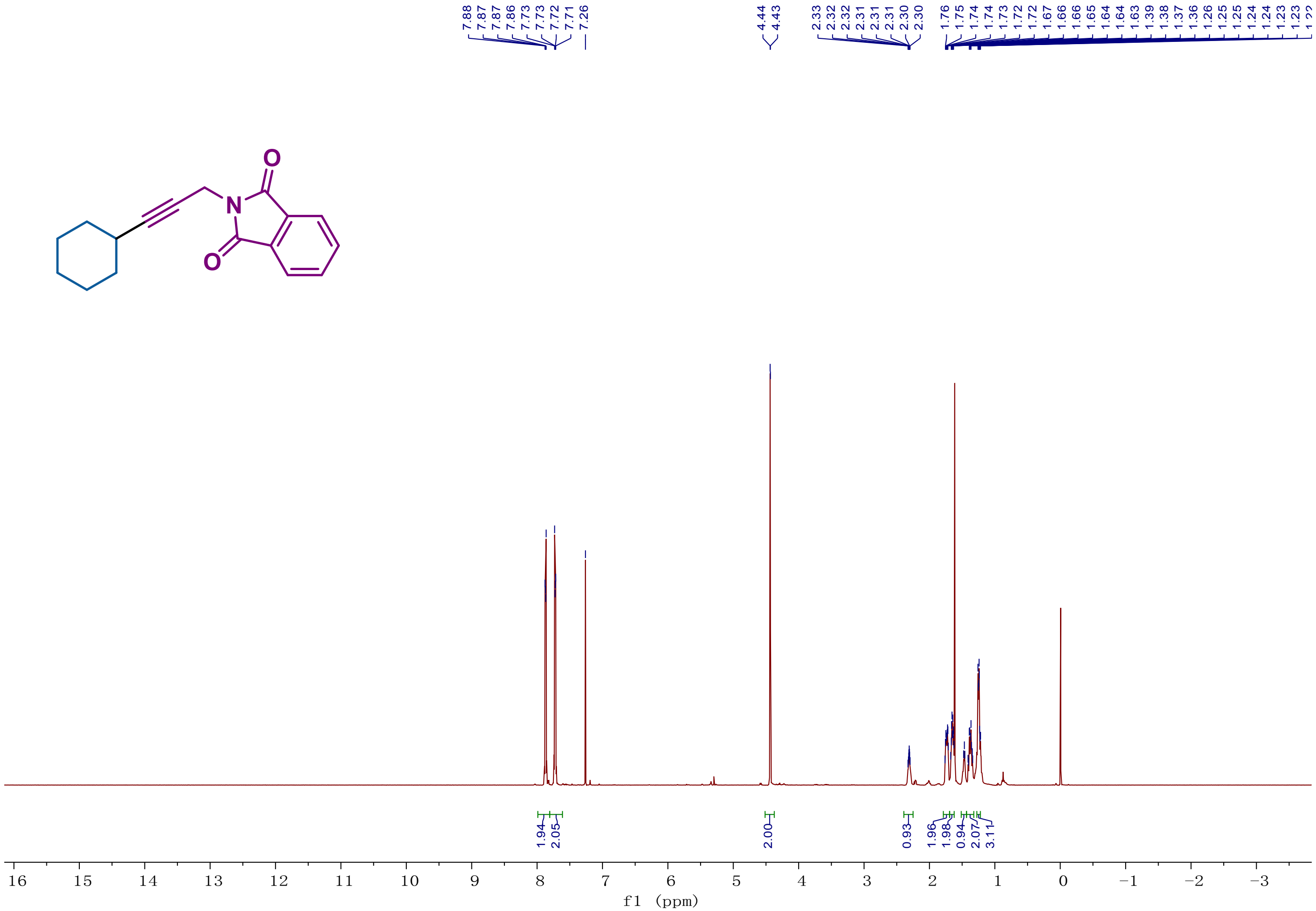


Compound 50 ^{13}C NMR

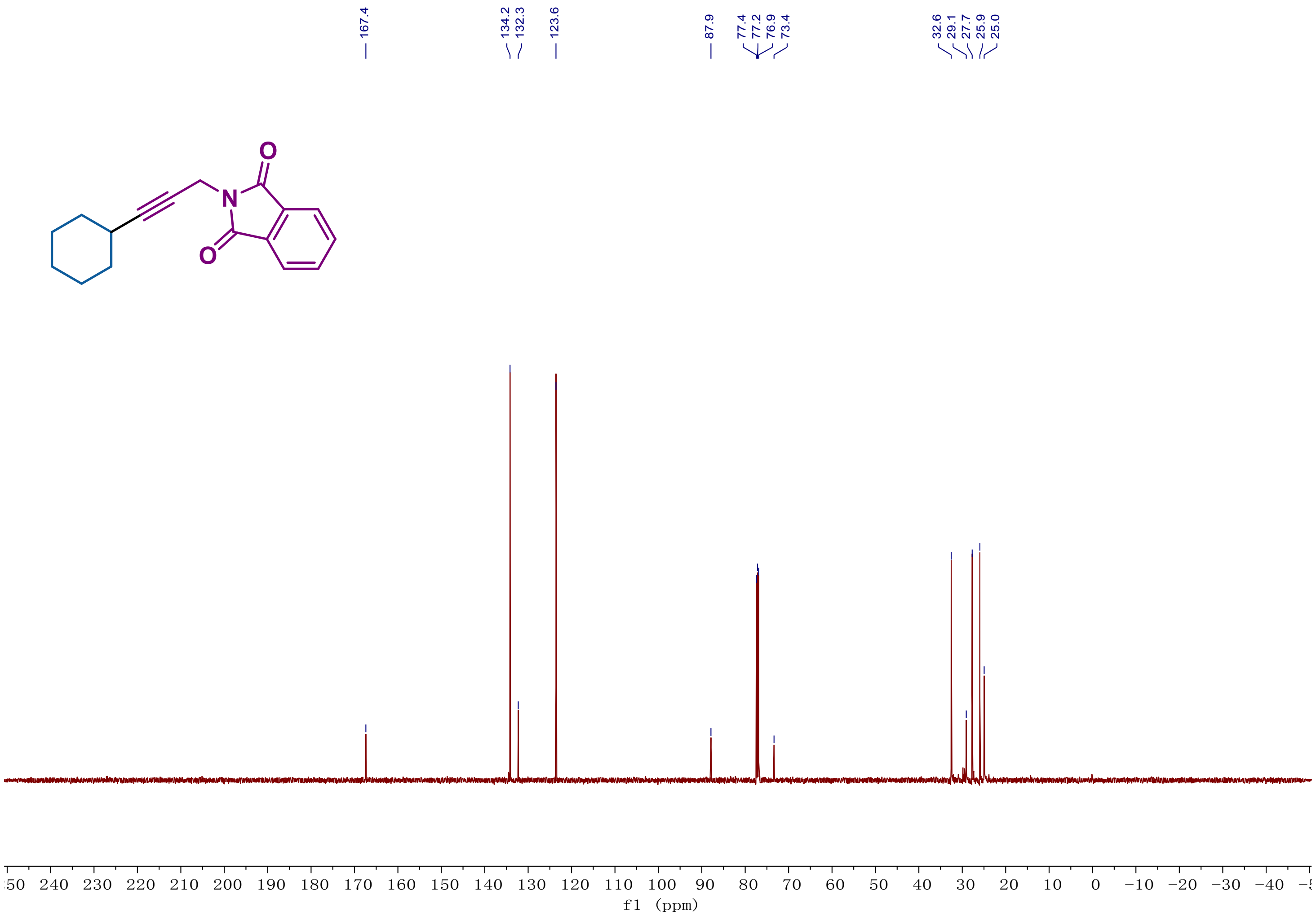




