Supporting Information

'Awaken' aryl sulfonyl fluoride: a new partner in the Suzuki–Miyaura coupling reaction

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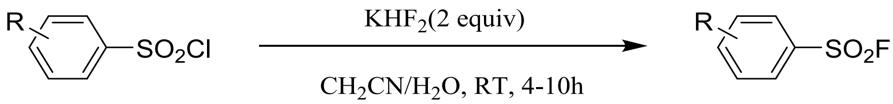
Table of Contents

Experimental Section

1: 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 or argon unless stated otherwise. 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 (300-400 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 500 MHz (^{1}HNMR) and 126 MHz (^{13}CNMR) instruments with TMS as the internal standard. High-resolution mass spectrometry analysis was performed on the ThermoFlisher ITQ1100.

2: Experimental Procedure for Compounds 1



Representative method for the synthesis of compound 1 (aryl sulfonyl fluoride).[1-3] 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 aryl sulfonyl chloride (17 mmol, 1 equivalent) 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. The yield for the formation of aryl sulfonyl fluoride ranges from 45 to 99%.

1. J. Dong, L. Krasnova, M. G. Finn and K. B. Sharpless, *Angew. Chem. Int. Ed.*, 2014, **53**, 9430-9448.

2. H. Mukherjee, J. Debreczeni, J. Breed, S. Tentarelli, B. Aquila, J. E. Dowling, A. Whitty and N. P. Grimster, *Org. Biomol. Chem.*, 2017, **15**, 9685-9695.

3. Y. Liu, D. Yu, Y. Guo, J. C. Xiao, Q. Y. Chen and C. Liu, *Org. Lett.*, 2020, **22**, 2281-2286.

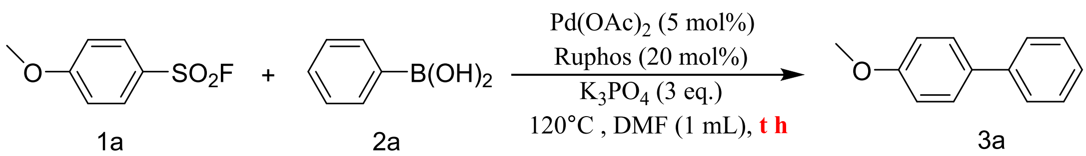
3: Optimization of reaction conditions

General Procedure for Reaction Optimization.

A Schlenk flask equipped with a stirring bar is filled with Aryl Sulfonyl fluoride (neat, 1.0 equiv.), base (typically, 3.0 equiv.), Organic Boron reagent (typically, 1.5 equiv.), palladium complex (typically, 5 mol%), ligand (typically, 20 mol%) under a positive pressure of nitrogen and five evacuations/backfilling cycles under high vacuum. The solvent (1 mL) was added under vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath and stirred for the indicated time. After the indicated time, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate (10 mL), filtered, and concentrated. It was purified by column chromatography on silica gel to obtain the pure product in yield and the samples were analyzed by ^{1}H NMR ($CDCl_3$, 500 MHz).

Optimization of the reaction conditions for Compounds 3.

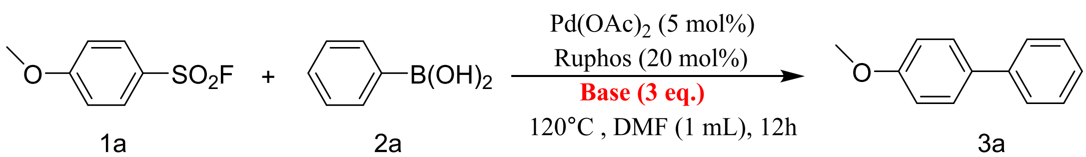
Table S1. Optimization of the reaction conditions: screening of time[a]



Entry	Time/h	Yield (%)[b]
1	4	47
2	8	55
3	12	64
4	16	63
5	24	59

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.01 mmol, 5 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1 mL), 120℃, t h; Under nitrogen atmosphere. [b] Isolated yield.

Table S2. Optimization of the reaction conditions: screening of base[a]

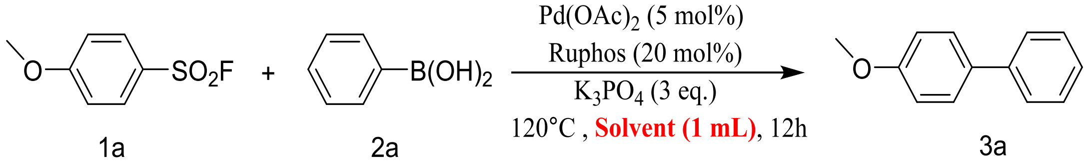


Entry	Base (3 eq.)	Yield (%)[b]
1	DMAP	none
2	Na_2CO_3	trace
3	$NaHCO_3$	trace

4	K_2CO_3	41
5	$KHCO_3$	51
6	KF	trace
7	Cs_2CO_3	45
8	t-BuOK	11
9	KH_2PO_4	trace
10	CH_3ONa	trace
11	DBU	none
12	DIPEA	trace
13	Et_3N	none
14	K_3PO_4	64
15[c]	-	none
16[d]	K_3PO_4	17
17[e]	K_3PO_4	48
18[f]	K_3PO_4	54

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.01 mmol, 5 mol%), Ruphos (0.04 mmol, 20 mol%), Base (0.6 mmol, 3.0 equiv.), DMF (1 mL), 120℃, 12.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] Base was omitted. [d] Base (0.2 mmol, 1.0 equiv.). [e] Base (0.4 mmol, 2.0 equiv.). [f] Base (0.8 mmol, 4.0 equiv.).

Table S3. Optimization of the reaction conditions: screening of solvent[a]

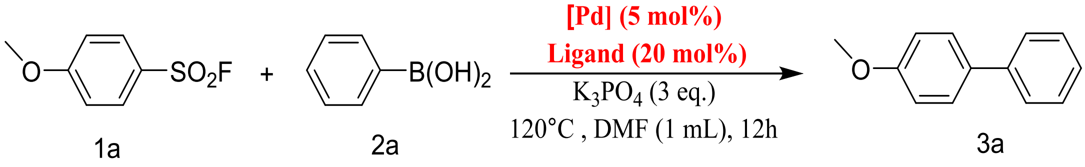


Entry	Solvent (1ml)	Yield (%)[b]
1	DMF	64
2	DMSO	54
3	DMAC	29
4	Toluene	62
5	Xylene	58
6	O-xylene	trace
7	Chlorobenzene	14
8	Ethylene glycol	trace
9	N-butanol	11
10	Glycerol	trace
11	Dioxane	38
12[c]	Water	none

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.01 mmol, 5 mol%), Ruphos (0.04 mmol, 20 mol%), Base (0.6

mmol, 3.0 equiv.), DMF (1 mL), 120℃, 12.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] The reaction was carried out at 80 ºC.

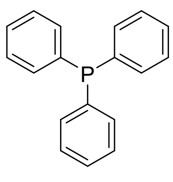
Table S4. Optimization of the reaction conditions: screening of palladium catalyst and ligand[a]



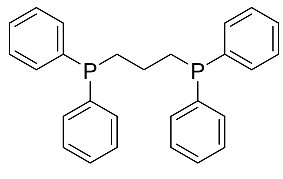
Entry	Cat. (mol%)	Ligand (mol%)	Yield (%)[b]
1	$Pd(acac)_2$	Ruphos	none
2	5 % Pd/C	Ruphos	none
3	$PdCl_2$	Ruphos	none
4	$Pd(PPh_3)Cl_2$	Ruphos	none
5	$Pd(TFA)_2$	Ruphos	57
6	$Pd(OAc)_2$	Ruphos	64
7	$Pd(OAc)_2$	PPh_3	none
8	$Pd(OAc)_2$	DPPP	none
9	$Pd(OAc)_2$	Xantphos	none
10	$Pd(OAc)_2$	TMTP	none
11	$Pd(OAc)_2$	(R)-BINAP	none
12	$Pd(OAc)_2$	SPhos	56
13	$Pd(OAc)_2$	BINAP	none
14	$Pd(OAc)_2$	DCPP	none
15	$Pd(OAc)_2$	DPEphos	none
16	$Pd(OAc)_2$	TDMPP	38
17	$Pd(OAc)_2$	NHC-Pd	none
18	$Pd(OAc)_2$	N-XantPhos	none
19	$Pd(OAc)_2$	$P(1\text{-}nap)_3$	14
20	$Pd(OAc)_2$	JohnPhos	none
21	Pd(OAc)2	BrettPhos	52
22	$Pd(OAc)_2$	Dppf	none
23	$Pd(OAc)_2$	Cphos	none
24	$Pd(OAc)_2$	PhDavephos	none
25[c]	-	Ruphos	none
26[d]	$Pd(OAc)_2$	-	none
27[e]	$Pd(OAc)_2$	Ruphos	41
28[f]	$Pd(OAc)_2$	Ruphos	74
29[g]	$Pd(OAc)_2$	Ruphos	74
30[h]	$Pd(OAc)_2$	Ruphos	39
31[i]	$Pd(OAc)_2$	Ruphos	15

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), [Pd] (0.01 mmol, 5 mol%), Ligand (0.04 mmol, 20 mol%), Base (0.6 mmol, 3.0 equiv.), DMF (1 mL), 120℃, 12.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] No Catalyst was used. [d] No Ligand was used. [e] $Pd(OAc)_2$ (0.004 mmol, 2 mol%). [f] $Pd(OAc)_2$ (0.02 mmol, 10 mol%). [g] $Pd(OAc)_2$ (0.04 mmol, 20 mol%). [h] Ruphos (0.02 mmol, 10 mol%). [i] Ruphos (0.08 mmol, 40 mol%).

