Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Alkyl/Aryl Carboxylic Acids Meet Sulfur Fluoride (SO_2F_2): A Platform for Decarboxylative Dehydrogenation and Decarboxylative Cross-Coupling

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I. Experimental Section

General Information

All source materials and reagents were purchased from commercial suppliers and are used without pretreatment unless otherwise indicated. All experiments involving palladium were performed using standard Schlenk techniques under nitrogen unless stated otherwise. All results were detected using thin-layer chromatography (TLC) on commercial silica gel plates. Visualization of the developed plates was performed under UV light (254 nm). Rapid column chromatography was performed on silica gel. Column chromatography was performed with silica gel (200-300 mesh) using various combinations of non-aqueous organic solvents as eluents.

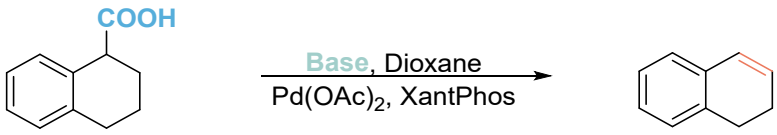
NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on Bruker AVANCE III 400/600 MHz (^{1}HNMR), 101 MHz (^{13}CNMR) and 377 MHz (^{19}FNMR) instruments with TMS as the internal standard and the following abbreviations were used to identify the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, dq = doublet of quartets, br = broad and all combinations thereof can be explained by their integral parts. Coupling constant (J) was reported in hertz unit (Hz). High-resolution mass spectrometry analysis was performed on the ThermoFlisher ITQ1100. Single crystals was selected and on a Bruker D8 VENTURE TXS PHOTON II diffractometer. DFT calculations were performed with Gaussian 16 program.

Reaction Conditions and Screening

General procedure for the optimization of decarboxylative dehydrogenation.

A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid (neat, 0.2 mmol, 1.0 equiv.), base (0.5~5.0 equiv.), Pd catalyst (typically, 5 mol%), ligand (typically, 6 mol%), solvent (0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at room temperature for 4 hours. Then increase to 100°C for 12 h. The mixture was allowed to react. After the reaction is completed, the reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

Table S1. Optimization of decarboxylative dehydrogenation conditions: screening of base[a]

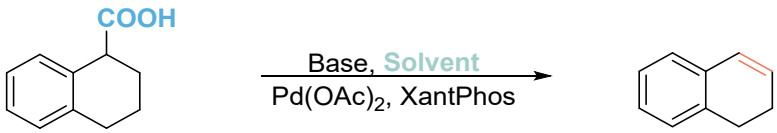


1a' **4a**

Entry	Base (x equiv.)	Yield 4a (%)
1	TEA (4.0)	75
2	DBU (4.0)	n.r.
3	DIPEA (4.0)	69
4	DMAP (4.0)	n.r.
5	DBACO (4.0)	n.r.
6	NaOAc (4.0)	41
7	KOAc (4.0)	59
8	K_3PO_4 (4.0)	28
9	Li^{t}OBu (4.0)	n.r.
10	TEA (5.0)	82
11	TEA (3.0)	77
12	TEA (2.0)	90
13	TEA (1.0)	87
14	TEA (0.5)	81

[a] Reaction conditions: **1a'** (0.2 mmol), **Base (x mmol, x eq.)**, dioxane (0.2 M), $Pd(OAc)_2$ (10 mol%), XantPhos (12 mol%), 45 ºC, 4 h, then 100 ºC, 18.0 h; Under SO_2F_2 gas atmosphere. n.r. = no reaction.

Table S2. Optimization of decarboxylative dehydrogenation conditions: screening of solvent[a]

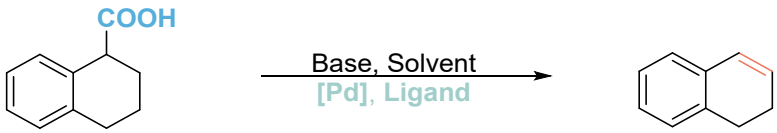


1a' **4a**

Entry	Solvent	Yield 4a (%)
1	Dioxane	90
2	CH_3CN	88
3	CH_3OH	n.r.
4	THF	n.r.
5	Toluene	90
6	DMF	59
7	DMSO	n.r.
8	NMP	n.r.
9	HFIP	n.r.
10	Octane	93
11	DCE	95

[a] Reaction conditions: **1a'** (0.2 mmol), TEA (0.4 mmol, 2 eq.), **Solvent (0.2 M)**, $Pd(OAc)_2$ (10 mol%), XantPhos (12 mol%), 45 ºC, 4 h, then 100 ºC, 18.0 h; Under SO_2F_2 gas atmosphere. n.r. = no reaction.

Table S3. Optimization of decarboxylative dehydrogenation conditions: screening of Pd catalysts and Ligands[a]



1a' **4a**

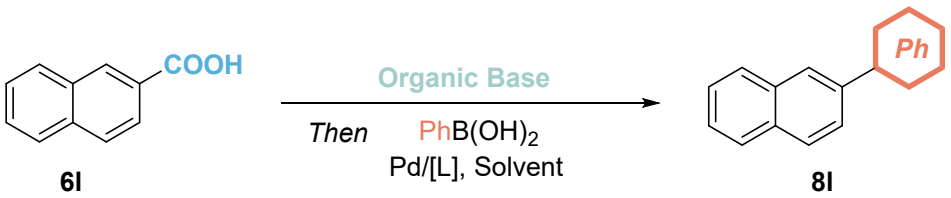
Entry	Pd catalysts (x mol%)	Ligand (x mol%)	Yield 4a[a] (%)
1	$Pd(OAc)_2$ (10)	L17 (12)	95
2	$PdCl_2$ (10)	L17 (12)	n.r.
3	$Pd(acac)_2$ (10)	L17 (12)	n.r.
4	$Pd(dba)_2$ (10)	L17 (12)	87
5	PdTEF (10)	L17 (12)	94
6	$Pd(PPh_3)_4Cl_2$ (10)	L17 (12)	87
7	$Pd(dppf)_2Cl_2$ (10)	L17 (12)	81
8	$Ni(DME)Cl_2$	L17 (12)	n.r.
9	$Cu(OAc)_2$	L17 (12)	n.r.
10	$Pd(OAc)_2$ (10)	L2 (10)	n.r.
11	$Pd(OAc)_2$ (10)	L6 (10)	61
12	$Pd(OAc)_2$ (10)	L7 (10)	52
13	$Pd(OAc)_2$ (10)	L11 (10)	73
14	$Pd(OAc)_2$ (10)	L13 (10)	90
15	$Pd(OAc)_2$ (10)	L19 (10)	65
16	$Pd(OAc)_2$ (10)	L22 (10)	57
17	$Pd(OAc)_2$ (5)	L17 (6)	96
18	$Pd(OAc)_2$ (2)	L17 (3)	81
19[b]	$Pd(OAc)_2$ (5)	L17 (6)	97
20[c]	$Pd(OAc)_2$ (5)	L17 (6)	93

[a] Reaction conditions: **1a'** (0.2 mmol), TEA (0.4 mmol, 2 eq.), DCE (0.2 M), **[Pd] (x mol%), Ligand (x mol%)**, 45 ºC, 4 h, then 100 ºC, 18.0 h; Under SO_2F_2 gas atmosphere. n.r. = no reaction. [b] 12.0 h instead of 18.0 h. [c] Reacts at 100°C for 12 h.

General procedure for the optimization of decarboxylative dehydrogenation.

A 25 mL Schlenk flask equipped with a stirring bar is filled with Arylcarboxylic acid (neat, 0.2 mmol, 1.0 equiv.), base (1.0~7.0 equiv.), solvent (1~2 mL). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45°C for few hours. After the reaction is completed, the reaction bottle is purged with nitrogen. Then a one-time addition Pd catalyst (typically, 6 mol%), ligand (typically, 8 mol%), arylboronic acid (1.0~3.0 equiv.), additives (0~2.0 equiv.), solvent (0~1 mL). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The mixture was allowed to react at T °C. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

Table S4. Optimization of decarboxylative cross-coupling conditions: screening of base[a]

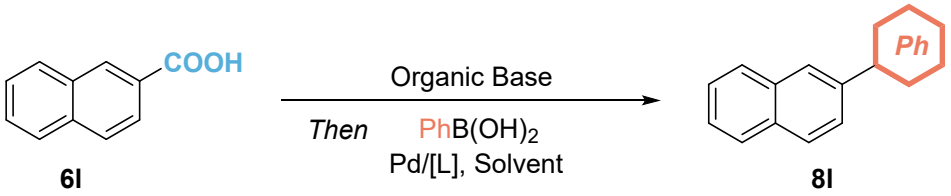


6l **8l**

Entry	Base (x equiv.)	Yield 8l (%)
1	DIPEA (3.0)	47
2	DBU (3.0)	10
3	TEA (3.0)	50
4	DMAP (3.0)	30
5	pyridine (3.0)	n.r.
6	^{t}BuONa (3.0)	n.r.
7	KF (3.0)	n.r.
8	CsF (3.0)	n.r.
9	TEA (1.0)	34
10	TEA (2.0)	37
11	TEA (4.0)	52
12	TEA (5.0)	47
13	TEA (7.0)	45

[a] Reaction conditions: **6l** (0.2 mmol), **Base (x mmol, x eq.)**, dioxane (0.2 M), 45 °C, 4 h, under SO_2F_2 gas atmosphere. Then add $PhB(OH)_2$ (0.4 mmol, 2.0 eq.), $Pd(OAc)_2$ (6 mol%), Ruphos (8 mol%), dioxane (0.2 M), 110 °C, 18.0 h; Under nitrogen atmosphere. n.r.=no reaction.

Table S5. Optimization of decarboxylative cross-coupling conditions: screening of time-1[a]

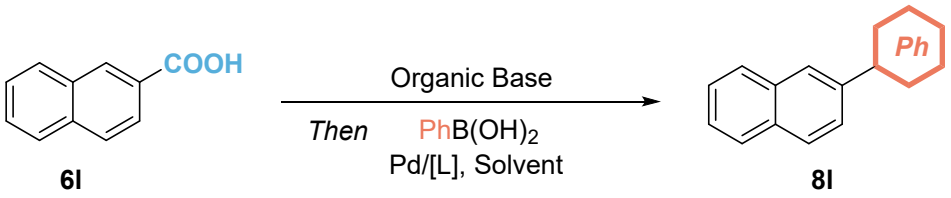


6l **8l**

Entry	Time-1 (h)	Yield 8l (%)
1	1.0	39
2	2.0	41
3	4.0	52
4	8.0	51

[a] Reaction conditions: **6l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), dioxane (0.2 M), 45 ºC, **x h**, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.4 mmol, 2.0 eq.), $Pd(OAc)_2$ (6 mol%), Ruphos (8 mol%) , dioxane (0.2 M), 110 ºC, 18.0 h; Under nitrogen atmosphere.

Table S6. Optimization of decarboxylative cross-coupling conditions: screening of temperature-2[a]

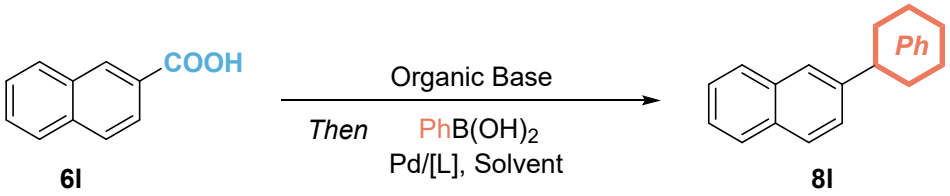


6l **8l**

Entry	Temperature-2 (ºC)	Yield 8l (%)
1	r.t.	trace
2	80	49
3	90	46
4	100	52
5	110	52
6	140	39

[a] Reaction conditions: **1l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), dioxane (0.2 M), 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.4 mmol, 2.0 eq.), $Pd(OAc)_2$ (6 mol%), Ruphos (8 mol%), dioxane (0.2 M), **x ºC**, 18.0 h; Under nitrogen atmosphere.

Table S7. Optimization of decarboxylative cross-coupling conditions: screening of [B] equivale.[a]

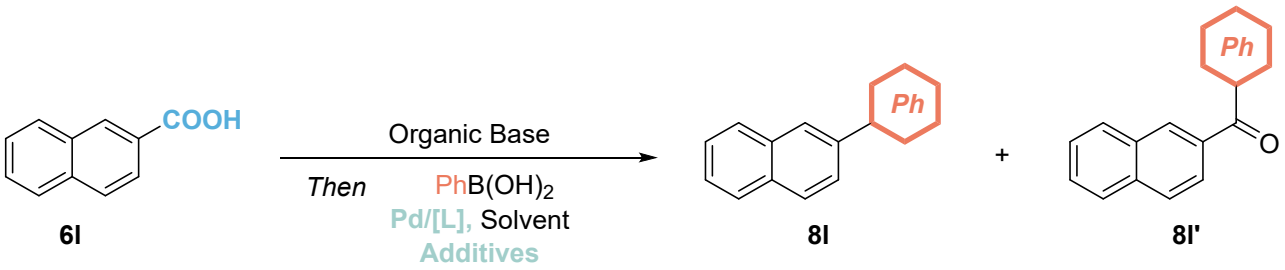


6l **8l**

Entry	[B] source (x equiv.)	Yield 8l (%)
1	$PhB(OH)_2$ (1.0)	30
2	$PhB(OH)_2$ (1.5)	39
3	$PhB(OH)_2$ (2.0)	52
4	$PhB(OH)_2$ (3.0)	56

[a] Reaction conditions: **1l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), dioxane (0.2 M), 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition **[B] (x mmol, x eq.)**, $Pd(OAc)_2$ (6 mol%), Ruphos (8 mol%) , dioxane (0.2 M), 100 ºC, 18.0 h; Under nitrogen atmosphere.

Table S8. Optimization of decarboxylative cross-coupling conditions: screening of Pd/Ligand and additives.[a]

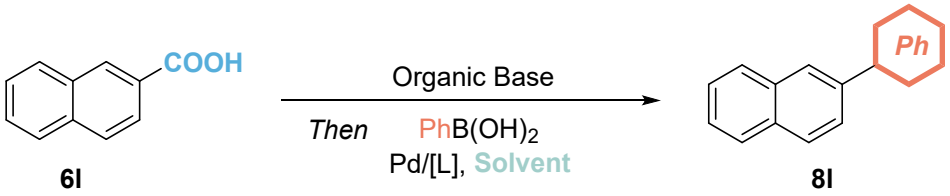


6l 8l 8l'

Entry	Pd (x mol%)	[L] (x mol%)	Additives (x mol%)	Yield 8l (%)	Yield 8l' (%)
1	$Pd(OAc)_2$ (6)	L1 (8)	-	12	14
2	$Pd(OAc)_2$ (6)	L2 (8)	-	22	22
3	$Pd(OAc)_2$ (6)	L3 (8)	-	28	22
4	$Pd(OAc)_2$ (6)	L4 (8)	-	n.r.	n.r.
5	$Pd(OAc)_2$ (6)	L5 (8)	-	7	n.r.
6	$Pd(OAc)_2$ (6)	L6 (8)	-	56	13
7	$Pd(OAc)_2$ (6)	L7 (8)	-	13	14
8	$Pd(OAc)_2$ (6)	L8 (8)	-	15	n.r.
9	$Pd(OAc)_2$ (6)	L9 (8)	-	39	20
10	$Pd(OAc)_2$ (6)	L10 (8)	-	29	16
11	$Pd(OAc)_2$ (6)	L11 (8)	-	40	19
12	$Pd(OAc)_2$ (6)	L12 (8)	-	n.r.	n.r.
13	$Pd(OAc)_2$ (6)	L13 (8)	-	39	n.r.
14	$Pd(OAc)_2$ (6)	L14 (8)	-	n.r.	n.r.
15	$Pd(OAc)_2$ (6)	L15 (8)	-	33	n.r.
16	$Pd(OAc)_2$ (6)	L16 (8)	-	43	11
17	$Pd(OAc)_2$ (6)	L17 (8)	-	73	13
18	$Pd(OAc)_2$ (6)	L18 (8)	-	48	9
19	$Pd(OAc)_2$ (6)	L19 (8)	-	30	n.r.
20	$Pd(OAc)_2$ (6)	L20 (8)	-	25	n.r.
21	$Pd(OAc)_2$ (6)	L21 (8)	-	34	n.r.
22	$Pd(OAc)_2$ (6)	L22 (8)	-	47	n.r.
23	$Pd(OAc)_2$ (6)	L23 (8)	-	43	19
24	$Pd(OAc)_2$ (6)	L24 (8)	-	21	13
25	$Pd(OAc)_2$ (6)	L25 (8)	-	23	10
26	$Pd(OAc)_2$ (6)	L26 (8)	-	n.r.	n.r.
27	$PdCl_2$ (6)	L17 (8)	-	10	n.r.
28	$Pd(acac)_2$ (6)	L17 (8)	-	64	11
29	$Pd(dba)_2$ (6)	L17 (8)	-	n.r.	n.r.
30	$Pd(TEF)_2$ (6)	L17 (8)	-	54	17
31	$Pd(OAc)_2$ (3)	L17 (6)	-	63	9
32	$Pd(OAc)_2$ (10)	L17 (15)	-	68	20
33	$Pd(OAc)_2$ (6)	L17 (8)	CuBr (10)	72	15
34	$Pd(OAc)_2$ (6)	L17 (8)	$Cu(OTf)_2$ (10)	78	2

[a] Reaction conditions: **6l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), dioxane (0.2 M), 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.6 mmol, 3.0 eq.), **[Pd] (x mol%), [L] (x mol%), Additives (10 mol%)**, dioxane (0.2 M), 100 ºC, 18.0 h; Under nitrogen atmosphere. n.r.=no reaction.

Table S9. Optimization of decarboxylative cross-coupling conditions: screening of solvent[a]



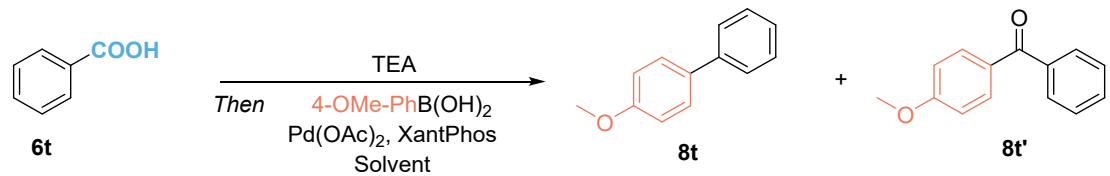
6l **8l**

Entry	Solvent-1 (x M)	Solvent-2 (x M)	Yield 8l (%)
1	ACN (0.2)	ACN (0.2)	NR
2	DMF (0.2)	dioxane (0.2)	10
3	DMSO (0.2)	dioxane (0.2)	NR
4	ACN (0.2)	dioxane (0.2)	25
5	ACN (0.2)	octane (0.2)	34
6	ACN (0.2)	fluorobenzene (0.2)	NR
7	dioxane (0.2)	dioxane (0.2)	78
8	dioxane (0.2)	-	65
9	THF (0.2)	-	50
10	octane (0.2)	-	54
11	heptane (0.2)	-	53
12	hexane (0.2)	-	44
13	MBTE (0.2)	-	38
14	toluene (0.2)	-	NR
15	xylol (0.2)	-	NR
16[b]	ACN (0.2)	-	37
17[b]	octane (0.2)	-	66
18[b]	ACN: dioxane=0.5:0.5 (0.2)	-	50
19[b]	dioxane:octane=8:2 (0.2)	-	72
20[b]	dioxane:octane=5:5 (0.2)	-	80
21[b]	dioxane:octane=3:7 (0.2)	-	87
22[b]	dioxane:octane=2:8 (0.2)	-	86
23[b]	dioxane:octane=1:9 (0.2)	-	85

[a] Reaction conditions: **6l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), **Solvent-1 (x M)**, 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.6 mmol, 3.0 eq.), $Pd(OAc)_2$ (6 mol%), Ruphos (8 mol%) , **Solvent-2 (x M)**, 100 ºC, 18.0 h; Under nitrogen atmosphere. NR=no reaction.

[b] Reaction conditions: **6l** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), **Solvent-1 (x M)**, 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.6 mmol, 3.0 eq.), $Pd(OAc)_2$ (6 mol%), XantPhos (8 mol%), $Cu(OTf)_2$ (10 mol%), 100 ºC, 18.0 h; Under nitrogen atmosphere.

Table S10. Optimization of decarboxylative cross-coupling conditions: screening of additive [a]

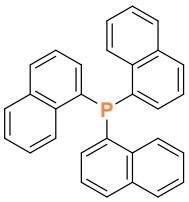


Entry	Additives	Yield 8t (%)	Yield 8t' (%)
1	CuBr	40	22
2	CuI	39	23
3	$CuBr_2$	40	34
4	$Cu(acac)_2$	36	32
5	$Cu(OAc)_2$	70	5
6	$Cu(OTf)_2$	77	0
7	Ag_2CO_3	11	15
8	AgOAc	15	11
9	AgOTf	21	15
10	$Co(OTf)_2$	44	35
11	$In(OTf)_3$	0	0
12	$Al(OTf)_3$	48	30
13	$Ba(OTf)_2$	43	37
14	$Ca(OTf)_2$	41	38
15	$Zn(OTf)_2$	46	34

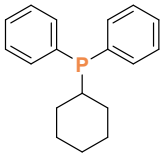
[a] Reaction conditions: **6t** (0.2 mmol), TEA (0.8 mmol, 4.0 eq.), octane : dioxane = 7 : 3 (0.2 M), 45 ºC, 4 h, under SO_2F_2 gas atmosphere. Then addition $PhB(OH)_2$ (0.6 mmol, 3.0 eq.), $Pd(OAc)_2$ (6 mol%), XantPhos (8 mol%), additive (10 mol%), 100 ºC, 18.0 h; Under nitrogen atmosphere.

List of ligands used.

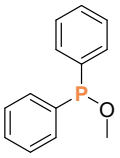
Monodentate phosphine



L1



L2



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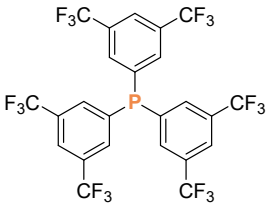
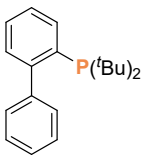
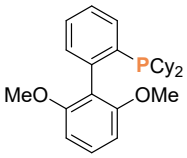


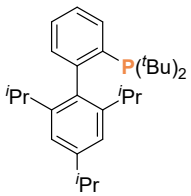
L4



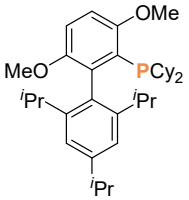
L5



L6

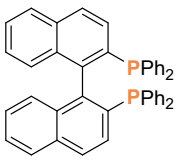


L7

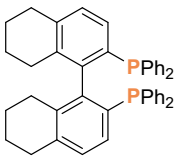


L8

Bidentate phosphine



L9



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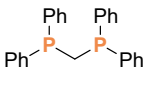

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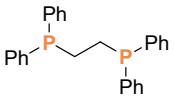

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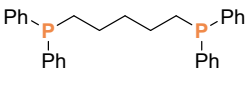

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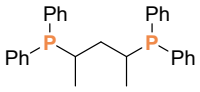

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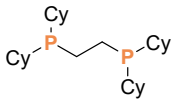

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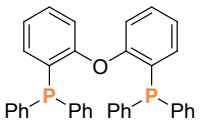

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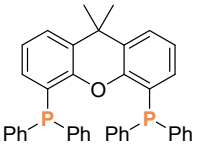

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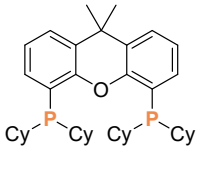

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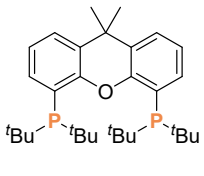

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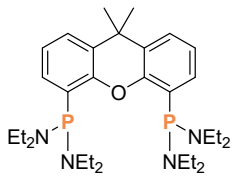

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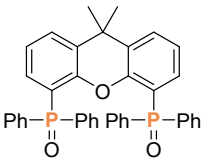

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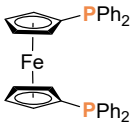
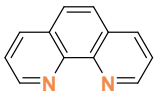


L22

Nitrogen containing ligand



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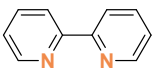
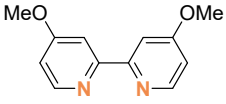
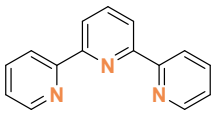


L24

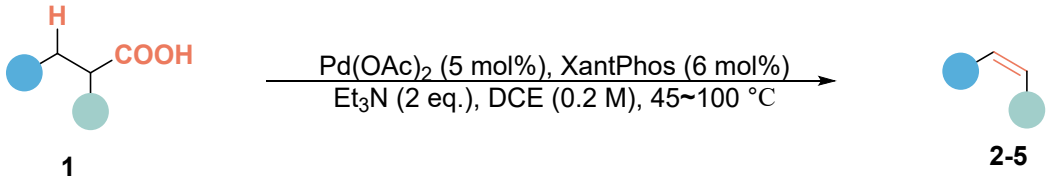


L25



L26

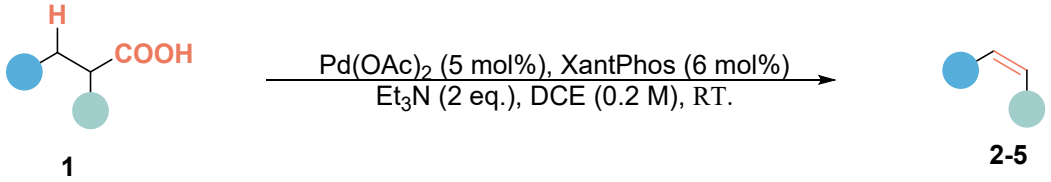
General procedure for decarboxylative dehydrogenation (standard conditions 1).



1 **2-5**

A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid **1** (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 4~8 hours. After the reaction is completed, the reaction bottle is purged with nitrogen. Then heat up to 100 ºC. The mixture was allowed to react for 12 h. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

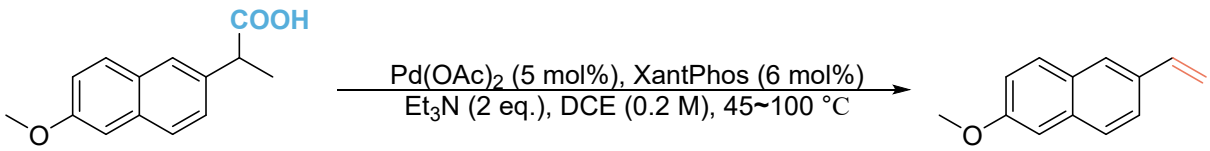
General procedure for decarboxylative dehydrogenation at room temperature.



1 **2-5**

A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid **1** (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 8 hours. After the reaction is completed, the reaction bottle is purged with nitrogen. Then heat up to 25 ºC. The mixture was allowed to react for 24 h. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

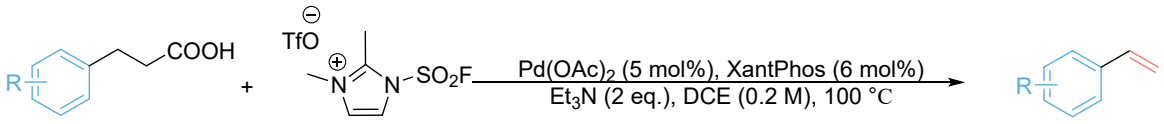
General procedure for decarboxylative dehydrogenation on a gram scale.



10 mmol **5e, 77%(1.42 g)**

A 25 mL Schlenk flask equipped with a stirring bar is filled with naproxen (neat, 10 mmol, 2.3 g), Et_3N (20 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (30 mL). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 12 hours under positive pressure of SO_2F_2 balloon. After the reaction is completed, the reaction bottle is purged with nitrogen. Then heat up to 100 ºC. The mixture was allowed to react for 12 h. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

General procedure for solid sulfuryl fluoride reagent-mediated decarboxylative dehydrogenation.

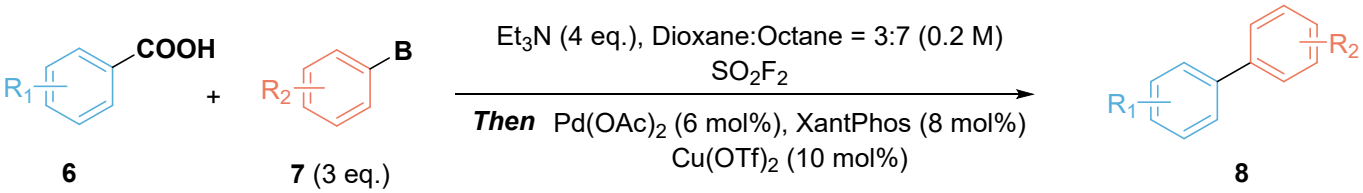


R = OMe **(1b)**
CN **(1h)**

2b, 92%
2h, 81%

A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid **1** (neat, 0.2 mmol, 1.0 equiv.), fluorosulfuryl imidazolium salt (0.4 mmol, 2.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (1 mL, 0.2 M). The heat up to 100 ºC. The mixture was allowed to react for 16 h. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

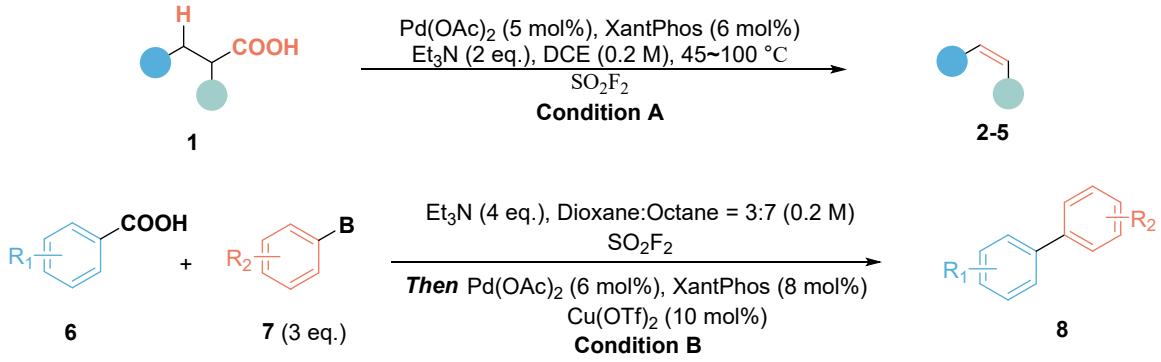
General procedure for decarboxylative cross-coupling (standard conditions 2).

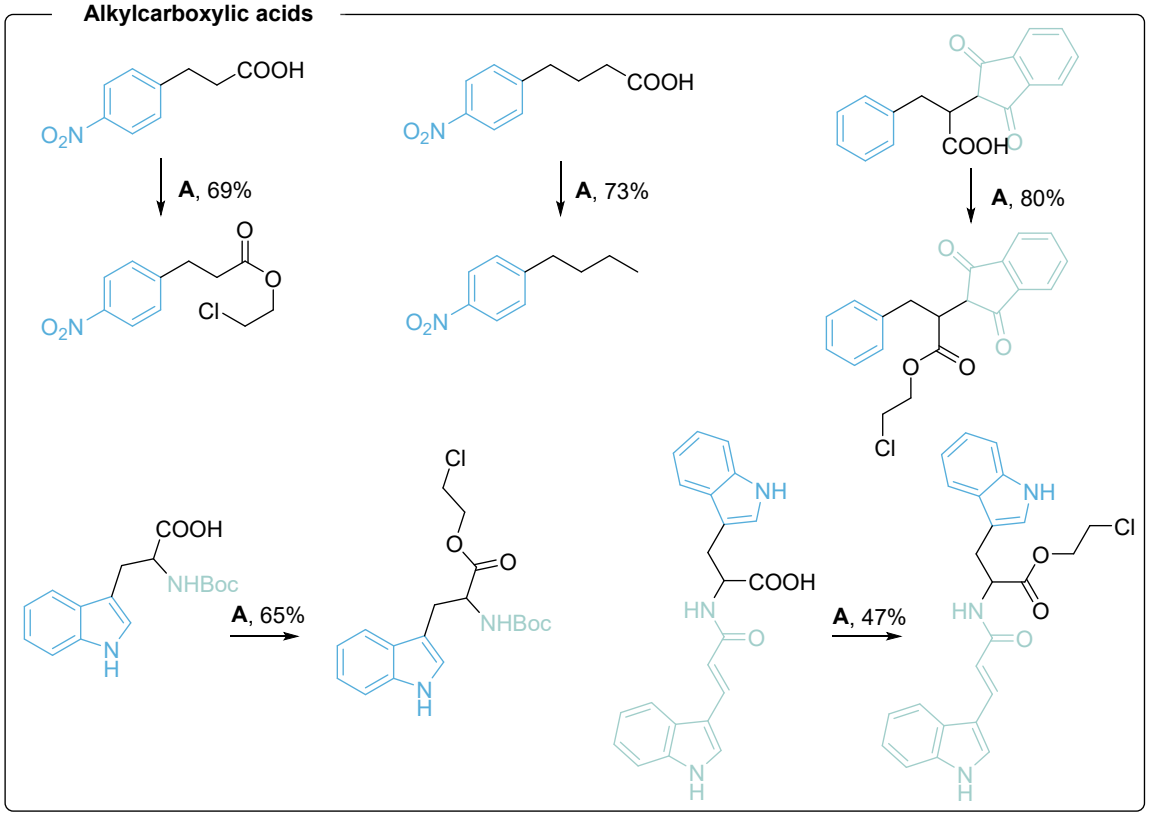


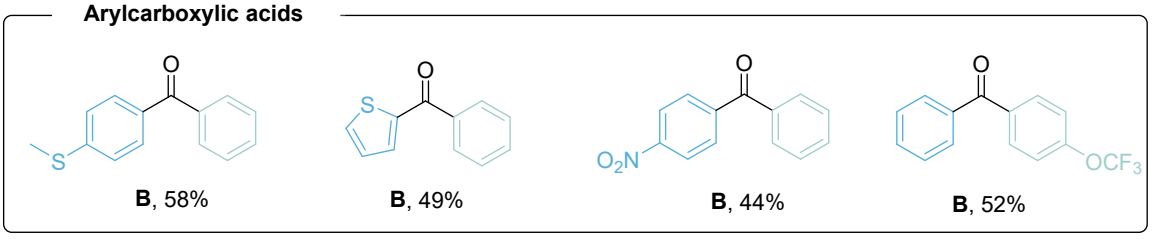
6 **7** (3 eq.) **8**

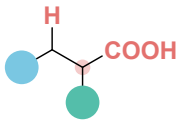
A 25 mL Schlenk flask equipped with a stirring bar is filled with Arylcarboxylic acid **6** (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.8 mmol, 4.0 equiv.), dioxane:octane=3:7 (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at room temperature for 4 hours. After the reaction is completed, the reaction bottle is purged with nitrogen. Then a one-time addition $Pd(OAc)_2$ catalyst (6 mol%), XantPhos (8 mol%), Arylboronic acid **7** (0.6 mmol, 3.0 equiv.), $Cu(OTf)_2$ (10 mol%). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The mixture was allowed to react for 18 h. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

Unsuccessful substrates



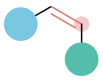




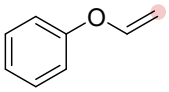


1S

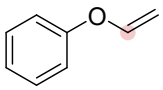
Condition A



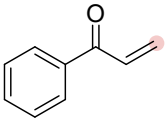
3S



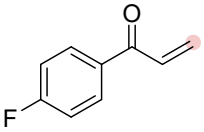
1S-a



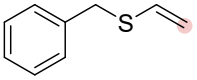
1S-b



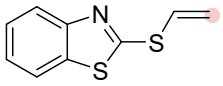
1S-c



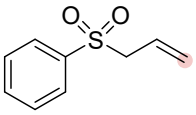
1S-d



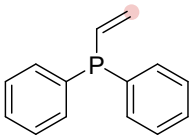
1S-e



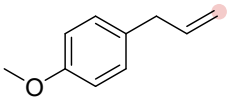
1S-f



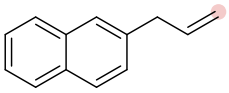
1S-g



1S-h



1S-i



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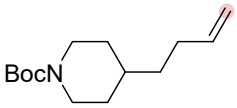
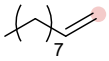
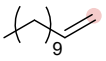


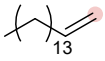
1S-k



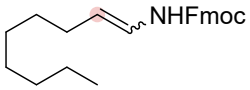
1S-l



1S-m

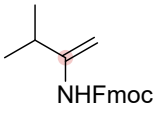


1S-n

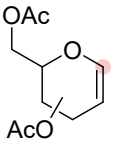


1S-o

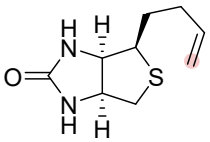
1S-p



1S-q



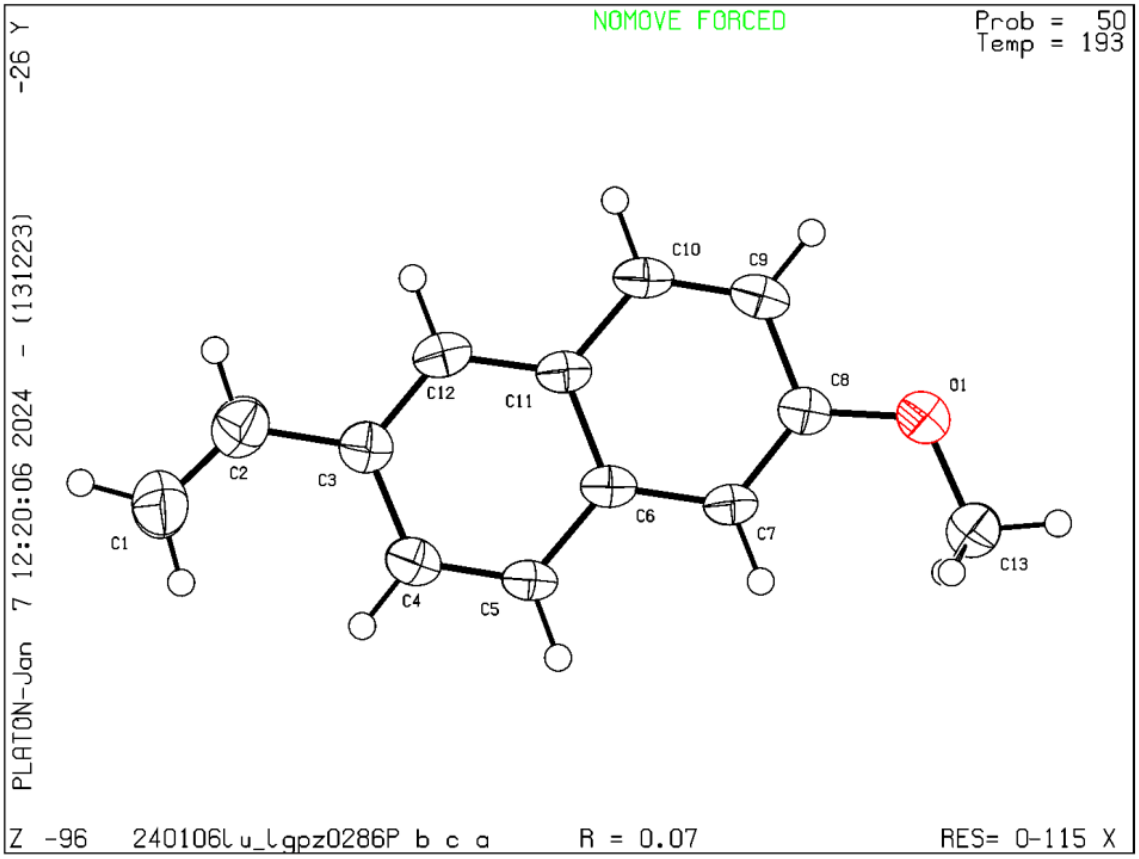
1S-r



1S-s

Sample (5e) Preparation for X-ray

For compound 5e: compound 5e (10 mg) was dissolved in ethyl acetate (0.5 mL) in a 10 mL vial at room temperature. Hexane (3.0 mL) was dropped carefully to the mixture. Then, the vial was capped with thin film. Finally, a lamellar crystal was obtained for 4 days.

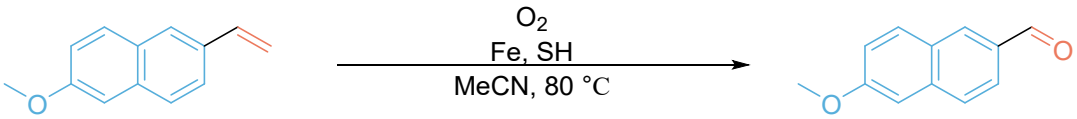


Crystal data and structure refinement for compound 5e.

Identification code	**5e**
CCDC number	2327303
Empirical formula	$C_{13}H_{12}O$
Formula weight	184.23
Temperature/K	193.00
Crystal system monoclinic	orthorhombic
Space group	Pbca
a/Å	5.9974(4)
b/Å	8.0073(6)
c/Å	41.526(3)
α/°	90
β/°	90
γ/°	90
Volume/Å3	1994.2(2)
Z	8
ρcalcg/cm3	1.227
μ/mm-1	0.076
F(000)	784.0

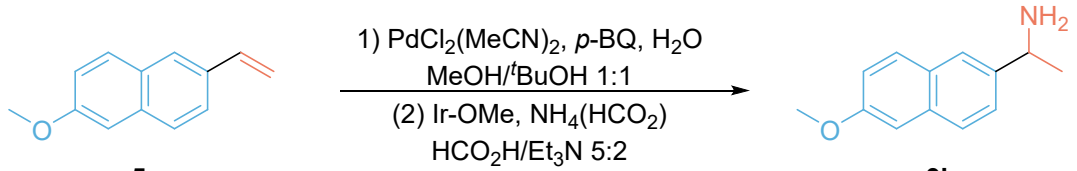
Crystal size/mm3	0.12 × 0.1 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.886 to 55.25
Index ranges	$-7 \leq h \leq 7$, $-10 \leq k \leq 10$, $-44 \leq l \leq 54$
Reflections collected	16218
Independent reflections	2311 [Rint = 0.0793, Rsigma = 0.0461]
Data/restraints/parameters	2311/0/129
Goodness-of-fit on F2	1.051
Final R indexes [I>=2σ (I)]	$R_1 = 0.0697$, $wR_2 = 0.1678$
Final R indexes [all data]	$R_1 = 0.1070$, $wR_2 = 0.1913$
Largest diff. peak/hole / e Å-3	0.31/-0.20

Synthetic Applications



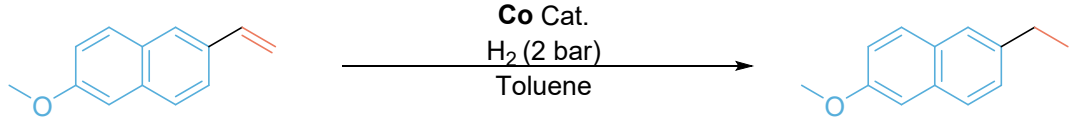
5e **9a**

Experimental procedure for the synthesis of 9a from 5e: A 25 mL Schlenk flask equipped with a stirring bar is filled with 1,1'-bis(diphenylphosphino)ferrocene (dppf) (16.6 mg, 0.03 mmol, 0.1 equiv) and bismuththiol (4.5 mg, 0.03 mmol, 0.1 equiv). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. Then 5e (0.30 mmol, 1 equiv) and anhydrous MeCN (0.5 mL) were added. The reaction mixture was heated to 80 ºC and allowed to react for 15 h. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.[1]



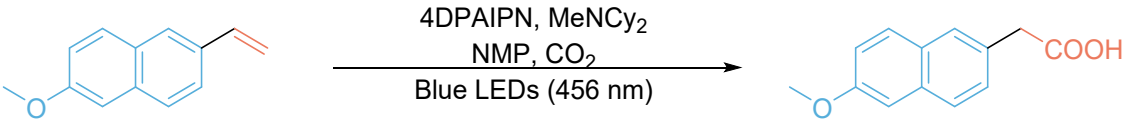
5e **9b**

Experimental procedure for the synthesis of 9b from 5e: A 25 mL Schlenk flask equipped with a stirring bar is filled with MeOH (3.6 mL), *t*BuOH (3.6 mL), $PdCl_2(MeCN)_2$ (1.6 mg, 0.006 mmol), *p*-benzoquinone (0.0973 g, 0.9 mmol), H_2O (27 µL) and the 5e (0.60 mmol). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The reaction mixture was heated to 70 ºC and allowed to react for 3 h. Then $HCOONH_4$ (380 mg, 6 mmol), Ir-OMe (3.7 mg, 0.006 mmol), and formic acid/triethylamine (5:2) complex (0.6 mL) were added. The mixture was stirred at 70 °C for another 8 h. The mixture was evaporated and NaHCO3 was added. The reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.[2]



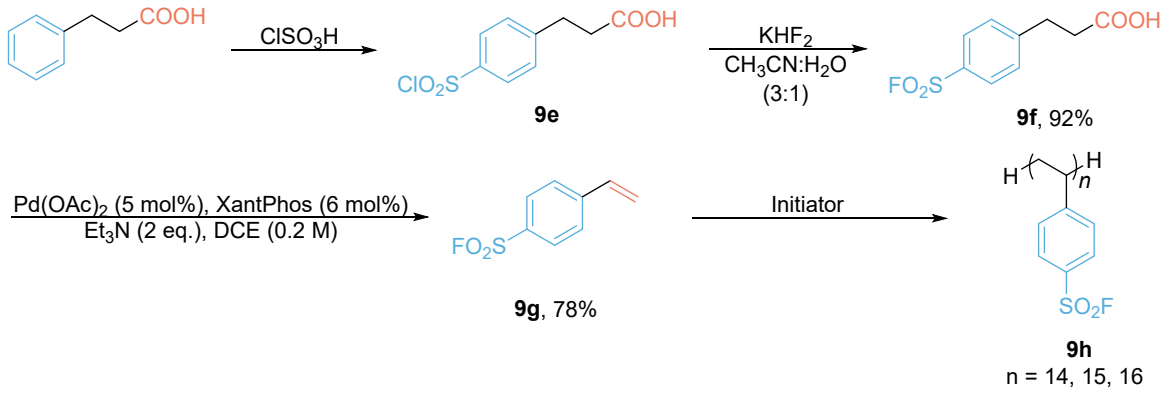
5e **9c**

Experimental procedure for the synthesis of 9c from 5e: A dry 5 mL vial with a screw cap and PTFE septum was charged with a magnetic stirrer bar and a solution of the potassium bis(anthracene)cobaltate (0.05 mmol) in Toluene (1 mL). After adding a solution of the 5e (0.5 mmol) in Toluene (1 mL) with a pipette, the vial was closed and the septum was punctured with a short needle. The vial was placed into a high-pressure reactor, which was sealed. After 6 h at room temperature under an atmosphere of hydrogen (2 bar), the pressure was released, the vial was removed, and the reaction was quenched with a saturated aqueous solution of $NaHCO_3$ (1 mL). The residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent. [3]



5e **9d**

Experimental procedure for the synthesis of 9d from 5e: A 25 mL Schlenk flask equipped with a stirring bar is filled with 5e (0.2 mmol, 1.0 equiv.) and 4DPAIPN (2.4 mg, 0.003 mmol). Under a positive pressure of CO_2 and five evacuations/backfilling cycles under high vacuum. Then anhydrous NMP (2.0 mL) and *N, N*-dicyclohexylmethylamine (0.3 mmol, 58.5 mg, 64 µL) were added. After that, under a positive pressure of CO_2 and five evacuations/backfilling cycles under high vacuum. The mixture was irradiated with a 40 W 456 nm Kessil LED (3 cm away, with a cooling fan to keep the reaction temperature at room temperature). After 24 hours, the reaction was quenched with HCl (2N) and extracted by ethyl acetate for 5 times. The combined organic layers were washed with brine and concentrated in vacuo. The residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent. [4]

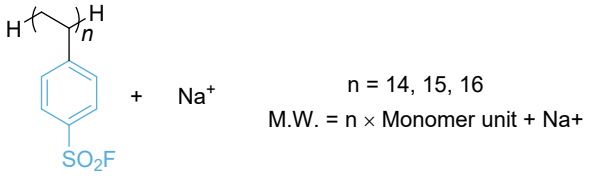


Experimental procedure for the synthesis of 9e: phenylpropanoic acid (22.5 g, 150 mmol, 1.0 eq.) was taken in a round bottle flask, and cooled to 10-15 °C. Chlorosulfonic acid (100 mL) was added to the reaction mass slowly in a dropwise manner at below 15 °C. The reaction mixture was stirred at 10-15 °C for 1 h slowly allowed to warm to room temperature and stirred for 2-3 h. The reaction mixture was added to cold water (300 mL) slowly in a dropwise manner at below 20 °C. The resulting mixture was allowed to room temperature, stirred for 2-3 h, filtered, washed with water (100 mL), and dried for 1 h. The wet product was dissolved in CH_2Cl_2 (500 mL) and washed with water (100 mL) followed by brine (100 mL). The organic layer was dried over Na_2SO_4 and concentrated to up to 100 mL. *n*-Hexane (200 mL) was added to the reaction mass at room temperature, and the resulting mixture was stirred for 1 h, filtered, and washed with n-hexane (100 mL). The wet product was taken into a round bottom flask, and dried at 40-45 °C under vacuum to give 12.3 g of 2-(4(chlorosulfonyl)phenyl)propanoic acid 9e (yellow solid, 49.5 mmol, 33% yield). [5]

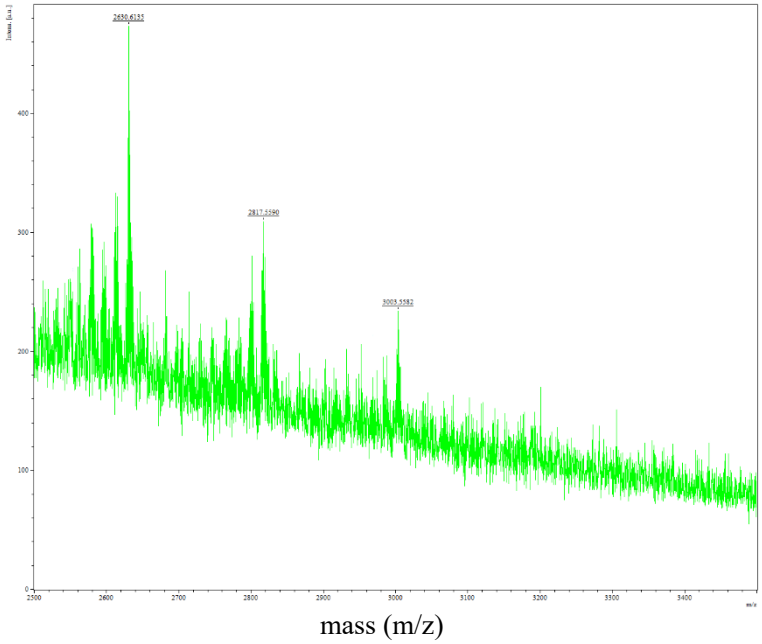
Experimental procedure for the synthesis of 9f: KHF_2 (42.5 mmol, 2.5 equiv.) was dissolved in H_2O (7 mL) to make a saturated solution, which was treated with a solution of 9e (17 mmol, 1 equiv.) in acetonitrile (20 mL). The reaction mixture was stirred at room temperature for 4-10 hours and was measured by HPLC. The aqueous phase was extracted with EtOAc (3 × 10 mL) and the combined organic extracts were washed with 10% NaCl aqueous solution (2x), saturated sodium chloride (1x), dried with sodium sulfate, filtered, and concentrated by rotary evaporation to obtain the crude product, which was purified by column chromatography on silica gel to obtain the pure product 9f (black solid, 3.6 g, 15.6 mmol, 92% yield). [6]

Experimental procedure for the synthesis of 9h: 0.6 g 4-vinylphenol sulfurofluoridate and 10 mg AIBN were added to a 25 mL round-bottomed flask containing 5 mL of DMSO. Then the flask was sealed and cycled between vacuum and argon three times before the reaction was allowed to stir at 85 ºC

for 24 h. Then, the mixture was washed petroleum ether (3 x 100 mL). The resulting polymer 9h was obtained. [7]



9h

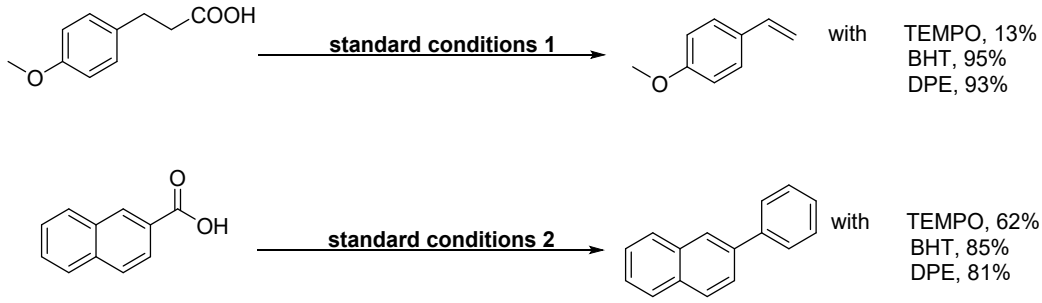


mass (m/z)

Figure S1. MALDI-TOF mass spectrum of **9h**.

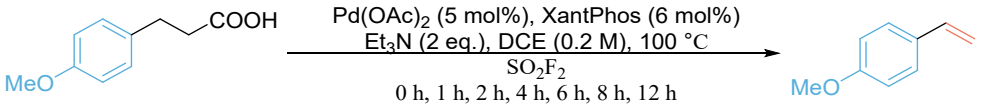
Mechanism Experiments

1. Free radical inhibition experiment.



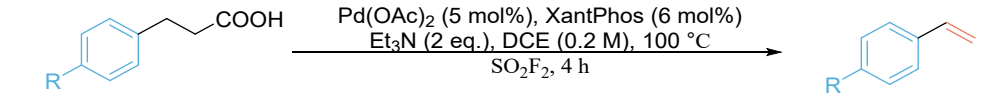
Free radical inhibitors 2,2,6,6-Tetramethylpiperidoxyl (TEMPO, 2.0 equiv.) or Butylated hydroxytoluene (BHT, 2.0 equiv.) or 1,1-Diphenylethene (DPE) (2.0 equiv.) were added to the reaction programme under standard conditions, respectively, and the yields were observed by ^{1}H NMR after completion of the reaction (1,3,5-trimethoxybenzene was used as an internal standard).

2. Reaction rate experiments.



A 25 mL Schlenk flask equipped with a stirring bar is filled with 4-Methoxyphenylpropionic acid (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 8 hours. After the reaction is completed, the reaction bottle is purged with nitrogen. Then heat up to 100 ºC. The mixture was allowed to react for 0 h, 1 h, 2 h, 4 h, 6 h, 8 h or 12 h. After completion of the reaction 0.5 mL of reaction solution was taken and mixed with the internal standard (1,3,5-Trimethoxybenzene) and the yield was detected by ^1H NMR. NMR analysis was used to determine the 4-nitrostyrene concentration and yields at the various timepoints.

3. Hammett Competition Experiments.



R = OMe, Me, H, F, Cl, CN

Procedure for Hammett Competition Experiments. A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 8 hours. The reaction bottle is purged with nitrogen. After $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%) were added. Then heat up to 100 ºC. The mixture was allowed to react for 4 h. After completion of the reaction 0.5 mL of reaction solution was taken and mixed with the internal standard (1,3,5-Trimethoxybenzene) and the yield was detected by ^1H NMR. A crude NMR spectrum of the residue was obtained in 0.6 mL $CDCl_3$.

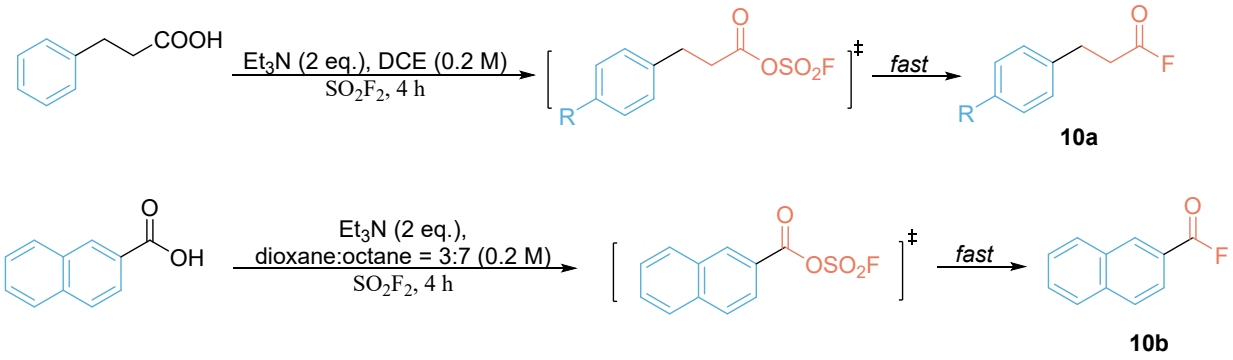
Data Analysis. ^1H NMR yield of each product was obtained by integration of the aromatic peak of the 1,3,5-trimethoxybenzene internal standard (6.08 ppm) and the product resonances. After the yields of each product were obtained by NMR spectroscopy, the ratios of substituted product (P_R, R = Ome, Me, F, Cl, CN) to unsubstituted product (P_H, R = H) were determined (P_R/P_H) and the logarithm of these value was calculated for use in the Hammett plot ($\log(P_R/P_H)$). The data was fit using the substituent constants, σ_p.

Table S11. Data for Hammett competition experiments

Entry	Substitution	Average (P_R/P_H)	Average $\log(P_R/P_H)$	σ_p
1	OMe	1.18	0.072	-0.27
2	Me	1.05	0.021	-0.17
3	H	1.00	0	0
4	F	0.95	-0.022	0.06
5	Cl	0.75	-0.125	0.23
6	CN	0.35	-0.456	0.66

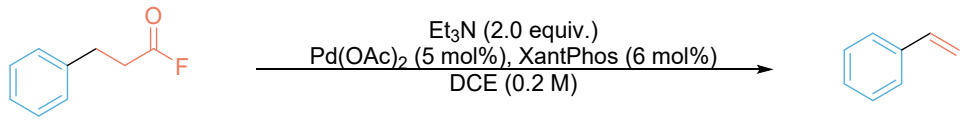
Entries 1-6 are comprised of an average of 3 trials each.

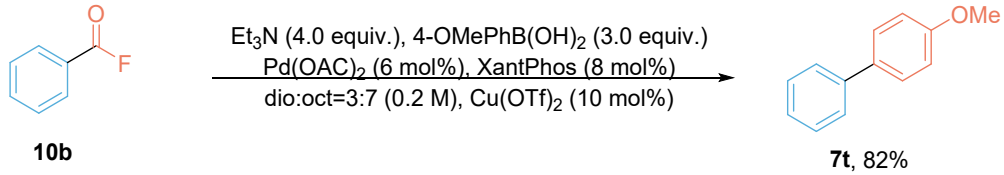
4. Possible intermediates.



Preparation of alkylcarboxylic acid activation intermediate 10a. A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid **1m** (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 4 hours. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

Preparation of arylcarboxylic acid activation intermediate 10b. A 25 mL Schlenk flask equipped with a stirring bar is filled with Arylcarboxylic acid **6l** (neat, 0.2 mmol, 1.0 equiv.), Et_3N (0.8 mmol, 4.0 equiv.), dioxane:octane=3:7 (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at room temperature for 4 hours. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

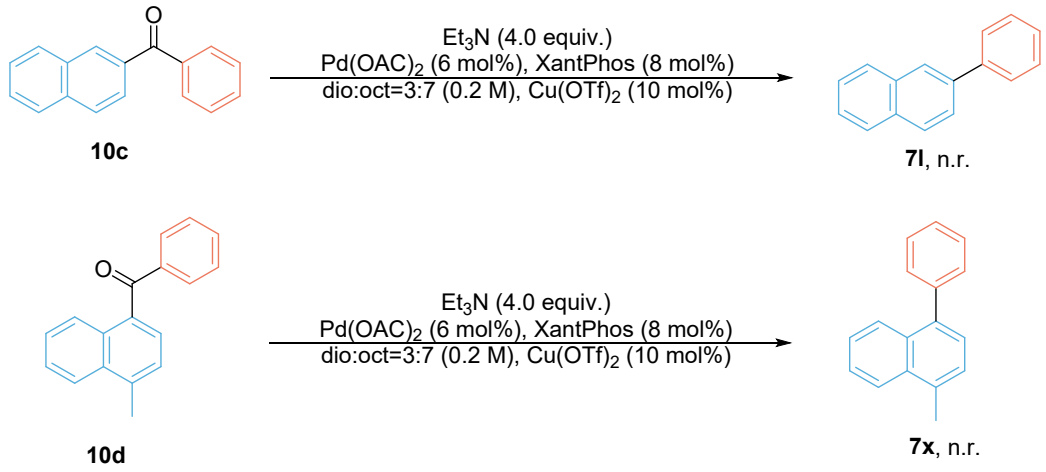




Experimental procedure for the preparation of 2m from intermediate 10a. A 25 mL Schlenk flask equipped with a stirring bar is filled with **10a** (0.2 mmol, 1.0 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%), dichloroethane (1 mL, 0.2 M). Then heat up to 100 ºC. The mixture was allowed to react for 12 h. The reaction was quenched with water and the reaction mixture was extracted with dichloromethane for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

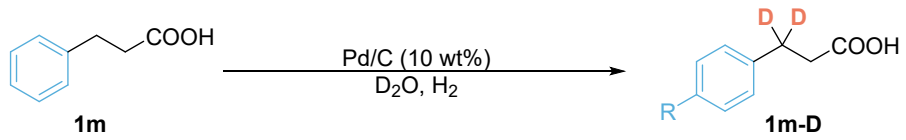
Experimental procedure for the preparation of 7t from intermediate 10b. A 25 mL Schlenk flask equipped with a stirring bar is filled with **10b** (0.2 mmol, 1.0 equiv.), Et_3N (0.8 mmol, 4.0 equiv.),

$Pd(OAc)_2$ catalyst (6 mol%), XantPhos (8 mol%), 4-methoxyphenylboronic acid (0.6 mmol, 3.0 equiv.), $Cu(OTf)_2$ (10 mol%), and dioxane:octane=3:7 (1 mL, 0.2 M). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The mixture was allowed to react for 18 h. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

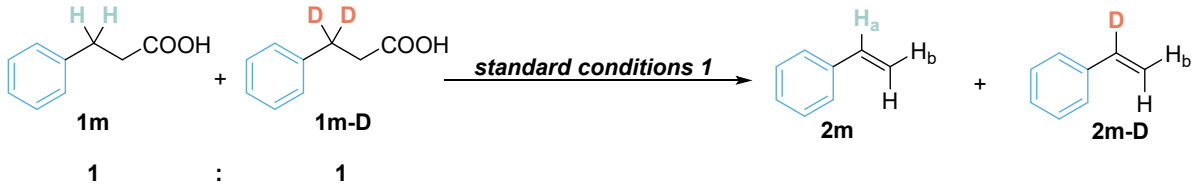


Experimental procedure for the preparation of 7l or 7x from intermediate 10c or 10d. A 25 mL Schlenk flask equipped with a stirring bar is filled with **10c** or **10d** (0.2 mmol, 1.0 equiv.), Et_3N (0.8 mmol, 4.0 equiv.), $Pd(OAc)_2$ catalyst (6 mol%), XantPhos (8 mol%), $Cu(OTf)_2$ (10 mol%), and dioxane:octane=3:7 (1 mL, 0.2 M). Under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The mixture was allowed to react for 18 h. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by a flash column chromatography on silica gel using ethyl acetate and petroleum as eluent.

5. Kinetic Isotope Effect Experiments.



Preparation of deuterated substrate 1m-D. A 25 mL Schlenk flask equipped with a stirring bar is filled with alkylcarboxylic acid **1m** (neat, 0.5 mmol, 1.0 equiv.), 10%Pd/C (7.5 mg, 10 wt%), heavy water (1 mL, 0.5 M). Under positive pressure of H_2, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 55 ºC for 24 hours. The reaction was quenched with water and the reaction mixture was extracted with ethyl acetate for three times. The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuum to give the product **1m-D** (D content 92%, ^{1}H NMR analysis was used to determine D content).[8]



Procedure for Kinetic Isotope Effect from Parallel Reactions. A 25 mL Schlenk flask equipped with a stirring bar is filled with 1m (0.1 mmol, 0.5 equiv.), 1m-D (0.1 mmol, 0.5 equiv.), Et_3N (0.4 mmol, 2.0 equiv.), dichloroethane (1 mL, 0.2 M). Under positive pressure of SO_2F_2 gas, five evacuation/backfill cycles are performed under high vacuum to fill the reaction tube and vigorous stirring at 45 ºC for 8 hours. The reaction bottle is purged with nitrogen. After $Pd(OAc)_2$ (5 mol%), XantPhos (6 mol%) were added. Then heat up to 100 ºC. The mixture was allowed to react for 4 h. After completion of the reaction 0.5 mL of reaction solution was taken and mixed with the internal standard (1,3,5-Trimethoxybenzene, 0.1 mmol) and the deuterated product content was detected by ^{1}H NMR. A crude NMR spectrum of the residue was obtained in 0.6 mL $CDCl_3$.

Data Analysis. After Fourier transform of the FID, an auto-baseline correction protocol was applied to the spectra and the spectra were manually integrated. The integration values of the aromatic peak of the methyl 1,3,5-Trimethoxybenzene standard (6.00 ppm, single-peak) and the H_b proton of the styrene product (5.17 ppm) were used to calculate the concentration of product (2m and 2m-D) in the reaction. Subsequently, based on the ratio of the peak areas of the two products ($P(Ha)/P(H_b\text{-}H_a)$), a KIE of 2.7 was obtained. (Calculated by taking the average of five experiments.)

Computational Details

DFT calculations were performed with Gaussian 16[9] program. All molecular geometries were optimized in gas phase at the B3LYP[10] /6-31G(d)[11] (SDD[12] basis set for Pd and Cu) level of theory at 298.15 K&337.15K and 1 atm with Grimme's D3[13] dispersion correction using SMD[14] as the solvation mode in Octane. Optimized minima and transition states (TSs) were verified by harmonic vibrational analysis to have no and one proper imaginary frequency, respectively. To refine calculated energies, single point calculations with larger basis set 6-311G(d,p)[15] were then performed based on these optimized structures by using the same B3LYP-D3BJ functional with SMD[14] as the solvation mode in Octane.

Table S12: Summary of barriers to each key step in acyl fluoride formation.

Barrier	Substrate (kcal/mol)
$Ph(C=O)OSO_2F$	103.6
Ph(C=O)F	102.9

Table S13: Summary of the barriers for each key step in the catalytic cycle.

Barrier	Substrate (kcal/mol)
Oxidative addition	13.1
Decarbonylation from Ph-[Pd^{II}]-(C=O)(F)	7.8
Transmetallisation	31.8
Reductive elimination	45.2

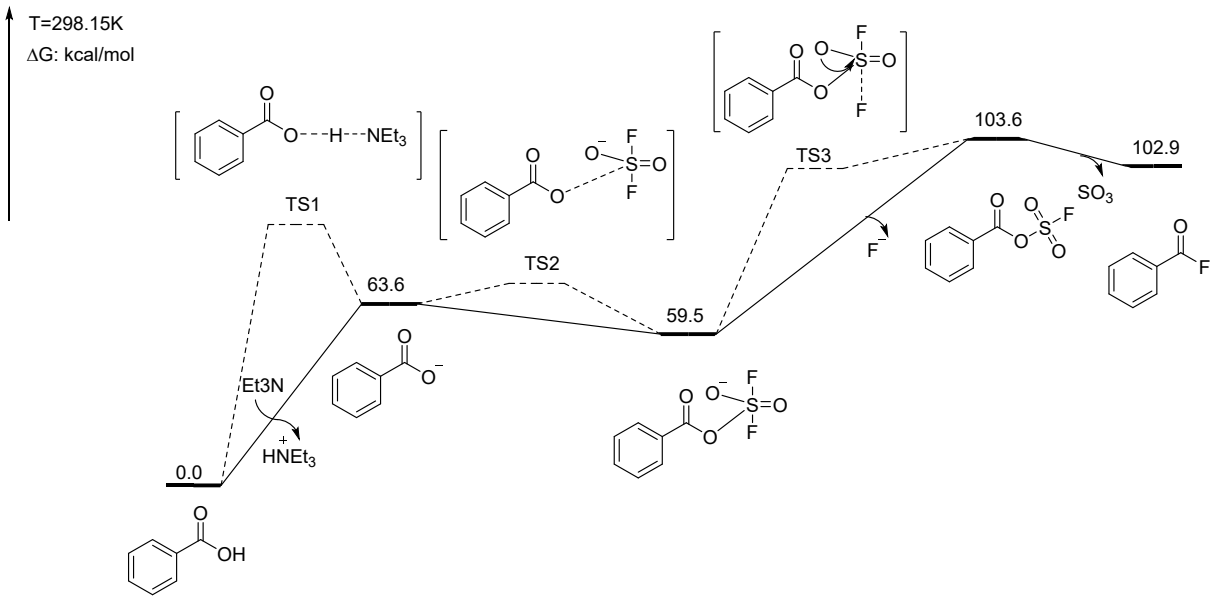


Figure S2. DFT calculations of aryl carboxylic acids activated by SO_2F_2.

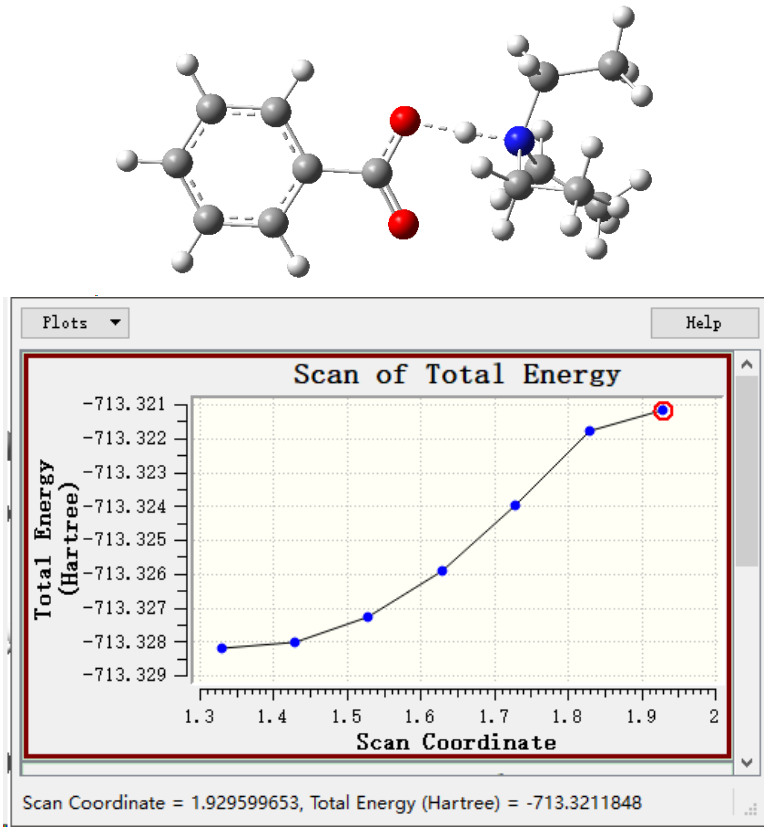
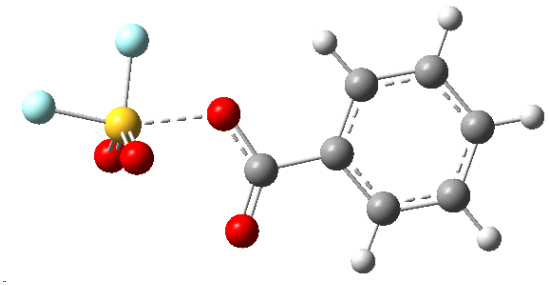


Figure S3. TS1s.log.



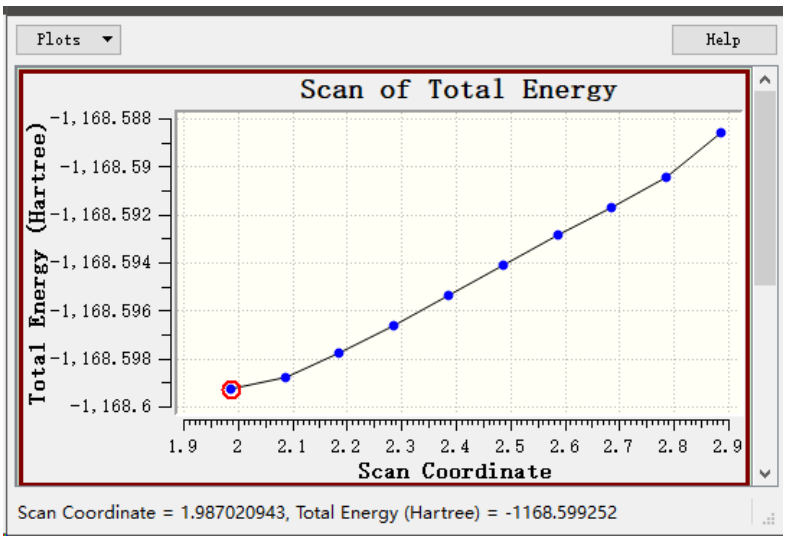


Figure S4. TS2s.log.

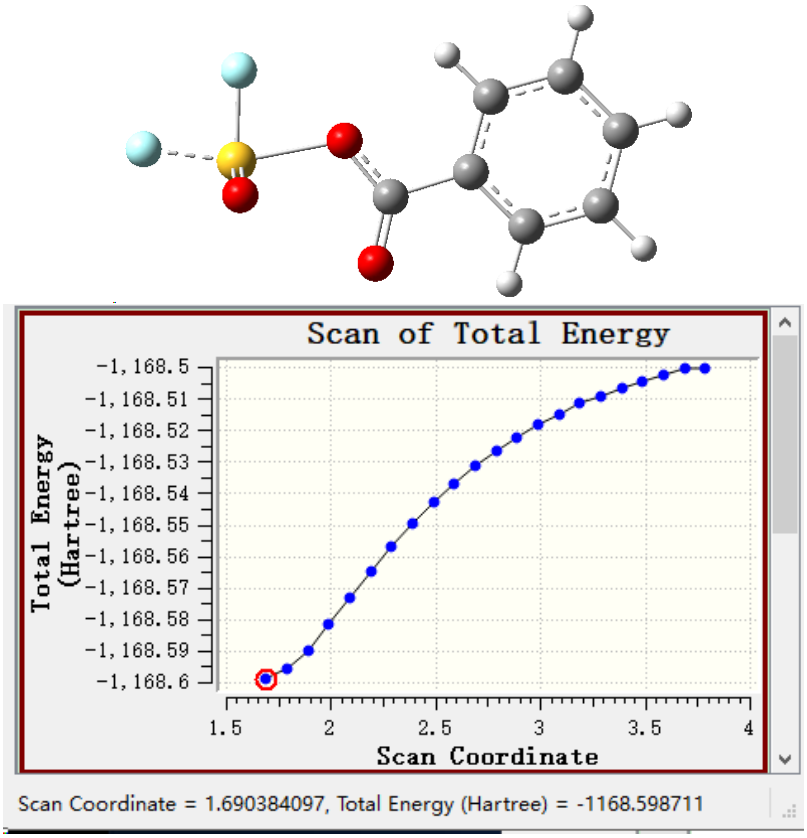
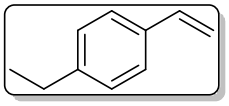


Figure S5. TS3s.log.

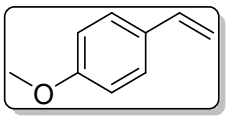
II. Experimental Characterization Data

Alkenylation Products of Alkyl Carboxylic Acids.



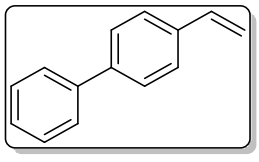
1-ethyl-4-vinylbenzene (2a)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Colourless oil, 93% yield, 24.6 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.1 Hz, 2H), 7.17 (d, J = 8.1 Hz, 2H), 6.70 (dd, J = 17.6, 10.9 Hz, 1H), 5.71 (d, J = 17.6 Hz, 1H), 5.19 (d, J = 10.9 Hz, 1H), 2.65 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.07, 136.73, 135.08, 128.05, 126.20, 112.87, 28.64, 15.61.
HRMS (EI-TOF) calcd for $C_{10}H_{12}$: 132.0939; Found：132.0940.
NMR spectroscopic data agreed with literature values.[16]



1-methoxy-4-vinylbenzene (2b)

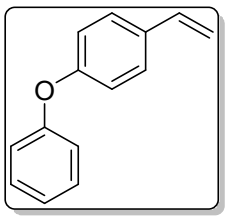
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 99% yield, 26.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.8 Hz, 2H), 6.89 (d, J = 8.8 Hz, 2H), 6.69 (dd, J = 17.6, 10.9 Hz, 1H), 5.64 (d, J = 17.6 Hz, 1H), 5.15 (d, J = 10.9 Hz, 1H), 3.84 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.36, 136.22, 130.44, 127.40, 111.60, 55.32.
HRMS (EI-TOF) calcd for $C_9H_{10}O$: 134.0732; Found：134.0735.
NMR spectroscopic data agreed with literature values.[16]



4-vinyl-1,1'-biphenyl (2c)

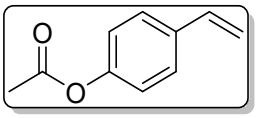
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). white solid, 97% yield, 26.0 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, J = 12.7, 7.7 Hz, 4H), 7.51 (d, J = 7.4 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 7.3 Hz, 1H), 6.89 – 6.69 (m, 1H), 5.82 (d, J = 17.6 Hz, 1H), 5.31 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.77, 140.62, 136.63, 136.44, 128.82, 127.35, 127.27, 127.01, 126.68, 113.94.
HRMS (EI-TOF) calcd for $C_9H_{10}O$: 134.0732; Found：134.0735.
NMR spectroscopic data agreed with literature values.[17]



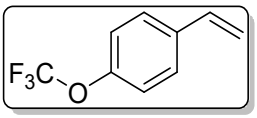
1-phenoxy-4-vinylbenzene (2d)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). Colourless oil, 94% yield, 36.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.34 (m, 4H), 7.18 (t, J = 7.4 Hz, 1H), 7.10 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 8.6 Hz, 2H), 6.77 (dd, J = 17.6, 10.9 Hz, 1H), 5.74 (d, J = 17.6 Hz, 1H), 5.27 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.24, 157.09, 136.14, 132.93, 129.88, 127.70, 123.45, 119.03, 118.96, 112.95.
HRMS (EI-TOF) calcd for $C_{14}H_{12}O$: 196.0888; Found：196.0889.
NMR spectroscopic data agreed with literature values.[18]



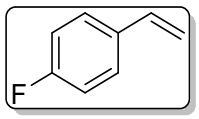
4-vinylphenyl acetate (2e)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 81% yield, 26.3 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.6 Hz, 2H), 7.05 (d, J = 8.6 Hz, 2H), 6.70 (dd, J = 17.6, 10.9 Hz, 1H), 5.70 (d, J = 17.6 Hz, 1H), 5.24 (d, J = 10.9 Hz, 1H), 2.30 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.50, 150.20, 135.90, 135.40, 127.20, 121.64, 114.07, 21.16.
HRMS (EI-TOF) calcd for $C_{10}H_{10}O_2$: 162.0681; Found：162.0686.
NMR spectroscopic data agreed with literature values.[19]



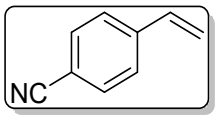
1-(trifluoromethoxy)-4-vinylbenzene (2f)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 83% yield, 31.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, J = 8.8 Hz, 2H), 7.17 (d, J = 8.5 Hz, 2H), 6.70 (dd, J = 17.5, 10.9 Hz, 1H), 5.73 (d, J = 17.6 Hz, 1H), 5.29 (d, J = 11.0 Hz, 1H).
^{19}F NMR (377 MHz, $CDCl_3$) δ -57.86.
HRMS (EI-TOF) calcd for $C_9H_7F_3O$: 188.0449; Found：188.0450.
NMR spectroscopic data agreed with literature values.[17]



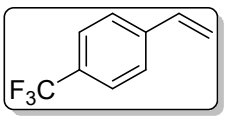
1-fluoro-4-vinylbenzene (2g)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Colourless oil, 87% yield, 21.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, J = 8.9, 5.4 Hz, 2H), 7.07 (t, J = 8.7 Hz, 2H), 6.74 (dd, J = 17.6, 10.9 Hz, 1H), 5.73 (d, J = 17.5 Hz, 1H), 5.28 (d, J = 11.0 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 163.76, 161.31, 135.75, 133.80 (d, J = 2.9 Hz), 127.79 (d, J = 8.0 Hz), 115.44 (d, J = 21.1 Hz), 113.52 (d, J = 2.2 Hz).
^{19}F NMR (377 MHz, $CDCl_3$) δ -114.25.
HRMS (EI-TOF) calcd for C_8H_7F: 122.0532; Found：122.0536.
NMR spectroscopic data agreed with literature values.[17]



4-vinylbenzonitrile (2h)

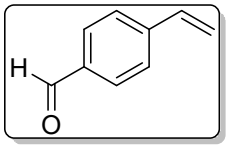
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). yellow oil, 96% yield, 24.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 6.72 (dd, J = 17.6, 10.9 Hz, 1H), 5.87 (d, J = 17.5 Hz, 1H), 5.44 (d, J = 11.0 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.90, 135.37, 132.41, 126.76, 118.95, 117.77, 111.11.
HRMS (EI-TOF) calcd for C_9H_7N: 129.0578; Found：129.0577.
NMR spectroscopic data agreed with literature values.[21]



1-(trifluoromethyl)-4-vinylbenzene (2i)

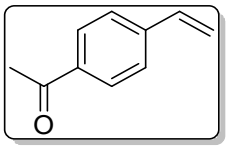
Reaction performed according to condition 1; purified by chromatography on silica gel

(Petroleum ether). Colourless oil, 99% yield, 34.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 6.75 (dd, J = 17.6, 10.9 Hz, 1H), 5.85 (d, J = 17.6 Hz, 1H), 5.39 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.94, 135.64, 129.87 (q, J = 32.3 Hz), 126.40, 125.51 (q, J = 4.0 Hz), 123.01, 116.50.
^{19}F NMR (377 MHz, $CDCl_3$) δ -62.51.
HRMS (EI-TOF) calcd for $C_9H_7F_3$: 172.0500; Found：172.0505.
NMR spectroscopic data agreed with literature values.[16]



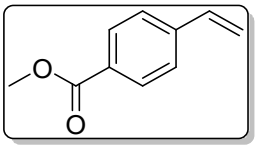
4-vinylbenzaldehyde (2j)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 90% yield, 23.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 7.83 (d, J = 8.3 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 6.76 (dd, J = 17.6, 10.9 Hz, 1H), 5.90 (d, J = 17.6 Hz, 1H), 5.43 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 191.70, 143.43, 135.88, 135.66, 130.08, 126.74, 117.46.
HRMS (EI-TOF) calcd for C_9H_8O: 132.0575; Found：132.0575.
NMR spectroscopic data agreed with literature values.[21]



1-(4-vinylphenyl)ethan-1-one (2k)

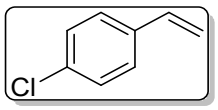
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). yellow solid, 84% yield, 24.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 6.76 (dd, J = 17.6, 10.9 Hz, 1H), 5.88 (d, J = 17.6 Hz, 1H), 5.40 (d, J = 10.9 Hz, 1H), 2.60 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 197.63, 142.10, 136.29, 135.94, 128.74, 126.32, 116.76, 26.64.
HRMS (EI-TOF) calcd for $C_{10}H_{10}O$: 146.0732; Found：146.0732.
NMR spectroscopic data agreed with literature values.[21]



methyl 4-vinylbenzoate (2l)

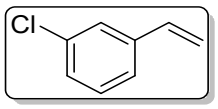
Reaction performed according to condition 1; purified by chromatography on silica gel

(Petroleum ether : Ethyl acetate = 10 : 1). White solid, 65% yield, 21.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 6.74 (dd, J = 17.6, 10.9 Hz, 1H), 5.85 (d, J = 17.5 Hz, 1H), 5.37 (d, J = 11.0 Hz, 1H), 3.90 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.81, 141.90, 136.01, 129.88, 129.27, 126.11, 116.44, 52.04.
HRMS (EI-TOF) calcd for $C_{10}H_{10}O_2$: 162.0681; Found：162.0686.
NMR spectroscopic data agreed with literature values.[21]



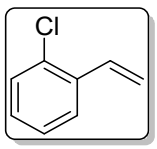
1-chloro-4-vinylbenzene (3a)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Yellow oil, 96% yield, 26.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (q, J = 8.6 Hz, 4H), 6.67 (dd, J = 17.6, 10.9 Hz, 1H), 5.73 (d, J = 17.6 Hz, 1H), 5.27 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.04, 135.68, 133.44, 128.70, 127.45, 114.49.
HRMS (EI-TOF) calcd for C_8H_7Cl: 138.0236; Found：138.0238.
NMR spectroscopic data agreed with literature values.[22]



1-chloro-3-vinylbenzene (3b)

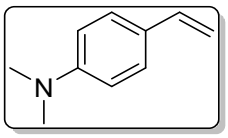
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Yellow oil, 89% yield, 24.6 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 δ 7.43 (s, 1H), 7.27 (t, J = 6.4 Hz, 3H), 6.69 (dd, J = 17.5, 10.9 Hz, 1H), 5.79 (d, J = 17.5 Hz, 1H), 5.34 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 139.46, 135.67, 134.57, 129.79, 127.81, 126.24, 124.52, 115.36.
HRMS (EI-TOF) calcd for C_8H_7Cl: 138.0236; Found：138.0238.
NMR spectroscopic data agreed with literature values.[22]



1-chloro-2-vinylbenzene (3c)

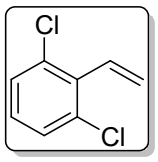
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Yellow oil, 81% yield, 22.4 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 7.6 Hz, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.29 – 7.13 (m, 3H), 5.79 (d, J = 17.6 Hz, 1H), 5.43 (d, J = 11.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.75, 133.23, 133.15, 129.68, 128.85, 126.85, 126.59, 116.56.
HRMS (EI-TOF) calcd for C_8H_7Cl: 138.0236; Found：138.0238.
NMR spectroscopic data agreed with literature values.[22]



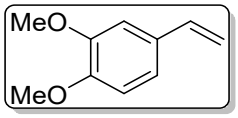
N,N-dimethyl-4-vinylaniline (3d)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow solid, 86% yield, 25.3 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, J = 8.9 Hz, 2H), 6.81 – 6.66 (m, 3H), 5.63 (d, J = 17.6 Hz, 1H), 5.11 (d, J = 10.9 Hz, 1H), 3.03 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.33, 136.71, 127.23, 126.28, 112.40, 109.40, 40.57.
HRMS (EI-TOF) calcd for $C_{10}H_{13}N$: 147.1048; Found：147.1058.
NMR spectroscopic data agreed with literature values.[21]



1,3-dichloro-2-vinylbenzene (3e)

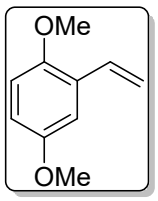
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Yellow oil, 64% yield, 22.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.0 Hz, 2H), 7.11 (t, J = 8.1 Hz, 1H), 6.75 (dd, J = 17.9, 11.7 Hz, 1H), 5.88 – 5.72 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.05, 134.29, 130.93, 128.44, 128.25, 122.94.
HRMS (EI-TOF) calcd for $C_8H_6Cl_2$: 171.9847; Found：171.9850.
NMR spectroscopic data agreed with literature values.[22]



1,2-dimethoxy-4-vinylbenzene (3f)

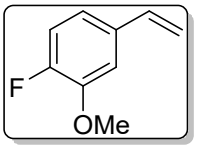
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 5 : 1). Yellow oil, 92% yield, 30.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 – 6.91 (m, 2H), 6.82 (d, J = 8.1 Hz, 1H), 6.65 (dd, J = 17.5, 10.9 Hz, 1H), 5.62 (d, J = 17.5 Hz, 1H), 5.15 (d, J = 10.8 Hz, 1H), 3.91 (s, 3H), 3.88 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.01, 148.97, 136.50, 130.73, 119.47, 111.84, 111.01, 108.49, 55.94, 55.83.

HRMS (EI-TOF) calcd for $C_{10}H_{12}O_2$: 164.0837; Found：164.0841.
NMR spectroscopic data agreed with literature values.[17]



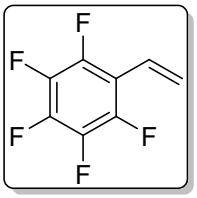
1,4-dimethoxy-2-vinylbenzene (3g)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 5 : 1). Yellow solid, 99% yield, 32.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 – 6.93 (m, 2H), 6.80 (d, J = 4.4 Hz, 2H), 5.73 (dt, J = 17.8, 1.2 Hz, 1H), 5.28 (dt, J = 11.1, 1.2 Hz, 1H), 3.80 (d, J = 6.8 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.69, 151.23, 131.52, 127.61, 114.72, 113.80, 112.25, 111.88, 56.26, 55.76.
HRMS (EI-TOF) calcd for $C_{10}H_{12}O_2$: 164.0837; Found：164.0841.
NMR spectroscopic data agreed with literature values.[23]



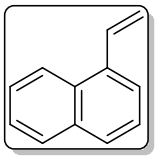
1-fluoro-2-methoxy-4-vinylbenzene (3h)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Pink oil, 73% yield, 22.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03 (dd, J = 10.9, 8.3 Hz, 2H), 6.96 – 6.90 (m, 1H), 6.66 (dd, J = 17.6, 10.9 Hz, 1H), 5.67 (d, J = 17.5 Hz, 1H), 5.23 (d, J = 10.9 Hz, 1H), 3.91 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.46, 151.01, 147.65 (d, J = 10.9 Hz), 136.03, 134.22 (d, J = 4.4 Hz), 119.08 (d, J = 7.3 Hz), 116.07, 115.88, 113.63 (d, J = 2.9 Hz), 110.84 (d, J = 2.2 Hz), 56.17.
^{19}F NMR (377 MHz, $CDCl_3$) δ -136.02.
HRMS (EI-TOF) calcd for C_9H_9FO: 152.0637; Found：152.0631.
NMR spectroscopic data agreed with literature values.



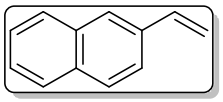
1,2,3,4,5-pentafluoro-6-vinylbenzene (3i)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 51% yield, 19.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.62 (dd, J = 18.1, 11.9 Hz, 1H), 6.07 (d, J = 18.0 Hz, 1H), 5.71 (d, J = 11.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.38 – 145.89 (m), 143.94 – 143.38 (m), 141.63 – 140.97 (m), 139.21 – 138.42 (m), 136.80 – 135.94 (m), 123.49 (td, J = 7.3, 2.9 Hz), 121.35 (d, J = 2.9 Hz), 112.17 (td, J = 13.8, 4.4 Hz).
^{19}F NMR (377 MHz, $CDCl_3$)
HRMS (EI-TOF) calcd for $C_8H_3F_5$: 194.0155; Found：194.0156.
NMR spectroscopic data agreed with literature values.[24]



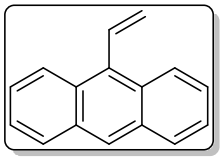
1-vinylnaphthalene (3j)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Colourless oil, 69% yield, 21.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 7.8 Hz, 1H), 7.83 (dd, J = 25.5, 7.9 Hz, 2H), 7.64 (d, J = 7.3 Hz, 1H), 7.57 – 7.38 (m, 4H), 5.80 (d, J = 18.8 Hz, 1H), 5.49 (d, J = 9.5 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.61, 134.39, 133.59, 131.11, 128.52, 128.10, 126.06, 125.76, 125.64, 123.77, 123.63, 117.12.
HRMS (EI-TOF) calcd for $C_{12}H_{10}$: 154.0783; Found：154.0788.
NMR spectroscopic data agreed with literature values.[18]



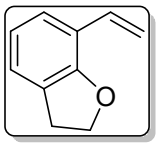
2-vinylnaphthalene (3k)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Colourless oil, 91% yield, 28.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, J = 7.9, 4.7 Hz, 3H), 7.81 (s, 1H), 7.70 (d, J = 8.6 Hz, 1H), 7.65 – 7.38 (m, 2H), 6.94 (dd, J = 17.5, 10.9 Hz, 1H), 5.94 (d, J = 17.5 Hz, 1H), 5.40 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 136.99, 135.06, 133.61, 133.21, 128.20, 128.10, 127.72, 126.44, 126.28, 125.96, 123.23, 114.23.
HRMS (EI-TOF) calcd for $C_{12}H_{10}$: 154.0783; Found：154.0788.
NMR spectroscopic data agreed with literature values.[18]



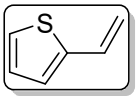
9-vinylanthracene (3l)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Yellow solid, 88% yield, 35.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.38 – 8.28 (m, 2H), 8.08 – 7.96 (m, 2H), 7.57 – 7.45 (m, 5H), 6.03 (d, J = 11.5 Hz, 1H), 5.66 (d, J = 17.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 133.68, 133.57, 131.45, 129.26, 128.63, 126.36, 126.03, 125.39, 125.14, 122.93.
HRMS (EI-TOF) calcd for $C_{16}H_{12}$: 204.0939; Found：204.0944.
NMR spectroscopic data agreed with literature values.[18]



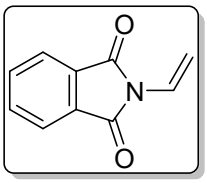
7-vinyl-2,3-dihydrobenzofuran (3m)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 77% yield, 22.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 (t, J = 7.8 Hz, 1H), 7.05 (d, J = 7.8 Hz, 1H), 6.77 (dd, J = 17.2, 9.6 Hz, 2H), 5.77 (d, J = 17.6 Hz, 1H), 5.40 (d, J = 11.1 Hz, 1H), 4.63 (t, J = 8.8 Hz, 2H), 3.29 (t, J = 8.8 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.37, 134.81, 134.46, 128.16, 124.92, 117.78, 115.64, 108.54, 71.08, 29.15.
HRMS (EI-TOF) calcd for $C_{10}H_{10}O$: 146.0732; Found：146.0736.
NMR spectroscopic data agreed with literature values.[25]



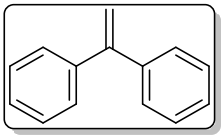
2-vinylthiophene (3n)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). Yellow oil, 86% yield, 18.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (d, J = 4.5 Hz, 1H), 6.97 (d, J = 4.6 Hz, 2H), 6.81 (dd, J = 17.3, 10.8 Hz, 1H), 5.57 (d, J = 17.3 Hz, 1H), 5.14 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.06, 129.87, 127.32, 125.79, 124.33, 113.26.
HRMS (EI-TOF) calcd for C_6H_6S: 110.0190; Found：110.0192.
NMR spectroscopic data agreed with literature values.[21]



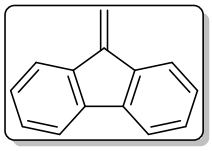
2-vinylisoindoline-1,3-dione (3o)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow solid, 60% yield, 20.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, J = 5.4, 3.1 Hz, 2H), 7.75 (dd, J = 5.6, 3.1 Hz, 2H), 6.88 (dd, J = 16.5, 9.9 Hz, 1H), 6.09 (d, J = 16.4 Hz, 1H), 5.05 (d, J = 9.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.46, 134.49, 131.62, 123.81, 123.64, 104.49.
HRMS (EI-TOF) calcd for $C_{10}H_7NO_2$: 173.0477; Found：173.0480.
NMR spectroscopic data agreed with literature values.[26]



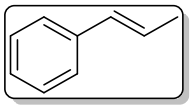
ethene-1,1-diyldibenzene (3p)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 92% yield, 33.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 10H), 5.48 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.08, 141.51, 128.30, 128.19, 127.74, 114.34.
HRMS (EI-TOF) calcd for $C_{14}H_{12}$: 180.0939; Found：180.0939.
NMR spectroscopic data agreed with literature values.[27]



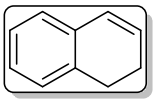
9-methylene-9H-fluorene (3q)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). White solid, 94% yield, 33.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, J = 17.4, 7.4 Hz, 4H), 7.45 (t, J = 7.4 Hz, 2H), 7.41 – 7.32 (m, 2H), 6.14 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 143.43, 140.23, 138.10, 128.80, 127.12, 121.08, 119.82, 107.84.
HRMS (EI-TOF) calcd for $C_{14}H_{10}$: 178.0783; Found：178.0788.
NMR spectroscopic data agreed with literature values.[27]



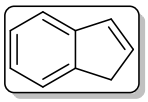
(*E*)-prop-1-en-1-ylbenzene (3r)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether). Colourless oil, 91% yield, 33.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (t, J = 6.8 Hz, 3H), 7.32 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 7.1 Hz, 1H), 6.45 (d, J = 16.0 Hz, 1H), 6.34 – 6.23 (m, 1H), 1.93 (d, J = 6.6 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 137.97, 131.06, 128.50, 126.76, 125.84, 125.72, 18.53.
HRMS (EI-TOF) calcd for C_9H_{10}: 118.0783; Found：118.0780.
NMR spectroscopic data agreed with literature values.[28]



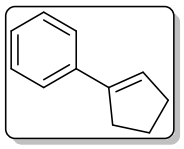
1,2-dihydronaphthalene (4a)

Reaction performed according to condition 1 (130 ºC instead of 100 ºC); purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Colourless oil, 97% yield, 25.2 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (dq, J = 14.6, 7.3 Hz, 3H), 7.24 (d, J = 6.8 Hz, 1H), 6.69 (d, J = 9.6 Hz, 1H), 6.24 (dt, J = 9.3, 4.4 Hz, 1H), 3.01 (t, J = 8.3 Hz, 2H), 2.57 – 2.49 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.64, 134.36, 128.81, 128.07, 127.76, 127.09, 126.67, 126.13, 27.73, 23.44.
HRMS (EI-TOF) calcd for $C_{10}H_{10}$: 130.0783; Found：130.0783.
NMR spectroscopic data agreed with literature values.[29]



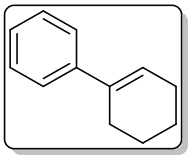
1H-indene (4b)

Reaction performed according to condition 1 (130 ºC instead of 100 ºC); purified by chromatography on silica gel (Petroleum ether). Colourless oil, 92% yield, 21.4 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 1H), 7.66 – 7.59 (m, 1H), 7.55 – 7.47 (m, 1H), 7.47 – 7.37 (m, 1H), 7.11 (s, 1H), 6.77 (s, 1H), 3.59 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.07, 143.88, 134.35, 132.31, 126.47, 124.78, 123.94, 121.19, 39.26.
HRMS (EI-TOF) calcd for C_9H_8: 116.0626; Found：116.0629.
NMR spectroscopic data agreed with literature values.[29]



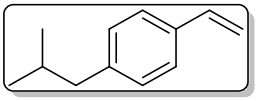
cyclopent-1-en-1-ylbenzene (4c)

Reaction performed according to condition 1 (130 ºC instead of 100 ºC); purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Colourless solid, 69% yield, 19.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.6 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.23 (q, J = 7.8 Hz, 1H), 6.20 (s, 1H), 2.73 (s, 2H), 2.55 (s, 2H), 2.04 (p, J = 7.5 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.45, 136.84, 128.28, 126.83, 126.12, 125.57, 33.37, 33.20, 23.39.
HRMS (EI-TOF) calcd for $C_{11}H_{12}$: 144.0939; Found：144.0944.
NMR spectroscopic data agreed with literature values.[30]



2,3,4,5-tetrahydro-1,1'-biphenyl (4d)

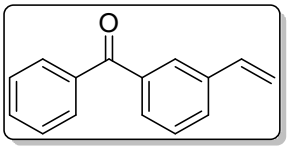
Reaction performed according to condition 1 (130 ºC instead of 100 ºC); purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 30 : 1). Colourless oil, 85% yield, 26.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 7.8 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 7.2 Hz, 1H), 6.20 (s, 1H), 2.49 (s, 2H), 2.28 (s, 2H), 1.85 (q, J = 5.8 Hz, 2H), 1.79 – 1.69 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 142.78, 136.68, 128.26, 126.59, 125.02, 124.83, 27.49, 25.99, 23.18, 22.28.
HRMS (EI-TOF) calcd for $C_{12}H_{14}$: 158.1096; Found：158.1102.
NMR spectroscopic data agreed with literature values.[29]



1-isobutyl-4-vinylbenzene (5a)

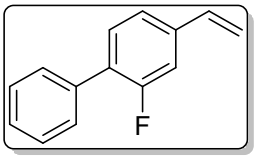
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). Colourless oil, 97% yield, 31.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.1 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 6.72 (dd, J = 17.6, 10.9 Hz, 1H), 5.73 (d, J = 17.6 Hz, 1H), 5.21 (d, J = 10.8 Hz, 1H), 2.48 (d, J = 7.3 Hz, 2H), 1.93 – 1.82 (m, 1H), 0.92 (d, J = 6.6 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.55, 136.78, 135.07, 129.31, 126.00, 112.82, 45.20, 30.27, 22.40.