Compound 51 ^{1}H NMR



Compound 51 ^{13}C NMR



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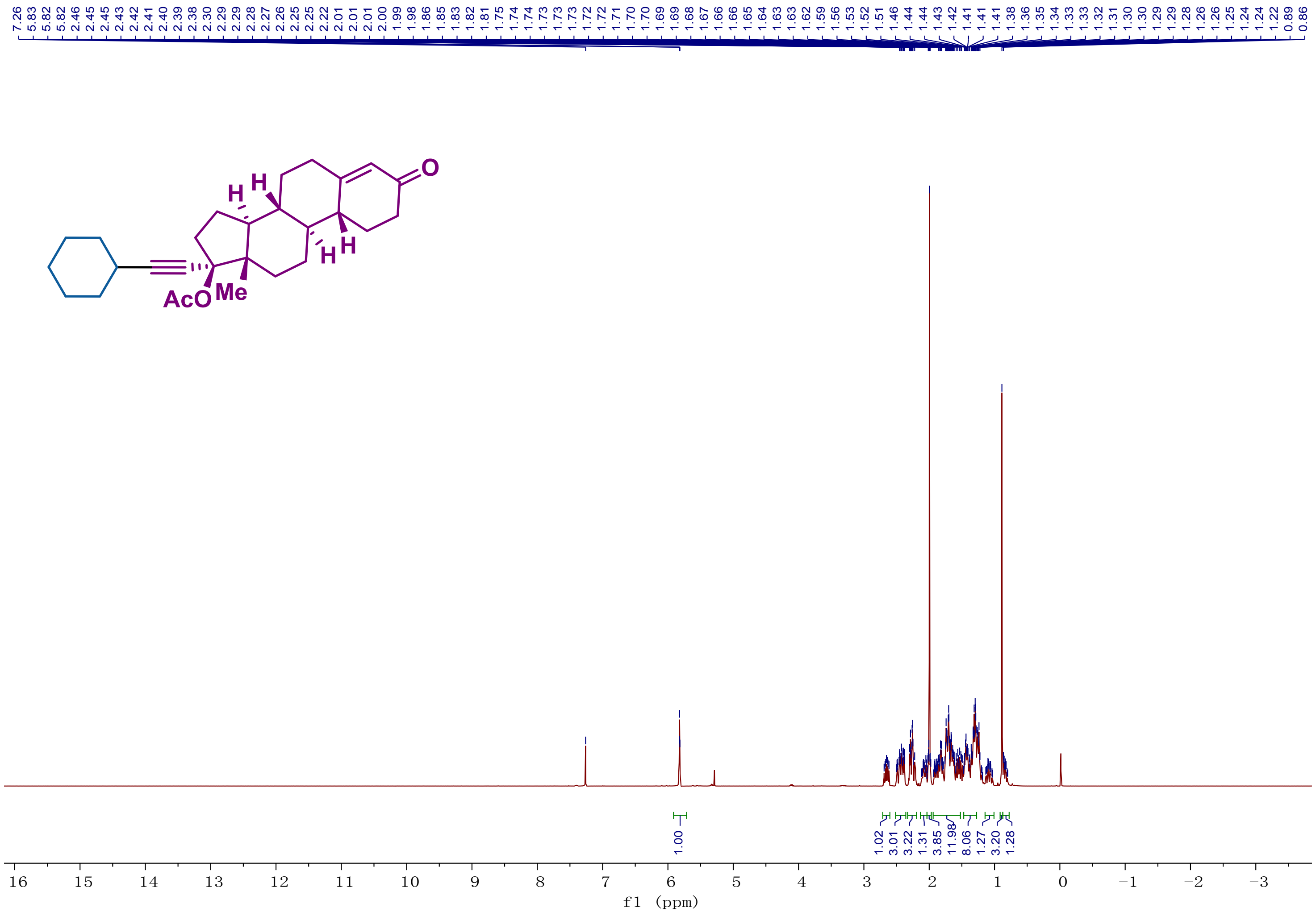

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