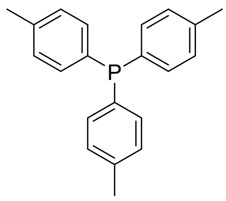
Phosphine ligands:



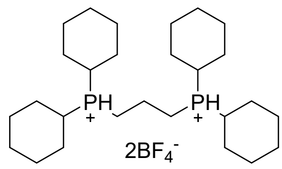
PPh_3



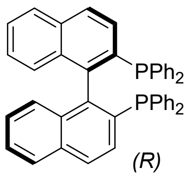
DPPP



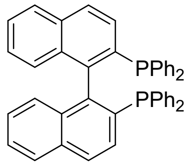
TMTP



DCPP



(R)-BINAP



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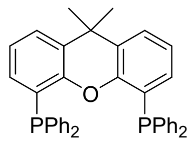
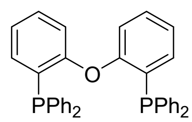
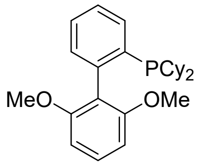


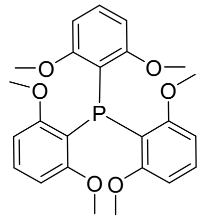
Xantphos



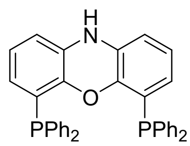
DPEphos



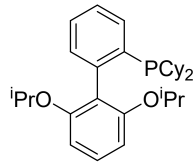
Sphos



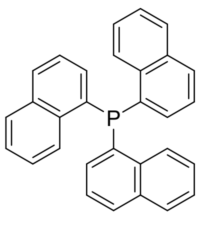
TDMPP



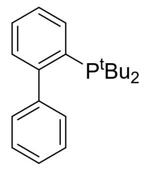
N-Xantphos



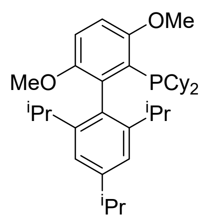
Ruphos



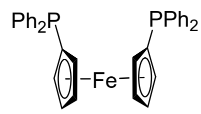
$P(1\text{-}nap)_3$



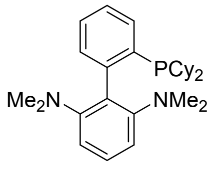
JohnPhos



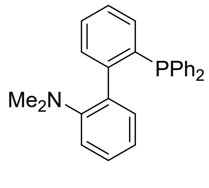
BrettPhos



Dppf

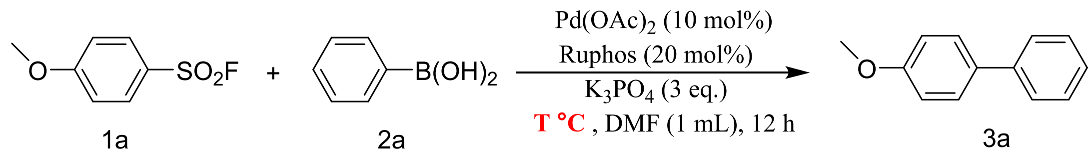


Cphos



PhDavephos

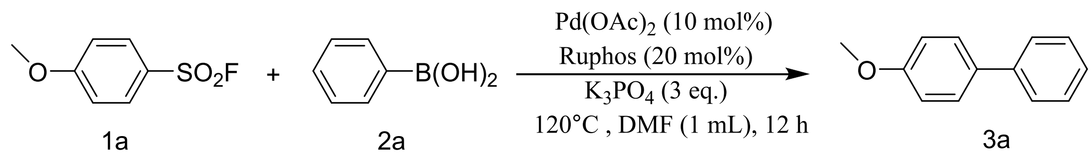
Table S5. Optimization of the reaction conditions: screening of temp[a]



Entry	Temp (°C)	Yield (%)[b]
1	100	45
2	120	74
3	140	37

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.02 mmol, 10 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1 mL), 12.0 h; Under nitrogen atmosphere. [b] Isolated yield.

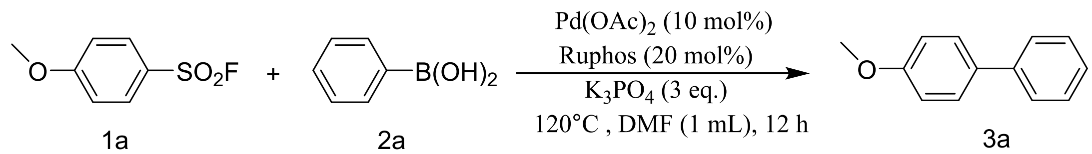
Table S6. Optimization of the reaction conditions: screening of the ratio of boronic acid[a]



Entry	2a (equiv)	Yield (%)[b]
1	1	47
2	1.5	74
3	2	50
4	4	50
5[c]	-	none

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids, $Pd(OAc)_2$ (0.02 mmol, 10 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1 mL), 120℃, 12.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] No Aryl boronic acids was used.

Table S7. Optimization of the reaction conditions: screening of atmosphere[a]

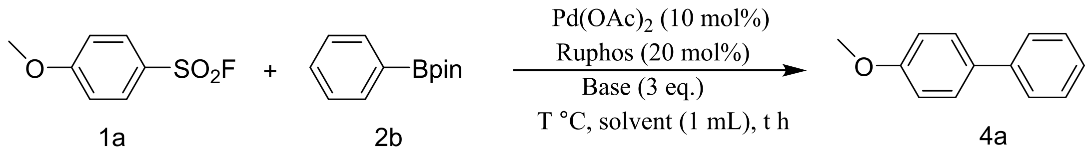


Entry	Atmosphere	Yield (%)
1	Air	12
2	N_2	74
3	O_2	none
4	SO_2F_2	none

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Aryl boronic acids (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.02 mmol, 10 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1ml), 120℃, 12.0 h. [b] Isolated yield.

Optimization of the reaction conditions for Compounds 4.

Table S8. Optimization of the reaction conditions.[a]

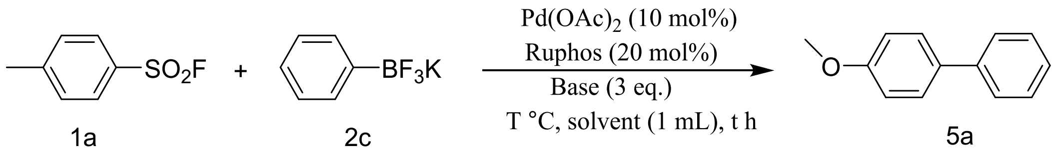


Entry	Base (3eq.)	Solvent	Temp (°C)	Time (h)	Yield (%)[b]
1	K_2CO_3	DMF	120	12	12
2	$KHCO_3$	DMF	120	12	trace
3	t-BuOK	DMF	120	12	none
4	Et_3N	DMF	120	12	11
5	Me_3SiOK	DMF	120	12	none
6	K_3PO_4	DMF	120	12	75
7	K_3PO_4	DMSO	120	12	58
8	K_3PO_4	Toluene	120	12	67
9	K_3PO_4	Dioxane	120	12	46
10	K_3PO_4	DMF	60	12	62
11	K_3PO_4	DMF	80	12	77
12	K_3PO_4	DMF	100	12	74
13	K_3PO_4	DMF	140	12	57
14	K_3PO_4	DMF	80	4	35
15	K_3PO_4	DMF	80	8	77
16	K_3PO_4	DMF	80	10	77
17	K_3PO_4	DMF	80	14	76
18[c]	K_3PO_4	DMF	80	8	61
19[d]	K_3PO_4	DMF	80	8	80

[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Arylboronic acid ester (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.02 mmol, 10 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1 mL), 80℃, 8.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] Arylboronic acid ester (0.2mmol, 1.0 equiv.). [d] Arylboronic acid ester (0.4mmol, 2.0 equiv.).

Optimization of the reaction conditions for Compounds 5.