HRMS (EI-TOF) calcd for $C_{12}H_{16}$: 160.1252; Found：160.1255.
NMR spectroscopic data agreed with literature values.[22]



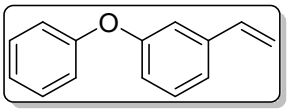
phenyl(3-vinylphenyl)methanone (5b)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White oil, 83% yield, 31.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.78 (m, 3H), 7.74 – 7.57 (m, 3H), 7.49 (dt, J = 20.4, 7.8 Hz, 3H), 6.79 (dd, J = 17.5, 10.9 Hz, 1H), 5.84 (d, J = 17.5 Hz, 1H), 5.36 (d, J = 11.0 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.72, 137.95, 137.81, 137.54, 135.99, 132.56, 130.10, 129.96, 129.44, 128.48, 128.36, 127.75, 115.34.
HRMS (EI-TOF) calcd for $C_{15}H_{12}O$: 208.0888; Found：208.0896.
NMR spectroscopic data agreed with literature values.[22]



2-fluoro-4-vinyl-1,1'-biphenyl (5c)

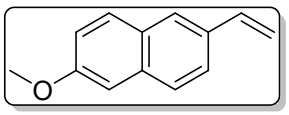
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow oil, 88% yield, 34.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.0 Hz, 2H), 7.43 (dt, J = 23.9, 7.1 Hz, 4H), 7.29 – 7.20 (m, 2H), 6.73 (dd, J = 17.6, 10.9 Hz, 1H), 5.81 (d, J = 17.6 Hz, 1H), 5.34 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.19, 158.73, 138.92 (d, J = 8.0 Hz), 135.60, 135.53 (d, J = 2.9 Hz), 130.75 (d, J = 4.4 Hz), 128.94 (d, J = 2.9 Hz), 128.49, 127.72, 122.43 (d, J = 2.9 Hz), 115.23, 113.43 (d, J = 23.3 Hz).
^{19}F NMR (377 MHz, $CDCl_3$) δ -118.37.
HRMS (EI-TOF) calcd for $C_{14}H_{11}F$: 198.0845; Found：198.0841.
NMR spectroscopic data agreed with literature values.[22]



1-phenoxy-3-vinylbenzene (5d)

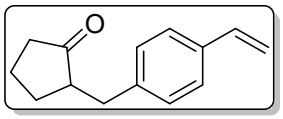
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Colourless oil, 95% yield, 37.3 mg.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dt, J = 22.1, 7.7 Hz, 3H), 7.20 – 7.08 (m, 3H), 7.04 (d, J = 7.8 Hz, 2H), 6.92 (d, J = 8.1 Hz, 1H), 6.69 (dd, J = 17.6, 10.9 Hz, 1H), 5.74 (d, J = 17.5 Hz, 1H), 5.27 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.51, 157.24, 139.53, 136.32, 129.82, 129.79, 123.27, 121.38, 118.88, 118.34, 116.55, 114.66.
HRMS (EI-TOF) calcd for $C_{14}H_{12}O$: 196.0888; Found：196.0892.
NMR spectroscopic data agreed with literature values.[32]



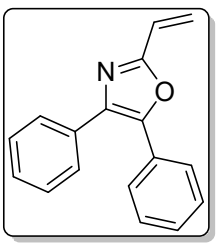
2-methoxy-6-vinylnaphthalene (5e)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solids, 92% yield, 33.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 3H), 7.61 (d, J = 8.6 Hz, 1H), 7.13 (d, J = 8.6 Hz, 2H), 6.85 (dd, J = 17.5, 10.9 Hz, 1H), 5.82 (d, J = 17.6 Hz, 1H), 5.28 (d, J = 10.9 Hz, 1H), 3.92 (d, J = 3.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.78, 136.95, 134.31, 132.97, 129.58, 127.02, 126.20, 123.76, 118.98, 113.13, 105.84, 55.34.
HRMS (EI-TOF) calcd for $C_{13}H_{12}O$: 184.0888; Found：184.0880.
NMR spectroscopic data agreed with literature values.[31]



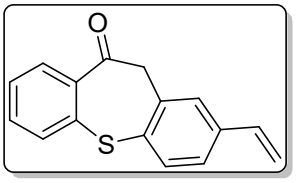
2-(4-vinylbenzyl)cyclopentan-1-one (5f)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 5 : 1). White solids, 97% yield, 38.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 6.69 (dd, J = 17.5, 10.9 Hz, 1H), 5.71 (d, J = 17.6 Hz, 1H), 5.21 (d, J = 11.0 Hz, 1H), 3.13 (dd, J = 13.9, 4.3 Hz, 1H), 2.34 (q, J = 7.4, 6.9 Hz, 2H), 2.16 – 2.04 (m, 2H), 2.00 – 1.91 (m, 1H), 1.79 – 1.68 (m, 1H), 1.62 – 1.48 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 220.27, 139.71, 136.54, 135.61, 129.11, 126.29, 113.29, 50.99, 38.25, 35.31, 29.12, 20.57.
HRMS (EI-TOF) calcd for $C_{14}H_{16}O$: 200.1201; Found：200.1206.
NMR spectroscopic data agreed with literature values.[31]



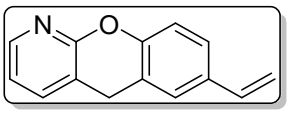
4,5-diphenyl-2-vinyloxazole (5g)

Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 5 : 1). White solids, 81% yield, 40.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, J = 12.9, 8.1 Hz, 4H), 7.36 (q, J = 8.1, 7.3 Hz, 6H), 6.68 (dd, J = 17.6, 11.3 Hz, 1H), 6.29 (d, J = 17.6 Hz, 1H), 5.69 (d, J = 11.3 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.51, 145.30, 136.50, 132.39, 128.83, 128.70, 128.62, 128.25, 128.03, 126.65, 123.37, 121.92.
HRMS (EI-TOF) calcd for $C_{14}H_{16}O$: 247.0997; Found：247.1003.
NMR spectroscopic data agreed with literature values.[31]



2-vinyldibenzo[b,f]thiepin-10(11*H*)-one (5h)

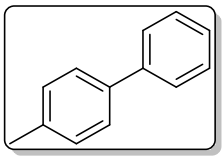
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solids, 73% yield, 36.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.0 Hz, 1H), 7.68 – 7.58 (m, 2H), 7.51 (s, 1H), 7.45 (t, J = 7.6 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.29 – 7.23 (m, 1H), 6.71 (dd, J = 17.6, 10.9 Hz, 1H), 5.81 (d, J = 17.5 Hz, 1H), 5.34 (d, J = 10.9 Hz, 1H), 4.39 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 191.47, 140.29, 139.45, 137.82, 136.13, 135.60, 133.63, 132.52, 131.56, 131.42, 130.80, 127.01, 126.83, 124.99, 115.56, 51.03.
HRMS (EI-TOF) calcd for $C_{16}H_{12}OS$: 252.0609; Found：252.0611.
NMR spectroscopic data agreed with literature values.[31]



7-vinyl-5*H*-chromeno[2,3-*b*]pyridine (5i)

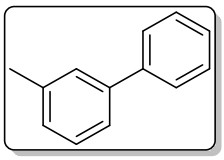
Reaction performed according to condition 1; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow solids, 83% yield, 34.7 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 5.1 Hz, 1H), 7.52 (d, J = 7.4 Hz, 1H), 7.27 (d, J = 11.0 Hz, 1H), 7.18 (s, 1H), 7.10 (d, J = 8.4 Hz, 1H), 7.06 – 6.96 (m, 1H), 6.64 (dd, J = 17.6, 10.9 Hz, 1H), 5.65 (d, J = 17.5 Hz, 1H), 5.19 (d, J = 10.9 Hz, 1H), 4.08 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.30, 151.25, 146.65, 138.47, 135.85, 133.39, 126.41, 125.87, 119.87, 119.37, 117.30, 115.31, 113.02, 28.03.
HRMS (EI-TOF) calcd for $C_{14}H_{11}NO$: 209.0841; Found：209.0840.

Biarylation Products of Aryl Carboxylic Acids



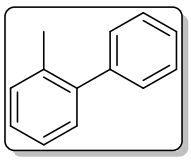
4-methyl-1,1'-biphenyl (8a)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether). White solid, 68% yield, 22.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.9 Hz, 2H), 7.67 (d, *J* = 8.1 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 2.56 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.32, 138.52, 137.15, 129.66, 128.89, 127.15 (d, *J* = 2.5 Hz), 21.27.
HRMS (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found：168.0940.
NMR spectroscopic data agreed with literature values.[33]



3-methyl-1,1'-biphenyl (8b)

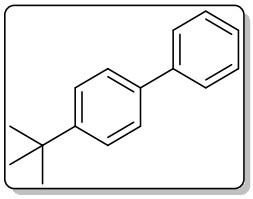
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether). White solid, 64% yield, 21.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.7 Hz, 2H), 7.68 (t, *J* = 7.6 Hz, 4H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 1H), 2.67 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.64, 141.51, 138.54, 128.97 (d, *J* = 1.7 Hz), 128.29, 128.24, 127.45, 124.57, 21.81.
HRMS (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found：168.0940.
NMR spectroscopic data agreed with literature values.[33]



2-methyl-1,1'-biphenyl (8c)

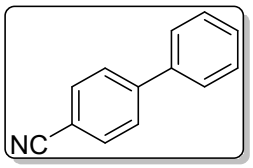
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether). White solid, 58% yield, 19.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.14 (m, 2H), 7.96 (dd, *J* = 16.7, 9.5 Hz, 4H), 7.87 (t, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 7.7 Hz, 1H), 2.94 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 142.00, 141.86, 138.79, 129.35, 128.67, 128.56, 127.79, 124.95, 22.10.
HRMS (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found：168.0940.
NMR spectroscopic data agreed with literature values.[33]



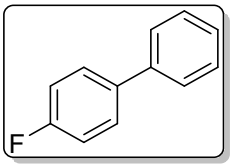
4-(tert-butyl)-1,1'-biphenyl (8d)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether). White solid, 62% yield, 26.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 1.46 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.31, 141.14, 138.40, 128.77, 127.10, 127.06, 126.87, 125.79, 34.60, 31.46.
HRMS (EI-TOF) calcd for $C_{16}H_{18}$: 210.1409; Found：210.1419.
NMR spectroscopic data agreed with literature values.[33]



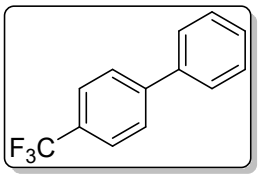
[1,1'-biphenyl]-4-carbonitrile (8e)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 45% yield, 16.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (q, *J* = 8.4 Hz, 4H), 7.62 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.71, 139.20, 132.62, 129.14, 128.68, 127.76, 127.25, 118.97, 110.93.
HRMS (EI-TOF) calcd for $C_{13}H_9N$: 179.0735; Found：179.0739.
NMR spectroscopic data agreed with literature values.[33]



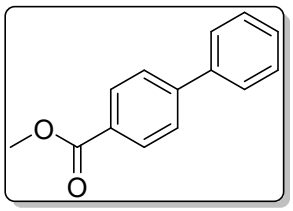
4-fluoro-1,1'-biphenyl (8f)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 63% yield, 21.7 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 4H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.17 (t, *J* = 8.7 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 162.54 (d, *J* = 246.3 Hz), 128.89, 128.75 (d, *J* = 8.0 Hz), 127.32, 127.09, 115.67 (d, *J* = 21.1 Hz).
^{19}F NMR (377 MHz, $CDCl_3$) δ -115.72.
HRMS (EI-TOF) calcd for $C_{12}H_9F$: 172.0688; Found：172.0690.
NMR spectroscopic data agreed with literature values.[34]



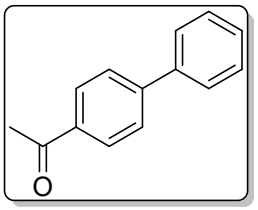
4-(trifluoromethyl)-1,1'-biphenyl (8g)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 70% yield, 31.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (s, 4H), 7.66 – 7.62 (m, 2H), 7.52 (t, *J* = 7.3 Hz, 2H), 7.48 – 7.43 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.76, 139.79, 129.02, 128.22, 127.45, 127.31, 125.74 (q, *J* = 4.0 Hz), 123.01.
^{19}F NMR (377 MHz, $CDCl_3$) δ -62.36.
HRMS (EI-TOF) calcd for $C_{13}H_9F_3$: 222.0656; Found：222.0659.
NMR spectroscopic data agreed with literature values.[33]



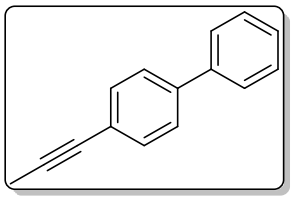
methyl [1,1'-biphenyl]-4-carboxylate (8h)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 66% yield, 28.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.4 Hz, 2H), 7.67 (dd, *J* = 14.9, 7.9 Hz, 4H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 3.97 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 167.03, 145.66, 140.02, 130.12, 128.95, 128.16, 127.30, 127.07, 52.16.
HRMS (EI-TOF) calcd for $C_{14}H_{12}O_2$: 212.0837; Found：212.0842.
NMR spectroscopic data agreed with literature values.[34]



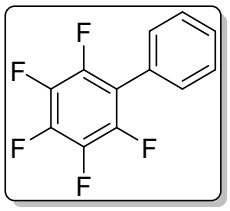
1-([1,1'-biphenyl]-4-yl)ethan-1-one (8i)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 75% yield, 29.4 mg.
^{1}H NMR (400 MHz, CDCl3) δ 8.06 (d, J = 8.5 Hz, 2H), 7.72 (d, J = 8.5 Hz, 2H), 7.66 (d, J = 7.0 Hz, 2H), 7.50 (d, J = 14.8 Hz, 2H), 7.43 (t, J = 7.3 Hz, 1H), 2.67 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 197.80, 145.81, 139.90, 135.87, 128.98, 128.94, 128.26, 127.30, 127.25, 26.71.
HRMS (EI-TOF) calcd for $C_{14}H_{12}O$: 196.0888; Found：196.0892.
NMR spectroscopic data agreed with literature values.[35]



4-(prop-1-yn-1-yl)-1,1'-biphenyl (8j)

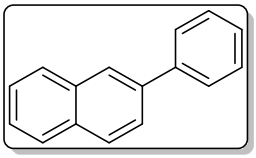
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 21% yield, 8.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.57 (m, 6H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 3.18 (s, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.61, 140.28, 132.60, 128.92, 127.78, 127.10, 127.05, 121.01, 83.60.
HRMS (EI-TOF) calcd for $C_{15}H_{12}$: 192.0939; Found：192.0944.
NMR spectroscopic data agreed with literature values.[36]



2,3,4,5,6-pentafluoro-1,1'-biphenyl (8k)

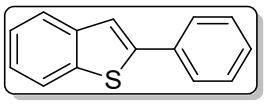
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 54% yield, 26.4 mg.

^{1}H NMR (400 MHz, CDCl3) δ 7.56 – 7.43 (m, 5H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.65 – 144.97 (m), 143.15 – 142.61 (m)., 141.99 – 141.32 (m), 139.50 – 138.78 (m), 137.06 – 136.22 (m), 130.16 , 129.31 , 128.74 , 126.41 , 116.11 – 115.75 (m).
^{19}F NMR (377 MHz, $CDCl_3$) δ -143.26 (dd, *J* = 23.6, 8.3 Hz), -155.62 (t, *J* = 21.5 Hz), -162.26 (td, *J* = 22.2, 7.6 Hz).
HRMS (EI-TOF) calcd for $C_{12}H_5F_5$: 244.0311; Found：244.0315.
NMR spectroscopic data agreed with literature values.[37]



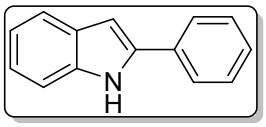
2-phenylnaphthalene (8l)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 87% yield, 35.5 mg.
^{1}H NMR (400 MHz, CDCl3) δ 8.13 (s, 1H), 8.02 – 7.91 (m, 3H), 7.88 – 7.77 (m, 3H), 7.64 – 7.52 (m, 4H), 7.50 – 7.38 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 141.23, 138.66, 133.80, 132.73, 128.98, 128.54, 128.33, 127.77, 127.55, 127.47, 126.41, 126.05, 125.92, 125.71.
HRMS (EI-TOF) calcd for $C_{16}H_{12}$: 204.0939; Found：204.0945.
NMR spectroscopic data agreed with literature values.[33]



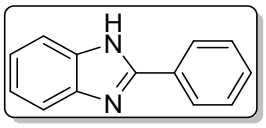
2-phenylbenzo[b]thiophene (8m)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 70% yield, 29.4 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.7 Hz, 1H), 7.81 (d, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 2H), 7.58 (s, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.32 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.27, 140.71, 139.52, 134.32, 128.98, 128.30, 126.52, 124.54, 124.34, 123.59, 122.30, 119.48.
HRMS (EI-TOF) calcd for $C_{14}H_{10}S$: 210.0503; Found：210.0504.
NMR spectroscopic data agreed with literature values.[38]



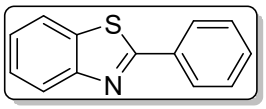
2-phenyl-1*H*-indole (8n)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 3 : 1). White solid, 64% yield, 24.7 mg.
^{1}H NMR (400 MHz, DMSO) δ 11.55 (s, 1H), 7.88 (d, *J* = 7.1 Hz, 2H), 7.54 (d, *J* = 7.1 Hz, 1H), 7.52 – 7.37 (m, 3H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.14 – 7.08 (m, 1H), 7.05 – 6.97 (m, 1H), 6.91 (d, *J* = 1.5 Hz, 1H).
^{13}C NMR (101 MHz, DMSO) δ 137.61, 137.13, 132.22, 128.90, 128.63, 127.39, 124.98, 121.57, 120.04, 119.37, 111.31, 98.67.
HRMS (EI-TOF) calcd for $C_{14}H_{11}N$: 193.0891; Found：193.0899.
NMR spectroscopic data agreed with literature values.[38]



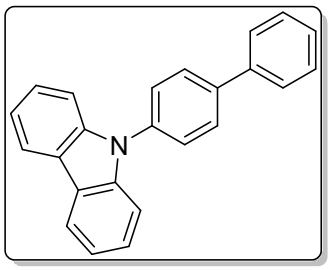
2-phenyl-1*H*-benzo[d]imidazole (8o)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 1 : 1). White solid, 49% yield, 19.0 mg.
^{1}H NMR (400 MHz, DMSO) δ 8.18 (d, *J* = 7.0 Hz, 2H), 7.67 – 7.43 (m, 5H), 7.21 (dd, *J* = 6.1, 3.2 Hz, 2H).
^{13}C NMR (101 MHz, DMSO) δ 156.42, 135.37, 135.07, 134.18, 131.65, 127.32.
HRMS (EI-TOF) calcd for $C_{13}H_{10}N_2$: 194.0844; Found：194.0846.
NMR spectroscopic data agreed with literature values.[40]



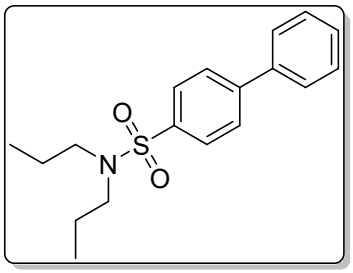
2-phenylbenzo[d]thiazole (8p)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 3 : 1). White solid, 62% yield, 26.1 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.00 (m, 3H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.55 – 7.47 (m, 4H), 7.39 (td, *J* = 7.7, 7.3, 1.3 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.13, 154.09, 135.05, 133.59, 131.04, 129.06, 127.61, 126.37, 125.24, 123.24, 121.66.
HRMS (EI-TOF) calcd for $C_{13}H_9NS$: 211.0456; Found：211.0457.
NMR spectroscopic data agreed with literature values.[40]



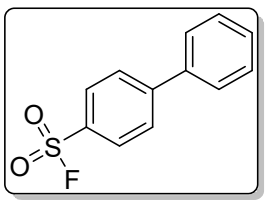
9-([1,1'-biphenyl]-4-yl)-9H-carbazole (8q)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 67% yield, 42.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.8 Hz, 2H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.74 – 7.70 (m, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.56 – 7.49 (m, 4H), 7.49 – 7.41 (m, 3H), 7.36 – 7.30 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 140.91, 140.33, 136.91, 129.01, 128.55, 127.69, 127.37, 127.19, 126.02, 123.48, 120.38, 120.02, 109.89.
HRMS (EI-TOF) calcd for $C_{24}H_{17}N$: 319.1361; Found：319.1366.
NMR spectroscopic data agreed with literature values.[41]



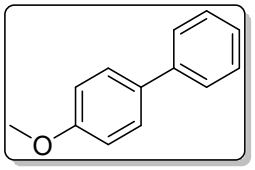
***N,N-dipropyl-[1,1'-biphenyl]-4-sulfonamide* (8r)**

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 5 : 1). White solid, 58% yield, 36.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.5 Hz, 2H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.3 Hz, 1H), 3.16 – 3.12 (m, 4H), 1.63 – 1.57 (m, 4H), 0.92 (t, *J* = 7.4 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.09, 139.42, 138.76, 129.04, 128.39, 127.58, 127.30, 50.13, 22.11, 11.23.
HRMS (EI-TOF) calcd for $C_{18}H_{23}NO_2S$: 317.1449; Found：317.1455.



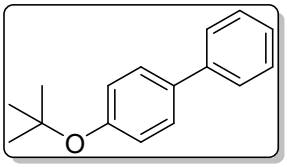
[1,1'-biphenyl]-4-sulfonyl fluoride (8s)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 61% yield, 28.8 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.5 Hz, 2H), 7.82 (d, *J* = 8.3 Hz, 2H), 7.64 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.57 – 7.46 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.66, 138.51, 129.31, 129.26, 129.02, 128.22, 127.48.
^{19}F NMR (377 MHz, $CDCl_3$) δ 66.61.
HRMS (EI-TOF) calcd for $C_{12}H_9FO_2S$: 236.0307; Found：236.0309.
NMR spectroscopic data agreed with literature values.[42]



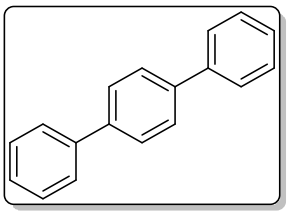
4-methoxy-1,1'-biphenyl (8t)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 77% yield, 28.3 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (t, *J* = 8.3 Hz, 4H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.15, 140.84, 133.79, 128.74, 128.18, 126.76, 126.67, 114.21, 55.37.
HRMS (EI-TOF) calcd for $C_{13}H_{12}O$: 184.0888; Found：184.0889.
NMR spectroscopic data agreed with literature values.[33]



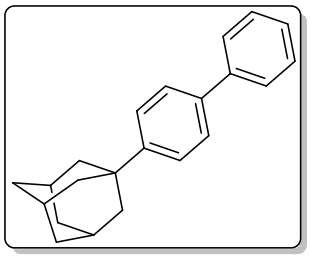
4-(tert-butoxy)-1,1'-biphenyl (8u)

Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 42% yield, 19.0 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.1 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.6 Hz, 2H), 1.41 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.94, 140.81, 136.20, 128.71, 127.53, 126.88, 126.85, 124.35, 28.91.
HRMS (EI-TOF) calcd for $C_{16}H_{18}O$: 226.1358; Found：226.1359.
NMR spectroscopic data agreed with literature values.[43]



1,1':4',1''-terphenyl (8v)

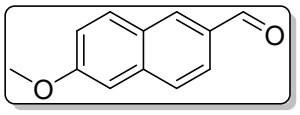
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 45% yield, 20.7 mg.
^{1}H NMR (400 MHz, DMSO) δ 7.72 – 7.64 (m, 8H), 7.48 (t, *J* = 7.6 Hz, 4H), 7.37 (d, *J* = 7.3 Hz, 2H).
^{13}C NMR (101 MHz, DMSO) δ 140.70, 140.13, 128.83, 127.51, 127.35, 127.06.
HRMS (EI-TOF) calcd for $C_{18}H_{14}$: 230.1096; Found：230.1098.
NMR spectroscopic data agreed with literature values.[44]



(3r,5r,7r)-1-([1,1'-biphenyl]-4-yl)adamantane (8w)

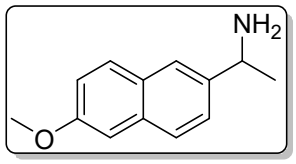
Reaction performed according to condition 2; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 20 : 1). White solid, 72% yield, 41.5 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.58 (m, 4H), 7.50 – 7.43 (m, 4H), 7.35 (t, *J* = 7.4 Hz, 1H), 2.16 (s, 3H), 2.00 (d, *J* = 3.3 Hz, 6H), 1.87 – 1.78 (m, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.53, 141.13, 138.38, 128.70, 127.06, 126.97, 126.85, 43.22, 36.83, 36.09, 28.98.
HRMS (EI-TOF) calcd for $C_{22}H_{24}$: 288.1878; Found：288.1880.
NMR spectroscopic data agreed with literature values.[45]

Other Products



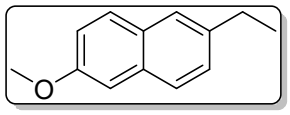
6-methoxy-2-naphthaldehyde (9a)

React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow solid, 62% yield, 34.6 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.26 (s, 1H), 7.92 (dd, J = 14.3, 8.8 Hz, 2H), 7.82 (d, J = 8.5 Hz, 1H), 7.25 (dd, J = 8.4, 3.1 Hz, 1H), 7.19 (d, J = 2.9 Hz, 1H), 3.98 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.07, 136.73, 135.08, 128.05, 126.20, 112.87, 28.64, 15.61.
HRMS (EI-TOF) calcd for $C_{12}H_{10}O_2$: 186.0681; Found：186.0680.



1-(6-methoxynaphthalen-2-yl)ethan-1-amine (9b)

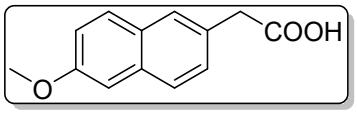
React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 3 : 1). Yellow solid, 80% yield, 96.5 mg.
^{1}H NMR (400 MHz, DMSO-d^6) δ 8.72 (s, 2H), 7.95 (s, 1H), 7.88 (d, J = 8.6 Hz, 1H), 7.82 (d, J = 9.0 Hz, 1H), 7.67 (d, J = 8.6 Hz, 1H), 7.35 (s, 1H), 7.21 (dd, J = 8.9, 2.6 Hz, 1H), 3.88 (s, 3H), 1.61 (d, J = 6.9 Hz, 3H).
^{13}C NMR (101 MHz, DMSO-d^6) δ 158.09, 134.86, 134.50, 129.85, 128.45, 127.71, 126.18, 125.60, 119.63, 106.29, 55.71, 50.54, 21.10.
HRMS (EI-TOF) calcd for $C_{13}H_{15}NO$: 201.1154; Found：201.1150.



2-ethyl-6-methoxynaphthalene (9c)

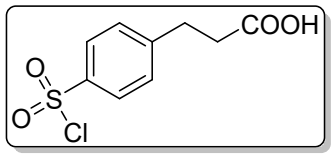
React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid, 74% yield, 68.9 mg.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.68 (m, 2H), 7.59 (s, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.16 (d, J = 7.9 Hz, 2H), 3.95 (s, 3H), 2.82 (q, J = 7.6 Hz, 2H), 1.35 (t, J = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.09, 139.48, 132.91, 129.19, 128.92, 127.57, 126.71, 125.44, 118.61, 105.68, 55.30, 28.86, 15.65.
HRMS (EI-TOF) calcd for $C_{13}H_{14}O$: 186.1045; Found：186.1049.



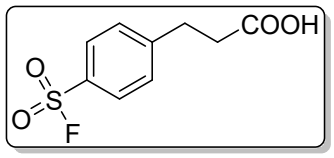
2-(6-methoxynaphthalen-2-yl)acetic acid (9d)

React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 1 : 1). Yellow solid, 47% yield, 20.3 mg.
^{1}H NMR (400 MHz, DMSO-d^6) δ 7.77 (dd, J = 8.7, 4.7 Hz, 2H), 7.69 (s, 1H), 7.38 (d, J = 8.5 Hz, 1H), 7.30 (d, J = 2.8 Hz, 1H), 7.15 (dd, J = 8.9, 2.6 Hz, 1H), 3.87 (s, 3H), 3.69 (s, 2H).
^{13}C NMR (101 MHz, DMSO-d^6) δ 173.41, 157.51, 133.53, 130.87, 129.41, 128.85, 127.96, 127.03, 119.08, 55.60, 41.33.
HRMS (EI-TOF) calcd for $C_{13}H_{12}O_3$: 216.0786; Found：216.0780.



3-(4-(chlorosulfonyl)phenyl)propanoic acid (9e)

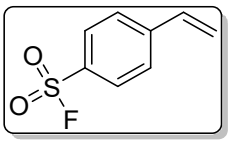
React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 1 : 1). Yellow solid, 33% yield, 12.8 g.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.5 Hz, 2H), 7.50 (d, J = 8.5 Hz, 2H), 3.11 (t, J = 7.5 Hz, 2H), 2.78 (t, J = 7.5 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.78, 148.58, 142.59, 129.67, 127.39, 34.37, 30.41.
HRMS (EI-TOF) calcd for $C_9H_9ClO_4S$: 247.9910; Found：247.9918.



3-(4-(fluorosulfonyl)phenyl)propanoic acid (9f)

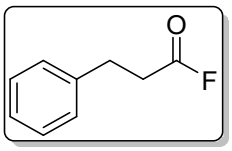
React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 1 : 1). Black solid, 92% yield, 3.6 g.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.3 Hz, 2H), 3.10 (t, J = 7.5 Hz, 2H), 2.76 (t, J = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.61, 148.95, 131.24, 130.99, 129.68, 128.79, 34.63, 30.48.
^{19}F NMR (377 MHz, $CDCl_3$) δ 66.16.
HRMS (EI-TOF) calcd for $C_9H_9FO_4S$: 232.0206; Found：232.0209.



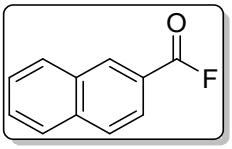
4-vinylbenzenesulfonyl fluoride (9g)

React according to the appropriate conditions in the synthetic application; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow oil, 78% yield, 12.8 g.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 8.4 Hz, 2H), 6.78 (dd, J = 17.6, 10.9 Hz, 1H), 5.97 (d, J = 17.5 Hz, 1H), 5.54 (d, J = 10.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.77, 134.84, 131.63, 128.85, 127.15, 119.36.
^{19}F NMR (377 MHz, $CDCl_3$) δ 66.31.
HRMS (EI-TOF) calcd for $C_8H_7FO_2S$: 186.0151; Found：186.0150.



3-phenylpropanoyl fluoride (10a)

React according to the appropriate conditions in the possible intermediates; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). Yellow oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (q, J = 8.1 Hz, 2H), 7.23 (q, J = 7.5, 6.7 Hz, 3H), 2.99 (dt, J = 14.4, 7.7 Hz, 2H), 2.80 (dt, J = 33.3, 7.6 Hz, 2H).
^{19}F NMR (377 MHz, $CDCl_3$) δ 45.39.
HRMS (EI-TOF) calcd for C_9H_9FO: 152.0637; Found：152.0644.



2-naphthoyl fluoride (10b)

React according to the appropriate conditions in the possible intermediates; purified by chromatography on silica gel (Petroleum ether : Ethyl acetate = 10 : 1). White solid.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.98 (dt, J = 24.9, 8.5 Hz, 4H), 7.71 (t, J = 7.6 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.38, 155.97, 136.45, 134.04 (d, J = 3.4 Hz), 132.29, 129.69 (d, J = 5.9 Hz), 129.07, 127.98, 127.40, 125.62 (d, J = 4.2 Hz), 122.31, 121.71.

^{19}F NMR (377 MHz, $CDCl_3$) δ 18.08.
HRMS (EI-TOF) calcd for $C_{11}H_7FO$: 174.0481; Found：174.0483.

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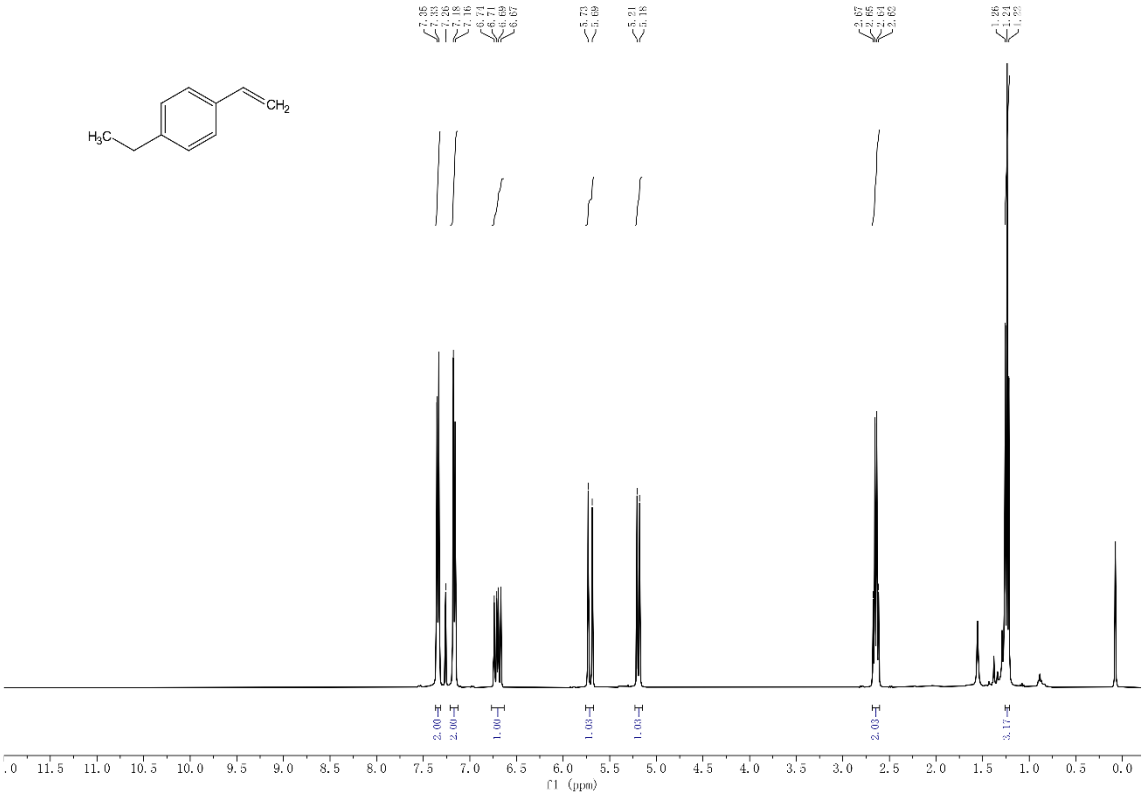
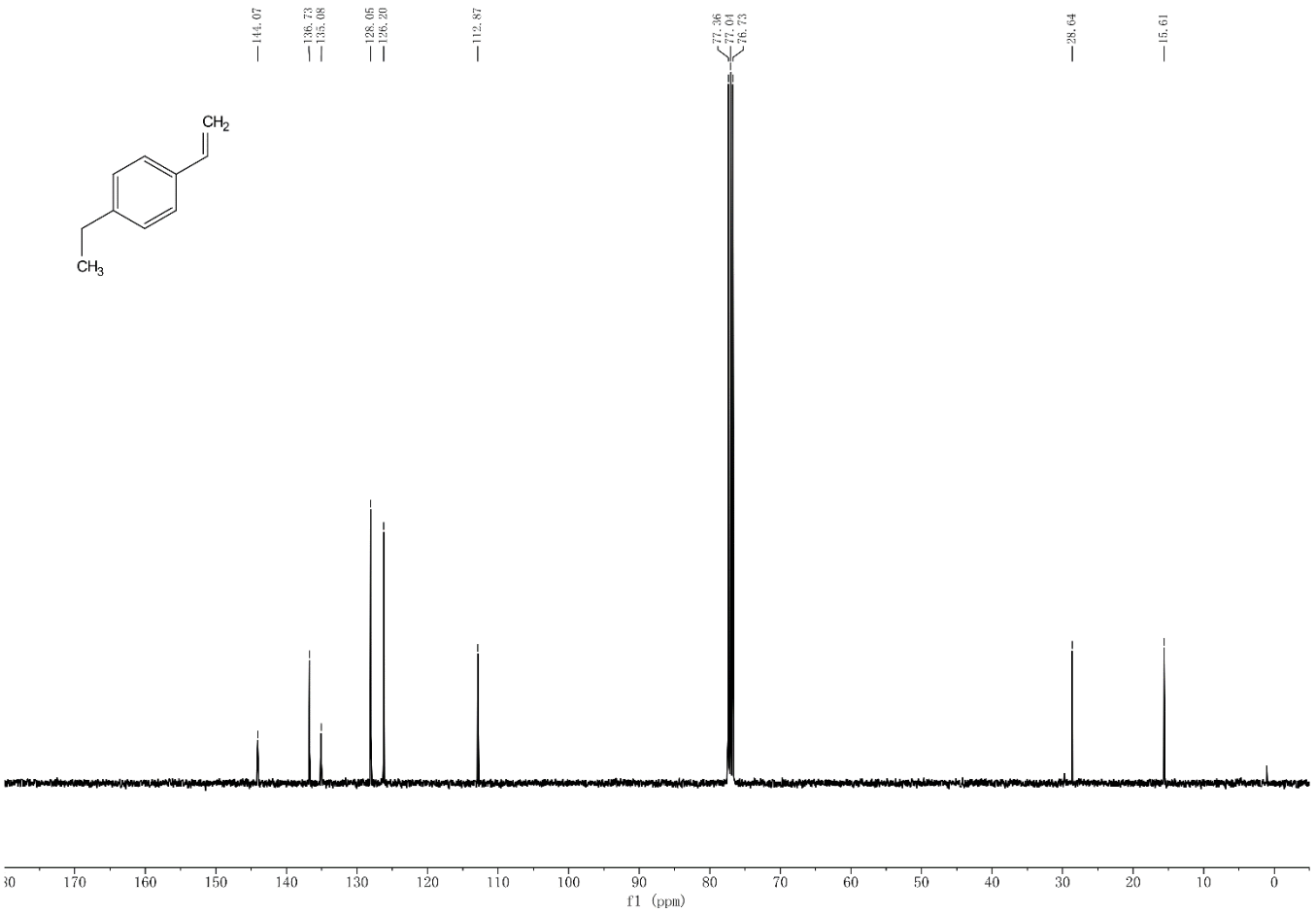
IV. Spectroscopic Data

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 2a



$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 2a



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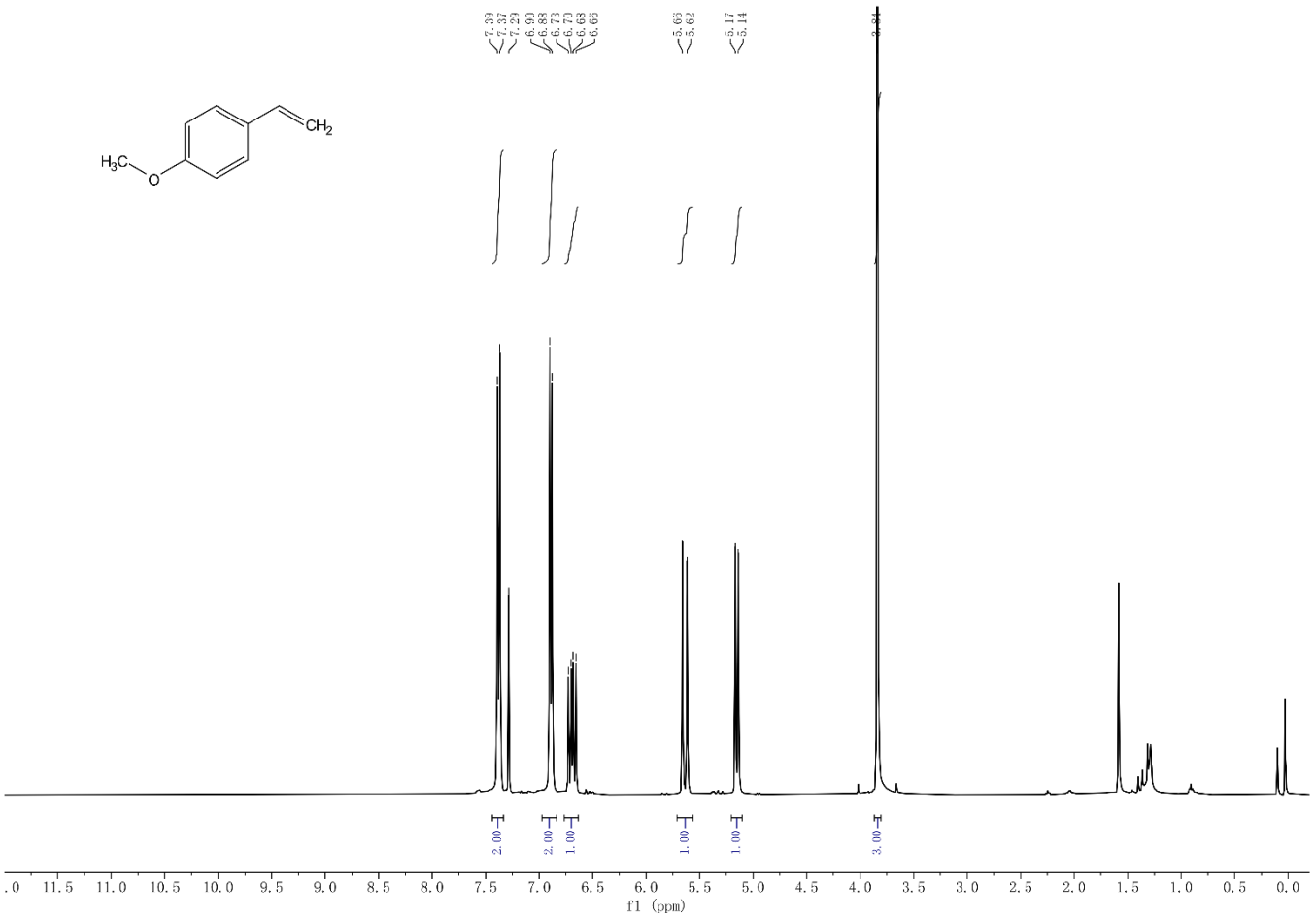

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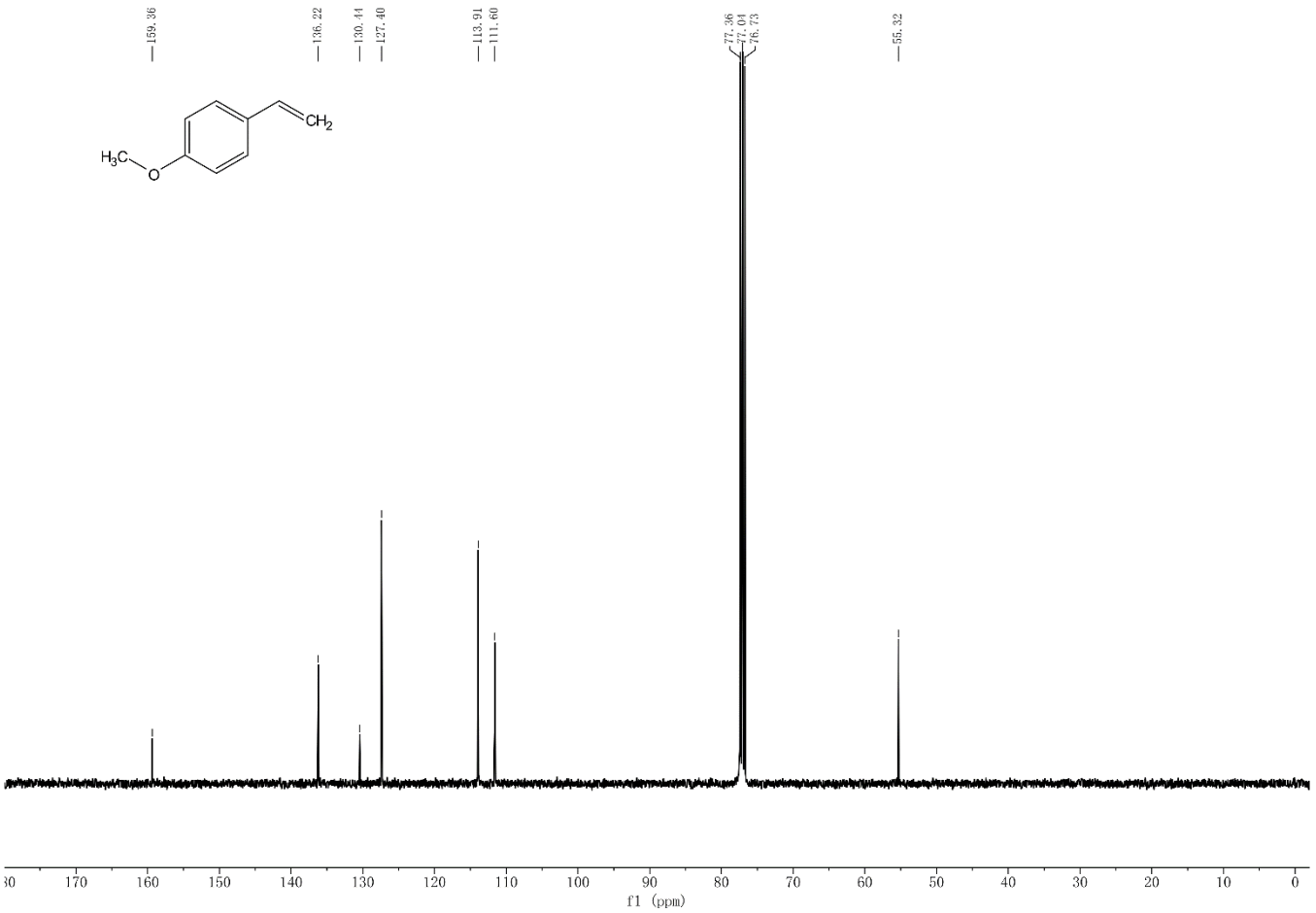

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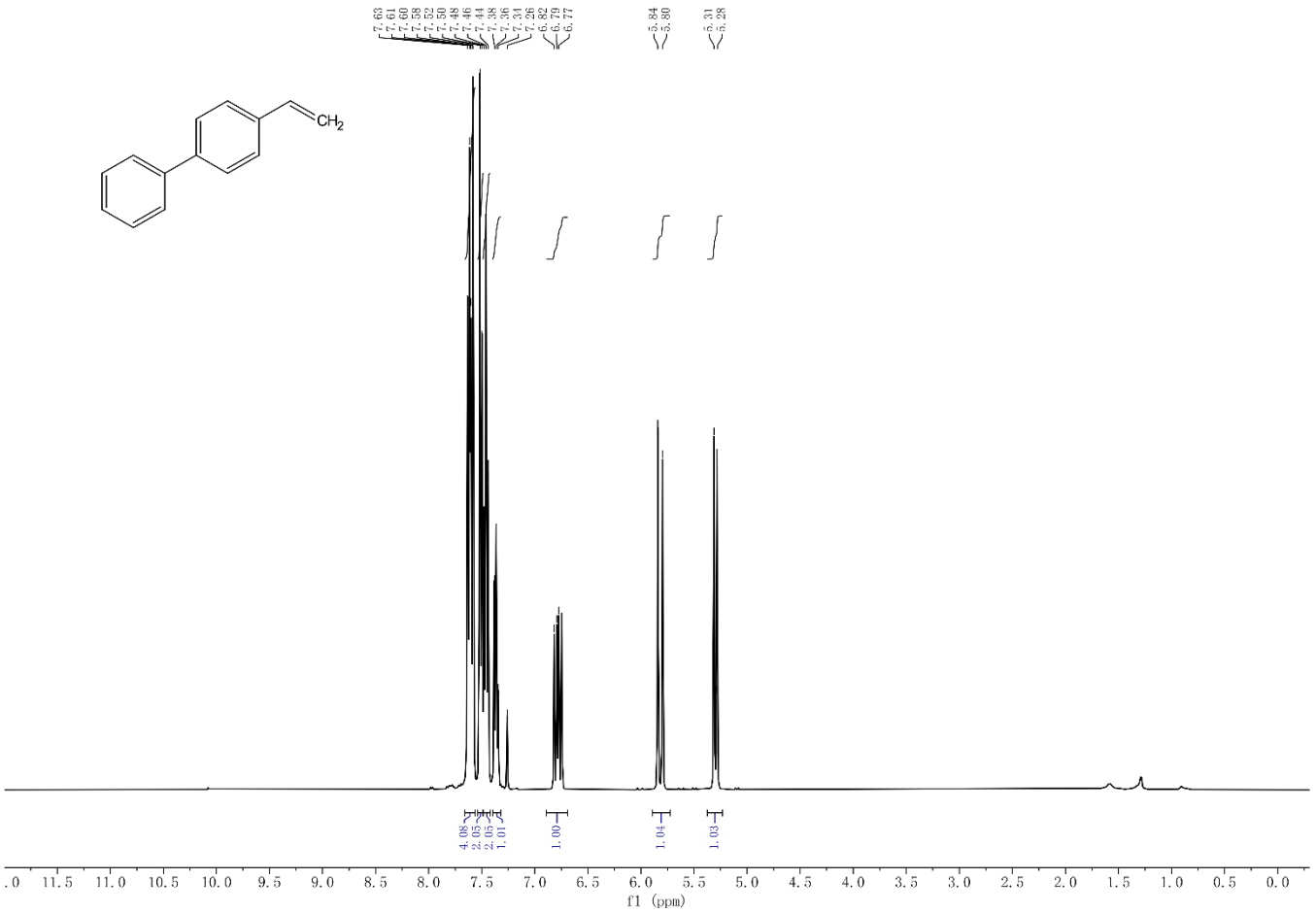

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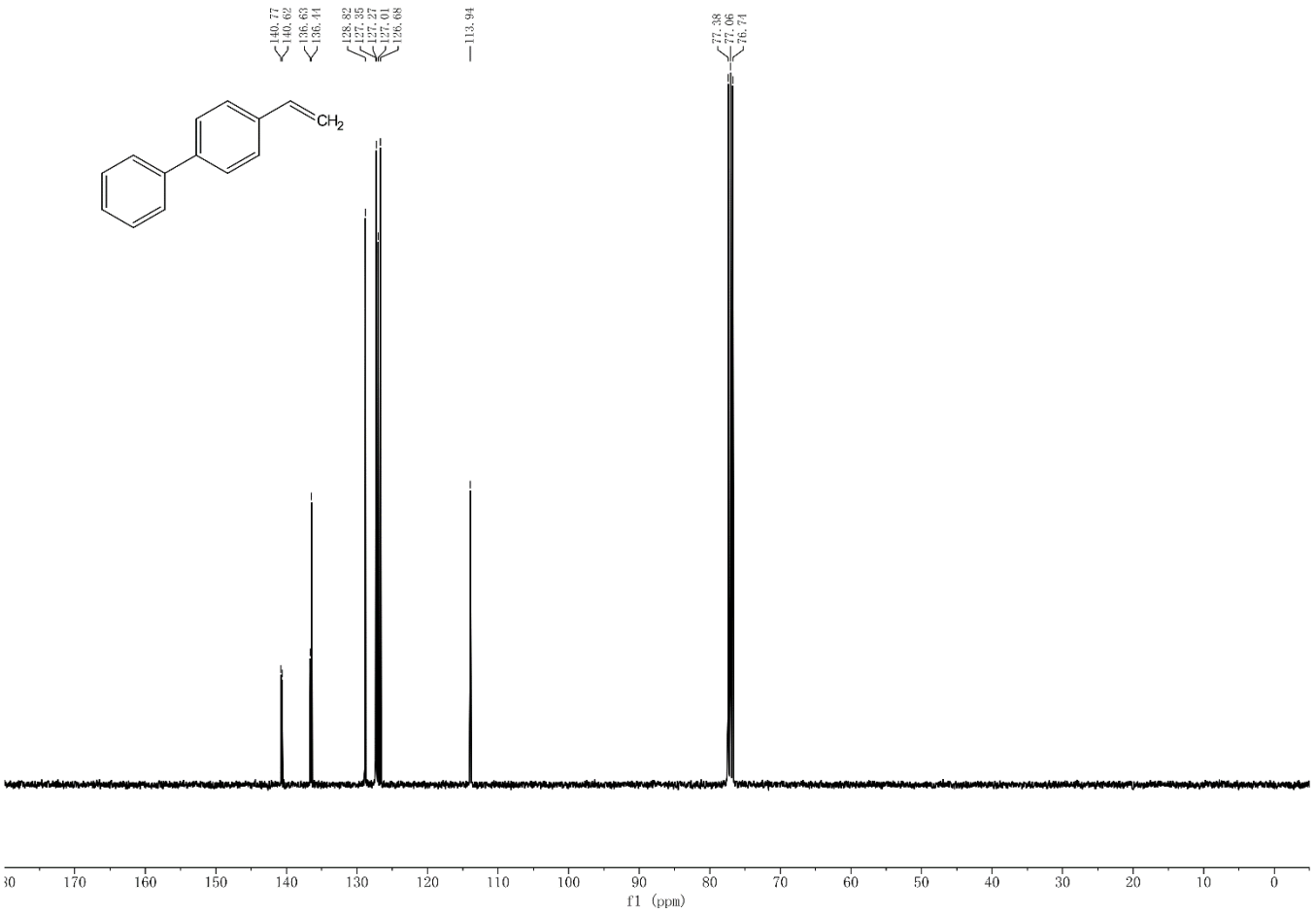

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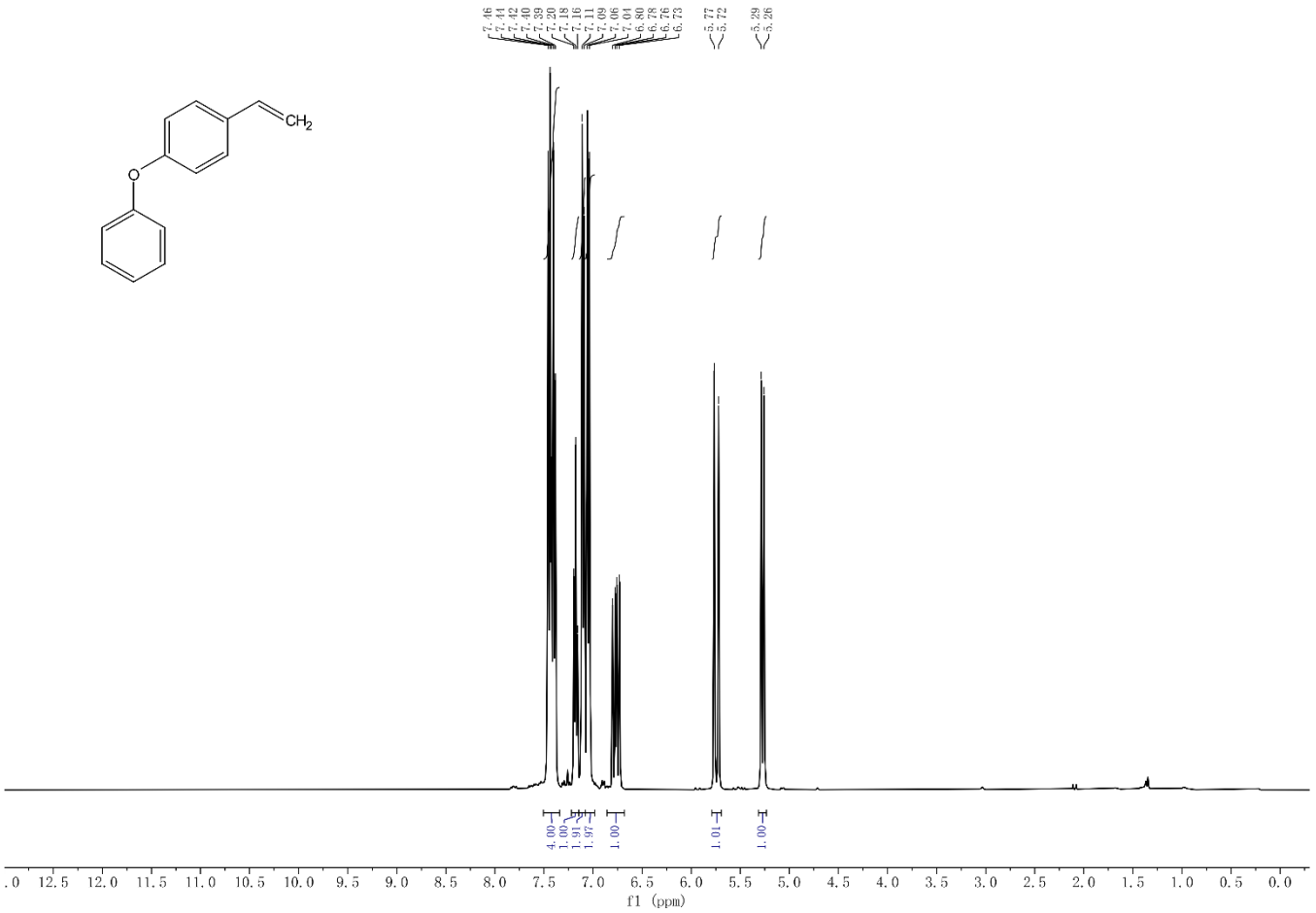

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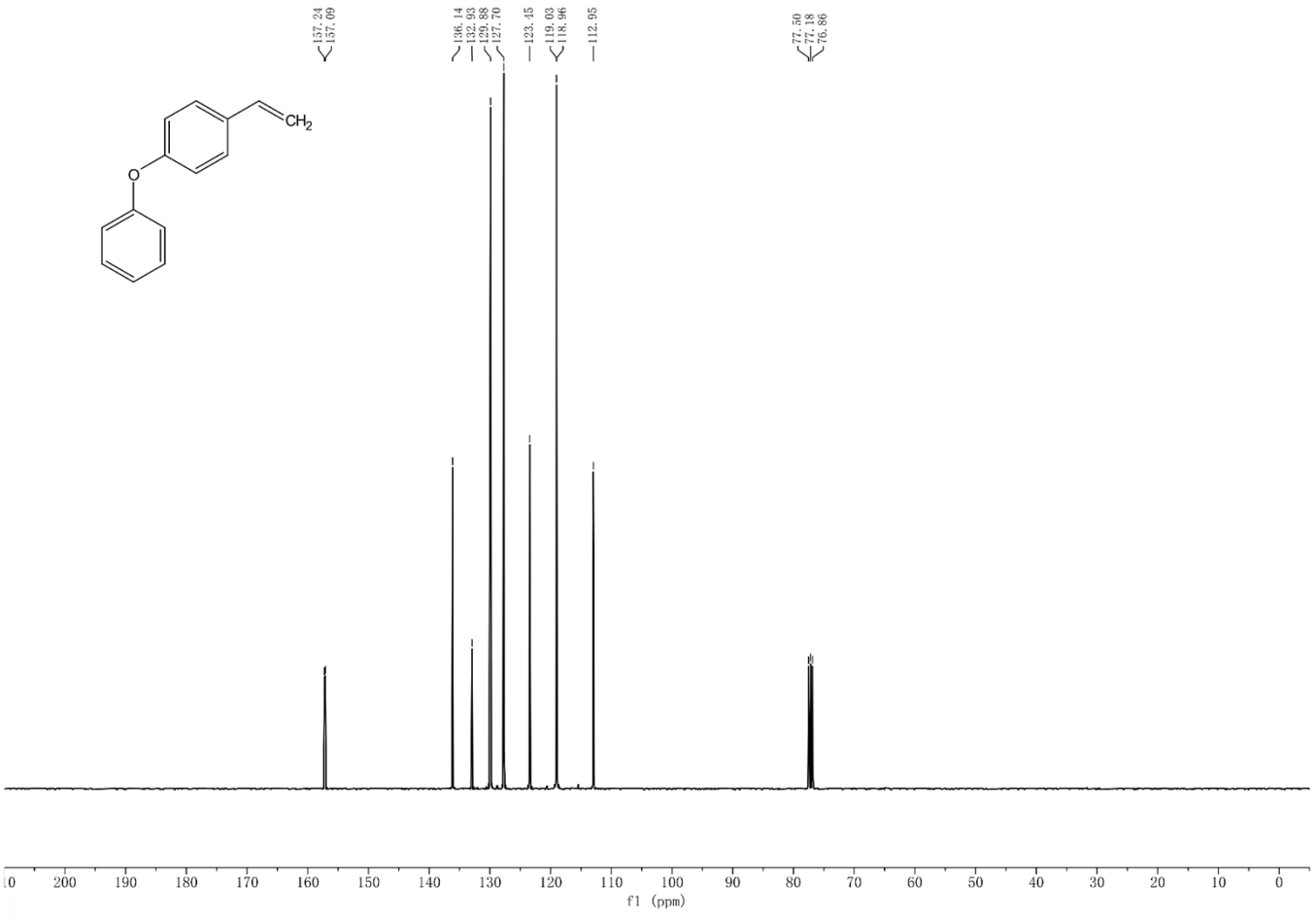

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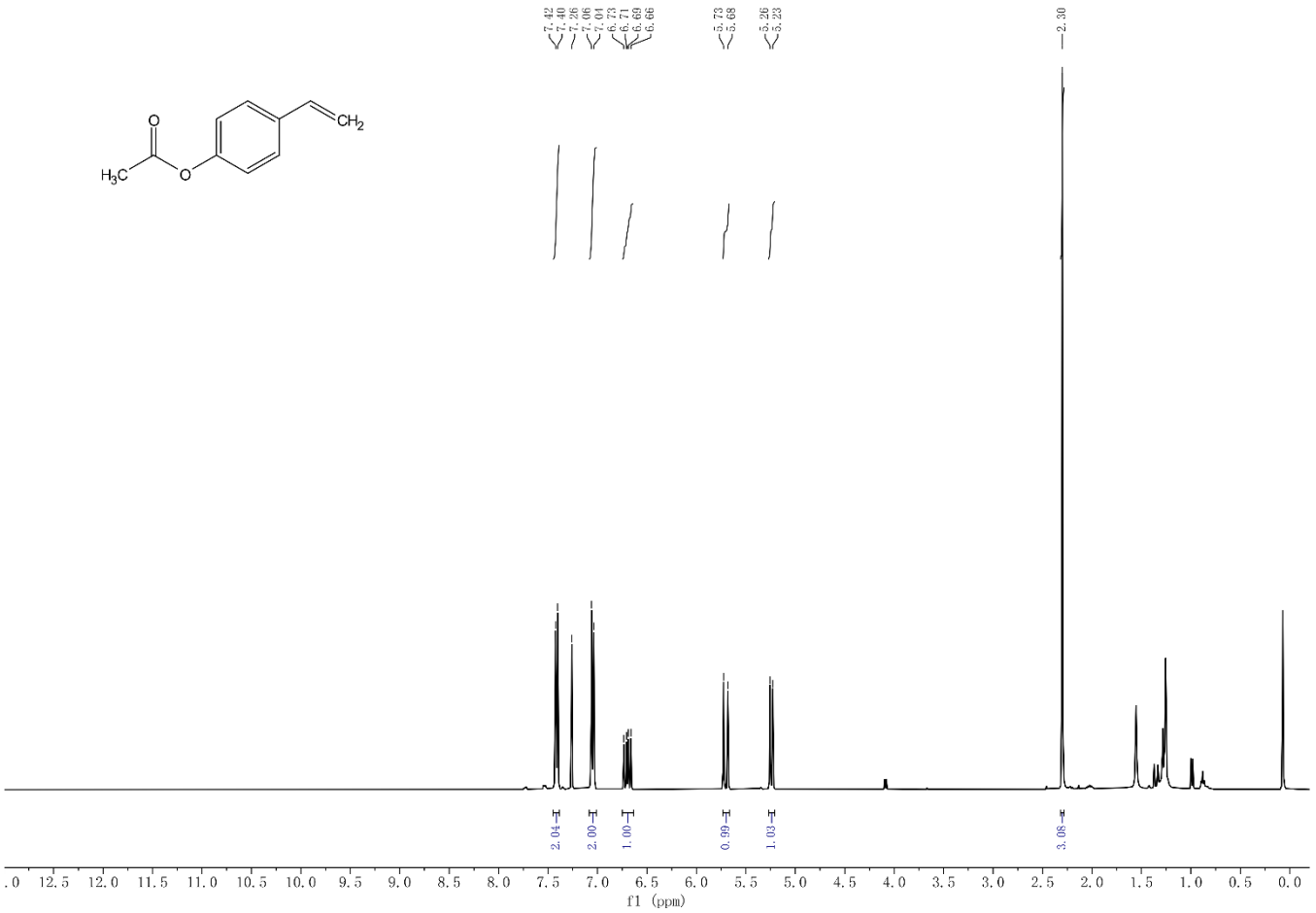

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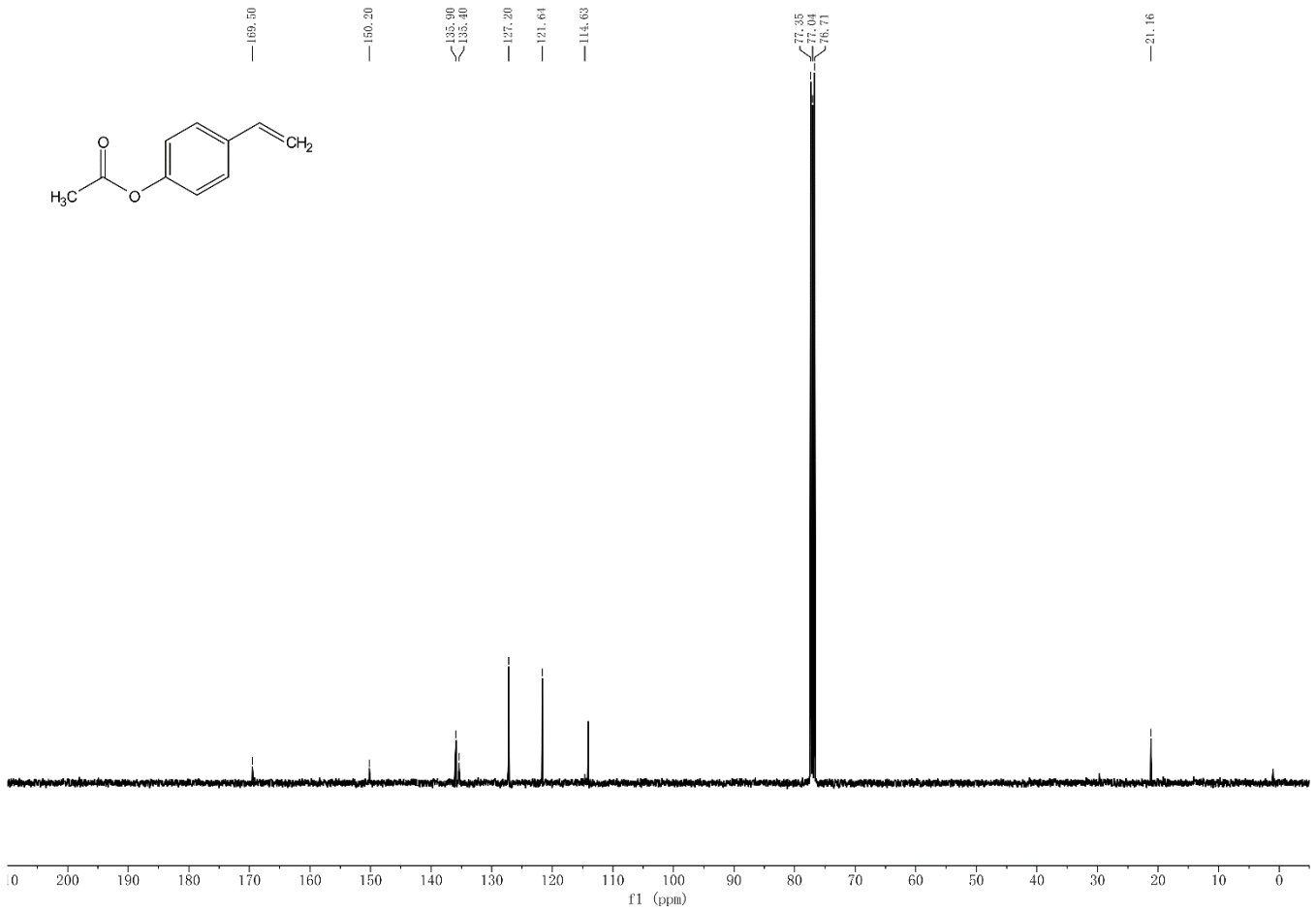

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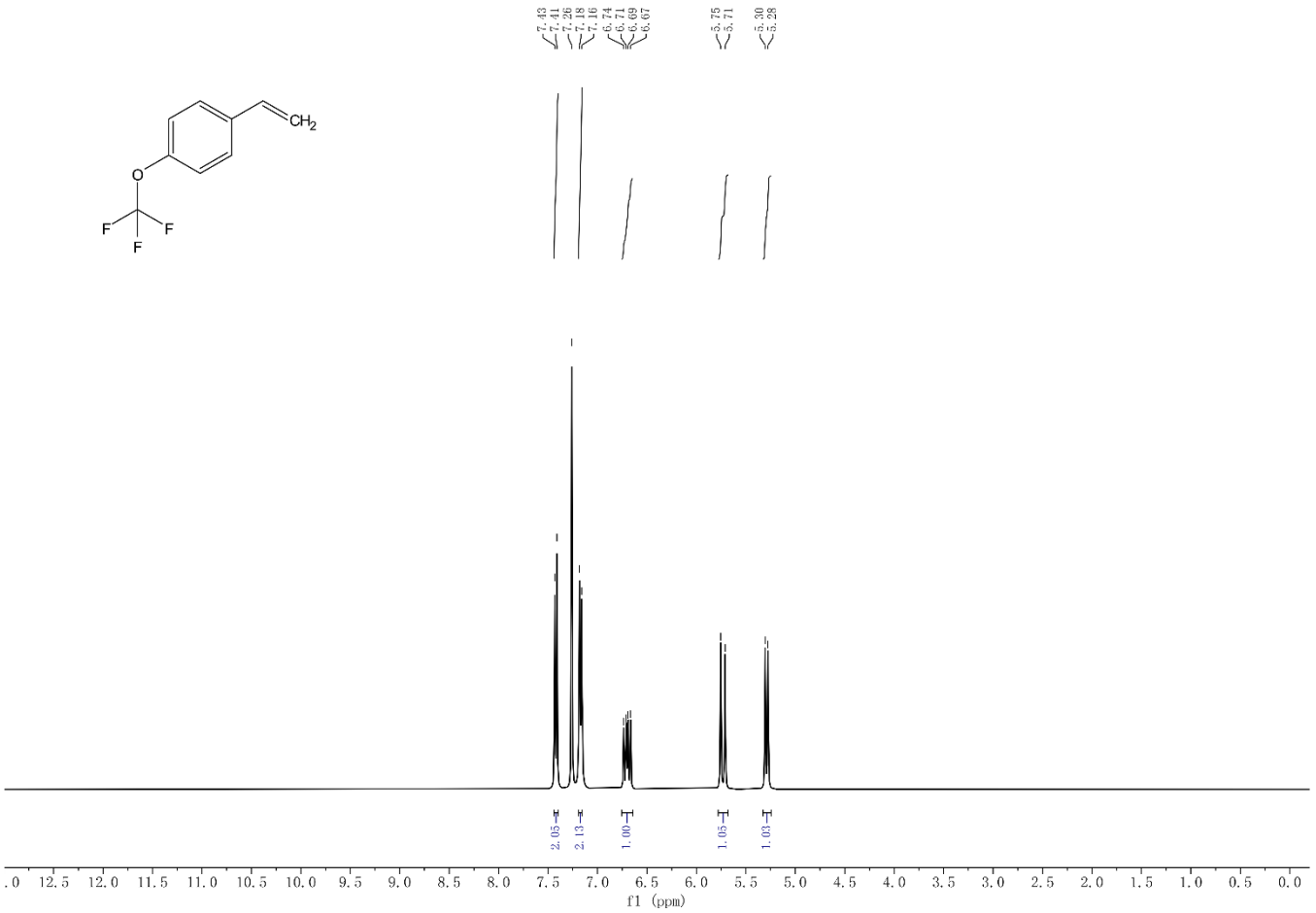
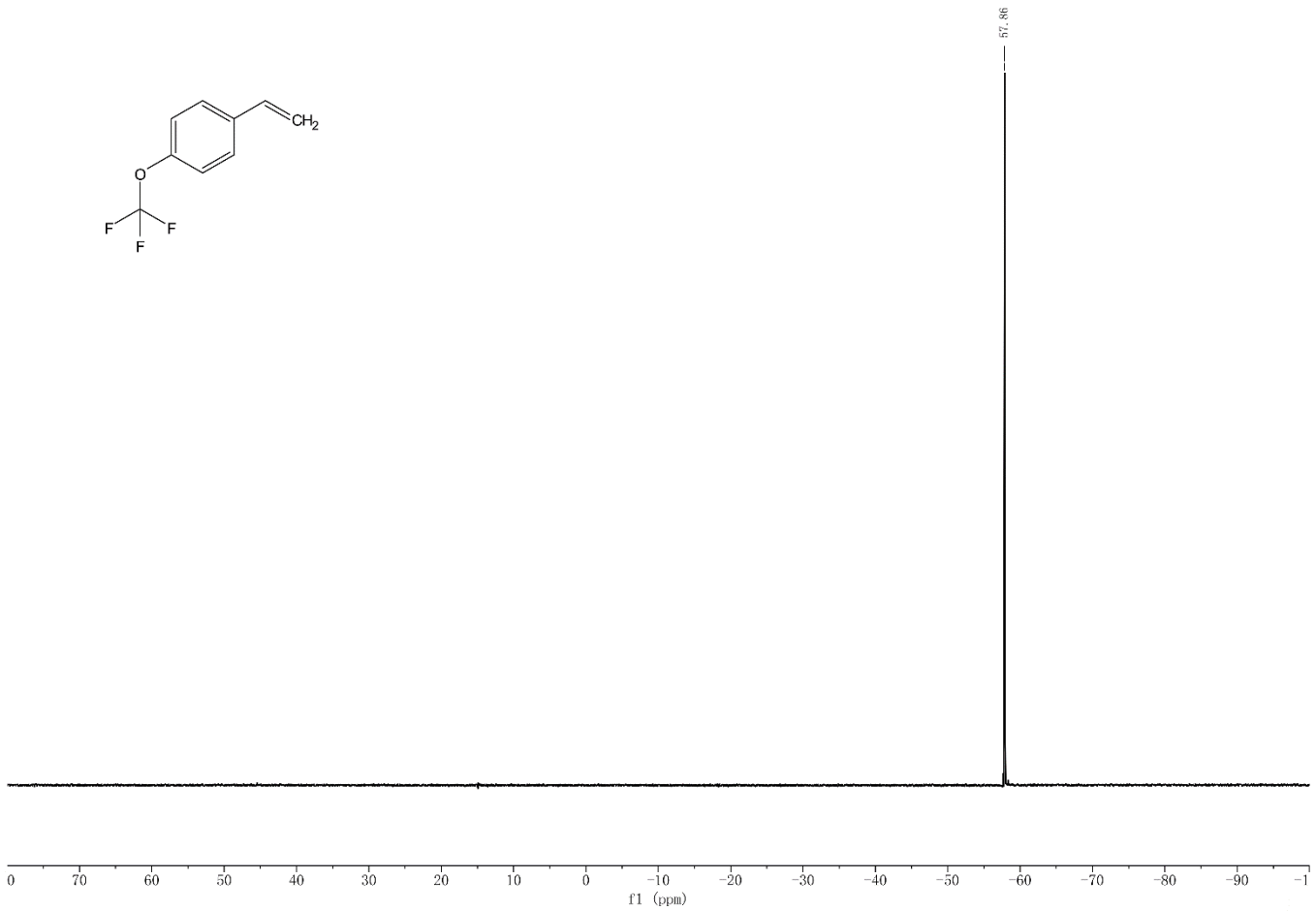


^{13}F NMR (377 MHz, $CDCl_3$) spectrum of 2f



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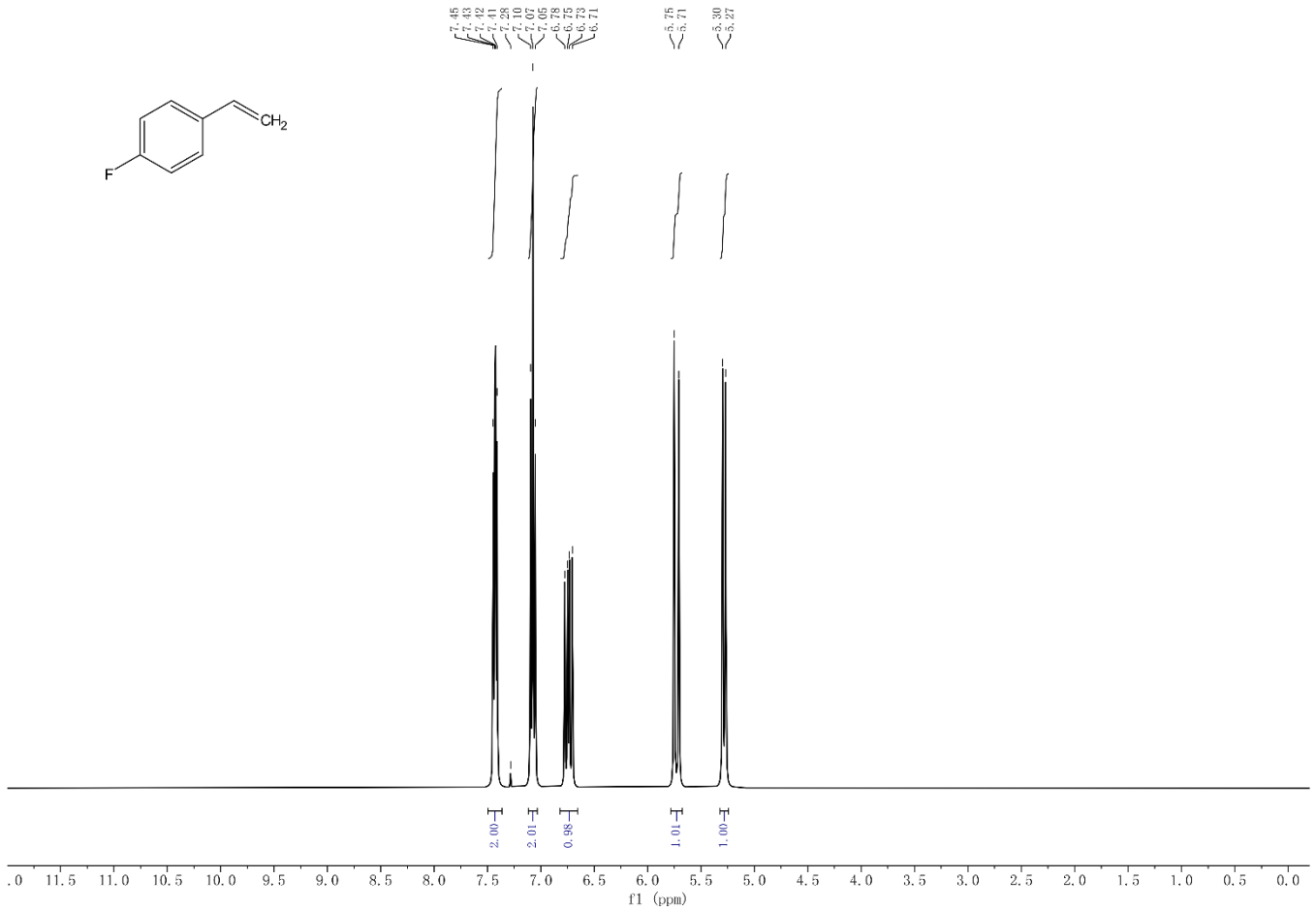
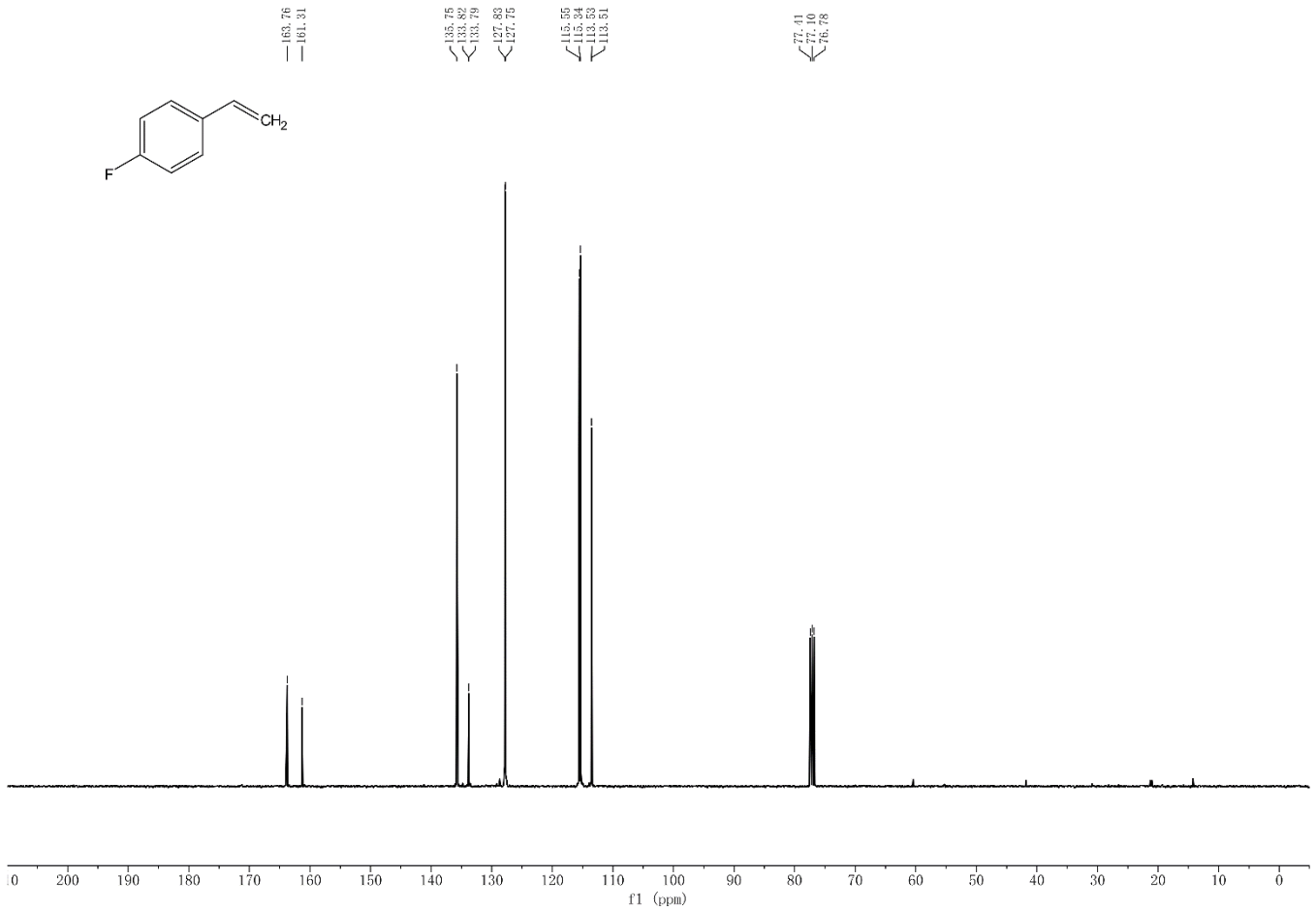
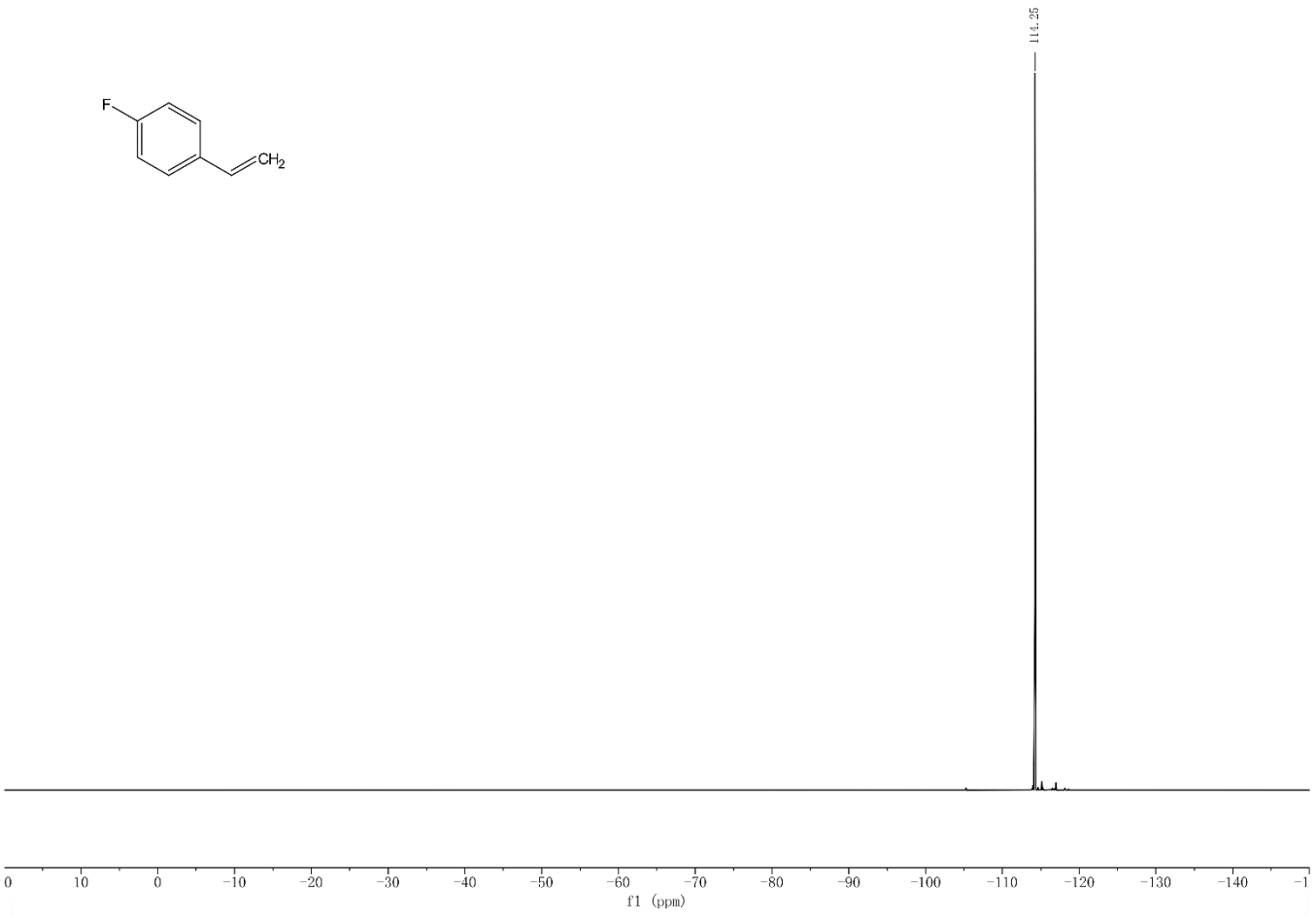


$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 2g



^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 2g



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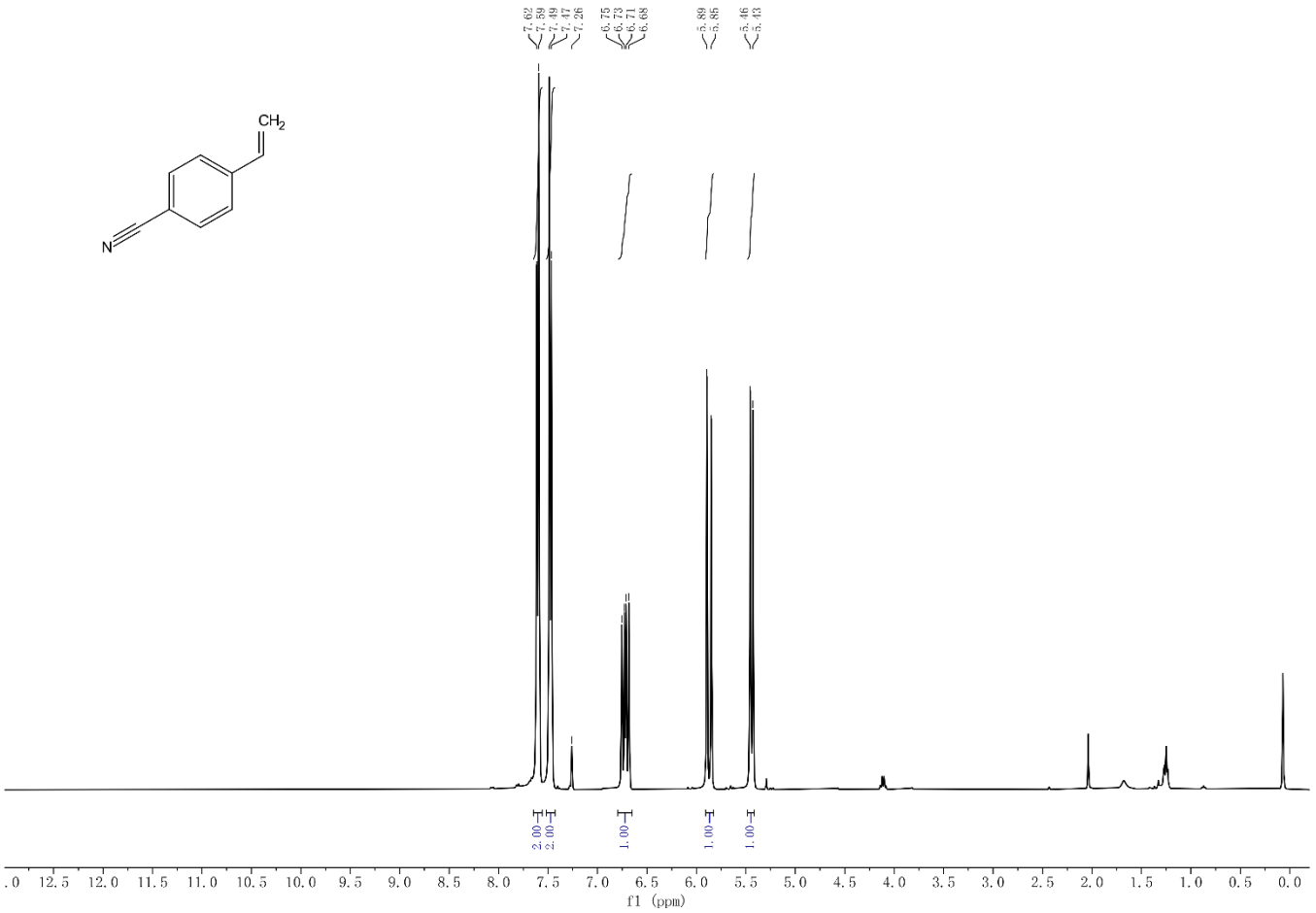
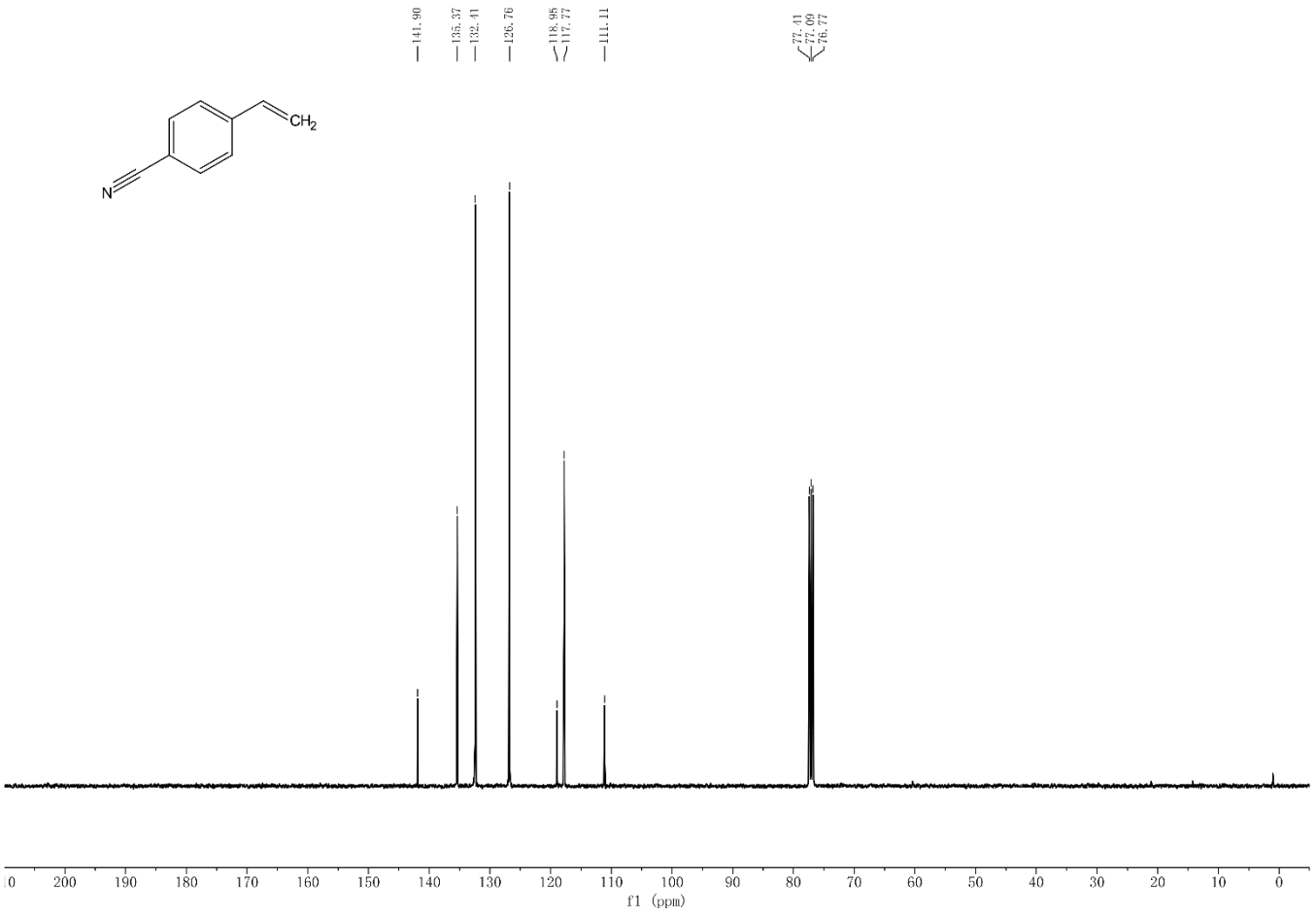
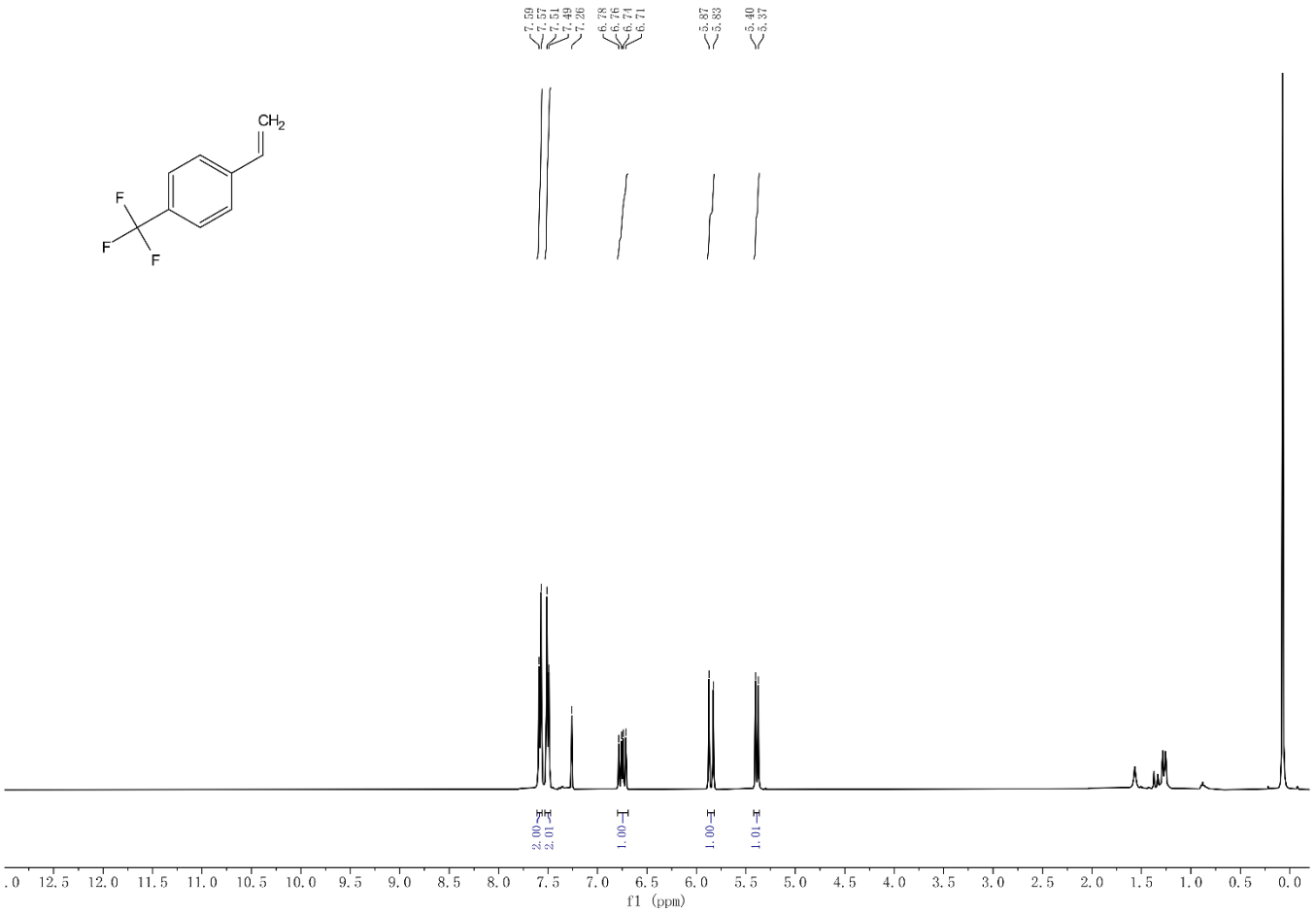


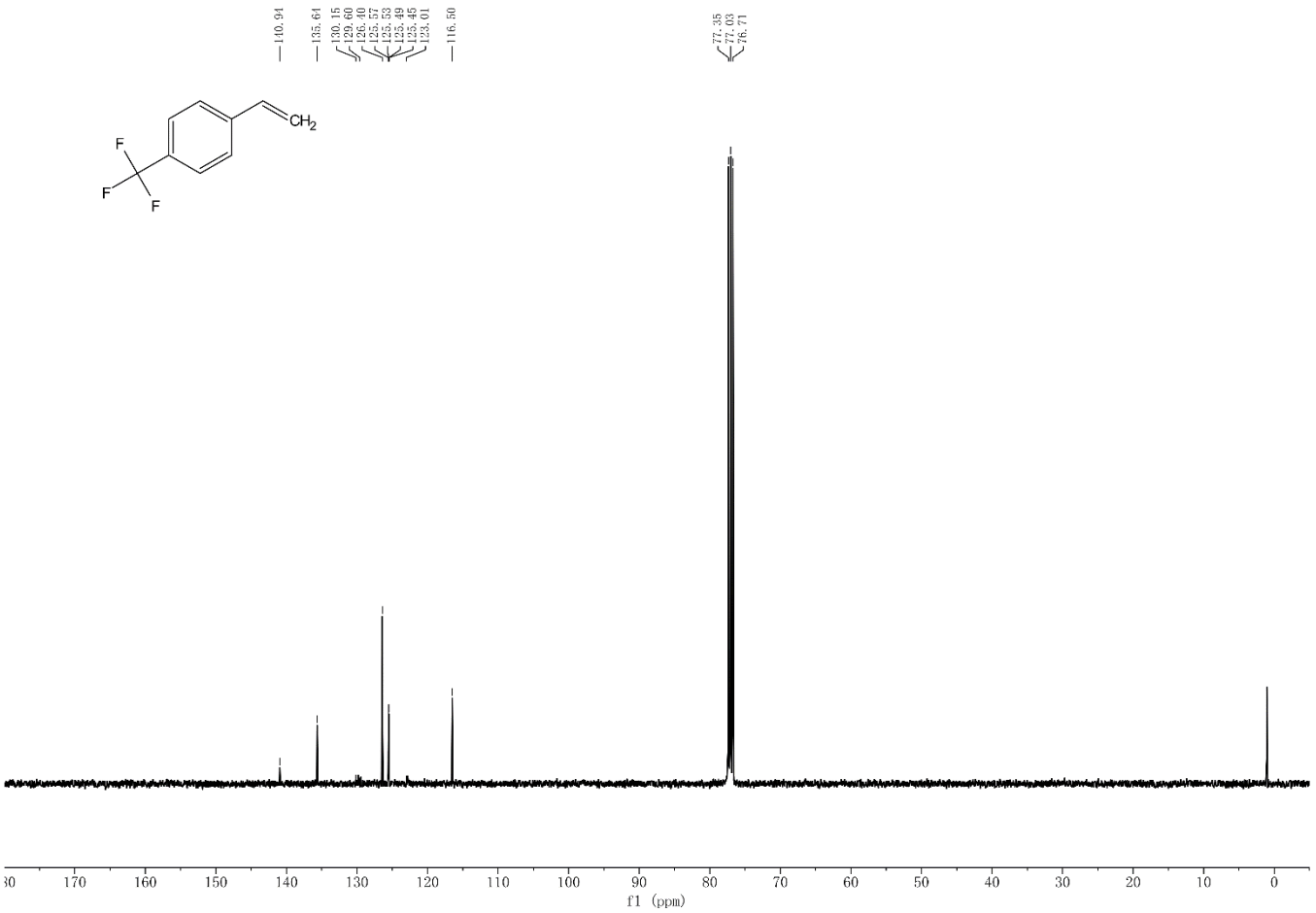
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 2h