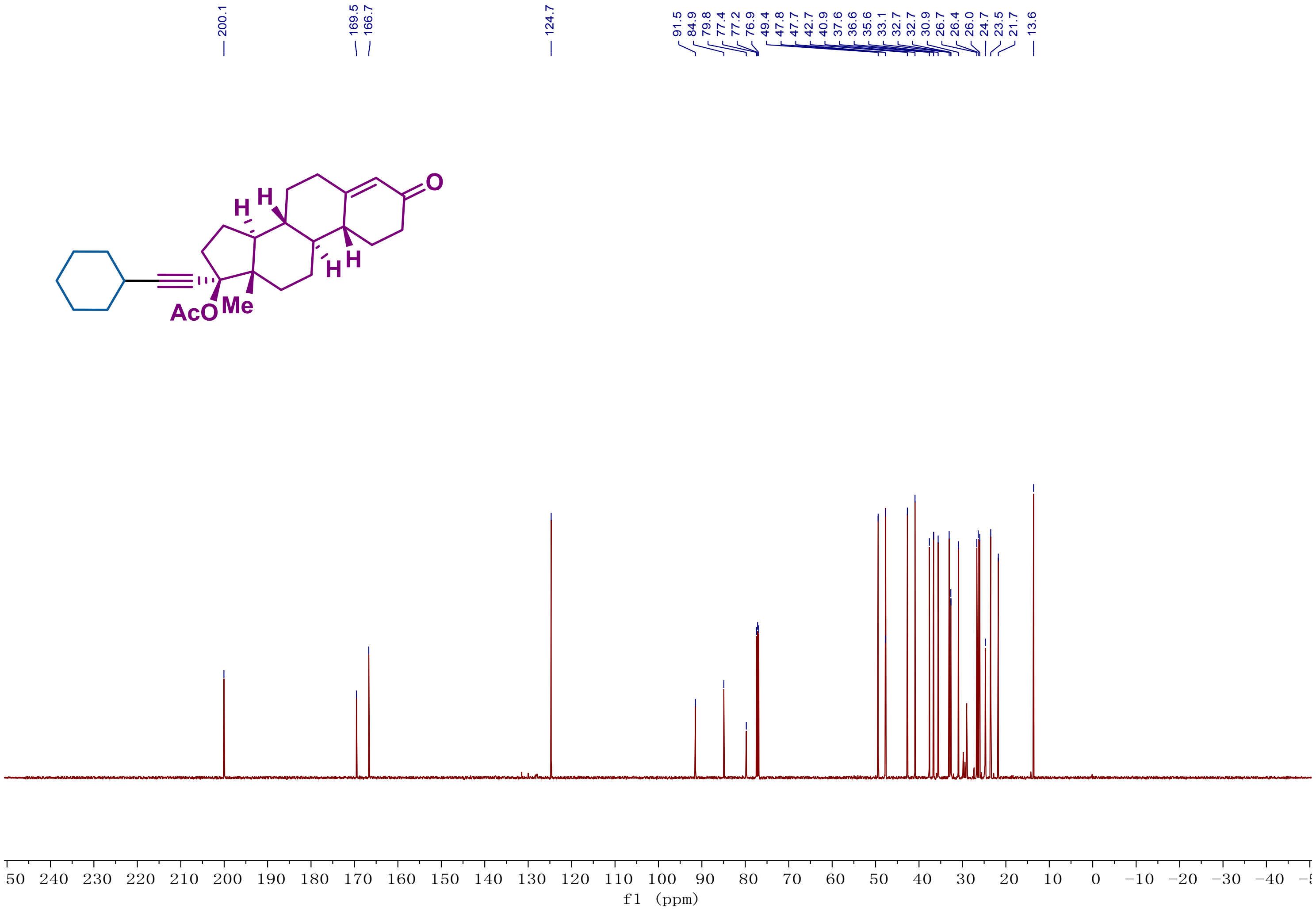
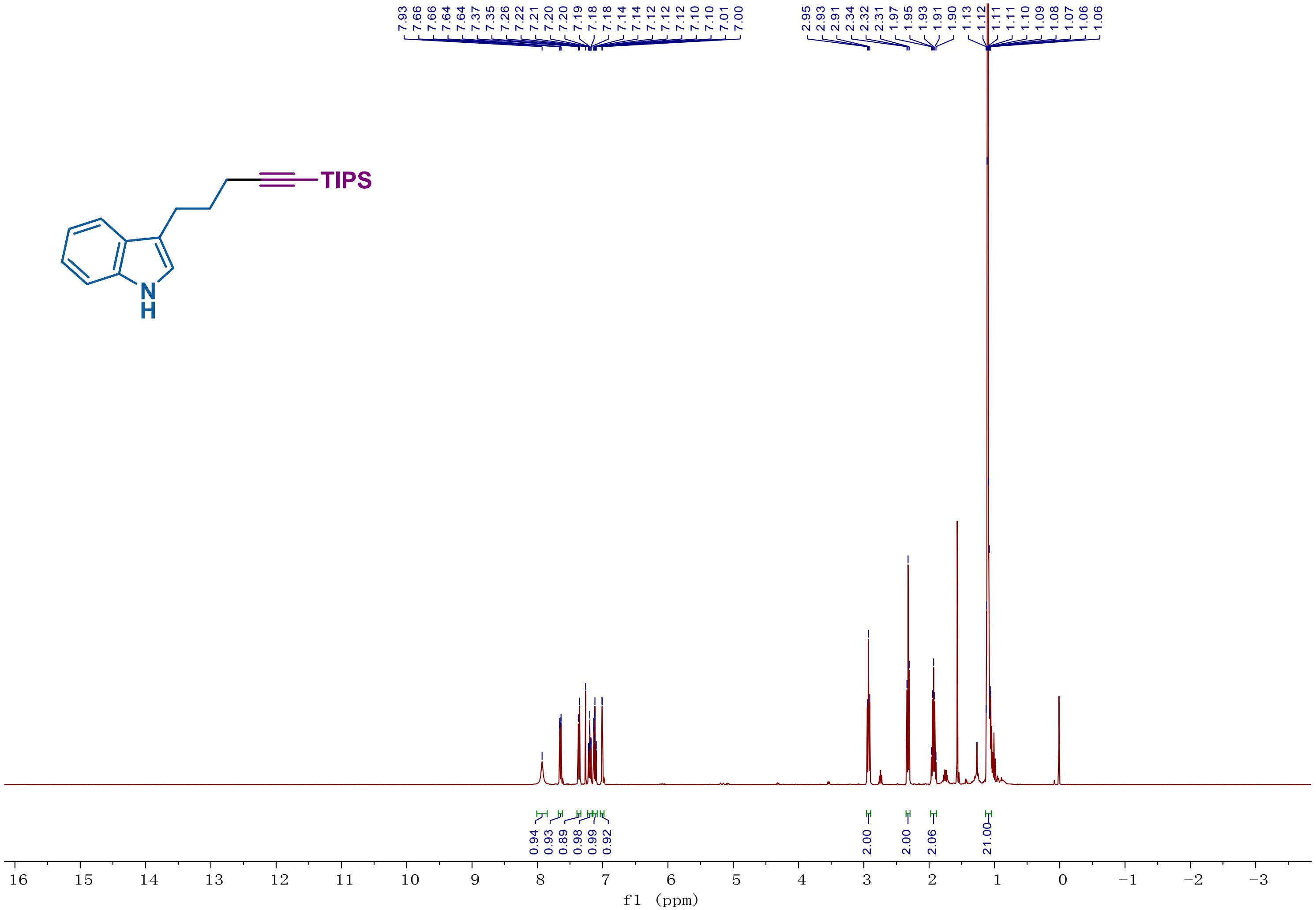