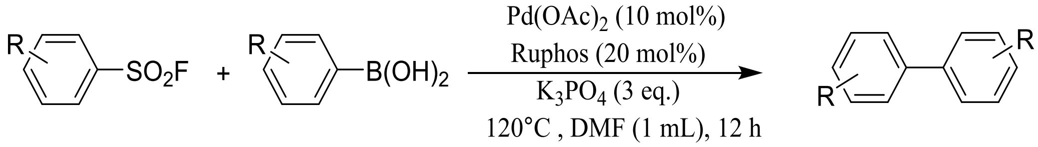
Table S9. Optimization of the reaction conditions.[a]



Entry	Base (3eq.)	Solvent	Temp (°C)	Time (h)	Yield (%)[b]
1	K_3PO_4	DMF	80	12	20
2	K_3PO_4	DMF	100	12	32
3	K_3PO_4	DMF	120	12	19
4	K_3PO_4	DMF	140	12	17
5	K_3PO_4	DMF	100	6	13
6	K_3PO_4	DMF	100	8	46
7	K_3PO_4	DMF	100	16	32
8	K_3PO_4	DMF	100	24	31
9	K_2CO_3	DMF	100	8	29
10	$KHCO_3$	DMF	100	8	16
11	t-BuOK	DMF	100	8	none
12	Et_3N	DMF	100	8	11
13	Me_3SiOK	DMF	100	8	none
14	K_3PO_4	DMSO	100	8	trace
15	K_3PO_4	Toluene	100	8	trace
16	K_3PO_4	Dioxane	100	8	27
17[c]	K_3PO_4	DMF	100	8	11
18[d]	K_3PO_4	DMF	100	8	35

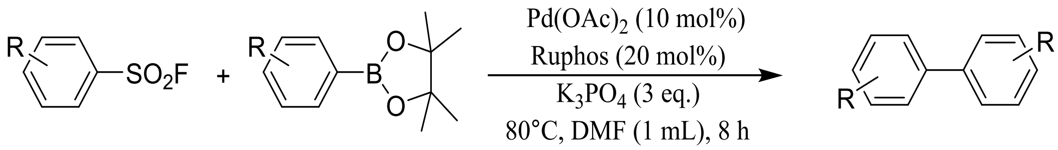
[a] Reaction conditions: 4-Methoxybenzenesulfonyl fluoride (0.2 mmol), Potassium phenyl trifluoroborate (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.02 mmol, 10 mol%), Ruphos (0.04 mmol, 20 mol%), K_3PO_4 (0.6 mmol, 3.0 equiv.), DMF (1 mL), 80℃, 8.0 h; Under nitrogen atmosphere. [b] Isolated yield. [c] Potassium phenyltrifluoroborate (0.2mmol, 1.0 equiv.). [d] Potassium phenyl trifluoroborate (0.4mmol, 2.0 equiv.)

4: Experimental Procedure for coupling products



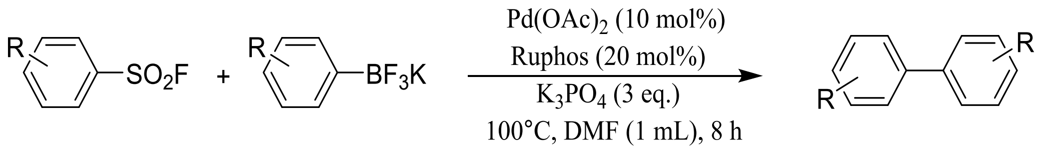
General procedure for Suzuki-Miyamura cross-coupling of aryl sulfonyl fluoride with aryl boronic acid.

Aryl sulfonyl fluoride (0.2 mmol, 1.0 equiv.), Aryl boronic acid (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (4.4 mg, 10 mol%), Ruphos (18.7mg, 20 mol%) and K_3PO_4 (0.6 mmol, 3.0 equiv.) were added to 10 mL Schlenk Flasks equipped with stirring bar. under a positive pressure of nitrogen and five evacuation/backfilling cycles under high vacuum. The DMF (1 mL) was added under vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath (120℃) and stirred for 12 hours. After 12 hours, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate (10 mL), filtered, and concentrated. Column chromatographic purification on silica gel (ethyl acetate/petroleum ether) to obtain pure product.



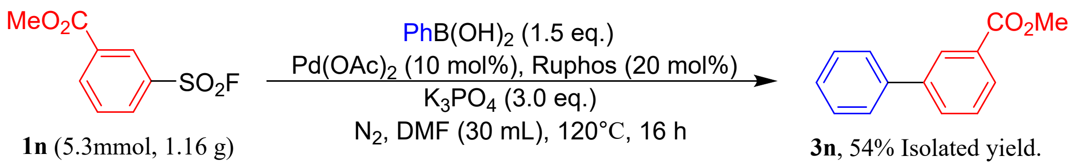
General procedure for Suzuki-Miyamura cross-coupling of aryl sulfonyl fluoride with aryl boronic acid ester.

Aryl sulfonyl fluoride (0.2 mmol, 1.0 equiv.), Aryl boronic acid ester (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (4.4 mg, 10 mol%), Ruphos (18.7mg, 20 mol%) and K_3PO_4 (0.6 mmol, 3.0 equiv.) were added to 10 mL Schlenk Flasks equipped with stirring bar. under a positive pressure of nitrogen and five evacuation/backfilling cycles under high vacuum. The DMF (1 mL) was added under vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath (80℃) and stirred for 8 hours. After 8 hours, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate (10 mL), filtered, and concentrated. Column chromatographic purification on silica gel (ethyl acetate/petroleum ether) to obtain pure product.



General procedure for Suzuki-Miyamura cross-coupling of aryl sulfonyl fluoride with potassium phenyl trifluoroborate.

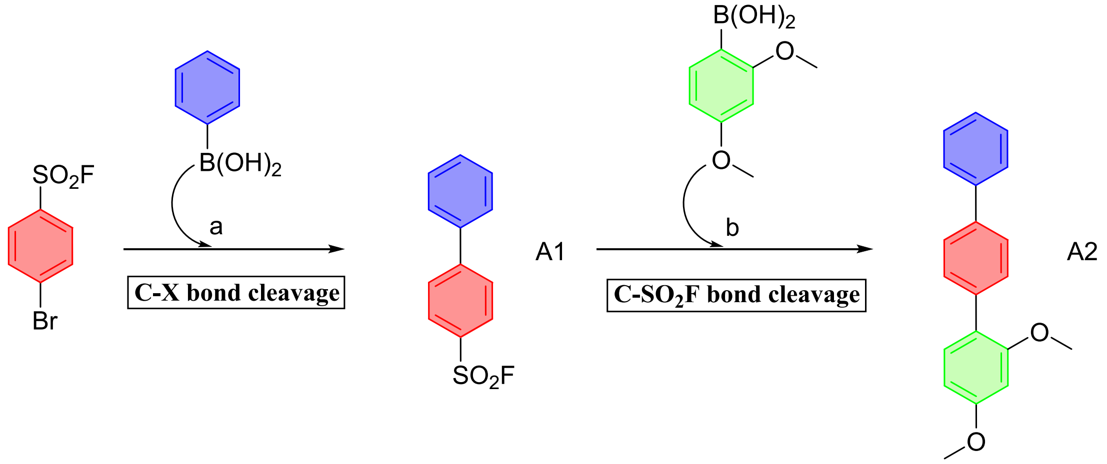
Aryl sulfonyl fluoride (0.2 mmol, 1.0 equiv.), Potassium phenyl trifluoroborate (0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (4.4 mg, 10 mol%), Ruphos (18.7mg, 20 mol%) and K_3PO_4 (0.6 mmol, 3.0 equiv.) were added to 10 mL Schlenk Flasks equipped with stirring bar. under a positive pressure of nitrogen and five evacuation/backfilling cycles under high vacuum. The DMF (1 mL) was added under vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath (100℃) and stirred for 8 hours. After 8 hours, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate (10 mL), filtered, and concentrated. Column chromatographic purification on silica gel (ethyl acetate/petroleum ether) to obtain pure product.



1n (5.3mmol, 1.16 g) **3n**, 54% Isolated yield.

General procedure for the gram-scale preparation.

methyl 3-(fluorosulfonyl)benzoate (5.3 mmol, 1.16g, 1.0 equiv.), Aryl boronic acid (8.0 mmol, 1.5 equiv.), $Pd(OAc)_2$ (130.0 mg, 10 mol%), Ruphos (494.6 mg, 20 mol%) and K_3PO_4 (15.9 mmol, 3.0 equiv.) were added to 100 mL Schlenk Flasks equipped with stirring bar. under a positive pressure of nitrogen and five evacuation/backfilling cycles under high vacuum. The DMF (30 mL) was added under vigorous stirring at room temperature, the reaction mixture was placed in a preheated oil bath (120℃) and stirred for 16 hours. After 16 hours, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate, filtered, and concentrated. Column chromatographic purification on silica gel (ethyl acetate/petroleum ether) to obtain pure product. Yield: 54% (607.4 mg).



Sequential synthesis of non-symmetric terphenyls.

4-Br-sulfonyl fluoride (49 mg, 0.2 mmol, 1.0 equiv.), aryl/alkenyl boronic acid (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (0.5 mg, 1 mol%), triethylamine (88 μL, 0.6 mmol, 3.0 equiv.), and water (2.5 mL) were added to a 10 mL Schlenk Flasks equipped with amagnetic stir bar. The resulting reaction mixture was stirred at room temperature in the open air. The reaction progress was monitored using TLC. Upon completion, the reaction mixture was diluted with ethylacetate (20 mL) and washed with water (3 × 15mL), followed by brine solution (3 × 15 mL). The organic layer was dried over anhydrous $MgSO_4$ and concentrated under vacuum. Column chromatographic purification on silica gel (EtOAc/hexanes = 1:50) to obtain pure product **A1**.