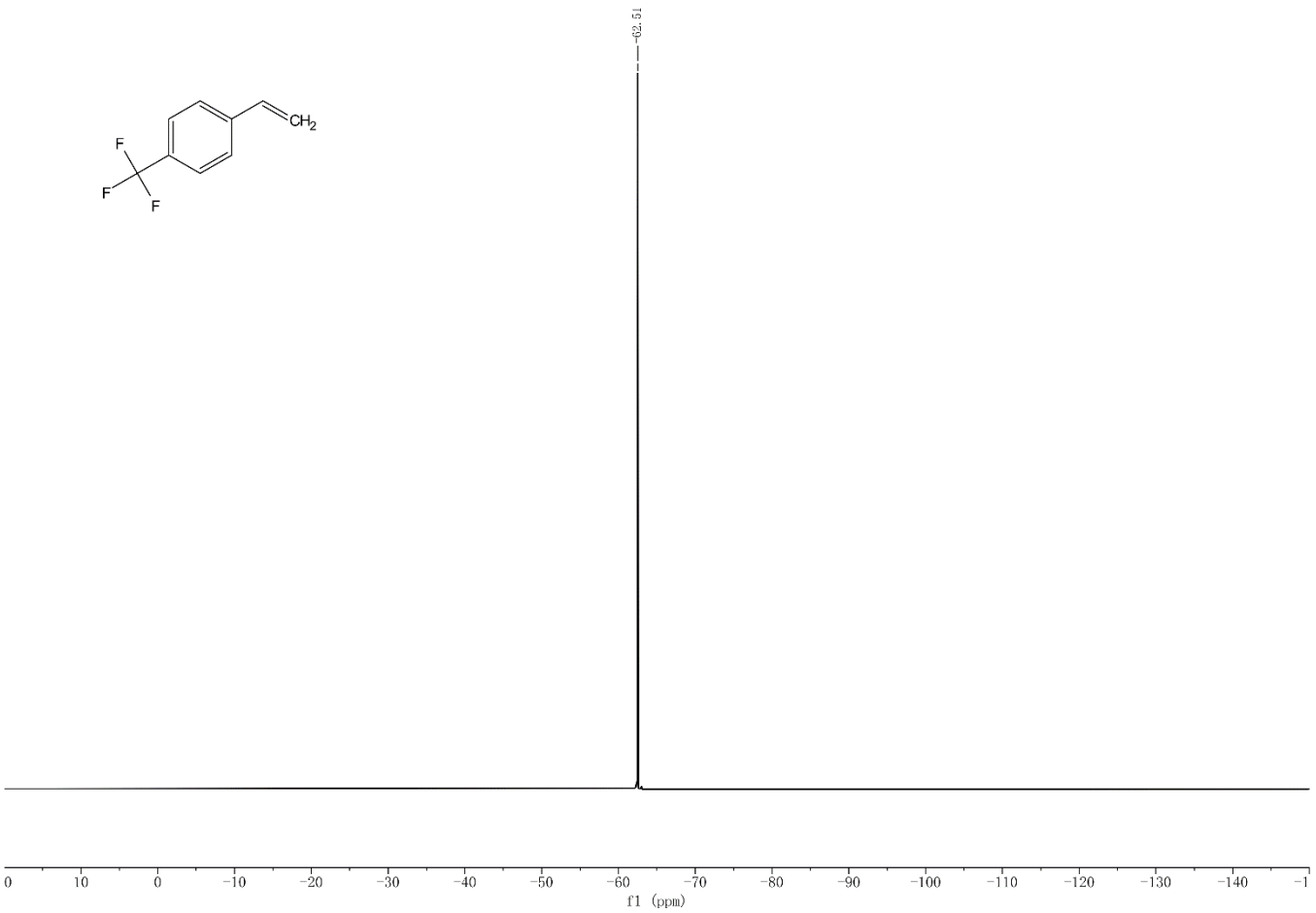
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 2i



$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 2i



^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 2i



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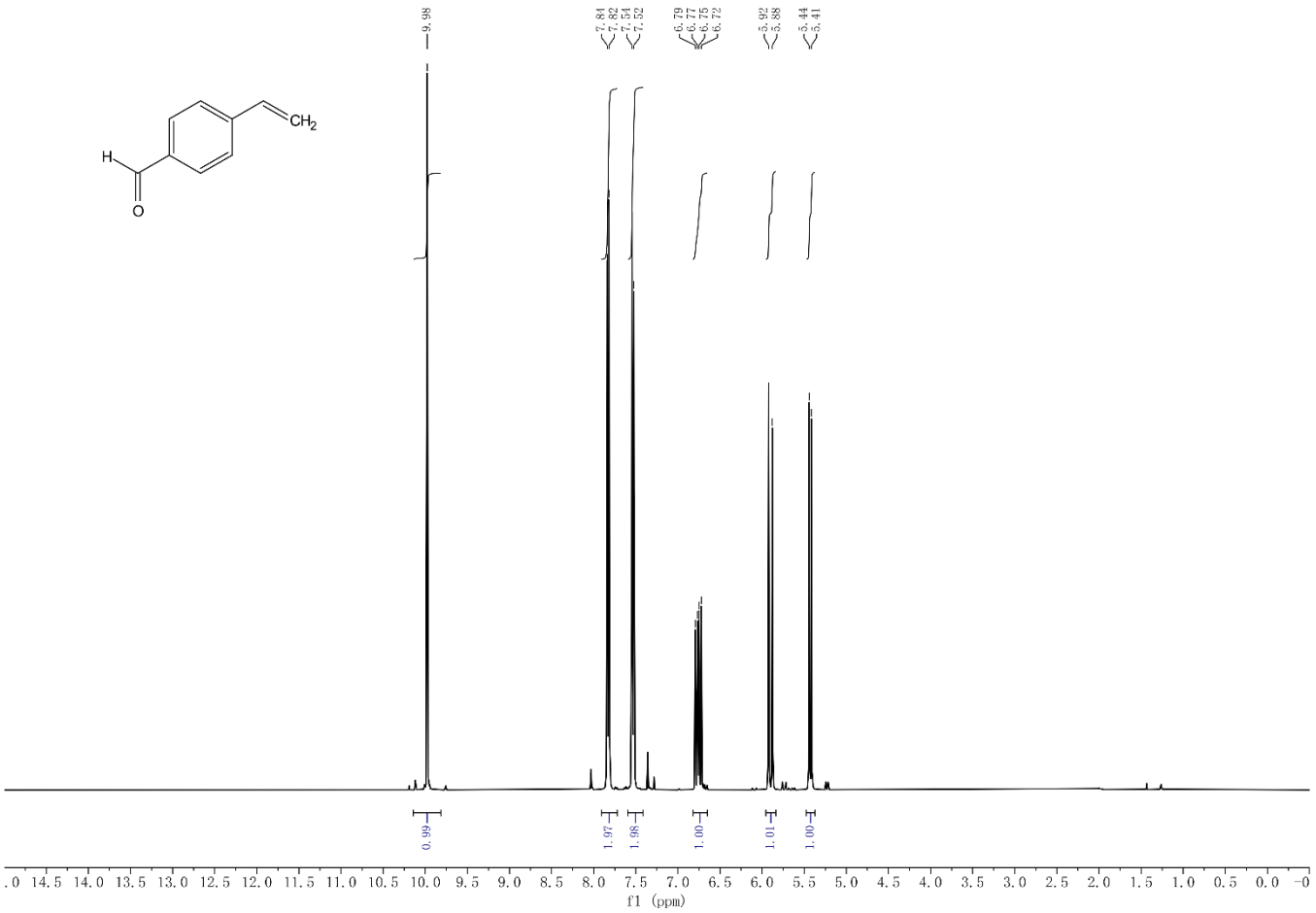

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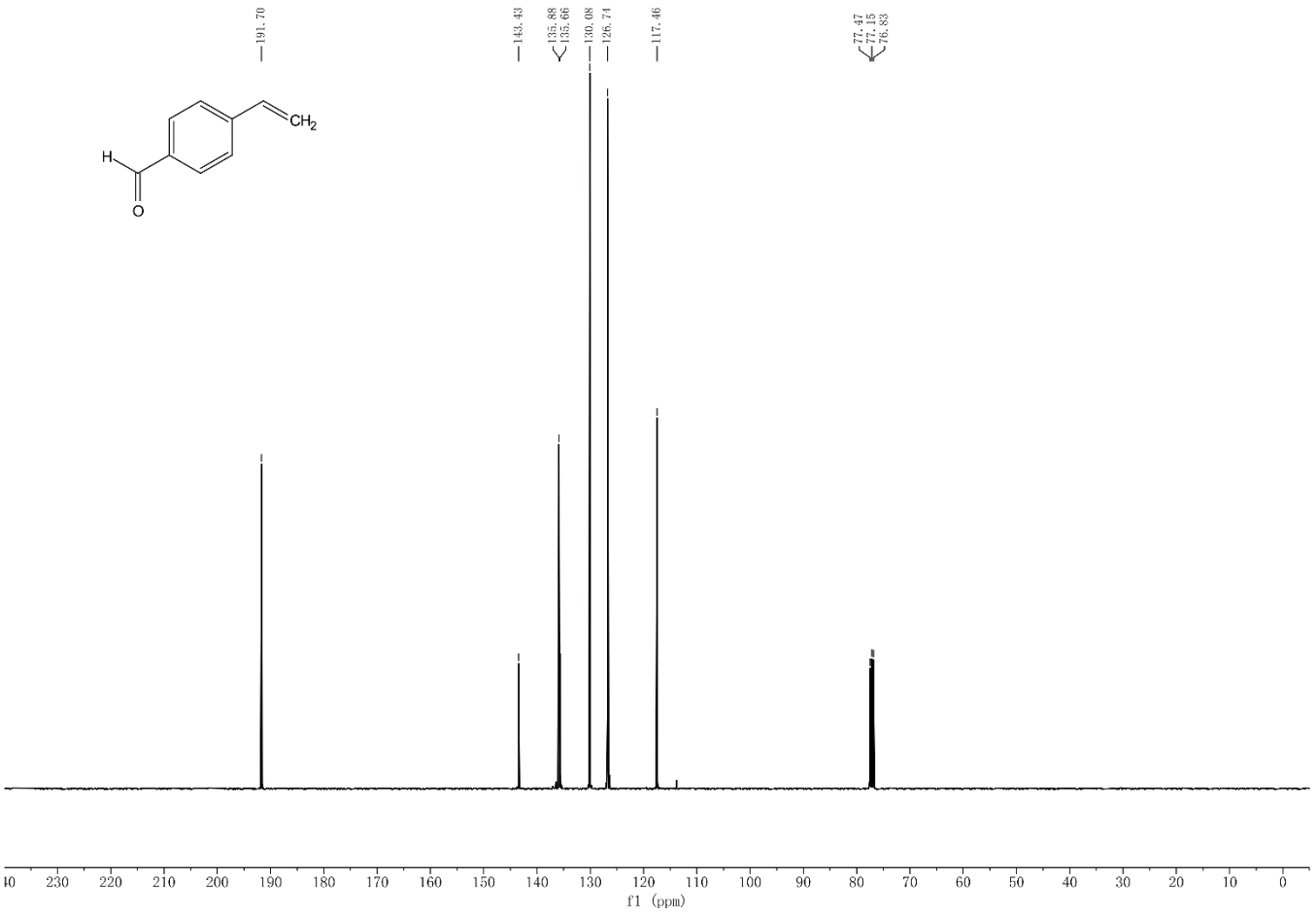

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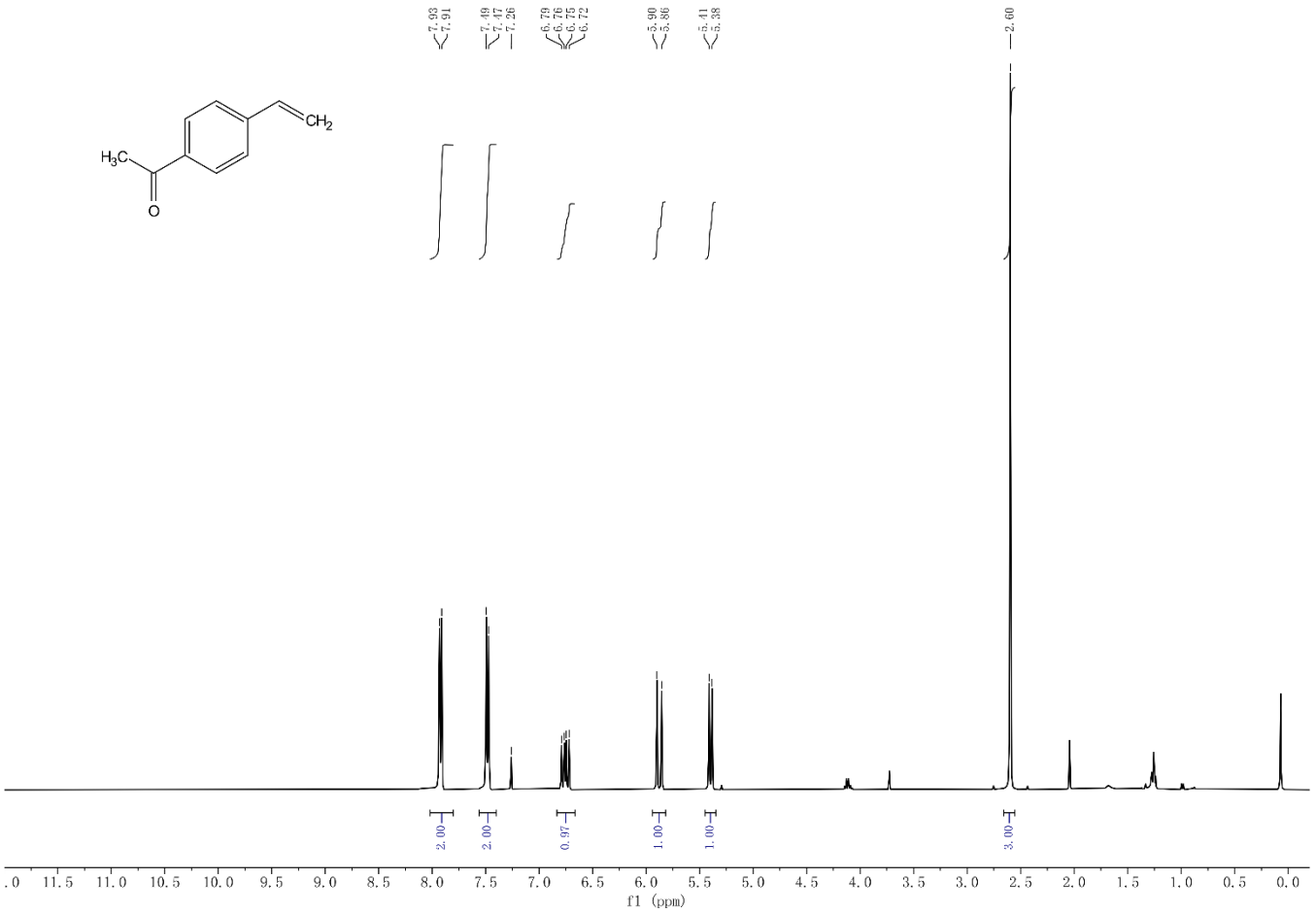

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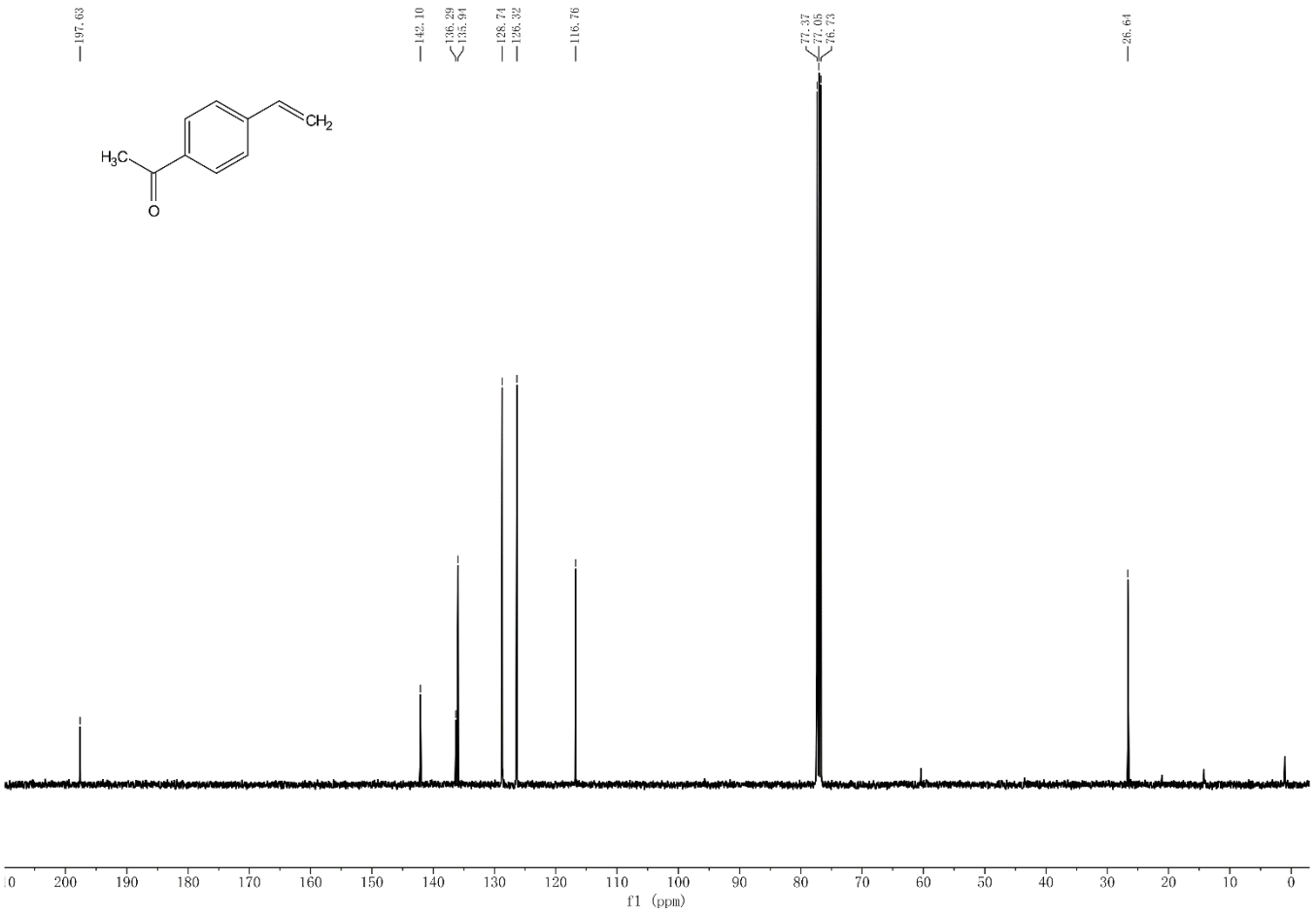

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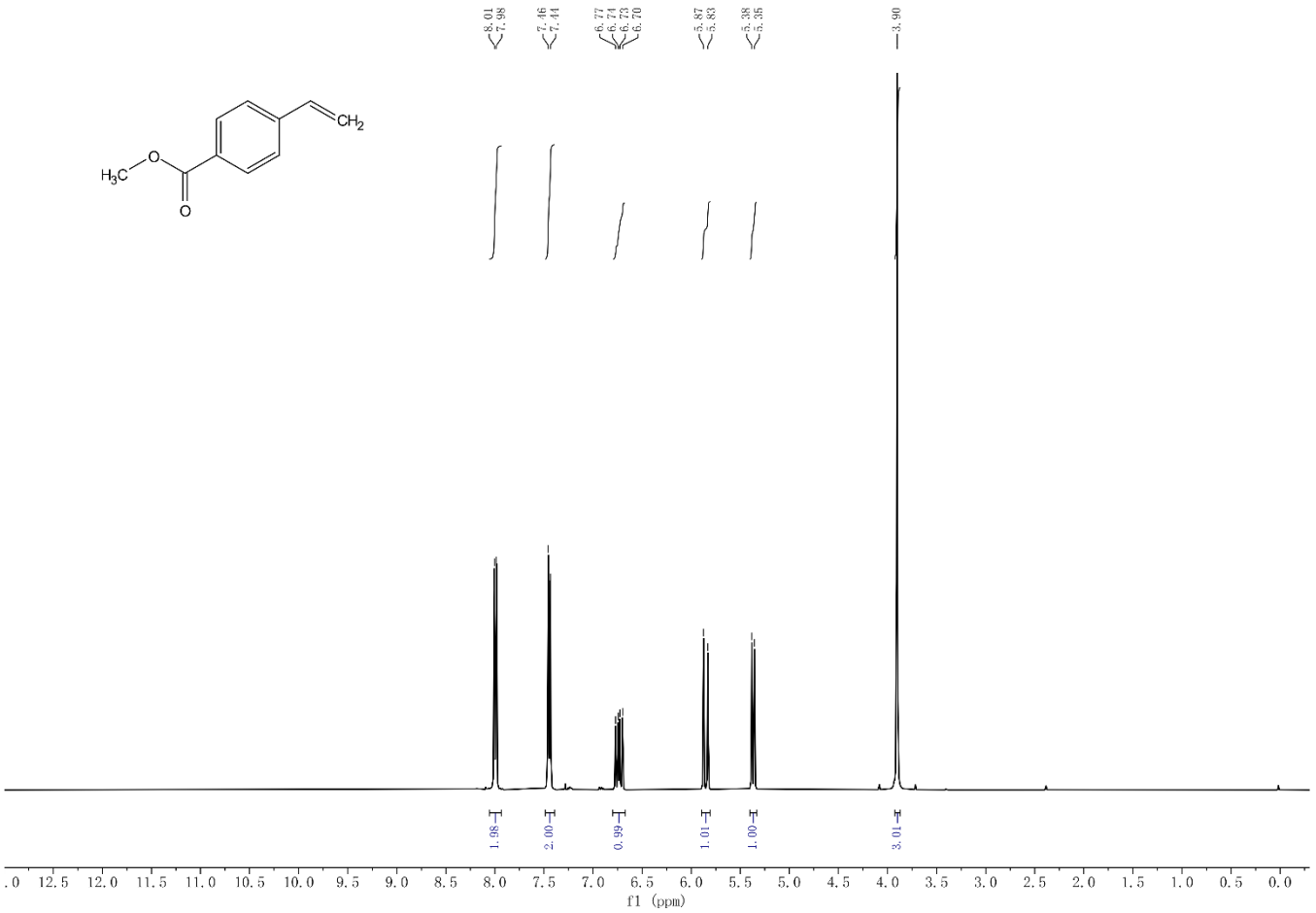

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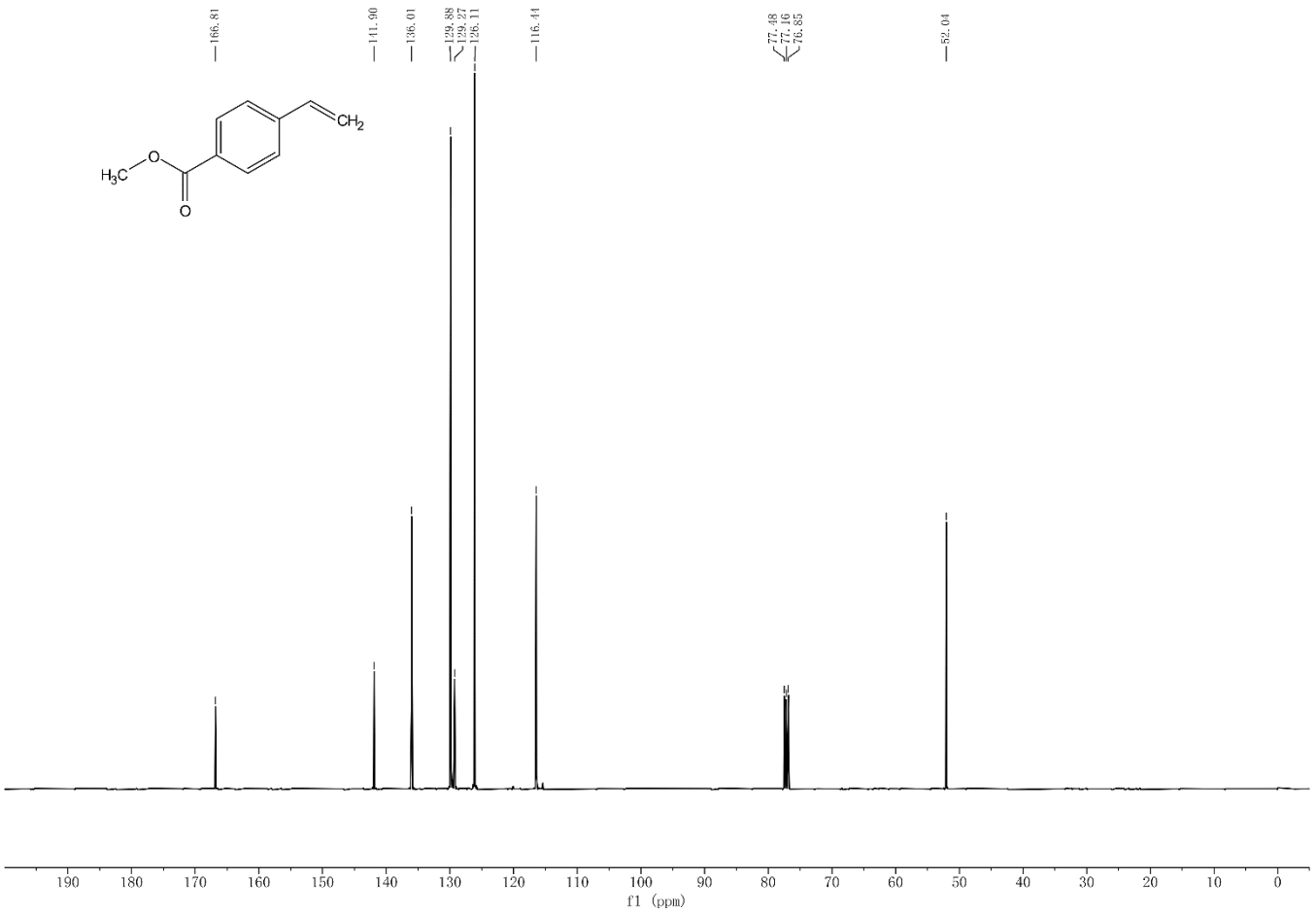

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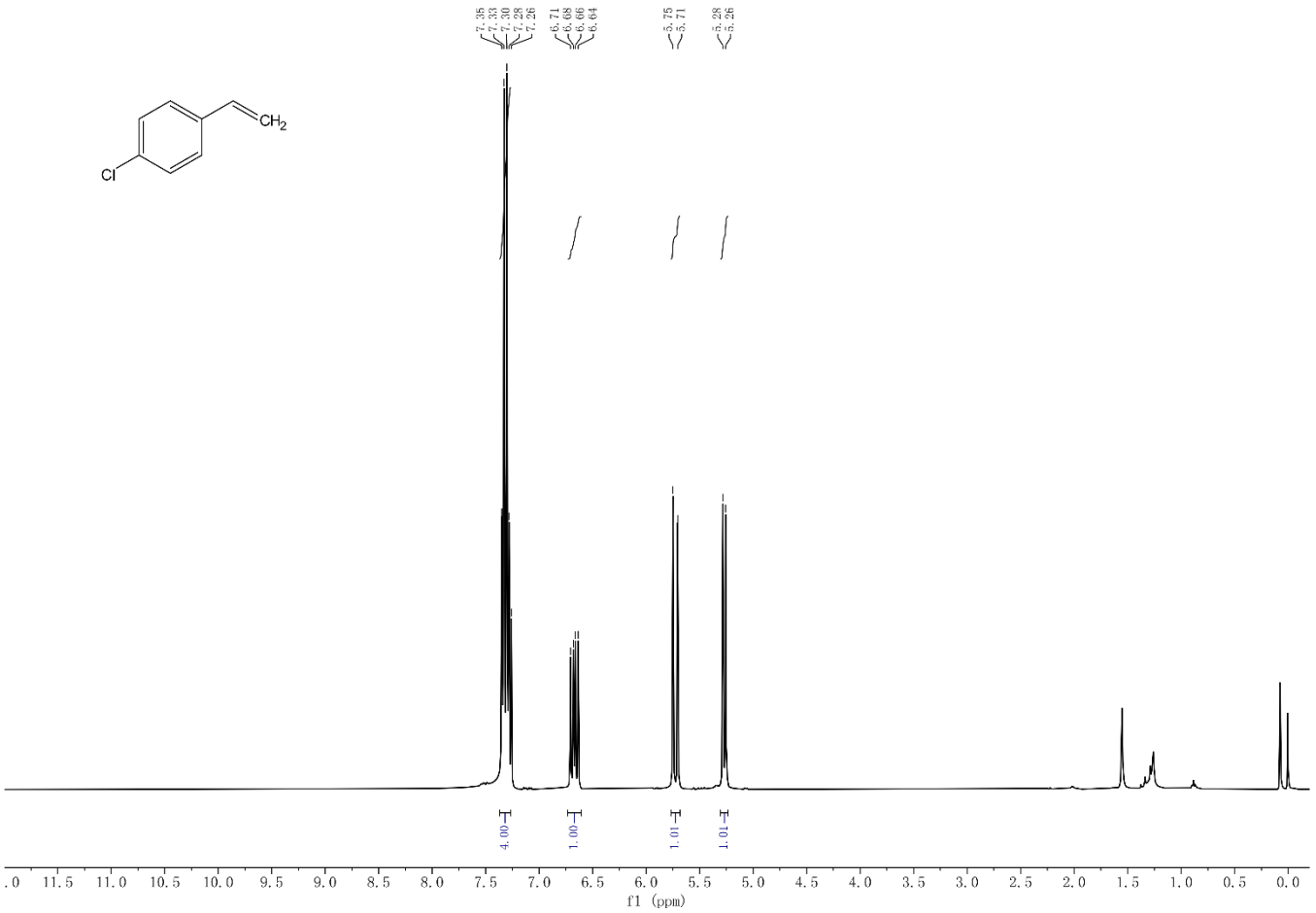

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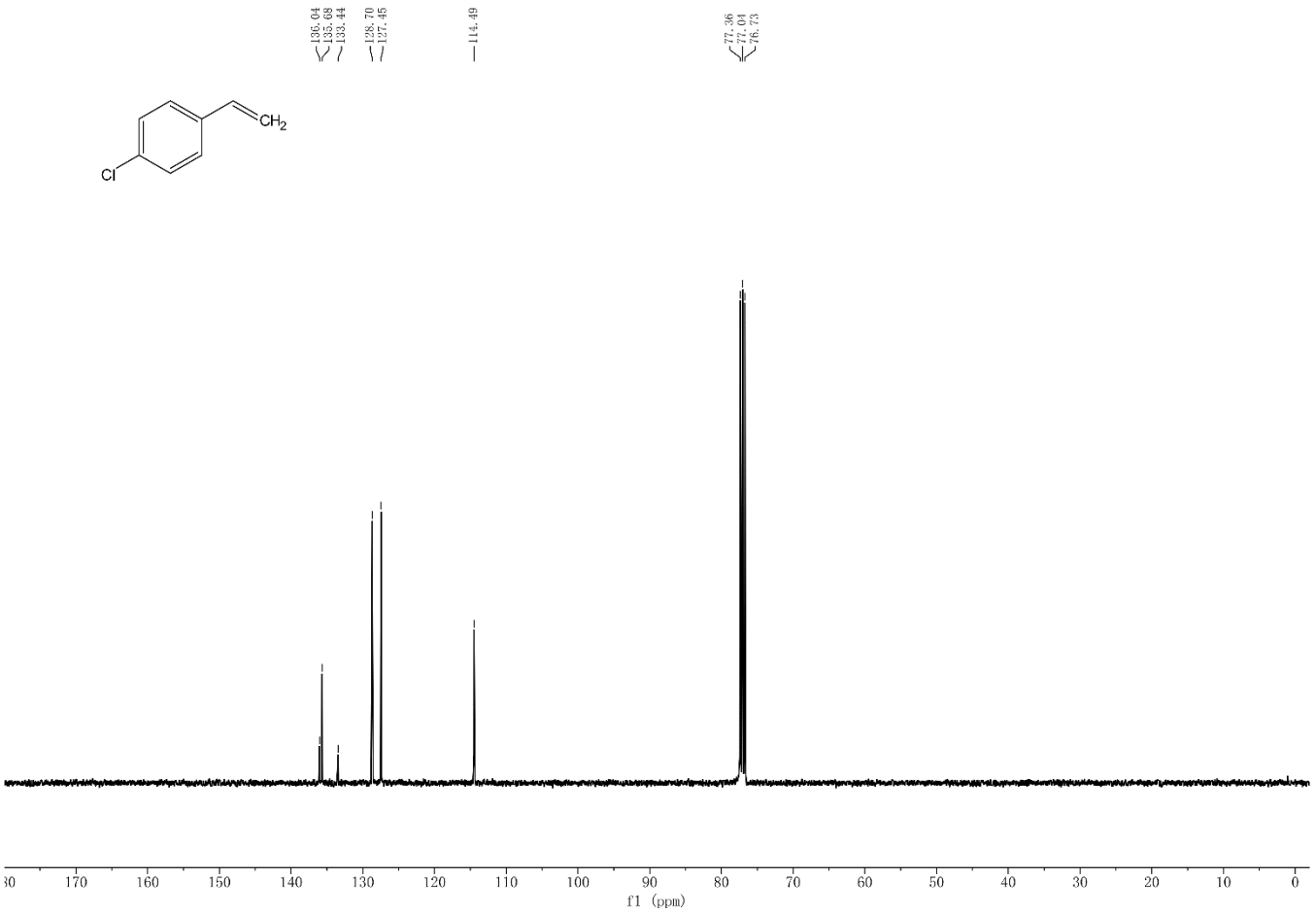

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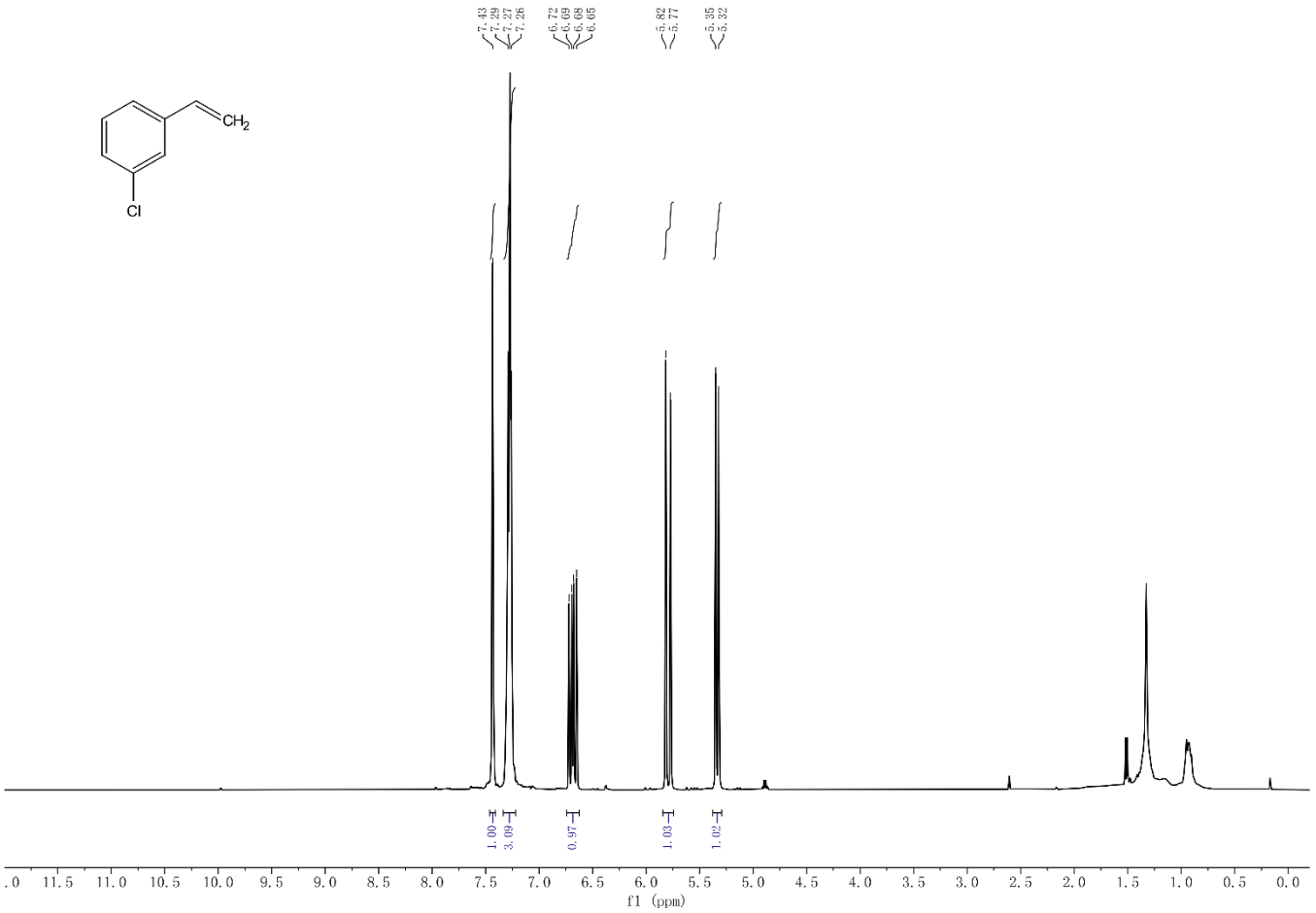

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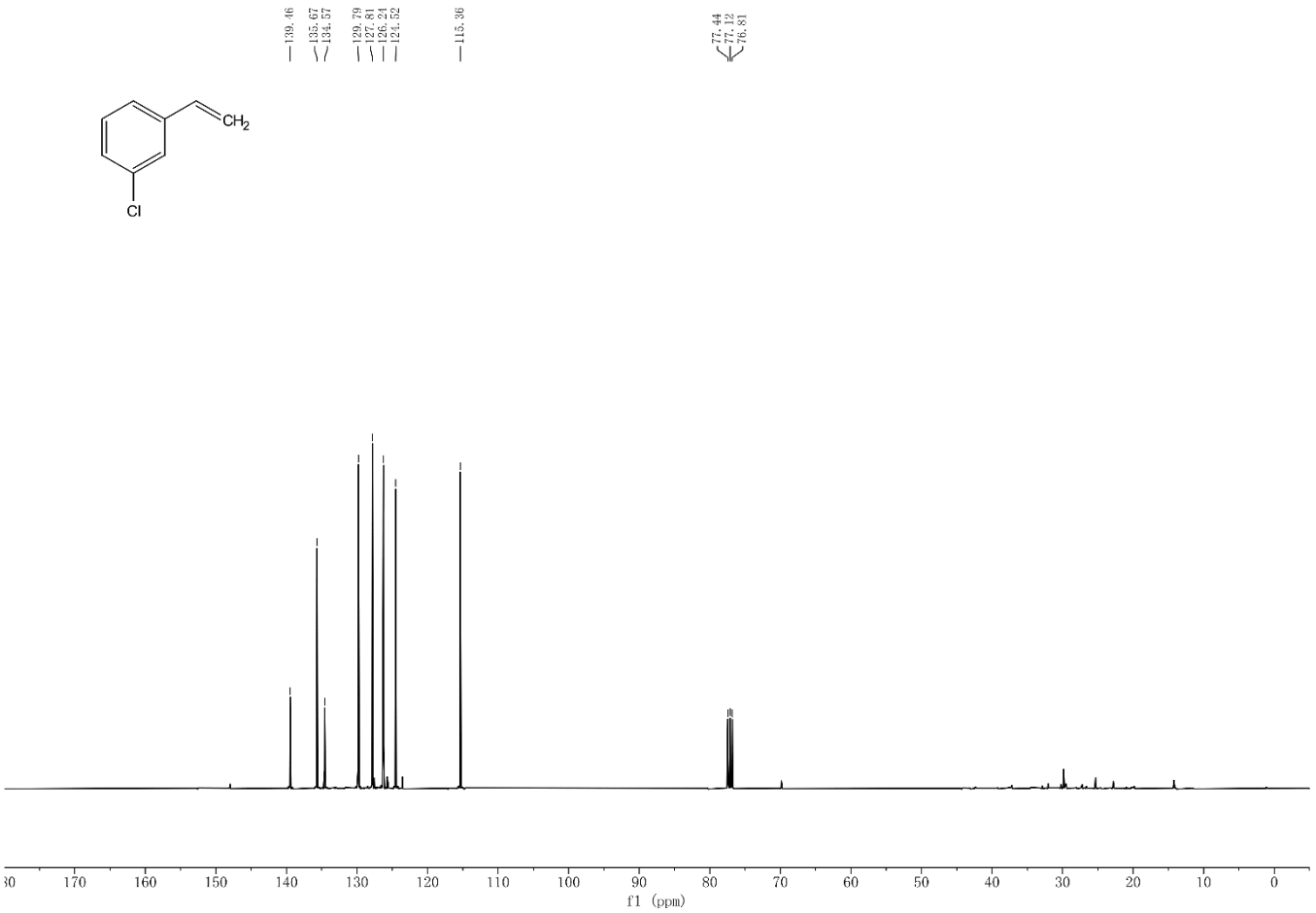

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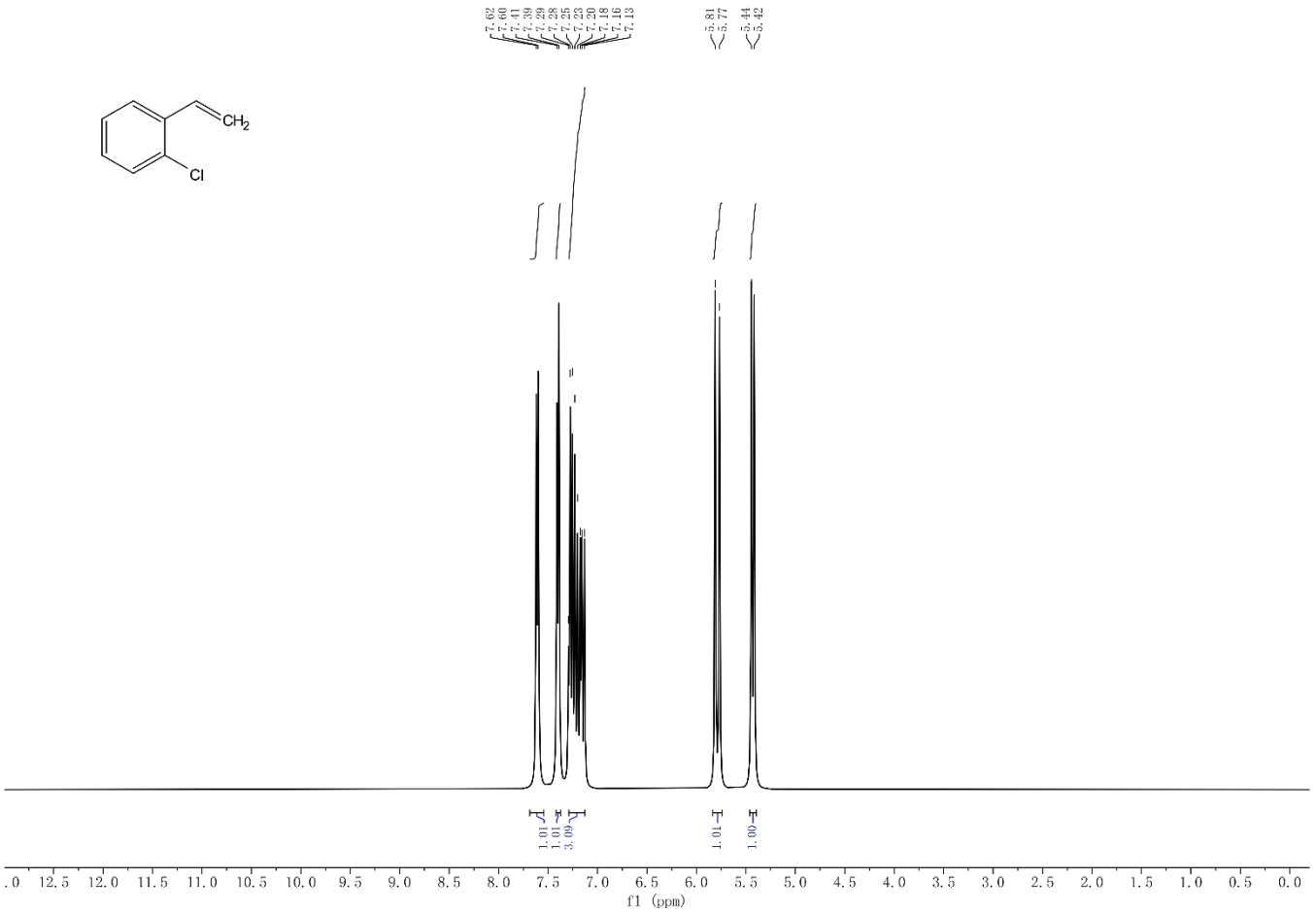

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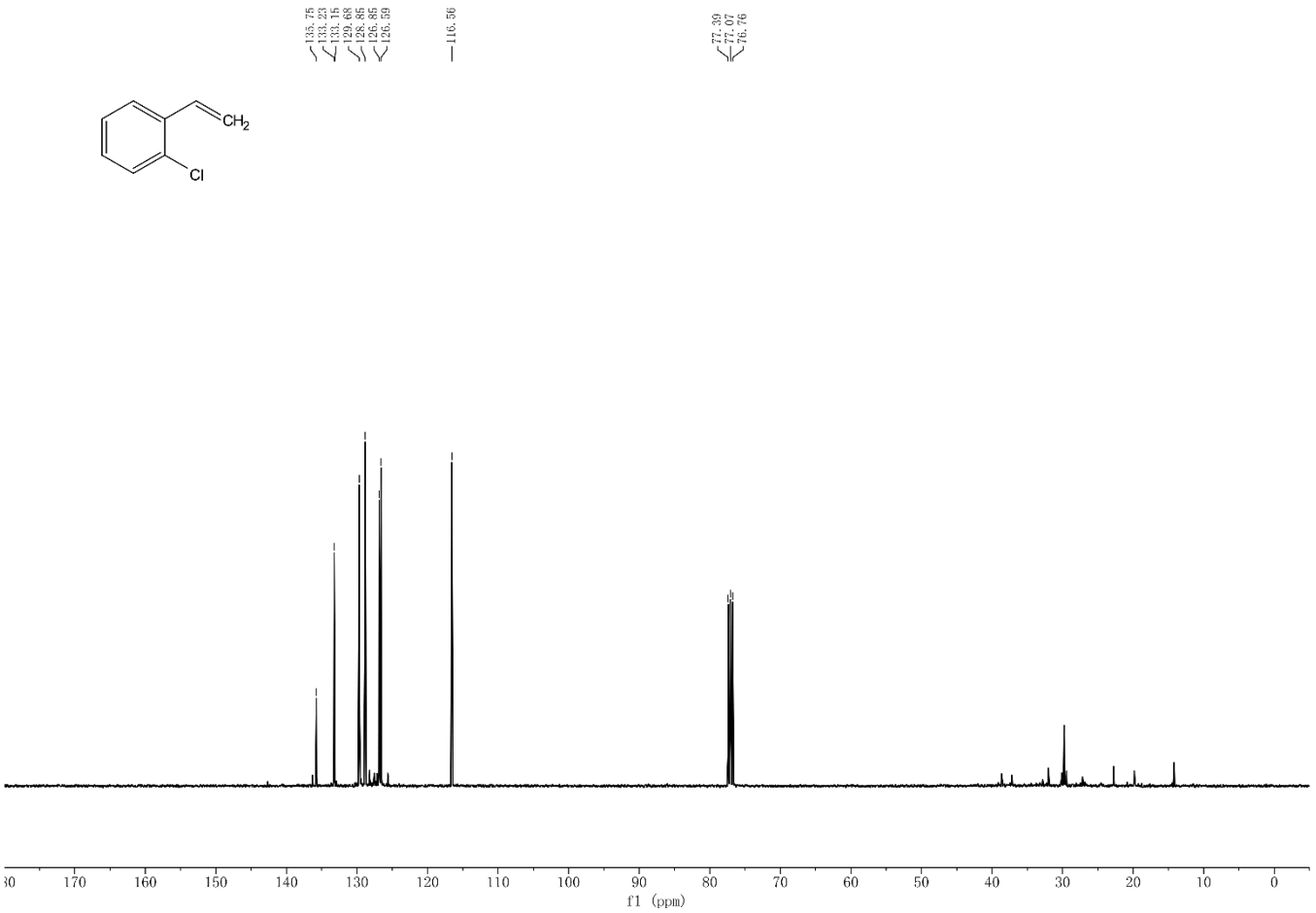

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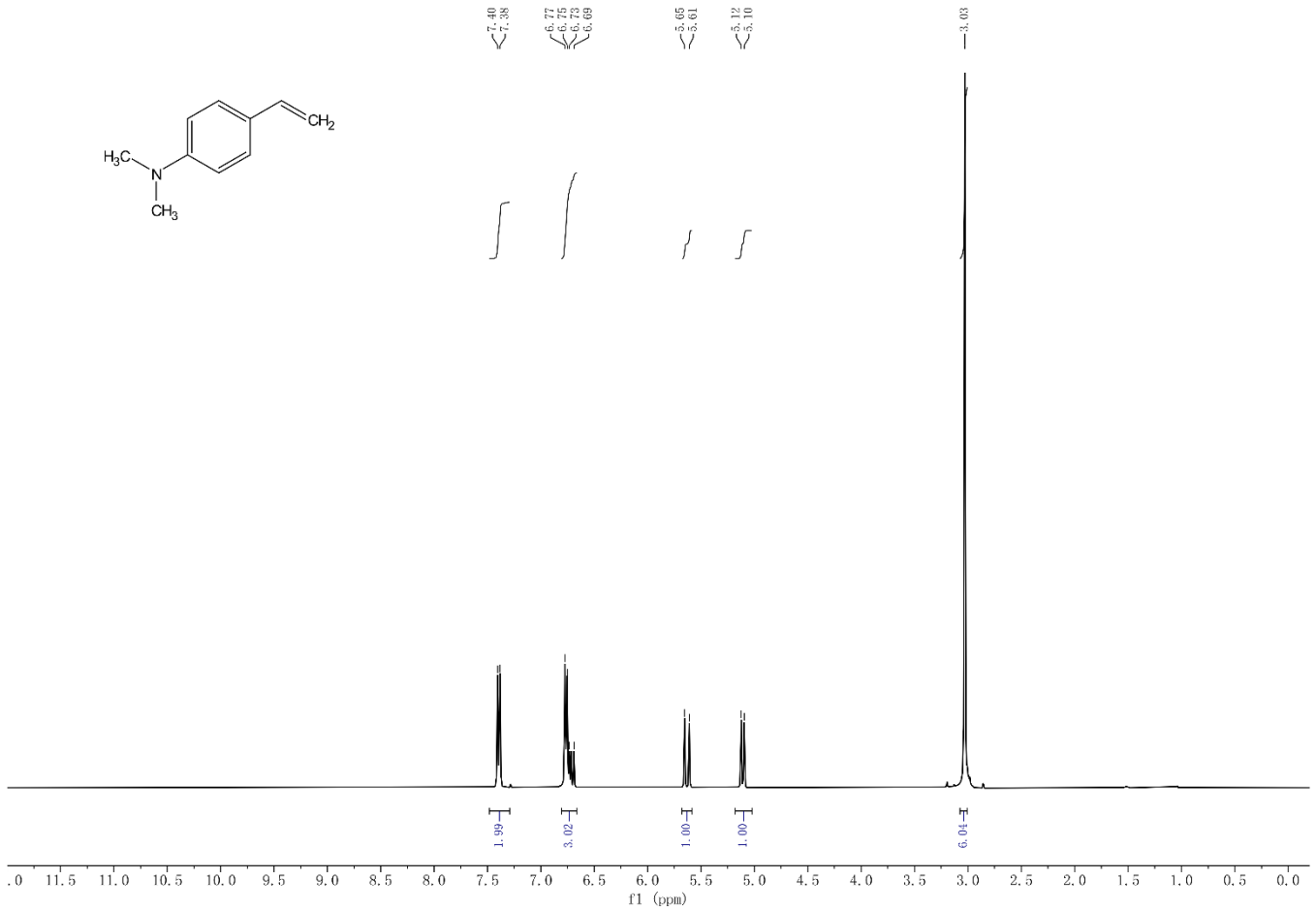

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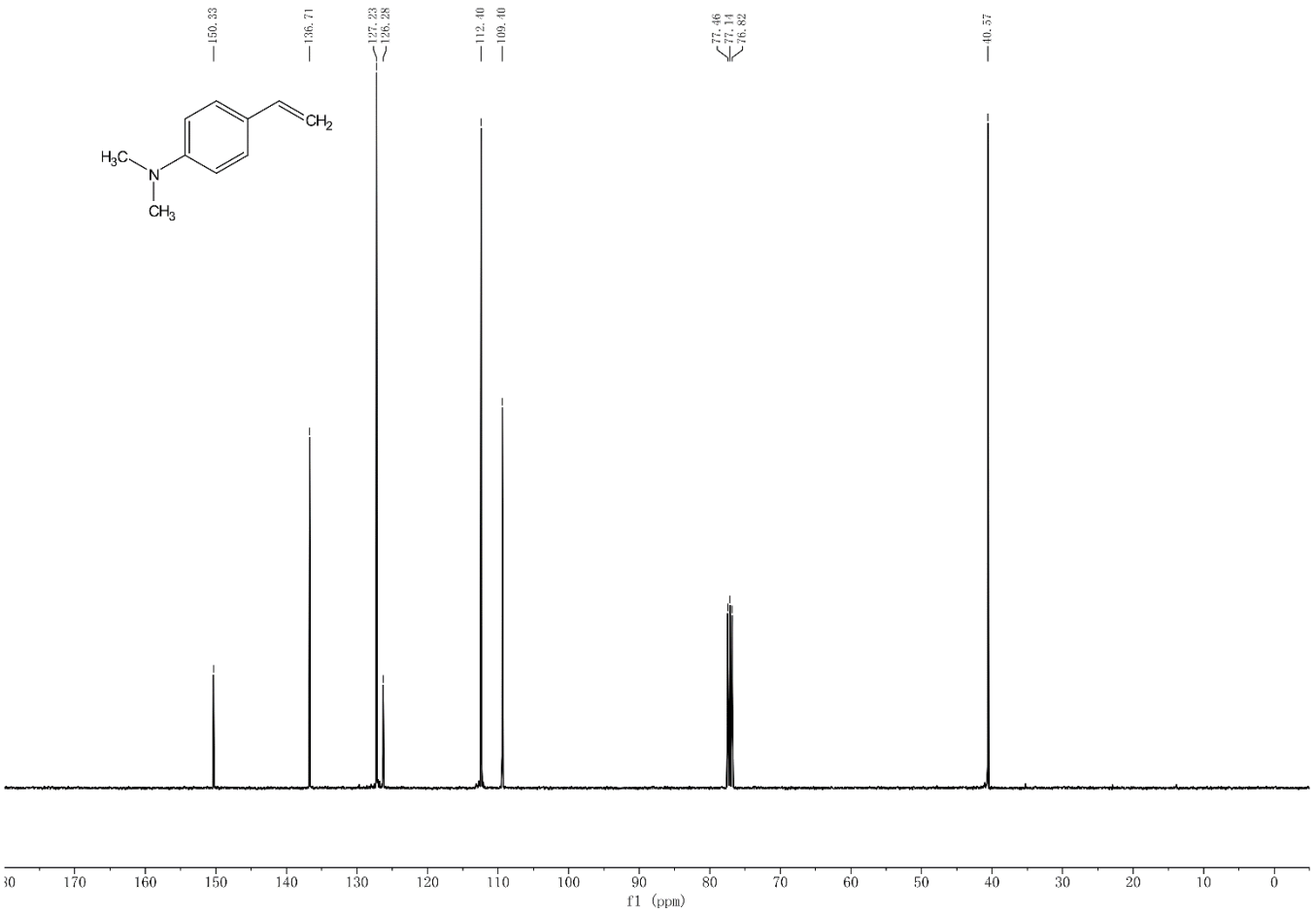

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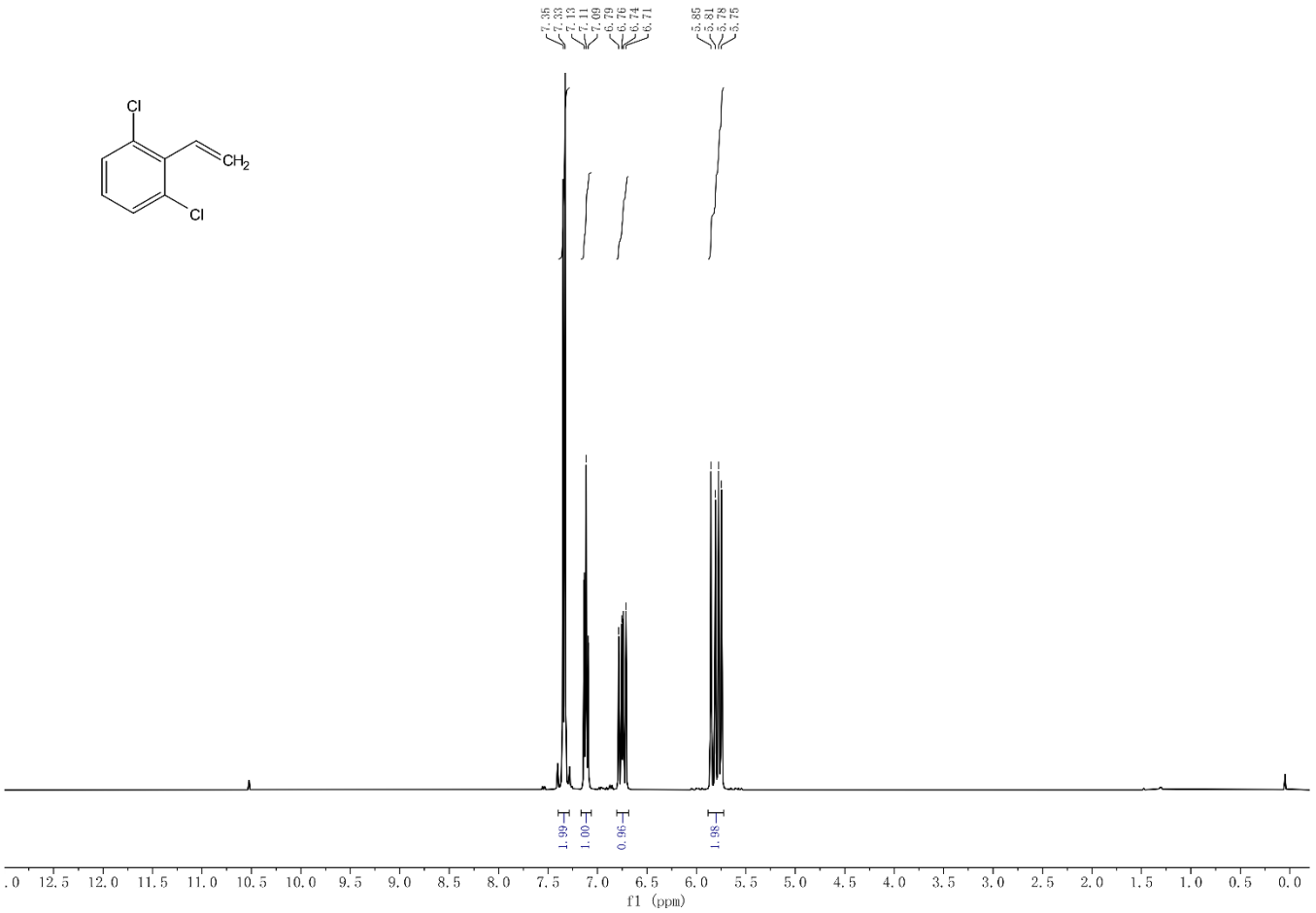

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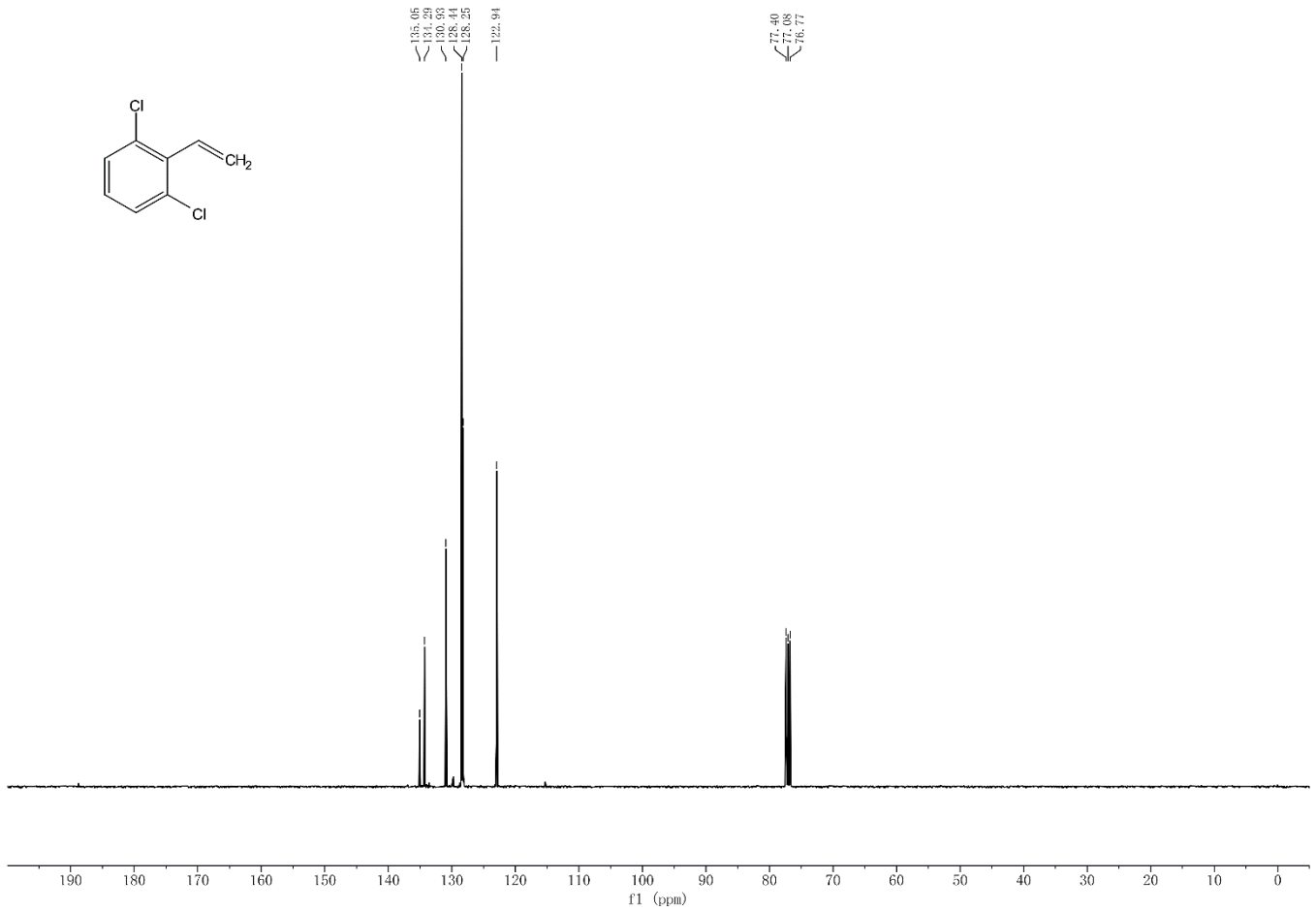

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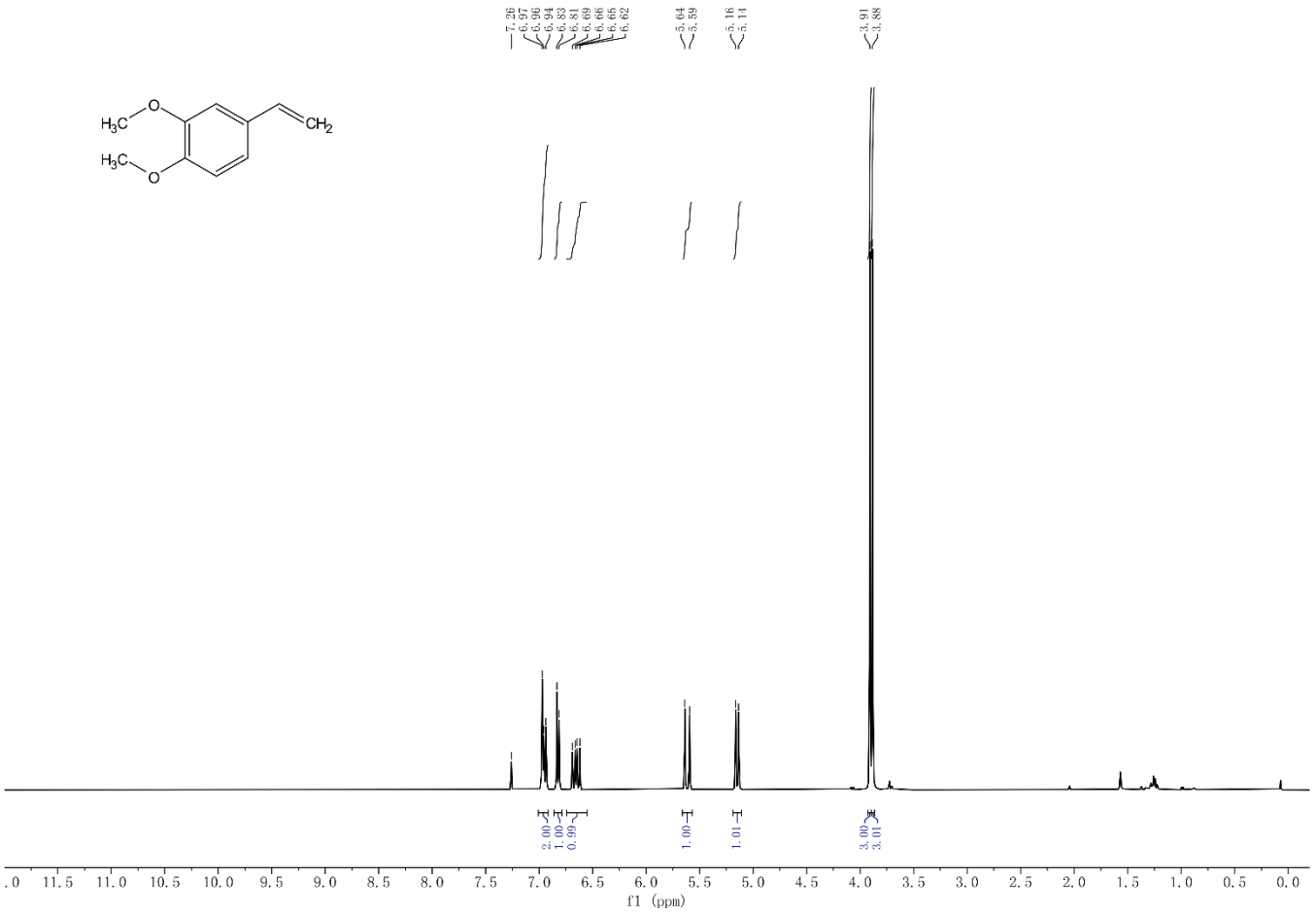

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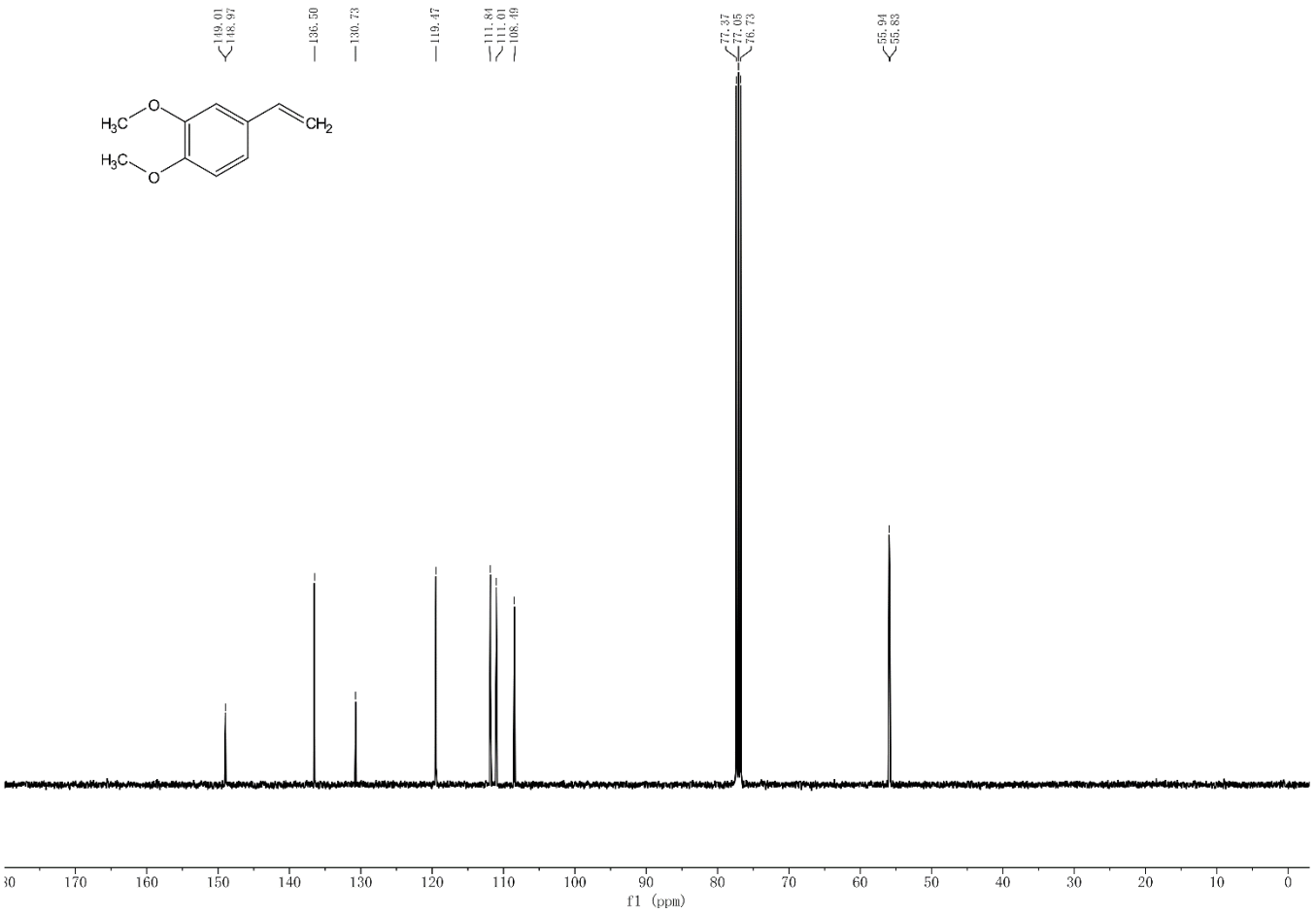

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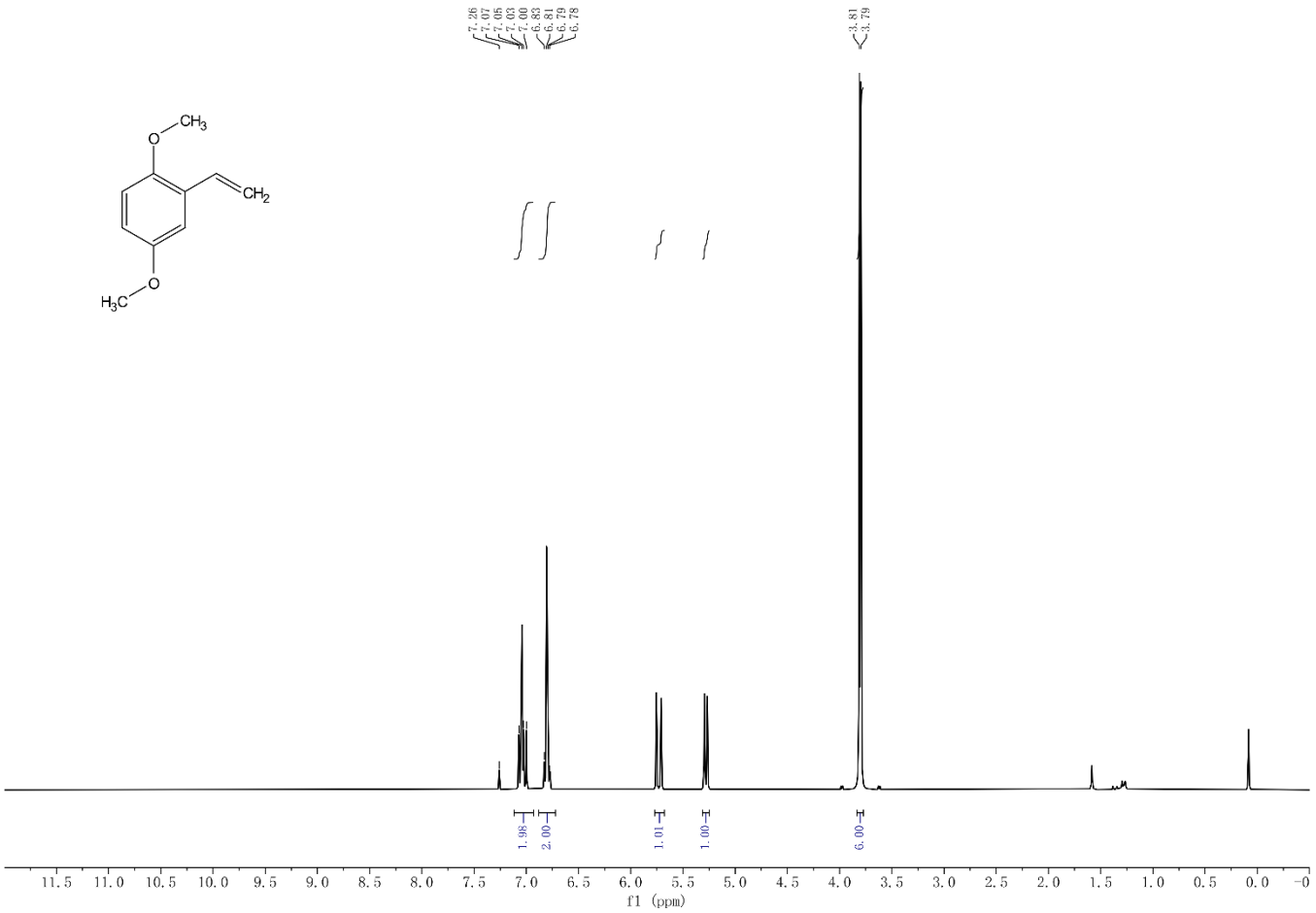
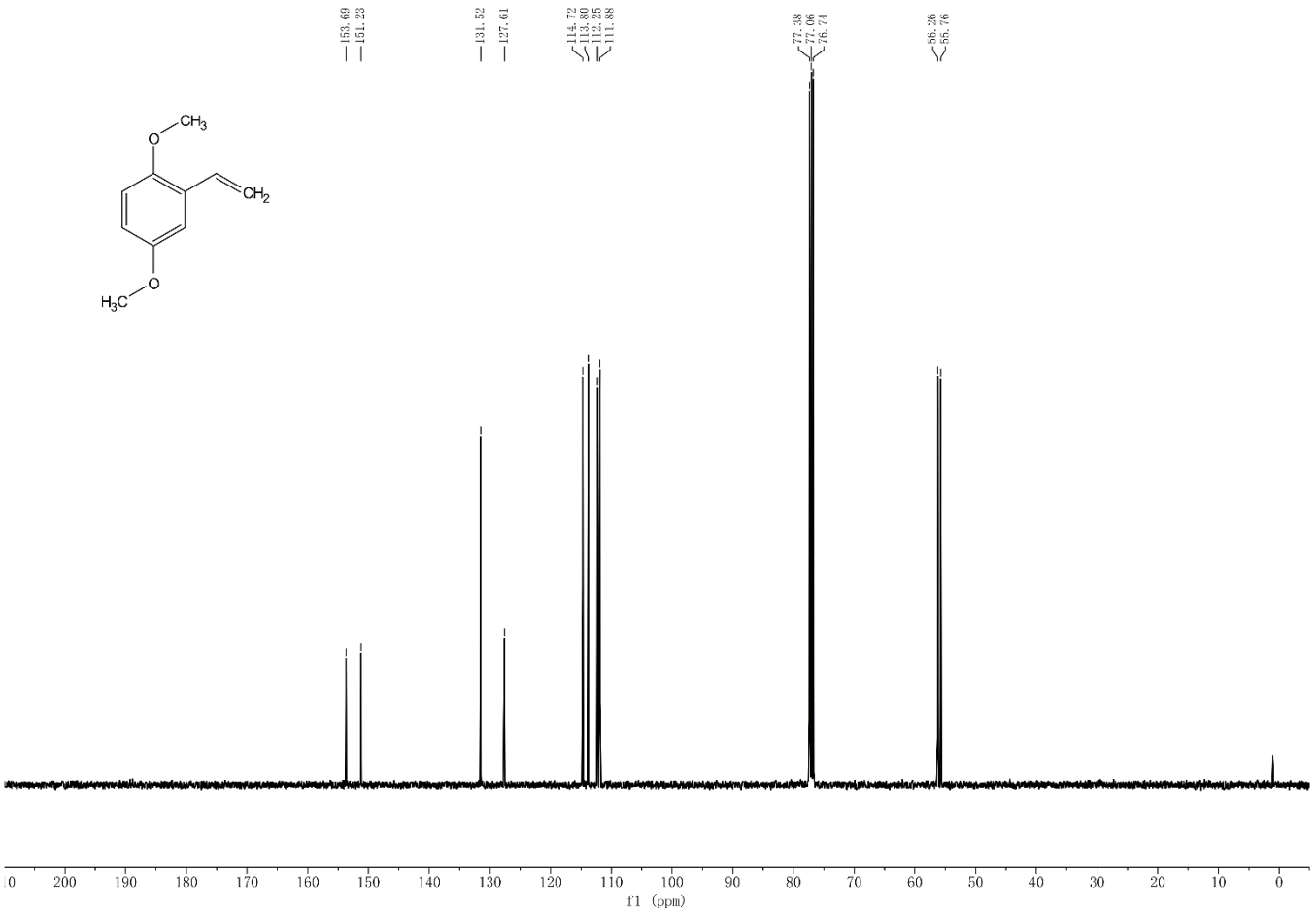
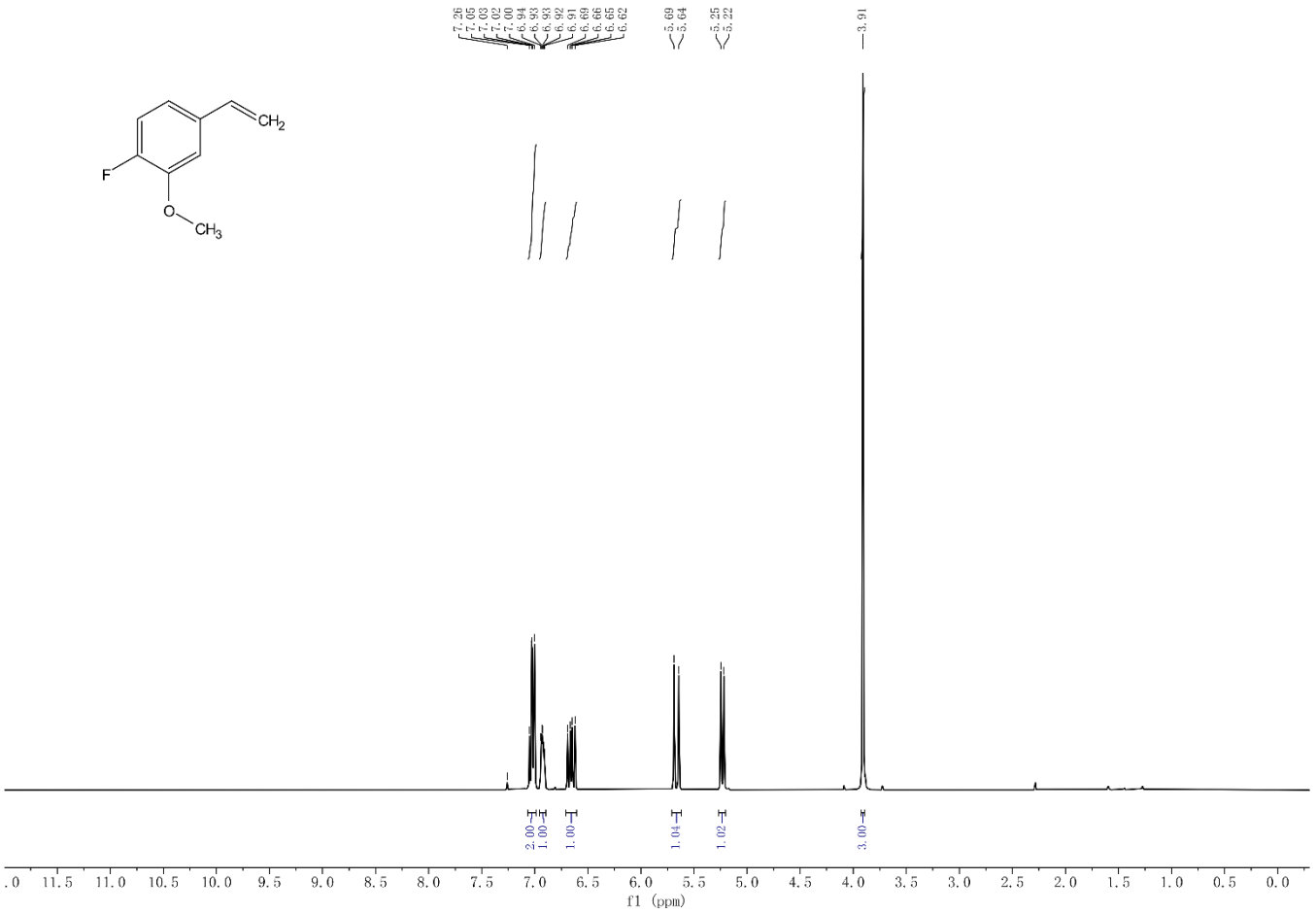


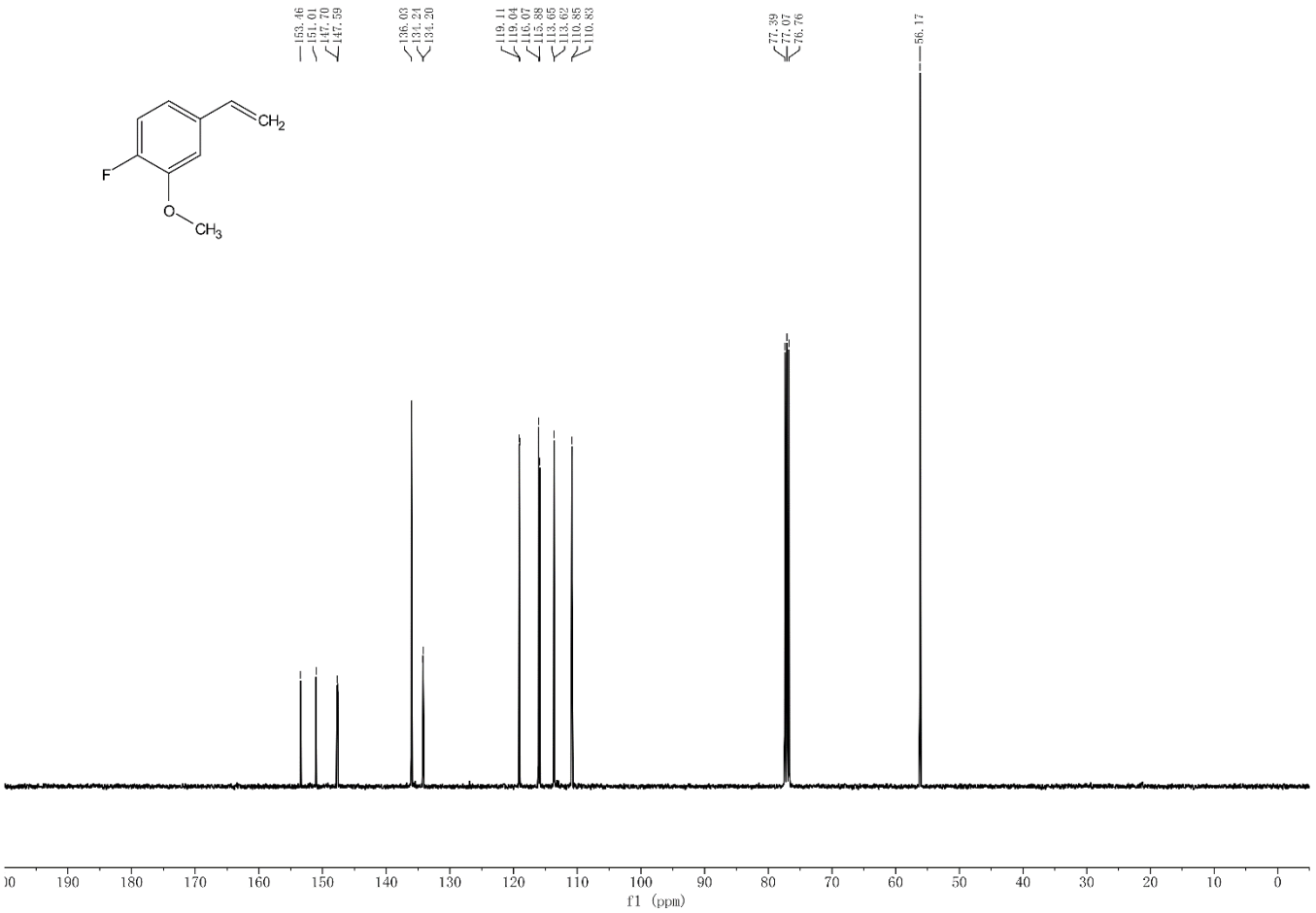
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3g



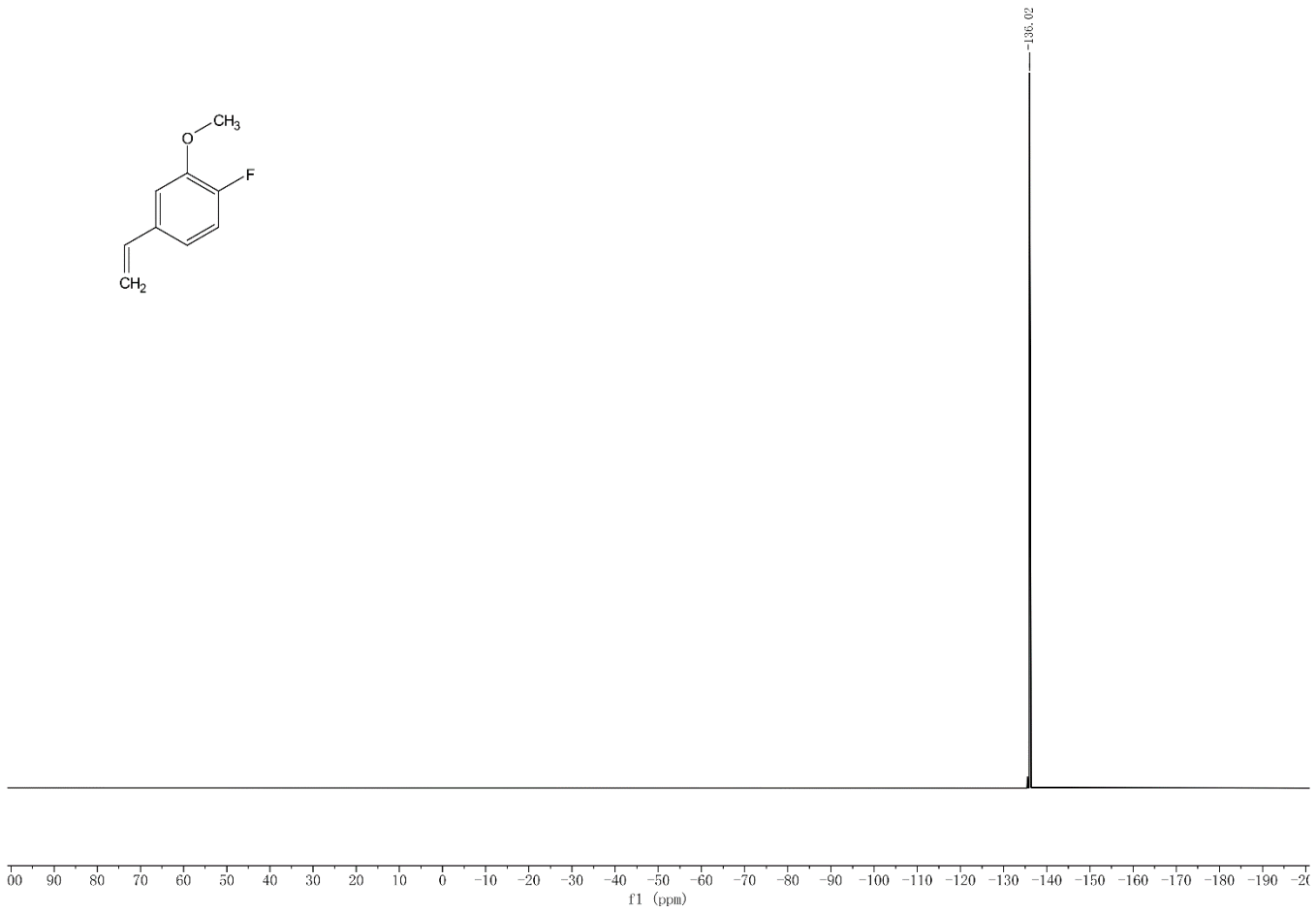
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3h



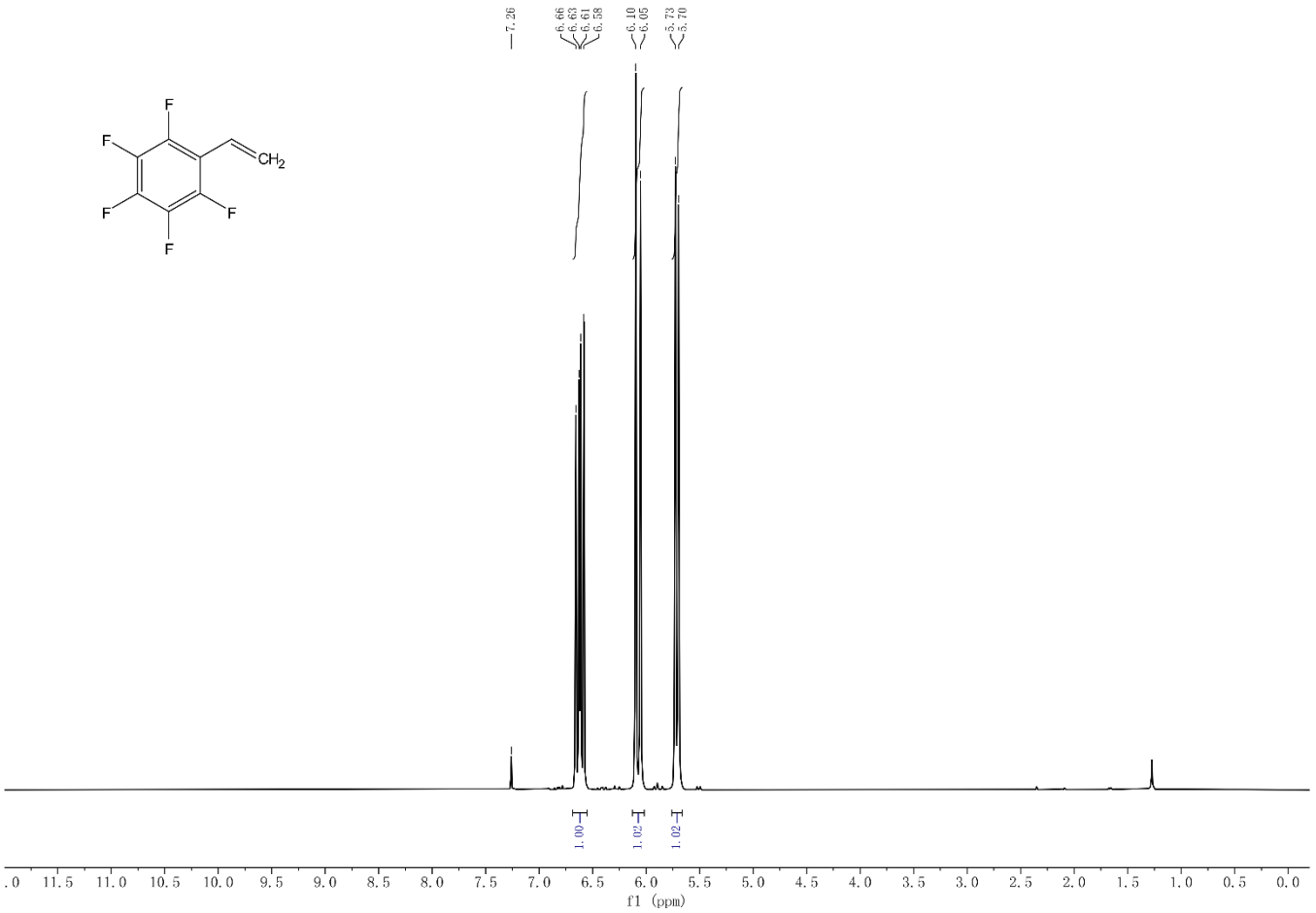
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3h



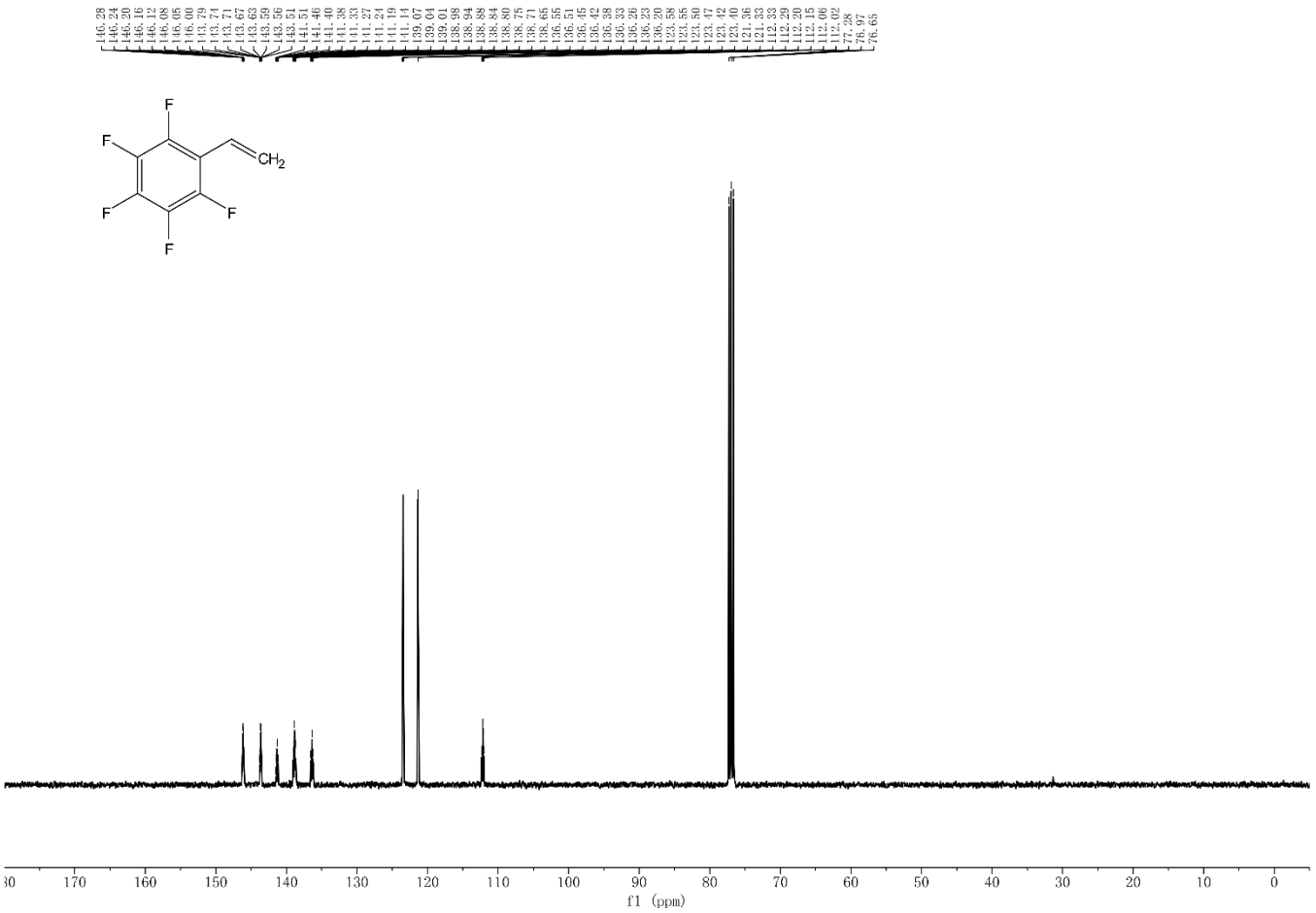
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 3h



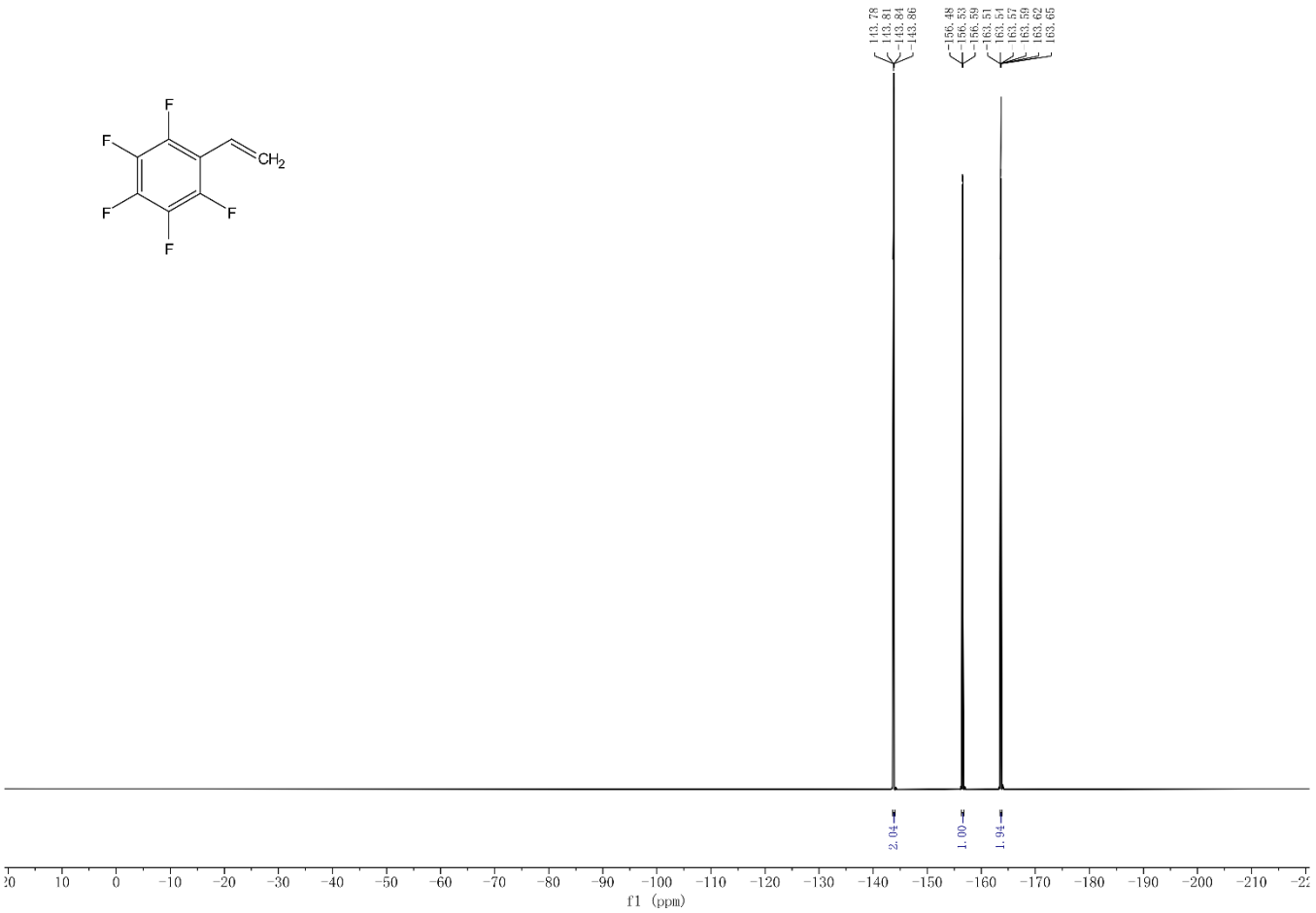
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3i