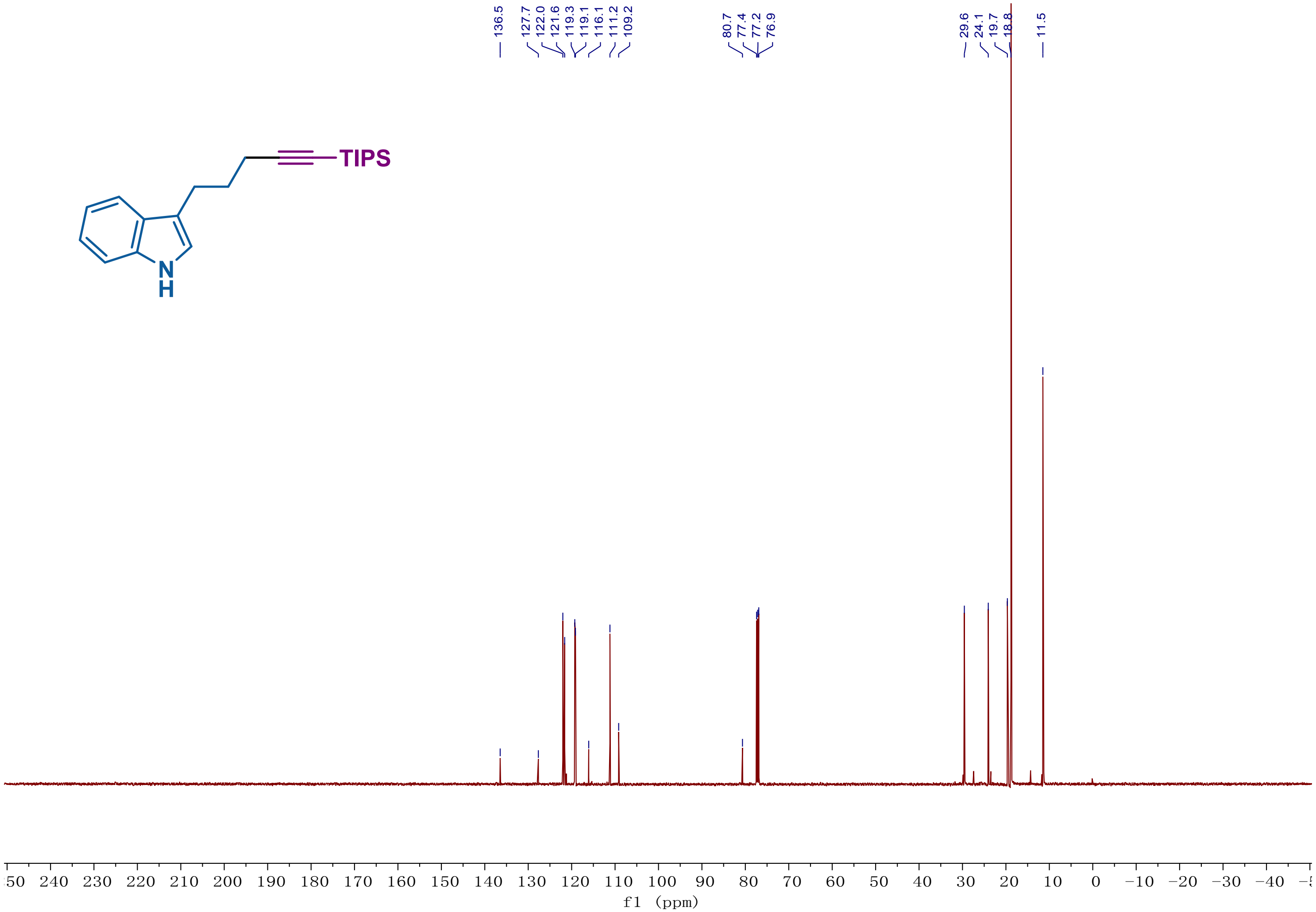


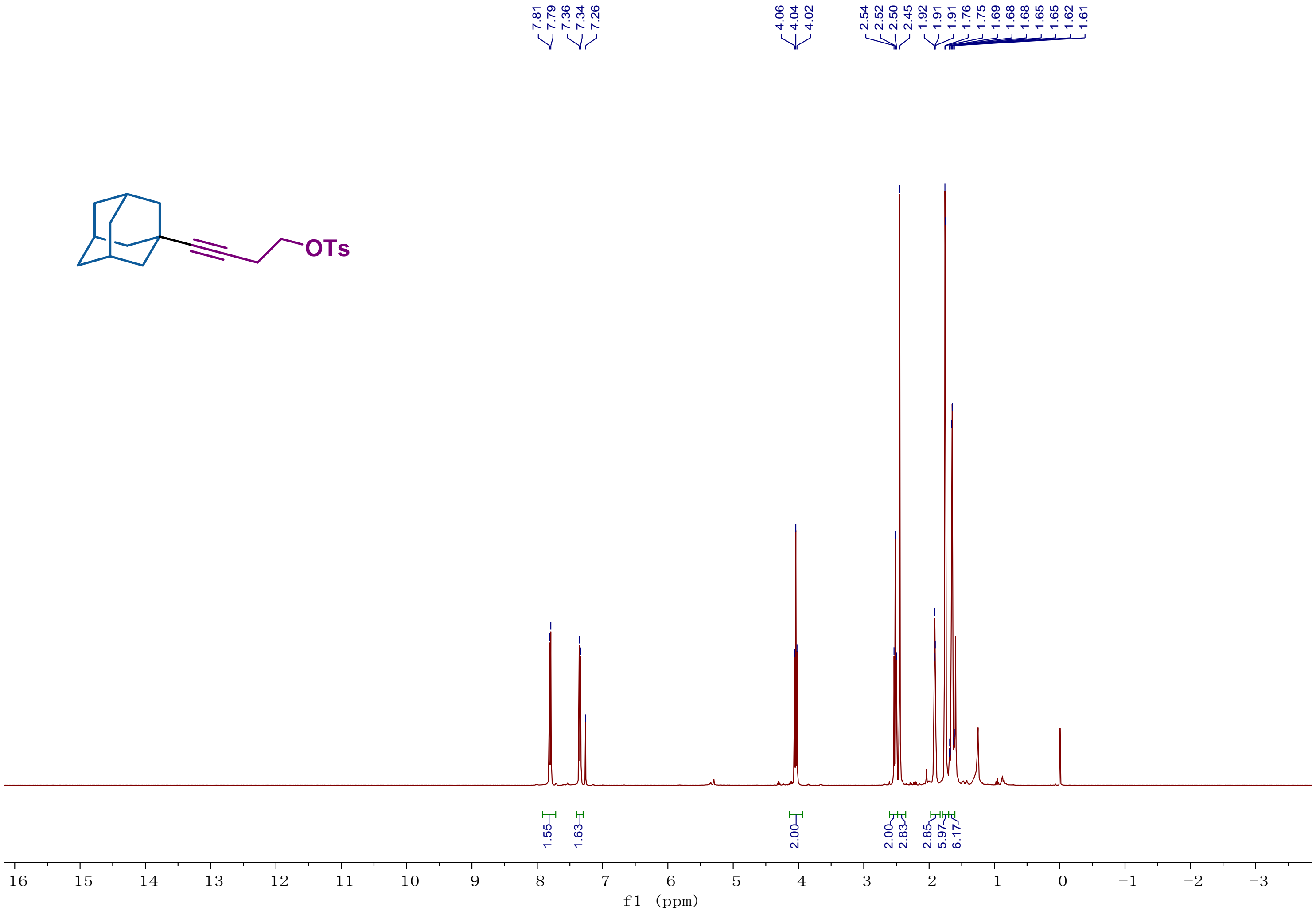