The **A1** (0.2 mmol, 1.0 equiv.), (3,4-dimethoxyphenyl)boronic acid (0.3 mmol, 1.5 equiv.), $Pd(OAc)_2$ (6.7 mg, 15 mol%), Ruphos (18.7mg, 20 mol%) and K_3PO_4 (0.6 mmol, 3.0 equiv.) were added in nitrogen. Under a positive pressure of nitrogen and five evacuation/backfilling cycles under high vacuum. The reaction mixture was placed in a preheated oil bath (120℃) and stirred for 12 hours. After 12 hours, the reaction mixture was cooled down to room temperature, diluted with ethyl acetate (10 mL), filtered, and concentrated. Column chromatographic purification on silica gel (EtOAc/hexanes = 1:20) to obtain pure product **A2**. Yield: 73% (42 mg).

5: Mechanistic Studies

Method

All calculations were carried out with the Gaussian 09 software[1]. The PBE0 functional[2] was adopted for all calculations in combination with the D3BJ dispersion correction[3]. For geometry optimization and frequency calculations, the LanL2DZ ECP and basis set[4] was used for Pd and 6-31G(d) for others[5,6]. The thermal correction to Gibbs free energy was calculated by the Shermo program[7], based on the vibrational analysis result, and the temperature was set as 393 K. The singlet point energy calculations were performed with a larger basis set combination, in which the def2-TZVP basis set[8] was used for Pd, and 6-311+G(d,p)[9,10] for others. The SMD implicit solvation model[11] was used to account for the solvation effect of DMF when performing single point energy calculations.

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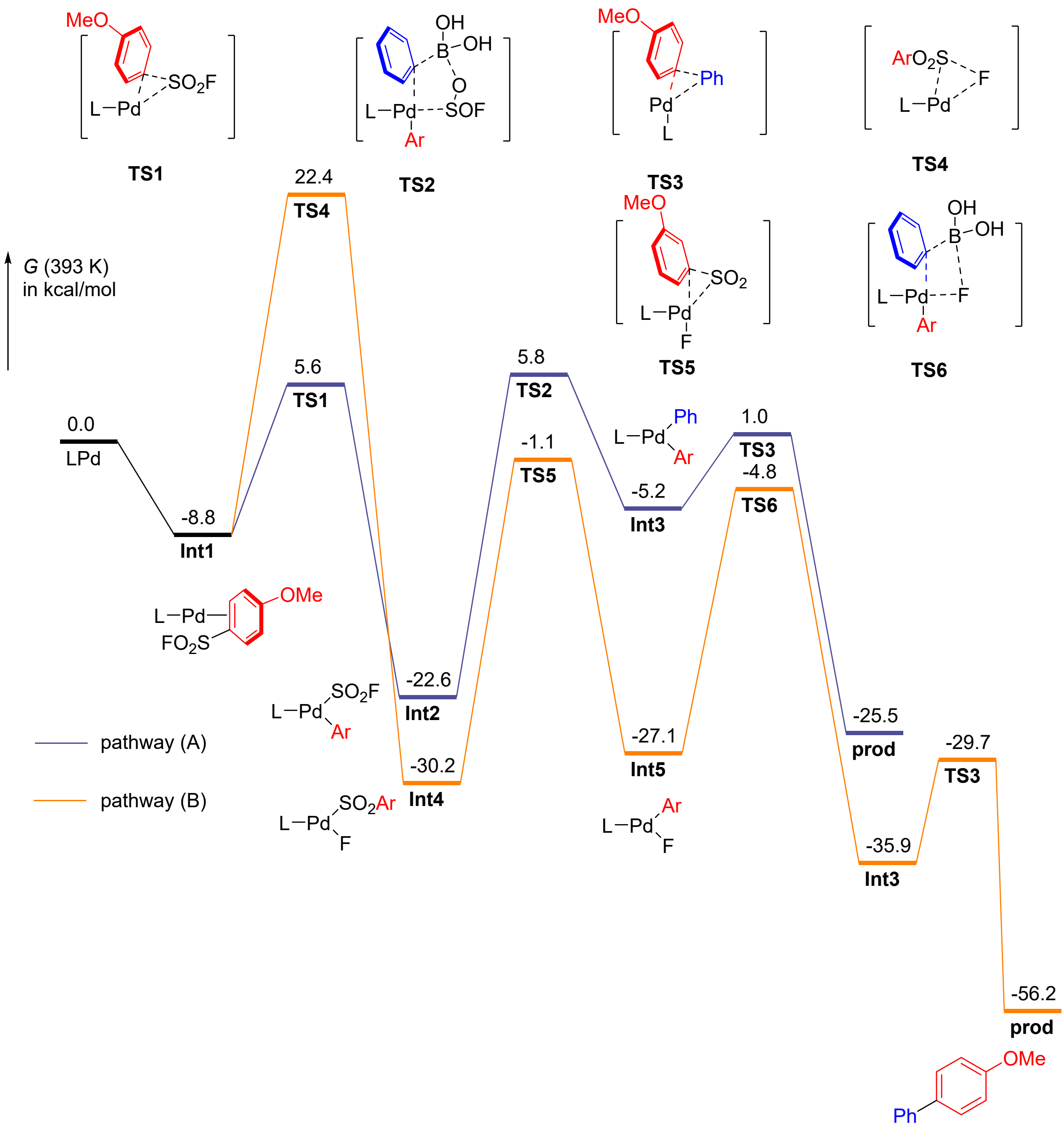
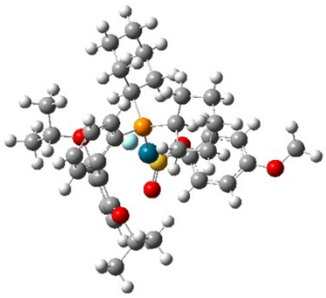
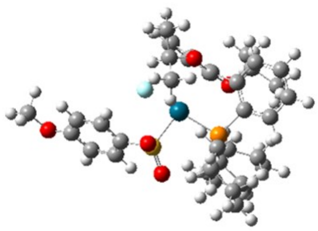
10. *J. Chem. Phys*., **72**, 650-654 (1980).
11. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *The Journal of Physical Chemistry B*, 2009, **113**, (18), 6378.

Possible pathways of (A) and (B) catalytic cycle.

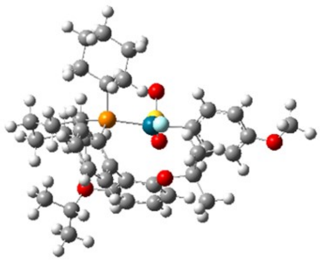




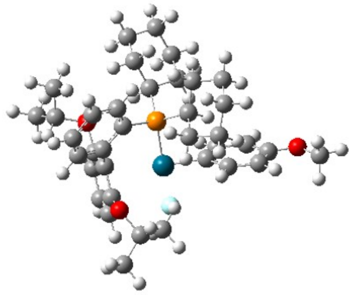
Int2



Int4

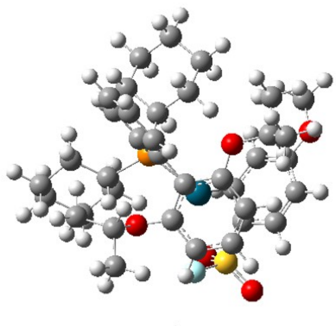


Ts5

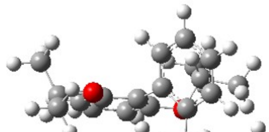


Int5

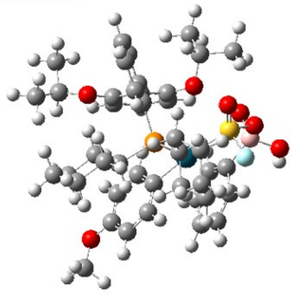
Oxidative addition：



Int1

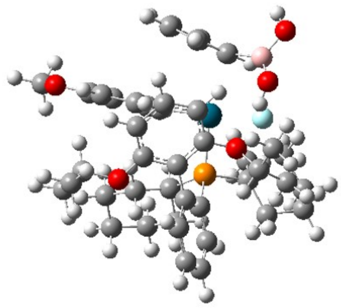


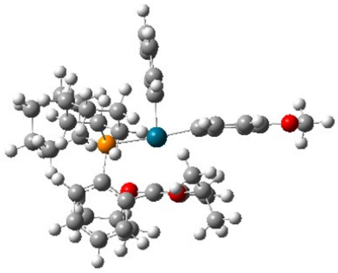
Transmetalation：



Ts2

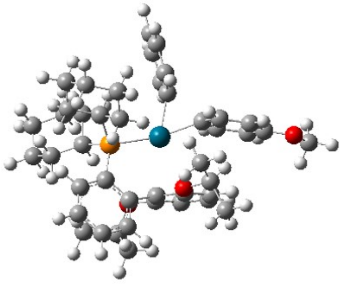
Ts6



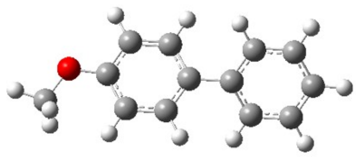


Int3

Reductive elimination：

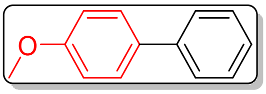


Ts3



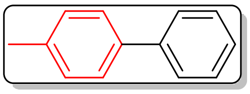
Prod.