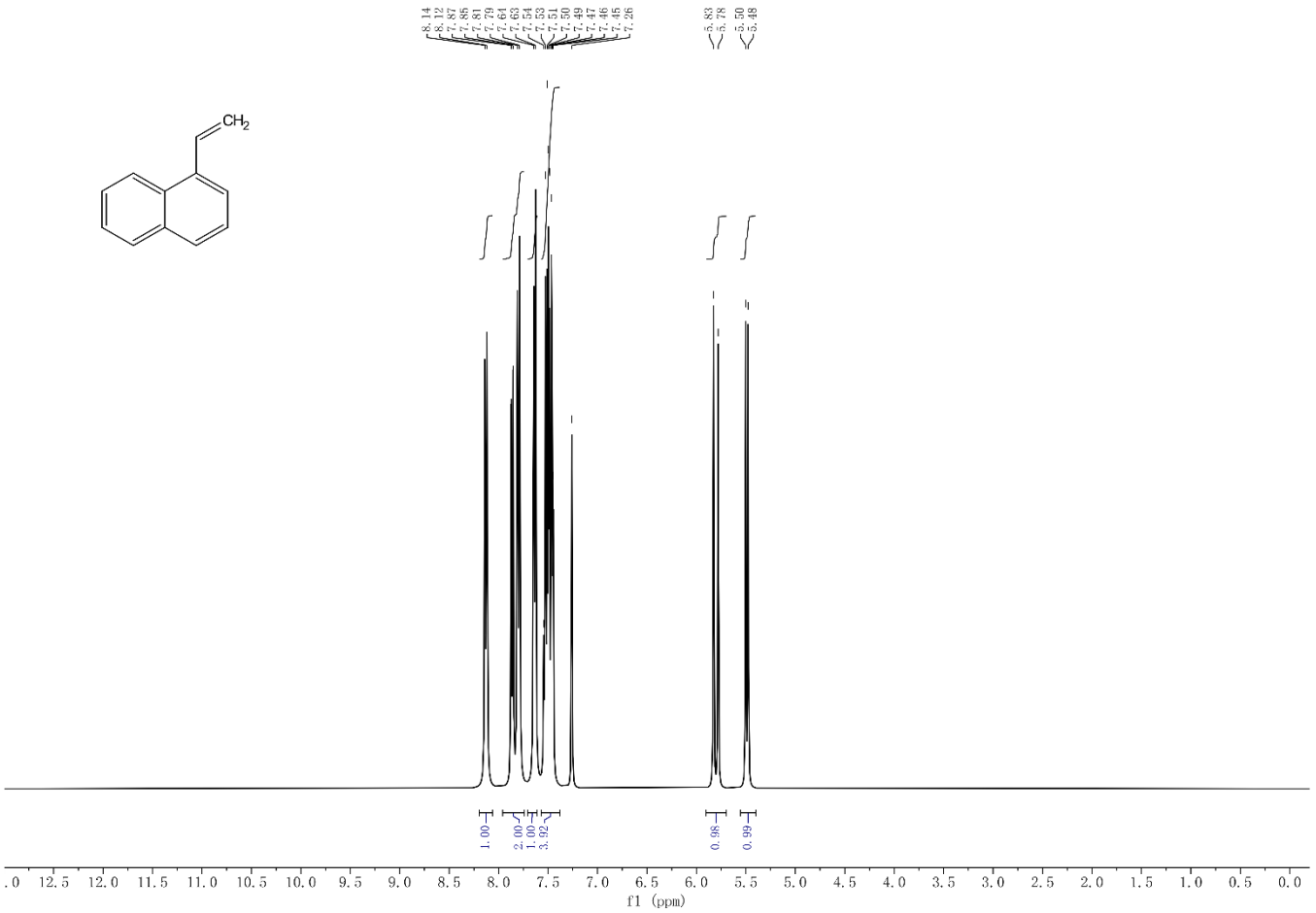
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3i



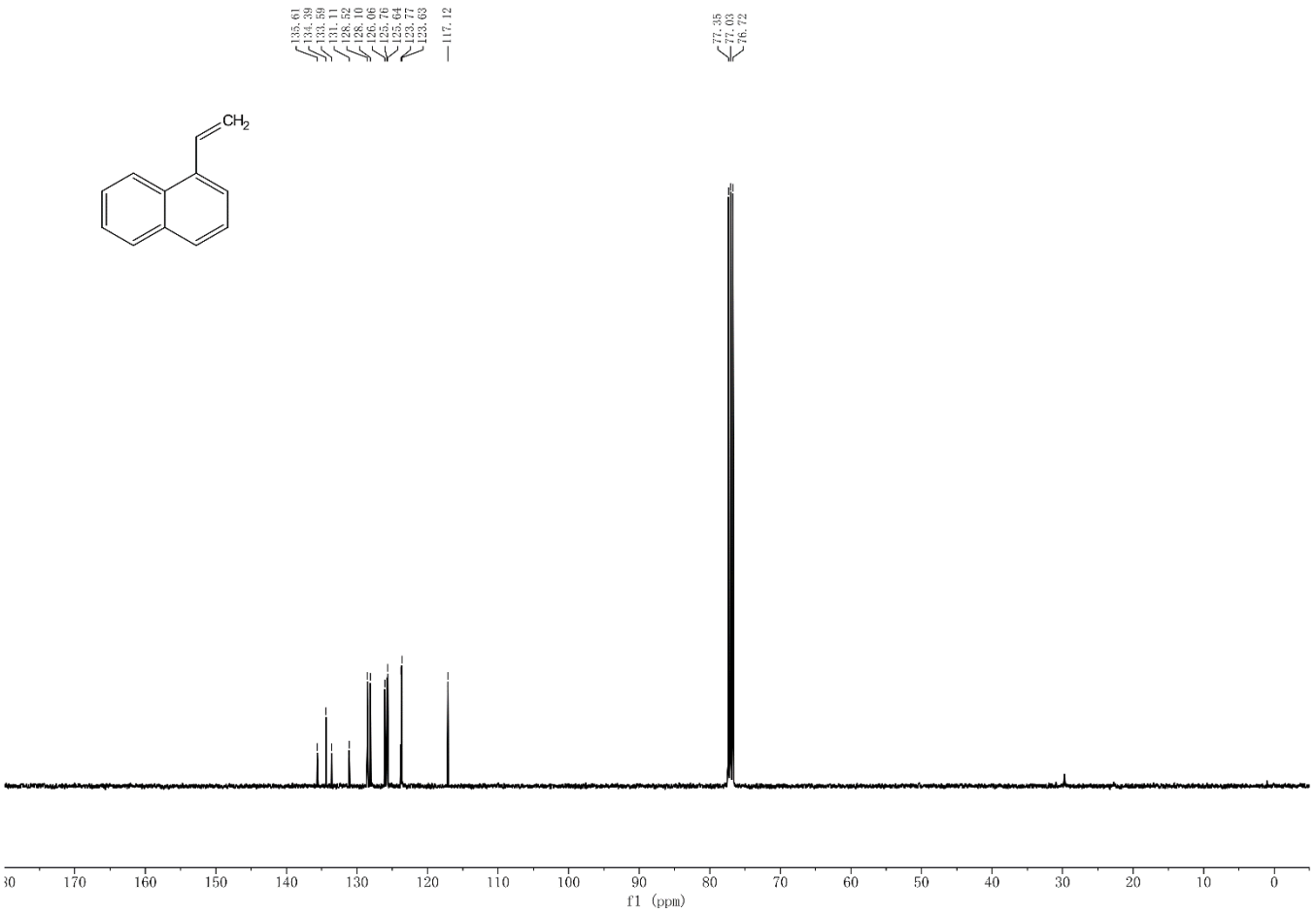
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 3i



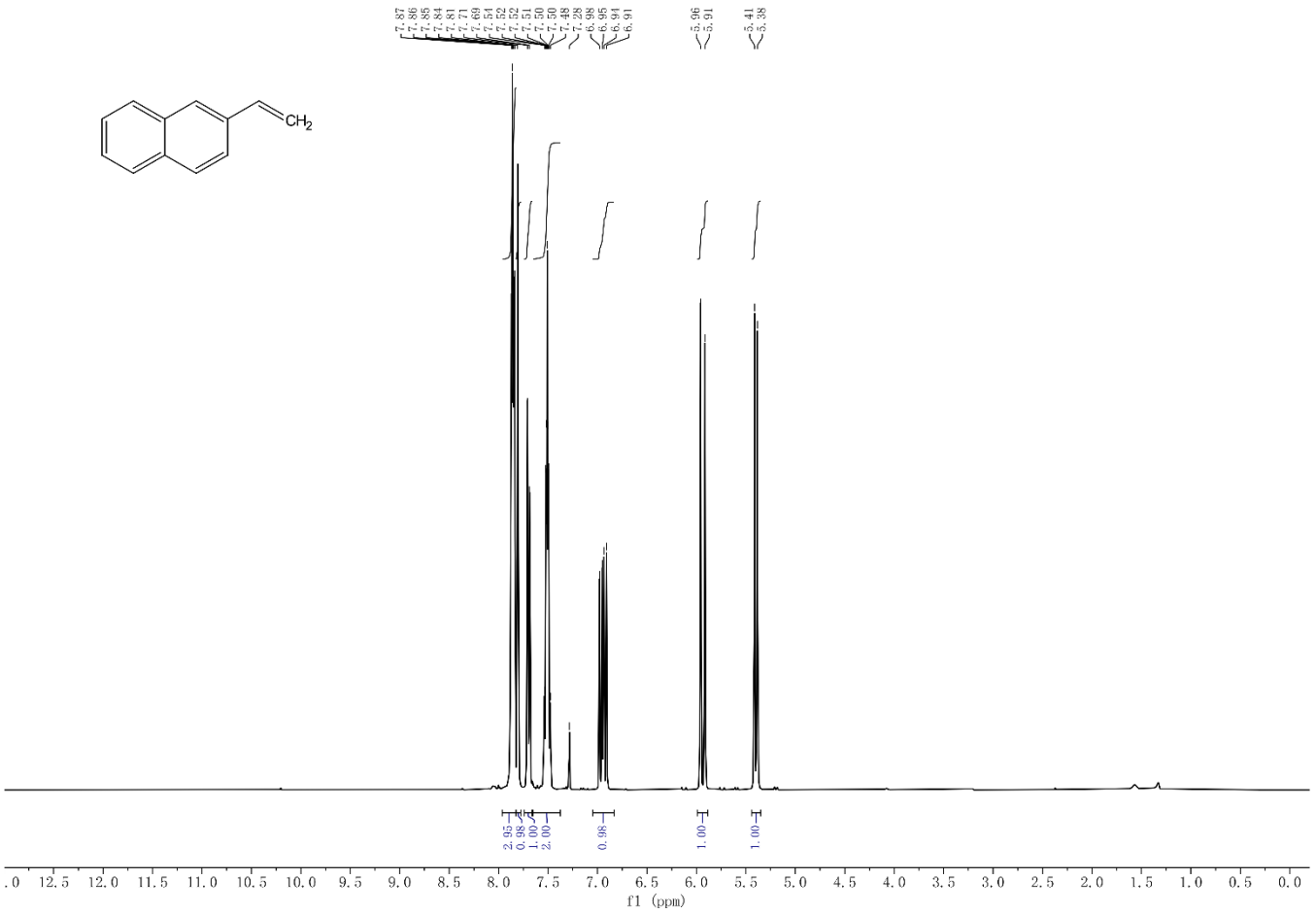
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3j



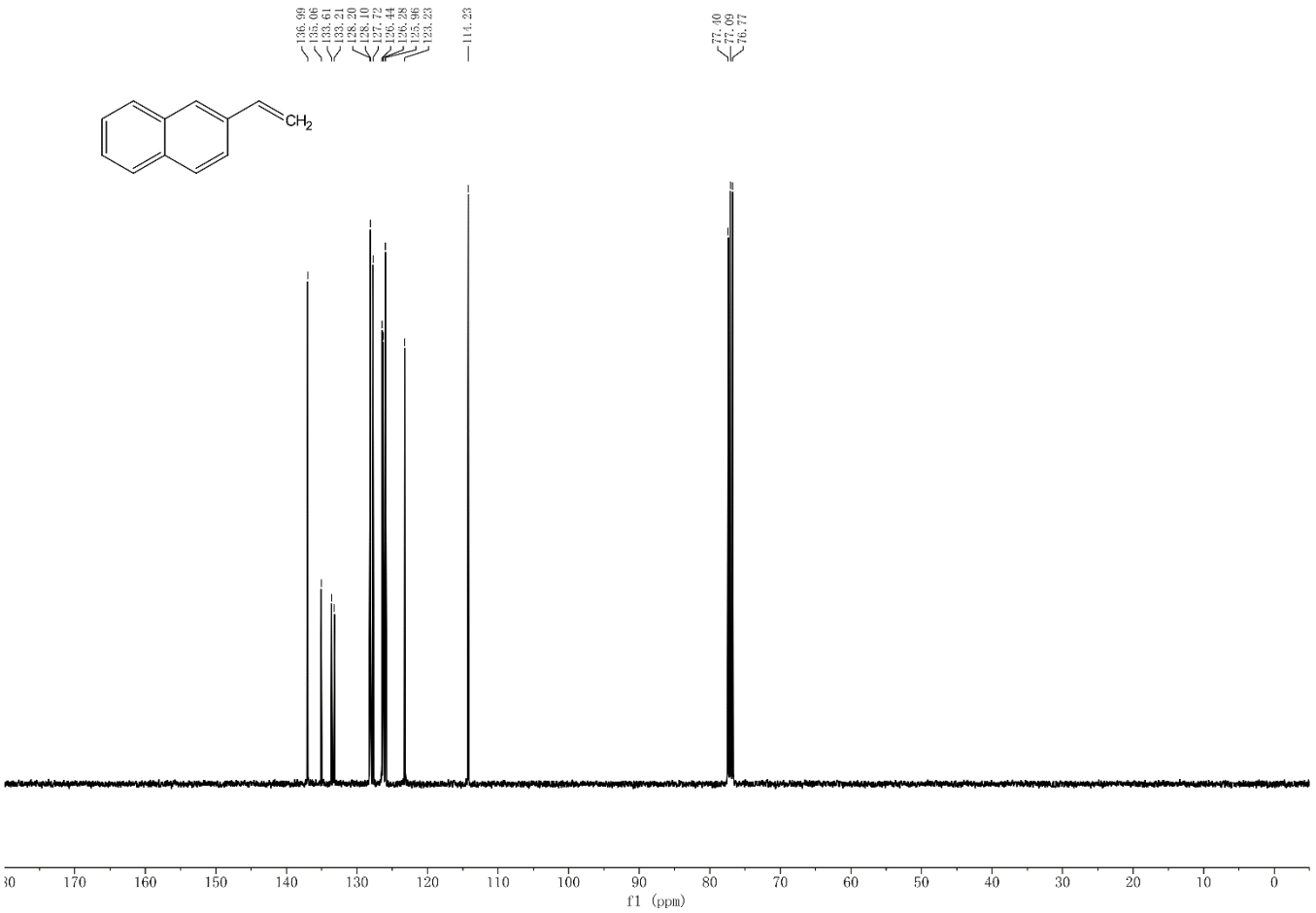
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3j



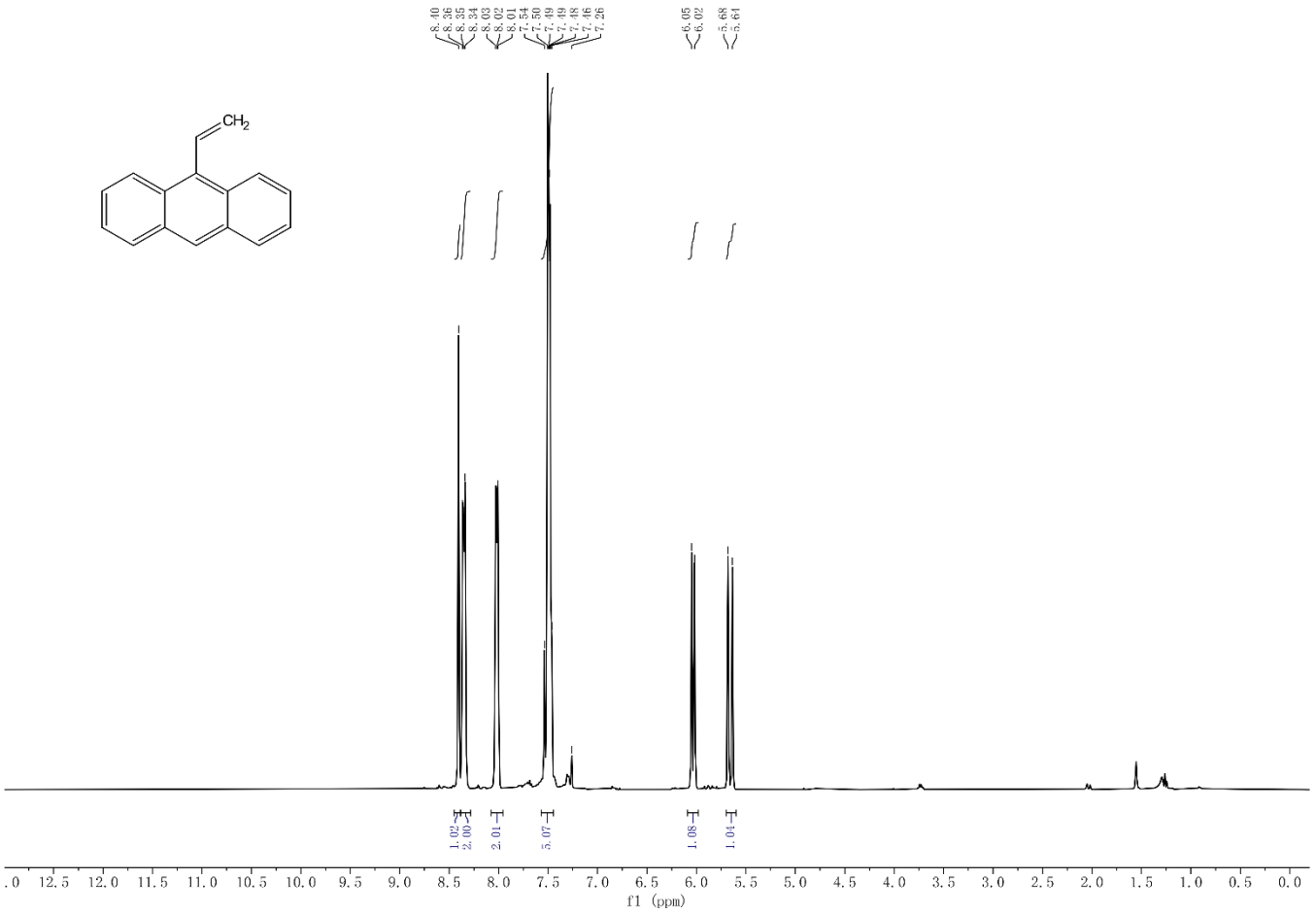
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3k



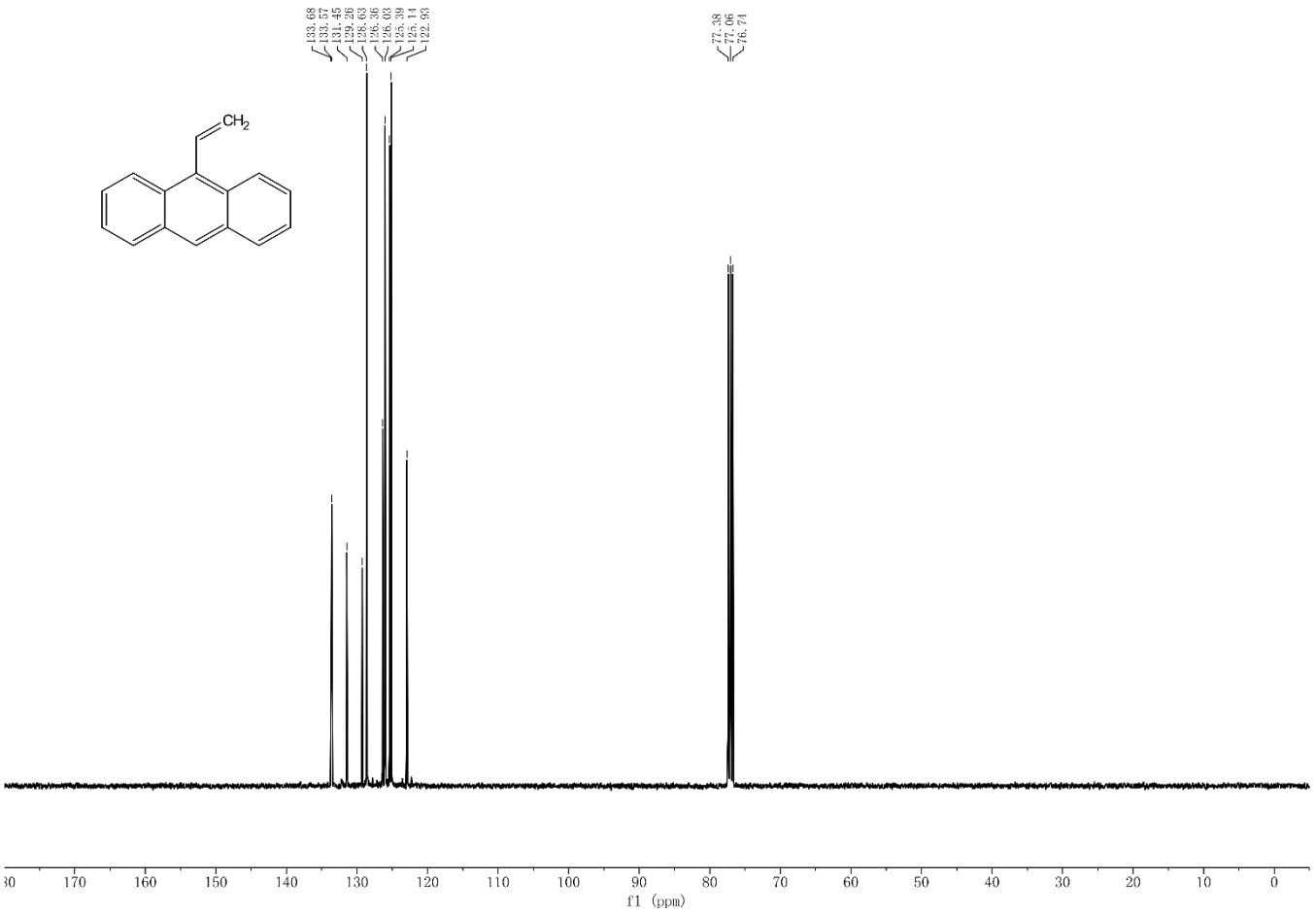
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3k



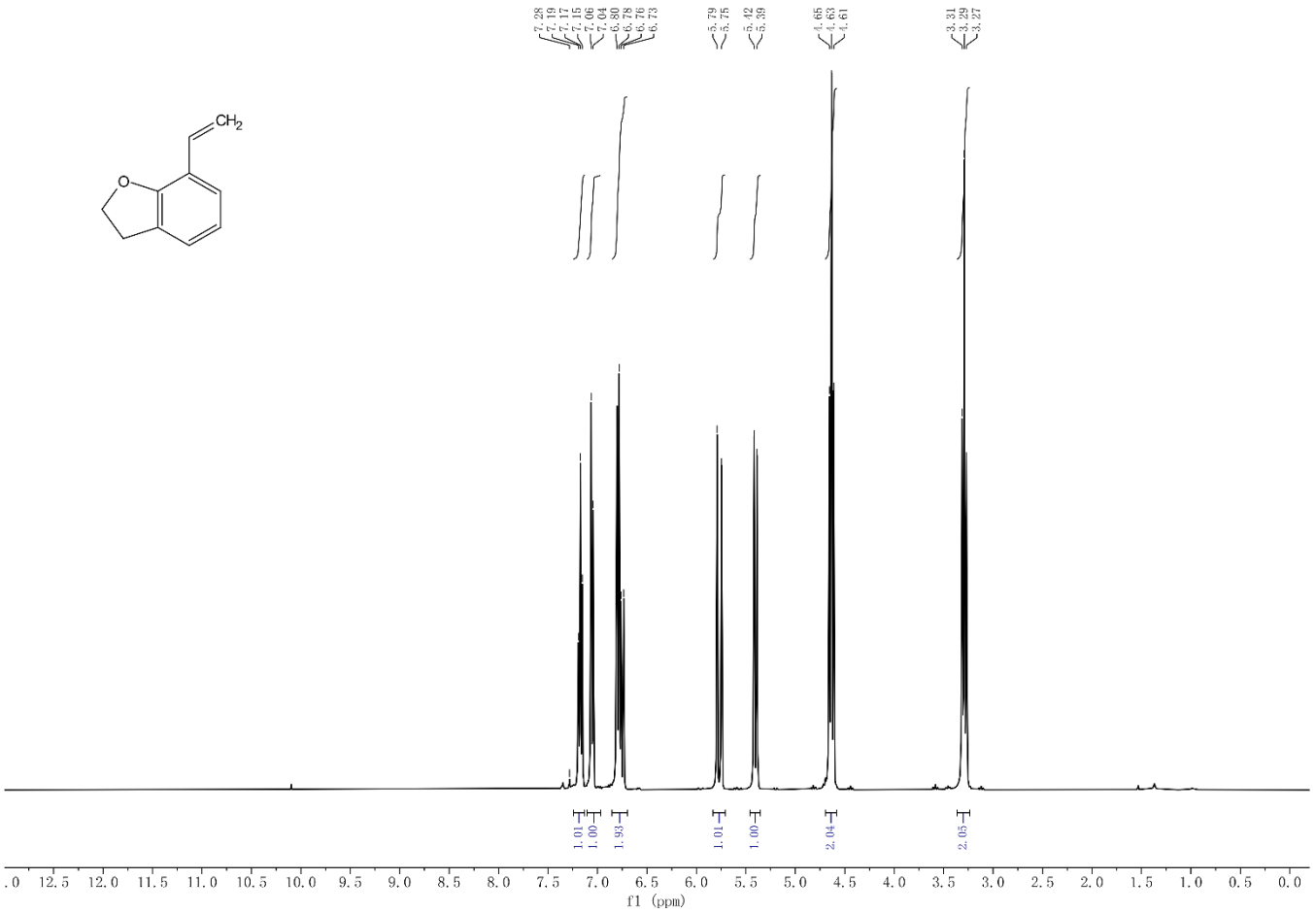
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3l



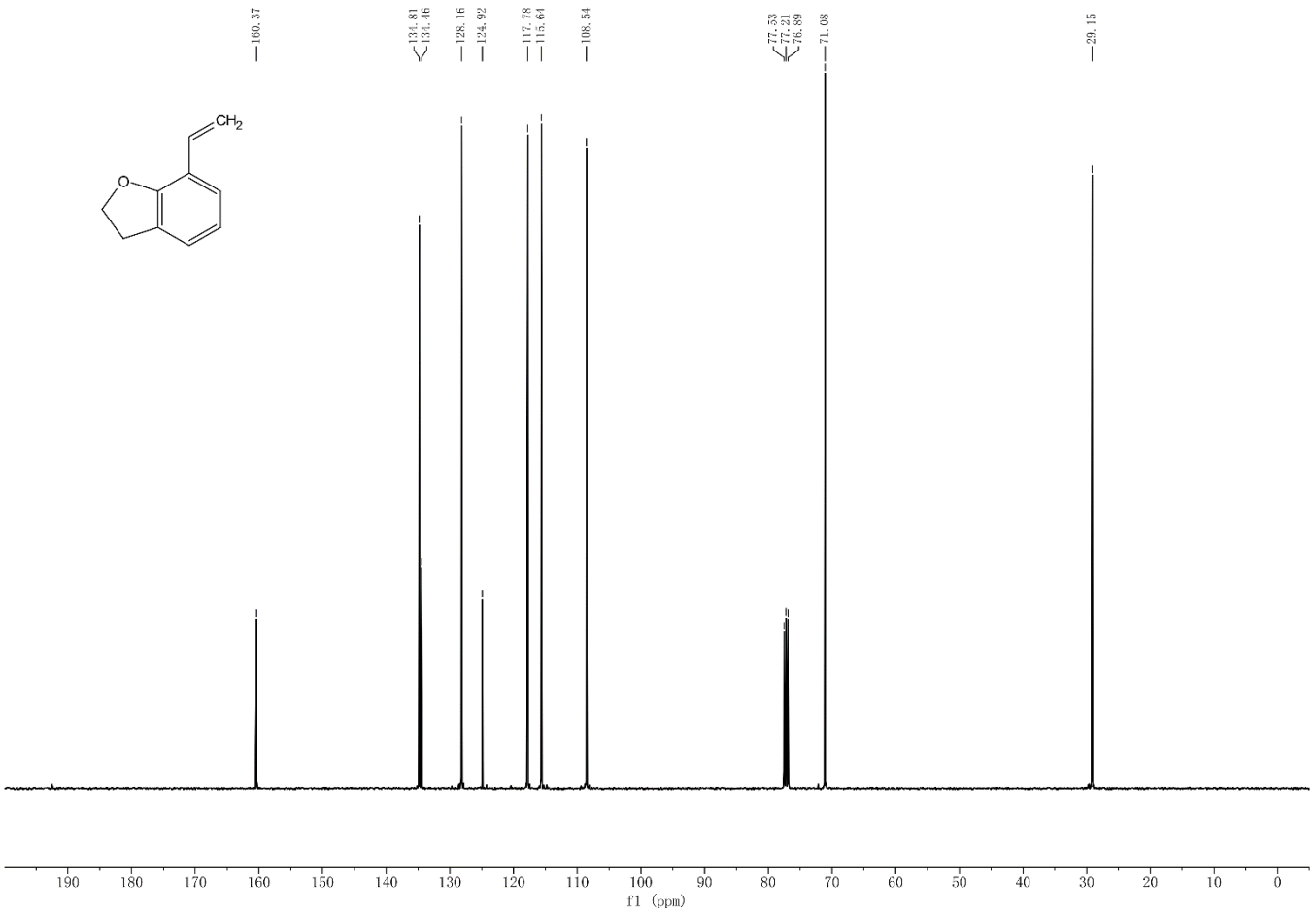
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3l



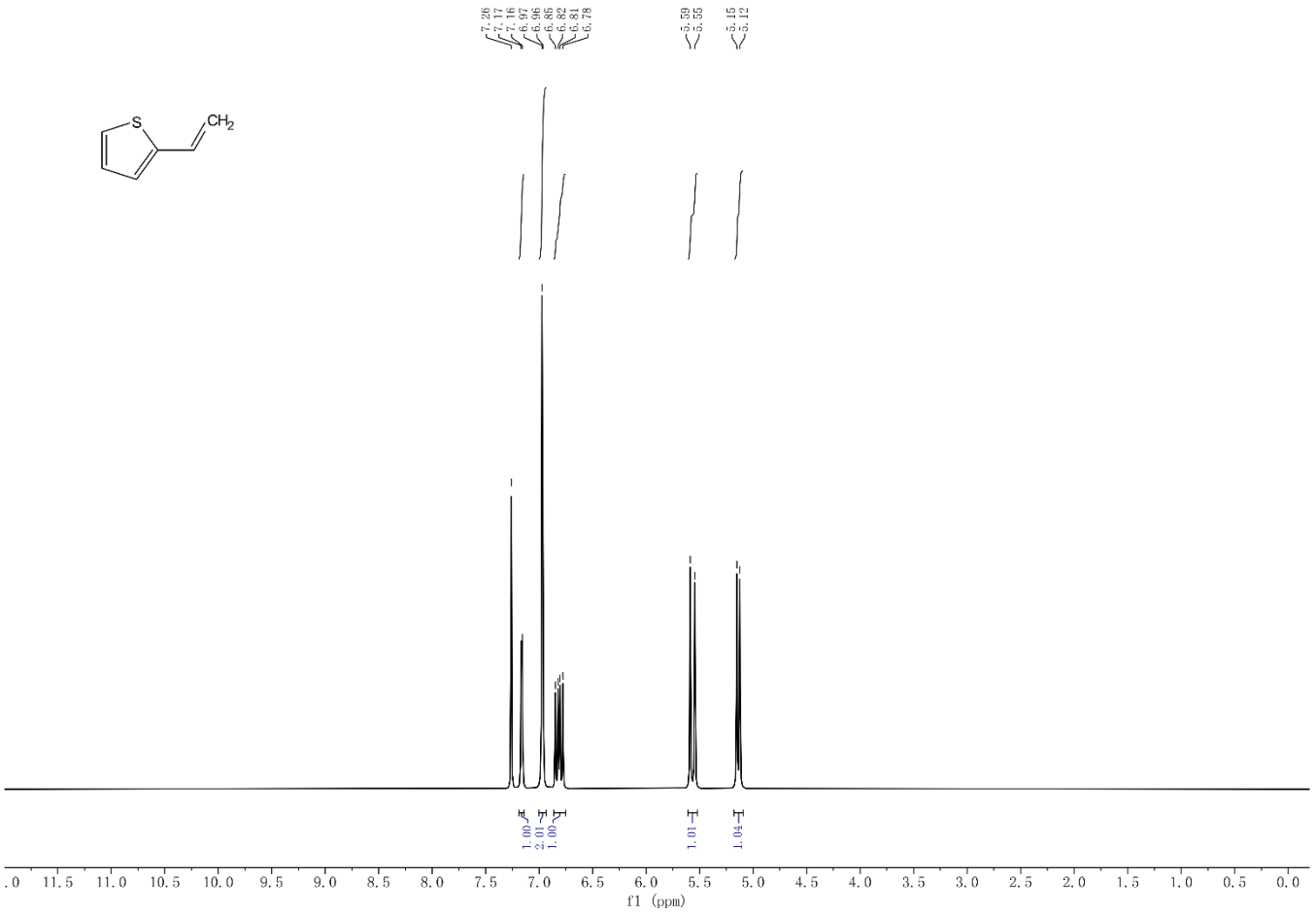
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3m



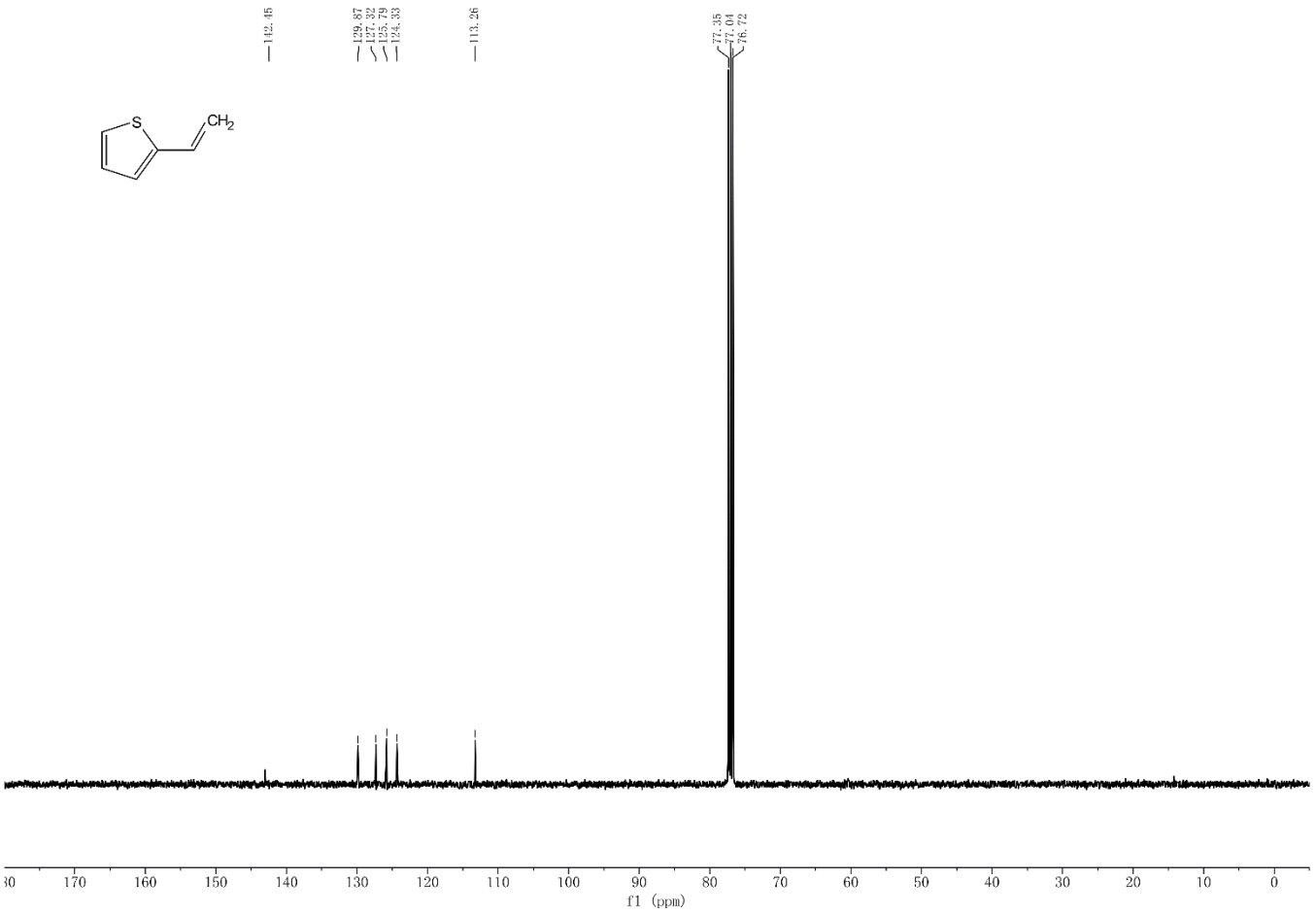
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3m



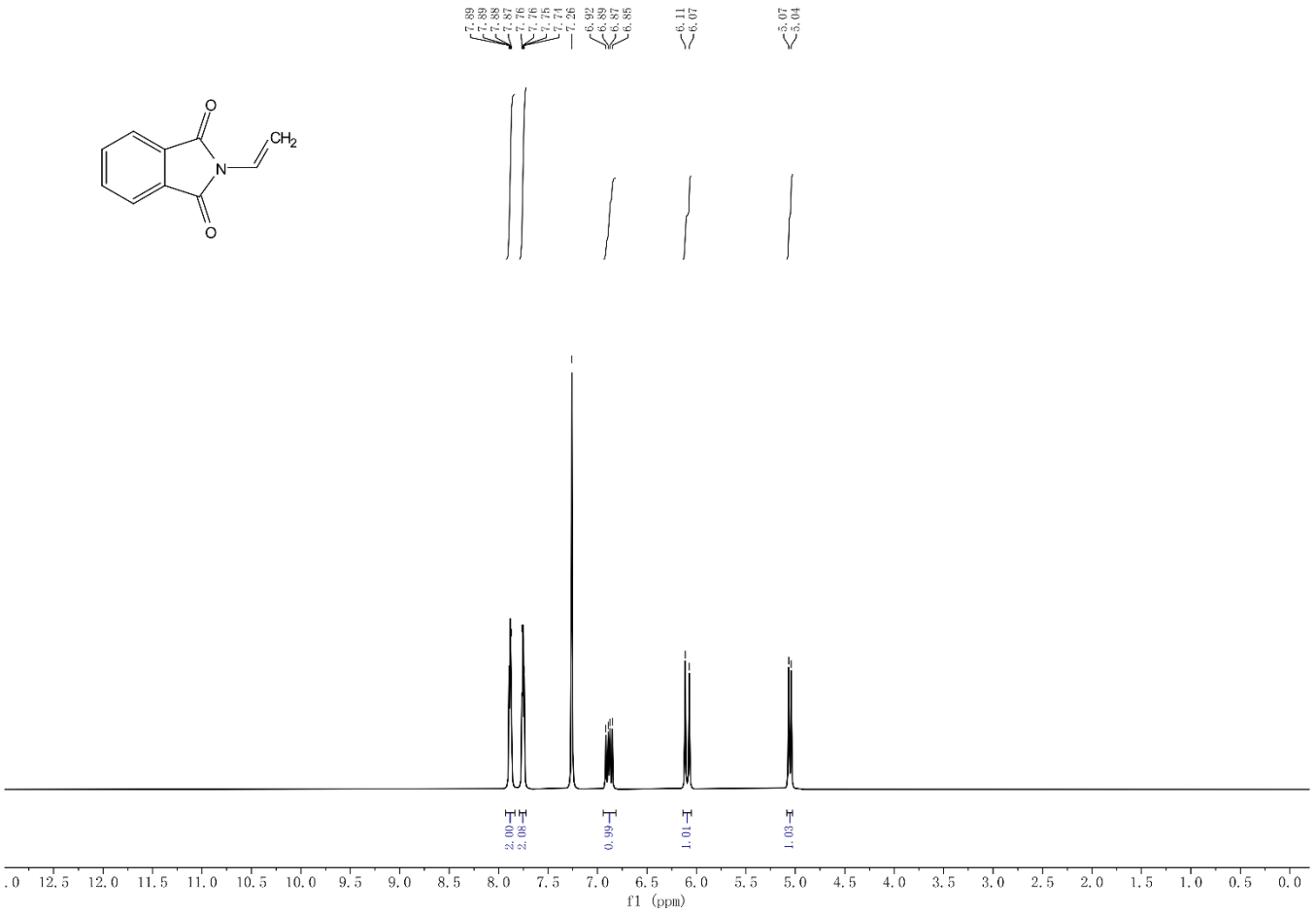
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3n



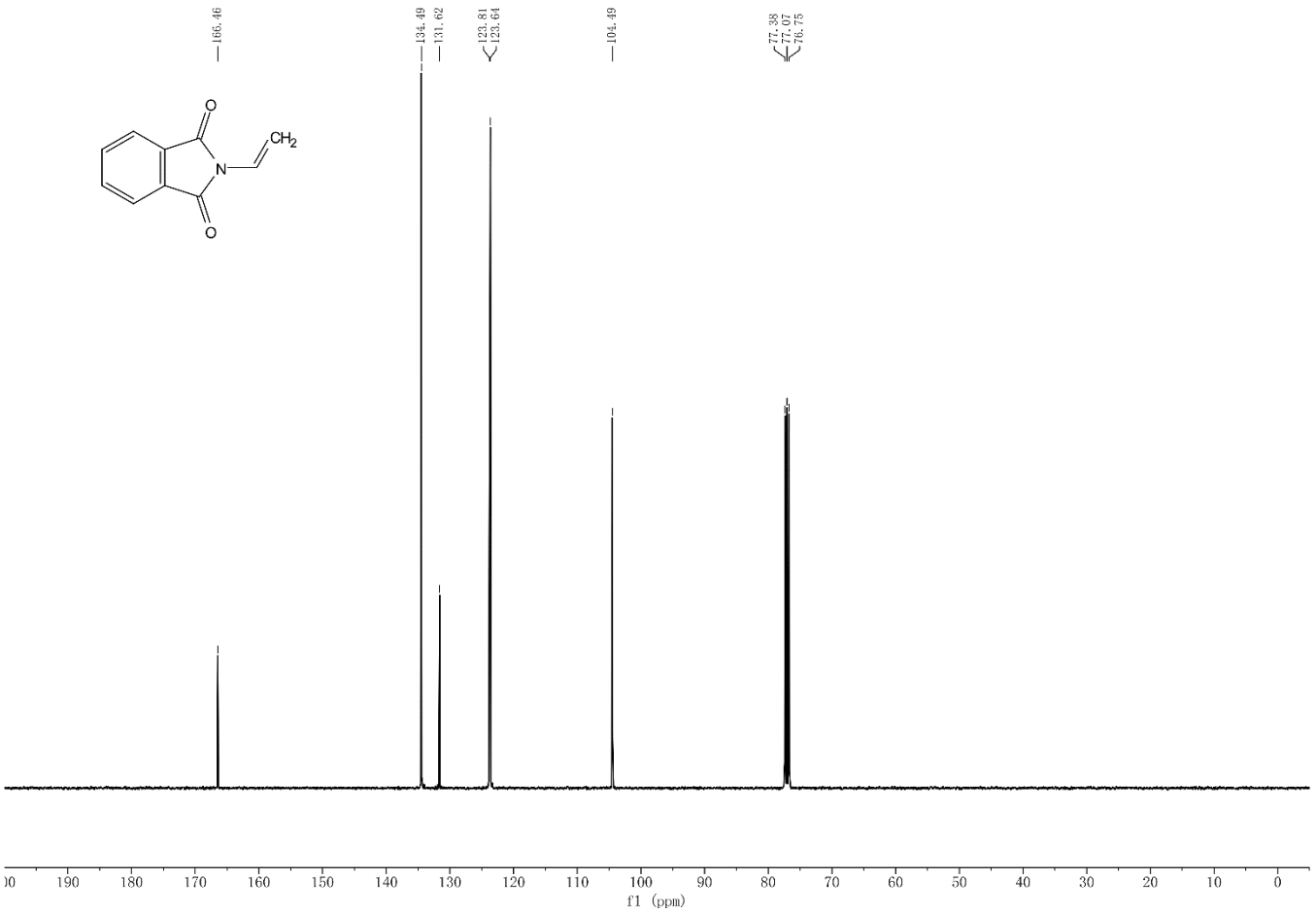
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3n



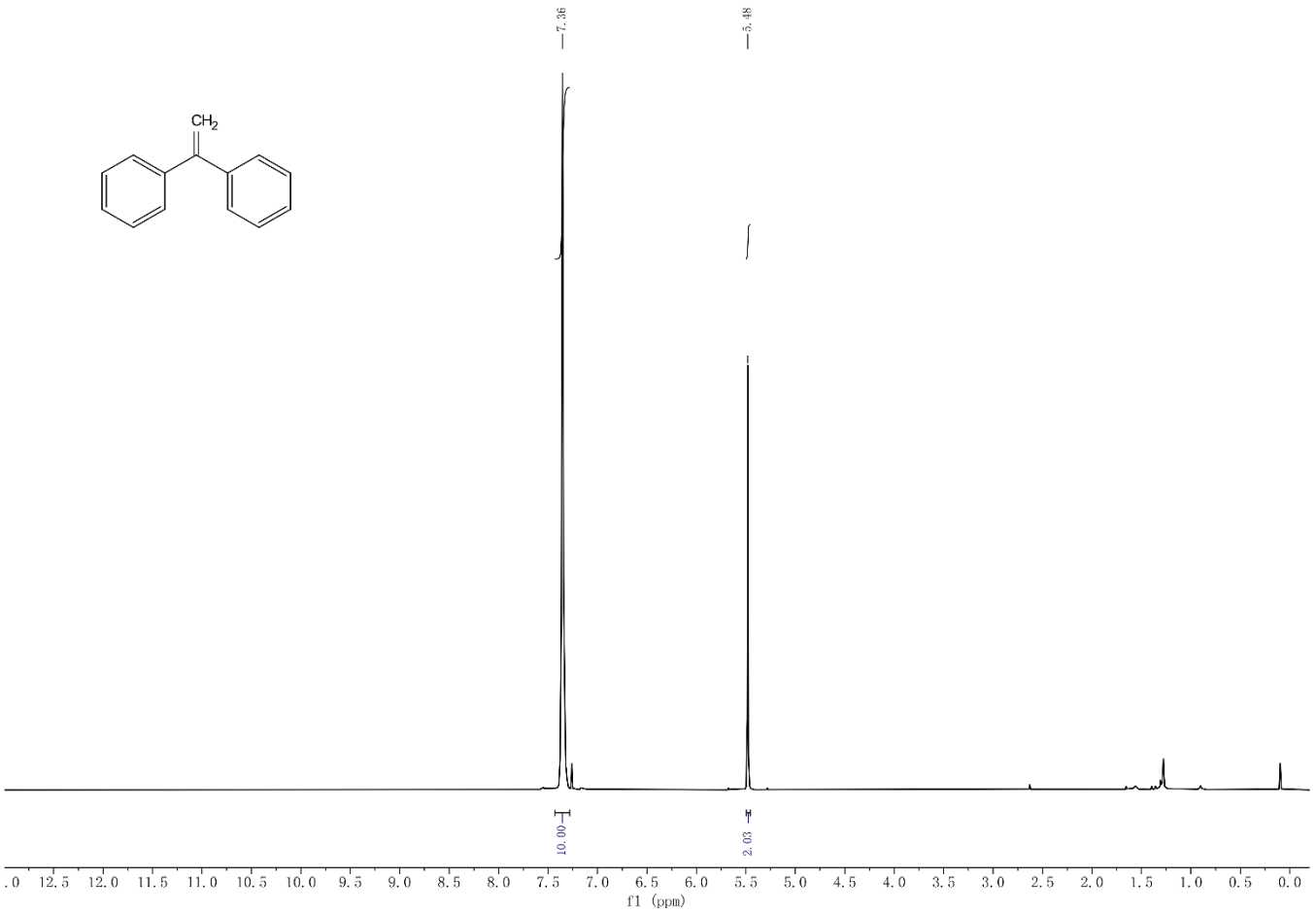
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3o



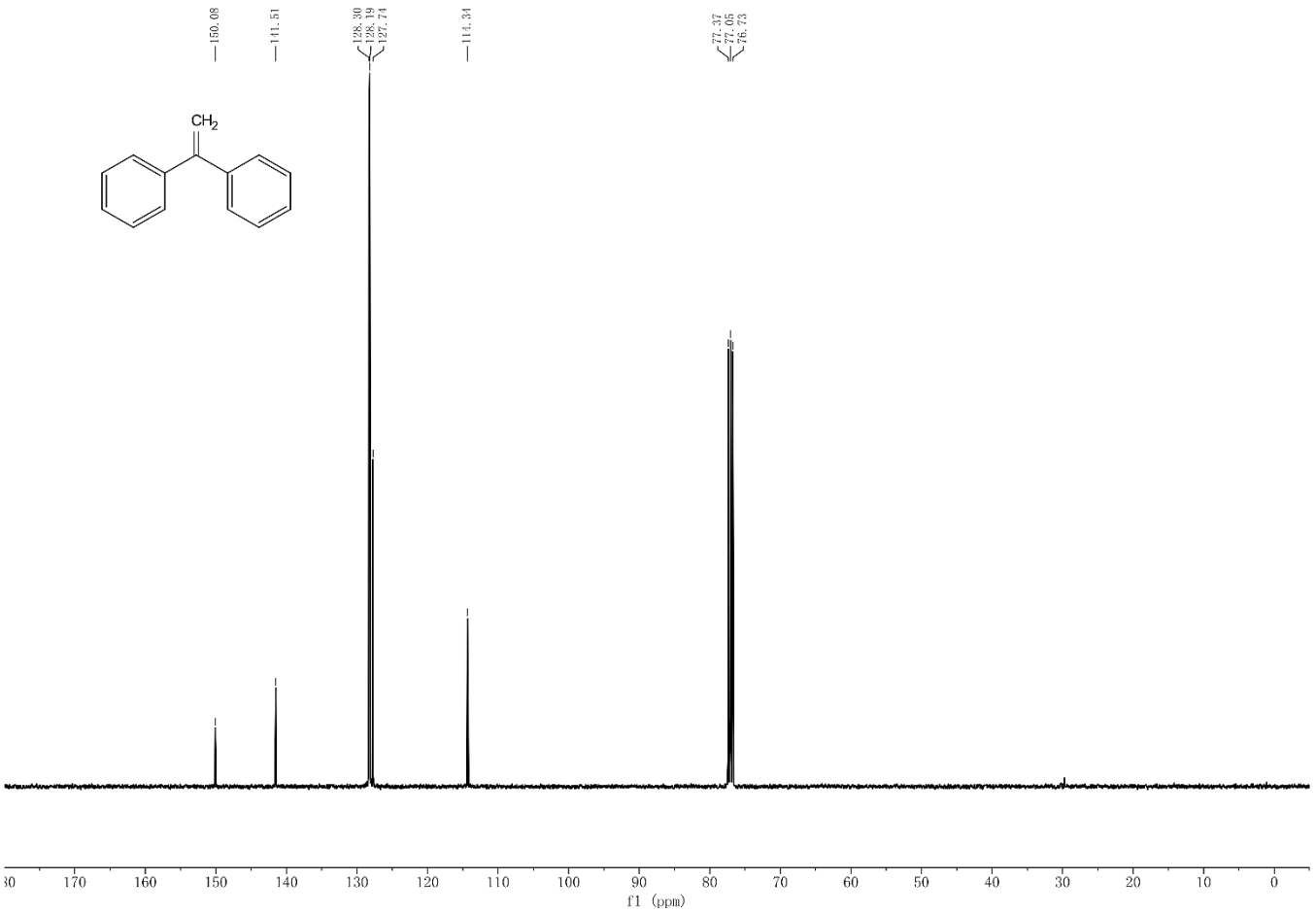
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3o



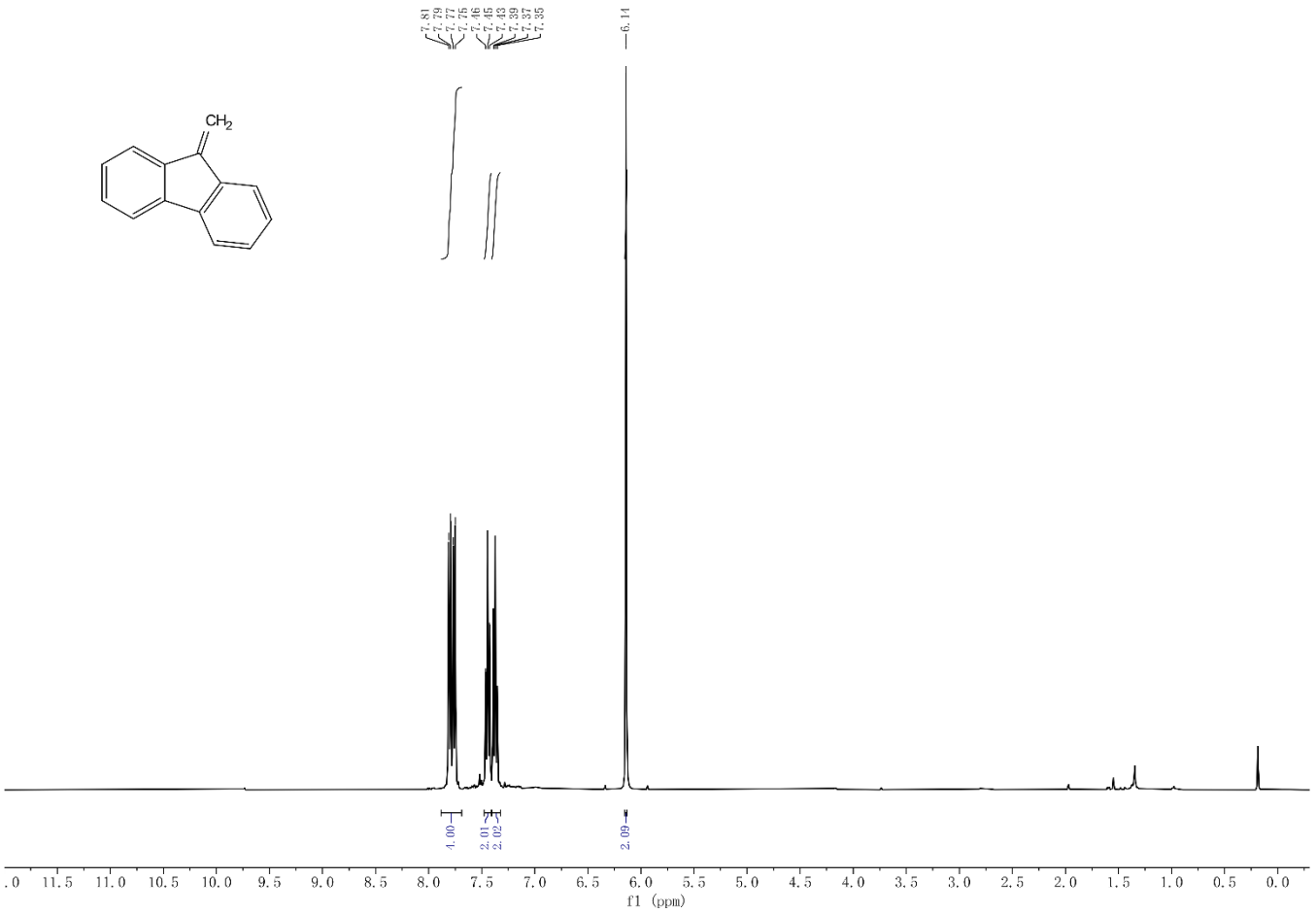
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3p



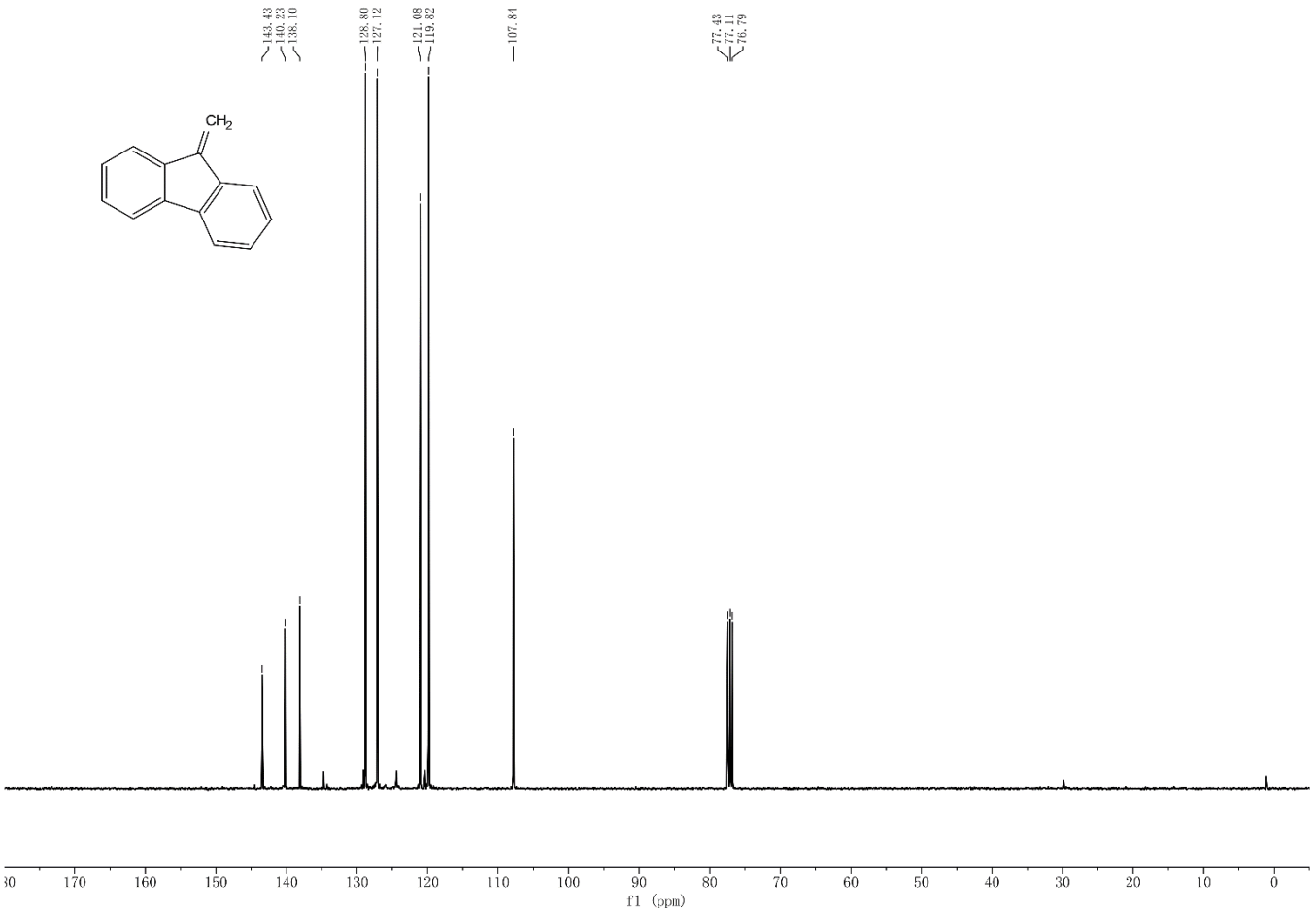
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3p



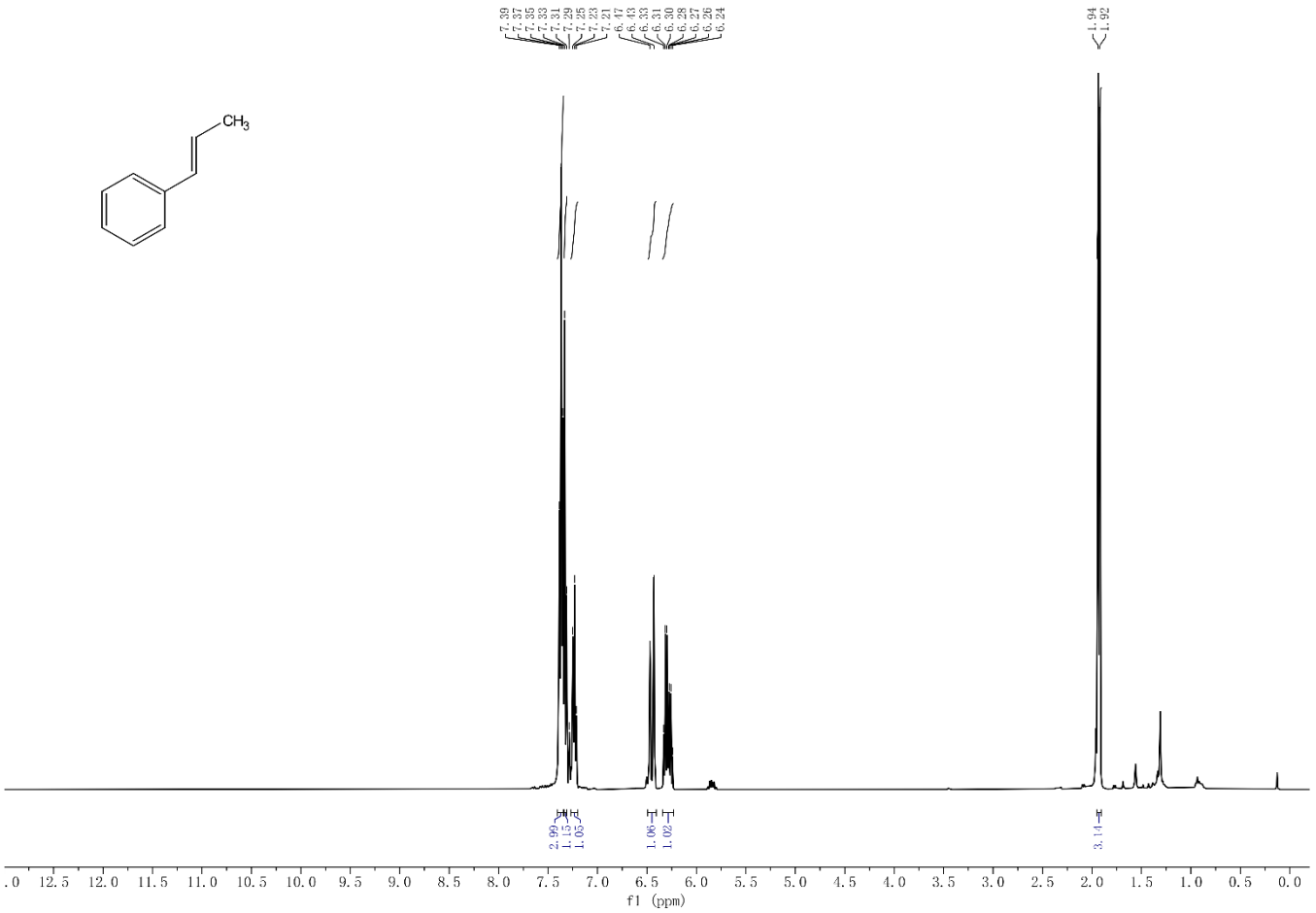
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3q



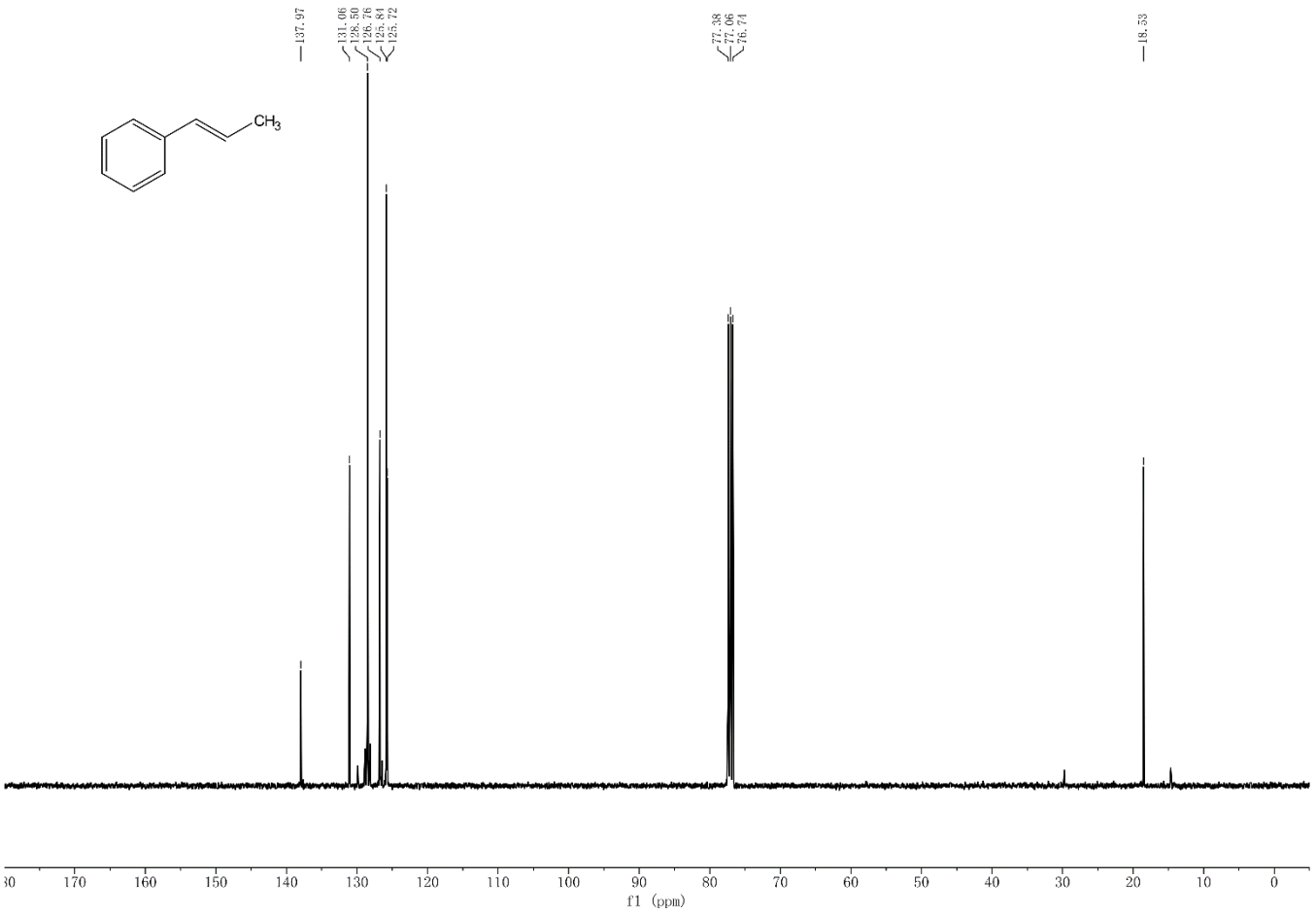
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3q



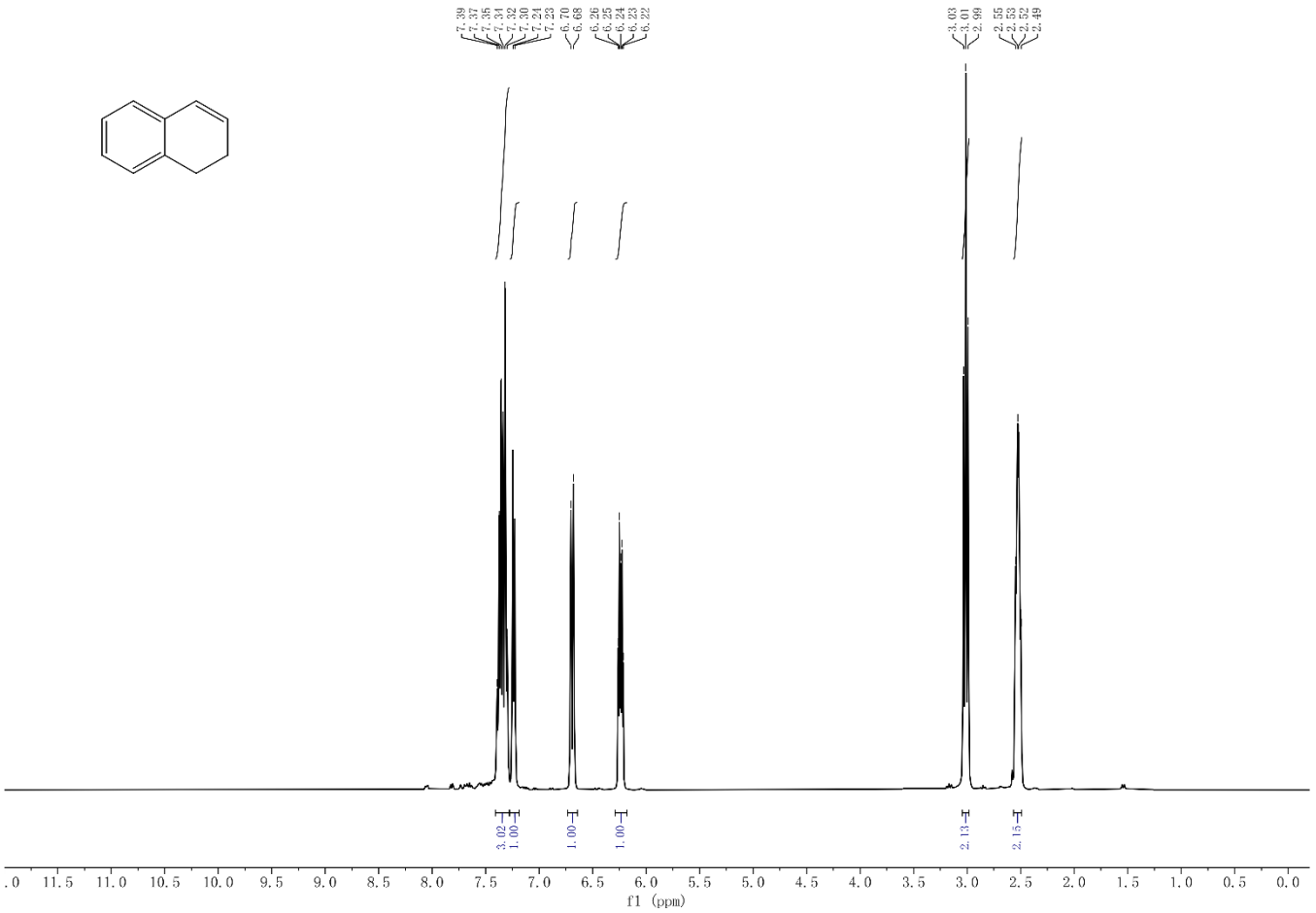
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3r



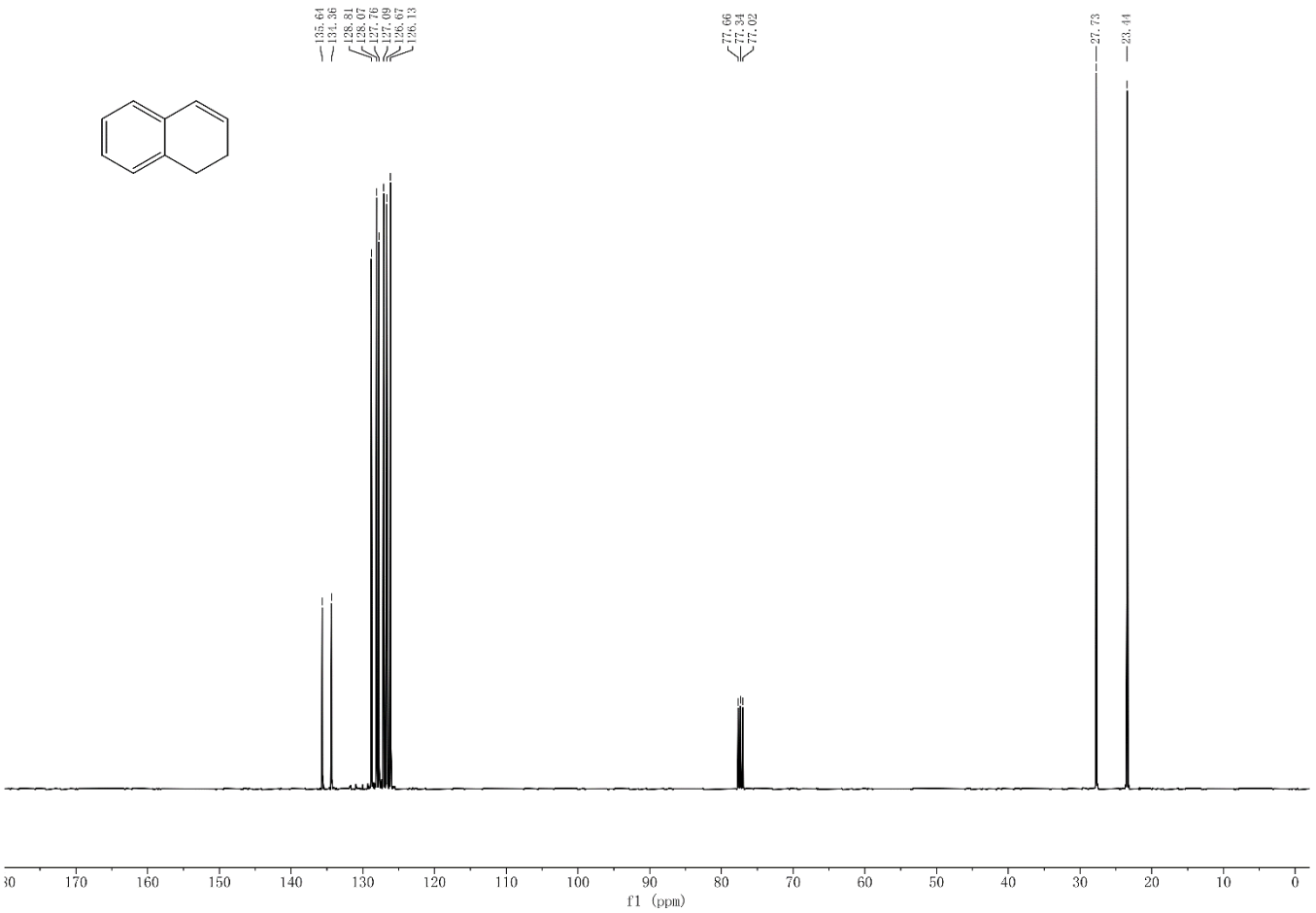
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 3r



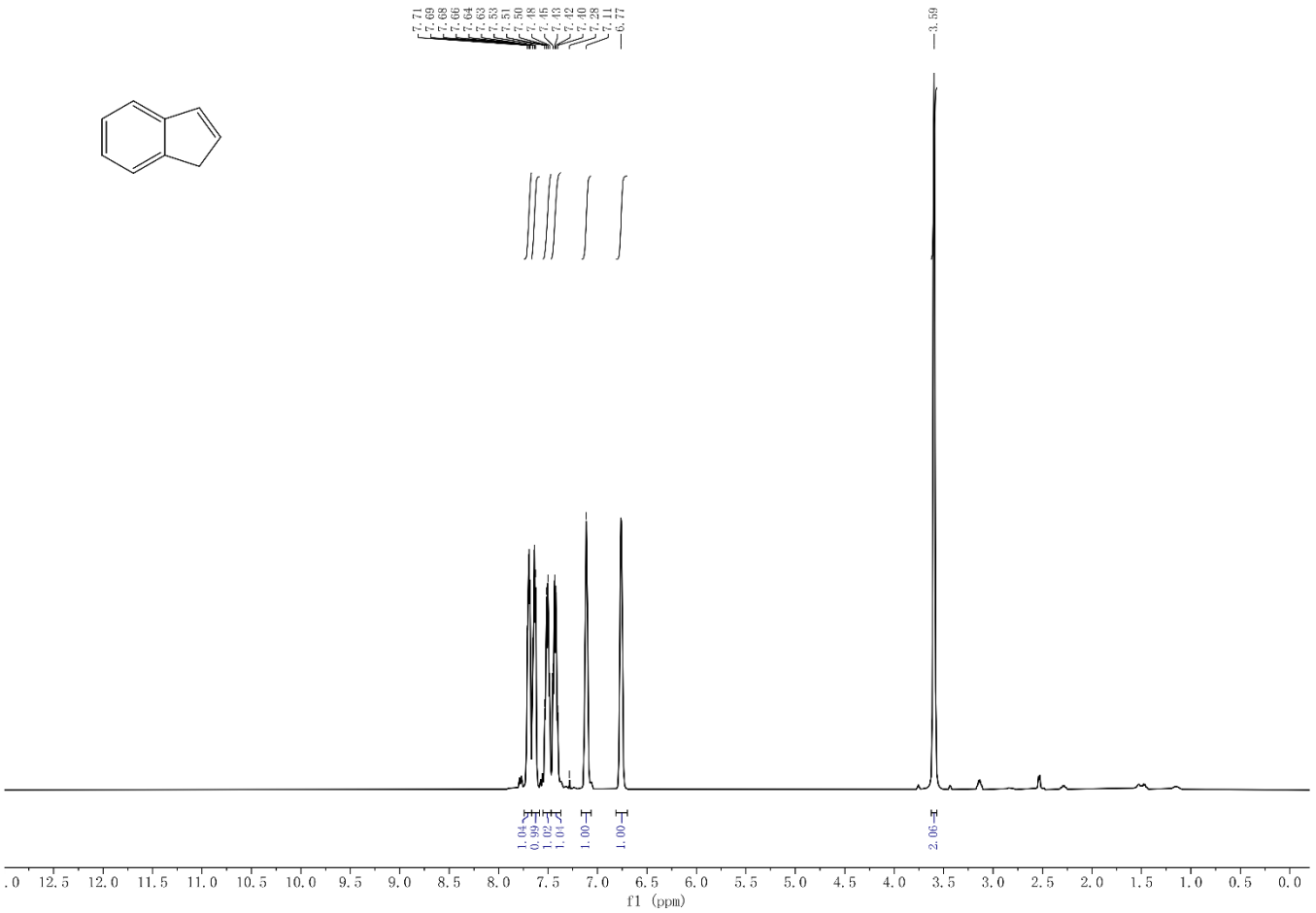
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4a



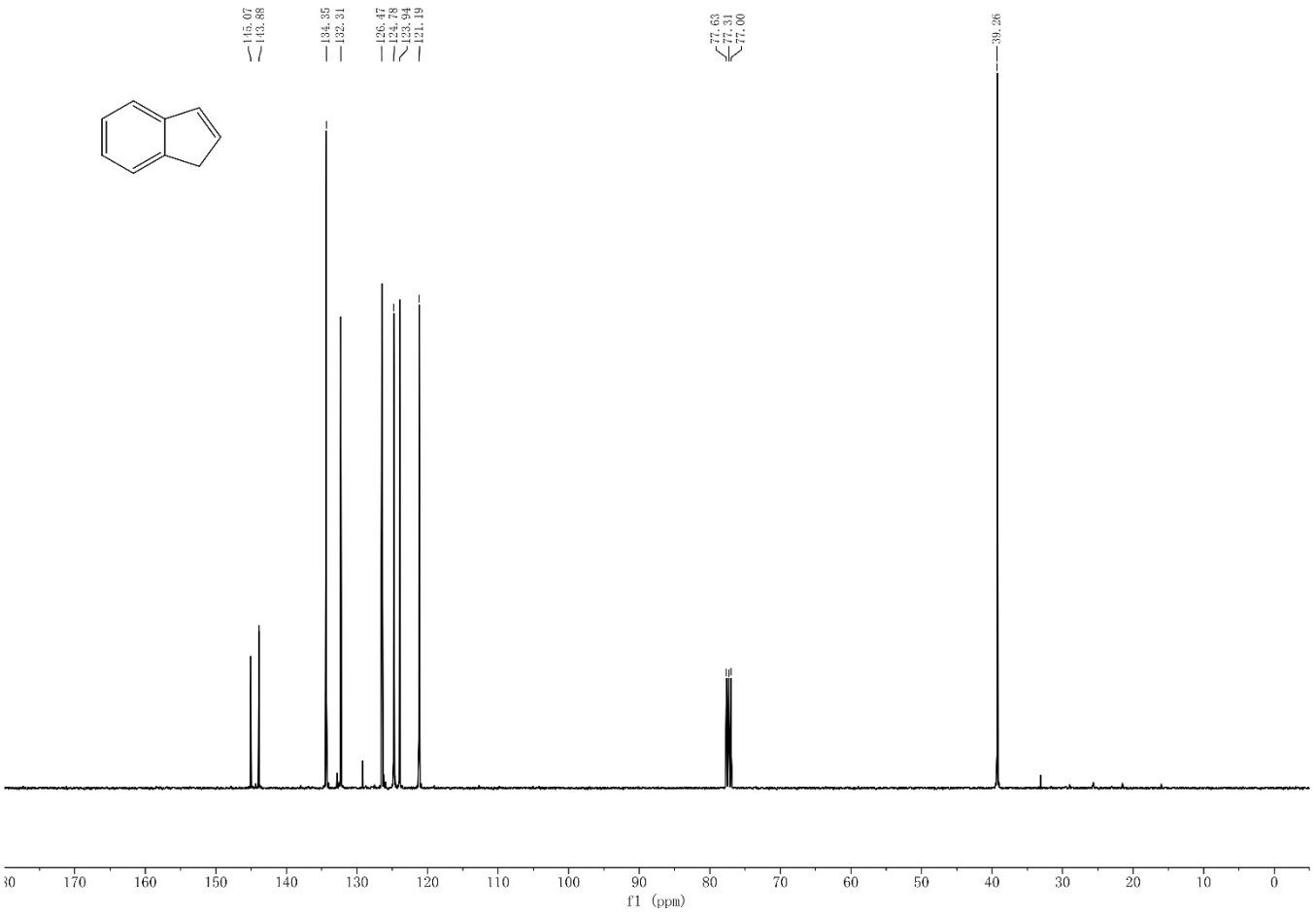
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 4a



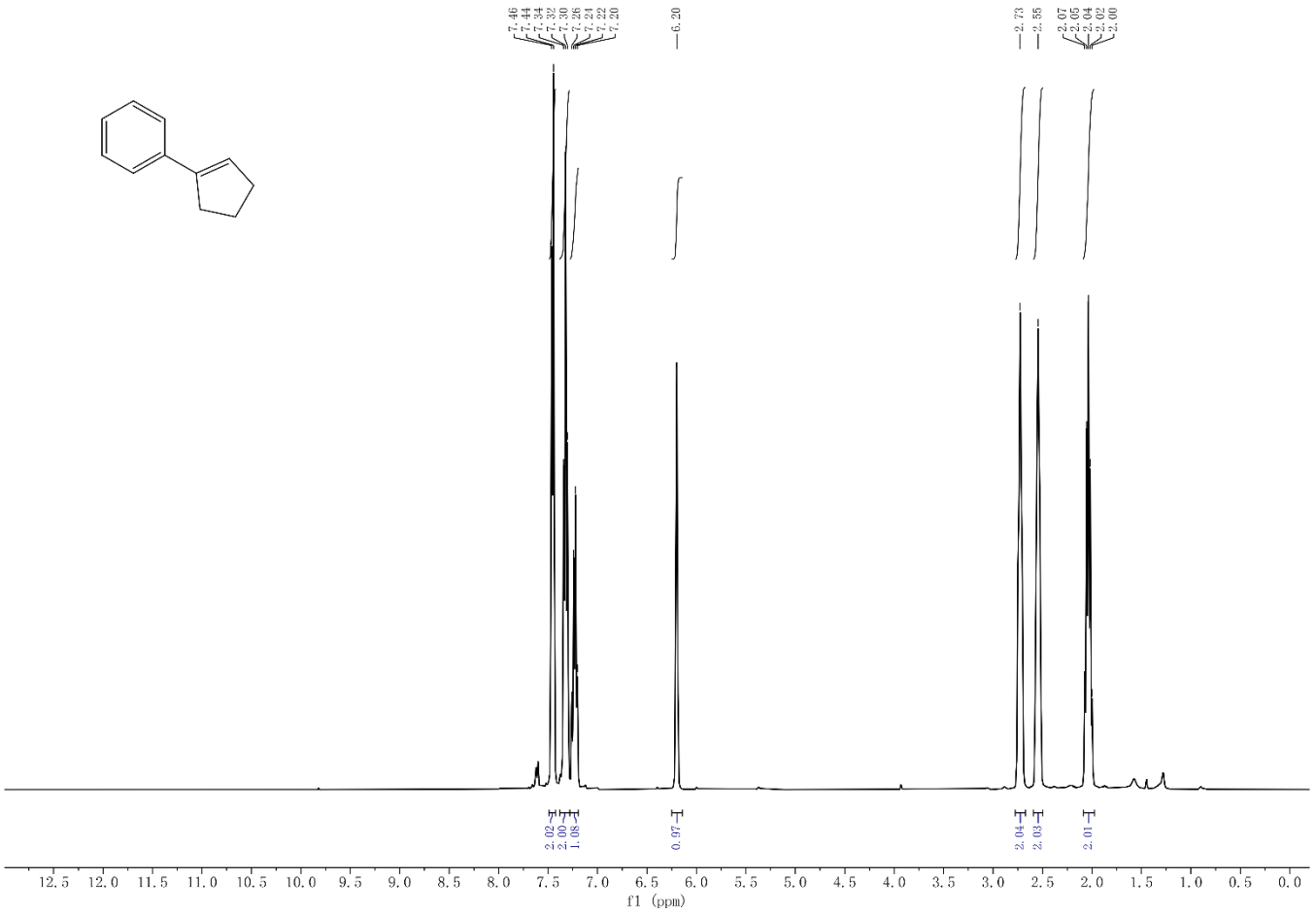
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4b



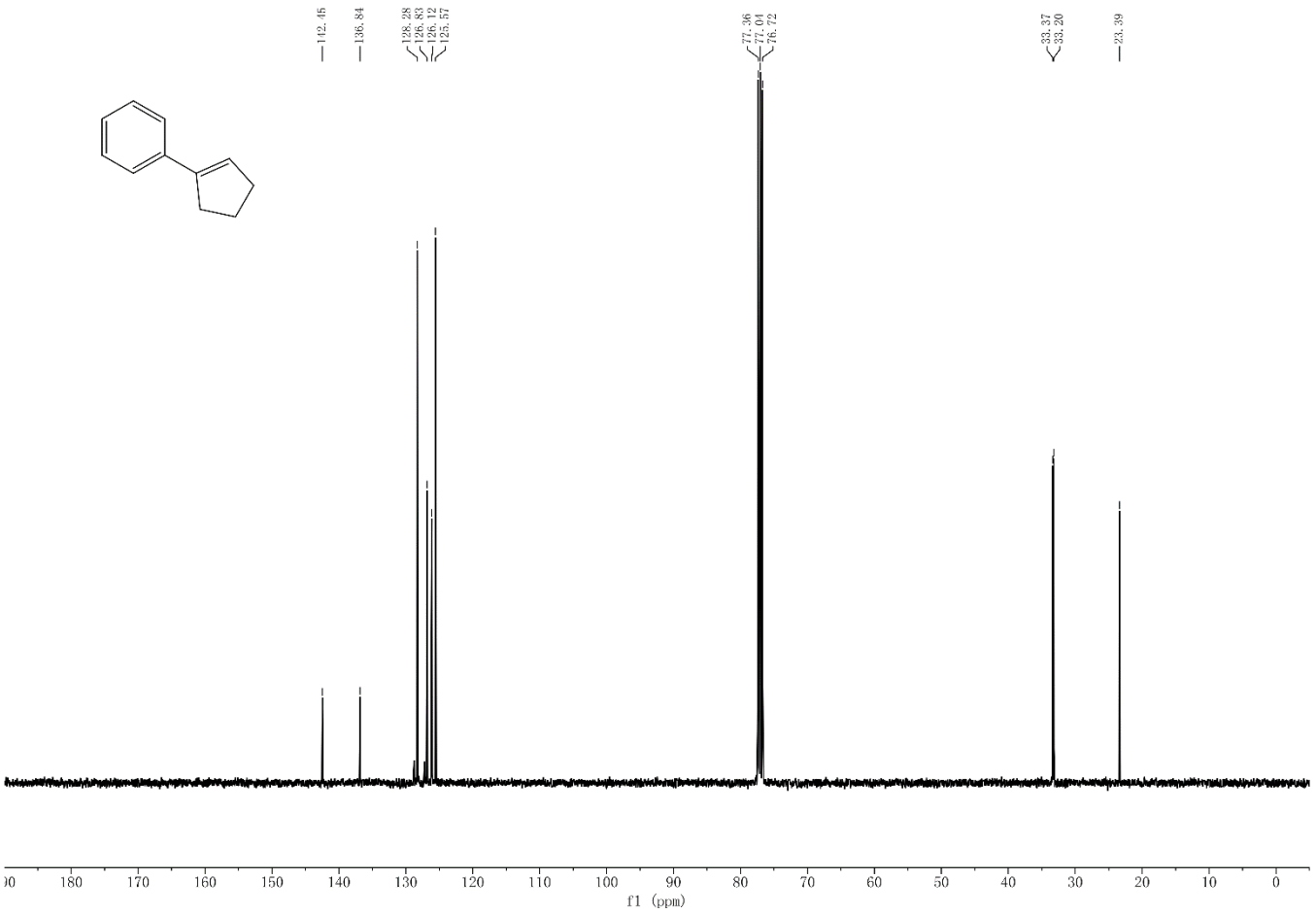
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 4b



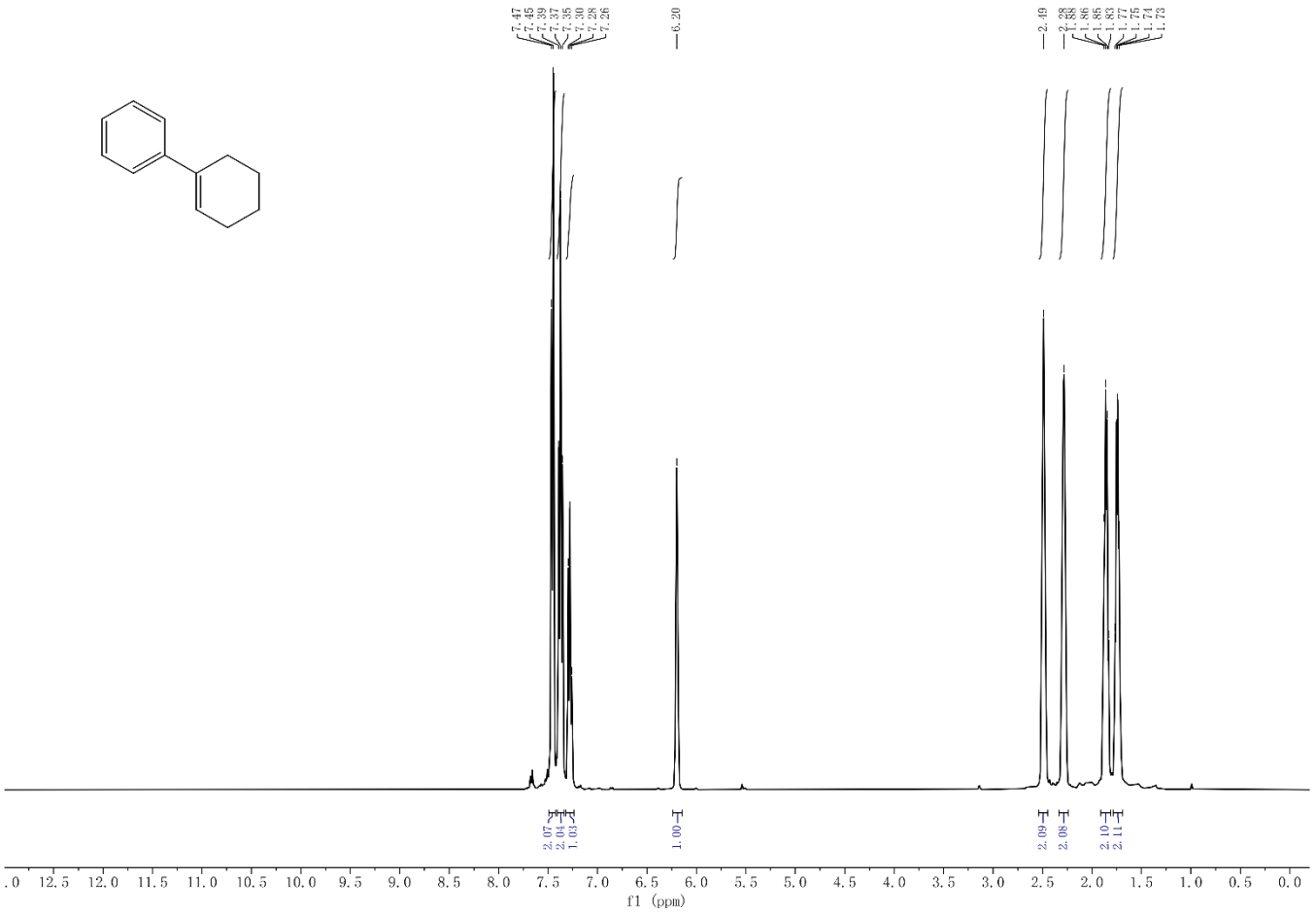
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4c



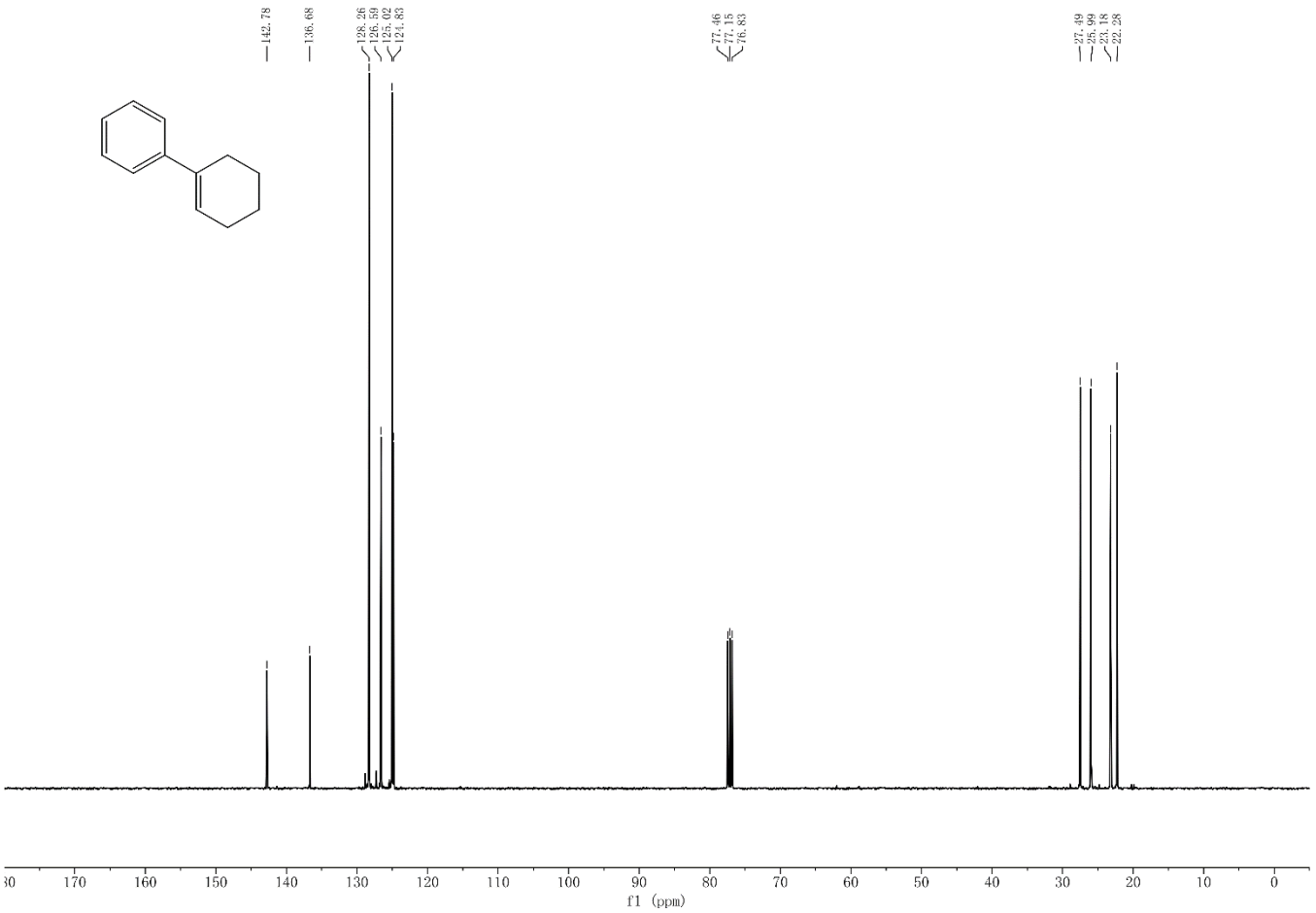
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 4c



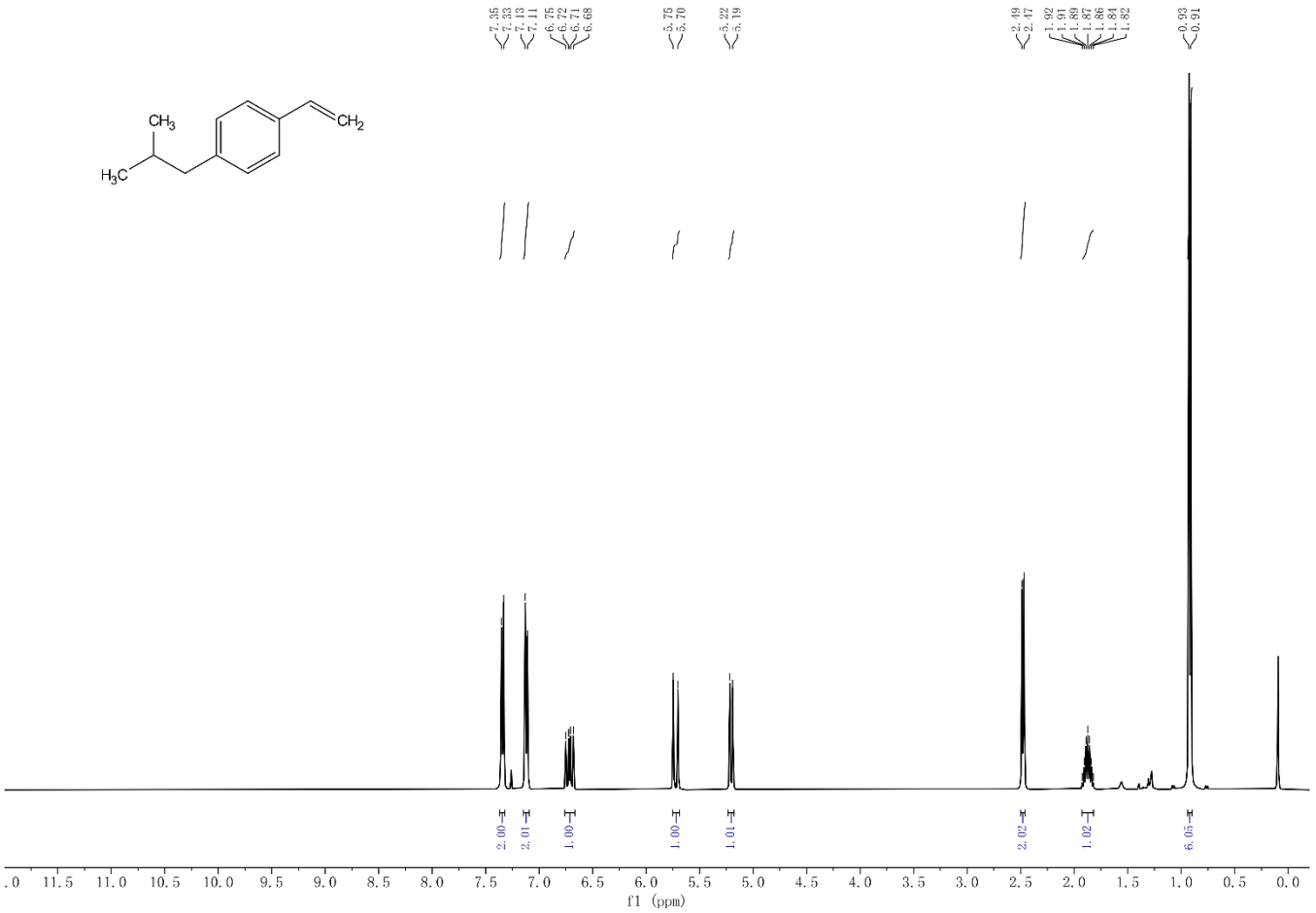
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4d