Compound 53 ^{1}H NMR



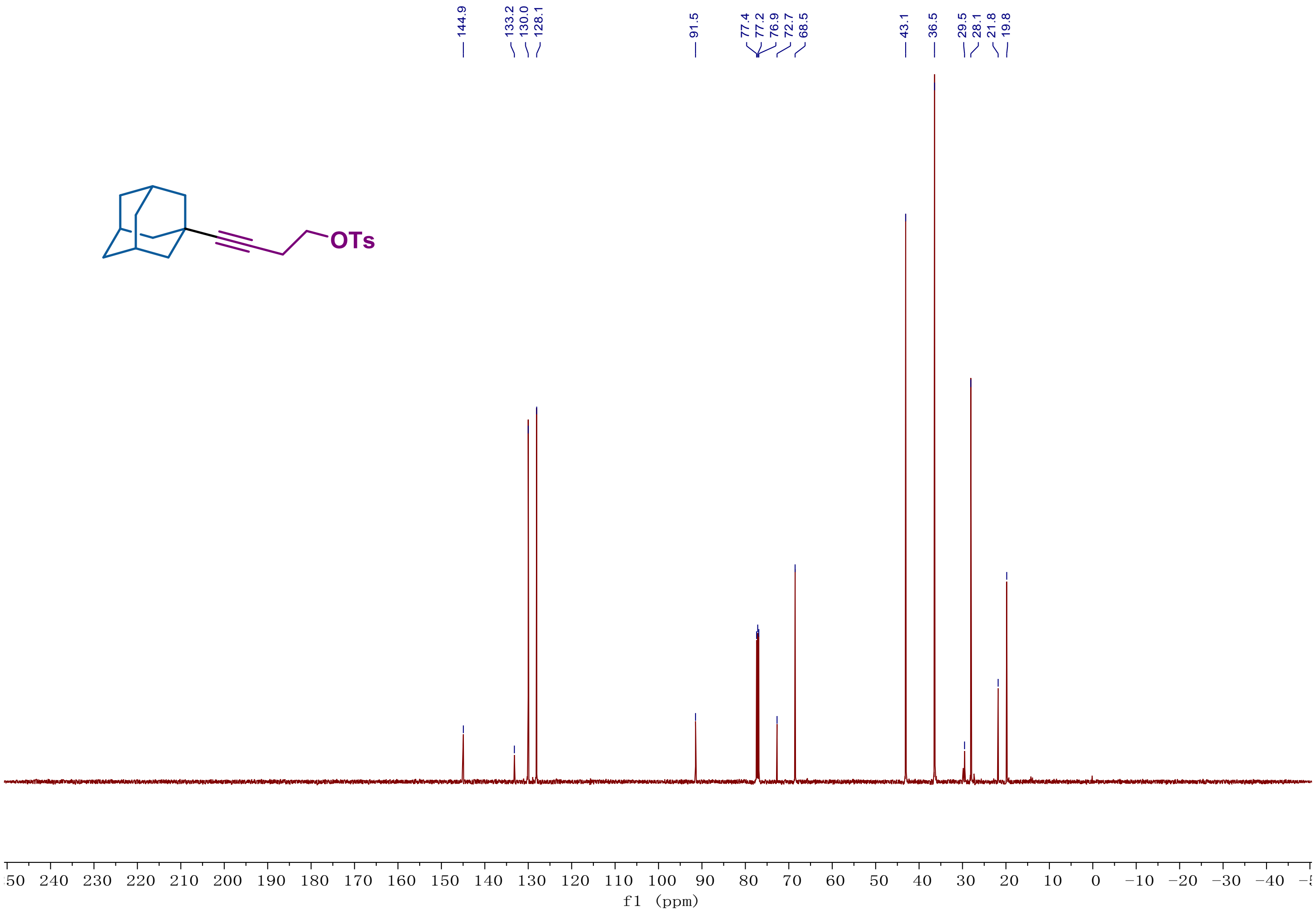
Compound 53 ^{13}C NMR



Compound 54 ^{1}H NMR