6: Experimental Characterization Data



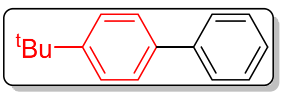
4-Methoxybiphenyl (**3a**)

White solid, 78% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 10.6, 8.1 Hz, 4H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.00 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.16 , 140.84 , 133.79 , 128.74 , 128.17 , 126.75 , 126.67 , 114.22 , 55.36 . **HRMS** (EI-TOF) calcd for $C_{13}H_{12}O$: 184.0888; Found： 184.0896. NMR spectroscopic data agreed with literature values.[1]



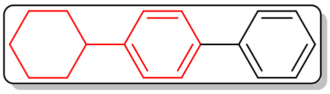
4-Methylbiphenyl (**3b**)

White solid, 78% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (d, J = 7.6 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.39 (t, J = 7.3 Hz, 1H), 7.32 (d, J = 8.0 Hz, 2H), 2.46 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.19 , 138.39 , 137.01 , 129.48 , 128.71 , 127.00 , 126.98 , 21.09 . **HRMS** (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found： 168.0940. NMR spectroscopic data agreed with literature values.[1]



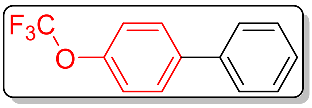
4-tert-Butylbiphenyl (**3c**)

White solid, 93% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 – 7.60 (m, 2H), 7.59 – 7.54 (m, 2H), 7.52 – 7.48 (m, 2H), 7.45 (t, J = 7.7 Hz, 2H), 7.37 – 7.32 (m, 1H), 1.39 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.29 , 141.11 , 138.35 , 128.71 , 127.04 , 126.99 , 126.81 , 125.73 , 34.55 , 31.40 . **HRMS** (EI-TOF) calcd for $C_{16}H_{18}$: 210.1409; Found：210.1419. NMR spectroscopic data agreed with literature values.[2]



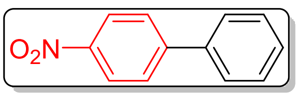
4-cyclohexyl-1,1'-biphenyl (**3d**)

White solid, 91% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.60 (d, J = 7.7 Hz, 2H), 7.54 (d, J = 8.2 Hz, 2H), 7.44 (dd, J = 15.3 Hz, 2H), 7.34 (dd, J = 7.4 Hz, 1H), 7.30 (d, J = 8.2 Hz, 2H), 2.60 – 2.53 (m, 1H), 1.97 – 1.85 (m, 4H), 1.82 – 1.76 (m, 1H), 1.51 – 1.38 (m, 5H). **^{13}C NMR** (126 MHz,) δ 147.23 , 141.20 , 138.73 , 128.66 , 127.00 , 126.91 , 44.25 , 34.47 , 26.92 , 26.18 . **HRMS** (EI-TOF) calcd for $C_{18}H_{20}$: 236.1565; Found：236.1563. NMR spectroscopic data agreed with literature values.[3]



4-(trifluoromethoxy)-1,1'-biphenyl (**3e**)

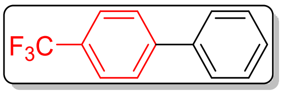
White solid, 82% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 4H), 7.47 (t, J = 7.6 Hz, 2H), 7.42 – 7.36 (m, 1H), 7.31 (d, J = 8.1 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.71 (q, 1.7 Hz), 140.02 , 139.89 , 128.91 , 128.48 , 127.68 , 127.13 , 121.23 , 120.58 (q, 257.0 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.51 . **HRMS** (EI-TOF) calcd for $C_{13}H_9F_3O$: 238.0605; Found：238.0601. NMR spectroscopic data agreed with literature values.[2]



4-nitro-1,1'-biphenyl (**3f**)

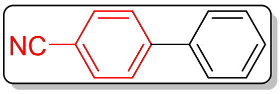
Yellow solid, 26% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 (d, J = 8.9 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H), 7.64 (d, J = 7.3 Hz, 2H), 7.55 – 7.44 (m, 3H). **^{13}C NMR** (126 MHz,

$CDCl_3$) δ 147.65 , 138.80 , 129.16 , 128.91 , 127.81 , 127.39 , 124.10 . **HRMS** (EI-TOF) calcd for $C_{12}H_9NO_2$: 199.0633; Found：199.0641. NMR spectroscopic data agreed with literature values.[4]



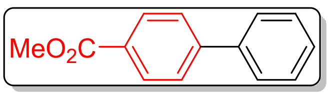
4-(trifluoromethyl)-1,1'-biphenyl (**3g**)

White solid, 92% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (s, 4H), 7.64 – 7.61 (m, 2H), 7.53 – 7.48 (m, 2H), 7.46 – 7.41 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.74 (q, J=1.0 Hz), 139.77 , 128.97 (q, J=32.5 Hz), 128.97 , 128.17 , 127.41 , 127.26 , 125.69 (q, J = 3.8 Hz), 124.32 (q, J = 271.9 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.41 . **HRMS** (EI-TOF) calcd for $C_{13}H_9F_3$: 222.0656; Found：222.0659. NMR spectroscopic data agreed with literature values.[1]



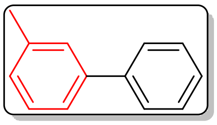
[1,1'-biphenyl]-4-carbonitrile (**3h**)

White solid, 70% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 – 7.73 (m, 2H), 7.72 – 7.69 (m, 2H), 7.63 – 7.58 (m, 2H), 7.52 – 7.48 (m, 2H), 7.47 – 7.42 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.73 , 139.23 , 132.62 , 129.13 , 128.68 , 127.76 , 127.25 , 118.93 , 110.98 . **HRMS** (EI-TOF) calcd for $C_{13}H_9N$: 179.0735; Found：179.0739. NMR spectroscopic data agreed with literature values.[1]



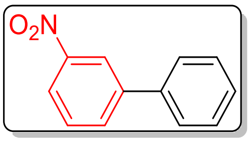
methyl [1,1'-biphenyl]-4-carboxylate (**3i**)

White solid, 72% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 2H), 7.68 (d, J = 8.5 Hz, 2H), 7.64 (d, J = 7.2 Hz, 2H), 7.49 (t, J = 7.5 Hz, 2H), 7.41 (t, J = 7.4 Hz, 1H), 3.96 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.02 , 145.67 , 140.04 , 130.11 , 128.93 , 128.14 , 127.29 , 127.06 , 52.11 . **HRMS** (EI-TOF) calcd for $C_{14}H_{12}O_2$: 212.0837; Found：212.0842. NMR spectroscopic data agreed with literature values.[1]



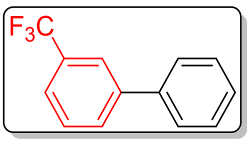
3-methyl-1,1'-biphenyl (**3j**)

White solid, 75% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.60 (dd, J = 8.3, 1.0 Hz, 2H), 7.50 – 7.31 (m, 6H), 7.18 (d, J = 7.5 Hz, 1H), 2.44 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.49 , 141.42 , 128.71 , 128.68 , 128.02 , 127.21 , 127.18 , 124.30 , 21.56 . **HRMS** (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found：168.0940. NMR spectroscopic data agreed with literature values.[5]



3-nitro-1,1'-biphenyl (**3k**)

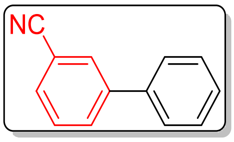
Yellow solid, 35% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.22 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H), 7.67 – 7.60 (m, 3H), 7.52 (t, J = 7.5 Hz, 2H), 7.45 (t, J = 7.4 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.95 , 138.74 , 129.72 , 129.20 , 128.57 , 127.20 , 122.06 , 122.01 . **HRMS** (EI-TOF) calcd for $C_{12}H_9NO_2$: 199.0633; Found：199.0641. NMR spectroscopic data agreed with literature values.[6]



3-(trifluoromethyl)-1,1'-biphenyl (**3l**)

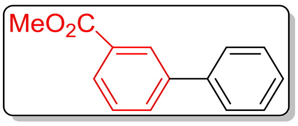
Yellow solid, 84% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.66 – 7.54 (m, 4H), 7.50 (t, J = 7.6 Hz, 2H), 7.42 (t, J = 7.3 Hz, 1H). **^{13}C**

NMR (126 MHz, $CDCl_3$) δ 142.05 , 139.80 , 131.21 (q, J = 32.2 Hz), 130.42 , 129.22 , 129.00 , 128.03 , 127.20 , 125.30 (q, J=272.2 Hz), 123.96 (q, J = 3.6 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.60 . **HRMS** (EI-TOF) calcd for $C_{13}H_9F_3$: 222.0656; Found：222.0659. NMR spectroscopic data agreed with literature values.[7]



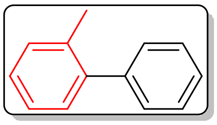
[1,1'-biphenyl]-3-carbonitrile (**3m**)

White solid, 65% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (dd, 1H, J=1.5 Hz, 2.0 Hz), 7.81 (m, 1H), 7.67 – 7.41 (m, 7H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.52 , 138.93 , 131.52 , 130.74 , 129.62 , 129.15 , 128.42 , 127.12 , 118.86 , 113.03 . **HRMS** (EI-TOF) calcd for $C_{13}H_9N$: 179.0735; Found：179.0739. NMR spectroscopic data agreed with literature values.[1]