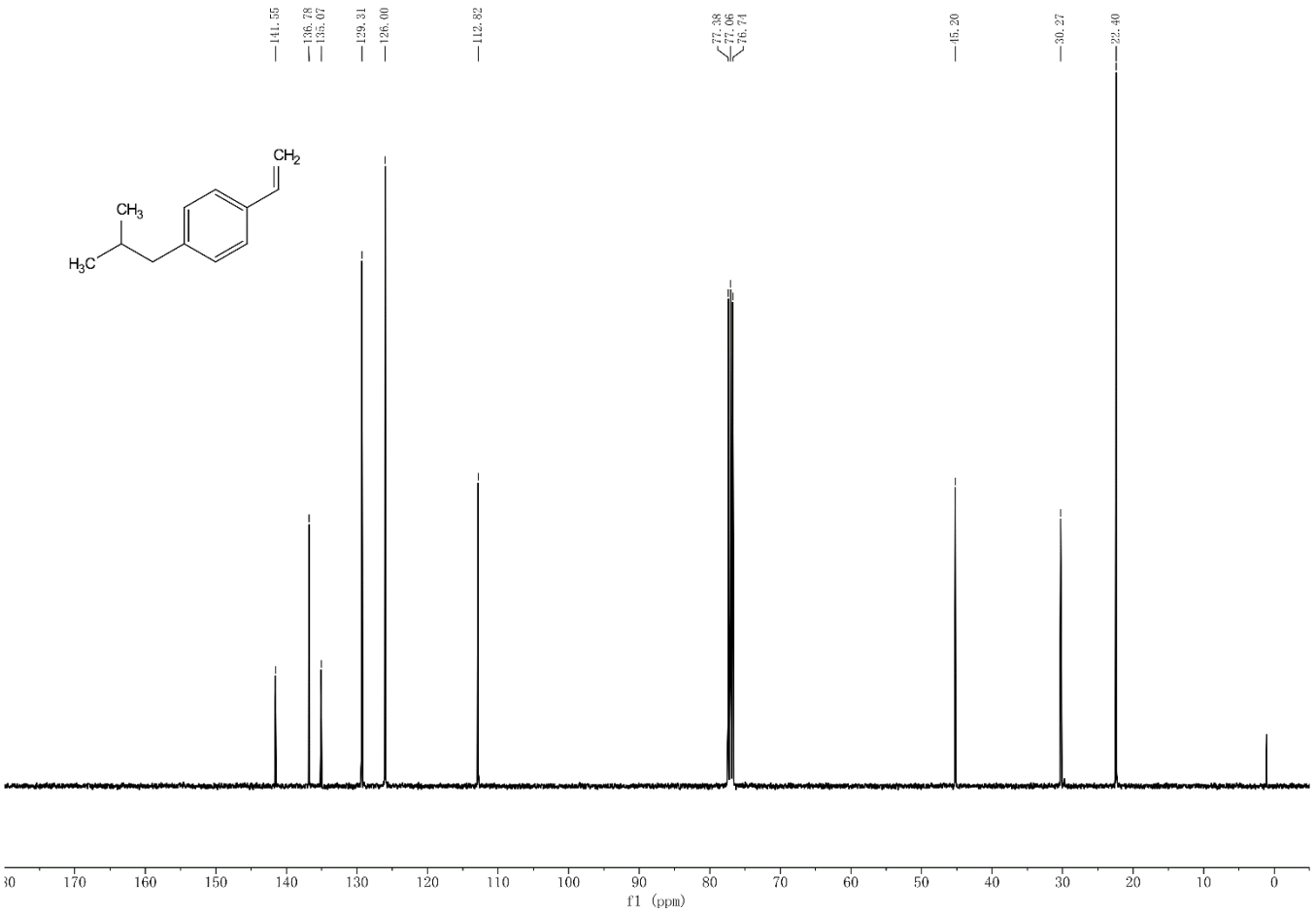
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 4d



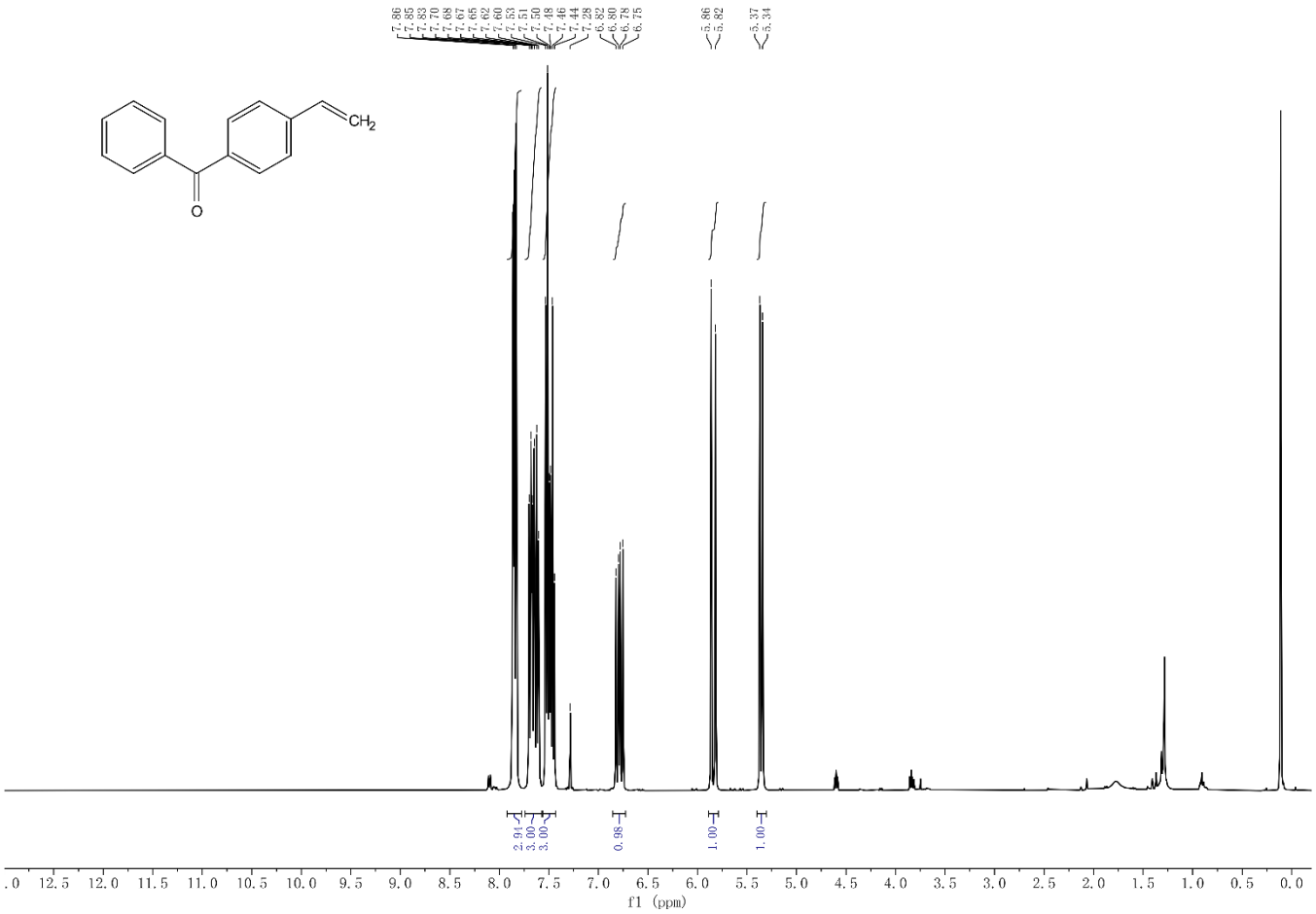
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5a



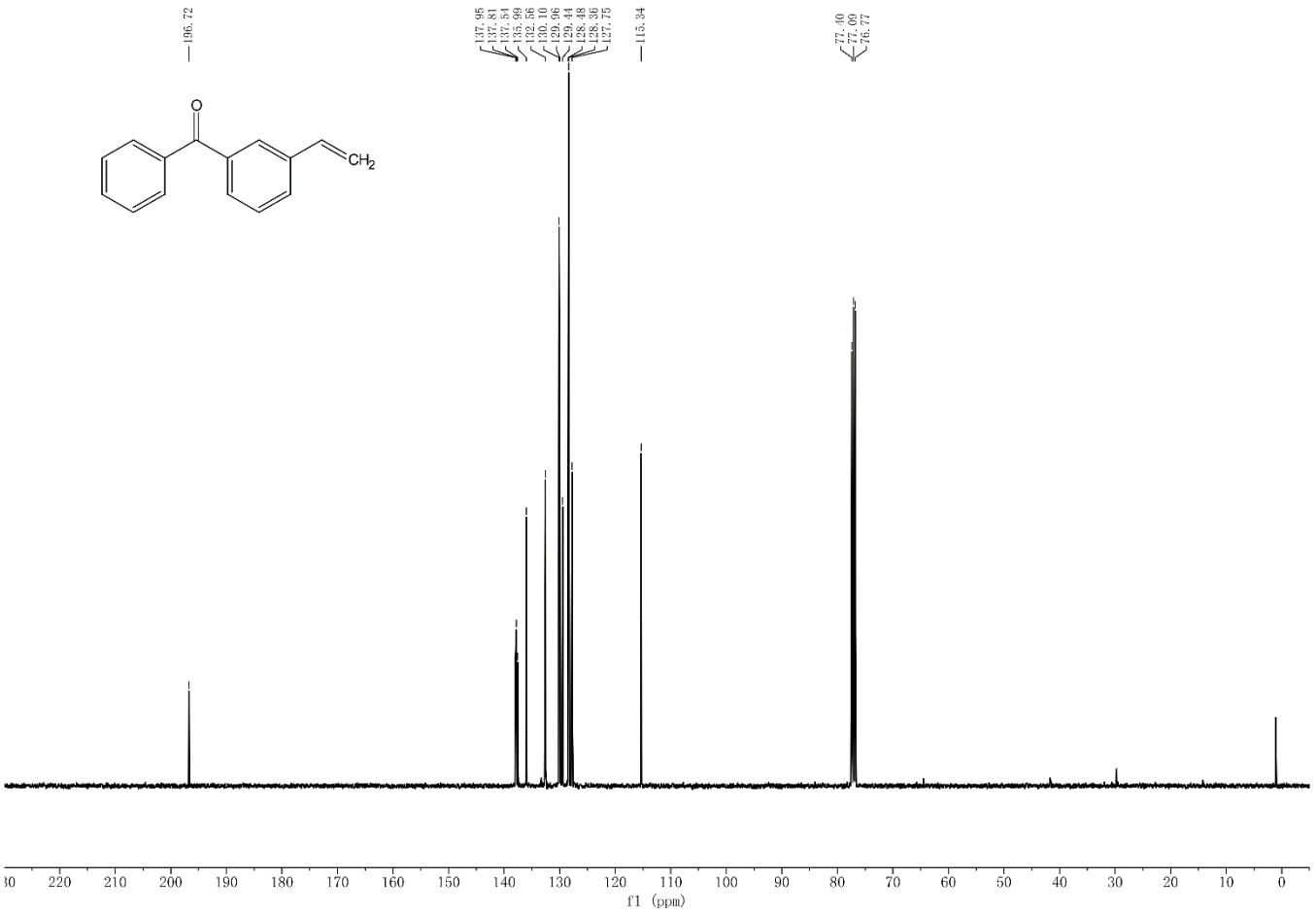
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5a



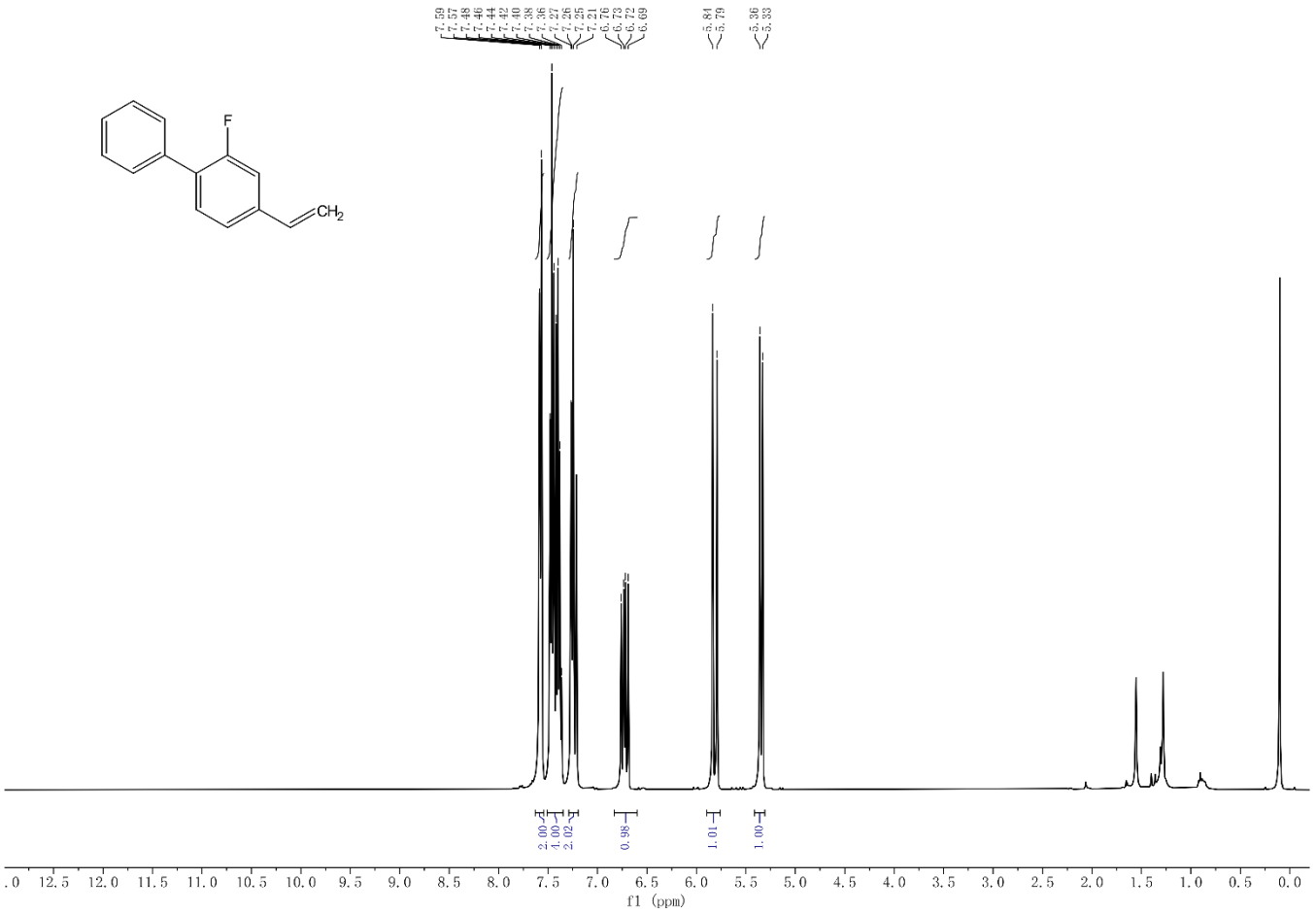
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5b



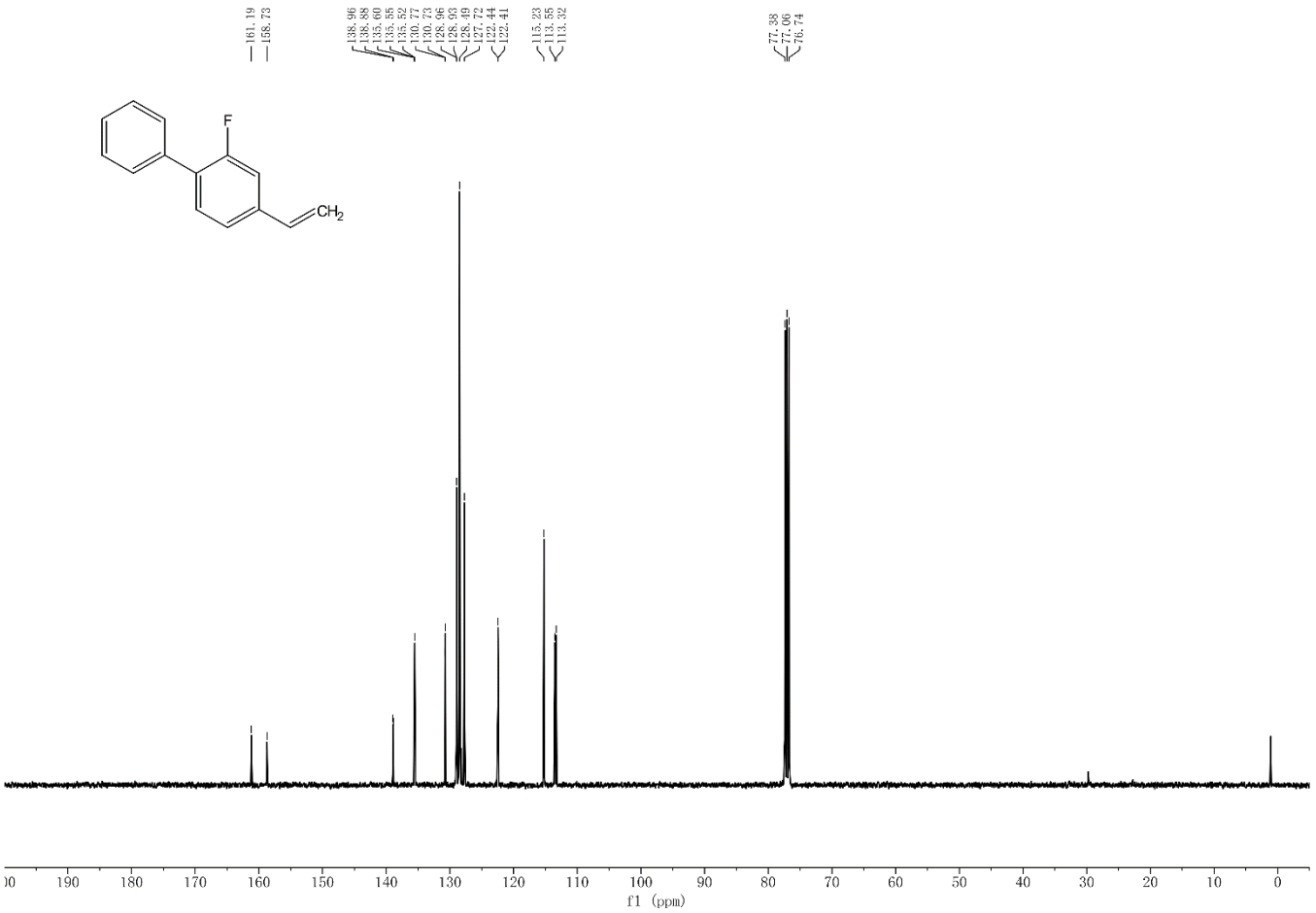
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5b



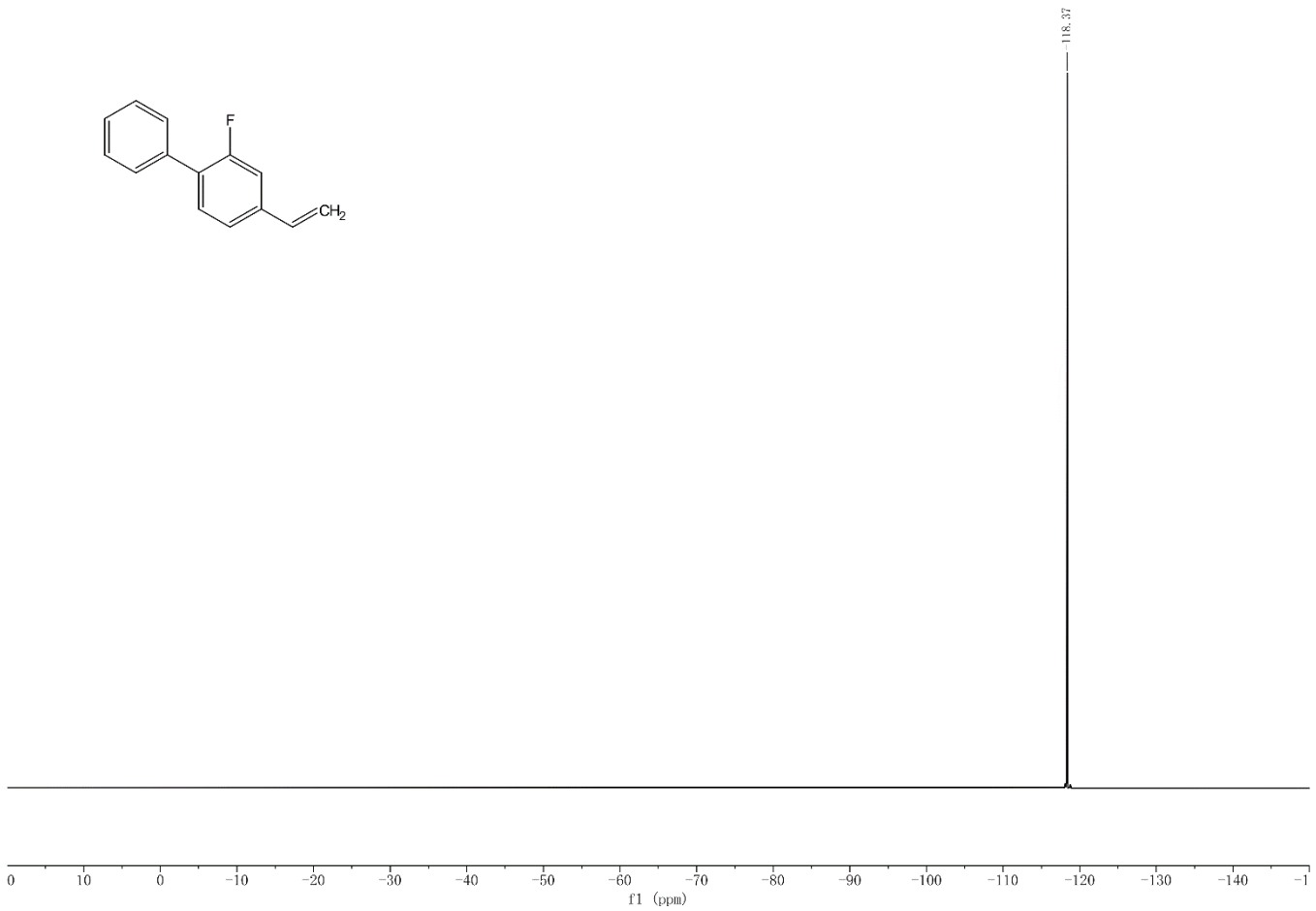
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5c



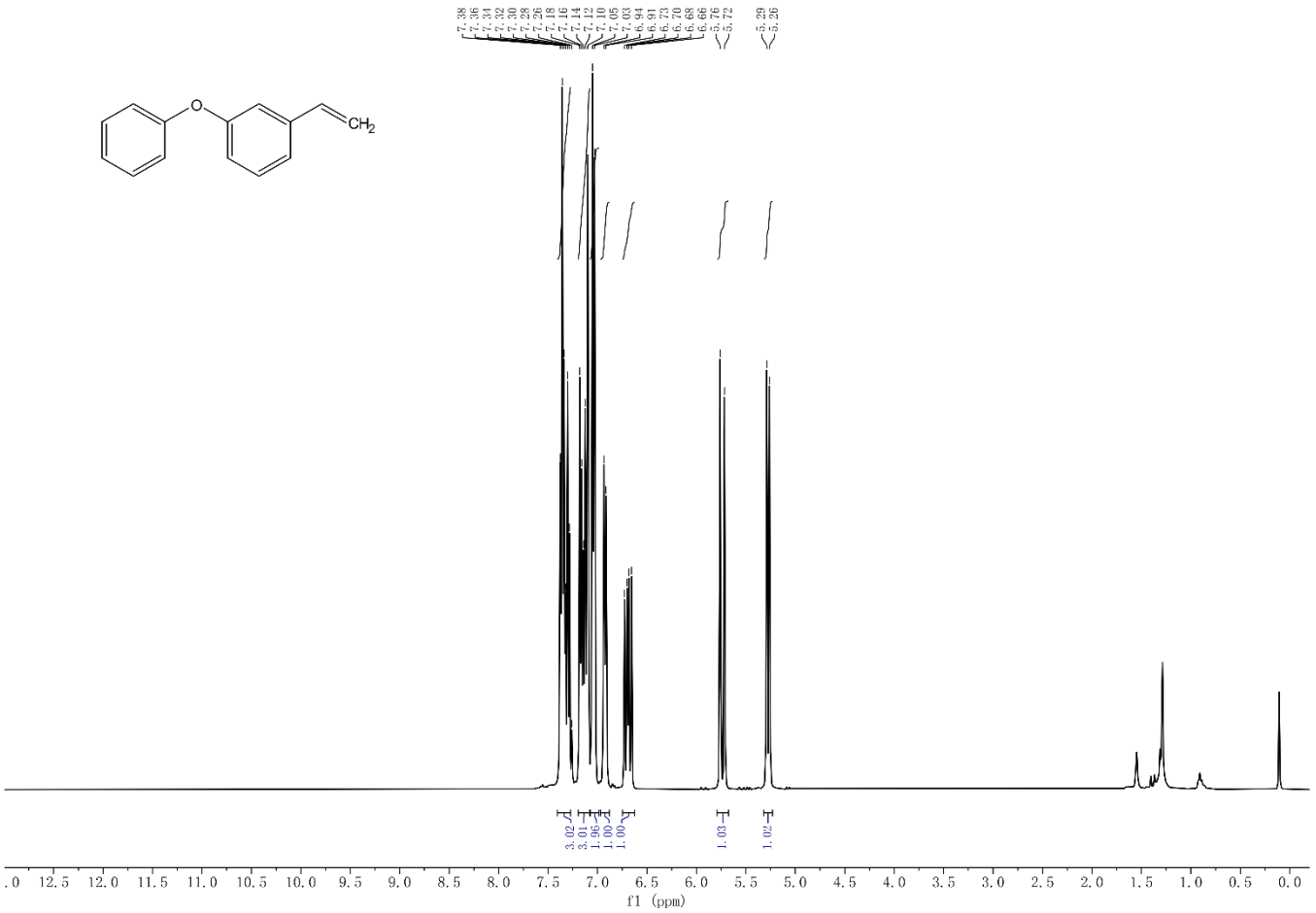
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5c



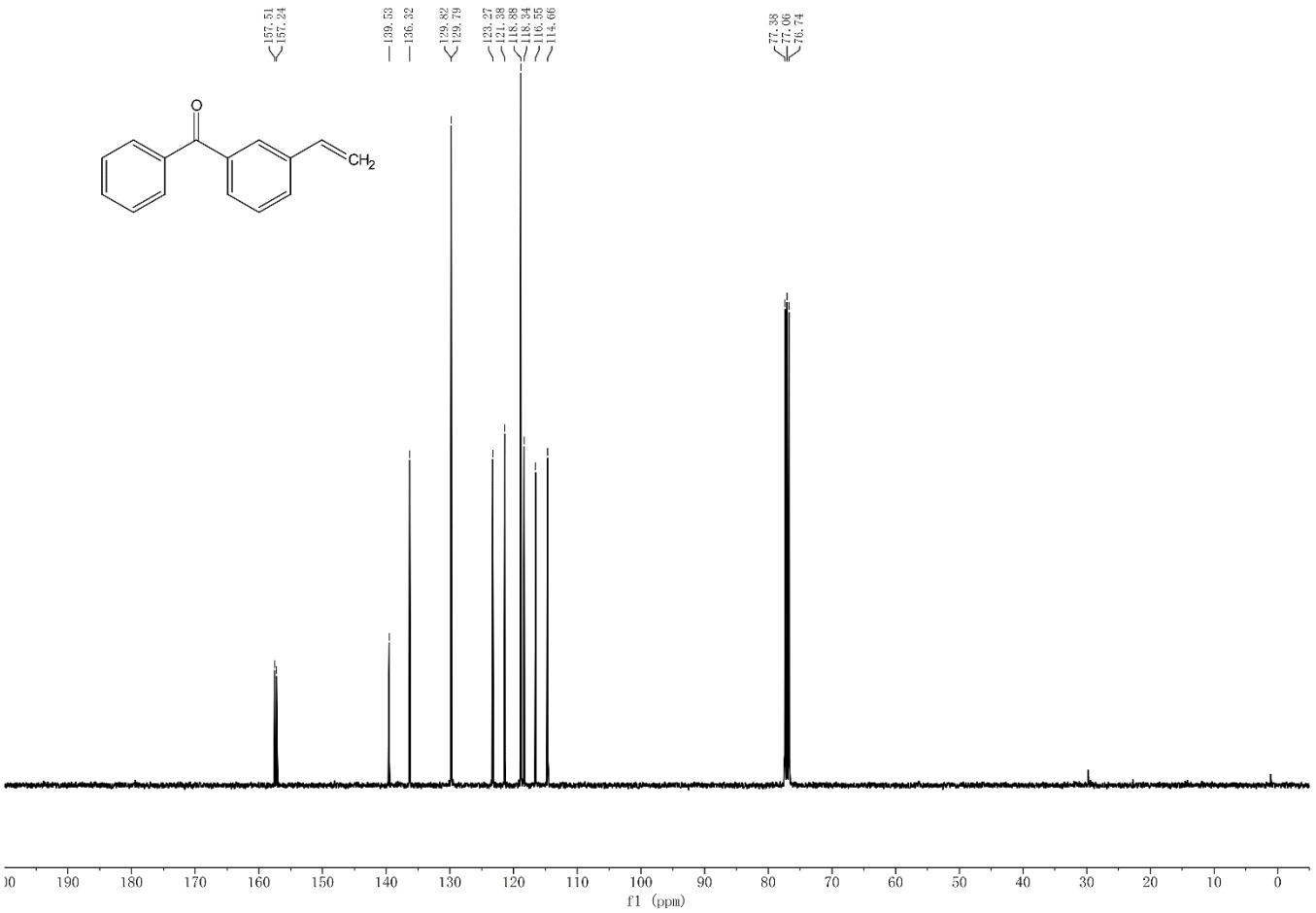
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 5c



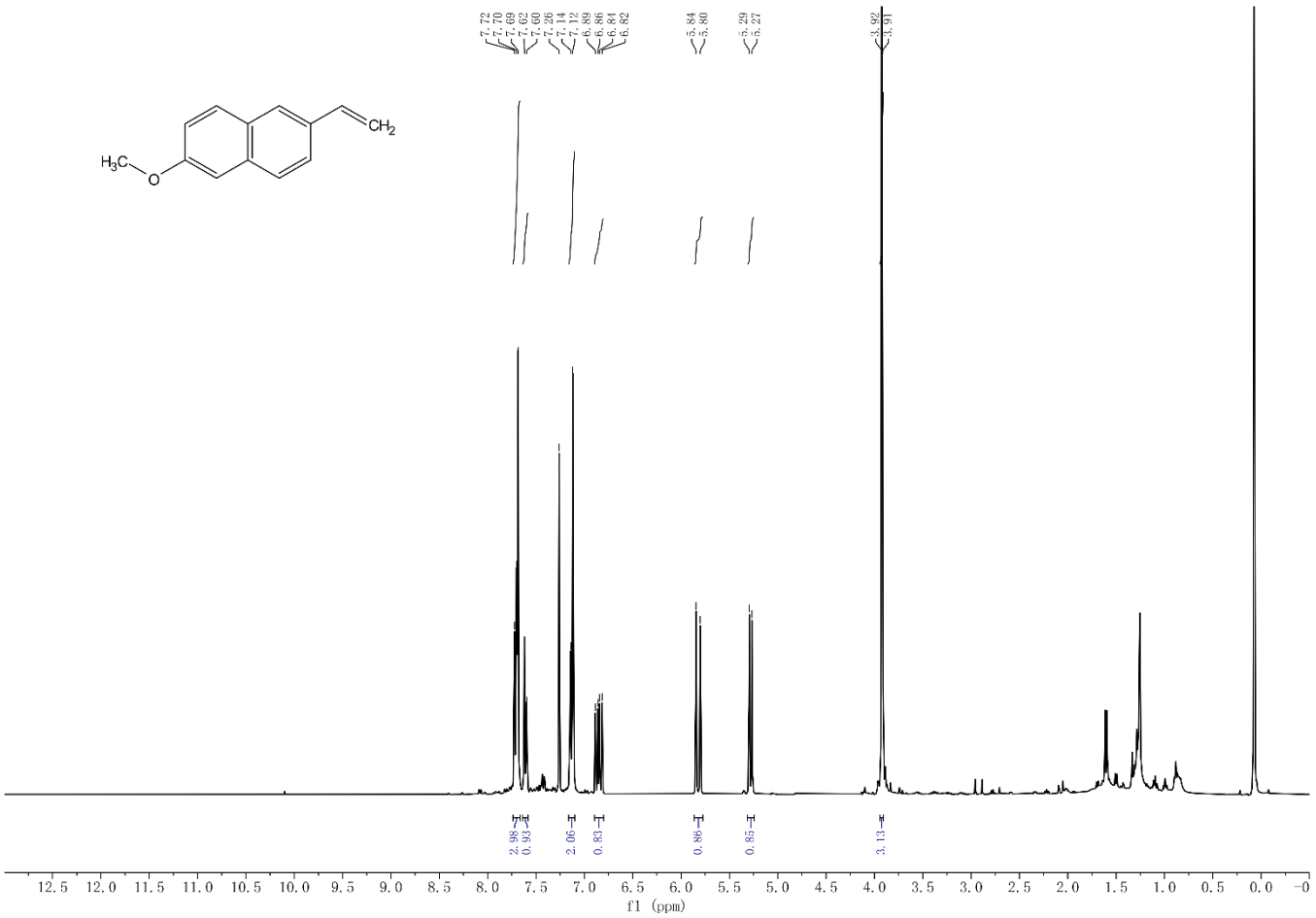
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5d



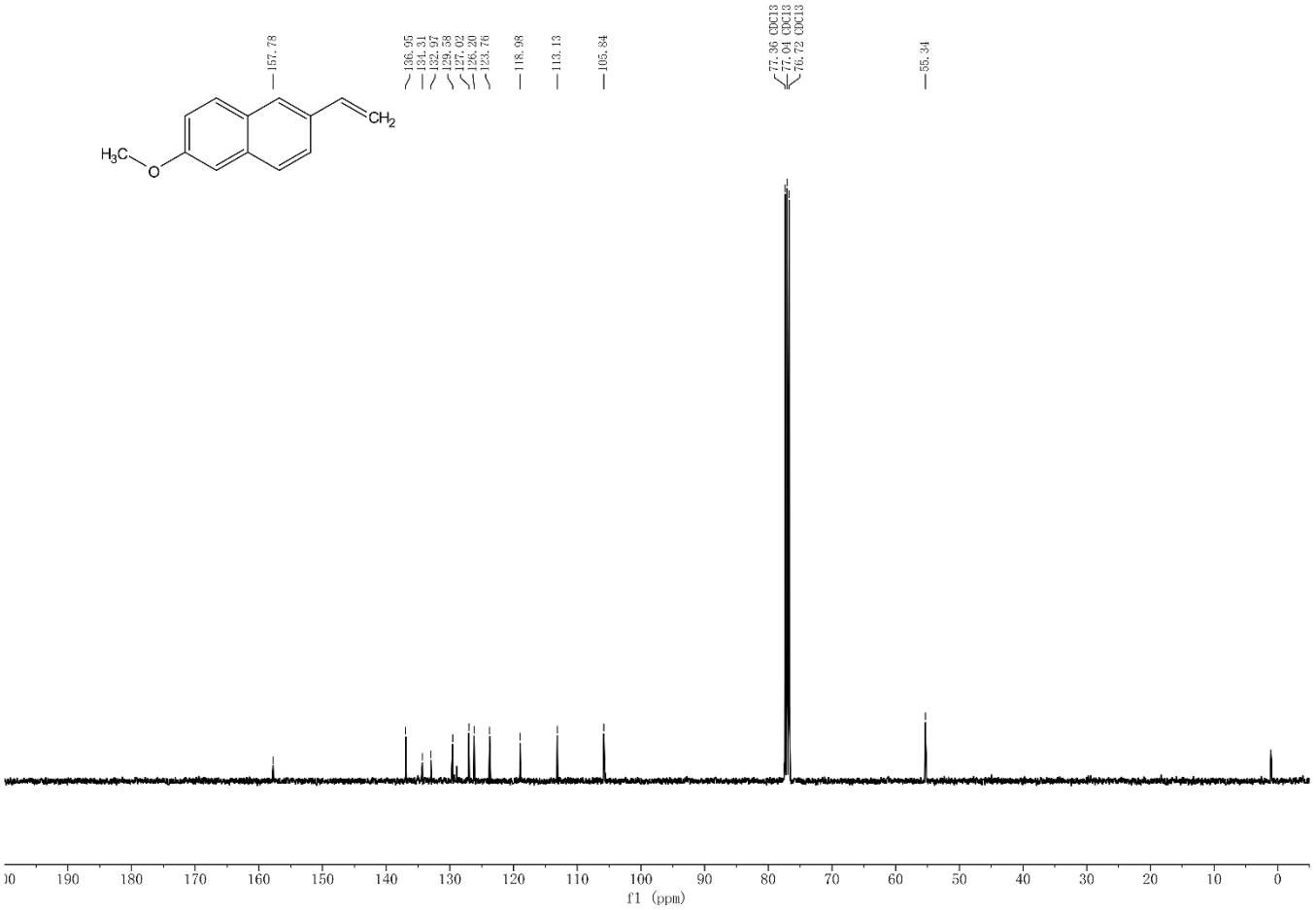
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5d



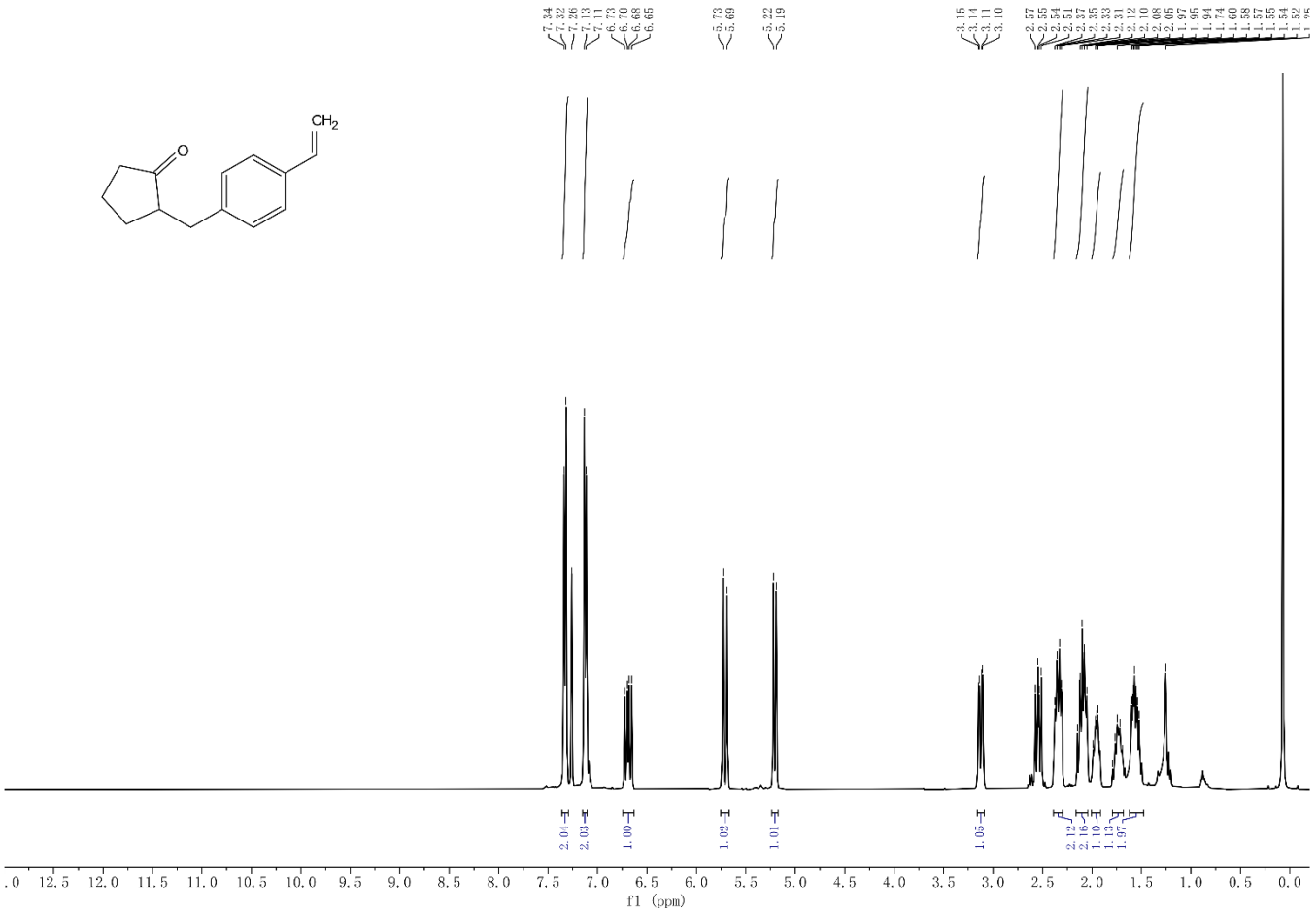
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5e



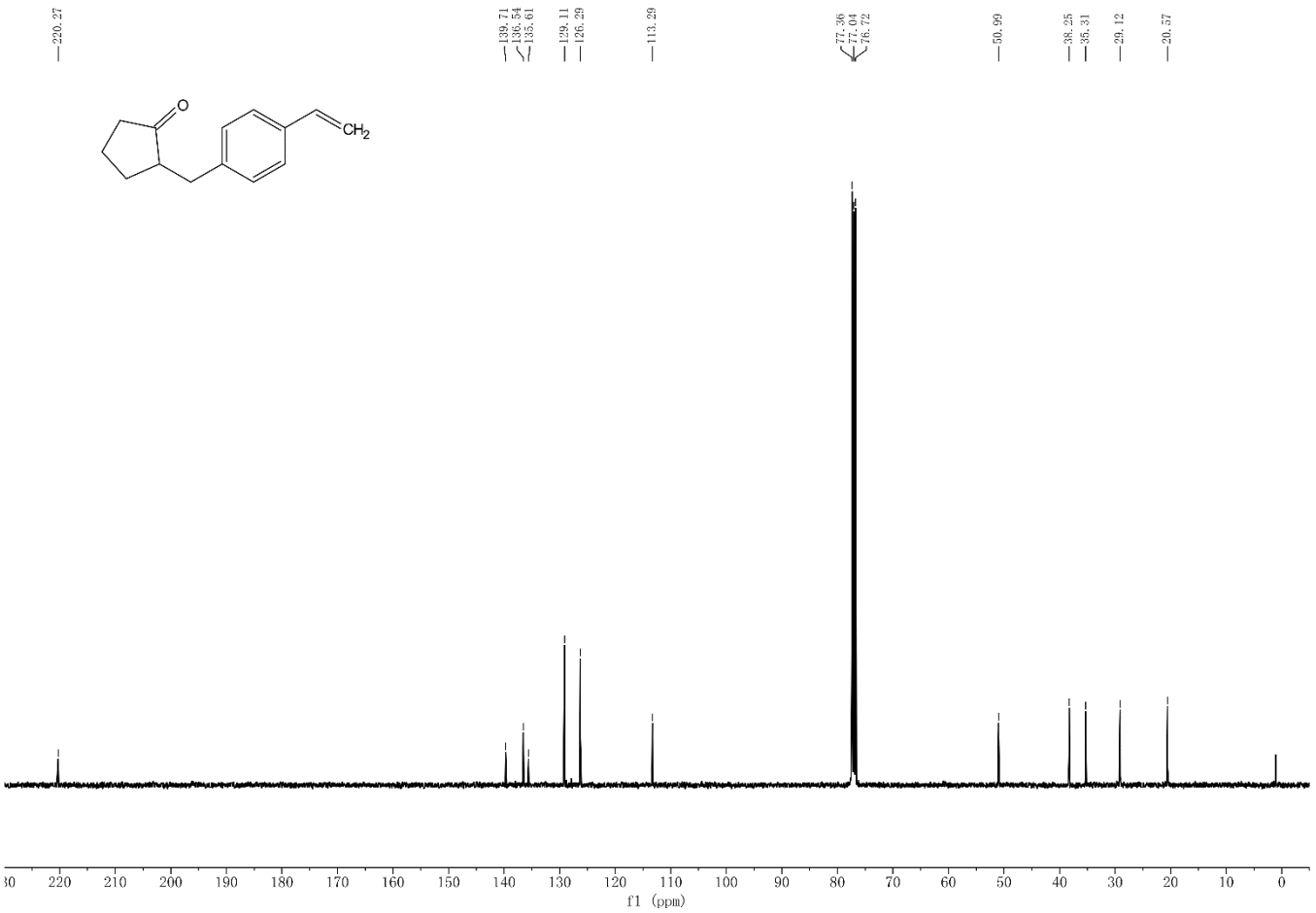
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5e



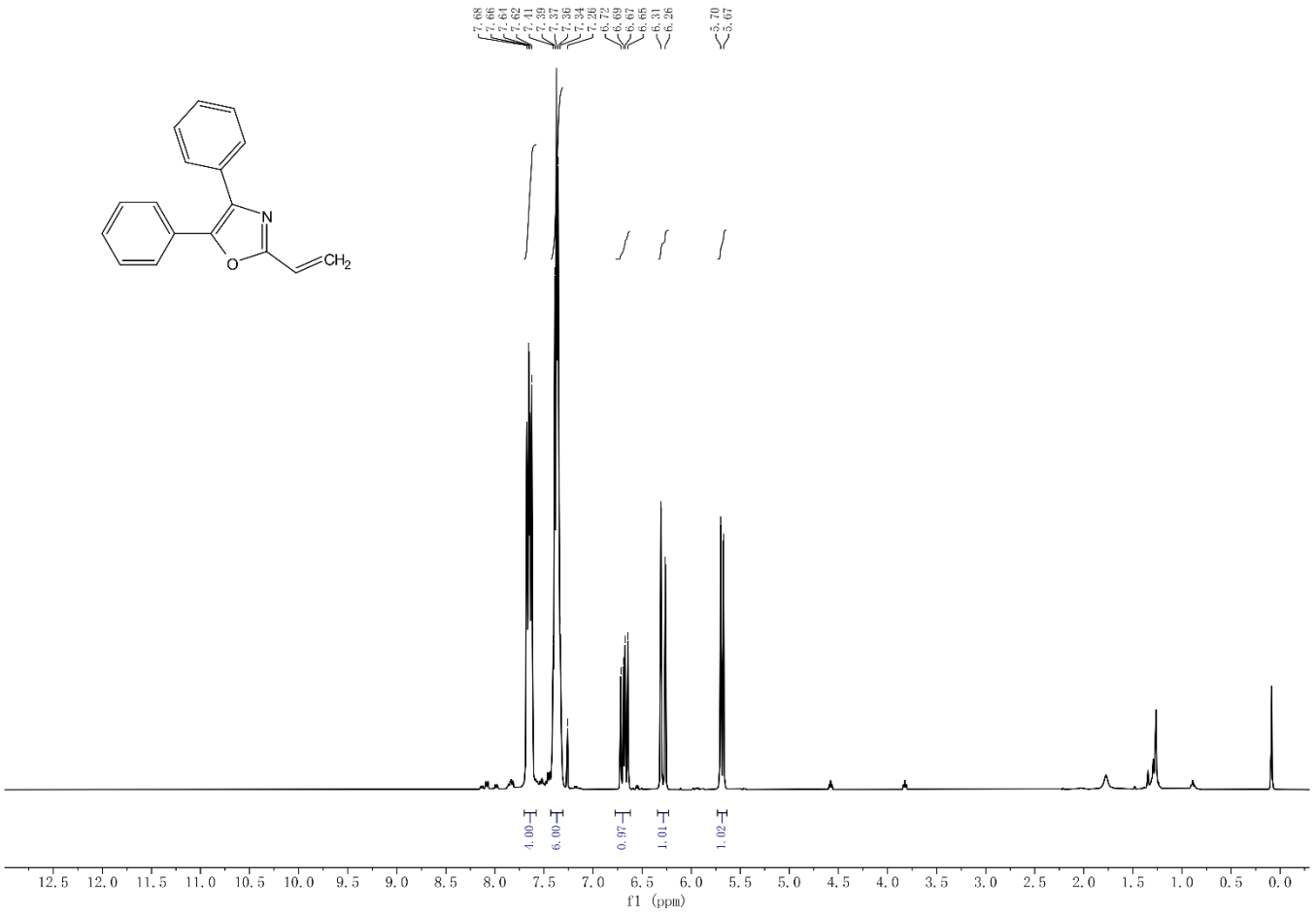
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5f



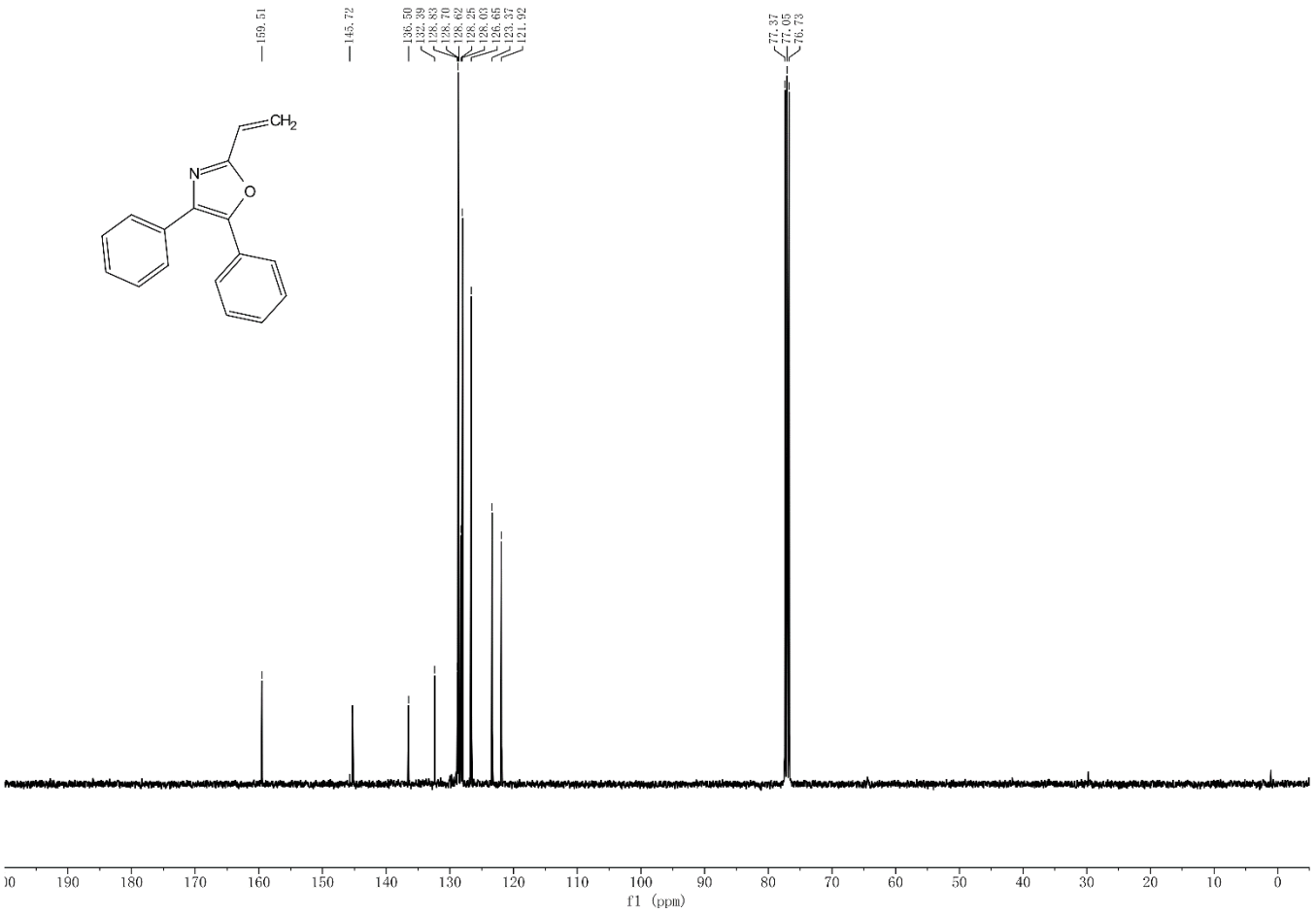
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5f



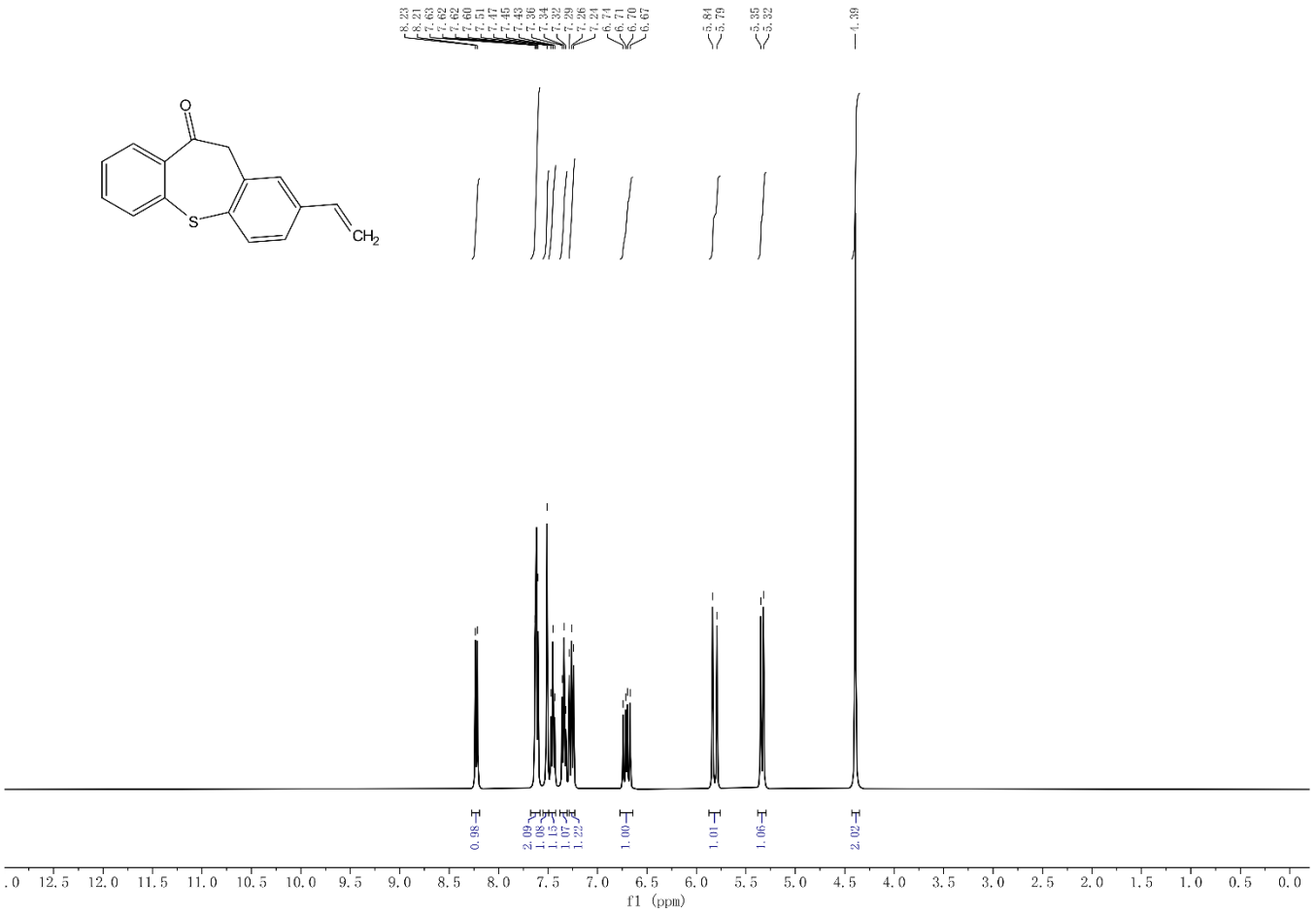
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5g



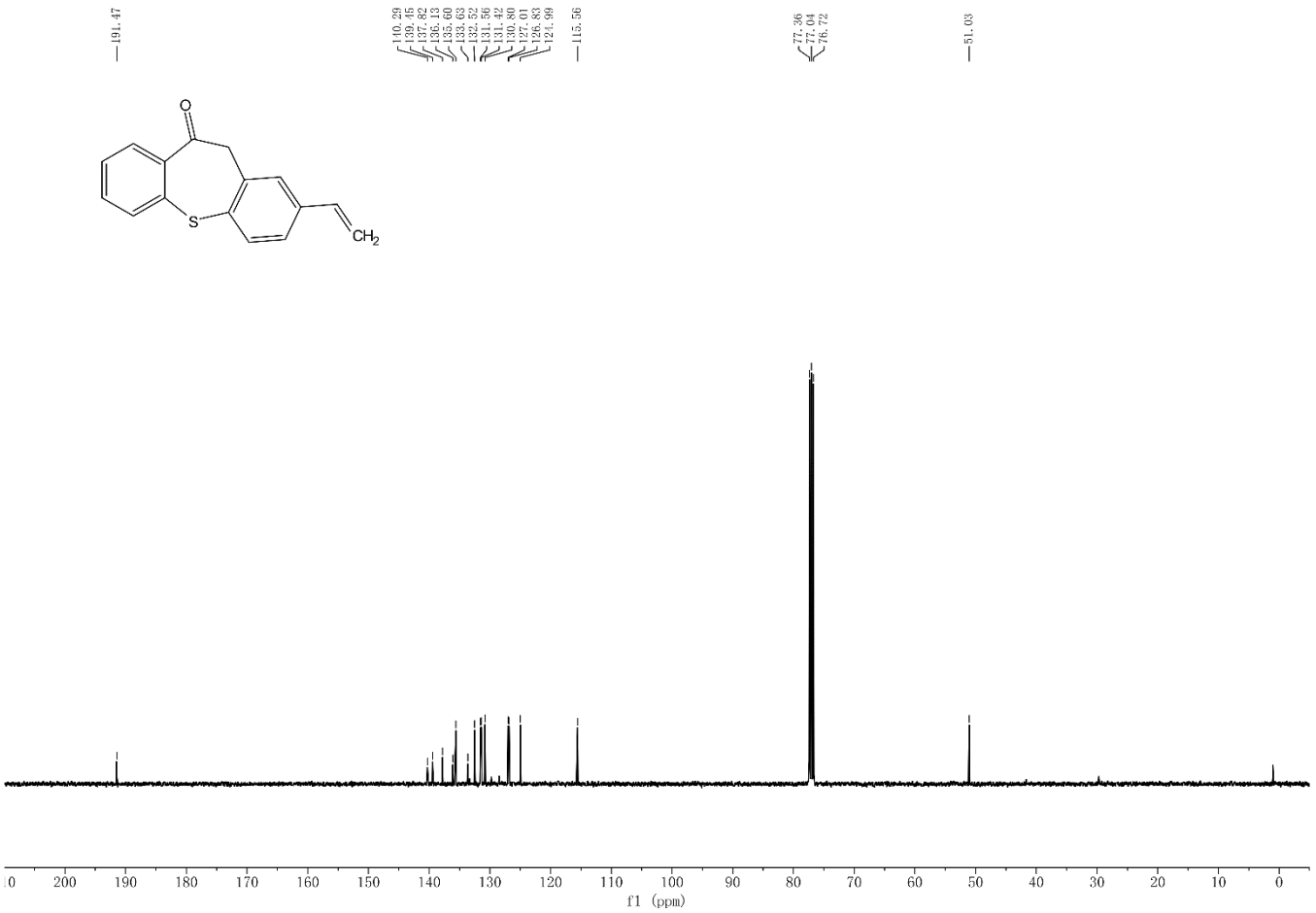
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5g



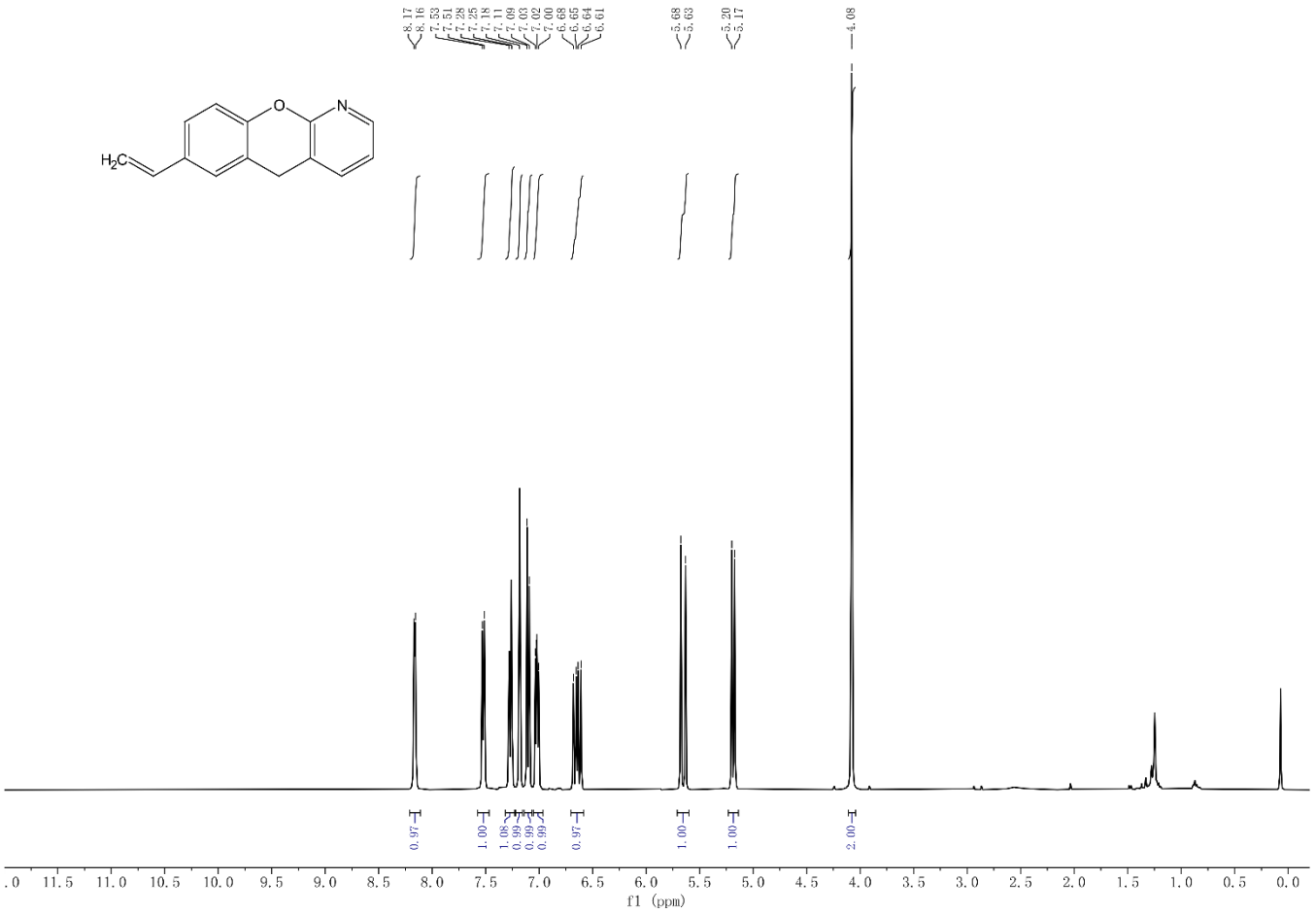
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5h



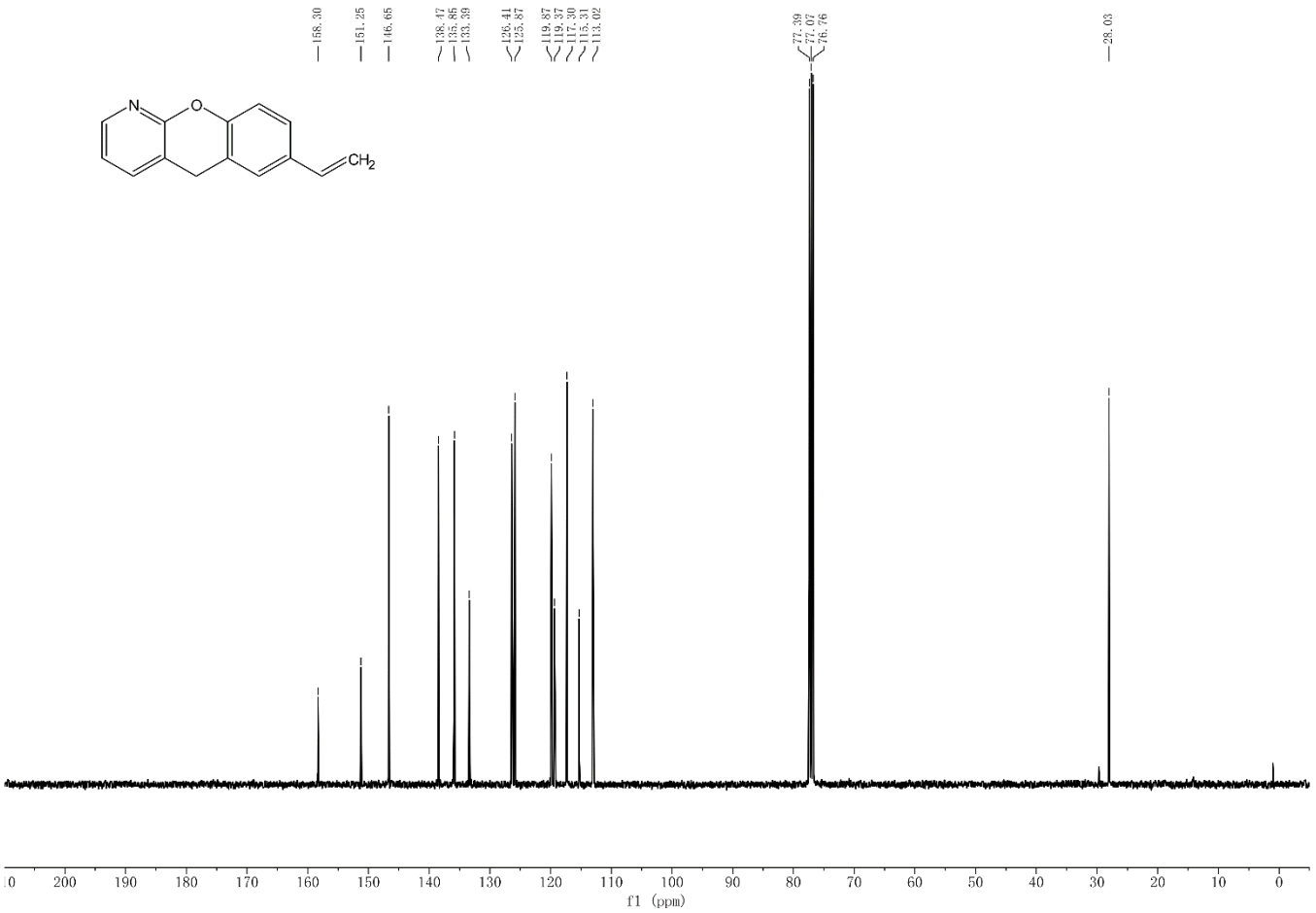
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5h



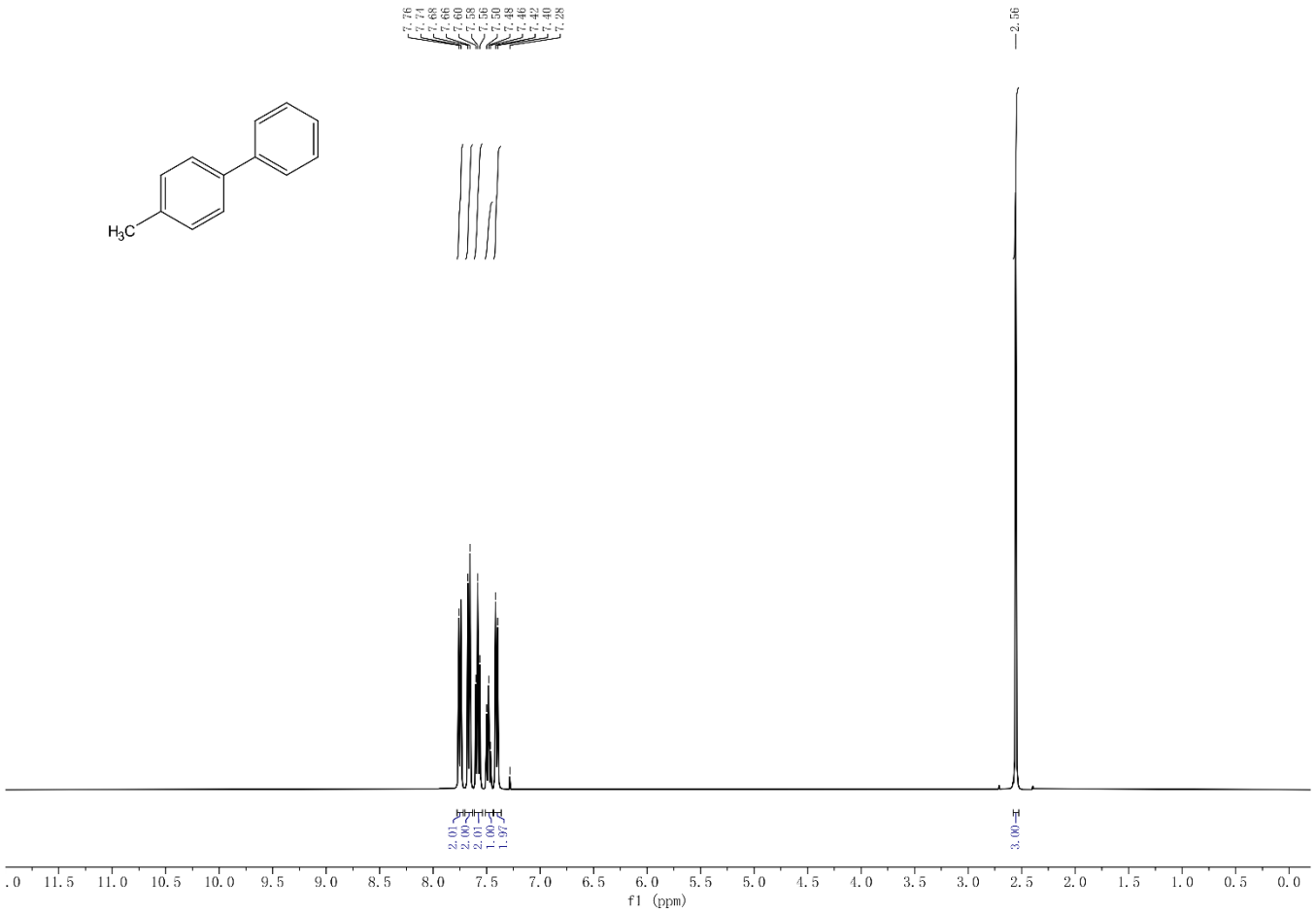
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 5i



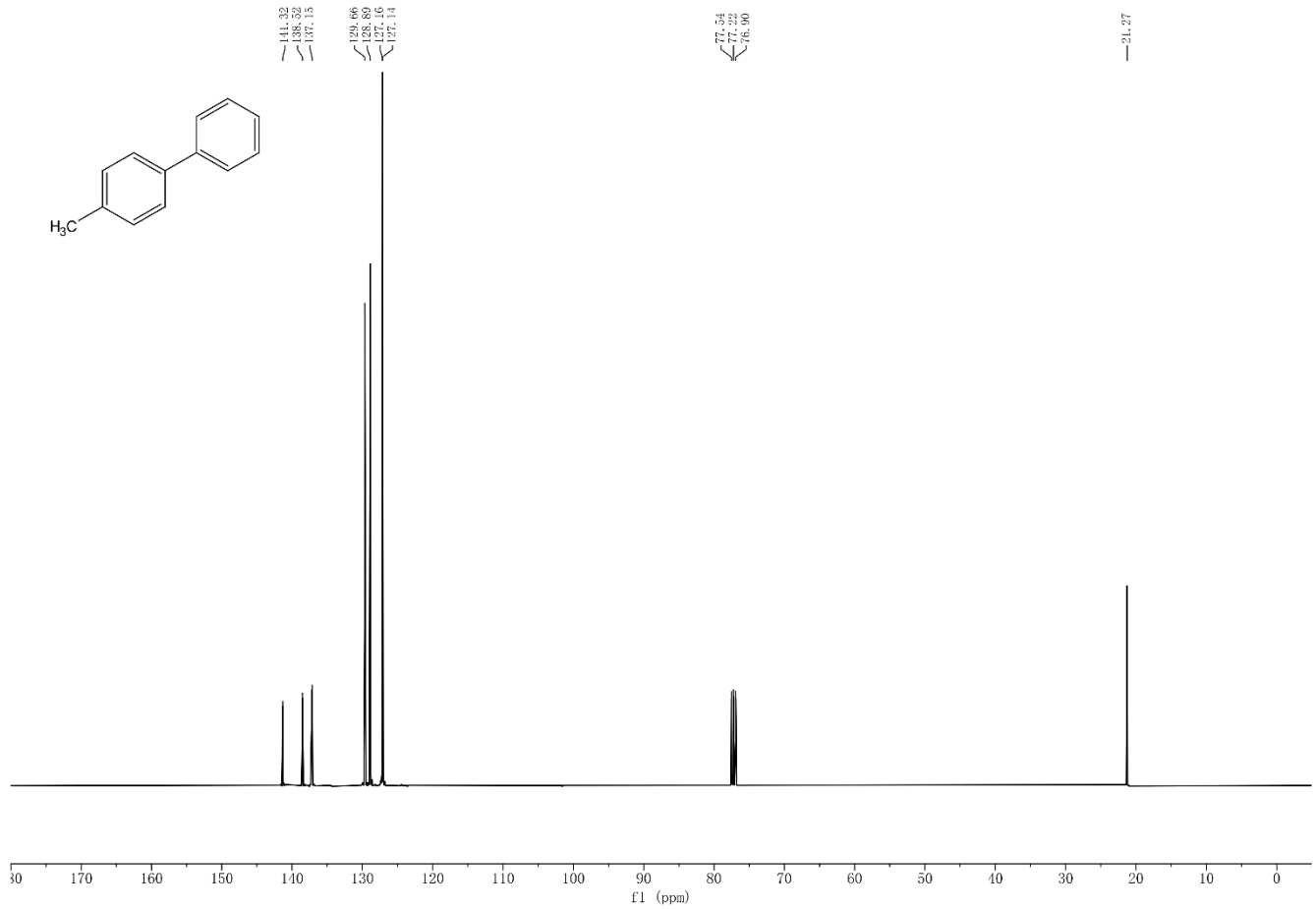
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 5i



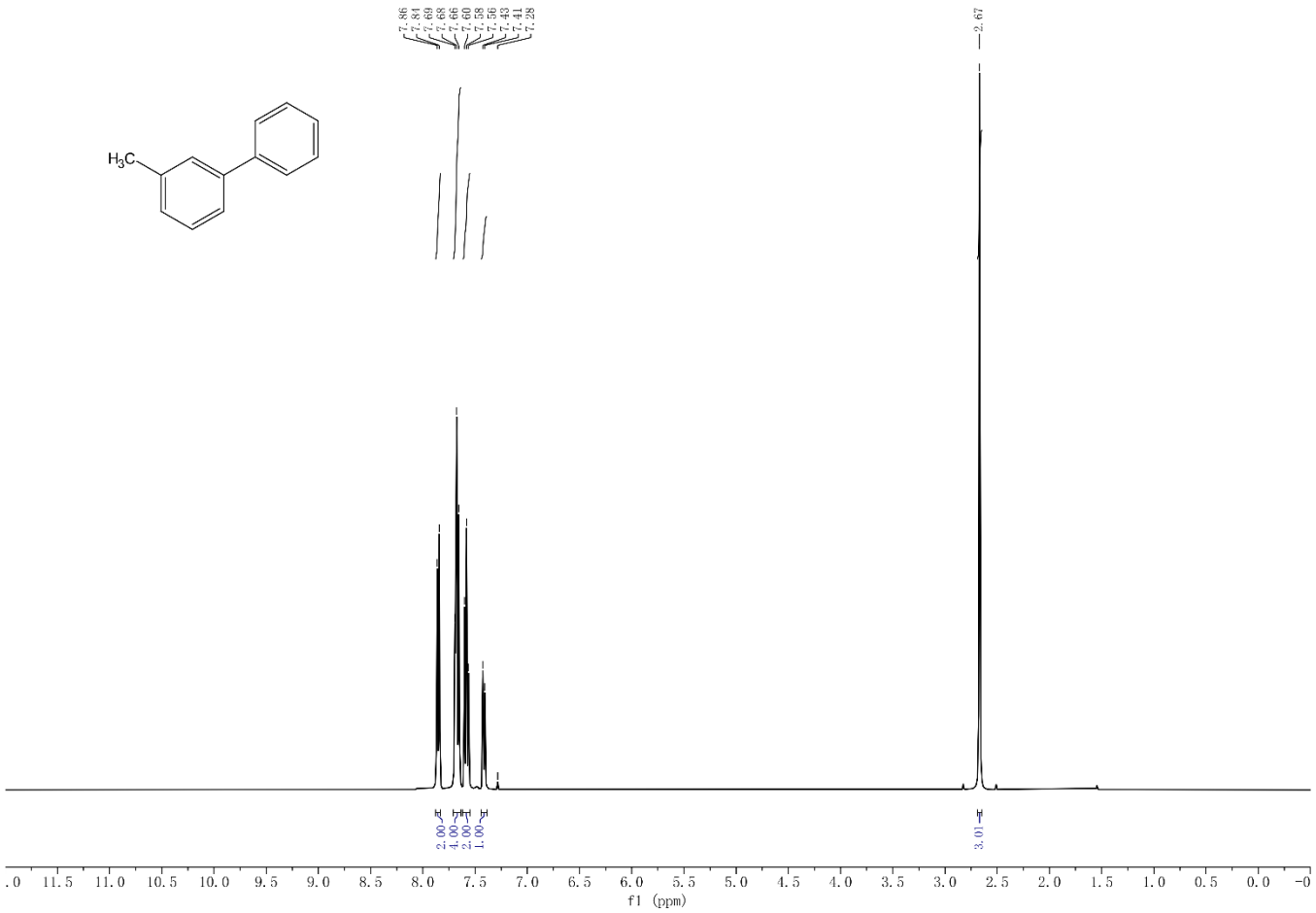
^{1}H NMR (400 MHz, CDCl3) spectrum of 8a



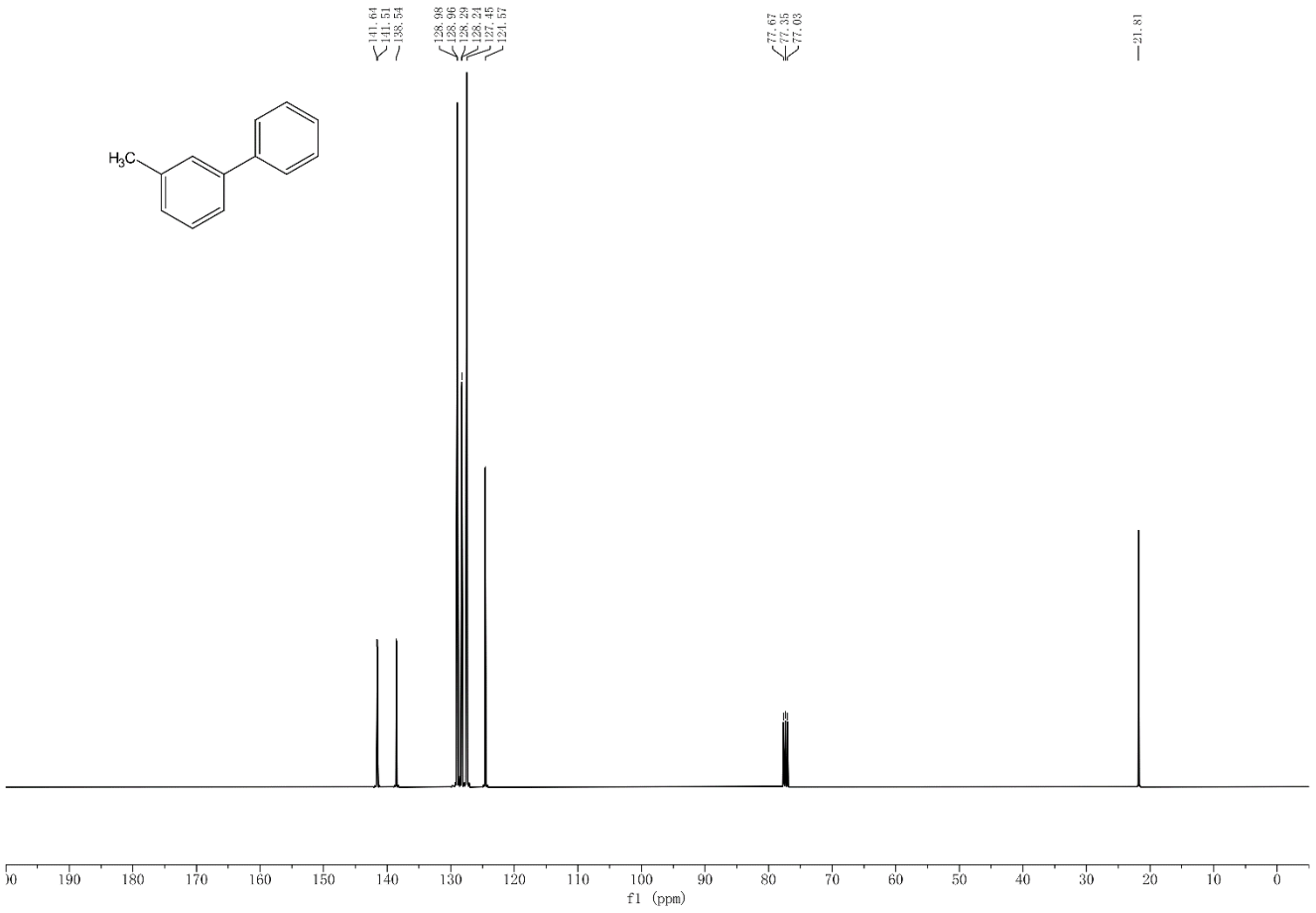
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8a



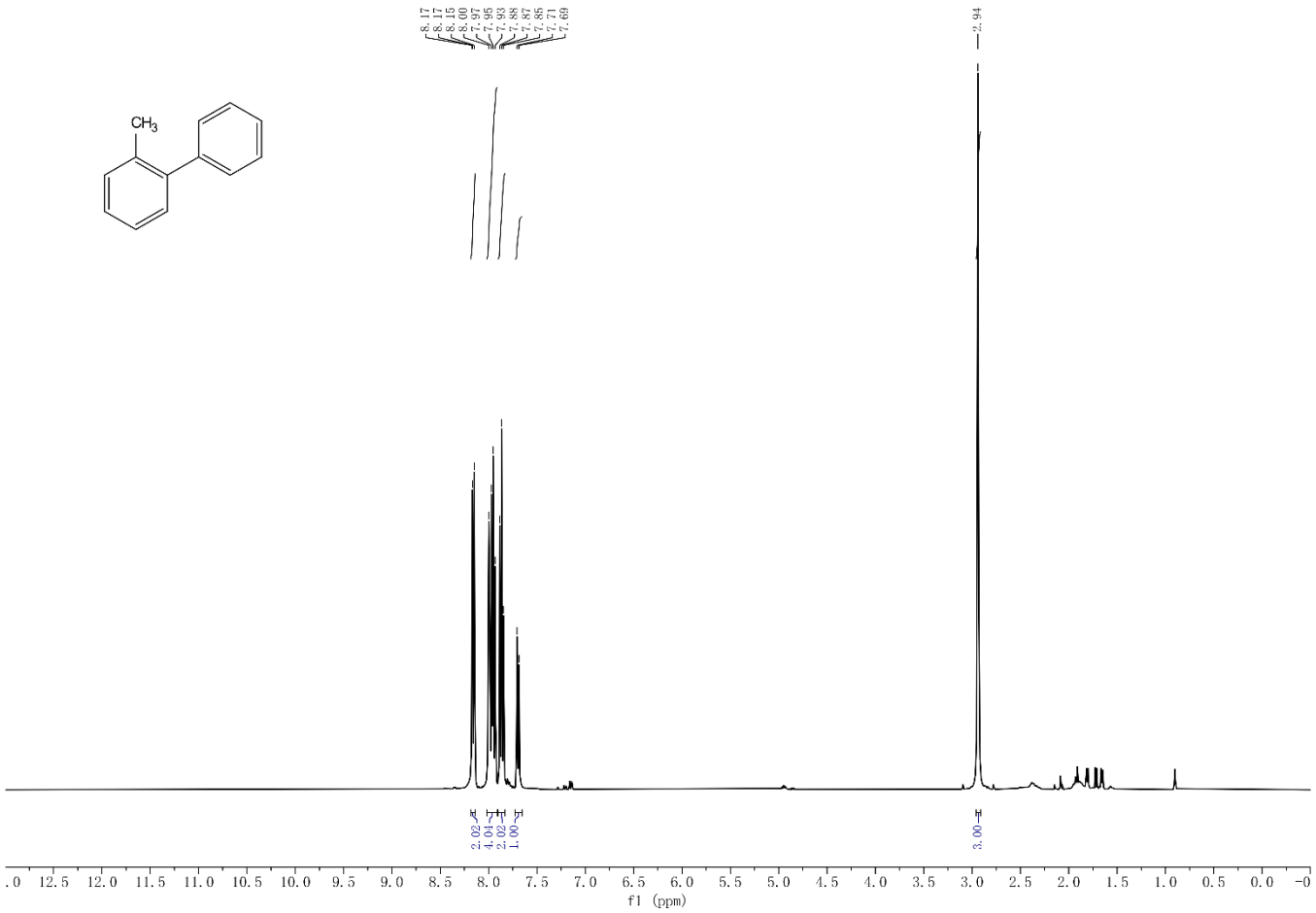
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8b



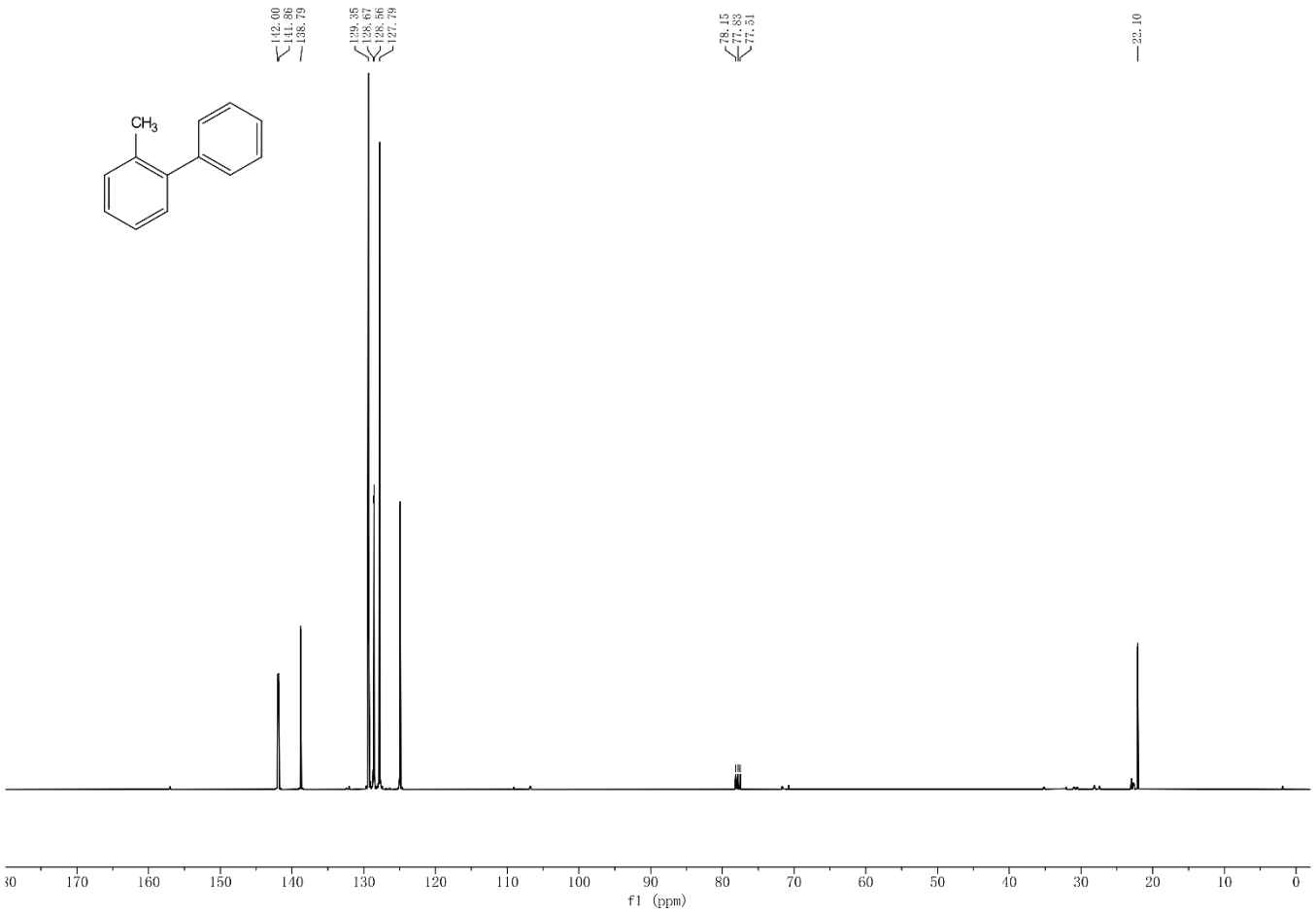
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8b



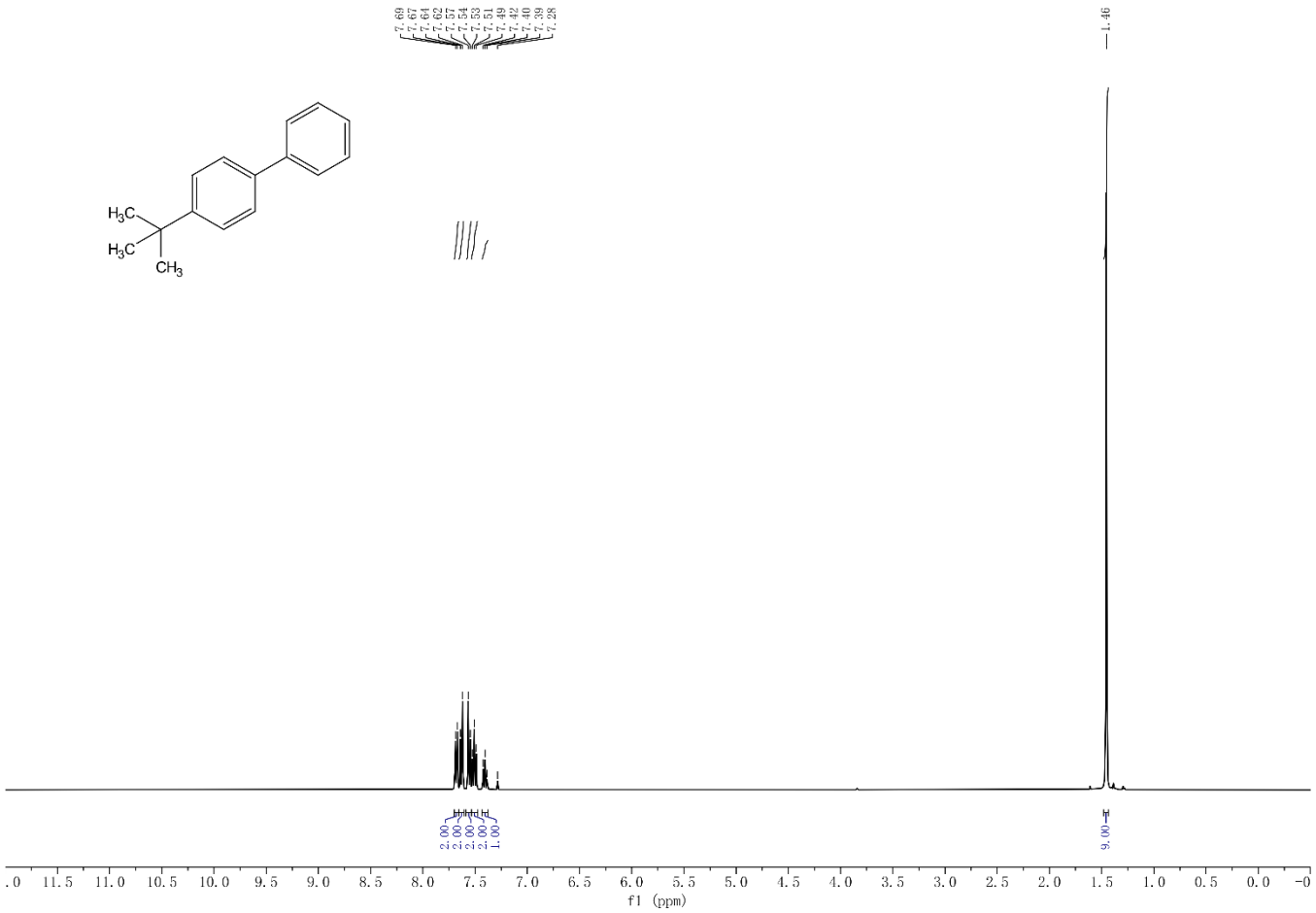
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8c



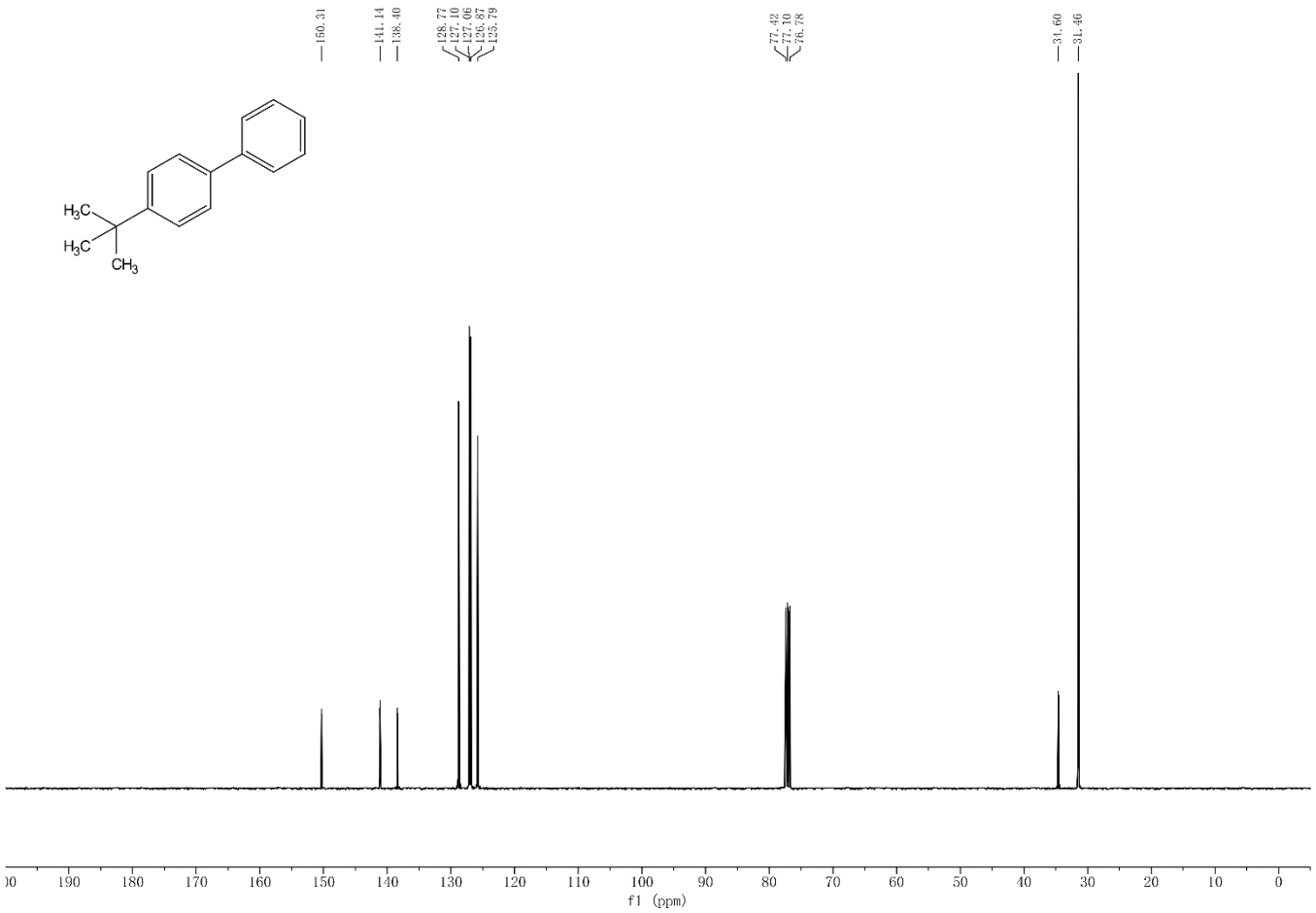
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8c



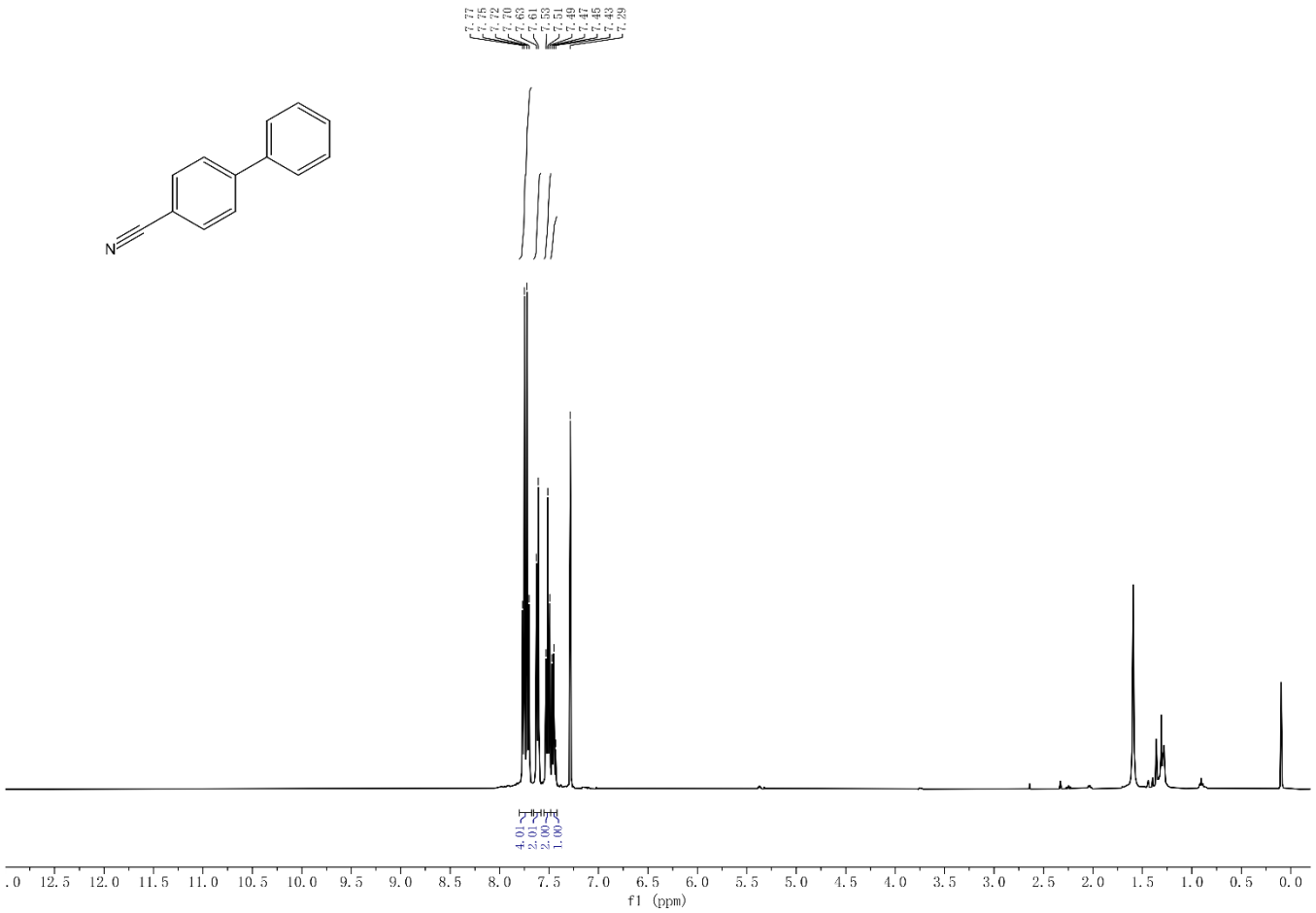
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8d



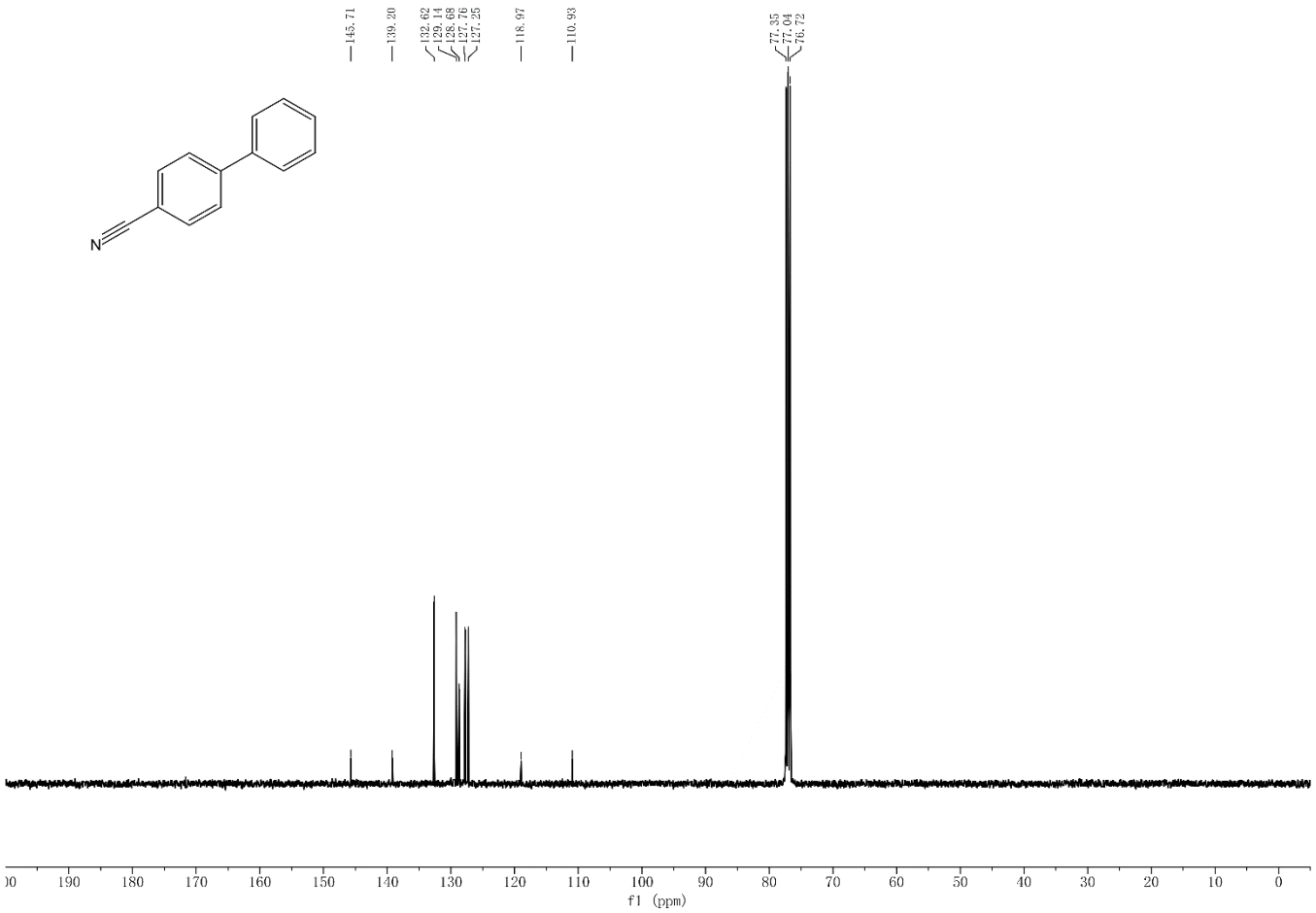
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8d