Compound 54 ^{13}C NMR



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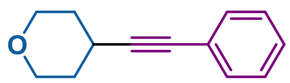

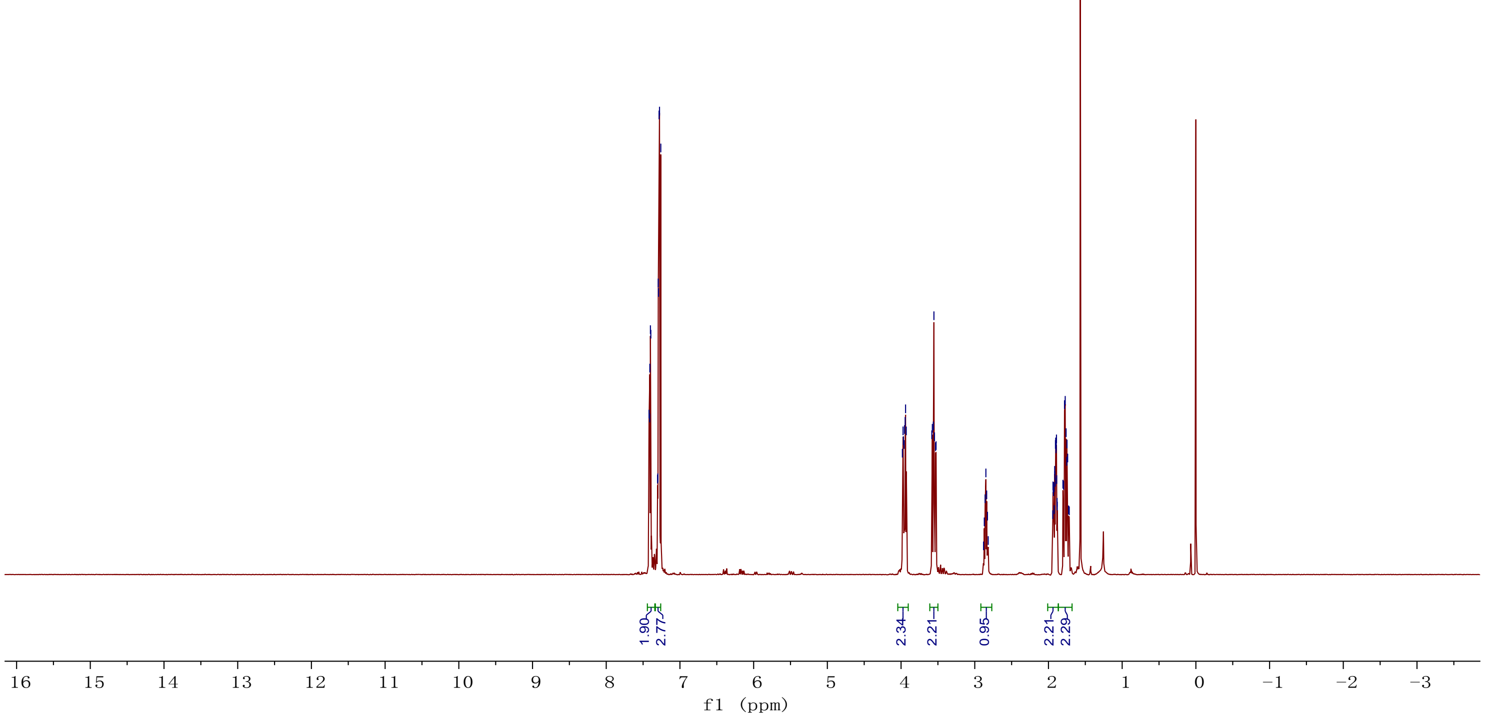

Compound 55 ^{13}C NMR