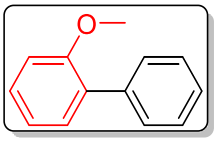
methyl [1,1'-biphenyl]-3-carboxylate (**3n**)

White solid, 77% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.04 (d, J = 7.8 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.67 – 7.62 (m, 2H), 7.56 – 7.45 (m, 3H), 7.43 – 7.38 (m, 1H), 3.97 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.06 , 141.50 , 140.14 , 131.53 , 130.73 , 128.89 , 128.85 , 128.35 , 128.28 , 127.75 , 127.17 , 52.18 . **HRMS** (EI-TOF) calcd for $C_{14}H_{12}O_2$: 212.0837; Found：212.0842. NMR spectroscopic data agreed with literature values.[8]



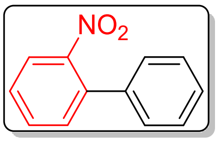
2-methyl-1,1'-biphenyl (**3o**)

White solid, 75% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.46 – 7.24 (m, 9H), 2.29 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 142.02 , 141.99 , 135.37 , 130.31 , 129.81 , 129.21 , 128.08 , 127.26 , 126.77 , 125.76 , 20.46 . **HRMS** (EI-TOF) calcd for $C_{13}H_{12}$: 168.0939; Found： 168.0940. NMR spectroscopic data agreed with literature values.[1]



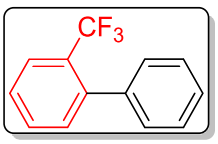
2-methoxy-1,1'-biphenyl (**3p**)

White solid, 91% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.60 – 7.53 (m, 2H), 7.47 – 7.41 (m, 2H), 7.40 – 7.32 (m, 3H), 7.09 – 7.01 (m, 2H), 3.84 (s, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 156.50 , 138.57 , 130.89 , 130.78 , 129.54 , 128.60 , 127.96 , 126.89 , 120.84 , 111.29 , 55.56 . **HRMS** (EI-TOF) calcd for $C_{14}H_{12}O_2$: 212.0837; Found： 212.0845. NMR spectroscopic data agreed with literature values.[1]



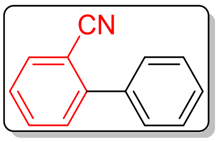
2-nitro-1,1'-biphenyl (**3q**)

Yellow oil, 52% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 8.1 Hz, 1H), 7.53 – 7.41 (m, 5H), 7.37 – 7.30 (m, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 149.34 , 137.39 , 136.36 , 132.24 , 131.95 , 128.67 , 128.22 , 128.14 , 127.89 , 124.05 . **HRMS** (EI-TOF) calcd for $C_{12}H_9NO_2$: 199.0633; Found： 199.0641. NMR spectroscopic data agreed with literature values.[9]



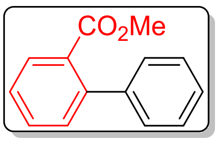
2-(trifluoromethyl)-1,1'-biphenyl (**3r**)

Yellow solid, 64% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.78 (d, J = 7.9 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.46 – 7.40 (m, 3H), 7.39 – 7.33 (m, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 141.44 (q, J = 2.6 Hz), 139.86 , 132.04 , 131.28 , 128.96 , 128.47 (q, J = 29.7 Hz), 127.74 , 127.61 , 127.32 , 126.05 (q, J = 5.3 Hz), 124.17 (q, J = 274.0 Hz). **^{19}F NMR** (565 MHz, $CDCl_3$) δ -56.85. **HRMS** (EI-TOF) calcd for $C_{13}H_9F_3$: 222.0656; Found：222.0661. NMR spectroscopic data agreed with literature values.[10]



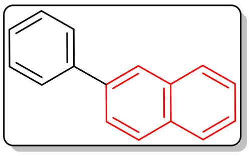
[1,1'-biphenyl]-2-carbonitrile (**3s**)

Yellow solid, 77% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (d, J = 7.8 Hz, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.55 – 7.44 (m, 5H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.53 , 138.16 , 133.75 , 132.79 , 130.08 , 128.76 , 128.73 , 128.72 , 127.53 , 118.69 , 111.34 . **HRMS** (EI-TOF) calcd for $C_{13}H_9N$: 179.0735; Found：179.0739. NMR spectroscopic data agreed with literature values.[11]



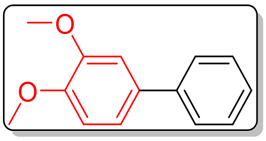
methyl [1,1'-biphenyl]-2-carboxylate (**3t**)

White solid, 79% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (dd, J = 7.7, 1.0 Hz, 1H), 7.55 (td, J = 7.6, 1.3 Hz, 1H), 7.47 – 7.31 (m, 7H), 3.65 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 169.15 , 142.50 , 141.34 , 131.24 , 130.90 , 130.71 , 129.77 , 128.32 , 128.03 , 127.22 , 127.15 , 51.91 . **HRMS** (EI-TOF) calcd for $C_{14}H_{12}O_2$: 212.0837; Found：212.0842. NMR spectroscopic data agreed with literature values.[12]



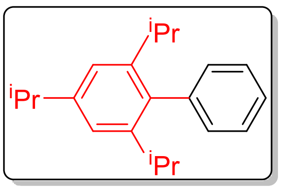
2-phenylnaphthalene (**3aa**)

White solid, 56% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.93 (t, J = 8.8 Hz, 2H), 7.89 (d, J = 7.4 Hz, 1H), 7.78 (dd, J = 8.5, 1.8 Hz, 1H), 7.75 (d, J = 7.1 Hz, 2H), 7.55 – 7.48 (m, 4H), 7.40 (t, J = 7.4 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.18 , 138.62 , 133.73 , 132.67 , 128.88 , 128.43 , 128.22 , 127.67 , 127.46 , 127.37 , 126.31 , 125.95 , 125.83 , 125.63 . **HRMS** (EI-TOF) calcd for $C_{16}H_{12}$: 204.0939; Found：204.0945. NMR spectroscopic data agreed with literature values.[1]



3,4-dimethoxy-1,1'-biphenyl (**3ab**)

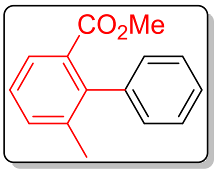
Yellow solid, 53% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 (d, J = 7.1 Hz, 2H), 7.44 (t, J = 7.7 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.97 (d, J = 8.3 Hz, 1H), 3.97 (s, 3H), 3.94 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.19 , 148.65 , 141.06 , 134.29 , 128.71 , 126.85 , 126.83 , 119.41 , 111.56 , 110.56 , 56.00 , 55.96 . **HRMS** (EI-TOF) calcd for $C_{14}H_{14}O_2$: 214.0994; Found：214.1004. NMR spectroscopic data agreed with literature values.[13]



2,4,6-triisopropyl-1,1'-biphenyl (**3ac**)

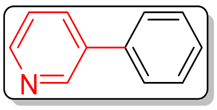
White solid, 67% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 3H), 7.21 (dd, J = 8.1, 1.3 Hz, 2H), 7.09 (s, 2H), 2.98 (hept, J = 7.0 Hz, 1H), 2.64 (hept, J = 6.9 Hz, 2H), 1.35 (d, J = 6.9 Hz, 6H), 1.11 (d, J = 6.9 Hz, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$)

δ 147.84 , 146.53 , 140.93 , 137.11 , 129.85 , 127.90 , 126.39 , 120.52 , 34.30 , 30.29 , 24.23 , 24.11 . **HRMS** (EI-TOF) calcd for $C_{21}H_{28}$: 280.2191; Found： 280.2204. NMR spectroscopic data agreed with literature values.[14]



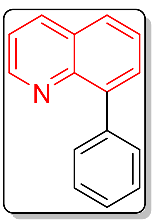
methyl 6-methyl-[1,1'-biphenyl]-2-carboxylate (**3ad**)

White solid, 53% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 (d, J = 7.7 Hz, 1H), 7.42 (t, J = 7.3 Hz, 3H), 7.39 – 7.31 (m, 2H), 7.19 (d, J = 6.9 Hz, 2H), 3.56 (s, 3H), 2.14 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.74 , 141.78 , 140.25 , 137.15 , 133.02 , 131.60 , 128.54 , 127.86 , 127.01 , 126.93 , 126.81 , 51.68 , 20.65 . **HRMS** (EI-TOF) calcd for $C_{15}H_{14}O_2$: 226.0994; Found： 226.0993. NMR spectroscopic data agreed with literature values.[15]



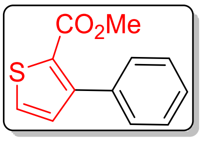
3-phenylpyridine (**3ae**)

Brown oil, 45% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.62 (d, J =4.0 Hz, 1H), 7.94 (dd, J =8.0, 1.5 Hz, 1H), 7.71 – 7.41 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.93 , 147.89 , 137.61 , 136.99 , 134.92 , 129.15 , 128.27 , 127.18 , 123.78 . **HRMS** (EI-TOF) calcd for $C_{11}H_9N$: 155.0735; Found： 155.0740. NMR spectroscopic data agreed with literature values.[16]