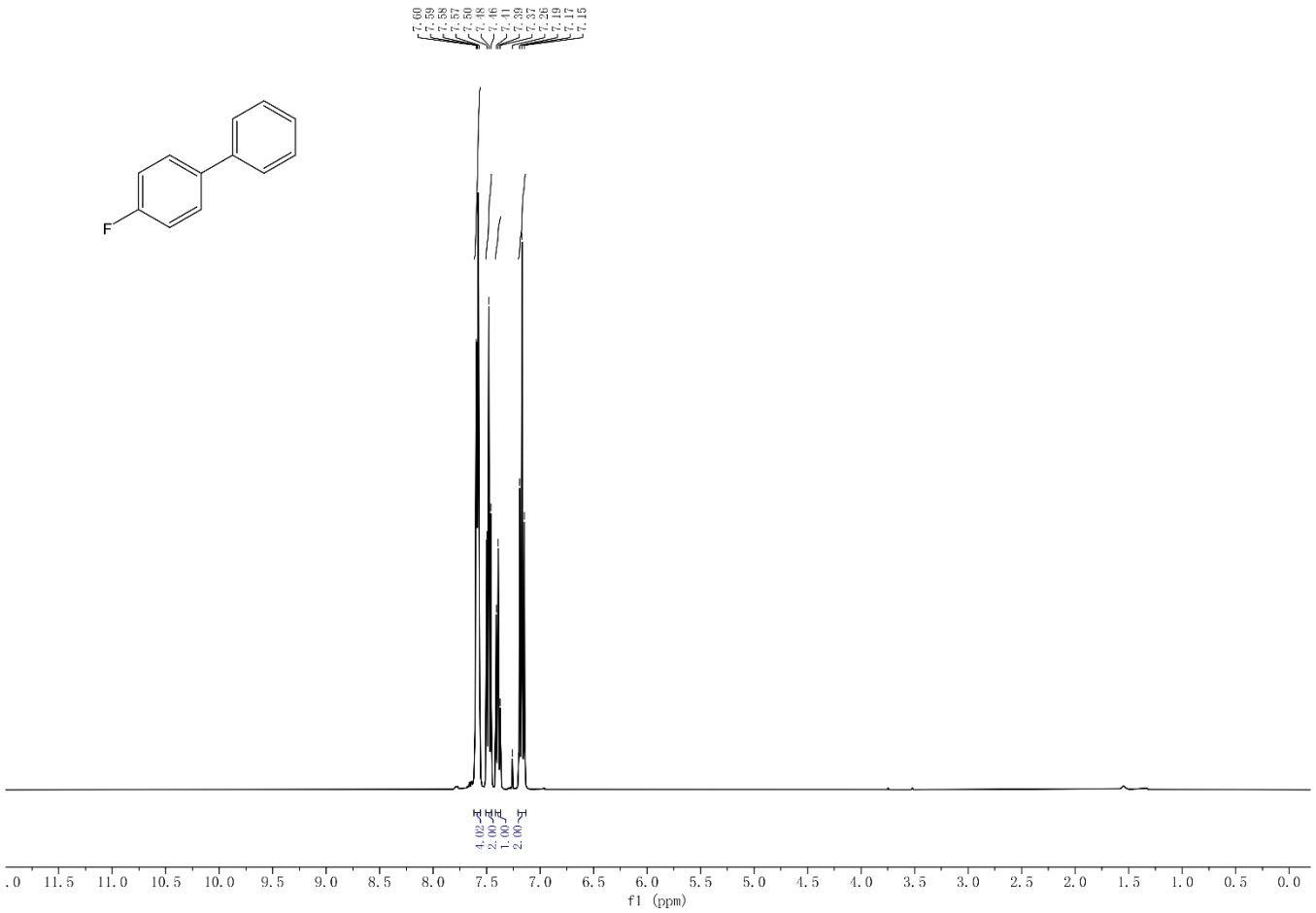
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8e



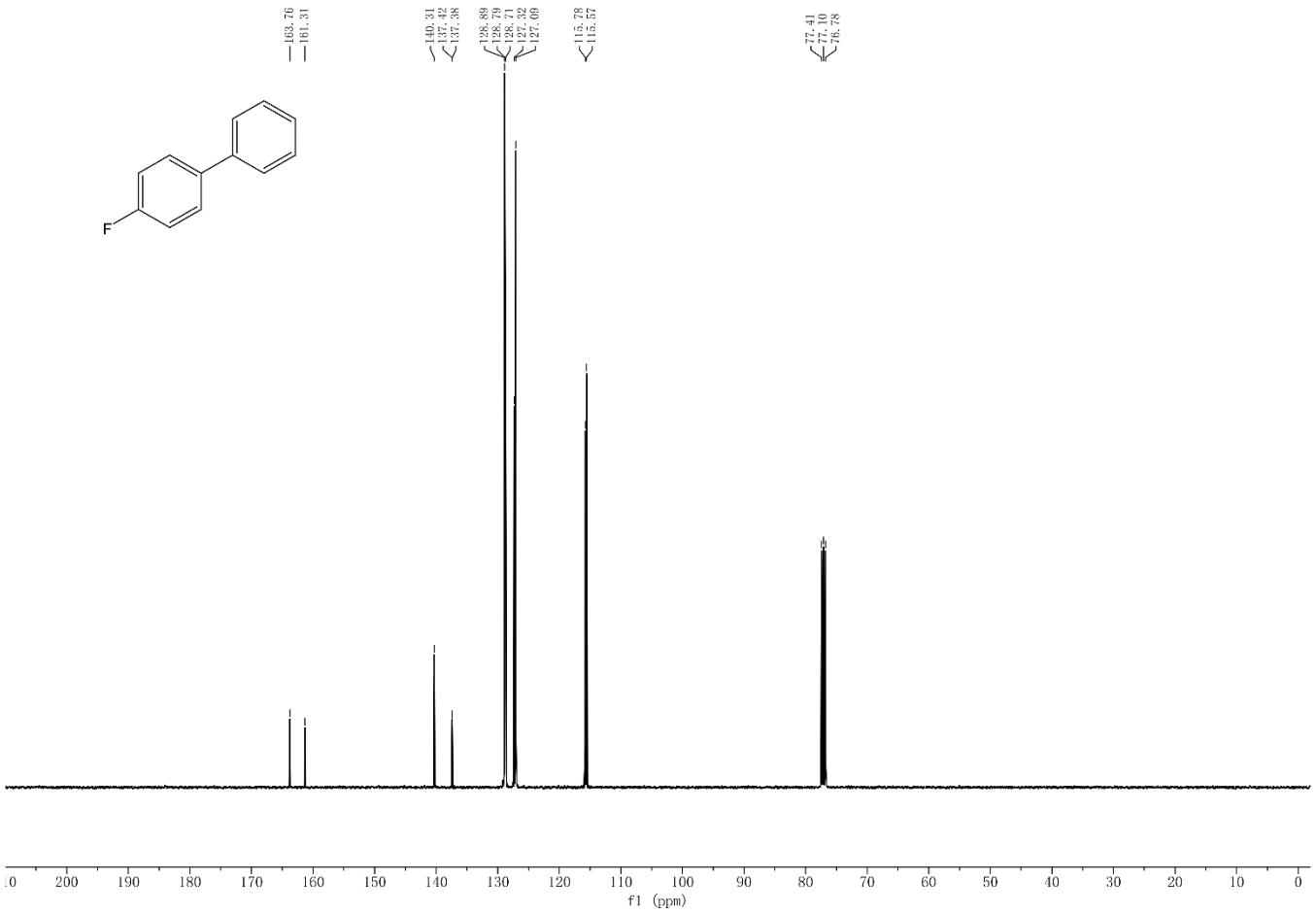
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8e



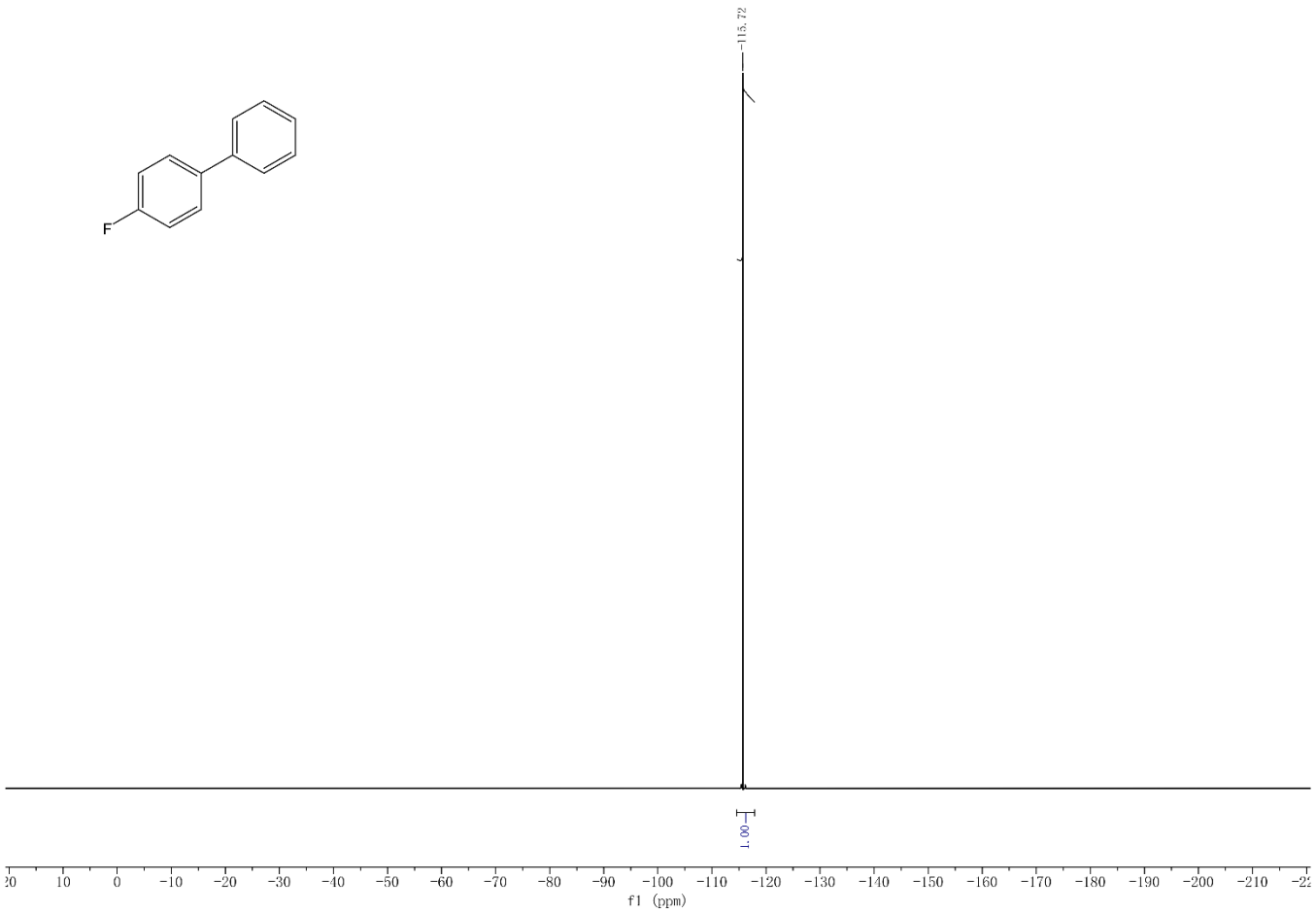
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8f



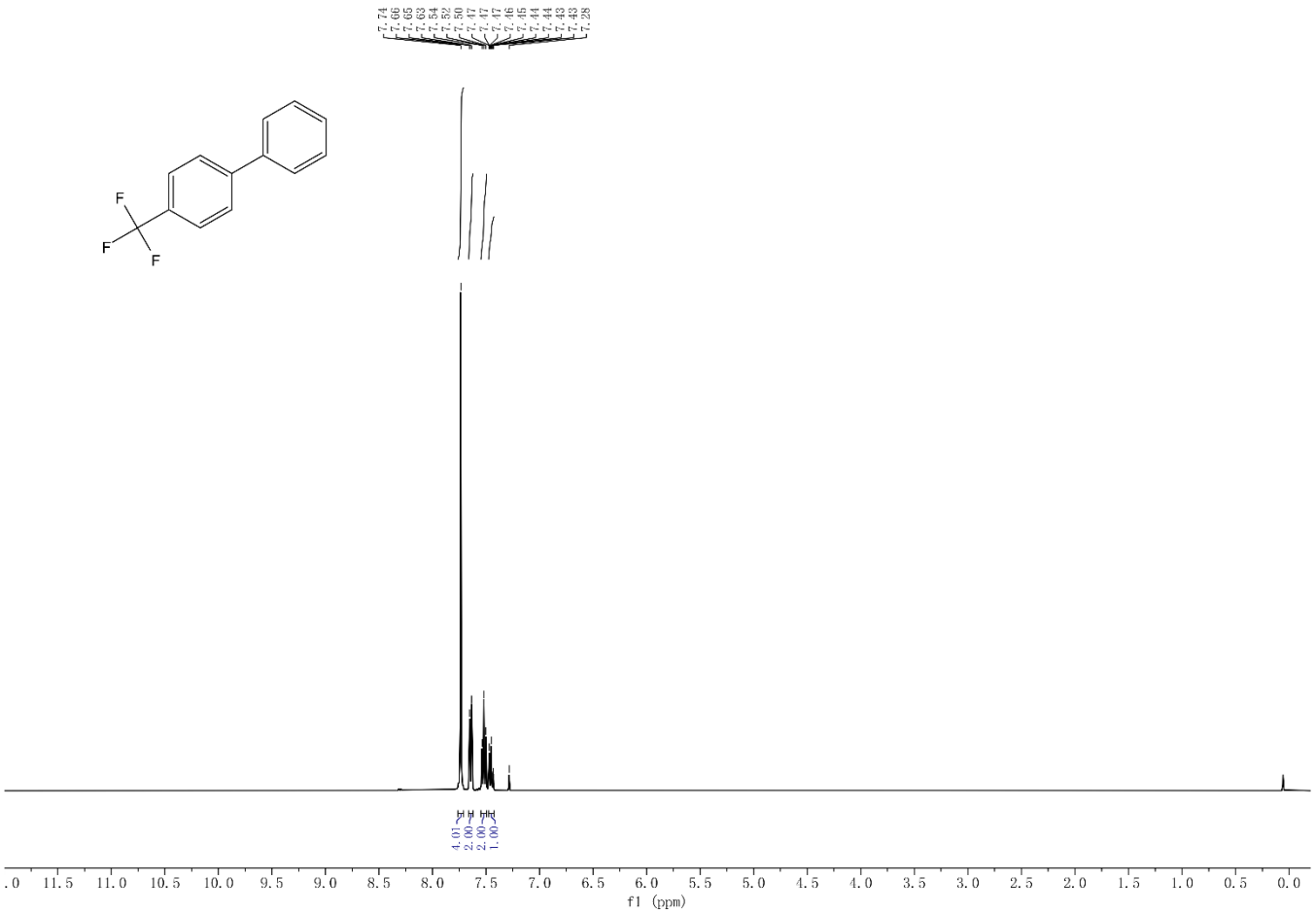
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8f



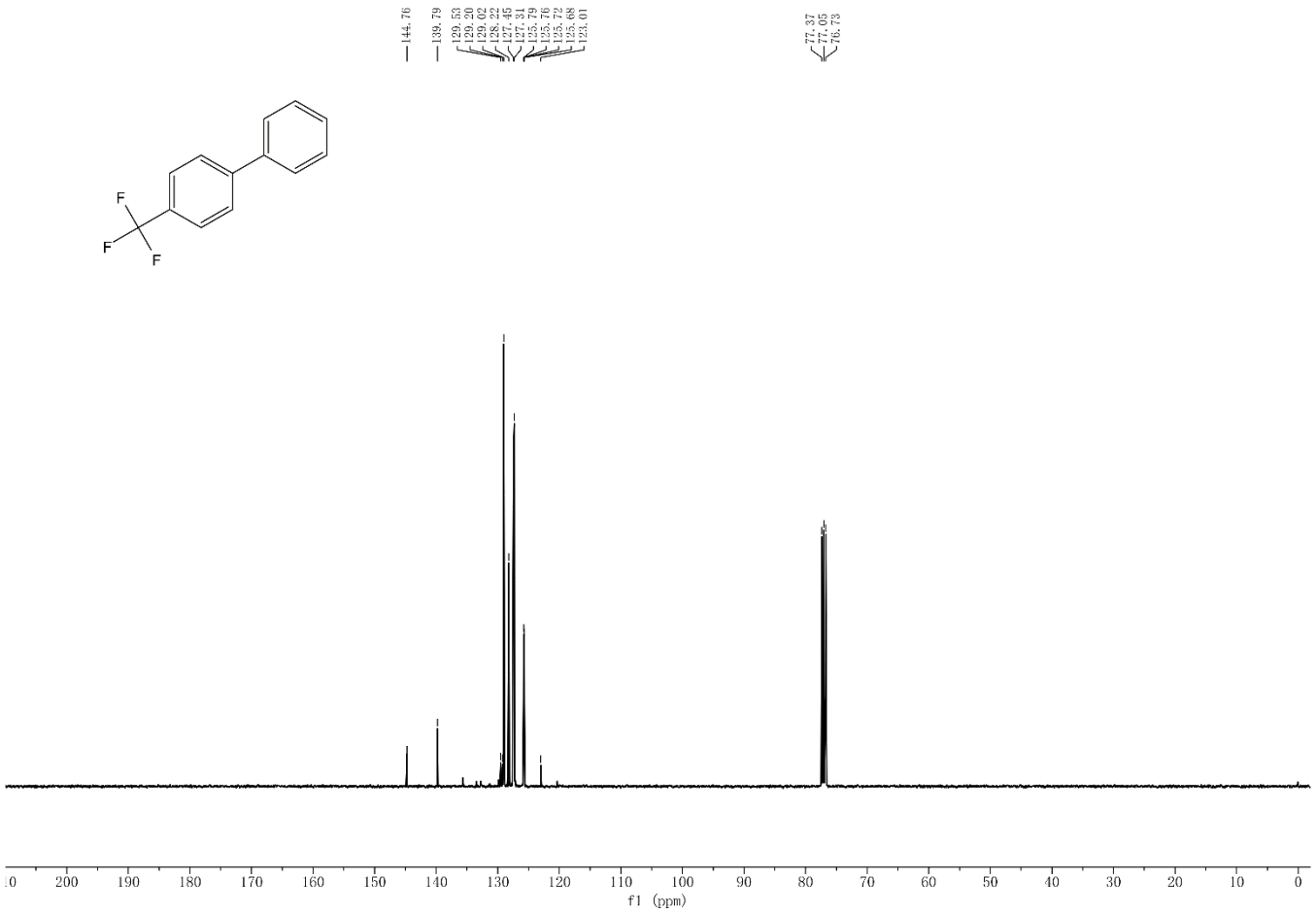
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 8f



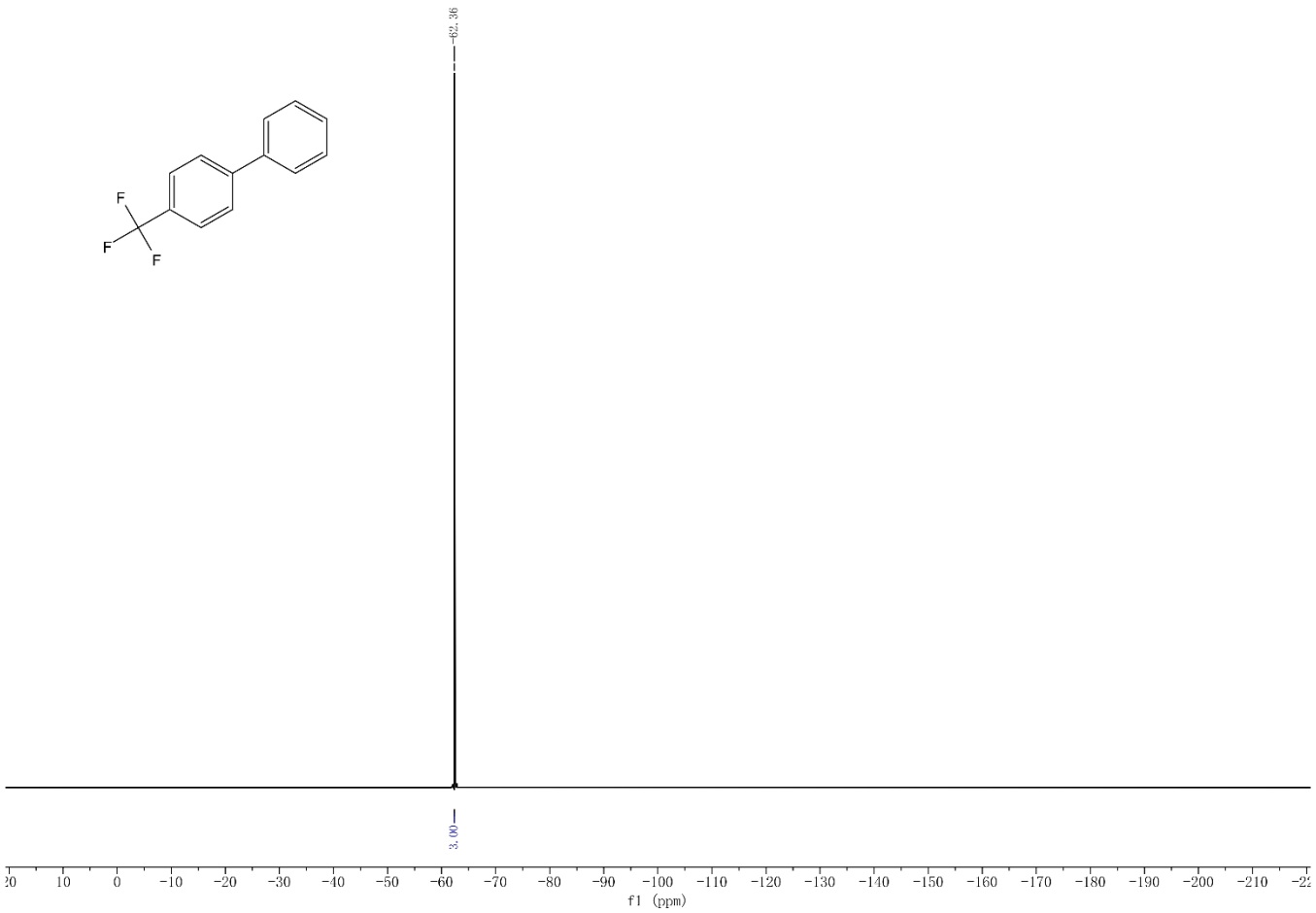
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8g



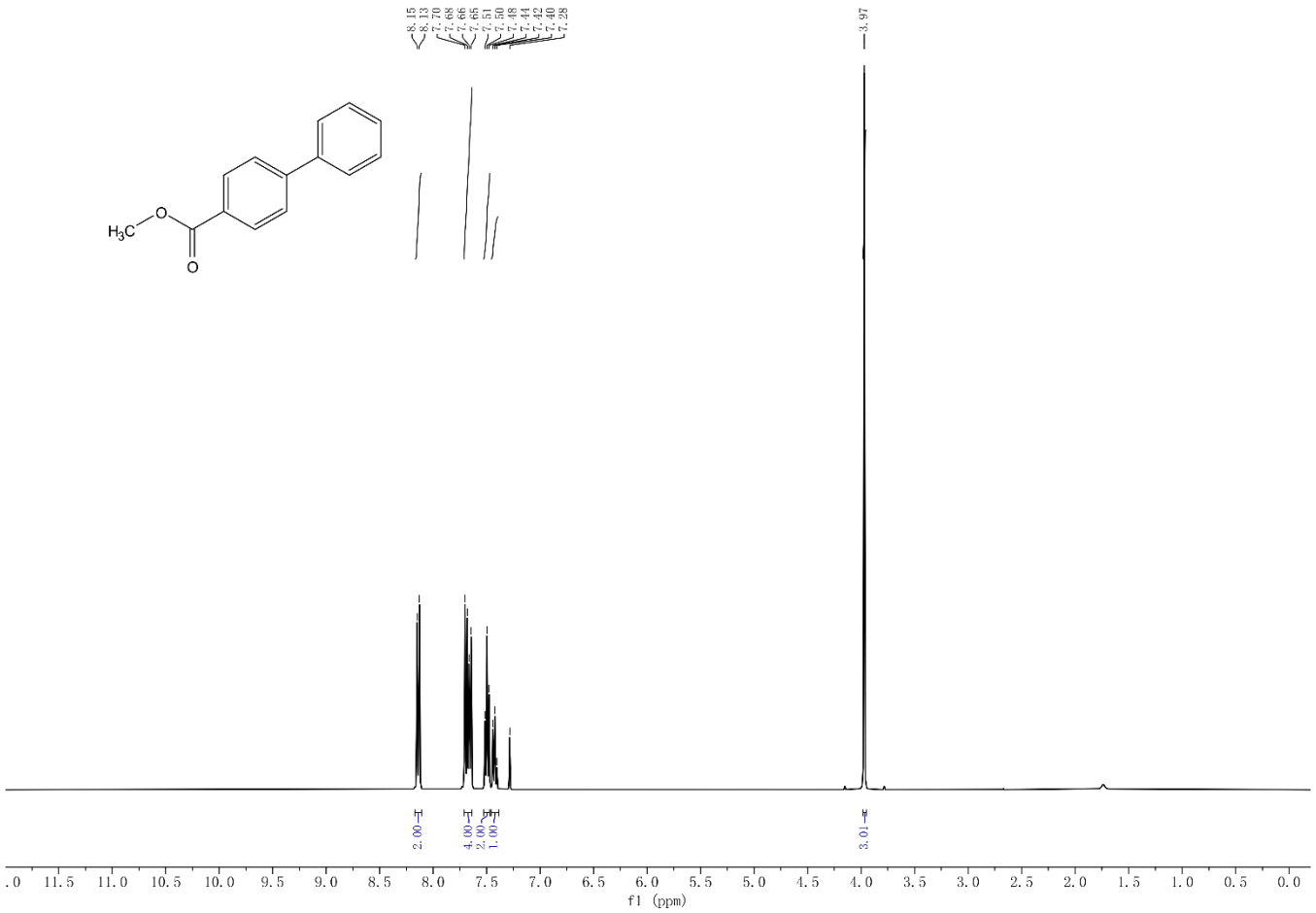
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8g



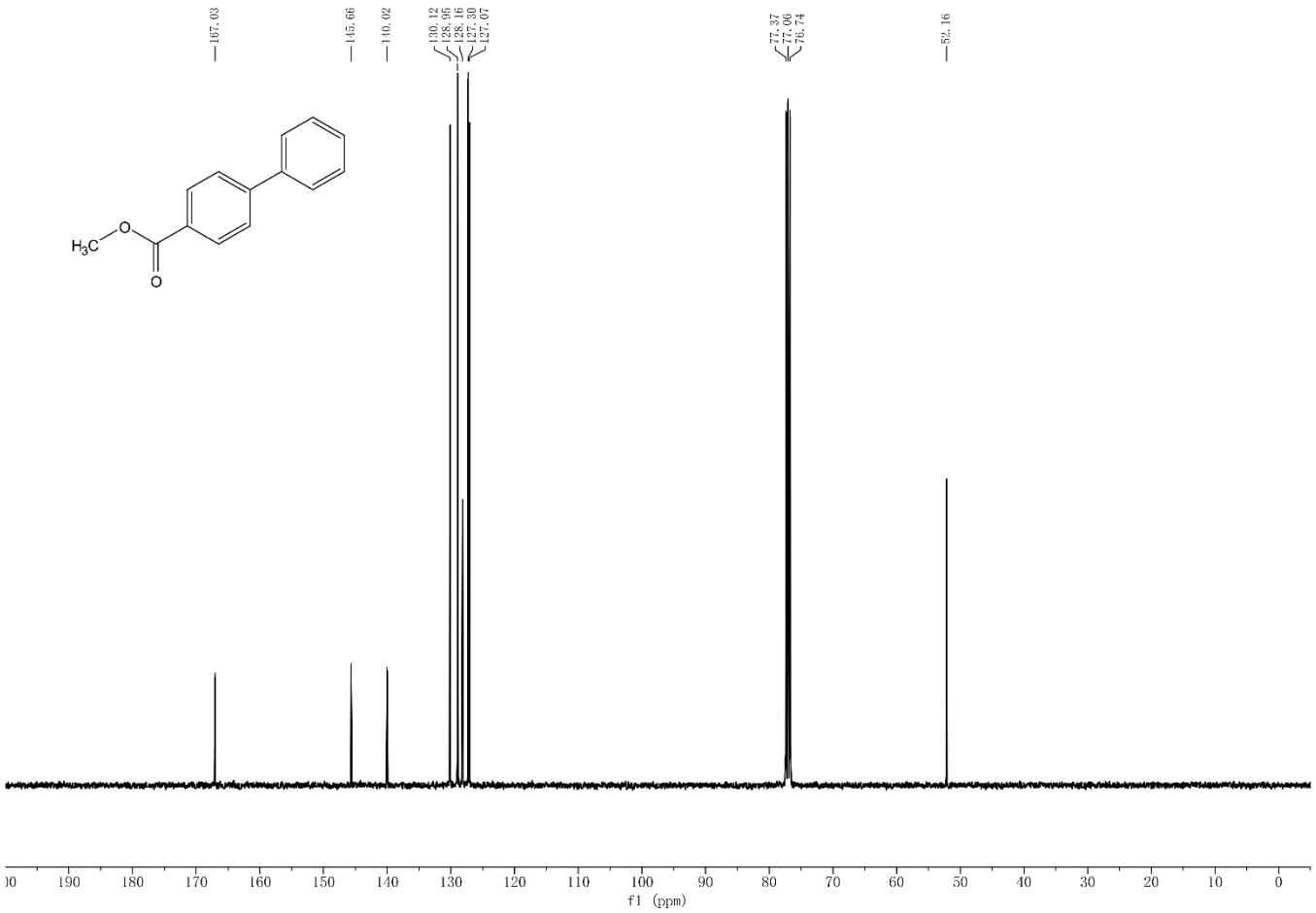
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 8g



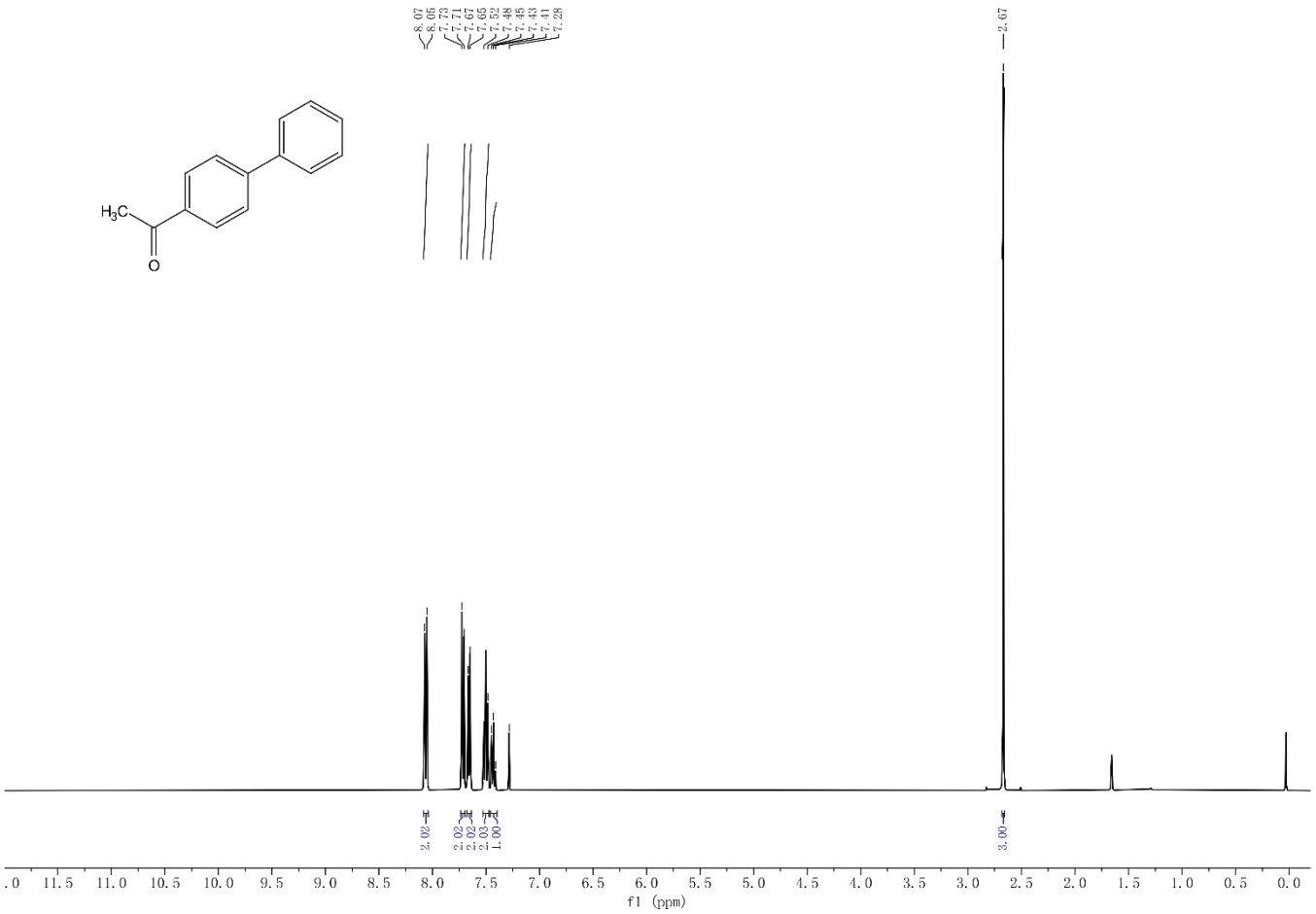
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8h



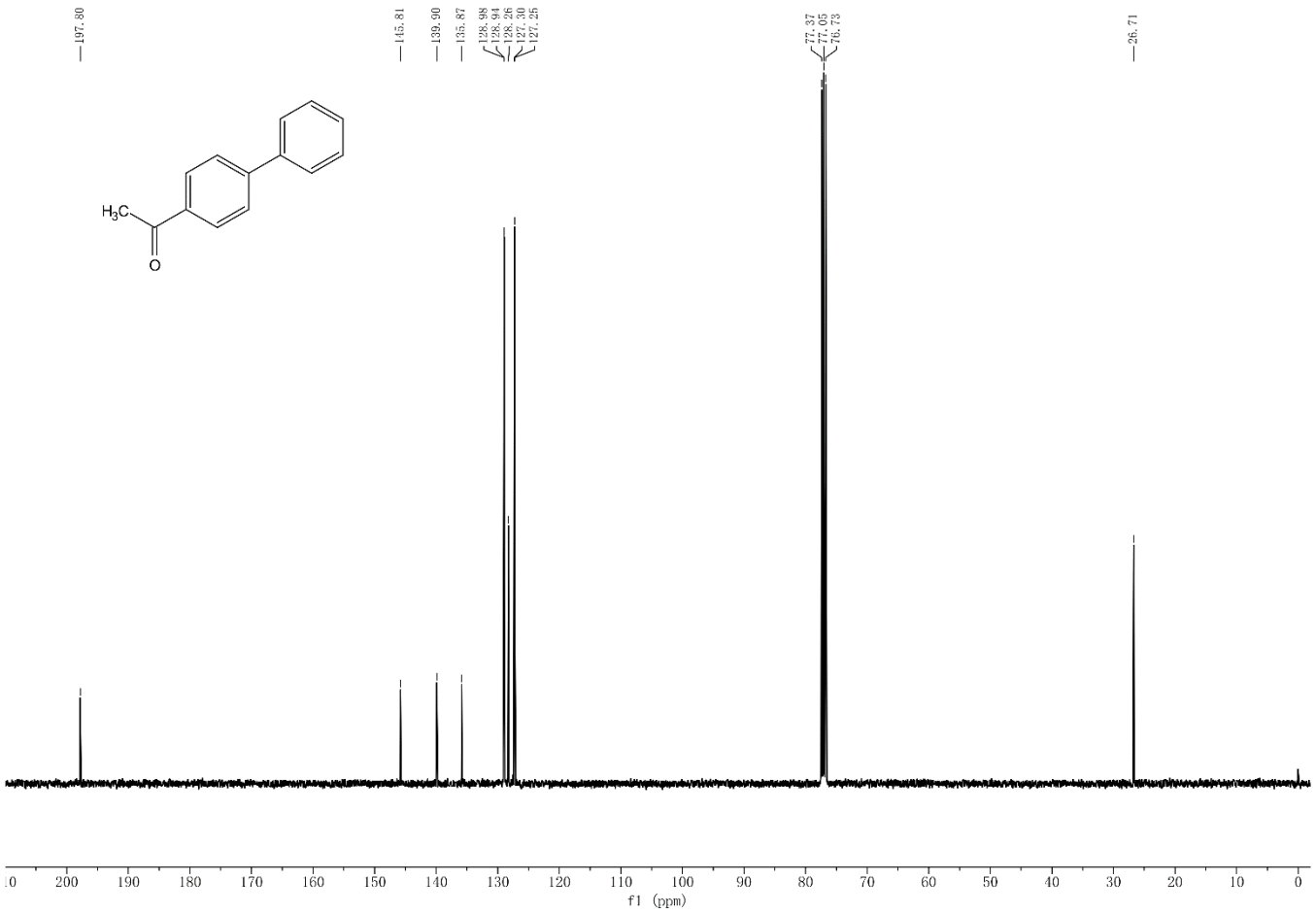
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8h



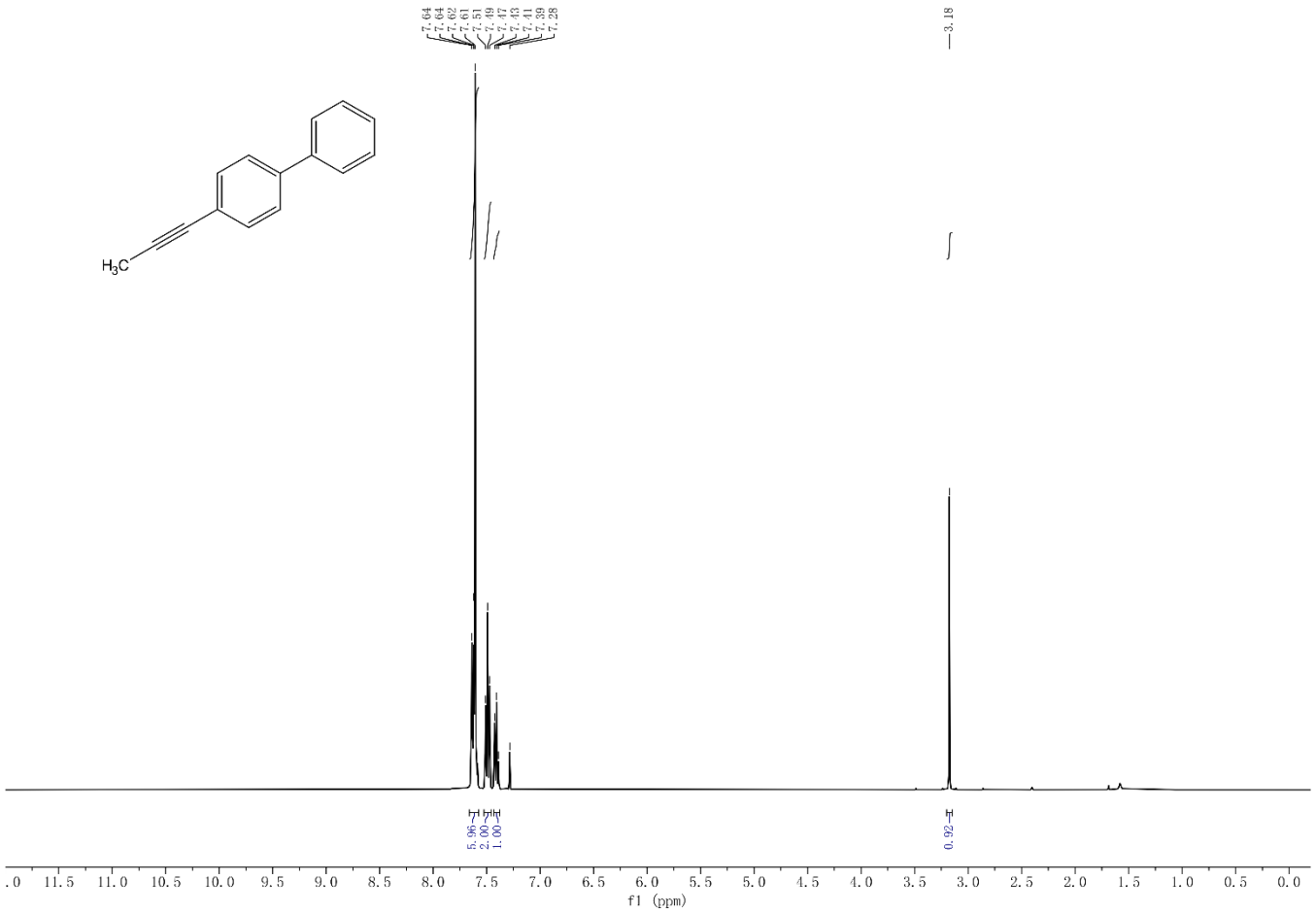
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8l



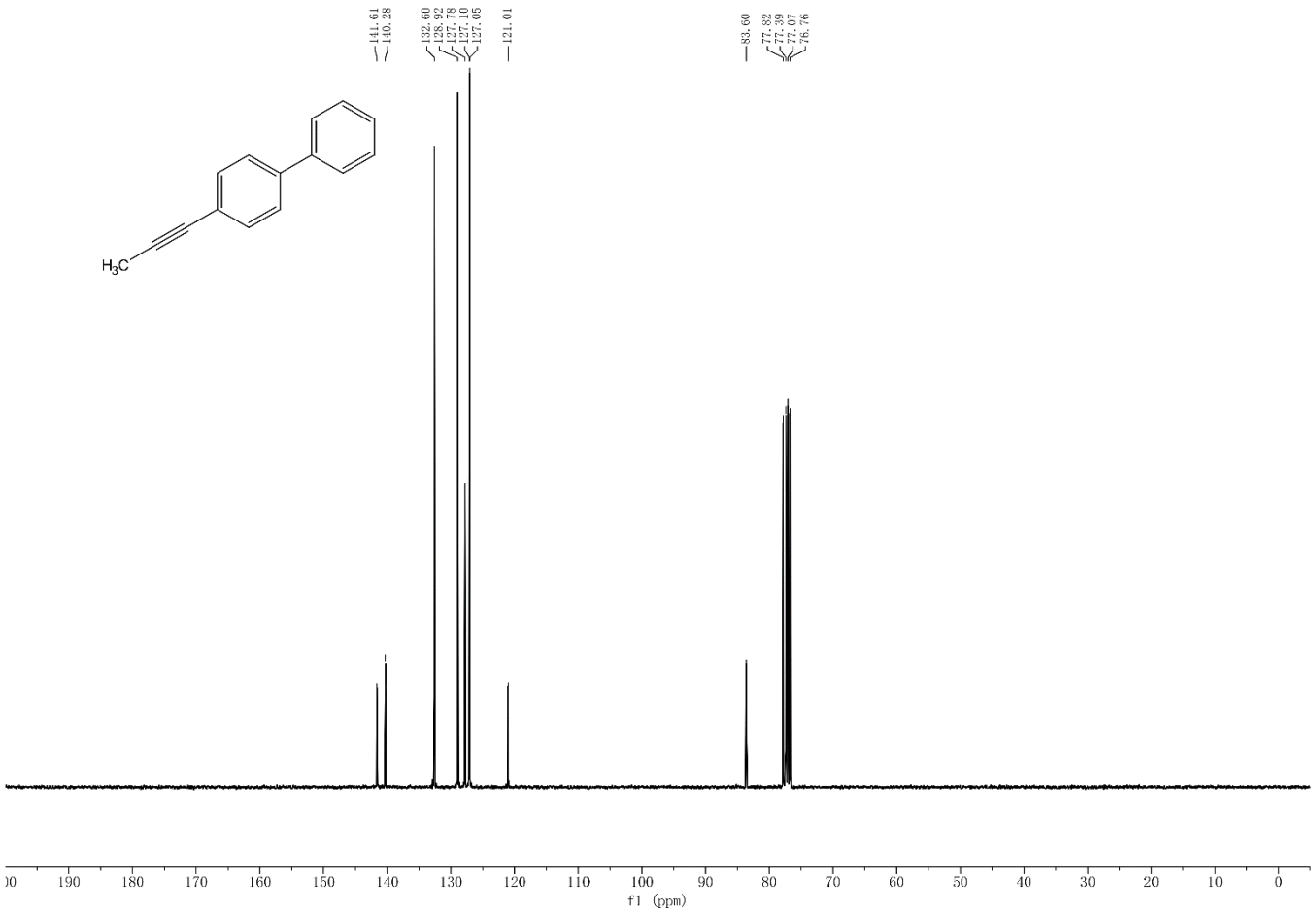
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8l



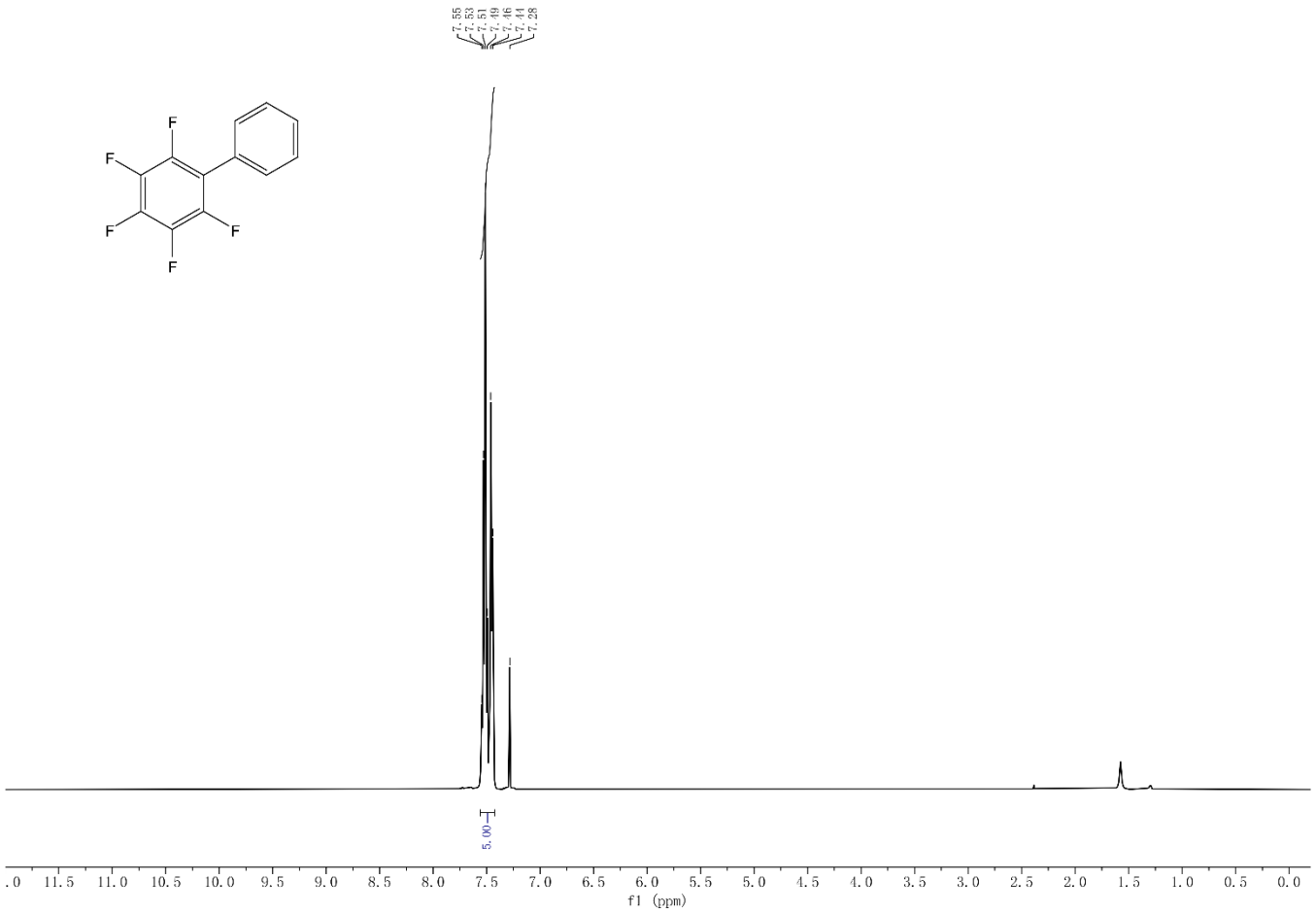
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8j



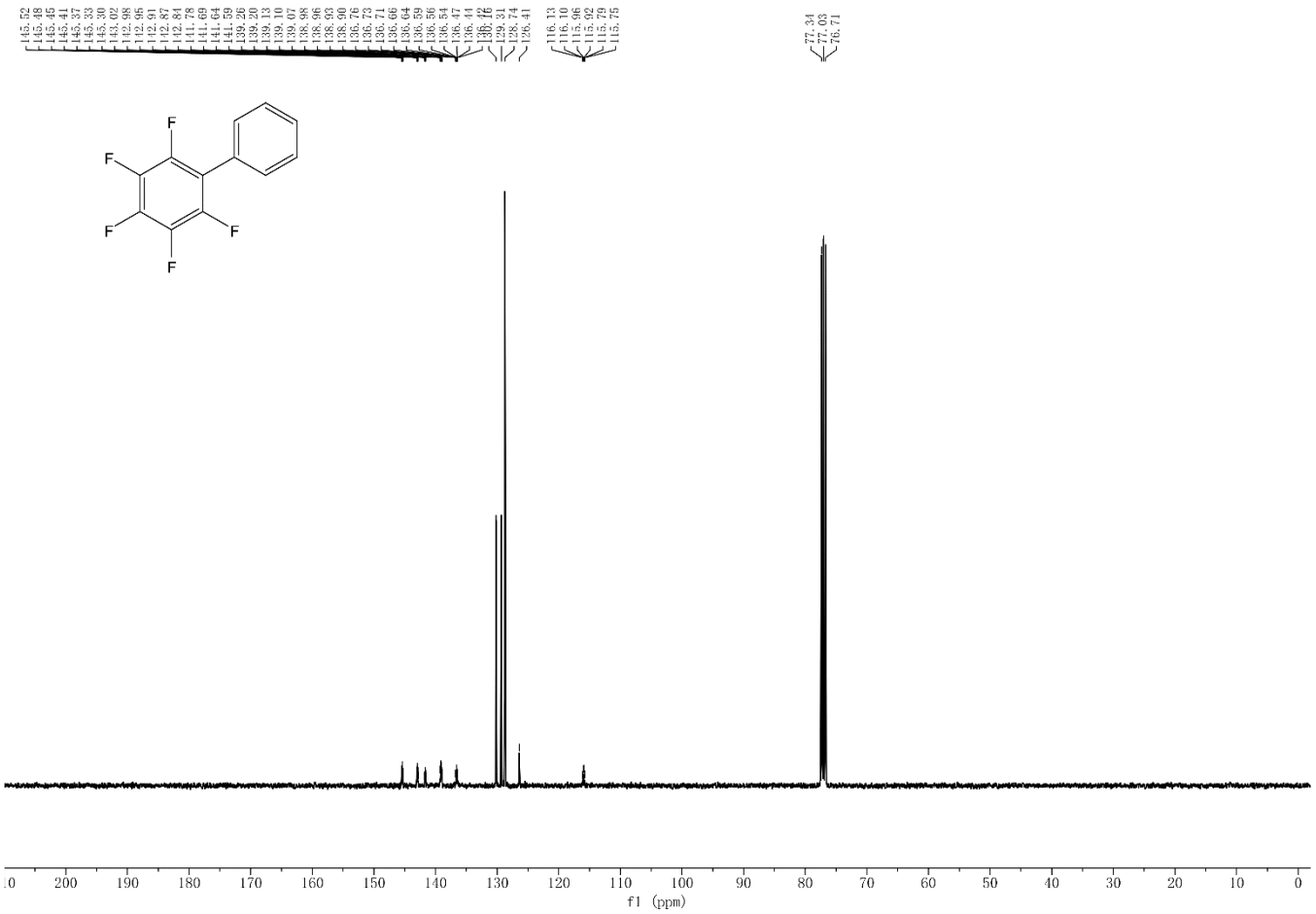
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8j



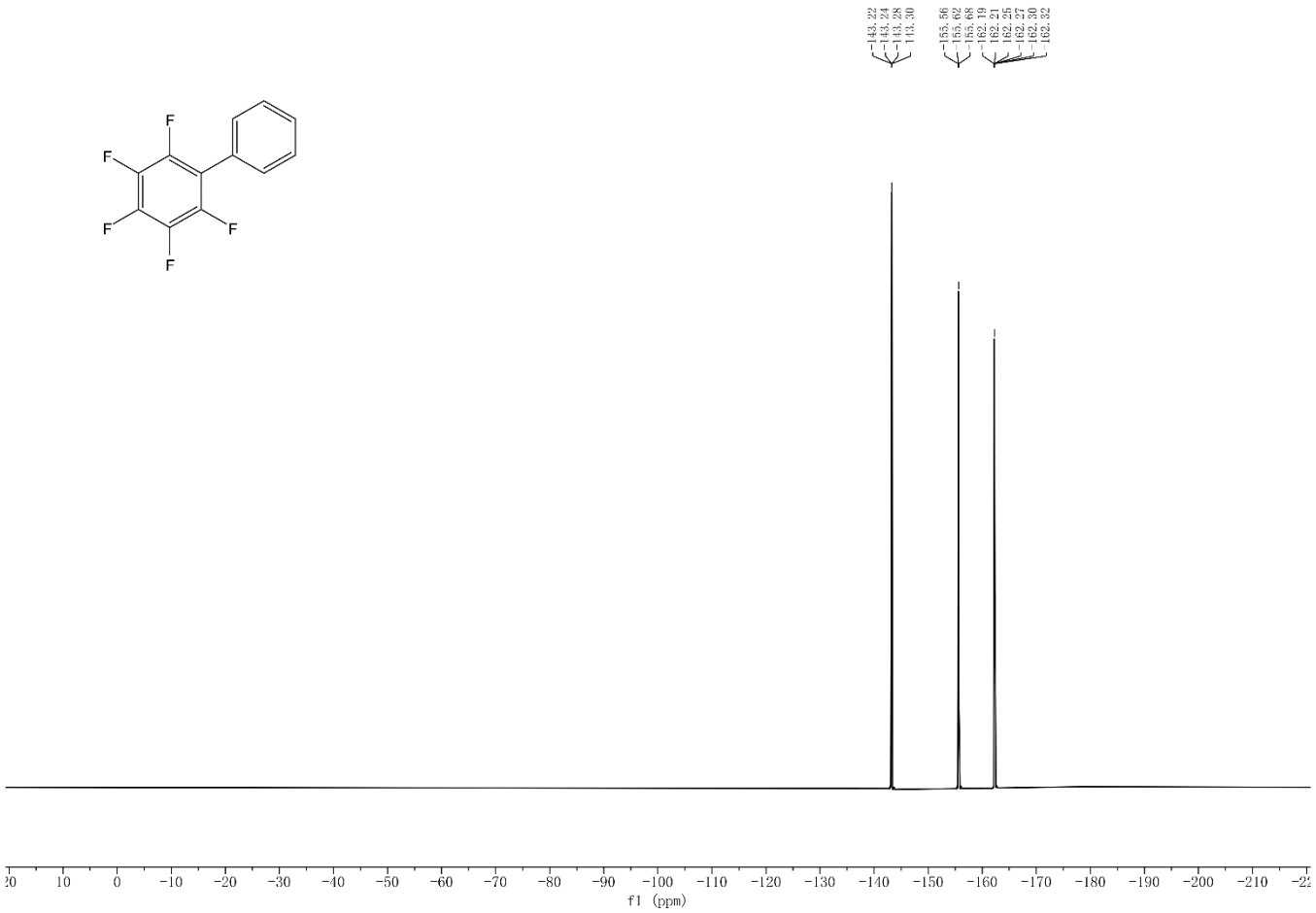
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8k



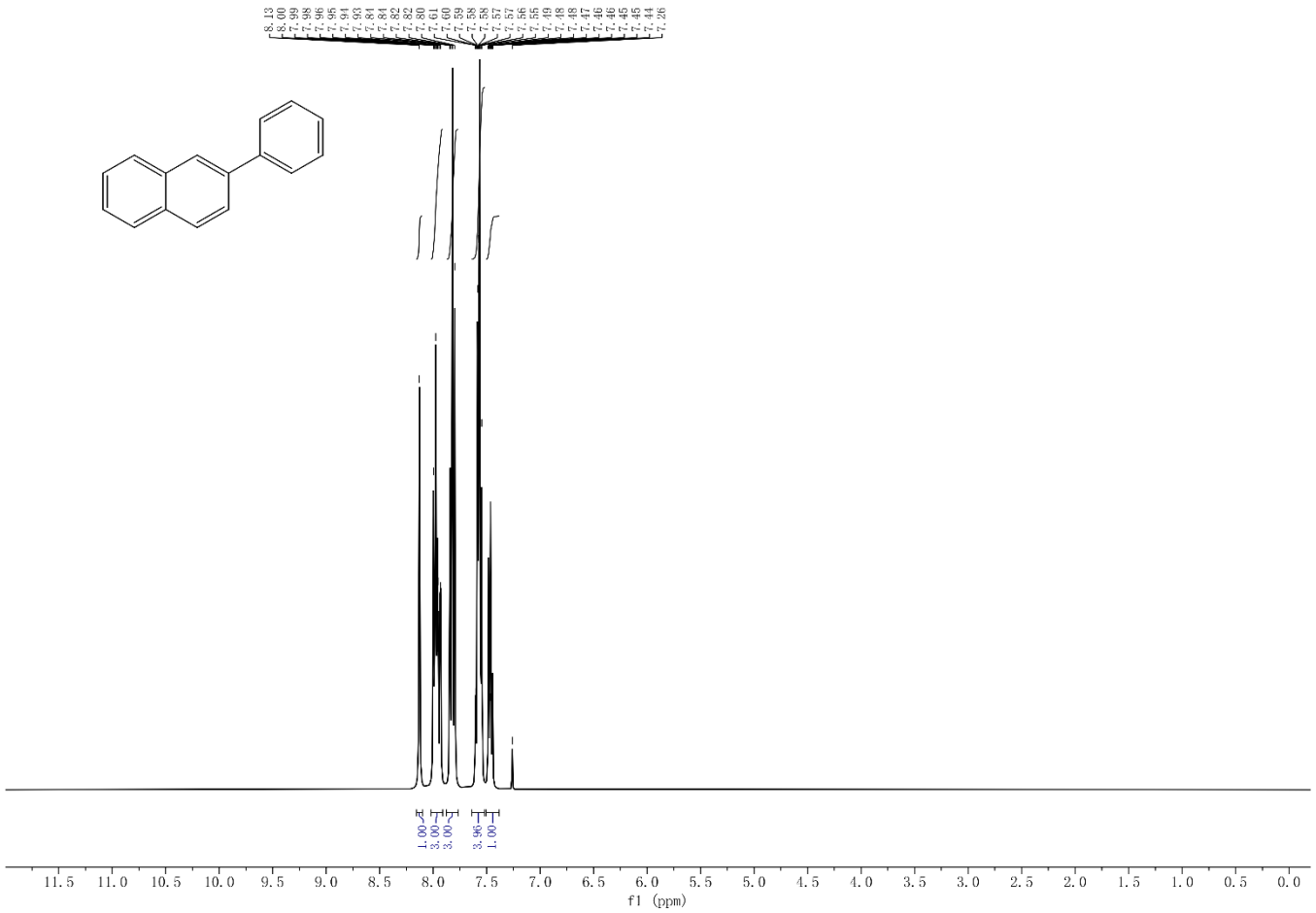
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8k



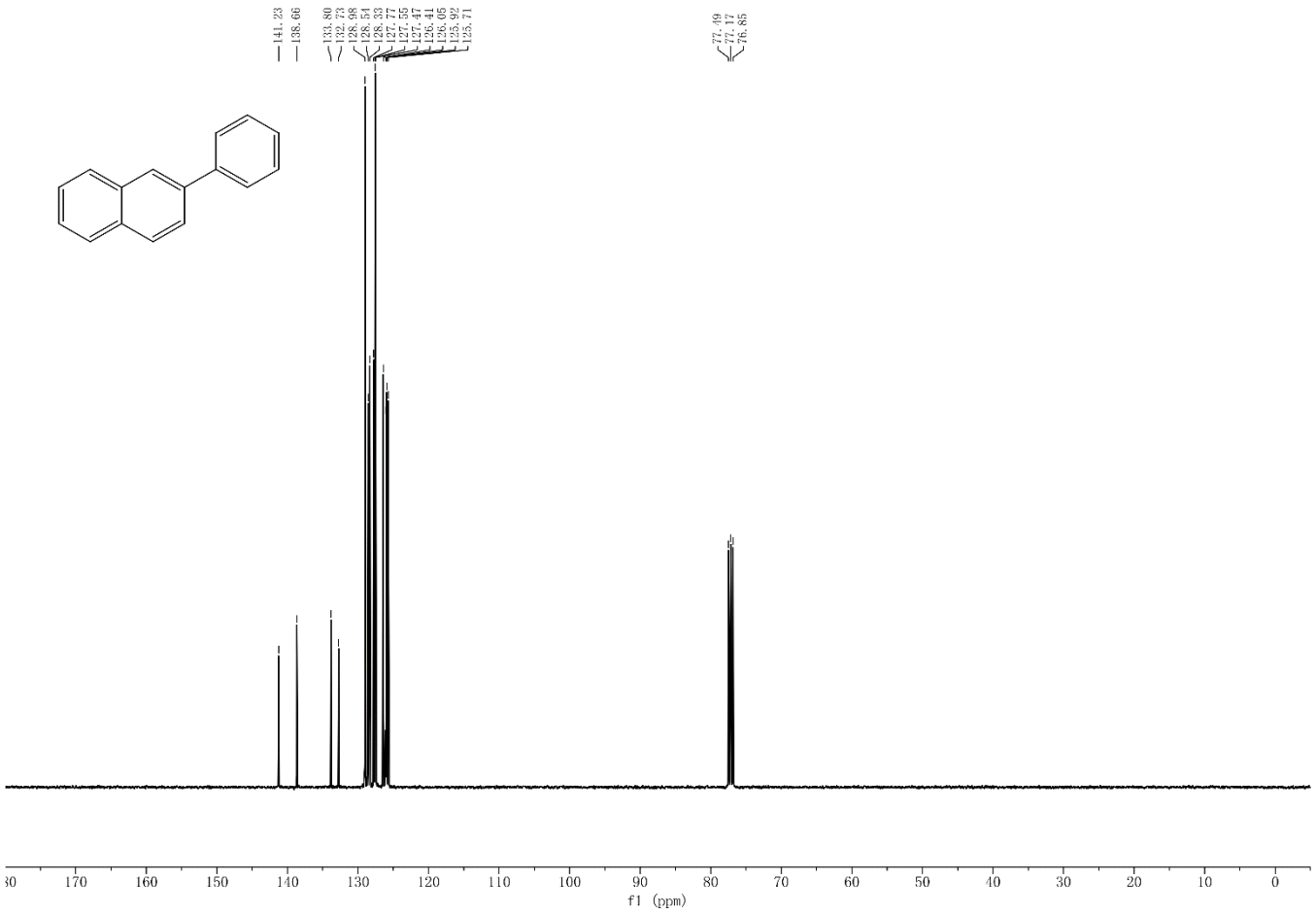
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 8k



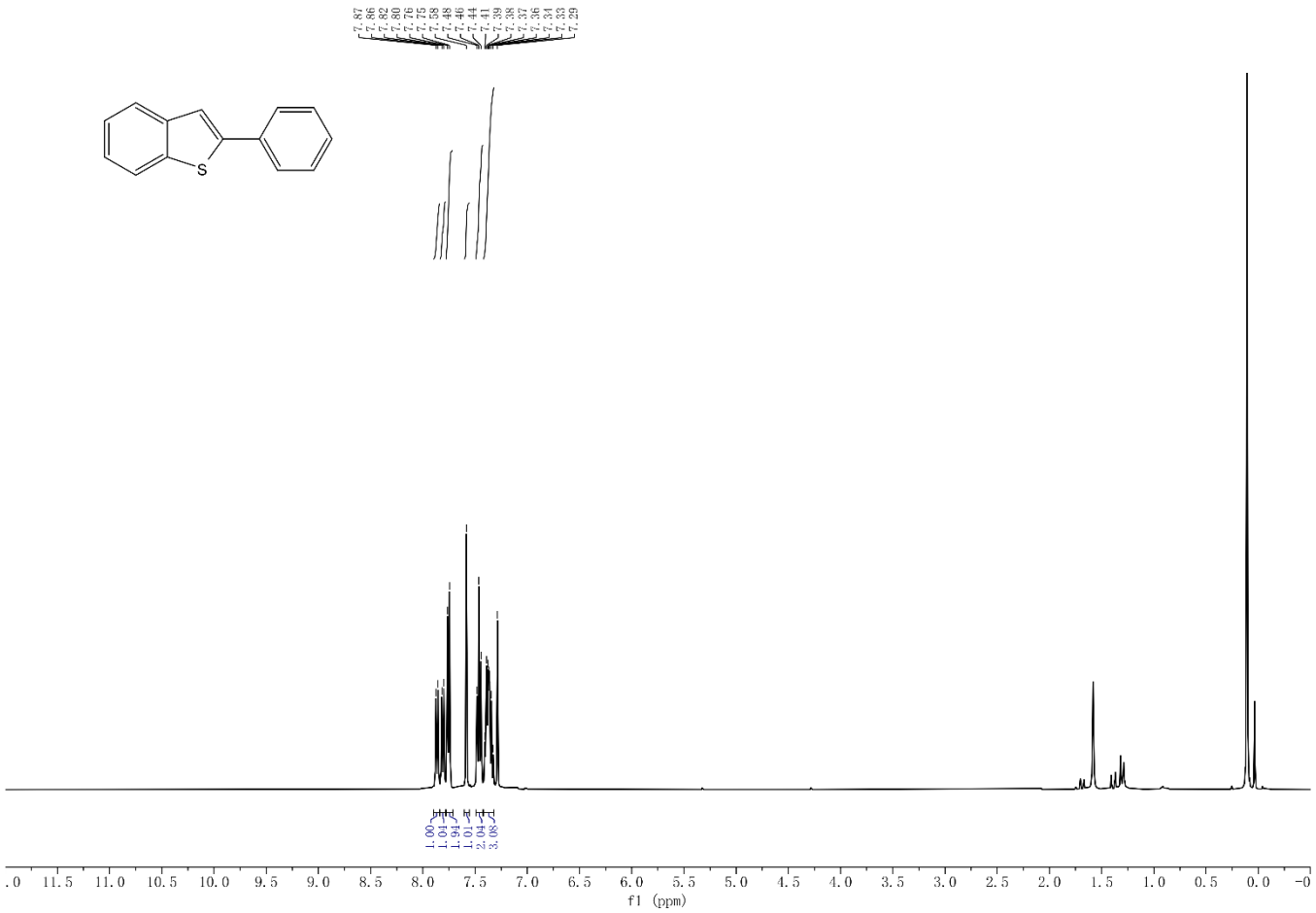
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8l



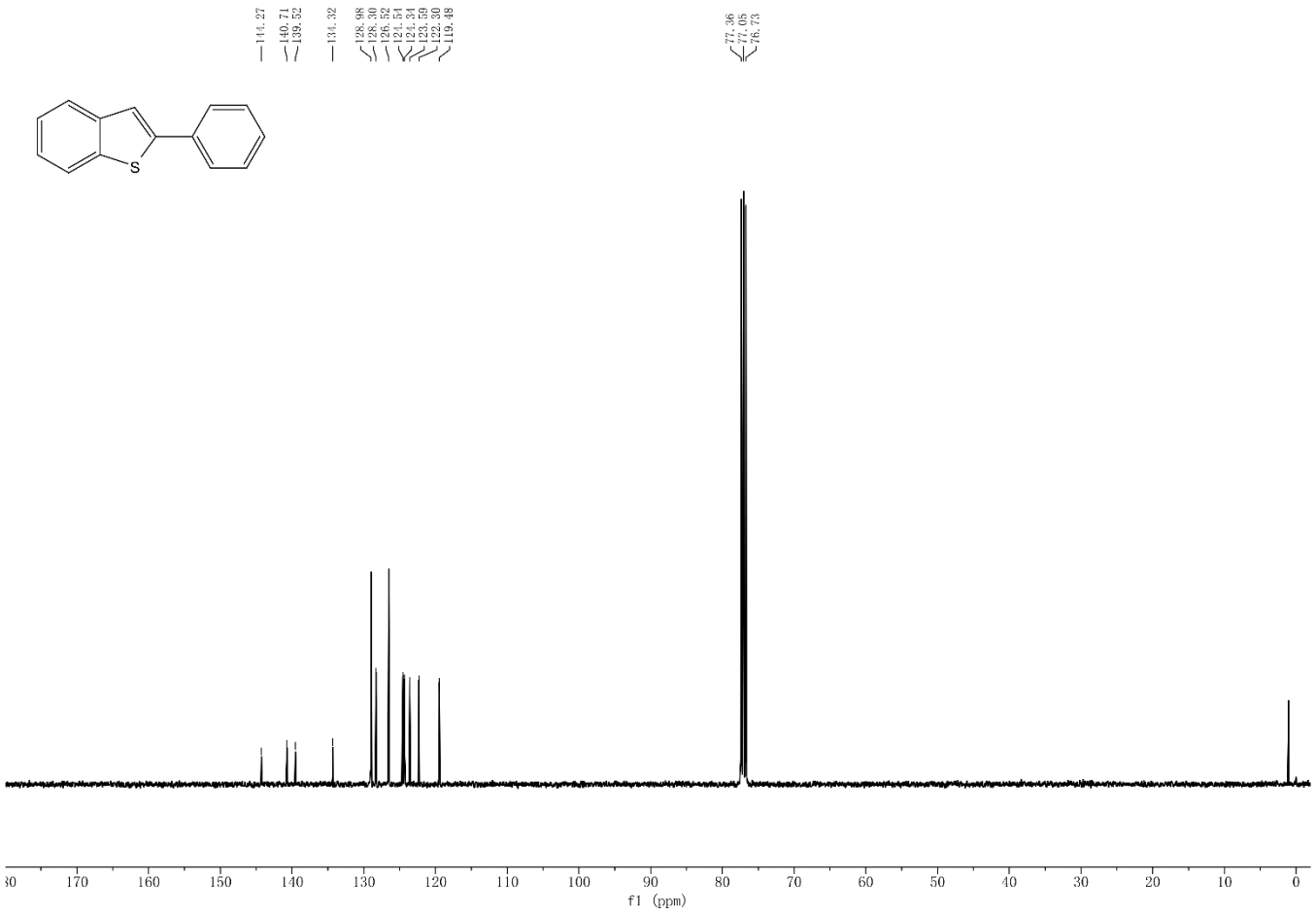
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8l



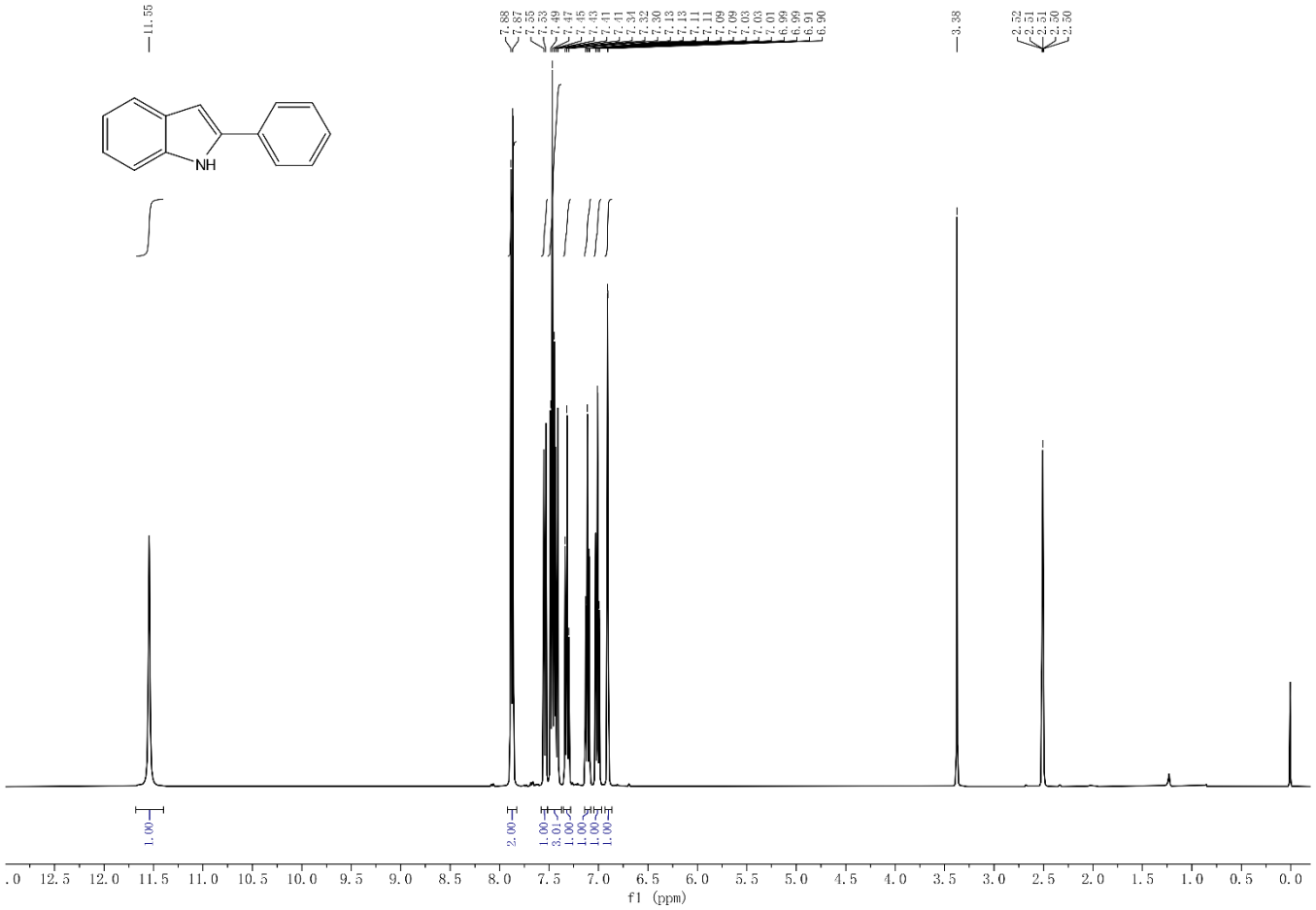
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8m



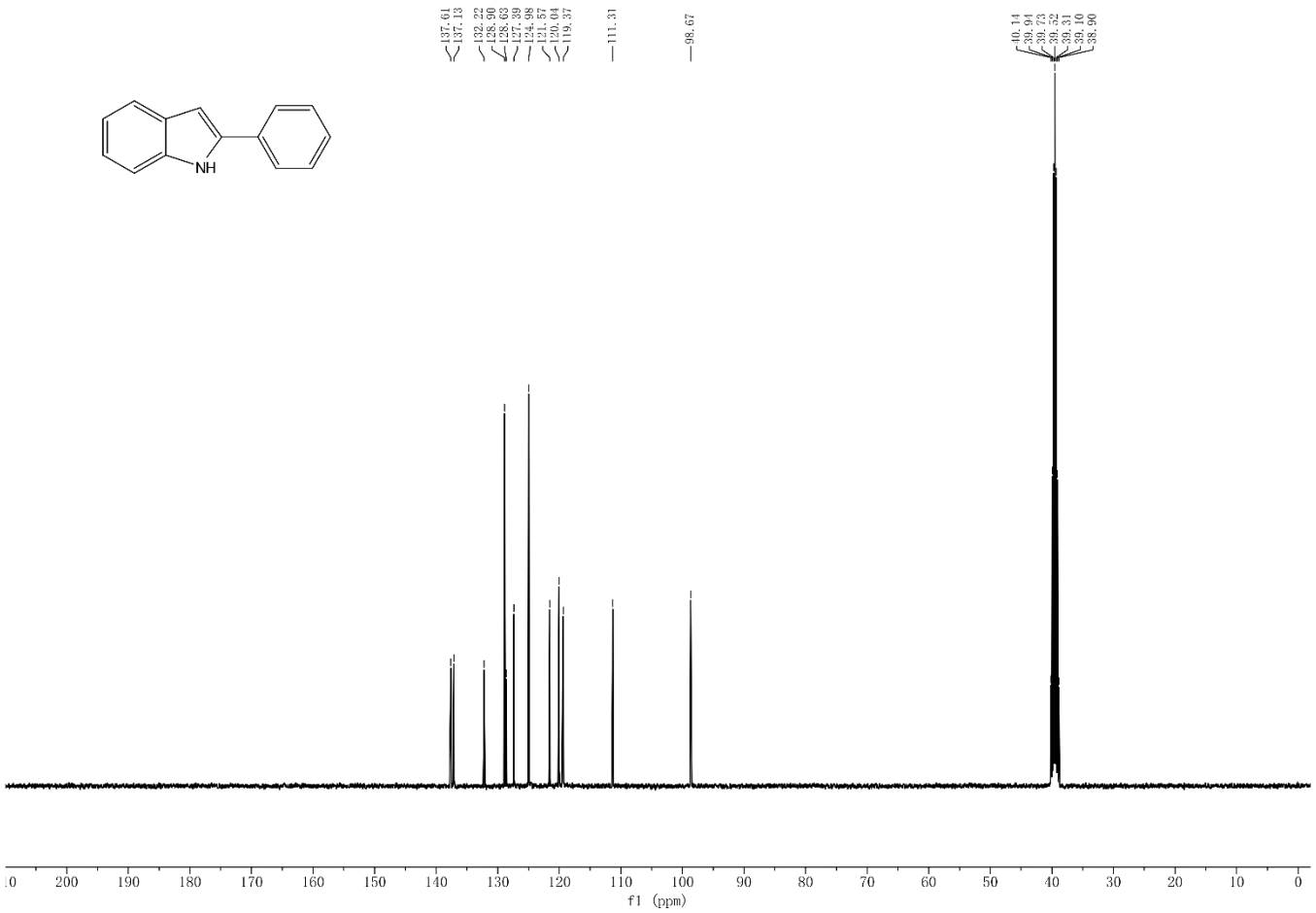
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8m



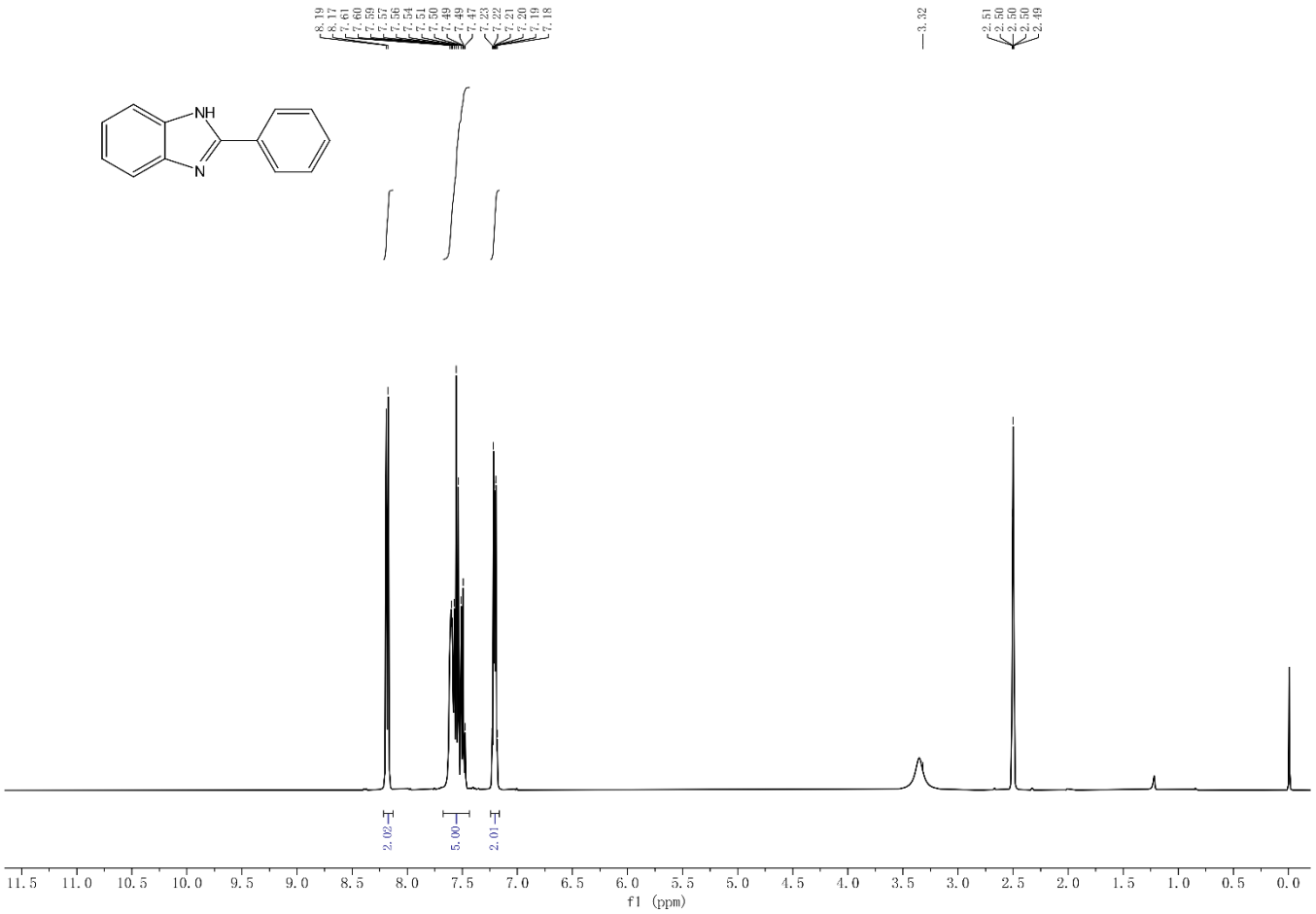
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8n



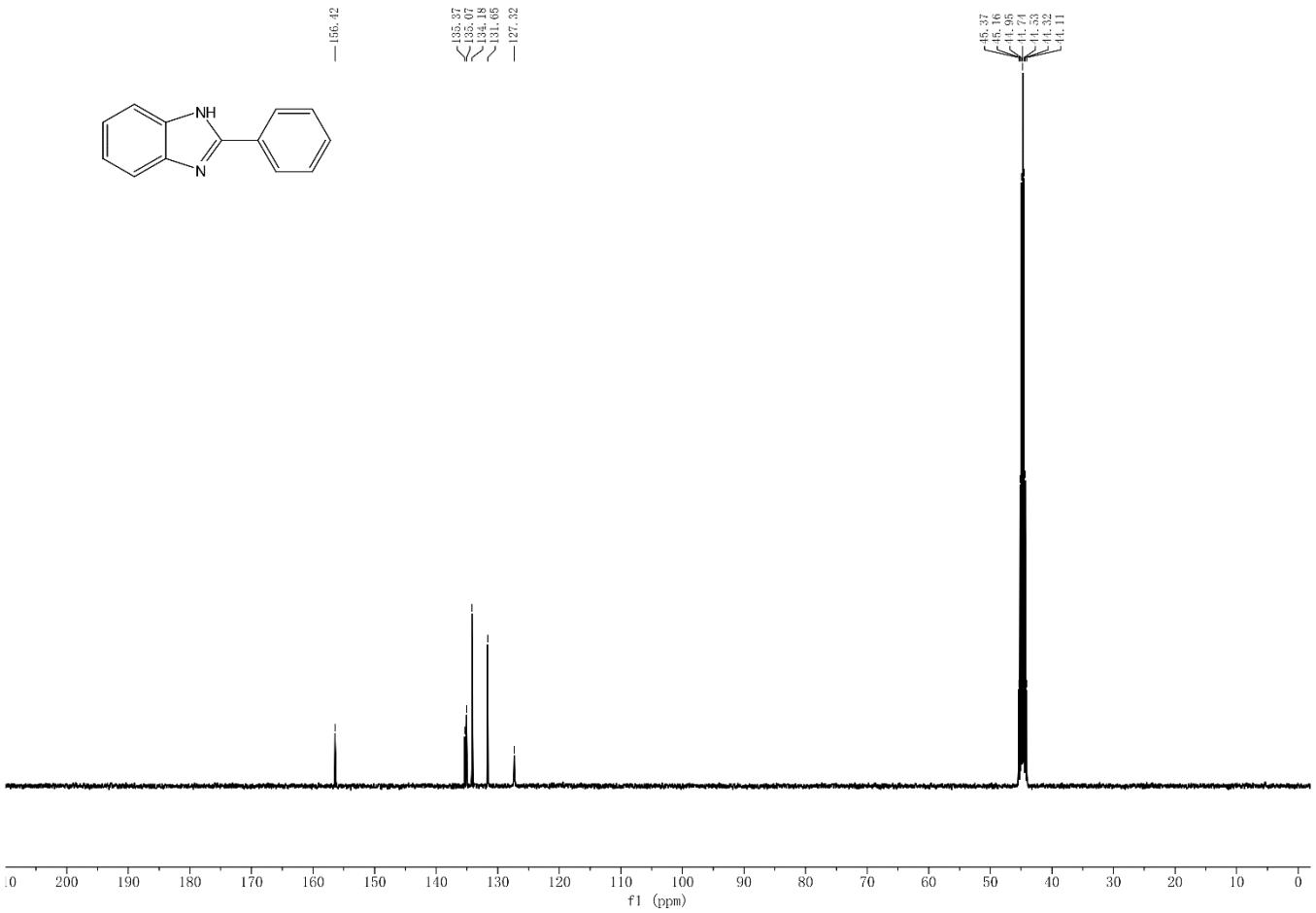
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8n



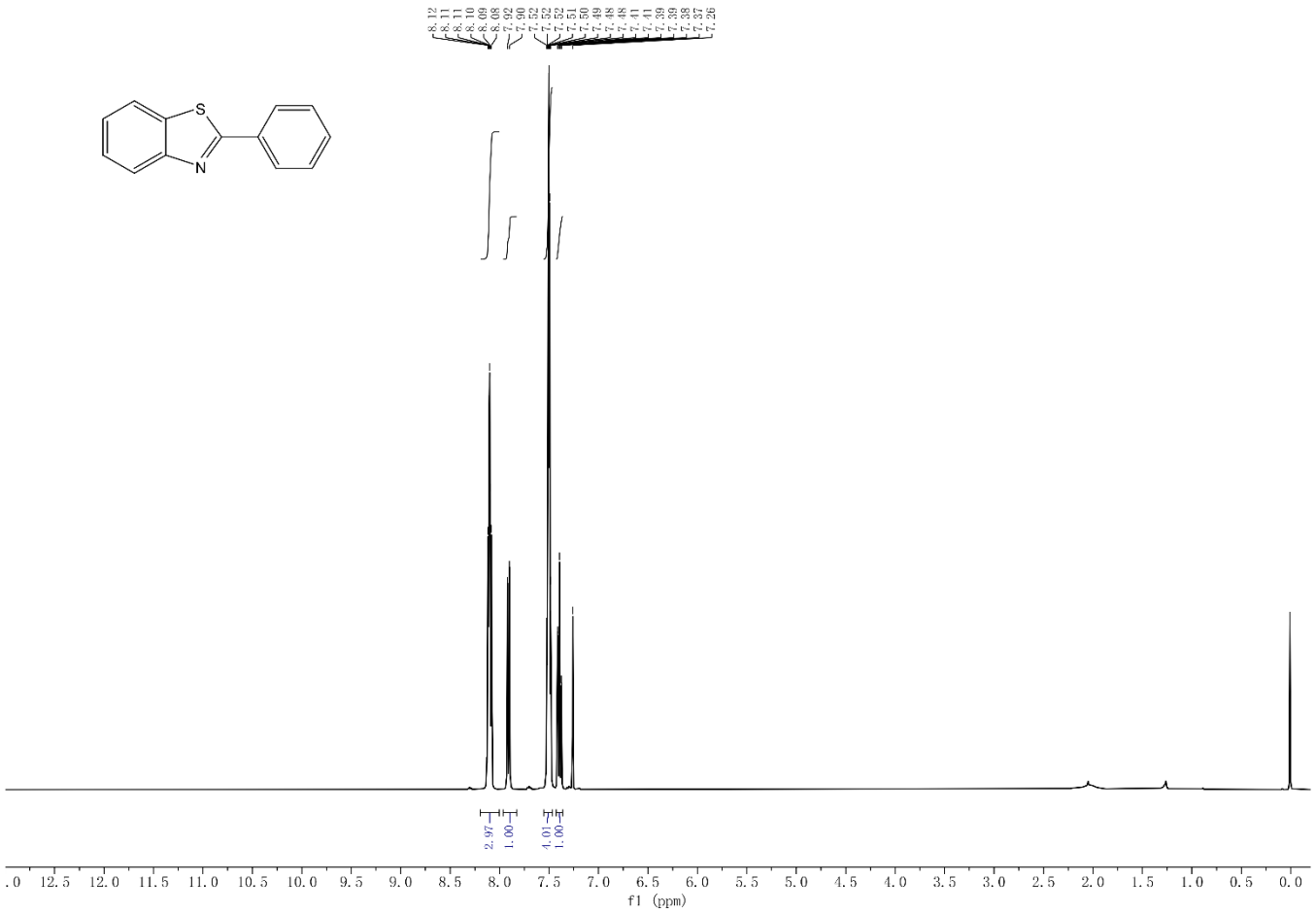
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8o



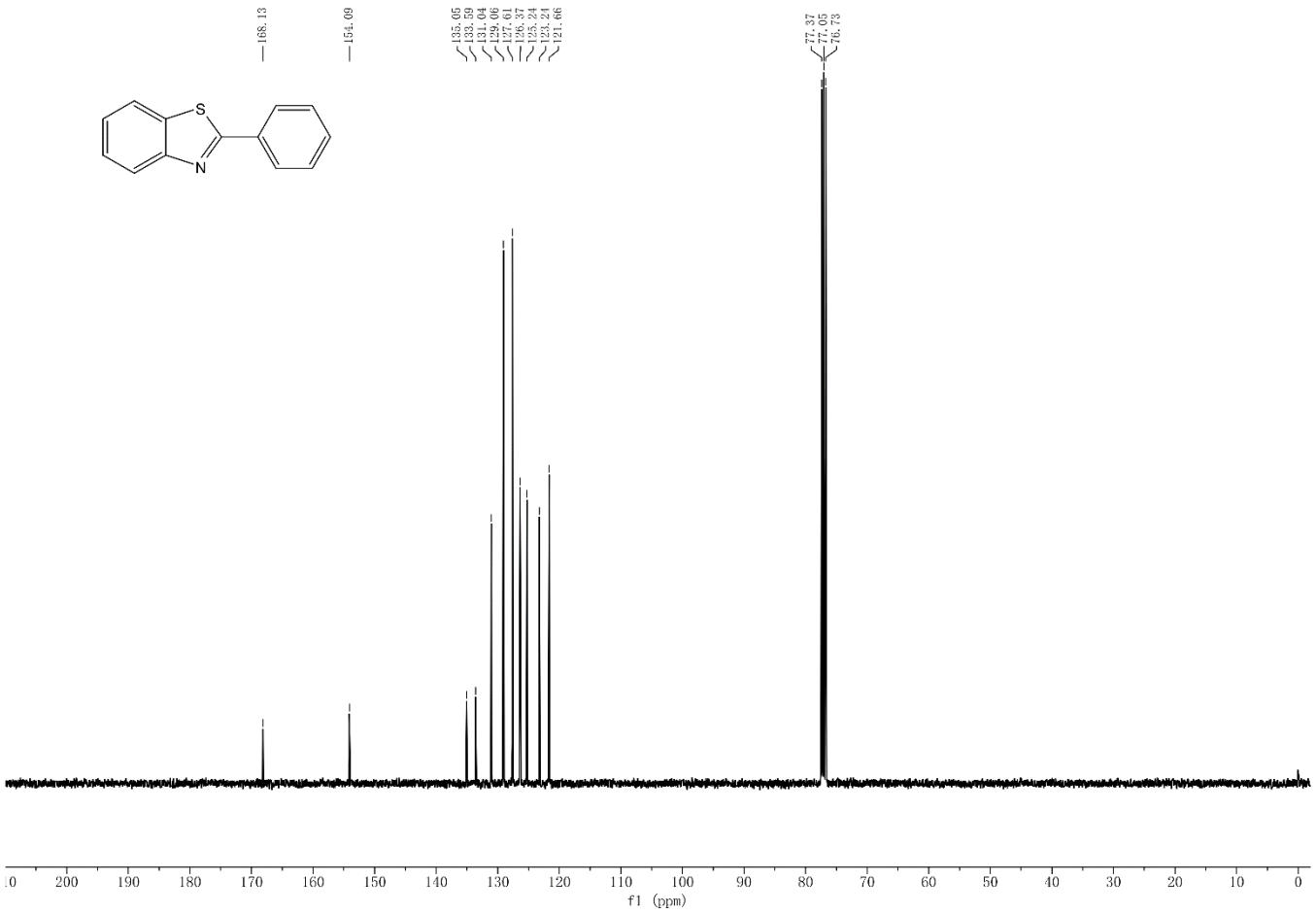
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8o



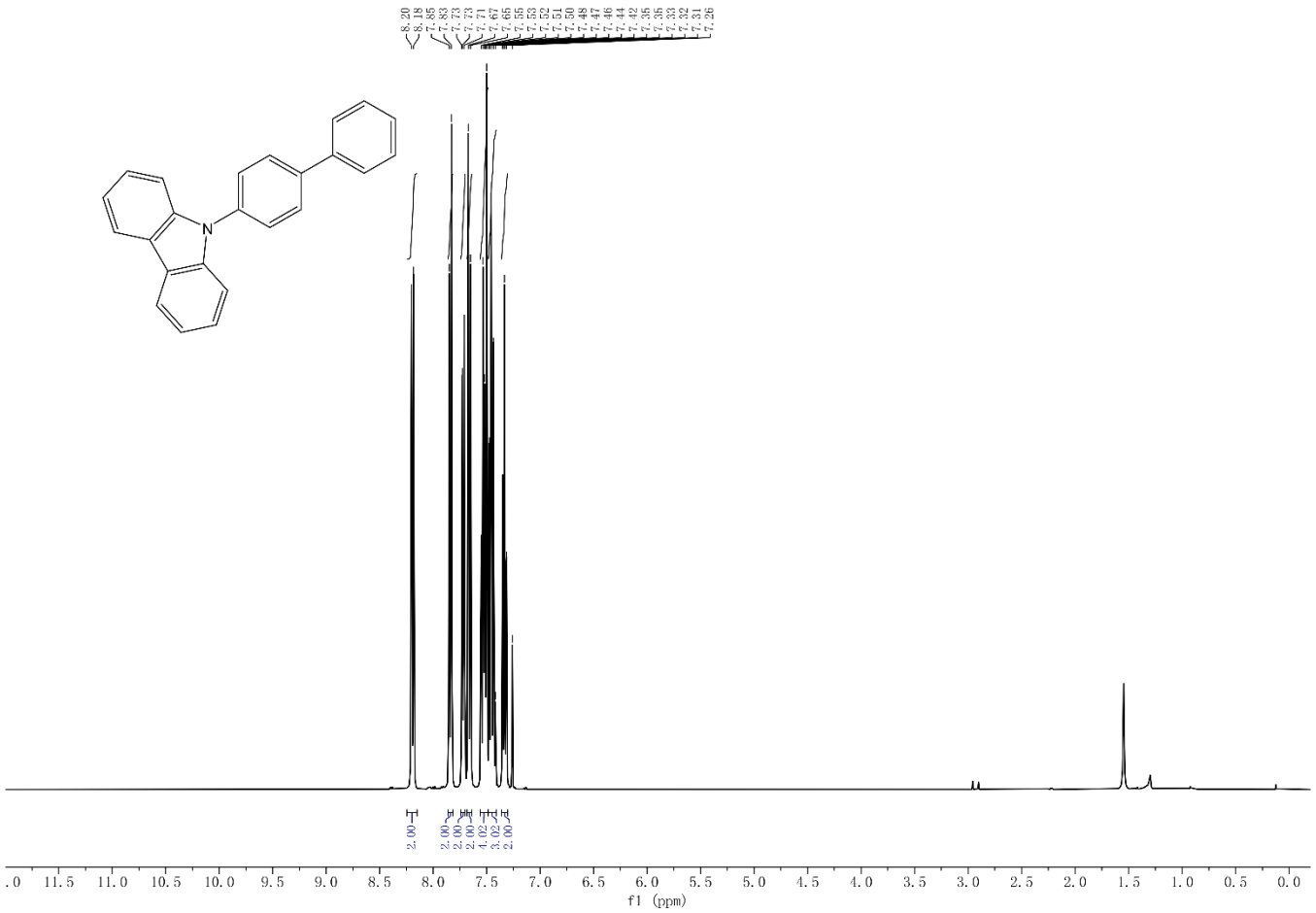
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8p



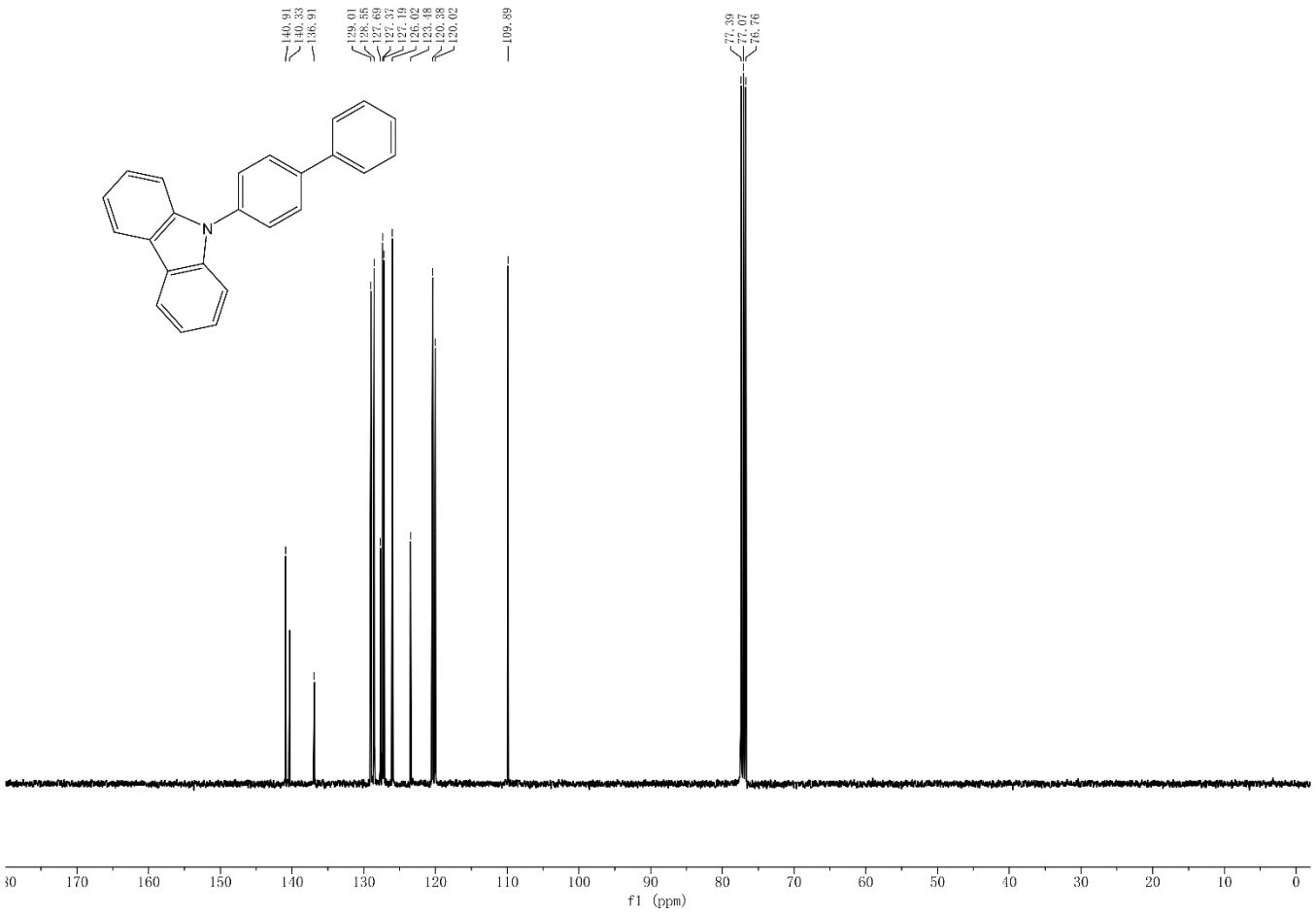
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8o