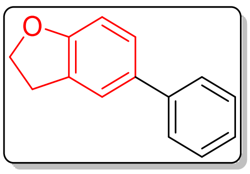
8-phenylquinoline (**3af**)

Yellow oil, 37% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.99 (dd, J = 4.1, 1.6 Hz, 1H), 8.24 (dd, J = 8.2, 1.6 Hz, 1H), 7.89 – 7.68 (m, 4H), 7.66 – 7.50 (m, 3H), 7.47 – 7.44 (m, 1H), 7.44 – 7.42 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.17 , 145.86 , 140.86 , 139.46 , 136.43 , 130.60 , 130.42 , 128.76 , 128.02 , 127.53 , 127.41 , 126.33 , 120.98 . **HRMS** (EI-TOF) calcd for $C_{15}H_{11}N$: 205.0891; Found：205.0897. NMR spectroscopic data agreed with literature values.[17]



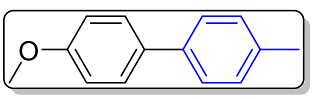
methyl 3-phenylthiophene-2-carboxylate (**3ag**)

Colorless solid, 37% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.52 (d, J = 5.1 Hz, 1H), 7.50 – 7.38 (m, 5H), 7.11 (d, J = 5.1 Hz, 1H), 3.79 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.48 , 148.71 , 135.70 , 131.58 , 130.19 , 129.23 , 127.93 , 127.84 , 126.96 , 51.90 . **HRMS** (EI-TOF) calcd for $C_{12}H_{10}O_2S$: 218.0402; Found：218.0416. NMR spectroscopic data agreed with literature values.[18]



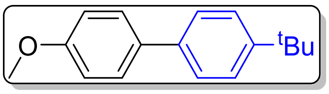
2,3-Dihydro-5-phenylbenzofuran (**3ah**)

Yellow oil, 65% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.56 (d, J = 7.1 Hz, 2H), 7.47 – 7.40 (m, 3H), 7.38 (d, J = 10.2 Hz, 1H), 7.32 (t, J = 7.4 Hz, 1H), 6.89 (d, J = 8.2 Hz, 1H), 4.64 (t, J = 8.7 Hz, 2H), 3.29 (t, J = 8.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.35 , 133.99 , 128.67 , 127.60 , 127.07 , 126.79 , 126.49 , 123.76 , 109.44 , 71.44 , 29.77 . **HRMS** (EI-TOF) calcd for $C_{14}H_{12}O$: 196.0888; Found： 196.0896. NMR spectroscopic data agreed with literature values.[2]



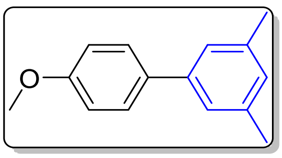
4-methoxy-4'-methyl-1,1'-biphenyl (**3ba**)

White solid, 61% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (d, J = 8.8 Hz, 2H), 7.47 (d, J = 8.1 Hz, 2H), 7.25 (d, J = 7.9 Hz, 2H), 6.99 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.99 , 138.02 , 136.37 , 133.81 , 129.46 , 127.98 , 126.61 , 114.21 , 55.37 , 21.06 . **HRMS** (EI-TOF) calcd for $C_{14}H_{14}O$: 198.1045; Found： 198.1054. NMR spectroscopic data agreed with literature values.[2]



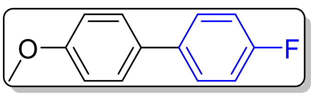
4-(tert-butyl)-4'-methoxy-1,1'-biphenyl (**3bb**)

White solid, 51% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.56 (d, J =8.0 Hz, 1H), 7.54 (d, J = 8.5 Hz, 1H), 7.52 (d, J = 2.1 Hz, 1H), 7.48 (d, J = 2.0 Hz, 1H), 7.46 (d, J = 2.0 Hz, 1H), 7.00 (d, J = 8.7 Hz, 1H), 3.87 (s, 3H), 1.39 (s, 8H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.97 , 149.63 , 137.95 , 133.68 , 128.01 , 126.37 , 125.67 , 114.17 , 55.34 , 34.49 , 31.40 . **HRMS** (EI-TOF) calcd for $C_{17}H_{20}O$: 240.1514; Found： 240.1525. NMR spectroscopic data agreed with literature values.[19]



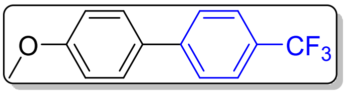
4'-methoxy-3,5-dimethyl-1,1'-biphenyl (**3bc**)

White solid, 61% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 (d, J = 8.7 Hz, 2H), 7.20 (s, 2H), 6.99 (d, J = 4.5 Hz, 3H), 3.87 (s, 3H), 2.40 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.04 , 140.86 , 138.19 , 134.04 , 128.32 , 128.16 , 124.71 , 114.10 , 55.34 , 21.42 . **HRMS** (EI-TOF) calcd for $C_{15}H_{16}O$: 212.1201; Found： 212.1213. NMR spectroscopic data agreed with literature values.[20]



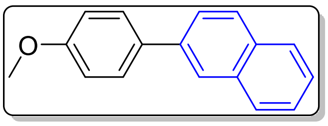
4-fluoro-4'-methoxy-1,1'-biphenyl (**3bd**)

White solid, 62% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.55 – 7.45 (m, 4H), 7.16 – 7.08 (m, 2H), 7.01 – 6.97 (m, 2H), 3.87 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.12 (d, J = 245.5 Hz), 159.15 , 136.99 , 132.88 , 128.23 (d, J = 8.0 Hz), 128.04 , 115.53 (d, J = 21.4 Hz), 114.28 , 55.37 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -116.76 . **HRMS** (EI-TOF) calcd for $C_{13}H_{11}OF$: 202.0794; Found：202.0803. NMR spectroscopic data agreed with literature values.[1]



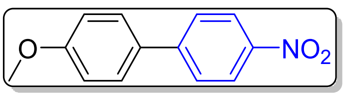
4-methoxy-4'-(trifluoromethyl)-1,1'-biphenyl (**3be**)

White solid, 56% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 – 7.63 (m, 4H), 7.56 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.88 , 144.33 , 132.22 , 128.73 (q, J = 32.5 Hz), 128.36 , 126.89 , 125.68 (q, J = 3.8 Hz), 124.40 (q, J = 272.2 Hz), 114.46 , 55.41 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.33 . **HRMS** (EI-TOF) calcd for $C_{14}H_{11}OF_3$: 252.0762; Found：252.0770. NMR spectroscopic data agreed with literature values.[1]



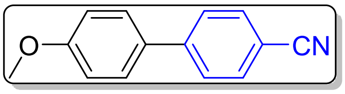
2-(4-methoxyphenyl)naphthalene (**3bf**)

White solid, 50% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.94 – 7.85 (m, 3H), 7.74 (dd, J = 8.5, 1.7 Hz, 1H), 7.69 (d, J = 8.7 Hz, 2H), 7.55 – 7.45 (m, 3H), 7.05 (d, J = 8.7 Hz, 2H), 3.90 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.31 , 138.20 , 133.80 , 133.69 , 132.36 , 128.45 , 128.35 , 128.07 , 127.64 , 126.24 , 125.66 , 125.46 , 125.06 , 114.37 , 55.41 . **HRMS** (EI-TOF) calcd for $C_{17}H_{14}O$: 234.1045; Found：234.1053. NMR spectroscopic data agreed with literature values.[19]



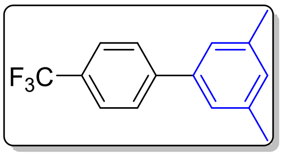
4-methoxy-4'-nitro-1,1'-biphenyl (**3bg**)

White solid, 37% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 (d, J = 8.9 Hz, 2H), 7.71 (d, J = 8.9 Hz, 2H), 7.62 – 7.58 (m, 2H), 7.04 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.48 , 147.23 , 146.59 , 131.12 , 128.58 , 127.08 , 124.15 , 114.64 , 55.44 . **HRMS** (EI-TOF) calcd for $C_{13}H_{11}NO_3$: 229.0739; Found：229.0753. NMR spectroscopic data agreed with literature values.[21]



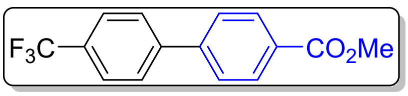
4'-methoxy-[1,1'-biphenyl]-4-carbonitrile (**3bh**)

White solid, 32% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 – 7.63 (m, 4H), 7.55 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.21 , 145.22 , 132.54 , 131.51 , 128.34 , 127.09 , 119.04 , 114.55 , 110.12 , 55.39 . **HRMS** (EI-TOF) calcd for $C_{14}H_{11}NO$: 209.0841; Found：209.0857. NMR spectroscopic data agreed with literature values.[1]



3,5-dimethyl-4'-(trifluoromethyl)-1,1'-biphenyl (**3ca**)