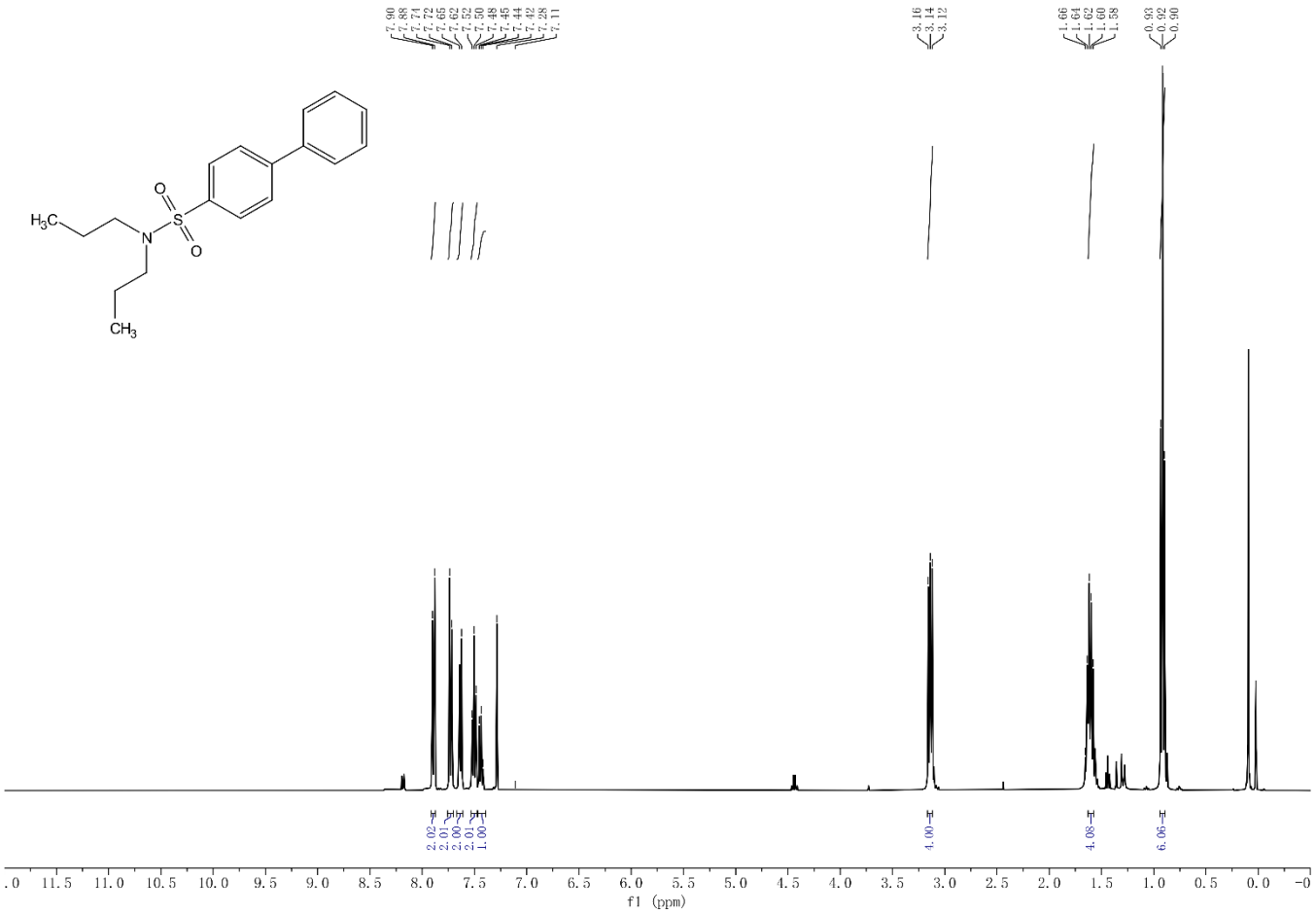
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8q



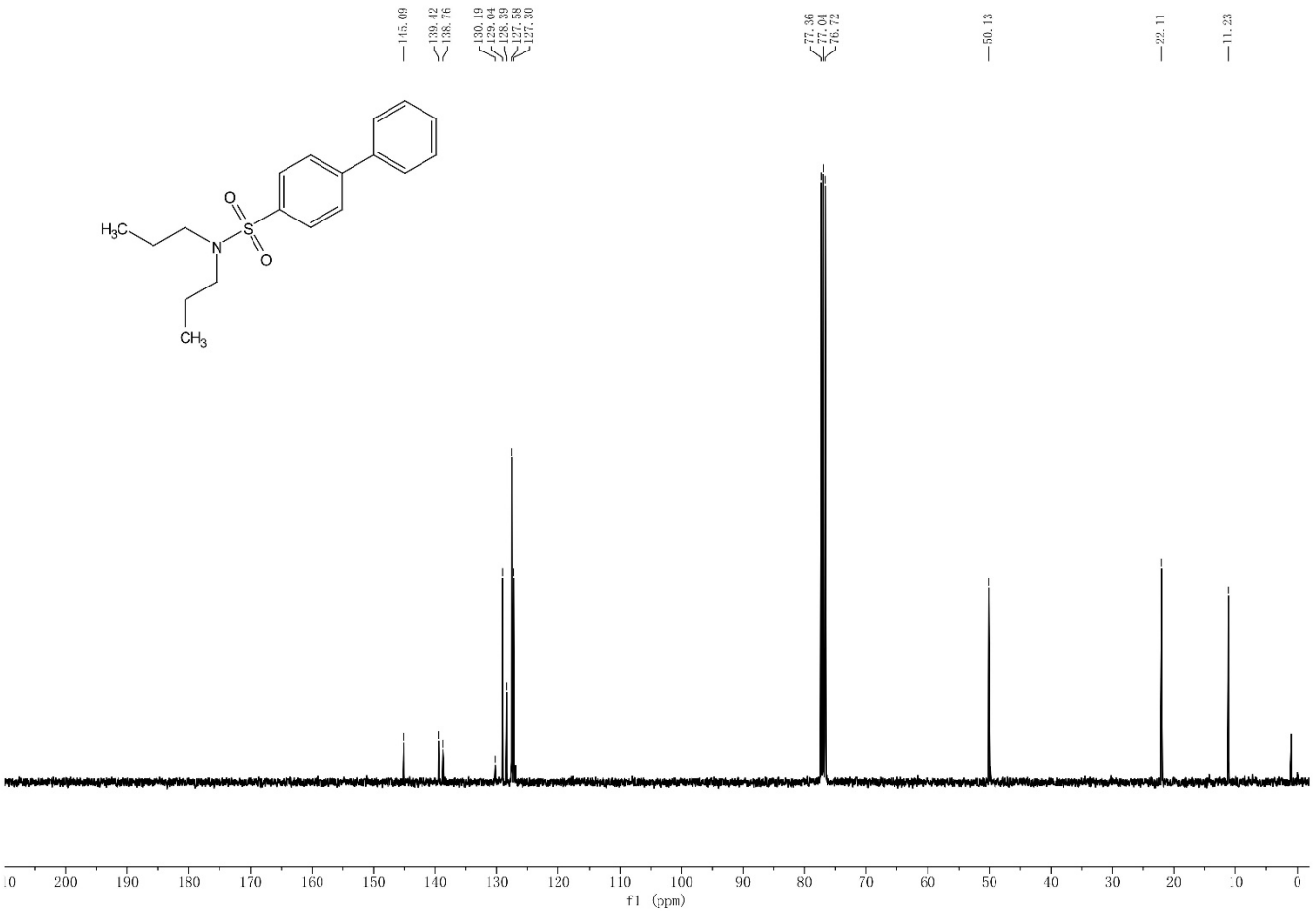
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8q



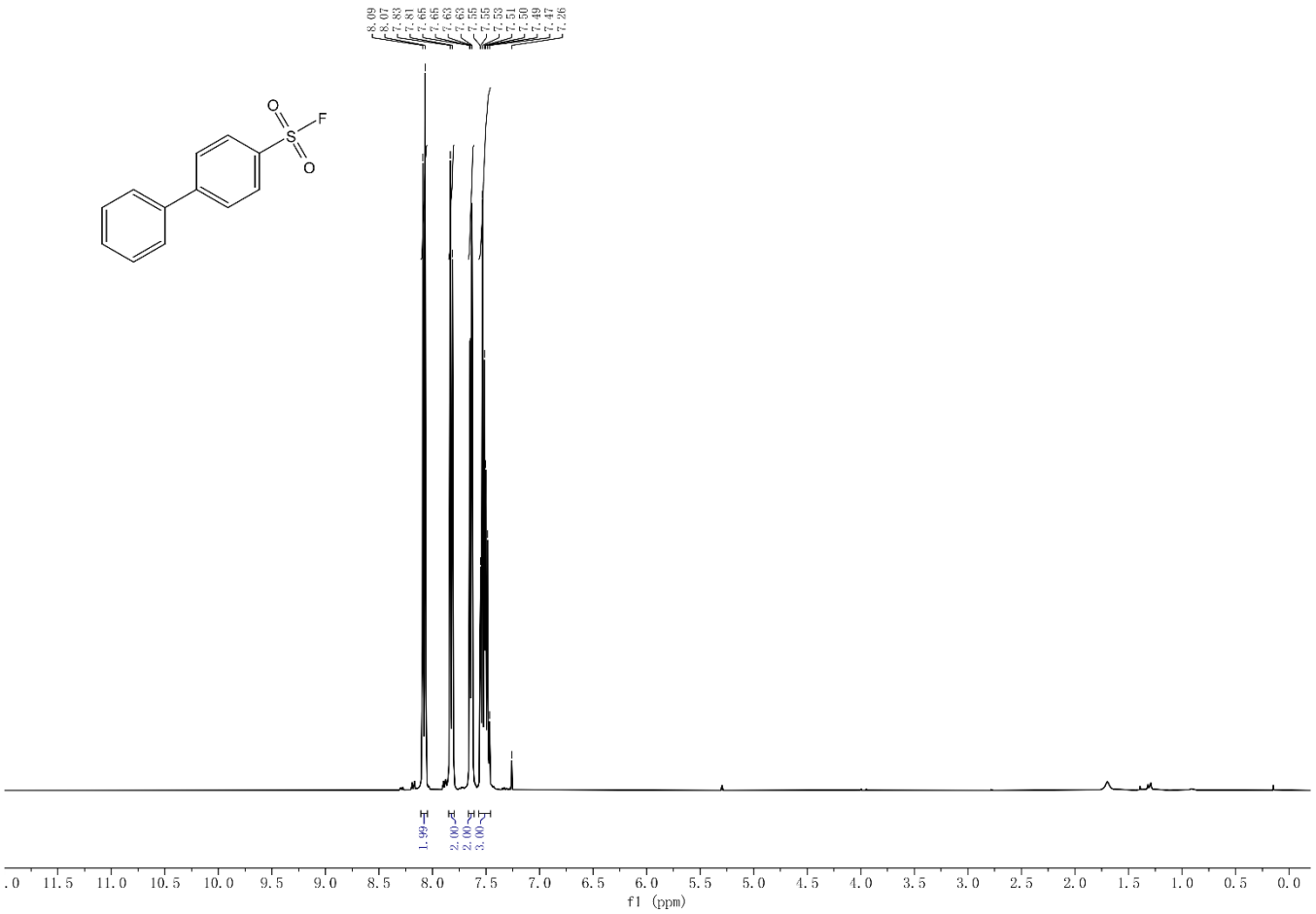
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8r



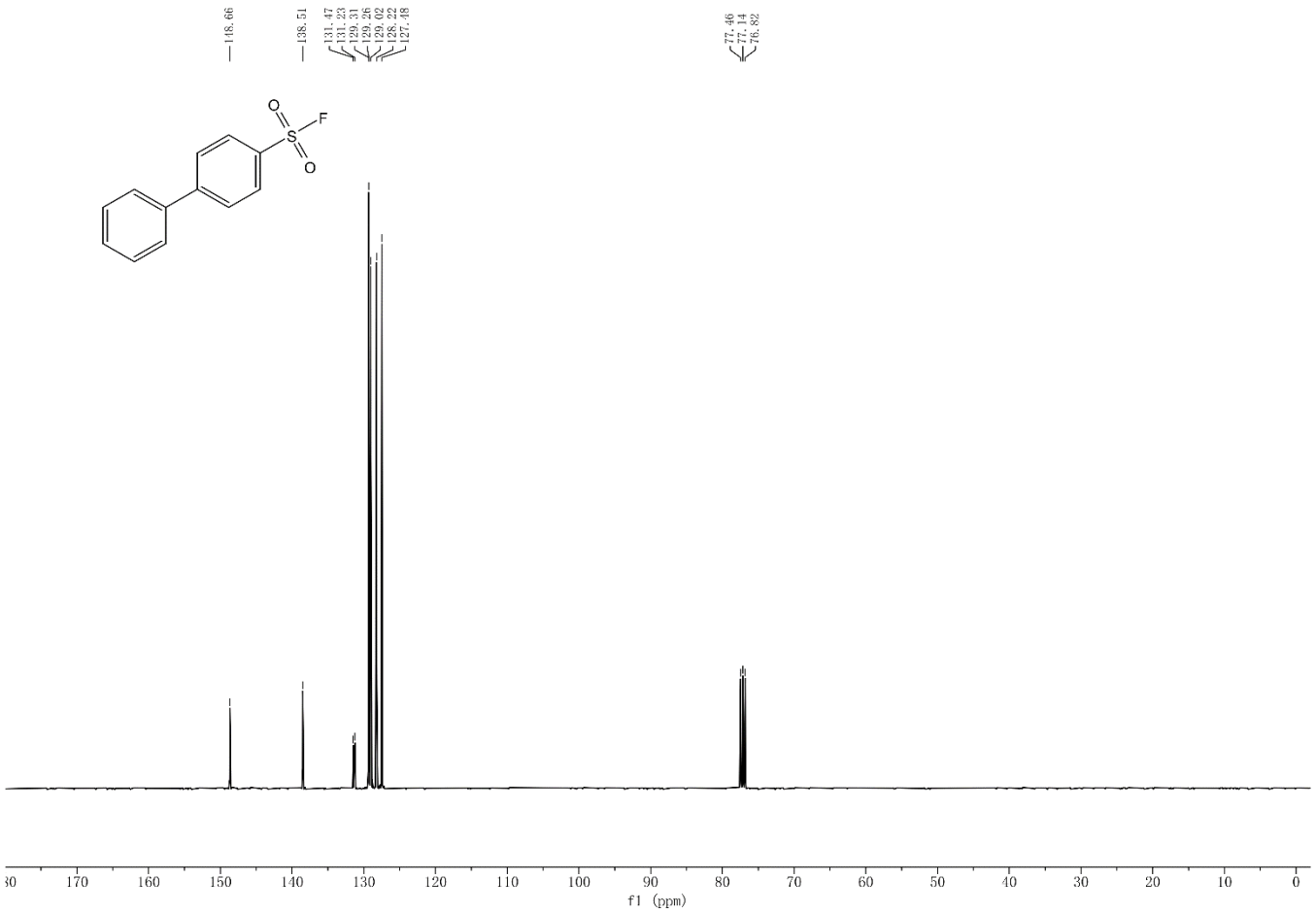
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8r



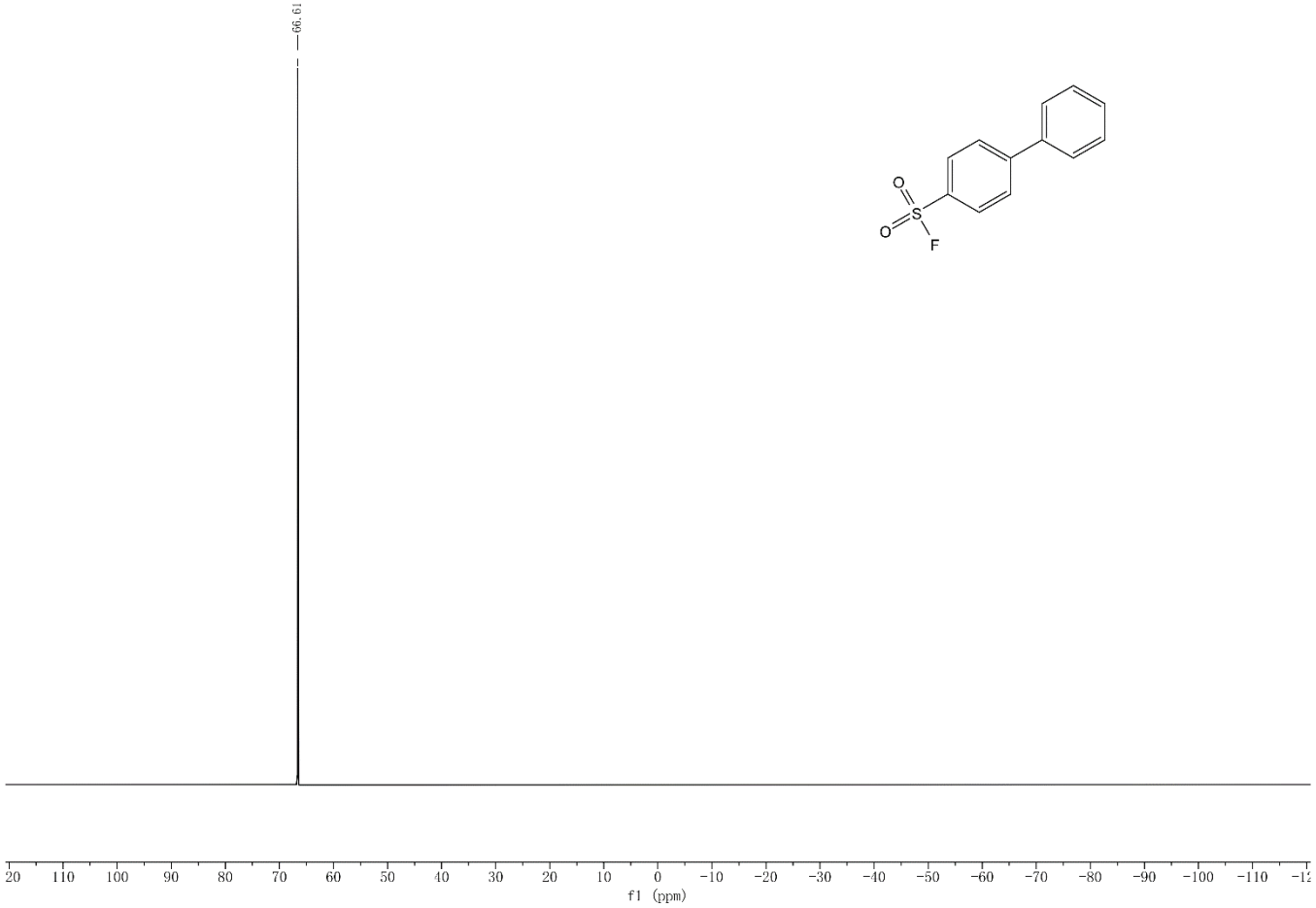
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8s



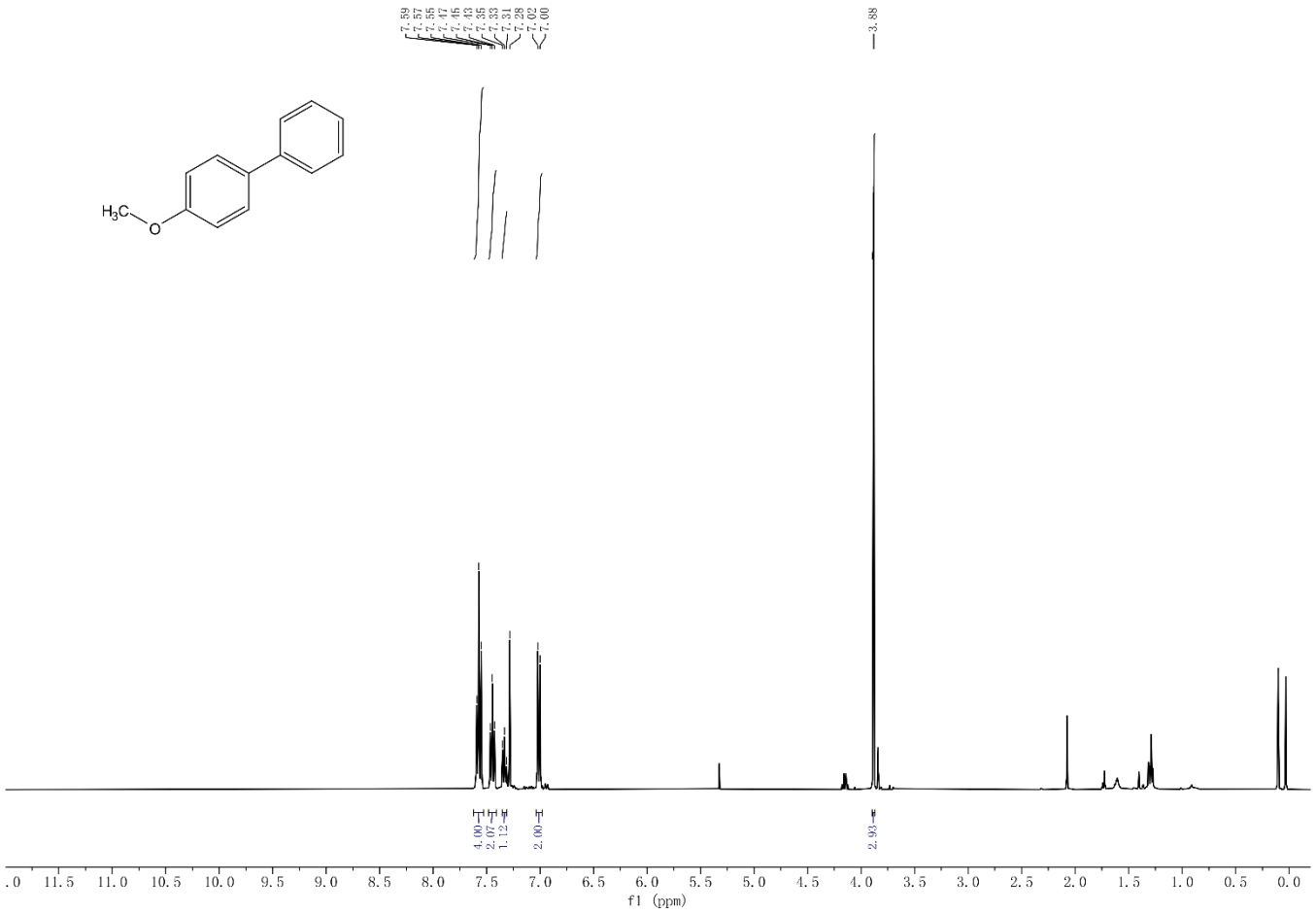
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8s



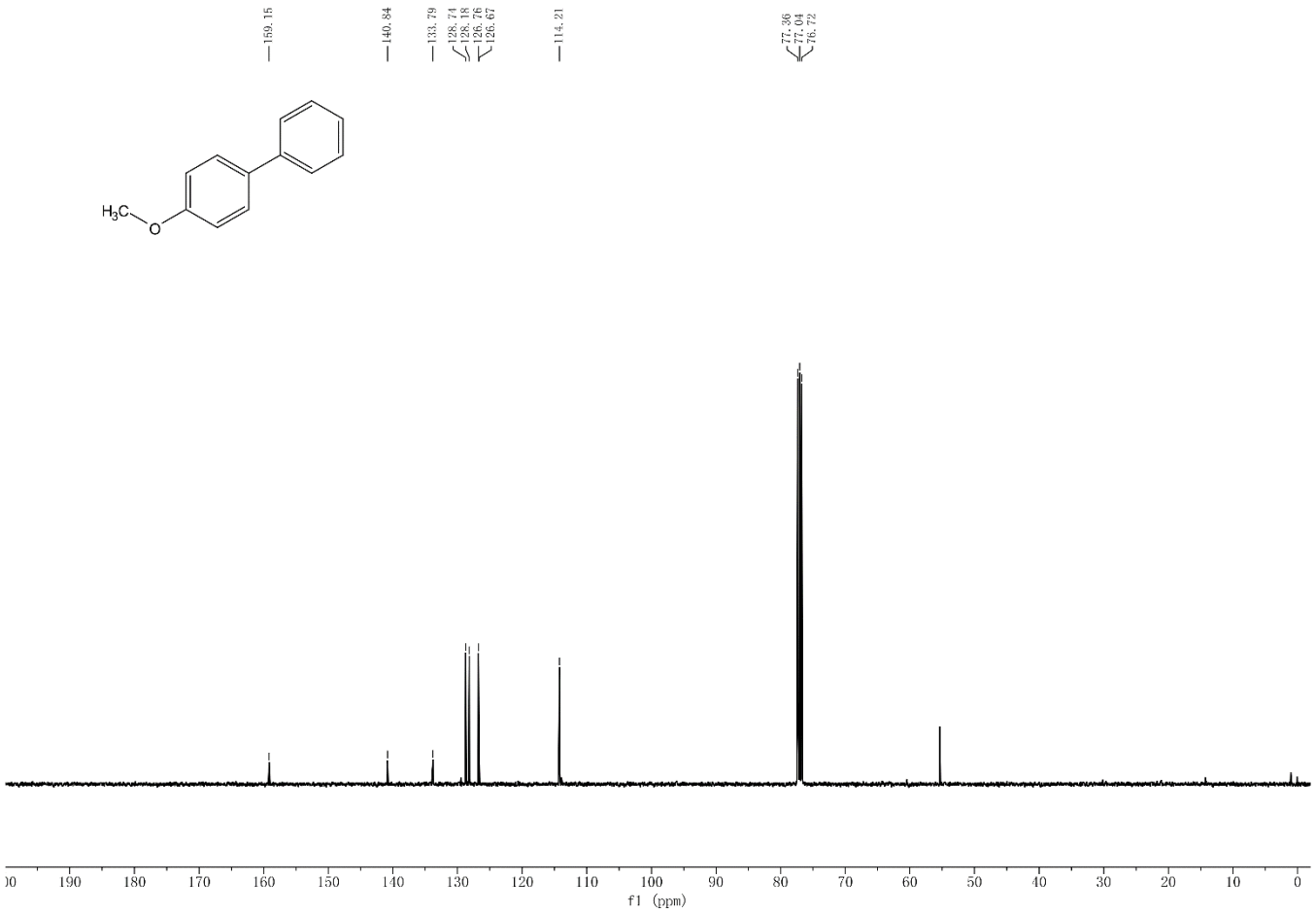
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 8s



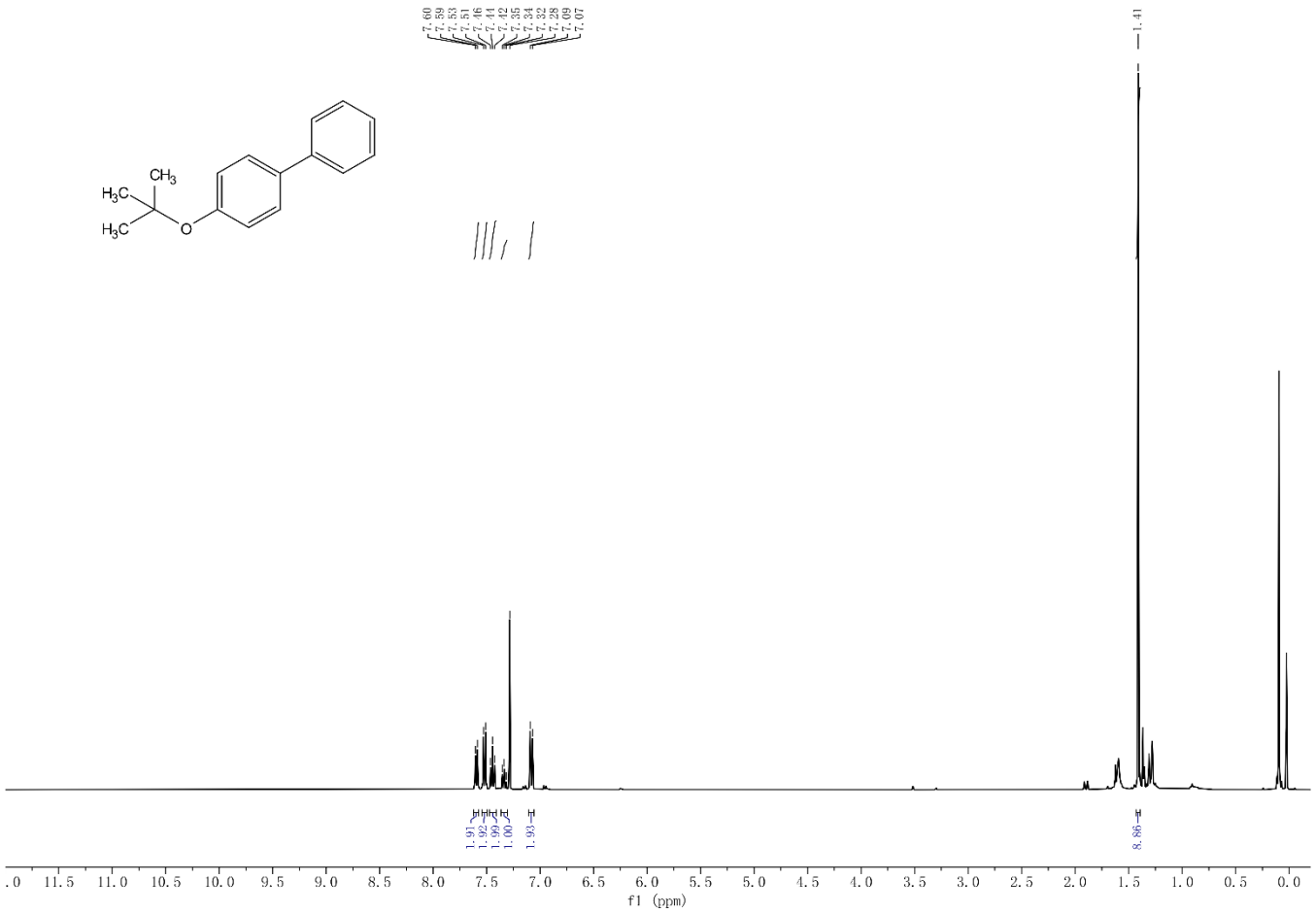
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8t



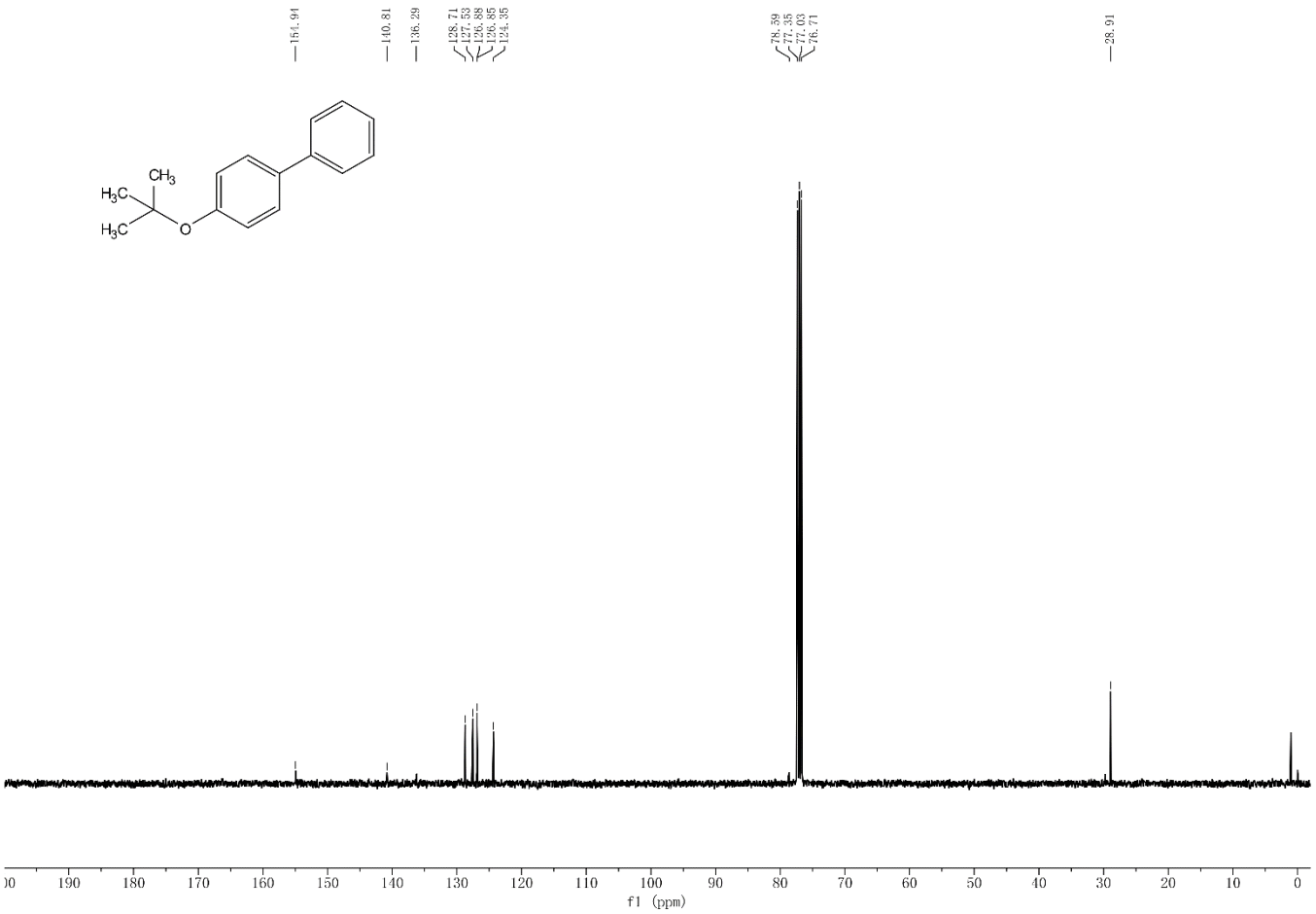
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8t



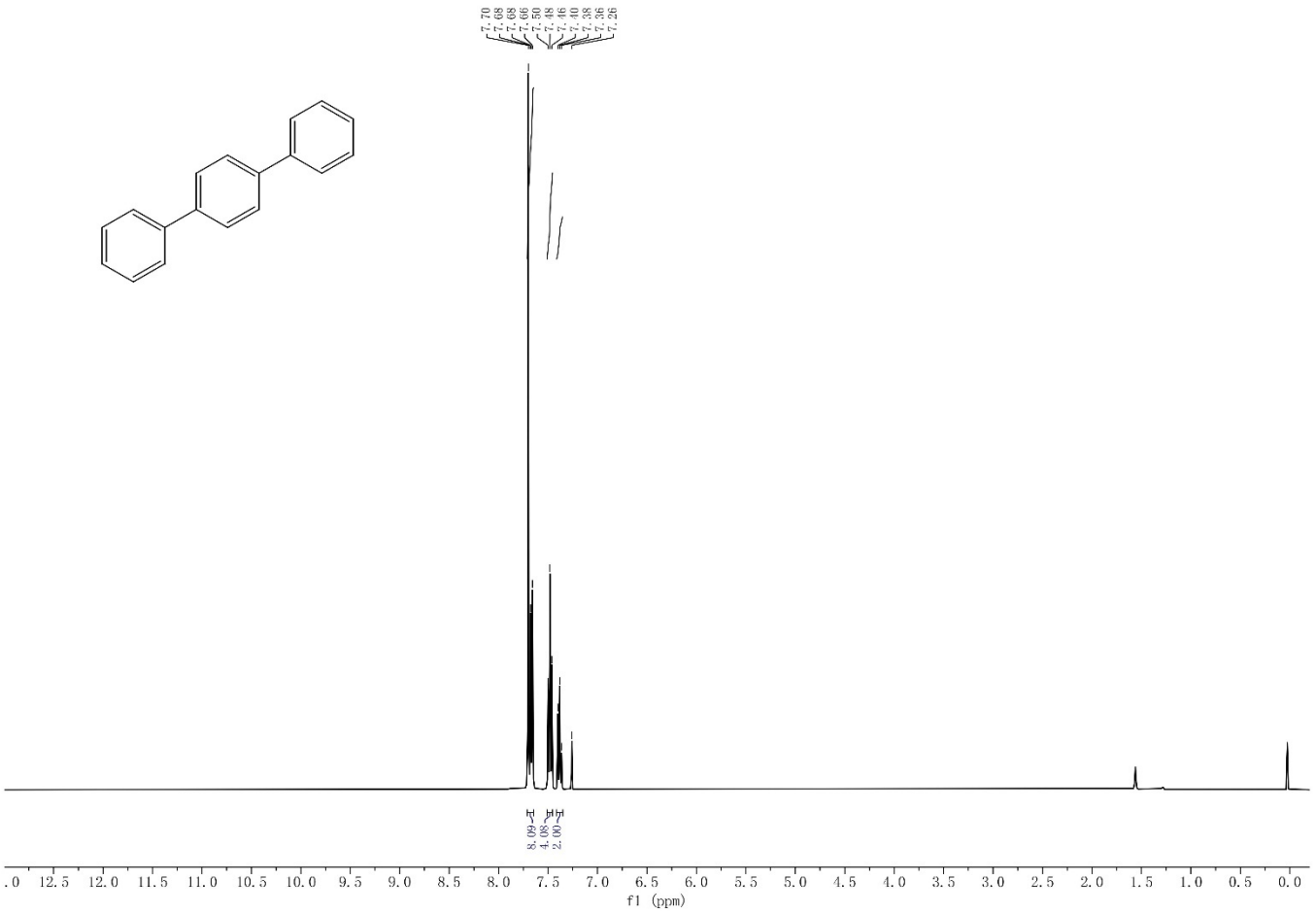
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8u



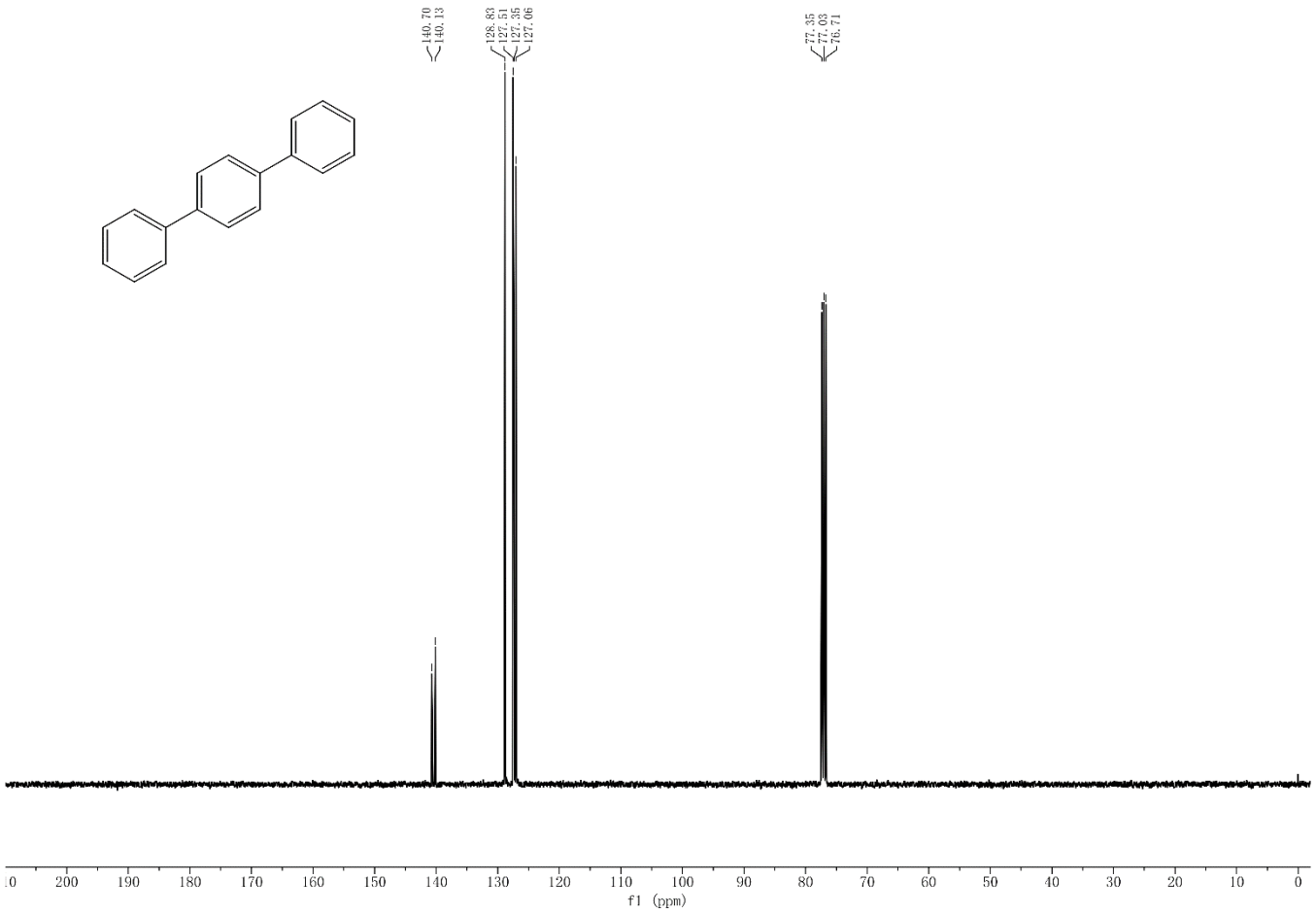
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8u



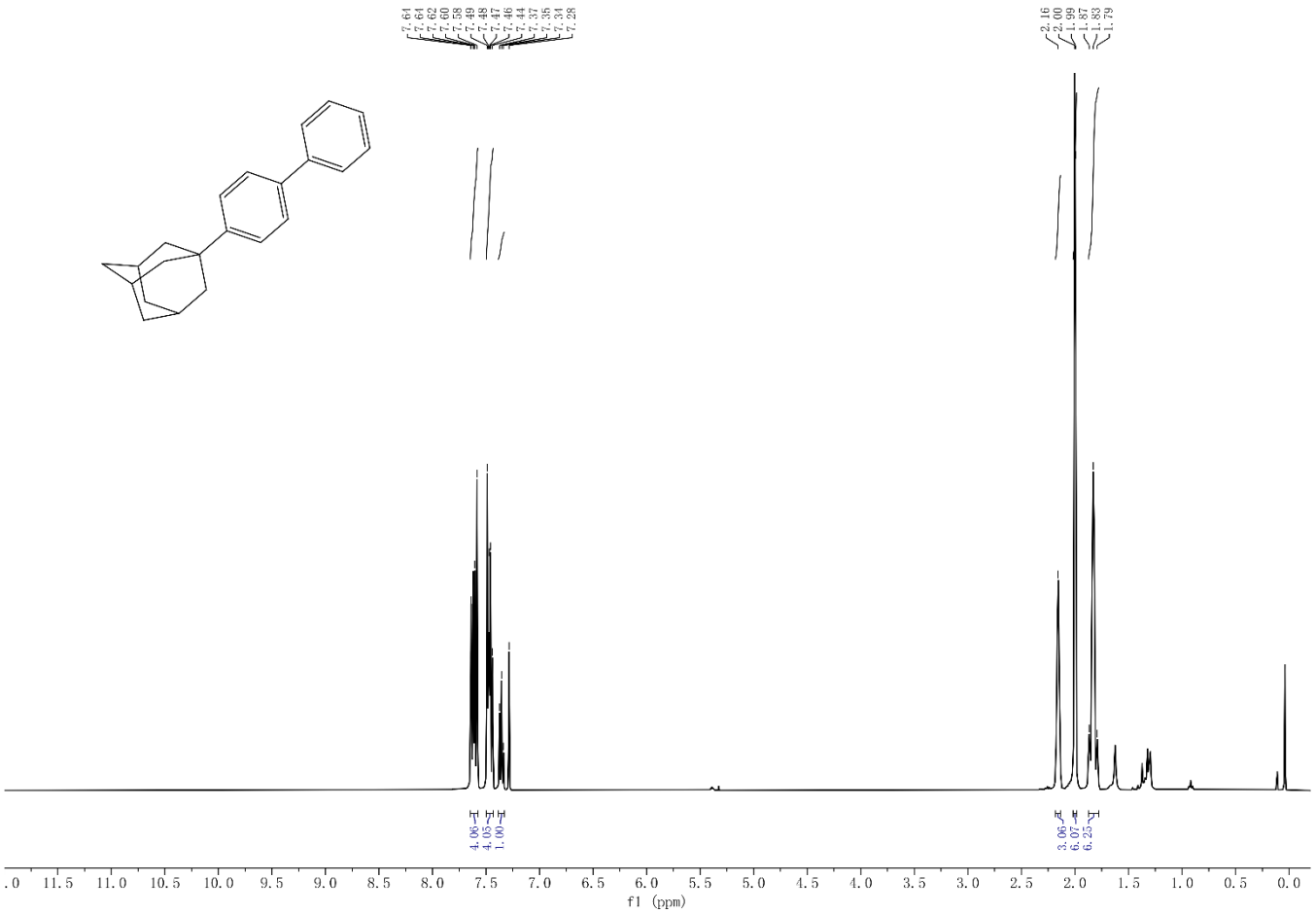
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8v



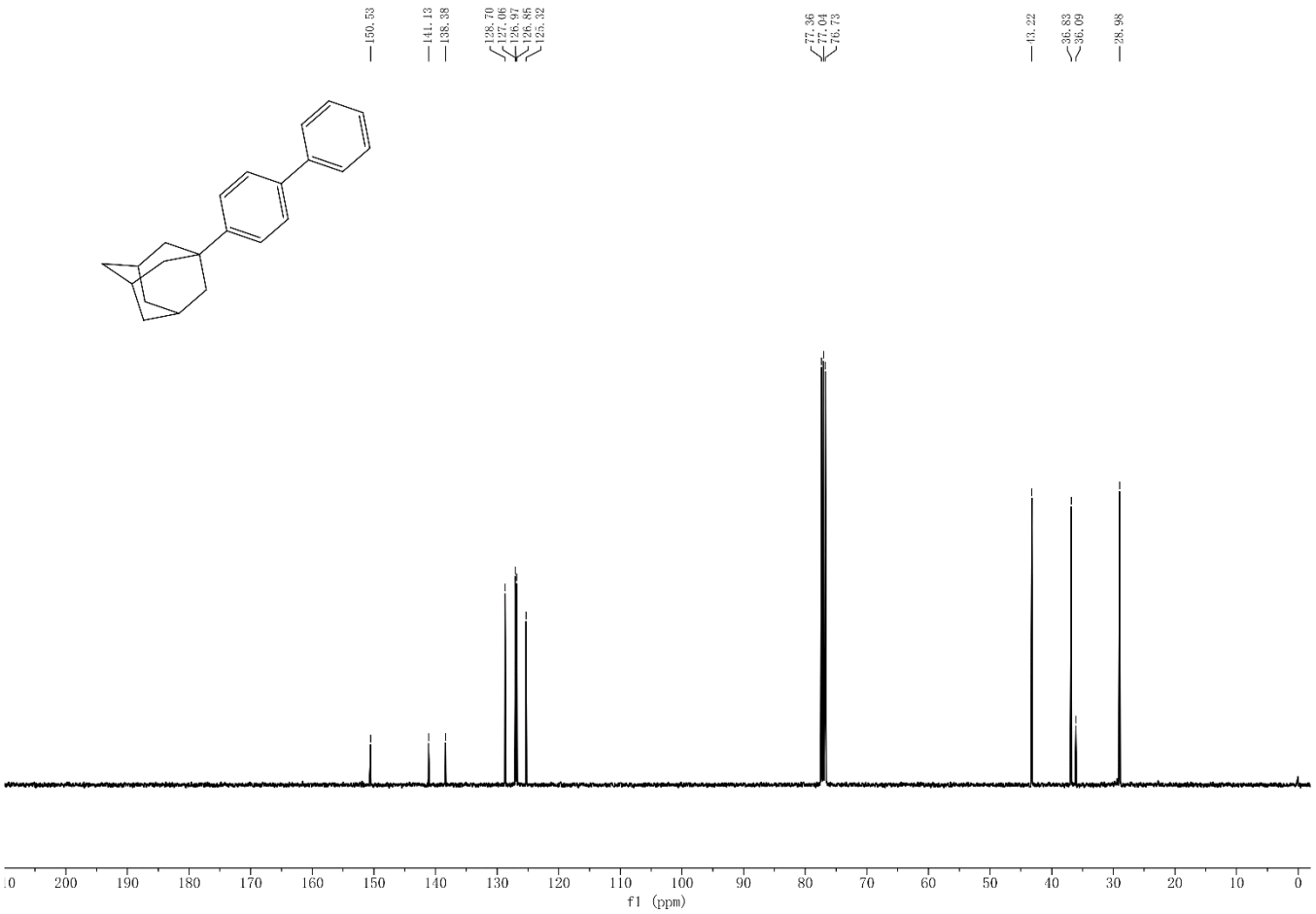
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8v



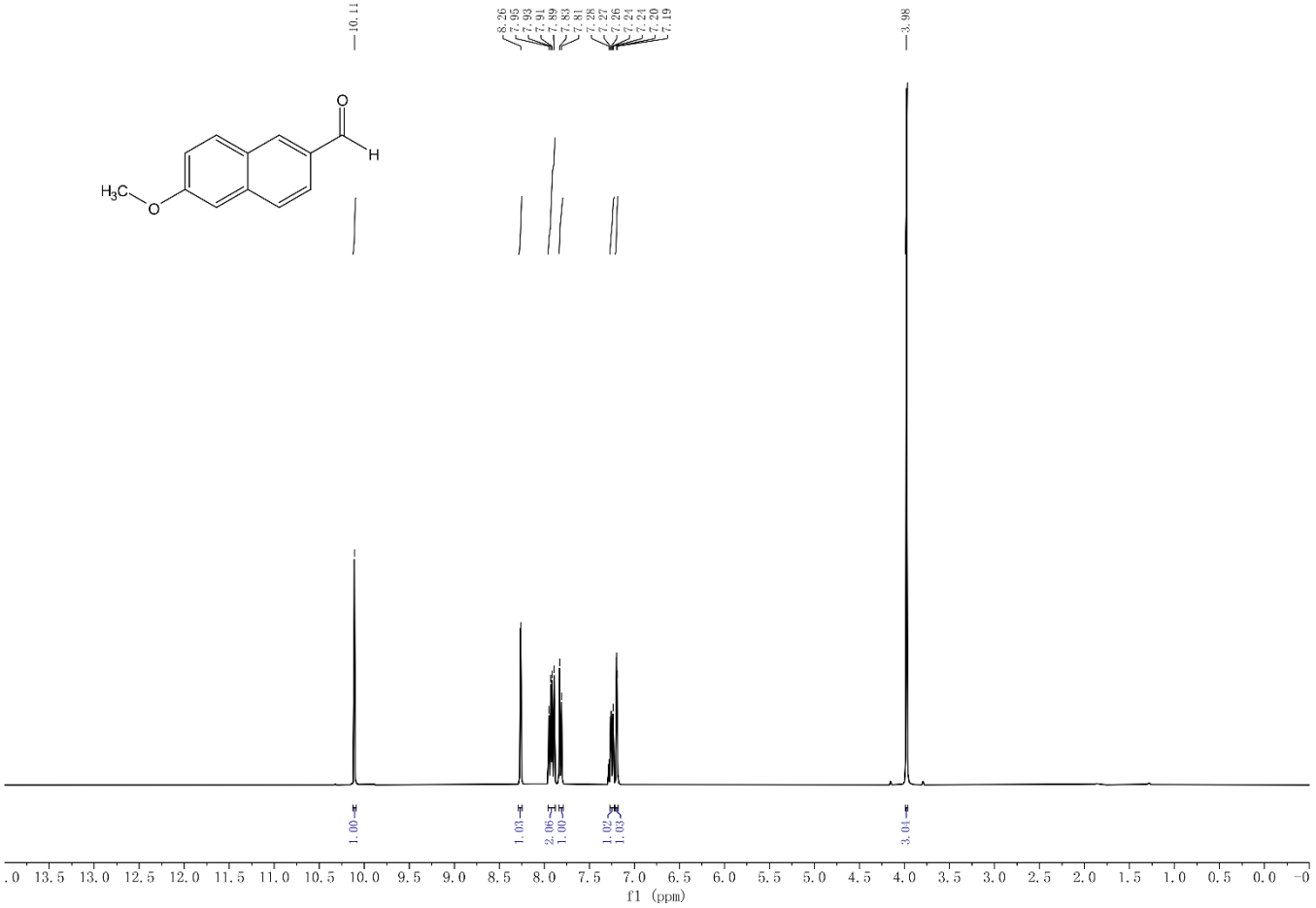
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 8w



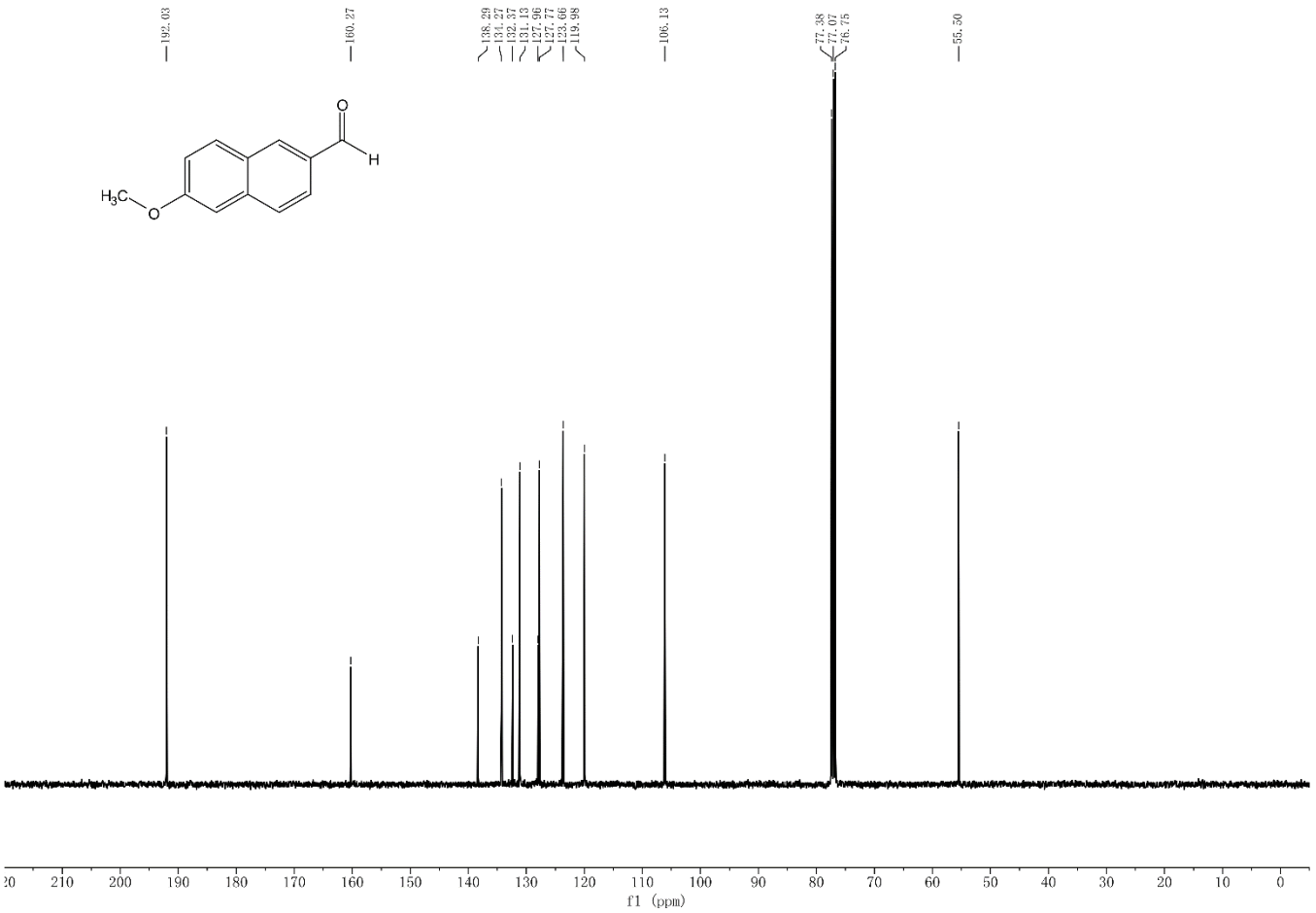
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 8v



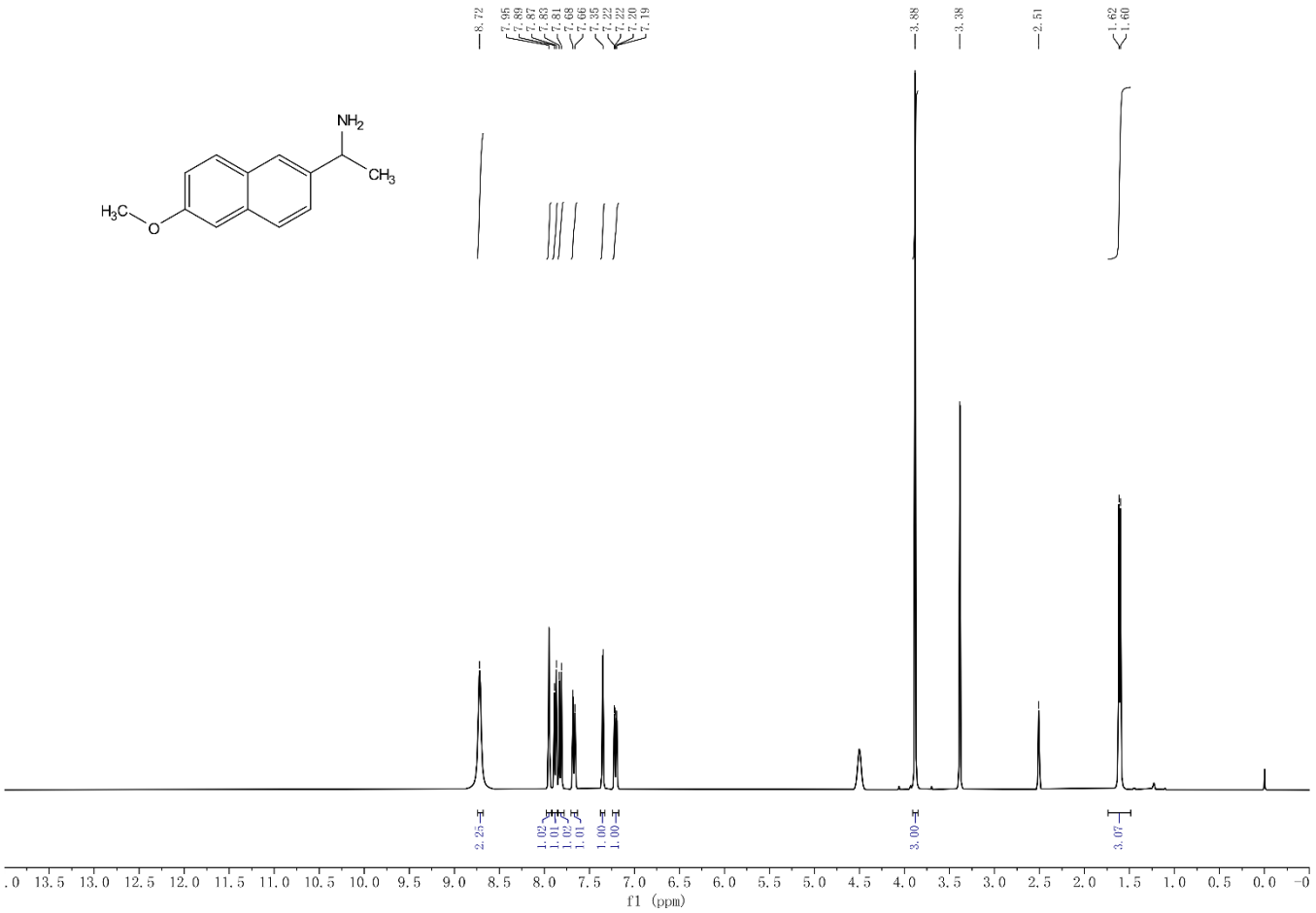
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9a



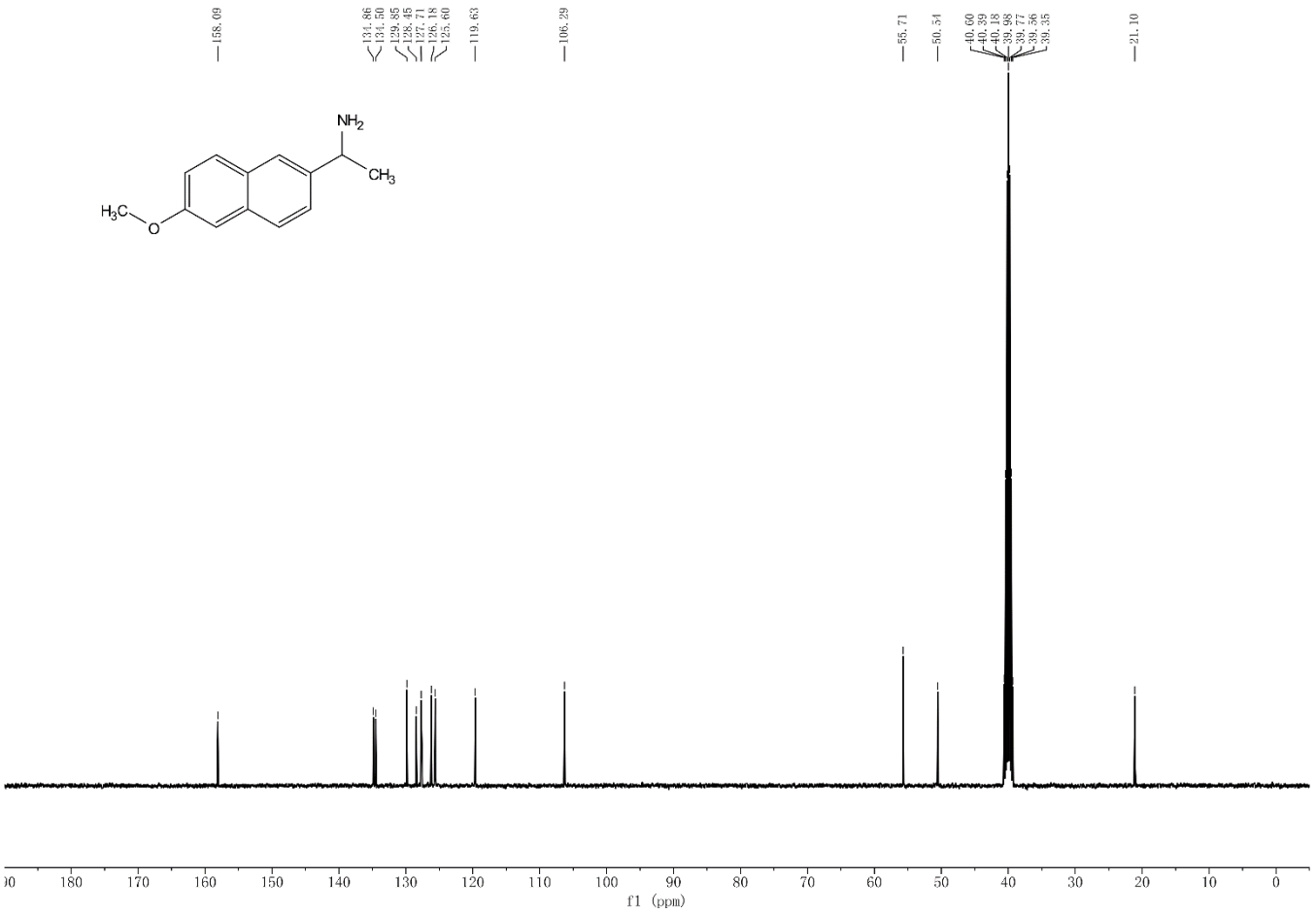
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 9a



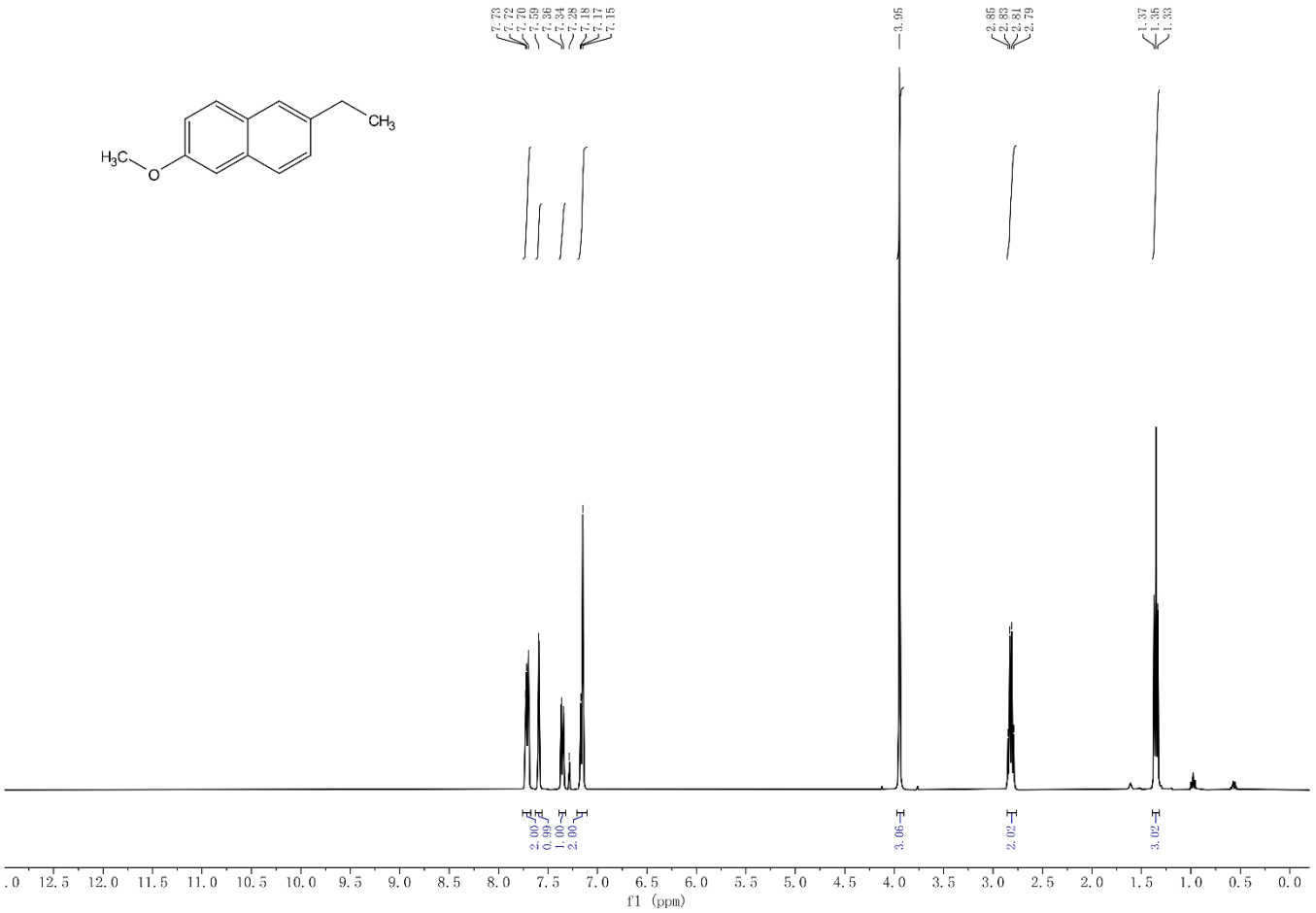
^{1}H NMR (400 MHz, DMSO-d^{6}) spectrum of 9b



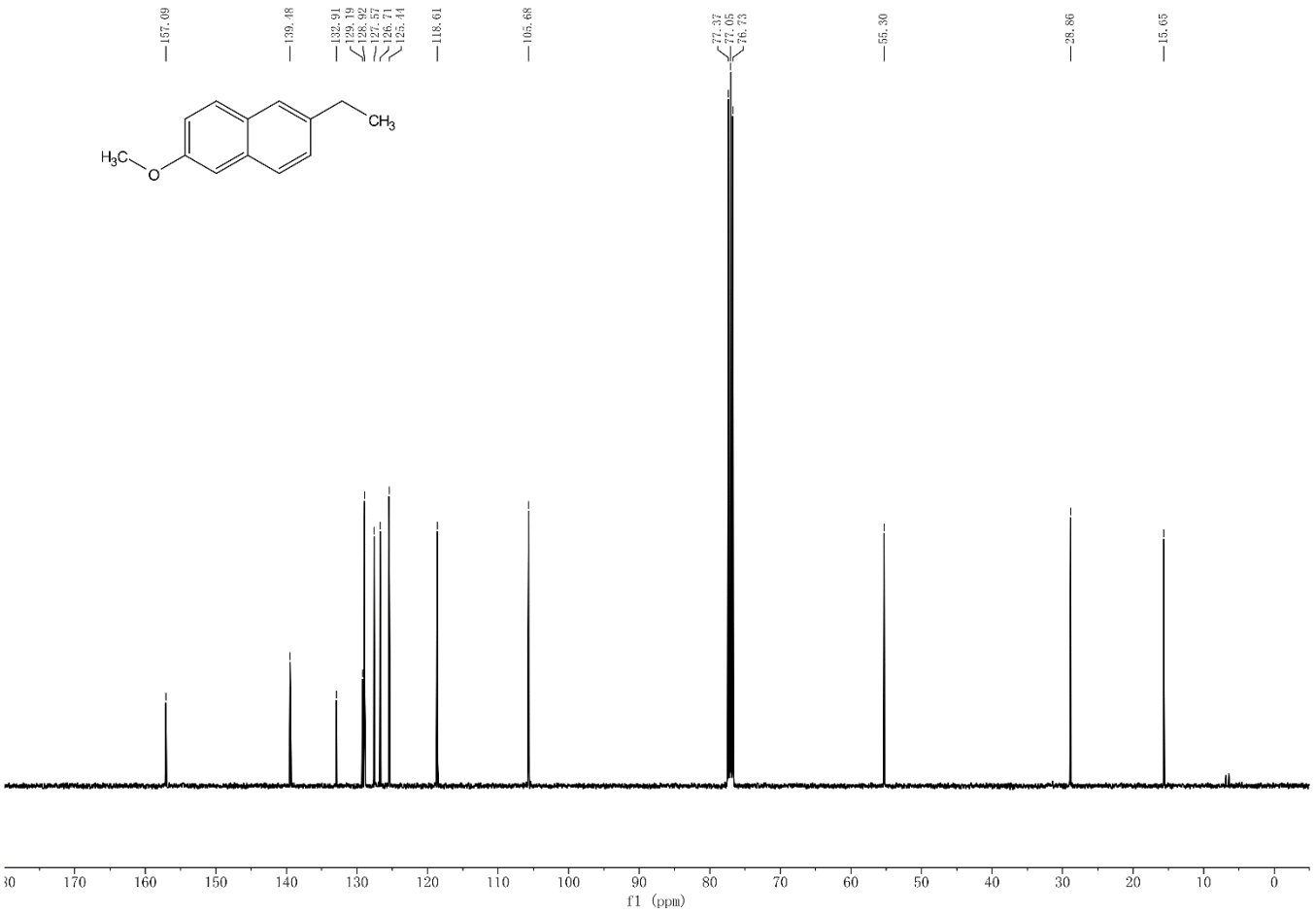
$^{13}C\{1H\}$ NMR (101 MHz, DMSO-d^6) spectrum of 9b



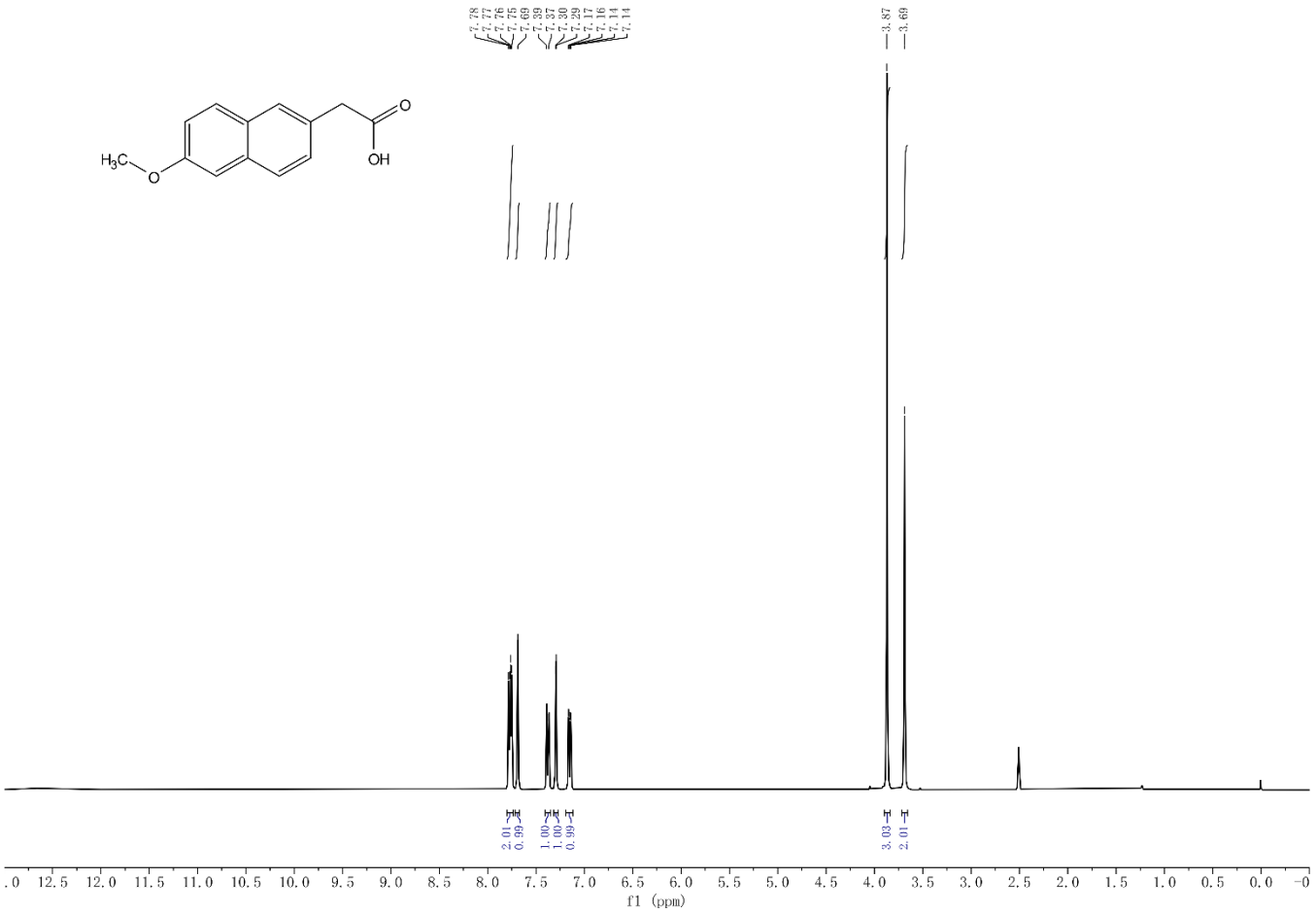
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9c



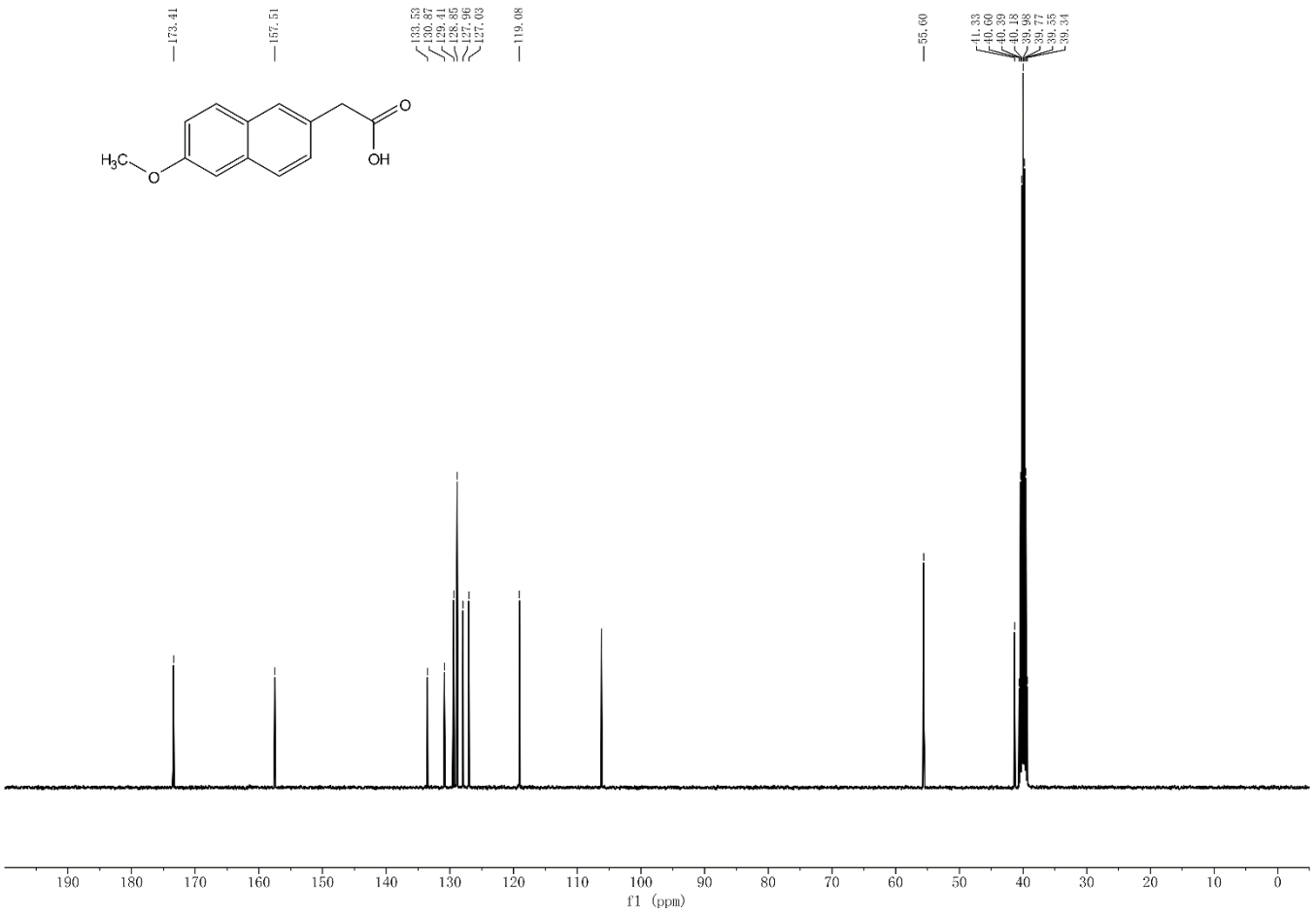
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 9c



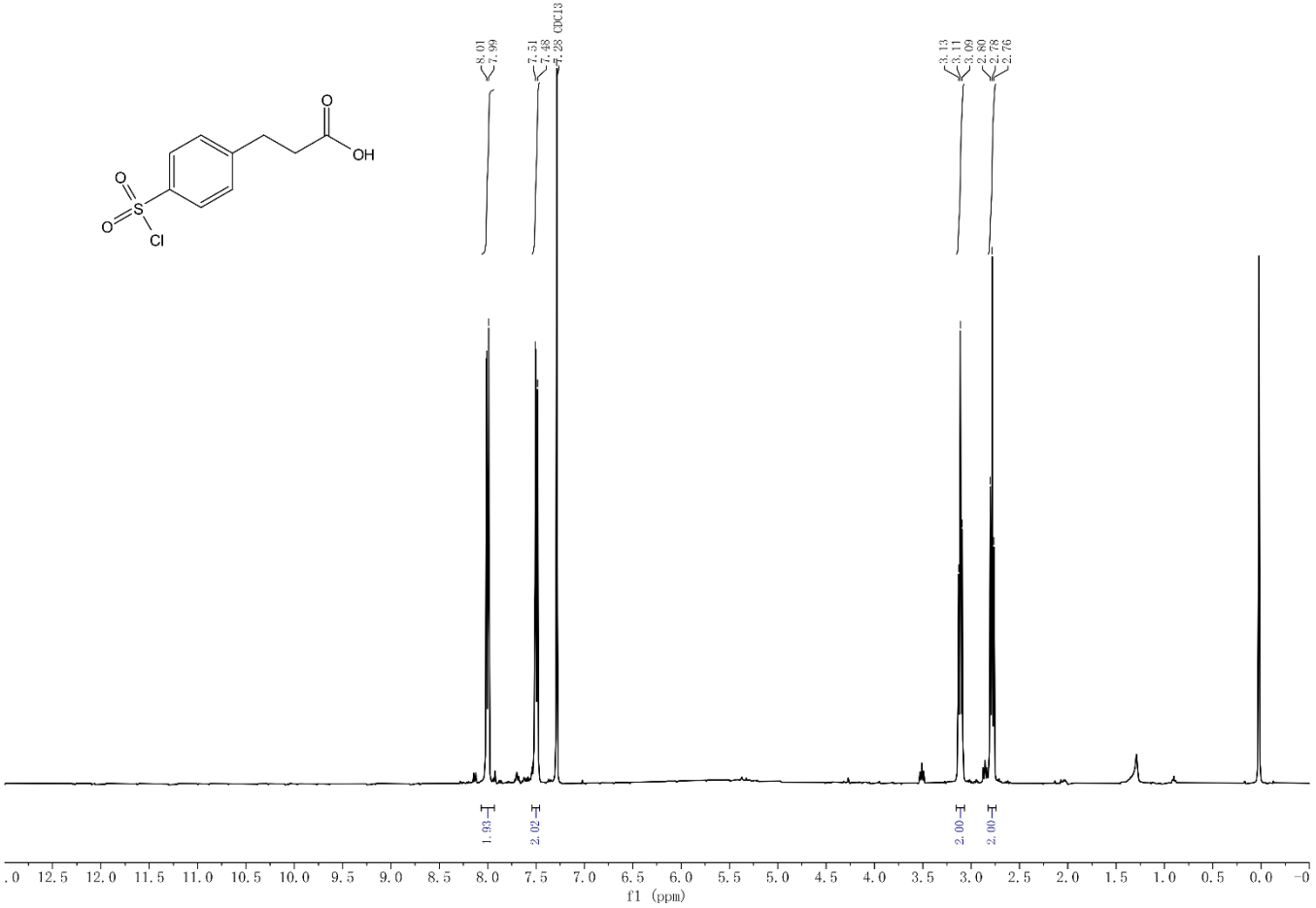
^{1}H NMR (400 MHz, DMSO-d^{6}) spectrum of 9d



$^{13}C\{1H\}$ NMR (101 MHz, DMSO-d^6) spectrum of 9d

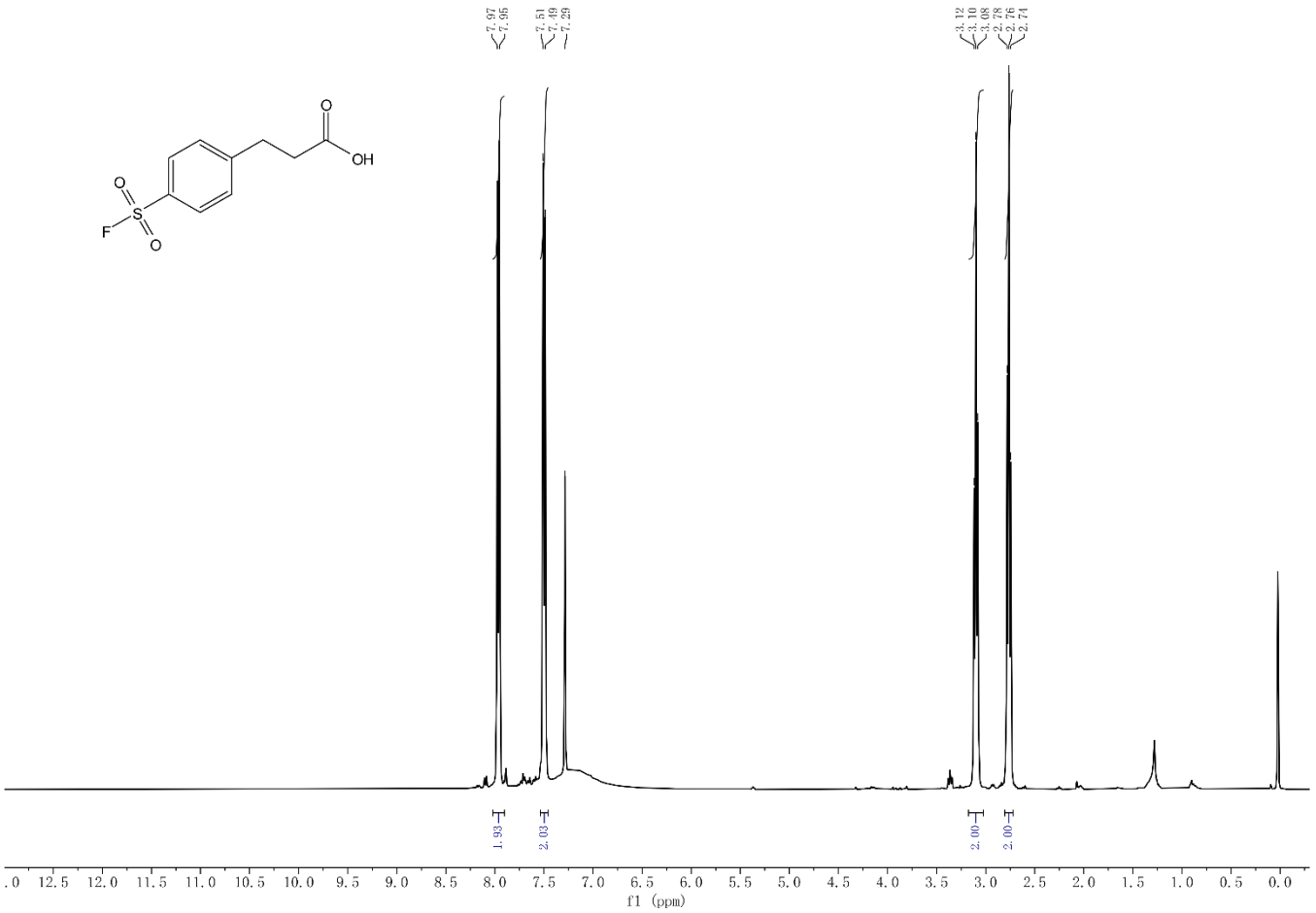


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9e

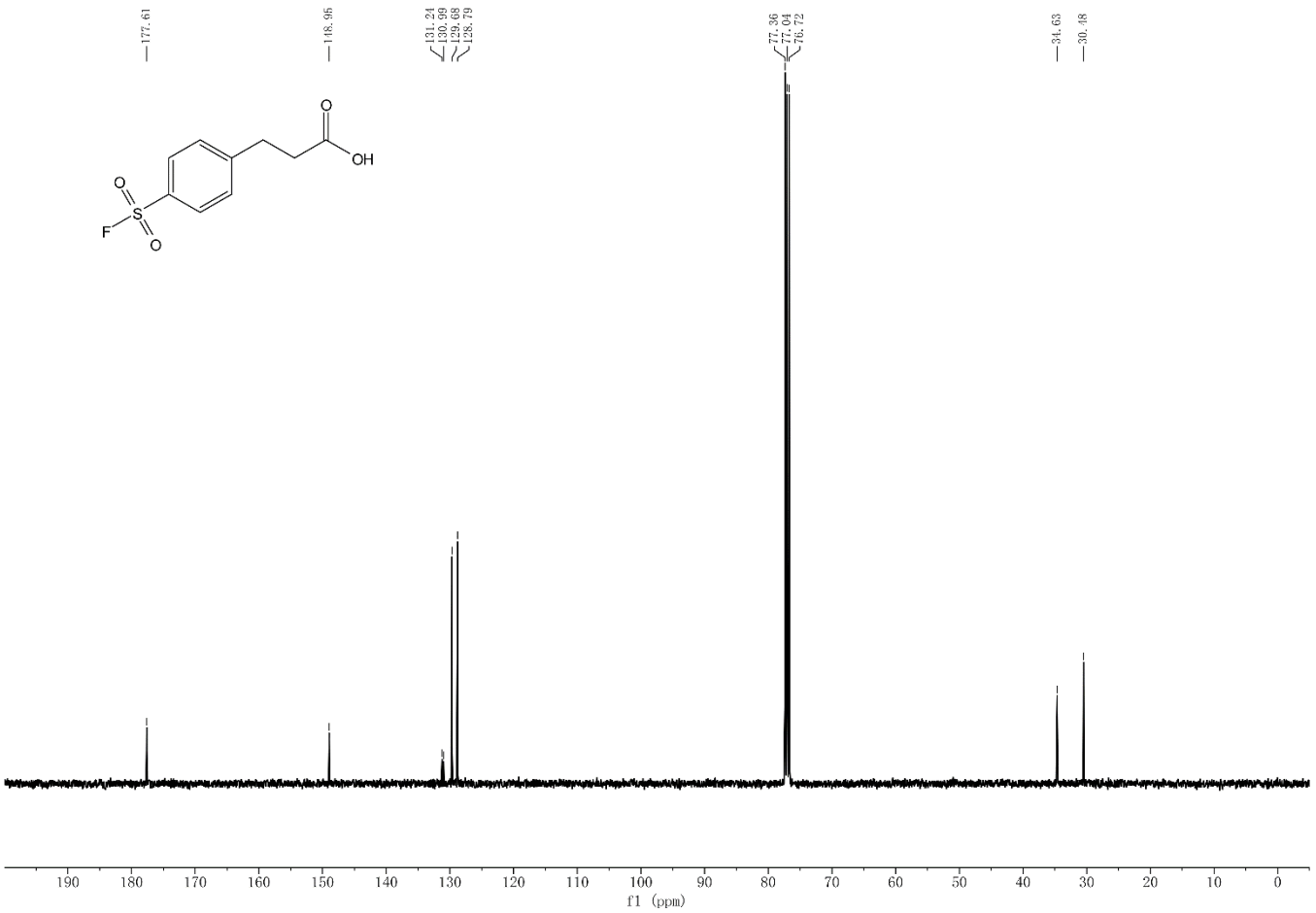


$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 9e

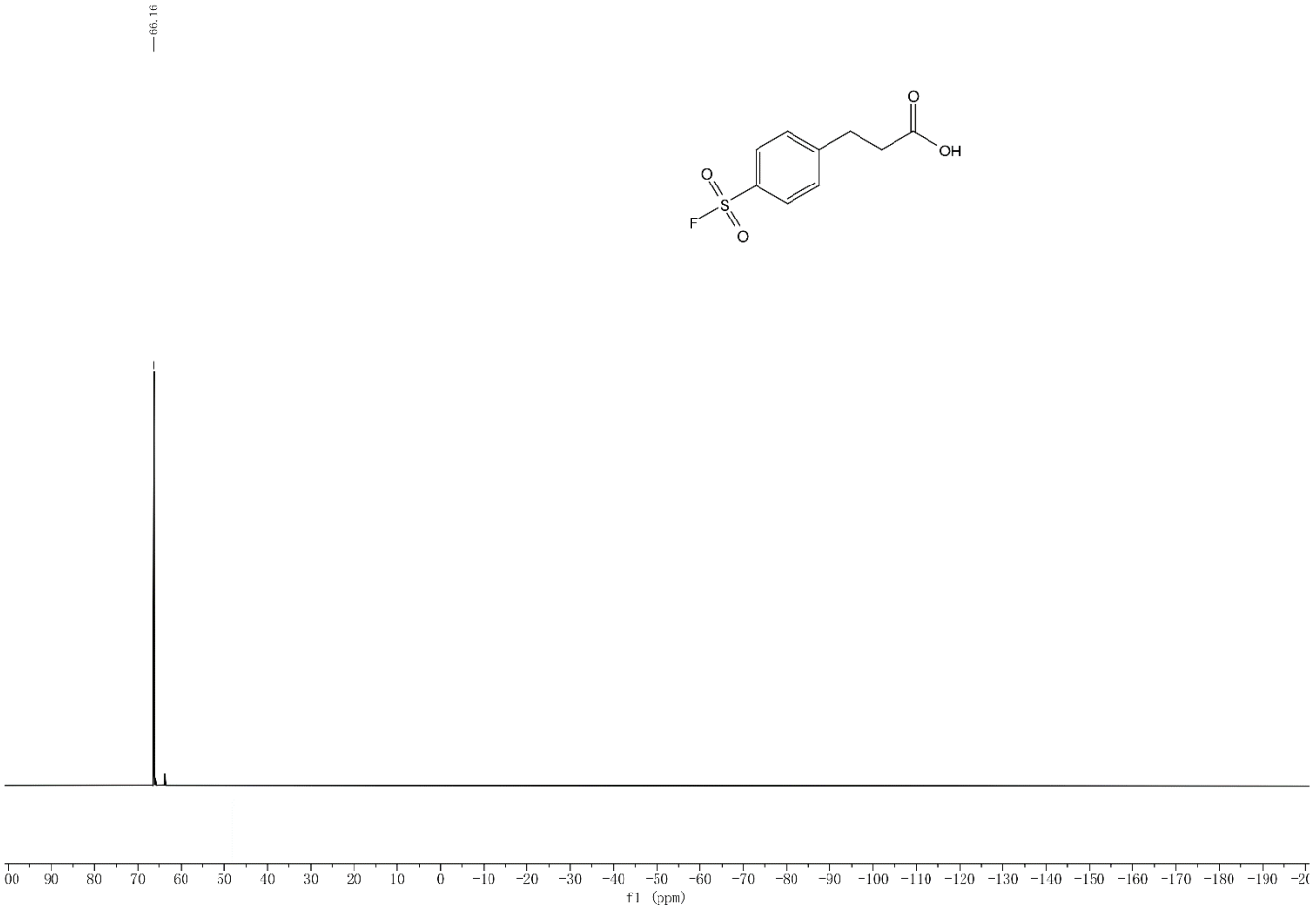
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9f



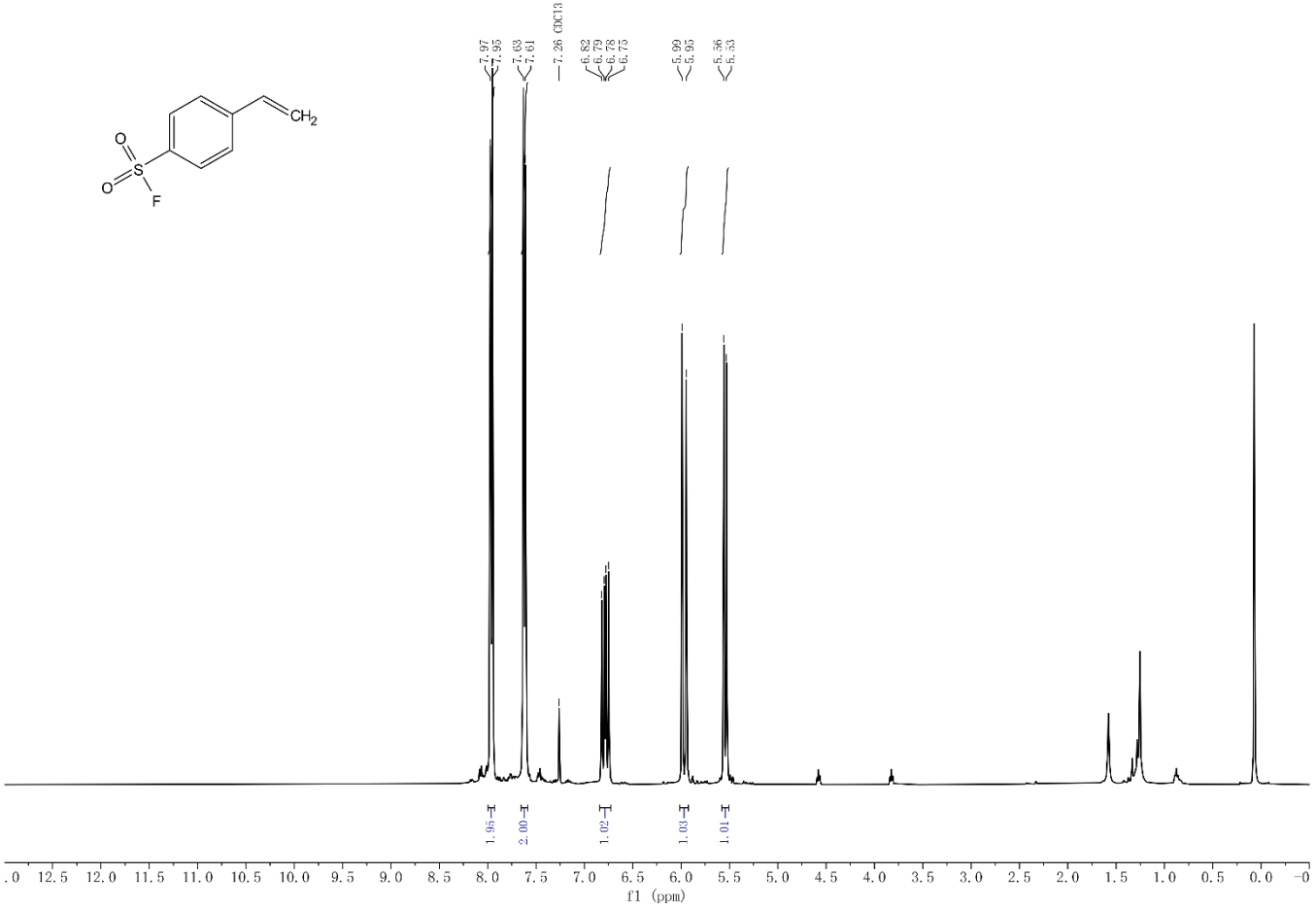
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 9f



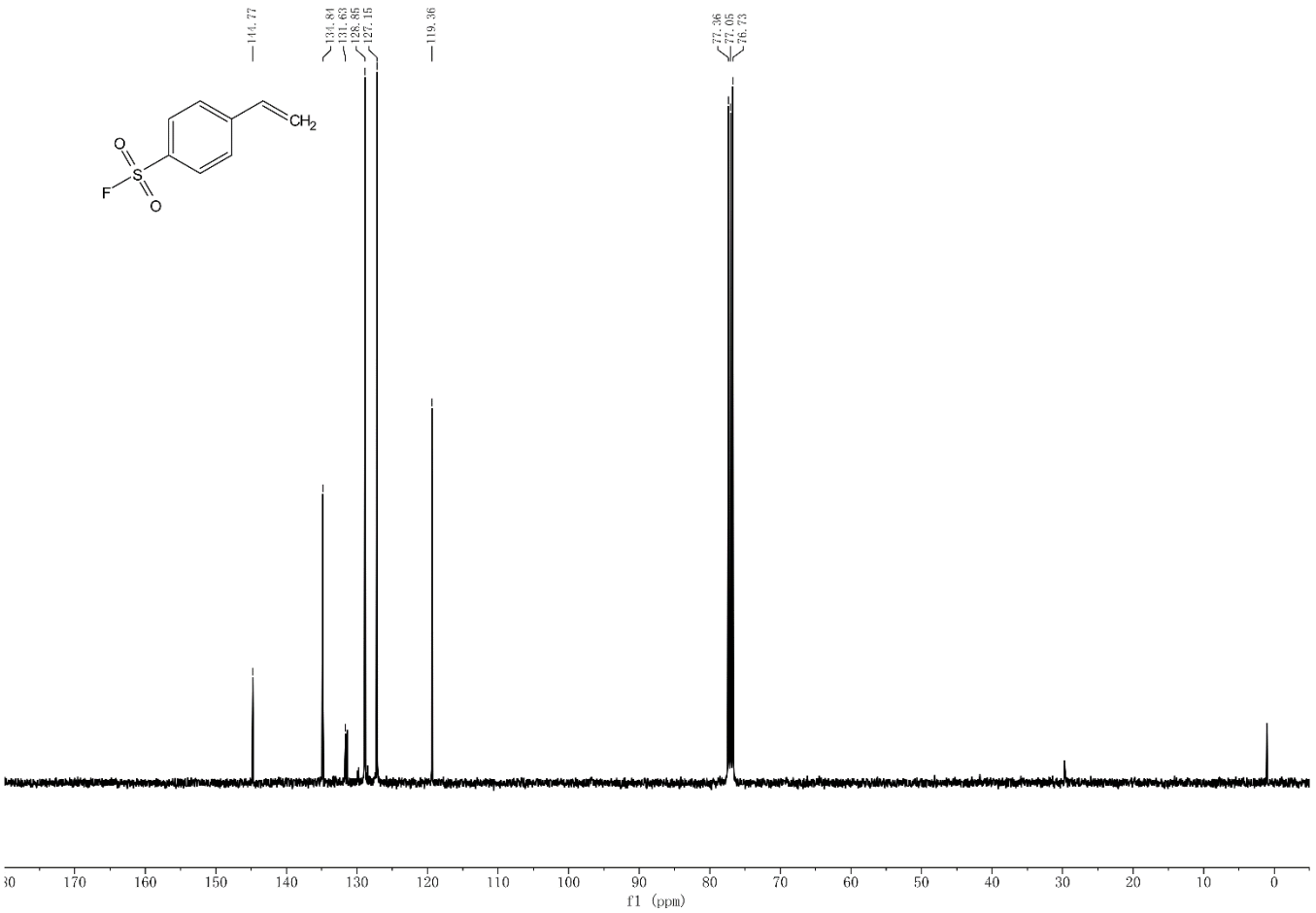
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 9f



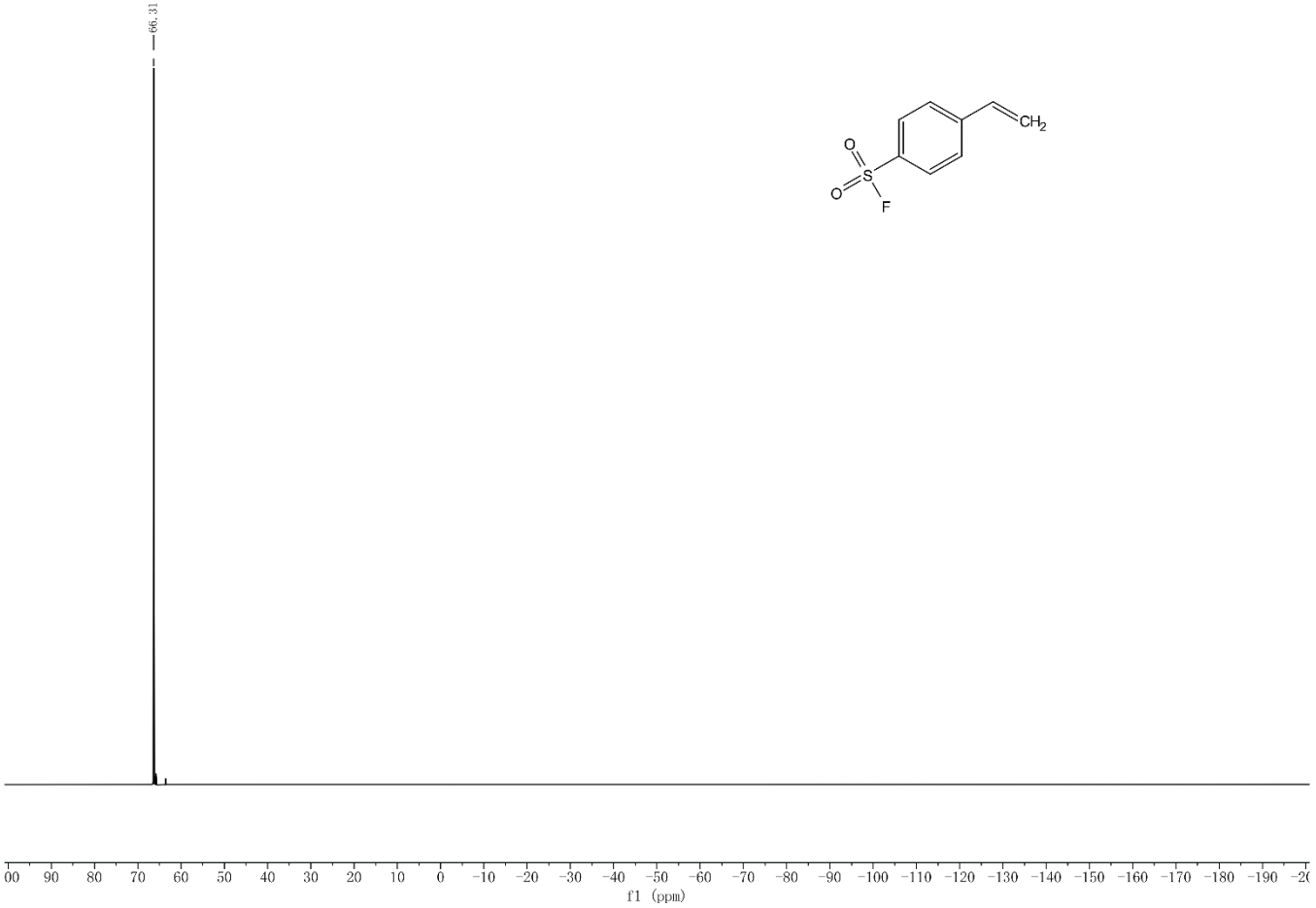
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 9g



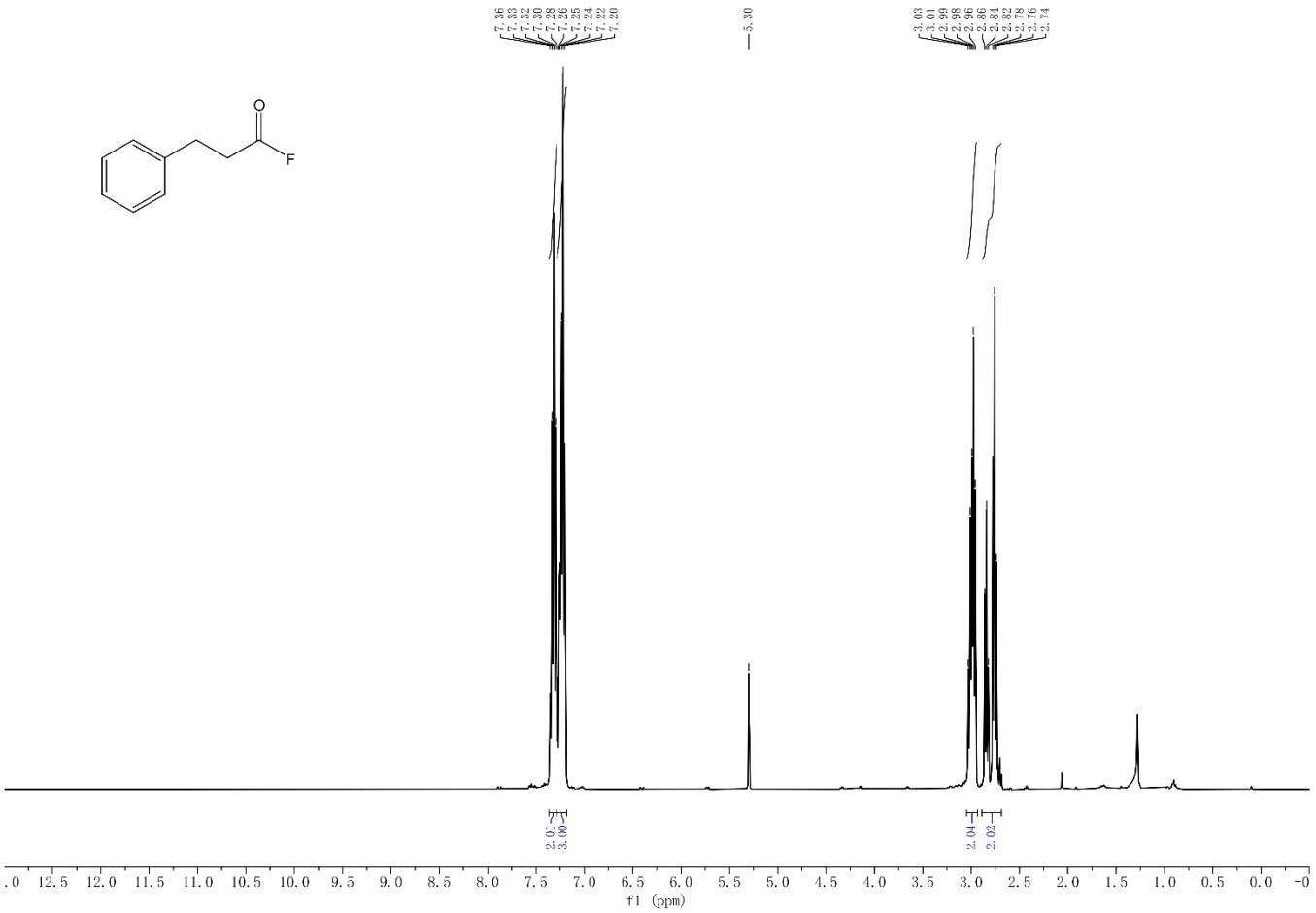
$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 9g



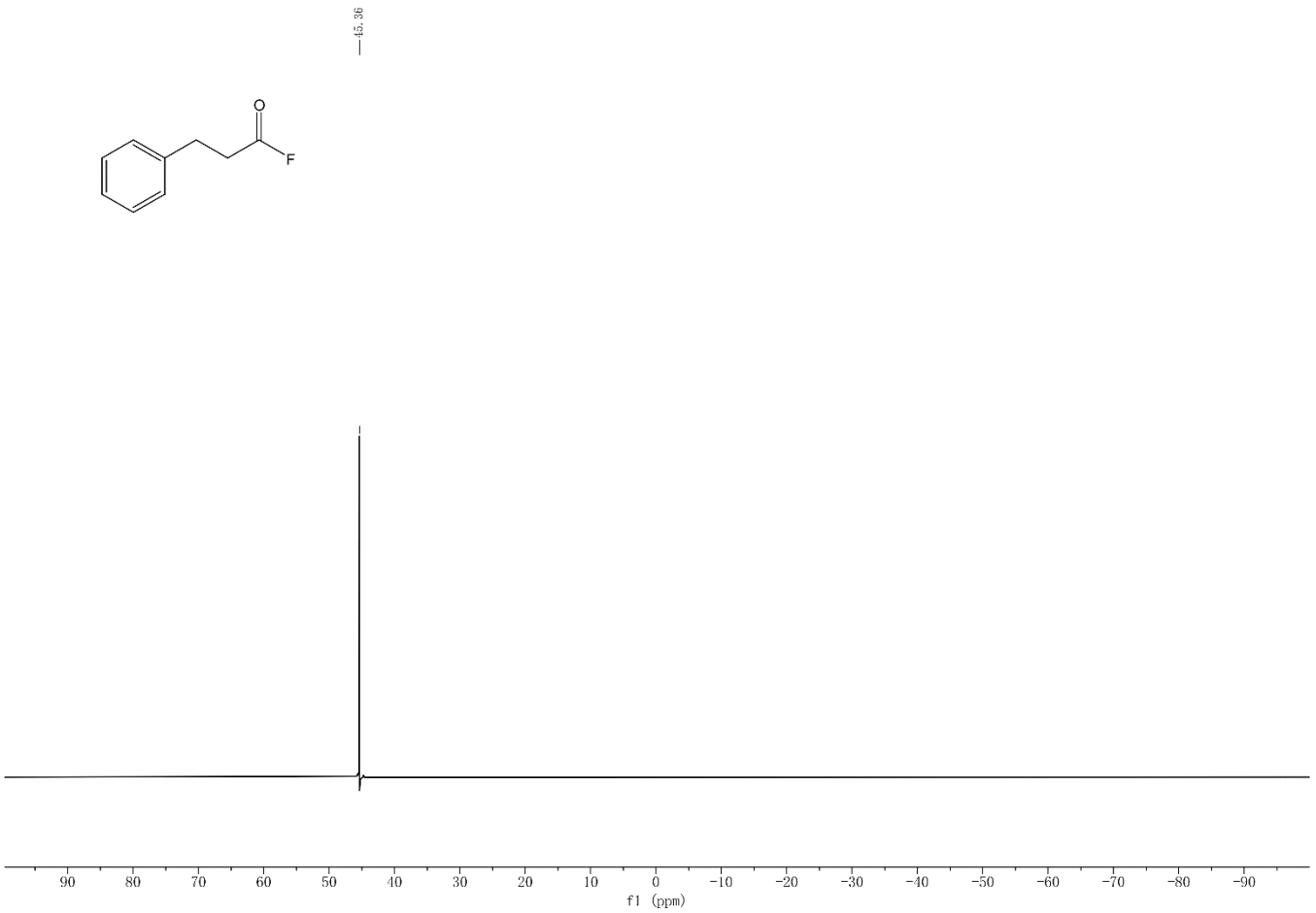
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 9g



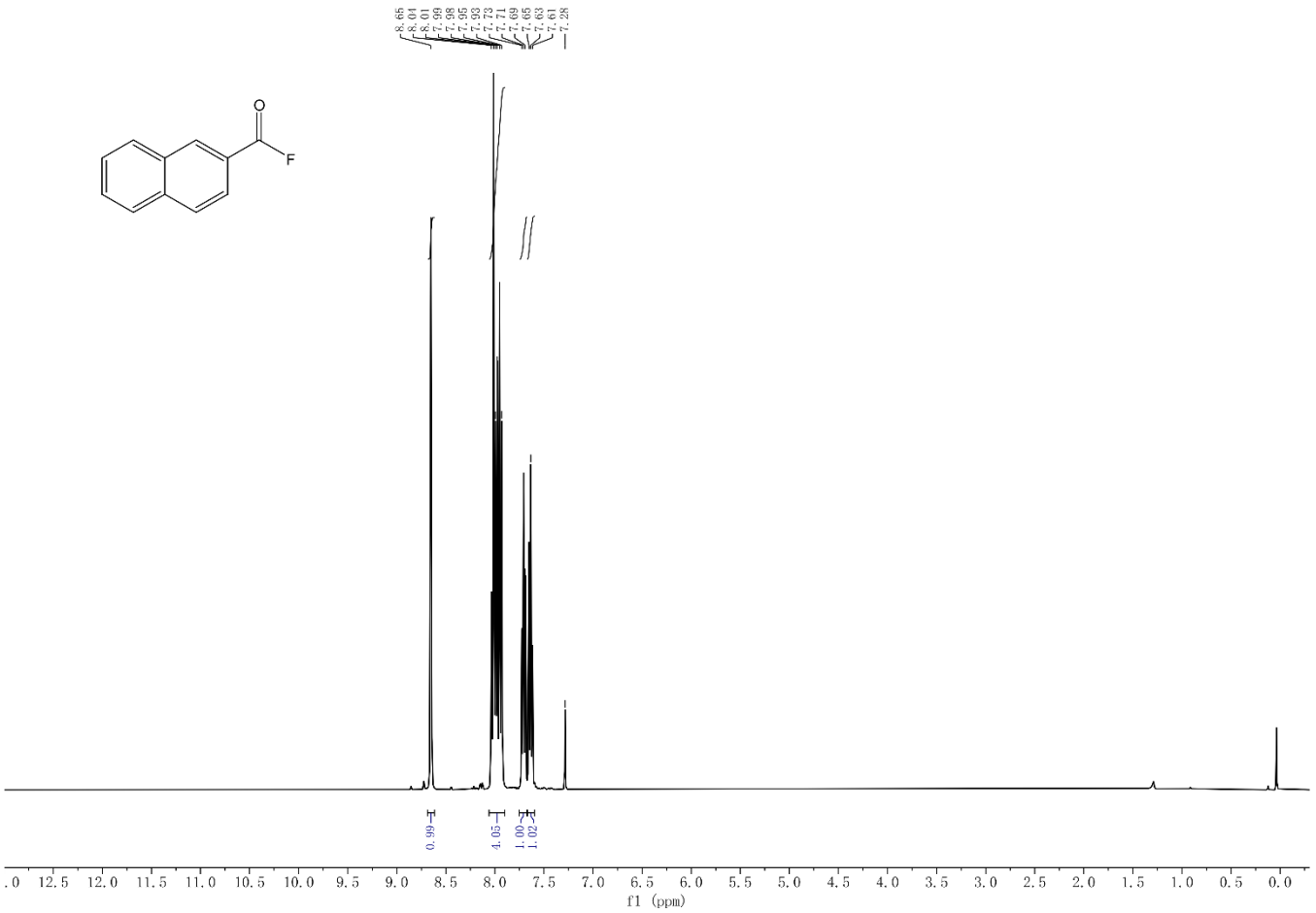
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 10a



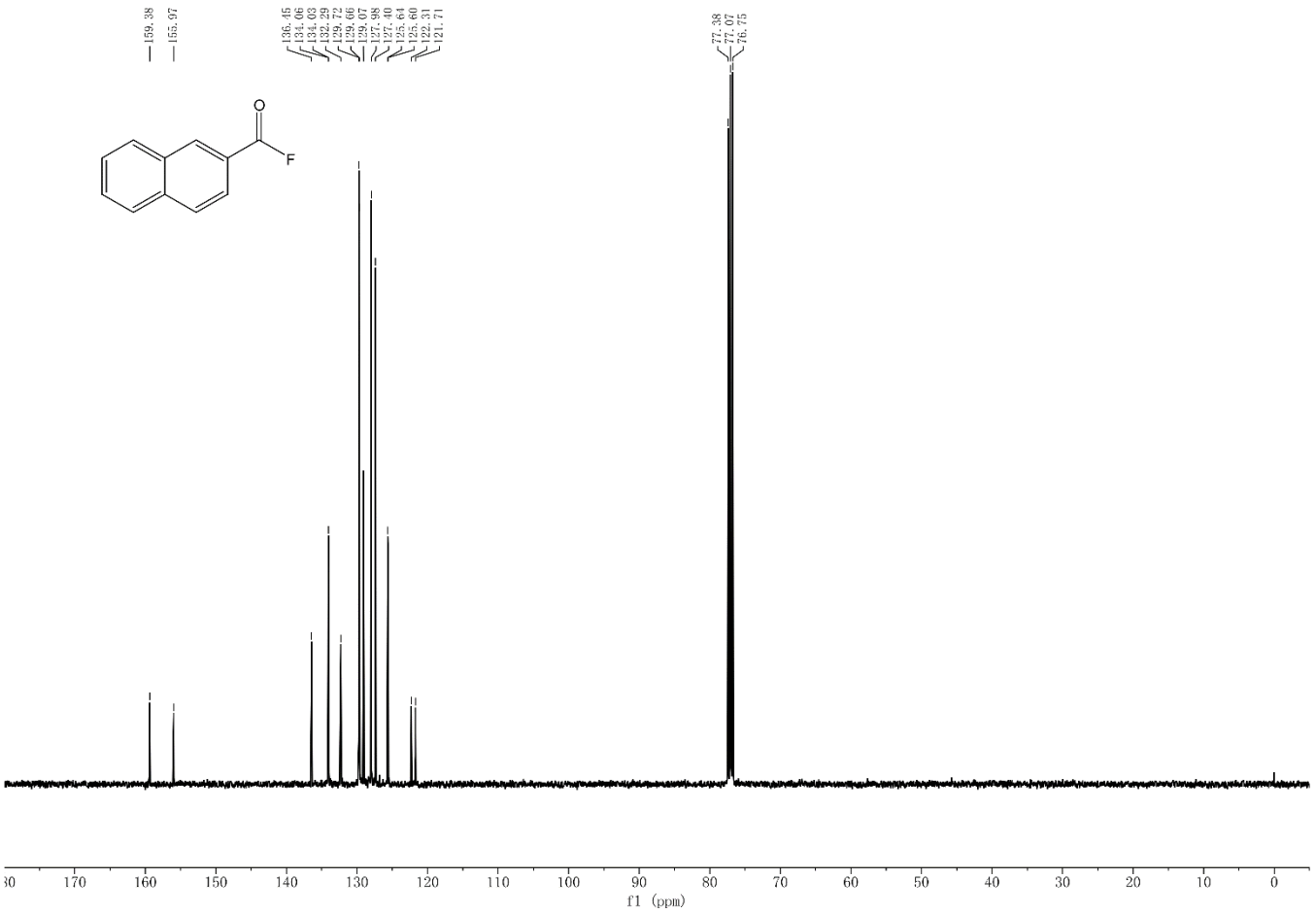
^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 10a



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 10b



$^{13}C\{1H\}$ NMR (101 MHz, $CDCl_3$) spectrum of 10b



^{19}F NMR (377 MHz, $CDCl_3$) spectrum of 10b

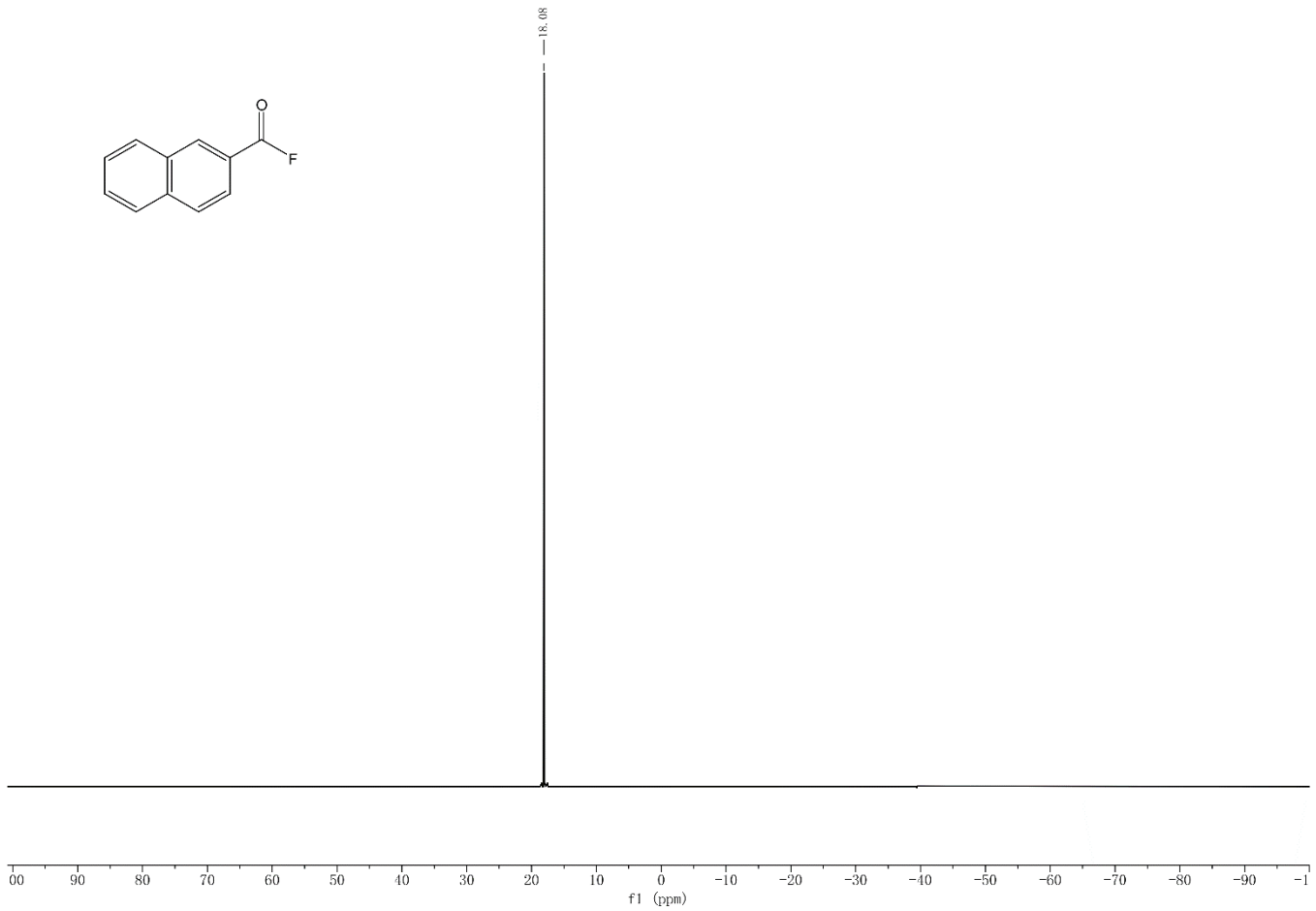


Table S13. Energies for all calculated species.

Structures	ZPE	tcH	tcG	E	H	G	Imaginary Frequency
PhCOOH	0.116039	0.124087	0.083949	-420.741641	-420.733592	-420.773730	
Et_3N	0.207095	0.217458	0.174120	-292.235201	-292.234257	-292.277595	
HEt_3N^+	0.224924	0.234574	0.192408	-292.652123	-292.651179	-292.693344	
$PhCOO^-$	0.102429	0.110304	0.070704	-420.216792	-420.215847	-420.255448	
SO_2F_2	0.014857	0.020209	-0.013072	-748.225989	-748.225045	-748.258325	
$PhCOOSO_2F_2^-$	0.119330	0.131787	0.080302	-1168.468409	-1168.467465	-1168.518950	
F^-	0.000000	0.002360	-0.014159	-99.825875	-99.824931	-99.841450	
$PhCOOSO_2F$	0.117591	0.129730	0.078473	-1068.533238	-1068.532294	-1068.583552	
SO_3	0.011763	0.016308	-0.014716	-623.752036	-623.751092	-623.782116	
PhCOF	0.103219	0.111101	0.071229	-444.756363	-444.755418	-444.795291	
PdP_2	0.599422	0.637685	0.527695	-2390.938055	-2390.937111	-2391.047100	
Ts4	0.702176	0.748501	0.621311	-2835.701219	-2835.700274	-2835.827464	153.30i
Int1	0.703235	0.750125	0.621744	-2835.717753	-2835.716808	-2835.845189	
Int1A	0.730651	0.784749	0.639831	-3697.295865	-3697.294921	-3697.439839	
Ts5	0.699921	0.747088	0.619061	-2835.674739	-2835.673795	-2835.801822	292.63i
Ts5A	0.728360	0.782444	0.639513	-3697.270839	-3697.269895	-3697.412826	331.53i
Ts5B	0.758791	0.825412	0.653486	-4955.862166	-4955.861222	-4956.033148	124.09i

Int2	0.700945	0.748619	0.619272	-2835.697821	-2835.696876	-2835.826223	
Int2A	0.729338	0.783911	0.640061	-3697.280438	-3697.279494	-3697.423344	
Ts6	0.699715	0.747443	0.618186	-2835.675479	-2835.674535	-2835.803792	27.48i
Ts6A	0.727036	0.782008	0.635268	-3697.256566	-3697.255622	-3697.402361	74.52i
CO	0.005039	0.008344	-0.014098	-113.296017	-113.295073	-113.317515	
Int3	0.693500	0.738259	0.616026	-2722.374240	-2722.373296	-2722.495529	
Int3A	0.720674	0.772889	0.631802	-3583.950022	-3583.949078	-3584.090165	
MeOPhB(OH)$_2$	0.156900	0.166903	0.122376	-522.645778	-522.644834	-522.689361	
Ts7	0.850595	0.907259	0.758134	-3245.027083	-3245.026139	-3245.175263	200.00i
FB(OH)$_2$	0.036157	0.041256	0.009767	-276.463773	-276.462829	-276.494318	
Int4	0.813988	0.865490	0.727590	-2968.578982	-2968.578037	-2968.715938	
Ts8	0.812628	0.863696	0.727042	-2968.566063	-2968.565119	-2968.701773	386.84i
product	0.215131	0.227500	0.177185	-577.666960	-577.666016	-577.716331	

V. Cartesian Coordinates of the Structures

PhCOOH

C	-1.49358	1.62495	0.60027
C	-0.18724	1.58964	0.09415
C	0.36613	2.73315	-0.49752
C	-0.38685	3.91198	-0.58309
C	-1.69318	3.94729	-0.07697
C	-2.24655	2.80378	0.51471
H	-1.91609	0.75185	1.05203
H	1.36354	2.70619	-0.88395
H	0.03566	4.78507	-1.03485
H	-2.26809	4.84736	-0.1423
H	-3.24397	2.83075	0.90114
C	0.6402	0.29422	0.18818
O	0.07553	-0.87263	0.79193
H	0.71706	-1.58648	0.77022
O	1.81323	0.26251	-0.2663

Et_3N

N	0.45509	-0.188	0.00375
C	0.99673	0.21773	-1.30121
H	0.63947	1.19587	-1.54716
H	2.0657	0.22946	-1.25565
C	0.89121	0.76621	1.03341
H	0.49695	0.47089	1.98328
H	1.96017	0.77794	1.07897
C	0.94591	-1.53181	0.34164
H	0.62847	-2.22636	-0.40784
H	2.01488	-1.52007	0.3872
C	0.37848	-1.95685	1.70874
H	0.73575	-2.93499	1.95469
H	0.69593	-1.26229	2.45822
H	-0.69048	-1.96858	1.66318
C	0.37701	2.17401	0.67942
H	0.69446	2.86857	1.4289
H	0.77127	2.46933	-0.27044
H	-0.69195	2.16228	0.63386
C	0.53985	-0.78192	-2.3799
H	0.9341	-0.4866	-3.32976
H	0.89711	-1.76006	-2.13395
H	-0.52912	-0.79365	-2.42546

HEt_3N^+

N	0.05142	0.06992	-0.31857
C	-1.24089	-0.55331	0.0015
H	-1.95334	-0.30729	-0.75796
H	-1.12253	-1.61569	0.04884
C	1.14248	-0.78864	0.1645
H	1.65561	-1.21727	-0.67089
H	1.82754	-0.20378	0.74203
C	0.13656	1.38432	0.3341

H	-0.11164	2.14959	-0.37136
H	-0.54888	1.42002	1.15495
C	1.56951	1.60855	0.85177
H	1.63149	2.56529	1.32685
H	1.81772	0.84328	1.55723
H	2.25495	1.57286	0.03092
C	0.56102	-1.91292	1.04171
H	1.3552	-2.53785	1.39333
H	0.0479	-1.48429	1.8771
H	-0.12403	-2.49778	0.46418
C	-1.73967	-0.03125	1.36175
H	-2.68032	-0.48489	1.59473
H	-1.02721	-0.27726	2.12121
H	-1.85802	1.03113	1.31441
H	0.13039	0.18377	-1.30893

$PhCOO^-$

C	-1.49358	1.62495	0.60027
C	-0.18724	1.58964	0.09415
C	0.36613	2.73315	-0.49752
C	-0.38685	3.91198	-0.58309
C	-1.69318	3.94729	-0.07697
C	-2.24655	2.80378	0.51471
H	-1.91609	0.75185	1.05203
H	1.36354	2.70619	-0.88395
H	0.03566	4.78507	-1.03485
H	-2.26809	4.84736	-0.1423
H	-3.24397	2.83075	0.90114
C	0.6402	0.29422	0.18818
O	0.07553	-0.87263	0.79193
O	1.81323	0.26251	-0.2663

SO_2F_2

S	-0.24769	2.59011	0.
O	0.30898	3.37735	1.36355
O	0.30895	1.01561	0.
F	-1.83769	2.59013	0.
F	0.28231	3.33964	-1.29823

$PhCOOSO_2F_2^-$

C	2.16179	-1.15796	-0.00145
C	1.79467	0.18193	-0.00024
C	2.77908	1.16294	0.00131
C	4.116	0.80917	0.0017
C	4.47799	-0.52858	0.00046
C	3.49983	-1.51027	-0.00114
H	1.38181	-1.90364	-0.00259
H	2.46744	2.19678	0.00215
H	4.88089	1.57427	0.00297
H	5.52389	-0.80645	0.00073
H	3.78539	-2.55371	-0.00213
C	0.33799	0.5976	-0.00072
O	0.04546	1.77569	-0.00279
O	-0.47577	-0.40474	0.00127
S	-2.28312	0.01148	0.00001

O	-2.26172	0.61219	-1.29091
O	-2.26243	0.61644	1.28898
F	-3.99905	-0.23027	0.00004
F	-2.32073	-1.63822	0.00293

F^-

F	-1.45564	3.32257	1.78112

$PhCOOSO_2F$

C	-1.48798	1.59713	0.56725
C	-0.18427	1.57344	0.05372
C	0.37164	2.73424	-0.50073
C	-0.37616	3.91874	-0.54166
C	-1.67987	3.94244	-0.02813
C	-2.23578	2.78163	0.52633
H	-1.91242	0.71083	0.99059
H	1.36705	2.71615	-0.89282
H	0.04828	4.80504	-0.96499
H	-2.25083	4.84683	-0.05938
H	-3.23118	2.79972	0.91842
C	0.63749	0.27179	0.0987
O	0.07024	-0.91271	0.66447
O	1.80816	0.25051	-0.36243
S	1.28386	-1.85008	1.3258
O	2.31778	-0.88031	2.20867
O	2.13547	-2.60257	0.10211
F	0.64416	-2.9494	2.27993

SO_3

S	0.04053	1.74221	-0.25759
O	0.77281	3.01637	-0.25759
O	0.87266	0.29429	-0.25759
O	-1.62947	1.74221	-0.25759

PhCOF

C	-1.48798	1.59713	0.56725
C	-0.18427	1.57344	0.05372
C	0.37164	2.73424	-0.50073
C	-0.37616	3.91874	-0.54166
C	-1.67987	3.94244	-0.02813
C	-2.23578	2.78163	0.52633
H	-1.91242	0.71083	0.99059
H	1.36705	2.71615	-0.89282
H	0.04828	4.80504	-0.96499
H	-2.25083	4.84683	-0.05938
H	-3.23118	2.79972	0.91842
C	0.63749	0.27179	0.0987
O	1.80816	0.25051	-0.36243
F	0.10197	-0.84644	0.63282

PdP_2

C	-3.50793	1.73308	0.85969
C	-2.31205	1.12305	0.45834
C	-1.27505	1.96321	0.0235

C	-1.38745	3.35531	-0.02999
C	-2.59007	3.92621	0.39752
C	-3.64117	3.12141	0.83852
C	-0.20866	4.13181	-0.62191
C	1.07428	3.44581	-0.14433
C	1.07011	2.04801	-0.07016
C	2.19661	1.29324	0.29833
C	3.37315	2.00102	0.58549
C	3.4042	3.39285	0.52658
C	2.2623	4.11056	0.16985
H	-4.33298	1.11679	1.19898
H	-2.71475	5.00315	0.37964
H	-4.57204	3.57843	1.16151
H	4.26512	1.45786	0.87451
H	4.32341	3.92156	0.7614
H	2.30391	5.19328	0.13152
C	-0.24577	5.61748	-0.24508
H	-0.19173	5.76355	0.83885
H	0.58634	6.15509	-0.70938
H	-1.16451	6.08464	-0.61174
C	-0.27937	4.00681	-2.168
H	0.57602	4.5134	-2.62923
H	-0.26849	2.95883	-2.48215
H	-1.20138	4.46552	-2.5428
O	-0.09272	1.36728	-0.37275
P	-2.01861	-0.69836	0.52469
P	2.06213	-0.53937	0.50955
C	3.74096	-0.97913	1.1296
C	4.86155	-1.10257	0.29434
C	3.88899	-1.19615	2.50626
C	6.10623	-1.4328	0.82999
H	4.75755	-0.94016	-0.77404
C	5.13632	-1.51769	3.04331
H	3.01709	-1.11621	3.15117
C	6.24605	-1.63863	2.20508
H	6.96772	-1.52888	0.17461
H	5.23902	-1.68342	4.1122
H	7.21614	-1.89801	2.62001
C	2.12379	-1.1801	-1.21652
C	2.25163	-2.56801	-1.39281
C	2.00014	-0.36273	-2.34512
C	2.277	-3.12081	-2.67047
H	2.33476	-3.21328	-0.52205
C	2.00301	-0.92103	-3.62551
H	1.90621	0.71138	-2.23041
C	2.14759	-2.29738	-3.79311
H	2.38786	-4.19518	-2.7911
H	1.89689	-0.27437	-4.49222
H	2.15445	-2.72873	-4.79026
C	-3.65359	-1.32257	1.10342
C	-4.73469	-1.58635	0.25068
C	-3.80344	-1.54054	2.48116
C	-5.9436	-2.05235	0.76929
H	-4.6309	-1.43003	-0.81823
C	-5.01612	-1.99337	3.00041
H	-2.95978	-1.35492	3.14195
C	-6.0883	-2.25248	2.14382

H	-6.77361	-2.25851	0.09879
H	-5.1203	-2.1548	4.06985
H	-7.03048	-2.61579	2.54482
C	-2.00776	-1.12801	-1.26728
C	-2.61669	-0.32408	-2.24104
C	-1.33973	-2.29394	-1.66659
C	-2.56338	-0.6847	-3.5884
H	-3.12716	0.58786	-1.94719
C	-1.29545	-2.65816	-3.01129
H	-0.83269	-2.89651	-0.91871
C	-1.90492	-1.85304	-3.97544
H	-3.03451	-0.05077	-4.33497
H	-0.76356	-3.55669	-3.30748
H	-1.85813	-2.12989	-5.02514
Pd	0.04871	-1.11819	1.39311

Ts4

C	1.54956	3.42953	-1.16185
C	0.72153	2.42579	-0.6393
C	-0.65883	2.58901	-0.80464
C	-1.23936	3.66988	-1.47578
C	-0.37706	4.6301	-2.01141
C	1.00422	4.51326	-1.84925
C	-2.76928	3.75041	-1.50116
C	-3.29544	2.32121	-1.65209
C	-2.60726	1.31129	-0.97597
C	-2.98915	-0.03352	-0.99029
C	-4.14414	-0.36999	-1.70915
C	-4.85699	0.61428	-2.39307
C	-4.43428	1.94579	-2.37045
H	2.62291	3.3587	-1.03757
H	-0.77998	5.48256	-2.54696
H	1.66146	5.27575	-2.25664
H	-4.47137	-1.403	-1.74686
H	-5.74724	0.34271	-2.95264
H	-5.00152	2.69251	-2.9151
C	-3.28385	4.67459	-2.61074
H	-2.96836	4.33346	-3.60233
H	-4.37661	4.72496	-2.59347
H	-2.92043	5.69591	-2.46342
C	-3.24271	4.29884	-0.12796
H	-4.33736	4.3327	-0.09032
H	-2.88976	3.66827	0.69378
H	-2.85555	5.3119	0.02872
O	-1.47176	1.62022	-0.25469
P	1.33966	0.94295	0.27286
P	-1.86945	-1.24089	-0.17961
C	-2.58028	-2.85329	-0.68576
C	-3.71836	-3.40719	-0.08058
C	-1.94993	-3.5475	-1.72782
C	-4.22127	-4.63125	-0.5199
H	-4.20474	-2.88112	0.73522
C	-2.45706	-4.77036	-2.16867
H	-1.05253	-3.13461	-2.17986
C	-3.59272	-5.31285	-1.5656
H	-5.10205	-5.05479	-0.04509
H	-1.95708	-5.30367	-2.97206

H	-3.98337	-6.26902	-1.90255
C	-2.30865	-1.14142	1.6002
C	-1.74103	-2.10192	2.45446
C	-3.11531	-0.13581	2.14227
C	-1.99687	-2.06554	3.82257
H	-1.09598	-2.87511	2.04516
C	-3.3535	-0.09086	3.51777
H	-3.5638	0.61111	1.49563
C	-2.80107	-1.05592	4.35916
H	-1.55704	-2.818	4.4713
H	-3.97658	0.69882	3.92857
H	-2.99121	-1.02067	5.42826
C	3.1539	1.20444	0.21534
C	3.91548	1.44066	1.36529
C	3.80081	1.11133	-1.02798
C	5.29998	1.60036	1.27066
H	3.42945	1.5023	2.33291
C	5.177	1.29572	-1.12225
H	3.22306	0.89298	-1.92098
C	5.93133	1.53966	0.02872
H	5.88153	1.78051	2.17065
H	5.66353	1.22361	-2.08985
H	7.00752	1.66999	-0.04332
C	0.87668	1.347	2.00407
C	0.63016	2.66172	2.4231
C	0.76432	0.29624	2.92579
C	0.26859	2.92065	3.745
H	0.71614	3.48174	1.71741
C	0.41206	0.56175	4.2488
H	0.95468	-0.72249	2.60496
C	0.15822	1.87113	4.65944
H	0.07268	3.9422	4.0596
H	0.31949	-0.25984	4.9519
H	-0.1276	2.07374	5.68803
Pd	0.57197	-1.15329	-0.24925
C	3.25848	-2.12198	-2.07035
C	3.4364	-2.14999	-0.68111
C	4.72534	-2.07343	-0.14356
C	5.83029	-1.98074	-0.9884
C	5.65375	-1.96021	-2.3722
C	4.36459	-2.02816	-2.91065
H	2.2564	-2.17497	-2.48151
H	4.84513	-2.08271	0.93394
H	6.82818	-1.9171	-0.5639
H	6.51497	-1.88857	-3.03104
H	4.22297	-2.01367	-3.9879
C	2.29433	-2.22142	0.27806
O	2.38433	-2.37644	1.48077
F	1.23555	-3.28168	-0.43791

Int1

C	-1.15097	-3.40618	-1.60722
C	-0.43892	-2.42681	-0.90144
C	0.95508	-2.47479	-0.96904
C	1.66918	-3.43091	-1.69564
C	0.92495	-4.37413	-2.40931
C	-0.47089	-4.36124	-2.3636

C	3.19727	-3.40034	-1.58248
C	3.61152	-1.92634	-1.55917
C	2.7804	-1.03819	-0.8718
C	3.00316	0.33695	-0.79333
C	4.17408	0.8332	-1.38508
C	5.04464	-0.02867	-2.05038
C	4.75861	-1.39301	-2.15199
H	-2.23329	-3.42067	-1.56853
H	1.43111	-5.13291	-2.99603
H	-1.0342	-5.10833	-2.9146
H	4.38621	1.89549	-1.34539
H	5.94541	0.36683	-2.51026
H	5.43583	-2.03907	-2.69985
C	3.87848	-4.17273	-2.71743
H	3.63312	-3.75311	-3.69866
H	4.96565	-4.15631	-2.59593
H	3.57613	-5.22414	-2.70454
C	3.59009	-4.04376	-0.22529
H	4.67616	-4.00056	-0.08644
H	3.11592	-3.52463	0.61306
H	3.276	-5.0932	-0.19932
O	1.63761	-1.51254	-0.25832
P	-1.20594	-1.15074	0.18542
P	1.68121	1.39042	-0.06484
C	2.15545	3.03879	-0.6994
C	3.06922	3.87147	-0.04281
C	1.60013	3.44954	-1.91862
C	3.42922	5.09755	-0.60506
H	3.49635	3.56399	0.90649
C	1.96586	4.6702	-2.48161
H	0.86673	2.81747	-2.41119
C	2.88108	5.49667	-1.82507
H	4.1365	5.74047	-0.08829
H	1.52497	4.98448	-3.42343
H	3.15932	6.45291	-2.25942
C	2.07353	1.44985	1.72455
C	1.30863	2.3215	2.52075
C	3.01663	0.60997	2.32576
C	1.50287	2.35252	3.89999
H	0.56354	2.95633	2.04793
C	3.19693	0.63783	3.71031
H	3.60909	-0.06653	1.71818
C	2.44417	1.50893	4.49834
H	0.91052	3.02986	4.50887
H	3.92798	-0.02112	4.17067
H	2.58833	1.5307	5.57518
C	-2.98474	-1.56681	0.04188
C	-3.72932	-2.05328	1.12162
C	-3.63061	-1.30629	-1.17744
C	-5.10056	-2.27634	0.9822
H	-3.24474	-2.24523	2.07252
C	-4.99543	-1.54439	-1.31824
H	-3.06646	-0.90025	-2.01148
C	-5.73458	-2.02591	-0.23515
H	-5.6722	-2.645	1.82923
H	-5.48397	-1.32798	-2.26342
H	-6.8024	-2.1968	-0.33846

C	-0.70022	-1.72977	1.84992
C	-0.49345	-3.09038	2.12141
C	-0.49329	-0.7832	2.86169
C	-0.0797	-3.49505	3.38958
H	-0.64939	-3.83039	1.34246
C	-0.07945	-1.19267	4.1293
H	-0.65027	0.26836	2.65336
C	0.13117	-2.54624	4.39366
H	0.08227	-4.55011	3.59258
H	0.09196	-0.44794	4.89959
H	0.46156	-2.86356	5.37898
Pd	-0.78587	1.10352	0.02478
C	-3.29224	2.03585	-1.78528
C	-3.68822	1.79401	-0.46493
C	-5.04709	1.84182	-0.12542
C	-6.00053	2.11569	-1.10155
C	-5.60155	2.35361	-2.42069
C	-4.24658	2.32008	-2.76017
H	-2.23537	1.999	-2.03409
H	-5.33439	1.64086	0.90116
H	-7.05473	2.13991	-0.83927
H	-6.34652	2.56721	-3.18258
H	-3.93599	2.51535	-3.78282
C	-2.69639	1.40892	0.58693
O	-2.99016	1.35546	1.76311
F	-0.72457	3.13698	0.14192

Int1

C	3.13887	-2.28189	-1.83454
C	2.53939	-1.49939	-0.84027
C	3.07317	-0.22872	-0.60117
C	4.17821	0.28959	-1.27637
C	4.7516	-0.51751	-2.2649
C	4.23522	-1.78612	-2.5419
C	4.67509	1.67149	-0.84269
C	3.43547	2.52285	-0.5432
C	2.33938	1.8911	0.0551
C	1.14507	2.53987	0.38134
C	1.09108	3.92316	0.14997
C	2.17062	4.5901	-0.42519
C	3.32673	3.89418	-0.78619
H	2.7374	-3.26158	-2.06748
H	5.60517	-0.15801	-2.82831
H	4.69098	-2.39324	-3.31789
H	0.18934	4.47079	0.39584
H	2.10762	5.65914	-0.60469
H	4.14706	4.42882	-1.25195
C	5.57697	2.31653	-1.90137
H	5.05173	2.45676	-2.85214
H	5.93885	3.29033	-1.55908
H	6.46153	1.69865	-2.08239
C	5.48089	1.50429	0.47335
H	5.82369	2.48082	0.83262
H	4.87008	1.04732	1.25786
H	6.3562	0.86709	0.30433
O	2.41047	0.54029	0.33076
P	0.98483	-1.90482	0.03075

P	-0.32741	1.56879	0.94571
C	-1.65222	2.79044	0.5995
C	-2.31069	3.53126	1.58618
C	-1.98959	2.98783	-0.74923
C	-3.30225	4.44739	1.2293
H	-2.05793	3.39444	2.63145
C	-2.97112	3.90915	-1.1017
H	-1.49172	2.41477	-1.52325
C	-3.63555	4.63682	-0.11173
H	-3.8152	5.01028	2.00412
H	-3.22979	4.0403	-2.1483
H	-4.41396	5.34365	-0.38478
C	-0.165	1.51736	2.76695
C	-1.26779	1.08548	3.52401
C	1.03177	1.84218	3.41644
C	-1.17583	1.01997	4.91302
H	-2.18737	0.80686	3.02022
C	1.12395	1.74887	4.8058
H	1.89155	2.17099	2.84244
C	0.01917	1.3487	5.55769
H	-2.03884	0.70131	5.49128
H	2.05918	1.99815	5.29937
H	0.08982	1.28799	6.64022
C	0.73823	-3.69879	-0.21758
C	1.79191	-4.5971	0.02137
C	-0.53315	-4.1908	-0.53185
C	1.57874	-5.96871	-0.0846
H	2.77229	-4.22376	0.30119
C	-0.7431	-5.56794	-0.62919
H	-1.35109	-3.50485	-0.70069
C	0.30977	-6.45571	-0.41351
H	2.39802	-6.65807	0.09872
H	-1.73264	-5.94118	-0.87601
H	0.14393	-7.52642	-0.49269
C	1.38406	-1.83396	1.81455
C	2.70031	-1.86058	2.29136
C	0.31565	-1.82351	2.72002
C	2.94348	-1.87437	3.66413
H	3.53358	-1.86675	1.59576
C	0.56435	-1.85221	4.09104
H	-0.70573	-1.78158	2.35194
C	1.87655	-1.8717	4.56479
H	3.96669	-1.88689	4.02933
H	-0.26772	-1.8323	4.78629
H	2.06729	-1.87788	5.63405
Pd	-0.69633	-0.4771	-0.52401
C	0.53224	0.77998	-3.04981
C	-0.63151	0.00848	-3.195
C	-1.68367	0.46568	-4.00177
C	-1.56576	1.69027	-4.65567
C	-0.40474	2.45696	-4.51413
C	0.64784	1.9968	-3.72
H	1.34058	0.4225	-2.42357
H	-2.59129	-0.12248	-4.07914
H	-2.38497	2.05144	-5.27047
H	-0.32321	3.41423	-5.02099
H	1.54992	2.5899	-3.60469

C	-0.84319	-1.23972	-2.38019
O	-1.20802	-2.30124	-2.80517
S	-3.90249	0.01221	-0.02491
O	-5.15028	0.70299	-0.36244
O	-3.41475	0.10517	1.36448
C	-4.29265	-1.79618	-0.22607
F	-4.48343	-2.10281	-1.51604
F	-5.39459	-2.12153	0.46053
F	-3.27592	-2.55645	0.23632
O	-2.8241	0.2073	-1.0671

Ts5

C	3.28633	1.97633	0.57827
C	2.14362	1.17387	0.70567
C	1.01676	1.7598	1.29569
C	0.97225	3.08096	1.74884
C	2.12825	3.85013	1.58989
C	3.27566	3.30087	1.01421
C	-0.31718	3.5639	2.42047
C	-1.49056	2.9111	1.68496
C	-1.32491	1.59872	1.24062
C	-2.3297	0.85775	0.60819
C	-3.57134	1.47892	0.42596
C	-3.77035	2.7924	0.85251
C	-2.73957	3.50323	1.47061
H	4.17846	1.57063	0.11571
H	2.14047	4.88357	1.91745
H	4.1676	3.91064	0.90368
H	-4.37292	0.94029	-0.0668
H	-4.73535	3.26728	0.70124
H	-2.91661	4.52412	1.79053
C	-0.42366	5.09321	2.43094
H	-0.41836	5.50558	1.41662
H	-1.34318	5.41216	2.93019
H	0.4059	5.53586	2.98991
C	-0.32189	3.04869	3.88454
H	-1.24391	3.35452	4.39163
H	-0.26029	1.9566	3.91979
H	0.53288	3.4585	4.43424
O	-0.10812	0.9656	1.39739
P	1.95485	-0.49259	-0.05872
P	-1.85103	-0.7727	-0.08035
C	-3.40534	-1.38347	-0.84297
C	-4.52778	-1.72329	-0.07243
C	-3.46453	-1.51623	-2.23637
C	-5.69698	-2.16402	-0.68997
H	-4.48179	-1.64829	1.01001
C	-4.63612	-1.95916	-2.85341
H	-2.58091	-1.29627	-2.82923
C	-5.75373	-2.27869	-2.08209
H	-6.56178	-2.42477	-0.08601
H	-4.6685	-2.06614	-3.93399
H	-6.66427	-2.6277	-2.56127
C	-1.66619	-1.85122	1.3826
C	-1.05724	-3.09714	1.16974
C	-2.12994	-1.50686	2.65812
C	-0.94389	-3.99793	2.22698

H	-0.66923	-3.33448	0.18185
C	-1.99926	-2.40948	3.71426
H	-2.5936	-0.53936	2.82564
C	-1.41287	-3.65744	3.49772
H	-0.46865	-4.95976	2.06205
H	-2.35833	-2.13869	4.70374
H	-1.31184	-4.36021	4.32035
C	3.58021	-0.73887	-0.88361
C	4.76545	-0.92722	-0.15324
C	3.63575	-0.74159	-2.28296
C	5.98143	-1.09284	-0.81296
H	4.73065	-0.94778	0.93179
C	4.85508	-0.9071	-2.94381
H	2.71786	-0.63974	-2.85306
C	6.02851	-1.07932	-2.21044
H	6.89239	-1.23703	-0.2385
H	4.88178	-0.91453	-4.02977
H	6.97685	-1.21384	-2.72327
C	2.08967	-1.67188	1.34019
C	1.86985	-1.31423	2.6752
C	2.39033	-3.00829	1.02827
C	1.96798	-2.27288	3.68468
H	1.62972	-0.28903	2.93339
C	2.50518	-3.95708	2.04093
H	2.53406	-3.30115	-0.00734
C	2.29575	-3.59202	3.37298
H	1.79156	-1.9837	4.717
H	2.74876	-4.98534	1.78788
H	2.37809	-4.33455	4.16188
Pd	-0.02103	-0.61394	-1.73569
C	0.91912	2.27759	-2.12727
C	-0.17134	1.43376	-2.39801
C	-1.47313	1.96311	-2.42493
C	-1.68222	3.30668	-2.12589
C	-0.59642	4.13327	-1.82503
C	0.70415	3.62149	-1.83432
H	1.92613	1.87593	-2.13549
H	-2.31162	1.31629	-2.6596
H	-2.69185	3.70484	-2.11328
H	-0.7644	5.18025	-1.58871
H	1.54804	4.26139	-1.59714
C	0.18782	0.04545	-3.46942
O	0.33758	0.06981	-4.63436
F	0.07249	-2.66849	-1.86035

Ts5A

C	1.62759	-3.5567	-1.81506
C	1.48675	-2.51481	-0.88904
C	2.60257	-1.70051	-0.6637
C	3.82235	-1.848	-1.32682
C	3.92081	-2.89339	-2.25058
C	2.83774	-3.74285	-2.48379
C	4.94945	-0.87369	-0.96524
C	4.30272	0.49558	-0.72826
C	3.067	0.51837	-0.08026
C	2.37133	1.68857	0.24283
C	2.96596	2.90689	-0.10511

C	4.20167	2.92329	-0.75436
C	4.86212	1.73262	-1.0668
H	0.78474	-4.20114	-2.03411
H	4.84484	-3.04939	-2.79595
H	2.93282	-4.54977	-3.20396
H	2.449	3.83649	0.10087
H	4.65159	3.87337	-1.02654
H	5.8178	1.77374	-1.57758
C	6.03277	-0.81852	-2.04823
H	5.6277	-0.49284	-3.01207
H	6.83287	-0.13128	-1.75801
H	6.4959	-1.80049	-2.18148
C	5.59143	-1.34212	0.36775
H	6.38468	-0.6496	0.67053
H	4.85057	-1.3846	1.17185
H	6.02596	-2.34071	0.24837
O	2.4423	-0.67099	0.24428
P	-0.12458	-2.01241	-0.15236
P	0.66645	1.46535	0.88653
C	0.04226	3.15747	1.19034
C	0.75226	4.05149	2.00884
C	-1.19174	3.54464	0.65536
C	0.25386	5.3298	2.24781
H	1.68721	3.74172	2.4663
C	-1.69092	4.82464	0.90305
H	-1.77505	2.83599	0.08465
C	-0.96673	5.72036	1.68846
H	0.81022	6.01724	2.87884
H	-2.6531	5.11205	0.48919
H	-1.35758	6.71562	1.88107
C	0.90522	0.84849	2.59281
C	-0.24511	0.53501	3.3317
C	2.16577	0.76054	3.19563
C	-0.12743	0.1559	4.66689
H	-1.21969	0.58929	2.85648
C	2.27543	0.37259	4.53143
H	3.06004	1.00469	2.63167
C	1.12969	0.07606	5.26985
H	-1.02109	-0.08816	5.23283
H	3.2565	0.30826	4.99438
H	1.21536	-0.22342	6.31075
C	-1.31354	-3.23652	-0.80438
C	-1.20263	-4.58652	-0.4296
C	-2.35158	-2.84171	-1.65274
C	-2.10033	-5.52716	-0.92725
H	-0.41822	-4.89668	0.2541
C	-3.25276	-3.78624	-2.14616
H	-2.4815	-1.79719	-1.89923
C	-3.12552	-5.12765	-1.79008
H	-2.00698	-6.56921	-0.63498
H	-4.06307	-3.46524	-2.79379
H	-3.8308	-5.86112	-2.17057
C	-0.06106	-2.45811	1.61727
C	1.13102	-2.75066	2.28877
C	-1.28764	-2.54357	2.29642
C	1.09587	-3.13903	3.62829
H	2.08224	-2.69116	1.7734

C	-1.31268	-2.94224	3.6304
H	-2.21363	-2.30545	1.78134
C	-0.12336	-3.24223	4.29821
H	2.02428	-3.36218	4.14609
H	-2.26514	-3.01199	4.14791
H	-0.1456	-3.54888	5.34025
Pd	-0.4492	0.20702	-0.8849
C	0.89111	2.28421	-2.69945
C	-0.3927	1.81909	-2.38677
C	-1.51191	2.63639	-2.58098
C	-1.3366	3.94206	-3.03978
C	-0.05414	4.42187	-3.31678
C	1.05825	3.59263	-3.15213
H	1.75244	1.63671	-2.5741
H	-2.50494	2.26571	-2.36238
H	-2.20177	4.58451	-3.17672
H	0.07755	5.44058	-3.6703
H	2.0556	3.96204	-3.37241
C	-0.67263	-0.05318	-2.73098
O	-0.73567	-0.49588	-3.8071
S	-3.77723	0.08619	0.82072
O	-4.6304	0.71858	1.83773
O	-3.88966	-1.37859	0.66599
C	-4.44905	0.73562	-0.78502
F	-4.34028	2.07894	-0.84148
F	-5.73542	0.41272	-0.94856
F	-3.76197	0.23604	-1.84434
O	-2.37279	0.59996	0.79131

Ts5B

C	2.59332	2.34007	-2.89222
C	2.5344	1.55071	-1.73982
C	2.89339	2.14089	-0.52307
C	3.25784	3.47618	-0.379
C	3.3036	4.23974	-1.55157
C	2.99016	3.67489	-2.79056
C	3.61663	3.96529	1.02943
C	2.72499	3.21175	2.02827
C	2.40687	1.88143	1.75139
C	1.62644	1.06783	2.57953
C	1.17103	1.62522	3.78264
C	1.4814	2.9469	4.10135
C	2.23862	3.73525	3.23094
H	2.30849	1.92484	-3.85171
H	3.58386	5.28614	-1.5041
H	3.03327	4.28896	-3.68472
H	0.55361	1.0339	4.44887
H	1.11828	3.37237	5.03162
H	2.44912	4.7647	3.49812
C	3.45949	5.48573	1.15587
H	2.42921	5.80217	0.96248
H	3.74364	5.82373	2.15638
H	4.11936	6.00147	0.45216
C	5.09274	3.57991	1.3127
H	5.37607	3.88316	2.32642
H	5.24438	2.4993	1.22504
H	5.75898	4.07799	0.59956

O	2.84982	1.30937	0.57433
P	1.90409	-0.15405	-1.6016
P	1.05203	-0.56832	1.95955
C	-0.19003	-1.08188	3.18848
C	0.17368	-1.74028	4.37541
C	-1.53525	-0.78033	2.94766
C	-0.80848	-2.09532	5.2968
H	1.21341	-1.97882	4.57289
C	-2.51658	-1.14559	3.86752
H	-1.84017	-0.26863	2.04476
C	-2.15231	-1.80428	5.04084
H	-0.52572	-2.6089	6.21153
H	-3.55426	-0.93902	3.63545
H	-2.9154	-2.10048	5.75496
C	2.41853	-1.75234	2.17627
C	2.10344	-3.12182	2.15251
C	3.74256	-1.34559	2.37584
C	3.10455	-4.06667	2.36133
H	1.08008	-3.44488	1.99098
C	4.74103	-2.29967	2.57057
H	3.99473	-0.29116	2.39285
C	4.4235	-3.65836	2.57317
H	2.8517	-5.12287	2.35531
H	5.767	-1.97841	2.72448
H	5.20289	-4.39791	2.73353
C	1.42656	-0.76232	-3.2502
C	2.33747	-0.71807	-4.31746
C	0.17552	-1.36728	-3.4275
C	1.97513	-1.2353	-5.55998
H	3.32678	-0.29365	-4.175
C	-0.17484	-1.89831	-4.66806
H	-0.51564	-1.43377	-2.59733
C	0.71942	-1.82333	-5.73667
H	2.67801	-1.19138	-6.38675
H	-1.14302	-2.37393	-4.78994
H	0.44511	-2.23346	-6.70415
C	3.364	-1.16379	-1.19228
C	4.65163	-0.60768	-1.15543
C	3.19149	-2.54435	-1.01032
C	5.75822	-1.43161	-0.95922
H	4.79618	0.45687	-1.29982
C	4.3045	-3.35764	-0.81435
H	2.19667	-2.97352	-1.01624
C	5.5869	-2.80639	-0.79123
H	6.75394	-0.99778	-0.9416
H	4.16514	-4.42373	-0.66818
H	6.45062	-3.44658	-0.63656
Pd	0.02254	-0.02597	-0.19299
C	-0.78998	1.73964	-2.75185
C	-0.91443	1.39283	-1.40001
C	-0.98235	2.39649	-0.40898
C	-0.72406	3.72816	-0.76079
C	-0.52398	4.06244	-2.0966
C	-0.57949	3.07128	-3.09002
H	-0.81231	0.98293	-3.52612
H	-1.28863	2.16511	0.60801
H	-0.75183	4.49543	0.00687

H	-0.35618	5.09776	-2.3776
H	-0.43705	3.34109	-4.1329
C	-3.02634	-0.01774	-1.72423
O	-3.28724	0.01267	-2.83957
S	-1.1508	-3.18523	-0.10658
O	0.12931	-3.35825	-0.81359
O	-1.60108	-1.70919	-0.18458
C	-2.40512	-3.97464	-1.23992
F	-2.01078	-5.21619	-1.5302
F	-2.47605	-3.26375	-2.38329
F	-3.6131	-4.01099	-0.68659
O	-1.29565	-3.80223	1.20964
Cu	-3.58431	-0.81109	-0.05678
O	-5.14076	0.6516	-0.05295
S	-4.65288	1.72694	0.8922
O	-3.26346	1.45782	1.34079
O	-5.61859	2.16417	1.90026
C	-4.47603	3.17953	-0.25848
F	-3.83244	2.81723	-1.38443
F	-3.76826	4.15573	0.33135
F	-5.67386	3.66281	-0.59907
F	-4.18024	-1.81951	1.32094

Int2

C	3.35303	1.92141	0.64048
C	2.16217	1.18877	0.72778
C	1.03074	1.85401	1.21693
C	1.01862	3.20326	1.57648
C	2.2225	3.90346	1.45365
C	3.38036	3.26686	1.00373
C	-0.28172	3.80068	2.1249
C	-1.45548	3.10404	1.43025
C	-1.31681	1.75853	1.09286
C	-2.33126	0.99239	0.50895
C	-3.56172	1.61563	0.275
C	-3.73658	2.96137	0.59763
C	-2.69316	3.69858	1.16063
H	4.24958	1.44815	0.25764
H	2.26475	4.95512	1.71315
H	4.30713	3.8274	0.92516
H	-4.36933	1.05666	-0.18413
H	-4.69097	3.44224	0.40455
H	-2.85232	4.74516	1.39471
C	-0.33197	5.32238	1.93205
H	-0.27537	5.59165	0.87234
H	-1.25543	5.7358	2.34753
H	0.49172	5.81024	2.46107
C	-0.36092	3.47553	3.63989
H	-1.2936	3.86467	4.0638
H	-0.33268	2.39493	3.81353
H	0.48262	3.92993	4.17176
O	-0.12216	1.1049	1.30551
P	1.93442	-0.48425	-0.00019
P	-1.86577	-0.6812	-0.07212
C	-3.41376	-1.30667	-0.83975
C	-4.54165	-1.63135	-0.07016
C	-3.46881	-1.45827	-2.23077

C	-5.70832	-2.07966	-0.68717
H	-4.50198	-1.53983	1.011
C	-4.638	-1.90642	-2.84786
H	-2.5849	-1.24301	-2.82339
C	-5.75941	-2.21442	-2.07747
H	-6.57617	-2.3298	-0.08317
H	-4.66632	-2.02503	-3.92735
H	-6.66824	-2.56872	-2.55587
C	-1.76227	-1.66492	1.46719
C	-1.22294	-2.95632	1.37218
C	-2.25125	-1.20037	2.69532
C	-1.20504	-3.78009	2.49617
H	-0.79599	-3.27918	0.4266
C	-2.21606	-2.02768	3.81858
H	-2.66289	-0.19905	2.77414
C	-1.7016	-3.32099	3.71784
H	-0.78204	-4.77696	2.42068
H	-2.59544	-1.66245	4.76934
H	-1.67773	-3.96612	4.59206
C	3.57154	-0.82807	-0.76171
C	4.70376	-1.108	0.0206
C	3.69722	-0.79826	-2.15587
C	5.93779	-1.3396	-0.58411
H	4.61479	-1.15002	1.10164
C	4.93417	-1.02856	-2.76081
H	2.81869	-0.61075	-2.76509
C	6.05554	-1.29771	-1.97634
H	6.80719	-1.55671	0.03024
H	5.0161	-1.00796	-3.84382
H	7.01738	-1.48305	-2.44624
C	1.94082	-1.64083	1.4175
C	1.72856	-1.22598	2.73698
C	2.17238	-2.99977	1.14832
C	1.76778	-2.1546	3.77775
H	1.53979	-0.18125	2.95708
C	2.22884	-3.91828	2.19334
H	2.29864	-3.33069	0.12367
C	2.02953	-3.49812	3.5106
H	1.59733	-1.82371	4.7983
H	2.41769	-4.96612	1.97678
H	2.06727	-4.21755	4.32393
Pd	0.07668	-0.74109	-1.64455
C	1.08661	2.06428	-2.10764
C	-0.05355	1.25405	-2.0455
C	-1.30047	1.84418	-2.28961
C	-1.41447	3.22197	-2.4916
C	-0.27726	4.0307	-2.48701
C	0.9754	3.4434	-2.30921
H	2.07379	1.63547	-1.98512
H	-2.1987	1.2374	-2.30555
H	-2.39771	3.65808	-2.64752
H	-0.36541	5.10353	-2.63629
H	1.87531	4.05297	-2.32094
C	0.14008	-0.94343	-3.56562
O	0.17762	-1.05254	-4.70911
F	0.20056	-2.77789	-1.33724

Int2A

C	1.66938	-3.5044	-1.82398
C	1.51163	-2.47354	-0.88748
C	2.62087	-1.65462	-0.64696
C	3.85357	-1.79772	-1.28755
C	3.9682	-2.83411	-2.21896
C	2.88841	-3.68002	-2.47904
C	4.97742	-0.83308	-0.8906
C	4.33324	0.53748	-0.65714
C	3.08027	0.56071	-0.04479
C	2.37646	1.73151	0.25542
C	2.98098	2.95054	-0.07155
C	4.23881	2.96591	-0.67595
C	4.9059	1.77482	-0.97132
H	0.83397	-4.15211	-2.05993
H	4.90156	-2.98609	-2.74938
H	2.9947	-4.47928	-3.20616
H	2.45388	3.87976	0.10623
H	4.69679	3.91573	-0.93431
H	5.87652	1.81573	-1.45302
C	6.0865	-0.77497	-1.94682
H	5.70698	-0.43688	-2.9167
H	6.88391	-0.09623	-1.63051
H	6.54602	-1.75889	-2.07825
C	5.58445	-1.31827	0.45288
H	6.37473	-0.63385	0.78067
H	4.82461	-1.36312	1.23906
H	6.01537	-2.31853	0.33463
O	2.44288	-0.62739	0.26002
P	-0.1065	-1.98955	-0.14507
P	0.64934	1.50346	0.82363
C	0.01505	3.16579	1.24237
C	0.7862	4.02897	2.03873
C	-1.2837	3.53836	0.87861
C	0.28324	5.27222	2.41389
H	1.77133	3.72436	2.37789
C	-1.7861	4.78134	1.26625
H	-1.90883	2.84577	0.3346
C	-1.00233	5.65376	2.02009
H	0.88902	5.93712	3.02304
H	-2.79718	5.05889	0.98312
H	-1.39614	6.62169	2.31735
C	0.8156	0.78077	2.49888
C	-0.35828	0.45803	3.19437
C	2.05723	0.6617	3.13604
C	-0.2824	0.02919	4.51746
H	-1.31882	0.54532	2.69793
C	2.12414	0.22901	4.4602
H	2.9704	0.91961	2.61098
C	0.95511	-0.08535	5.15316
H	-1.19474	-0.22509	5.0477
H	3.09077	0.14148	4.94883
H	1.00732	-0.42311	6.18439
C	-1.2778	-3.22086	-0.82447
C	-1.11559	-4.5821	-0.51179
C	-2.35666	-2.82671	-1.62118
C	-1.9946	-5.53065	-1.02663

H	-0.30348	-4.89488	0.1375
C	-3.23998	-3.77936	-2.1323
H	-2.54663	-1.77864	-1.80387
C	-3.05647	-5.12996	-1.84365
H	-1.85813	-6.58049	-0.78338
H	-4.0817	-3.45688	-2.73771
H	-3.74704	-5.86997	-2.23805
C	-0.05129	-2.49736	1.61018
C	1.14052	-2.78512	2.28363
C	-1.28325	-2.65323	2.26726
C	1.10016	-3.24464	3.60034
H	2.09608	-2.66772	1.7866
C	-1.31263	-3.12047	3.5787
H	-2.20968	-2.41487	1.75272
C	-0.12349	-3.42058	4.24658
H	2.02863	-3.46643	4.1187
H	-2.26889	-3.24506	4.07862
H	-0.14965	-3.78361	5.27026
Pd	-0.38544	0.28758	-0.97559
C	0.91846	2.52412	-2.5485
C	-0.29862	2.08968	-2.01582
C	-1.45823	2.83106	-2.26021
C	-1.38537	4.03449	-2.96712
C	-0.16057	4.49267	-3.45637
C	0.98956	3.72992	-3.25414
H	1.81989	1.93765	-2.40872
H	-2.41842	2.48701	-1.89706
H	-2.29149	4.61128	-3.13451
H	-0.10672	5.42987	-4.00356
H	1.94687	4.06489	-3.6459
C	-0.64918	-0.34074	-2.76816
O	-0.68549	-0.6474	-3.87024
S	-3.77099	0.066	0.75205
O	-4.61795	0.68059	1.78488
O	-3.83828	-1.404	0.61741
C	-4.49793	0.67554	-0.84447
F	-4.49658	2.02243	-0.88508
F	-5.75565	0.25241	-1.00582
F	-3.77674	0.24096	-1.90849
O	-2.38476	0.62336	0.6807

Ts6

C	3.59303	1.64356	-0.63948
C	2.44078	1.07237	-0.09052
C	1.48988	1.93599	0.47521
C	1.67727	3.31501	0.57449
C	2.83948	3.85122	0.01015
C	3.78209	3.02517	-0.60255
C	0.63927	4.10768	1.37139
C	-0.7353	3.51452	1.0521
C	-0.82326	2.12843	0.87309
C	-2.0341	1.47415	0.58604
C	-3.19726	2.2573	0.5403
C	-3.13861	3.63526	0.73085
C	-1.91401	4.25927	0.96827
H	4.33593	1.00666	-1.10629
H	3.01752	4.91988	0.05063

H	4.67523	3.45897	-1.04209
H	-4.14834	1.78594	0.32179
H	-4.04796	4.2266	0.68225
H	-1.88215	5.3355	1.09415
C	0.70622	5.60995	1.07263
H	0.50693	5.8228	0.01717
H	-0.01734	6.16029	1.68101
H	1.69342	6.00663	1.32657
C	0.9241	3.88267	2.8812
H	0.17615	4.40361	3.48957
H	0.89439	2.8192	3.13731
H	1.91641	4.26854	3.14046
O	0.32299	1.36714	0.95454
P	2.04702	-0.71239	-0.11081
P	-2.07552	-0.30581	0.11017
C	-3.72927	-0.50046	-0.65285
C	-4.87735	-0.81331	0.08683
C	-3.82568	-0.34347	-2.04407
C	-6.10628	-0.96278	-0.55754
H	-4.80852	-0.94692	1.16154
C	-5.05658	-0.48411	-2.68263
H	-2.93396	-0.11925	-2.62239
C	-6.19816	-0.7965	-1.94076
H	-6.99122	-1.21118	0.02174
H	-5.12104	-0.36301	-3.76024
H	-7.15531	-0.91717	-2.44028
C	-2.18517	-1.19099	1.7046
C	-2.44583	-2.57099	1.68712
C	-1.96819	-0.54391	2.9274
C	-2.5046	-3.28229	2.88323
H	-2.59086	-3.07913	0.74186
C	-2.01746	-1.26446	4.12093
H	-1.76303	0.52063	2.95196
C	-2.28943	-2.63246	4.10183
H	-2.7098	-4.34886	2.86216
H	-1.8427	-0.7541	5.06381
H	-2.32996	-3.19257	5.03212
C	3.53425	-1.56412	-0.75315
C	4.80329	-1.42216	-0.17065
C	3.36624	-2.44427	-1.83016
C	5.89077	-2.12863	-0.68032
H	4.93729	-0.76966	0.68653
C	4.45658	-3.15386	-2.33671
H	2.37527	-2.58546	-2.25281
C	5.71924	-2.99196	-1.76656
H	6.87078	-2.01281	-0.22585
H	4.31546	-3.83715	-3.16915
H	6.56824	-3.54489	-2.15869
C	2.04375	-1.11276	1.68476
C	2.78524	-0.35108	2.60091
C	1.2867	-2.20191	2.13754
C	2.77403	-0.67996	3.95597
H	3.35935	0.50561	2.26241
C	1.28671	-2.52694	3.49475
H	0.68219	-2.7573	1.42464
C	2.02583	-1.77066	4.40499
H	3.34766	-0.08267	4.65984

H	0.68674	-3.36334	3.83929
H	2.01434	-2.02339	5.462
Pd	-0.12069	-1.02912	-0.97331
C	-0.75424	1.63573	-2.40635
C	0.08691	0.52548	-2.2367
C	1.12521	0.35961	-3.17489
C	1.30718	1.25234	-4.23377
C	0.46271	2.35345	-4.37912
C	-0.56884	2.53723	-3.4597
H	-1.57315	1.82129	-1.72526
H	1.81339	-0.47535	-3.08379
H	2.12109	1.08849	-4.93636
H	0.60853	3.0569	-5.19449
H	-1.24329	3.38526	-3.55635
C	-2.32083	-3.23741	-2.00819
O	-1.78577	-3.29646	-3.01298
F	-0.246	-2.95458	-0.25186

Ts6A

C	-3.65357	2.25212	-0.65486
C	-2.69531	1.39466	-0.10127
C	-3.04808	0.04777	0.06997
C	-4.29733	-0.46682	-0.28056
C	-5.21796	0.41603	-0.85461
C	-4.90134	1.76237	-1.03797
C	-4.59524	-1.92673	0.06725
C	-3.30175	-2.72822	-0.10114
C	-2.09338	-2.10853	0.22965
C	-0.85582	-2.77098	0.18823
C	-0.85442	-4.11996	-0.1897
C	-2.0423	-4.76038	-0.53363
C	-3.25198	-4.06743	-0.49828
H	-3.41156	3.29807	-0.80649
H	-6.19581	0.05697	-1.1546
H	-5.63301	2.43383	-1.47715
H	0.08332	-4.65961	-0.24673
H	-2.02493	-5.80273	-0.83693
H	-4.16471	-4.58202	-0.776
C	-5.73949	-2.4968	-0.78037
H	-5.4977	-2.4784	-1.84811
H	-5.9612	-3.52788	-0.49098
H	-6.65858	-1.92587	-0.62117
C	-5.00135	-1.98255	1.56478
H	-5.18931	-3.01793	1.87023
H	-4.21183	-1.5749	2.20423
H	-5.91181	-1.39629	1.73245
O	-2.08579	-0.782	0.60935
P	-0.96684	1.89567	0.24865
P	0.70282	-1.82505	0.41659
C	2.04398	-3.00448	0.04421
C	2.32155	-4.09652	0.8818
C	2.83094	-2.78734	-1.09291
C	3.35868	-4.97164	0.56575
H	1.73387	-4.25342	1.7812
C	3.86682	-3.66678	-1.40763
H	2.64756	-1.91546	-1.7122
C	4.12898	-4.75957	-0.58138

H	3.57149	-5.81403	1.2177
H	4.47864	-3.48527	-2.28627
H	4.94152	-5.43947	-0.82134
C	0.84068	-1.55357	2.22302
C	2.10576	-1.27255	2.76227
C	-0.27414	-1.61125	3.07025
C	2.24785	-1.06229	4.1322
H	2.9725	-1.21749	2.11407
C	-0.12311	-1.39879	4.43954
H	-1.2571	-1.82707	2.67239
C	1.13622	-1.12551	4.97399
H	3.23193	-0.84575	4.538
H	-0.9943	-1.44151	5.0864
H	1.24933	-0.95642	6.04125
C	-0.91233	3.67438	-0.18313
C	-1.54008	4.6604	0.59316
C	-0.19747	4.0476	-1.32888
C	-1.46753	5.99931	0.21335
H	-2.07635	4.3782	1.49409
C	-0.12757	5.38944	-1.70689
H	0.31599	3.28756	-1.9096
C	-0.76392	6.36456	-0.93826
H	-1.95334	6.75949	0.81868
H	0.43419	5.67194	-2.5927
H	-0.7037	7.4099	-1.22782
C	-0.91553	1.9048	2.086
C	-2.08568	1.82432	2.85536
C	0.32285	2.05121	2.72921
C	-2.0183	1.89825	4.24718
H	-3.05047	1.71292	2.37201
C	0.38129	2.13003	4.11945
H	1.23443	2.08616	2.14475
C	-0.78574	2.05568	4.88142
H	-2.93163	1.8372	4.83306
H	1.34645	2.23516	4.60536
H	-0.73395	2.1123	5.96529
Pd	0.62457	0.2348	-0.68973
C	-0.3804	-1.74266	-2.69932
C	-0.56906	-0.47013	-2.13846
C	-1.4667	0.40083	-2.7753
C	-2.17811	0.00187	-3.90931
C	-2.00184	-1.27558	-4.43966
C	-1.0908	-2.14067	-3.83501
H	0.32465	-2.4433	-2.27131
H	-1.61476	1.40732	-2.4089
H	-2.8699	0.70079	-4.3724
H	-2.56038	-1.58953	-5.31704
H	-0.92516	-3.13549	-4.24056
C	1.39455	1.41111	-3.39503
O	1.63411	1.00749	-4.43153
S	3.75768	1.05029	0.4382
O	4.18706	-0.35507	0.53707
O	4.45991	2.04699	1.2526
C	4.16729	1.49322	-1.31992
F	3.72885	0.52891	-2.15912
F	5.48871	1.61013	-1.47931
F	3.58763	2.64923	-1.67837

O	2.25808	1.24626	0.48111

CO

C	0.	0.	-0.65
O	0.	0.	0.4875

Int3

C	1.73943	3.19987	-1.55866
C	0.93934	2.30286	-0.83837
C	-0.4083	2.62984	-0.68199
C	-0.99843	3.78726	-1.194
C	-0.17571	4.64635	-1.92791
C	1.17847	4.35379	-2.10742
C	-2.47048	4.03659	-0.84451
C	-3.17497	2.67706	-0.89564
C	-2.4575	1.56642	-0.4434
C	-2.93548	0.25738	-0.479
C	-4.25402	0.0696	-0.92066
C	-5.01743	1.15922	-1.33656
C	-4.4782	2.44891	-1.34348
H	2.79458	2.99502	-1.69337
H	-0.58498	5.55462	-2.35672
H	1.80516	5.03618	-2.67362
H	-4.6691	-0.93045	-0.9652
H	-6.03532	1.00122	-1.68031
H	-5.08113	3.27542	-1.70331
C	-3.12154	5.05959	-1.78192
H	-3.09901	4.72708	-2.82496
H	-4.1631	5.23593	-1.49729
H	-2.60949	6.02417	-1.71414
C	-2.53501	4.57162	0.61126
H	-3.57758	4.72278	0.91257
H	-2.07339	3.87126	1.31376
H	-2.00761	5.52921	0.68584
O	-1.17365	1.73506	0.03187
P	1.5516	0.76161	-0.03269
P	-1.76295	-1.11518	-0.10077
C	-2.63308	-2.51272	-0.90024
C	-3.6053	-3.27459	-0.24369
C	-2.3418	-2.77444	-2.24572
C	-4.28506	-4.28382	-0.9293
H	-3.83034	-3.08269	0.80055
C	-3.02602	-3.77625	-2.92964
H	-1.563	-2.20431	-2.74409
C	-3.99933	-4.53323	-2.27201
H	-5.03647	-4.87436	-0.41225
H	-2.78907	-3.97819	-3.97042
H	-4.52684	-5.32064	-2.80327
C	-1.96102	-1.40526	1.69676
C	-1.33529	-2.54032	2.24298
C	-2.62685	-0.50907	2.53924
C	-1.39493	-2.77297	3.61538
H	-0.8073	-3.22334	1.583
C	-2.67173	-0.74245	3.9153
H	-3.10979	0.37064	2.12612
C	-2.0607	-1.87431	4.45505

H	-0.91598	-3.65568	4.03022
H	-3.18772	-0.03912	4.56307
H	-2.101	-2.05664	5.52554
C	3.36126	0.9535	-0.26179
C	4.20233	1.38198	0.76981
C	3.91195	0.63965	-1.51385
C	5.57904	1.48292	0.55613
H	3.79055	1.62454	1.74315
C	5.28332	0.74489	-1.72505
H	3.26865	0.28208	-2.3108
C	6.12149	1.16272	-0.68736
H	6.22539	1.80677	1.36713
H	5.7	0.48208	-2.69281
H	7.1936	1.23108	-0.84874
C	1.27264	1.1146	1.74693
C	1.2361	2.4245	2.24638
C	1.08598	0.03885	2.6255
C	1.01222	2.65162	3.60382
H	1.37622	3.26573	1.57477
C	0.86591	0.26914	3.98343
H	1.0845	-0.97603	2.24152
C	0.82559	1.57461	4.4738
H	0.98052	3.67002	3.98108
H	0.70349	-0.57296	4.64792
H	0.6433	1.75431	5.52967
Pd	0.67409	-1.31552	-0.4636
C	2.55038	-2.02611	-0.66392
C	2.90067	-2.54862	-1.91447
C	3.47265	-2.10296	0.38448
C	4.16809	-3.10026	-2.12353
H	2.18426	-2.5259	-2.73192
C	4.73672	-2.6632	0.17883
H	3.22648	-1.70107	1.36362
C	5.0927	-3.15334	-1.07846
H	4.42938	-3.49392	-3.10348
H	5.44618	-2.70557	1.00215
H	6.07947	-3.5792	-1.24093
F	0.10883	-3.25237	-0.52962

Int3A

C	-3.68401	1.95311	-0.76086
C	-2.67177	1.19138	-0.16685
C	-2.94123	-0.16025	0.09989
C	-4.17568	-0.75634	-0.16351
C	-5.15543	0.03218	-0.77535
C	-4.91096	1.37204	-1.07665
C	-4.38924	-2.18959	0.32601
C	-3.07351	-2.94931	0.13917
C	-1.87589	-2.25497	0.34548
C	-0.61287	-2.86383	0.24121
C	-0.58132	-4.23641	-0.04611
C	-1.75826	-4.95217	-0.24734
C	-2.99275	-4.30961	-0.16858
H	-3.50252	2.99641	-0.99292
H	-6.12235	-0.39653	-1.01223
H	-5.68446	1.96849	-1.55081
H	0.37259	-4.73909	-0.14776

H	-1.71237	-6.01222	-0.47765
H	-3.89893	-4.87807	-0.34296
C	-5.55923	-2.8753	-0.39079
H	-5.38821	-2.94435	-1.47005
H	-5.71749	-3.88367	0.00185
H	-6.49006	-2.32658	-0.22072
C	-4.69864	-2.13017	1.84655
H	-4.82913	-3.14148	2.24762
H	-3.88612	-1.64672	2.39779
H	-5.61813	-1.56132	2.02444
O	-1.92254	-0.90977	0.65817
P	-0.99068	1.82818	0.17199
P	0.93677	-1.8635	0.25057
C	2.23086	-3.00898	-0.33163
C	2.73425	-4.04054	0.47588
C	2.73471	-2.83365	-1.62634
C	3.71713	-4.89662	-0.01768
H	2.36279	-4.1653	1.48833
C	3.71412	-3.69583	-2.11855
H	2.37534	-2.00972	-2.23402
C	4.20424	-4.72722	-1.31657
H	4.10678	-5.69133	0.61214
H	4.10588	-3.54932	-3.12078
H	4.97433	-5.39218	-1.69733
C	1.32137	-1.57554	2.01425
C	2.64927	-1.31764	2.38917
C	0.30522	-1.50639	2.97661
C	2.95206	-1.01208	3.71407
H	3.43793	-1.34501	1.64573
C	0.61576	-1.19986	4.30034
H	-0.72662	-1.67951	2.69696
C	1.93775	-0.95281	4.67212
H	3.98219	-0.81063	3.99309
H	-0.17978	-1.14272	5.0368
H	2.17645	-0.70806	5.70341
C	-1.02521	3.5948	-0.29991
C	-1.82089	4.53097	0.3792
C	-0.19226	4.02268	-1.34166
C	-1.79961	5.87134	-0.00025
H	-2.44538	4.21013	1.20774
C	-0.17123	5.36682	-1.71761
H	0.45318	3.30745	-1.84112
C	-0.9774	6.28957	-1.05114
H	-2.41711	6.59208	0.5283
H	0.48317	5.69105	-2.52142
H	-0.95799	7.33656	-1.34
C	-0.92311	1.88282	2.00694
C	-2.0518	1.62706	2.79875
C	0.2903	2.22151	2.62486
C	-1.96711	1.71079	4.1891
H	-2.99804	1.37012	2.33538
C	0.36659	2.30558	4.01358
H	1.17619	2.38542	2.02378
C	-0.75937	2.05242	4.79905
H	-2.84852	1.51251	4.79307
H	1.31489	2.55501	4.47999
H	-0.69449	2.11486	5.88188

Pd	0.60213	0.26784	-0.67123
C	-0.64655	-1.61143	-2.70236
C	-0.5605	-0.30239	-2.20591
C	-1.16739	0.72163	-2.95511
C	-1.83714	0.44517	-4.14933
C	-1.92608	-0.8635	-4.62232
C	-1.32324	-1.88782	-3.89445
H	-0.19132	-2.44019	-2.1793
H	-1.12812	1.75159	-2.62077
H	-2.29675	1.26183	-4.70047
H	-2.45636	-1.08094	-5.54533
H	-1.37062	-2.91481	-4.24815
S	3.67015	1.1731	0.02436
O	4.05169	-0.16092	-0.47029
O	4.62469	1.898	0.86884
C	3.53113	2.20537	-1.51884
F	2.66075	1.64777	-2.39481
F	4.71531	2.31505	-2.12738
F	3.07907	3.43496	-1.22862
O	2.25627	1.24071	0.56226

MeOPhB(OH)$_2$

C	-1.60697	-0.2077	0.27566
C	-0.21181	-0.2077	0.27566
C	0.48572	1.00005	0.27566
C	-0.21193	2.20856	0.27446
C	-1.60676	2.20848	0.27398
C	-2.30436	1.00027	0.27498
H	-2.15673	-1.16002	0.27611
H	1.5854	1.00013	0.2763
H	0.33827	3.1607	0.2744
H	-3.40396	1.00046	0.2748
O	-2.32207	3.44671	0.27274
C	-2.55899	3.85977	-1.07565
H	-3.09545	4.78557	-1.07604
H	-1.62349	3.98941	-1.57856
H	-3.13532	3.11338	-1.58127
B	0.61271	-1.63692	0.27763
O	0.9967	-2.3025	1.61223
H	1.46865	-3.12021	1.43842
O	0.99827	-2.30528	-1.05512
H	1.47027	-3.12247	-0.87905

Ts7

C	-3.44051	-2.30219	1.3975
C	-2.63014	-1.28649	0.88882
C	-2.44501	-0.12542	1.65959
C	-3.05846	0.06318	2.8965
C	-3.86528	-0.97941	3.37232
C	-4.05408	-2.14911	2.64175
C	-2.87097	1.35207	3.6951
C	-1.88983	2.28777	2.98403
C	-1.30013	1.9577	1.75975
C	-0.33018	2.76211	1.13462
C	-0.0137	3.98501	1.73838
C	-0.61915	4.36866	2.93405

C	-1.5329	3.5169	3.55144
H	-3.58876	-3.21081	0.82509
H	-4.35665	-0.86982	4.33415
H	-4.68218	-2.94118	3.03773
H	0.72671	4.62779	1.27419
H	-0.36911	5.3213	3.39149
H	-1.98003	3.81202	4.4958
C	-2.31239	1.0018	5.09427
H	-1.35868	0.47449	5.00197
H	-2.15542	1.90521	5.69219
H	-3.00765	0.35789	5.64245
C	-4.23926	2.05917	3.84085
H	-4.14302	2.98165	4.42309
H	-4.64981	2.31688	2.85896
H	-4.95921	1.41223	4.35343
O	-1.63432	0.81283	1.08491
P	-1.73455	-1.4022	-0.70004
P	0.54725	2.0989	-0.35671
C	2.21513	2.86427	-0.09054
C	2.93045	3.51383	-1.10589
C	2.86348	2.6436	1.13874
C	4.25209	3.91889	-0.90457
H	2.45631	3.7114	-2.06036
C	4.17914	3.05561	1.343
H	2.33401	2.15042	1.94795
C	4.88475	3.68933	0.31727
H	4.7842	4.42233	-1.7076
H	4.65348	2.87721	2.30453
H	5.91279	4.00488	0.47149
C	-0.15235	3.11041	-1.72957
C	0.3319	2.86873	-3.02835
C	-1.16995	4.05736	-1.55408
C	-0.1489	3.60618	-4.10982
H	1.0844	2.10078	-3.18103
C	-1.6724	4.76864	-2.6454
H	-1.57026	4.24465	-0.56347
C	-1.15354	4.55809	-3.92333
H	0.25038	3.42163	-5.1039
H	-2.46405	5.49745	-2.49167
H	-1.53586	5.12371	-4.76885
C	-2.34745	-2.96654	-1.43542
C	-1.47843	-4.06331	-1.51082
C	-3.65677	-3.09051	-1.92302
C	-1.91594	-5.27326	-2.05169
H	-0.45753	-3.95322	-1.15498
C	-4.0913	-4.29932	-2.46421
H	-4.33049	-2.23992	-1.88337
C	-3.22248	-5.39249	-2.52693
H	-1.23434	-6.11727	-2.10853
H	-5.10625	-4.3878	-2.84139
H	-3.56282	-6.33222	-2.95272
C	-2.50544	-0.11575	-1.75006
C	-3.67899	0.5577	-1.38581
C	-1.89021	0.17998	-2.97455
C	-4.22779	1.51686	-2.23654
H	-4.16167	0.33732	-0.43939
C	-2.45315	1.12672	-3.82811

H	-0.96337	-0.31343	-3.24939
C	-3.61661	1.80226	-3.45845
H	-5.13191	2.0428	-1.94213
H	-1.96502	1.35717	-4.76876
H	-4.03905	2.55579	-4.1164
Pd	0.59308	-1.38279	-0.65831
C	0.55108	-1.71038	1.30565
C	0.89019	-0.67234	2.18031
C	0.16492	-2.9445	1.84374
C	0.82679	-0.85436	3.56361
H	1.19769	0.28495	1.77948
C	0.10256	-3.12724	3.22928
H	-0.10962	-3.76634	1.18864
C	0.42832	-2.08313	4.09541
H	1.09151	-0.03139	4.22406
H	-0.20945	-4.08994	3.62764
H	0.37449	-2.22496	5.17149
F	1.18034	-1.24025	-2.90953
C	3.14952	-2.97324	-0.59417
C	2.74448	-1.61341	-0.66023
C	3.54199	-0.70725	0.0653
C	4.67235	-1.09017	0.78514
C	5.03655	-2.44282	0.81447
C	4.26636	-3.38819	0.11432
H	2.56624	-3.72921	-1.11973
H	3.27904	0.34511	0.05474
H	5.25319	-0.34122	1.31176
H	4.56577	-4.43157	0.15553
O	6.11357	-2.93691	1.4803
C	6.90687	-2.03084	2.23394
H	7.69456	-2.6323	2.69231
H	7.36333	-1.26547	1.59321
H	6.31954	-1.54169	3.02153
B	2.51808	-0.82587	-2.60362
O	3.53504	-1.4757	-3.29543
H	3.48011	-2.43362	-3.17651
O	2.58444	0.56174	-2.5066
H	3.49777	0.85333	-2.3782

$FB(OH)_2$

B	0.61271	-1.63692	0.27763
O	0.9967	-2.3025	1.61223
H	1.46865	-3.12021	1.43842
O	0.99827	-2.30528	-1.05512
H	1.47027	-3.12247	-0.87905
F	-0.11687	-0.37228	0.27589

Int4

C	-3.94437	1.05378	-1.9187
C	-2.95834	0.42181	-1.146
C	-3.00294	-0.97188	-1.07621
C	-3.93439	-1.75926	-1.76059
C	-4.88143	-1.09315	-2.54194
C	-4.89154	0.30136	-2.61185
C	-3.87994	-3.27454	-1.544
C	-2.4037	-3.66177	-1.4241

C	-1.55755	-2.77334	-0.7556
C	-0.20168	-3.01198	-0.52368
C	0.32217	-4.23351	-0.9692
C	-0.49165	-5.14255	-1.64439
C	-1.83949	-4.85792	-1.87607
H	-3.95838	2.1343	-1.9922
H	-5.62398	-1.65936	-3.0931
H	-5.64261	0.80529	-3.21295
H	1.36767	-4.46291	-0.80126
H	-0.07294	-6.08182	-1.99334
H	-2.45136	-5.57974	-2.40581
C	-4.58895	-4.04576	-2.66364
H	-4.13289	-3.85471	-3.64069
H	-4.55635	-5.12207	-2.47038
H	-5.64604	-3.76876	-2.71442
C	-4.5756	-3.59441	-0.19357
H	-4.52146	-4.66869	0.01578
H	-4.10085	-3.05843	0.6338
H	-5.62965	-3.29759	-0.2312
O	-2.05408	-1.57814	-0.28068
P	-1.64414	1.31263	-0.19192
P	0.78768	-1.68748	0.29248
C	2.46546	-2.43105	0.21963
C	3.07472	-3.06522	1.30786
C	3.16201	-2.33679	-0.99461
C	4.37007	-3.57477	1.19059
H	2.54639	-3.15674	2.25035
C	4.45201	-2.84604	-1.10996
H	2.70152	-1.83934	-1.84081
C	5.06303	-3.46045	-0.01381
H	4.83633	-4.05762	2.04508
H	4.98703	-2.74698	-2.04975
H	6.07604	-3.84346	-0.09917
C	0.32595	-1.85897	2.06613
C	0.99818	-1.05039	2.99826
C	-0.68177	-2.71776	2.51779
C	0.67413	-1.10797	4.35205
H	1.77788	-0.37729	2.6587
C	-1.01858	-2.76092	3.87256
H	-1.20455	-3.3597	1.81754
C	-0.34261	-1.95999	4.79253
H	1.20954	-0.48165	5.06029
H	-1.80894	-3.42706	4.20706
H	-0.60354	-1.99928	5.84636
C	-1.80993	2.99771	-0.90062
C	-2.02988	4.12569	-0.10462
C	-1.57821	3.1657	-2.27504
C	-2.02522	5.40006	-0.67473
H	-2.18449	4.0156	0.96251
C	-1.59466	4.43595	-2.84517
H	-1.38239	2.29809	-2.89975
C	-1.81543	5.55883	-2.0438
H	-2.17962	6.26914	-0.04175
H	-1.42065	4.55074	-3.91156
H	-1.81335	6.55197	-2.48414
C	-2.44478	1.4275	1.45752
C	-3.78994	1.79933	1.60438

C	-1.69394	1.11271	2.5944
C	-4.36605	1.8624	2.8713
H	-4.3854	2.03752	0.72838
C	-2.27249	1.17086	3.86311
H	-0.66145	0.80785	2.48059
C	-3.60773	1.54774	4.00321
H	-5.40773	2.15294	2.97667
H	-1.67898	0.91025	4.73389
H	-4.0611	1.5927	4.98966
Pd	0.72581	0.72475	-0.10615
C	1.0917	2.72109	0.1616
C	1.3633	3.60857	-0.88842
C	1.02621	3.24917	1.46015
C	1.52521	4.97598	-0.65968
H	1.44126	3.23342	-1.90478
C	1.1899	4.61868	1.69705
H	0.8349	2.59473	2.30673
C	1.43534	5.49017	0.63623
H	1.71813	5.64246	-1.4974
H	1.12528	5.00037	2.71419
H	1.55986	6.55517	0.81541
C	2.76208	0.73874	-0.31437
C	3.26719	0.8406	-1.61566
C	3.7012	0.59117	0.71783
C	4.63636	0.74229	-1.89903
H	2.58549	0.99	-2.45105
C	5.06581	0.48767	0.46182
H	3.37343	0.545	1.75285
C	5.54227	0.54888	-0.85289
H	4.97438	0.81609	-2.92716
H	5.78097	0.35273	1.26842
O	6.89866	0.41664	-1.00789
C	7.41309	0.45744	-2.3245
H	7.2143	1.42168	-2.81269
H	8.49345	0.32042	-2.234
H	7.00059	-0.34815	-2.94876

Ts8

C	-3.85618	0.96224	-2.12589
C	-2.92172	0.37079	-1.26456
C	-2.94989	-1.02297	-1.15482
C	-3.82483	-1.84559	-1.86866
C	-4.72099	-1.21952	-2.73992
C	-4.73983	0.17144	-2.86126
C	-3.77759	-3.34935	-1.58014
C	-2.31187	-3.72279	-1.33784
C	-1.5118	-2.79766	-0.66071
C	-0.16745	-3.01341	-0.3421
C	0.38262	-4.25432	-0.69503
C	-0.3876	-5.20312	-1.36597
C	-1.71919	-4.93715	-1.69413
H	-3.8843	2.04042	-2.22965
H	-5.41735	-1.81447	-3.32051
H	-5.45217	0.64346	-3.53166
H	1.41897	-4.46743	-0.46002
H	0.05333	-6.15709	-1.64007
H	-2.29508	-5.68672	-2.22566

C	-4.40388	-4.17413	-2.71076
H	-3.87857	-4.02597	-3.66007
H	-4.38529	-5.24045	-2.46706
H	-5.45447	-3.90277	-2.85023
C	-4.56729	-3.61129	-0.26958
H	-4.52058	-4.67355	-0.00432
H	-4.15722	-3.03087	0.56244
H	-5.61814	-3.32794	-0.39715
O	-2.04681	-1.58568	-0.27764
P	-1.65389	1.27183	-0.2675
P	0.80131	-1.62038	0.38672
C	2.49483	-2.33109	0.33543
C	3.09156	-3.01528	1.40218
C	3.2091	-2.17647	-0.86126
C	4.38576	-3.52394	1.2764
H	2.54813	-3.1506	2.33134
C	4.49513	-2.69567	-0.98965
H	2.7639	-1.62375	-1.68157
C	5.0898	-3.36495	0.08175
H	4.84187	-4.04698	2.1127
H	5.0424	-2.55664	-1.91718
H	6.09978	-3.75419	-0.01189
C	0.3674	-1.68535	2.17338
C	1.13897	-0.91777	3.06303
C	-0.7335	-2.39099	2.67052
C	0.82461	-0.87238	4.41893
H	1.99512	-0.36565	2.68818
C	-1.05919	-2.32924	4.02708
H	-1.34	-2.99345	2.00355
C	-0.28148	-1.57559	4.9052
H	1.43899	-0.28352	5.09485
H	-1.92215	-2.87664	4.39593
H	-0.53434	-1.53357	5.96092
C	-1.92133	3.00268	-0.81969
C	-2.29078	4.02543	0.06013
C	-1.64133	3.32567	-2.15806
C	-2.39382	5.3423	-0.39248
H	-2.49116	3.79763	1.10128
C	-1.77307	4.63476	-2.61503
H	-1.32277	2.54476	-2.84414
C	-2.1476	5.64927	-1.73012
H	-2.67128	6.128	0.30479
H	-1.56642	4.86625	-3.65647
H	-2.23641	6.67371	-2.08102
C	-2.42788	1.22918	1.40076
C	-3.81791	1.18688	1.58075
C	-1.59357	1.25218	2.52526
C	-4.36115	1.16679	2.86486
H	-4.47462	1.16747	0.71654
C	-2.13827	1.24147	3.80943
H	-0.51899	1.26881	2.38745
C	-3.52209	1.19564	3.98159
H	-5.43959	1.1298	2.99368
H	-1.47894	1.25057	4.6714
H	-3.94662	1.1783	4.98173
Pd	0.68454	0.71322	-0.204
C	1.46528	2.65714	0.03048

C	1.35949	3.65508	-0.95584
C	1.4763	3.07332	1.37831
C	1.2346	4.99914	-0.6127
H	1.37169	3.3753	-2.00484
C	1.3373	4.41821	1.72187
H	1.59615	2.33685	2.16863
C	1.2162	5.39248	0.72855
H	1.13675	5.7432	-1.39875
H	1.33215	4.70507	2.77132
H	1.1151	6.44125	0.99347
C	2.73162	1.19464	-0.40489
C	3.18022	1.16897	-1.73594
C	3.68757	0.92096	0.59517
C	4.49868	0.83979	-2.06894
H	2.49195	1.41512	-2.5406
C	4.9991	0.59733	0.28294
H	3.40092	0.97234	1.64156
C	5.41483	0.54231	-1.05566
H	4.79297	0.82217	-3.1126
H	5.72116	0.36794	1.06093
O	6.72182	0.19388	-1.26282
C	7.17956	0.12802	-2.60062
H	7.10443	1.10087	-3.10542
H	8.23009	-0.16708	-2.54803
H	6.62548	-0.61985	-3.18507

Product

C	-0.56134	0.39711	1.48409
C	-0.21155	-0.20755	0.2764
C	-0.5579	0.3964	-0.93212
C	-1.25542	1.60498	-0.9333
C	-1.60551	2.2092	0.27413
C	-1.25812	1.60543	1.48293
H	-0.28779	-0.07899	2.43679
H	-0.28167	-0.07982	-1.88407
H	-1.52845	2.08095	-1.8863
H	-1.53405	2.08205	2.43469
O	-2.32032	3.44772	0.27335
C	-2.55767	3.86102	-1.07489
H	-3.09376	4.78705	-1.07493
H	-1.62234	3.99035	-1.5782
H	-3.13453	3.11493	-1.58035
C	0.55869	-1.54109	0.27815
C	0.90636	-2.14421	1.48722
C	0.90865	-2.14603	-0.92896
C	1.60442	-3.35165	1.48908
H	0.63098	-1.66664	2.43871
C	1.60607	-3.35435	-0.92727
H	0.63456	-1.67091	-1.88199
C	1.9541	-3.95714	0.28147
H	1.87904	-3.82678	2.44204
H	1.8815	-3.83129	-1.87918
H	2.50445	-4.90919	0.28319