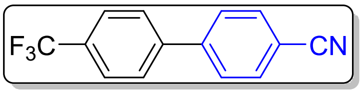
White solid, 72% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 4H), 7.23 (s, 2H), 7.07 (s, 1H), 2.41 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.04 , 139.82 , 138.57 , 129.81 , 127.43 , 125.59 (q, J = 3.8 Hz), 125.21 , 21.39 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.35 . **HRMS** (EI-TOF) calcd for $C_{15}H_{13}F_3$: 250.0969; Found：250.0980. NMR spectroscopic data agreed with literature values.[22]



methyl 4'-(trifluoromethyl)-[1,1'-biphenyl]-4-carboxylate (**3cb**)

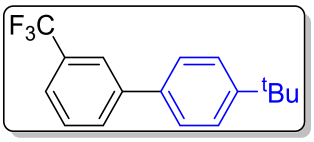
White solid, 64% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, J = 8.4 Hz, 2H), 7.74

(s, 4H), 7.68 (d, J = 8.4 Hz, 2H), 3.97 (s, 3H). **[13]C NMR** (126 MHz, $CDCl_3$) δ 166.77 , 144.10 , 143.57 , 130.35 (q, J = 32.8 Hz), 130.29 , 129.87 , 127.64 , 127.28 , 125.89 (q, J = 3.8 Hz), 125.25 (q, J = 272.4 Hz), 52.25 . **[19]F NMR** (565 MHz, $CDCl_3$) δ -62.54 . **HRMS** (EI-TOF) calcd for $C_{15}H_{11}O_2F_3$: 280.0711; Found：280.0719. NMR spectroscopic data agreed with literature values.[23]



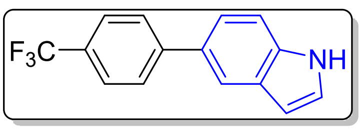
4'-(trifluoromethyl)-[1,1'-biphenyl]-4-carbonitrile (**3cc**)

White solid, 85% yield, **[1]H NMR** (500 MHz, $CDCl_3$) δ 7.79 (d, J = 8.3 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.73 – 7.70 (m, 4H). **[13]C NMR** (126 MHz, $CDCl_3$) δ 144.17 , 142.70 , 132.80 , 130.76 (q, J = 32.8 Hz), 127.98 , 127.64 , 126.09 (q, J = 3.8 Hz), 125.10 (q, J = 272.7 Hz), 118.55 , 112.06 . **[19]F NMR** (565 MHz, $CDCl_3$) δ -62.64 . **HRMS** (EI-TOF) calcd for $C_{14}H_8NF_3$: 247.0609; Found：247.0604. NMR spectroscopic data agreed with literature values.[24]



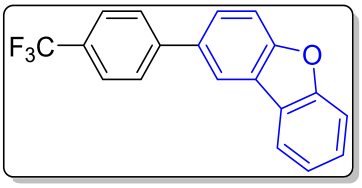
4'-(tert-butyl)-3-(trifluoromethyl)-1,1'-biphenyl (**3cd**)

Yellow solid, 80% yield, **[1]H NMR** (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.78 (s, 1H), 7.61 – 7.50 (m, 6H), 1.39 (s, 9H). **[13]C NMR** (126 MHz, $CDCl_3$) δ 151.22 , 141.90 , 136.88 , 131.27 (q, J = 32.1 Hz), 130.24 , 129.16 , 126.86 , 125.97 , 123.82 (q, J = 3.7 Hz), 123.66 (q, J = 3.6 Hz), 34.64 , 31.35 . **[19]F NMR** (565 MHz, $CDCl_3$) δ -62.16 . **HRMS** (EI-TOF) calcd for $C_{17}H_{17}F_3$: 278.1282; Found：278.1287. NMR spectroscopic data agreed with literature values.[25]



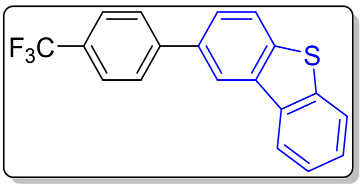
5-(4-(trifluoromethyl)phenyl)-1*H*-indole (**3ce**)

Yellow oil, 57% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (dd, J = 8.3, 3.9 Hz, 3H), 7.71 (d, J = 8.4 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.36 (t, J = 7.6 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 6.73 (d, J = 3.7 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.61 , 135.40 (q, J = 33.2 Hz), 134.83 , 130.87 , 127.28 , 126.46 (q, J = 3.7 Hz), 126.11 , 125.05 , 123.85 , 122.91 (q, J = 273.0 Hz), 121.68 , 113.46 , 110.16 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -63.37 . **HRMS** (EI-TOF) calcd for $C_{15}H_{10}NF_3$: 261.0765; Found：261.0778.



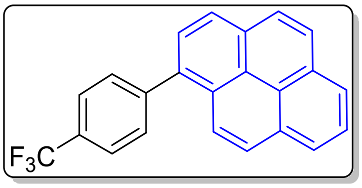
2-(4-(trifluoromethyl)phenyl)dibenzo[b,d]furan (**3cf**)

White solid, 78% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 7.98 (m, 4H), 7.82 (d, J = 8.2 Hz, 2H), 7.66 – 7.60 (m, 2H), 7.53 – 7.46 (m, 2H), 7.41 (t, J = 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.21 , 153.32 , 140.06 , 129.08 , 127.52 , 126.82 , 125.60 (q, J = 3.8 Hz), 125.42 (q, J = 272.5 Hz), 125.23 , 124.21 (q, J = 46.6 Hz), 123.36 , 123.03 , 120.78 , 120.63 , 111.87 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.48 . **HRMS** (EI-TOF) calcd for $C_{19}H_{11}OF_3$: 312.0762; Found：312.0768.



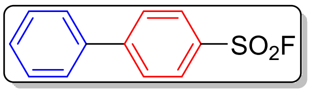
2-(4-(trifluoromethyl)phenyl)dibenzo[b,d]thiophene (**3cg**)

White solid, 71% yield, **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.26 – 8.20 (m, 2H), 7.90 – 7.84 (m, 3H), 7.80 (d, J = 8.2 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.53 – 7.48 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.17 , 139.38 , 138.47 , 136.52 , 135.64 , 135.56 , 130.10 (q, J = 32.8 Hz), 128.67 , 127.07 , 126.98 , 125.81 (q, J = 3.7 Hz), 125.22 , 124.61 , 123.12 (q, J = 272.4 Hz), 122.67 , 121.83 , 121.22 . **^{19}F NMR** (565 MHz, $CDCl_3$) δ -62.48 . **HRMS** (EI-TOF) calcd for $C_{19}H_{11}F_3S$: 328.0534; Found：328.0530.



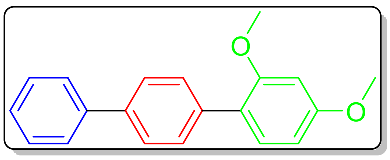
1-(4-(trifluoromethyl)phenyl)pyrene (**3ch**)

White solid, 82% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.28 – 8.20 (m, 3H), 8.14 (d, J = 2.0 Hz, 2H), 8.10 – 8.04 (m, 3H), 7.97 (d, J = 7.8 Hz, 1H), 7.85 (d, J = 8.0 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 144.99 , 136.02 , 131.48 , 131.12 , 130.91 , 129.63 , 129.38 , 128.45 , 128.01 , 127.88 , 127.36 , 126.22 , 125.47 , 125.36 (q, J = 3.7 Hz), 125.15 , 124.89 (q, J = 16.1 Hz), 124.71 , 124.64 , 122.34 (q, J = 297.6 Hz). ^{19}**F NMR** (565 MHz, $CDCl_3$) δ -62.31 . **HRMS** (EI-TOF) calcd for $C_{23}H_{13}F_3$: 346.0969; Found：346.0976. NMR spectroscopic data agreed with literature values.[26]



[1,1'-biphenyl]-4-sulfonyl fluoride (**A1**)

White solid, 82% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.09 (d, J = 8.5 Hz, 2H), 7.84 (d, J = 8.3 Hz, 2H), 7.67 – 7.63 (m, 2H), 7.58 – 7.46 (m, 3H). ^{13}**C NMR** (126 MHz, $CDCl_3$) δ 148.64 , 138.50 , 131.37 (d, J = 24.5 Hz), 129.26 , 129.21 , 128.98 , 128.19 , 127.45 . ^{19}**F NMR** (565 MHz, $CDCl_3$) δ 66.51 . **HRMS** (EI-TOF) calcd for $C_{12}H_9FO_2S$: 236.0307; Found：236.0302. NMR spectroscopic data agreed with literature values.[27]



2,4-dimethoxy-1,1':4',1''-terphenyl (**A2**)

White solid, 73% yield, ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.69 – 7.58 (m, 6H), 7.50 – 7.43 (m, 2H), 7.40 – 7.34 (m, 1H), 7.34 – 7.30 (m, 1H), 6.62 (s, 1H), 6.61 (s, 1H), 3.89 (s, 3H), 3.85 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.50 , 157.65 , 141.20 , 139.40 , 137.49 , 131.28 , 129.87 , 128.80 , 127.16 , 126.83 , 123.25 , 104.84 , 99.17 , 55.67 , 55.52 . **HRMS** (EI-TOF) calcd for $C_{20}H_{18}O_2$: 290.1307; Found：290.1312.

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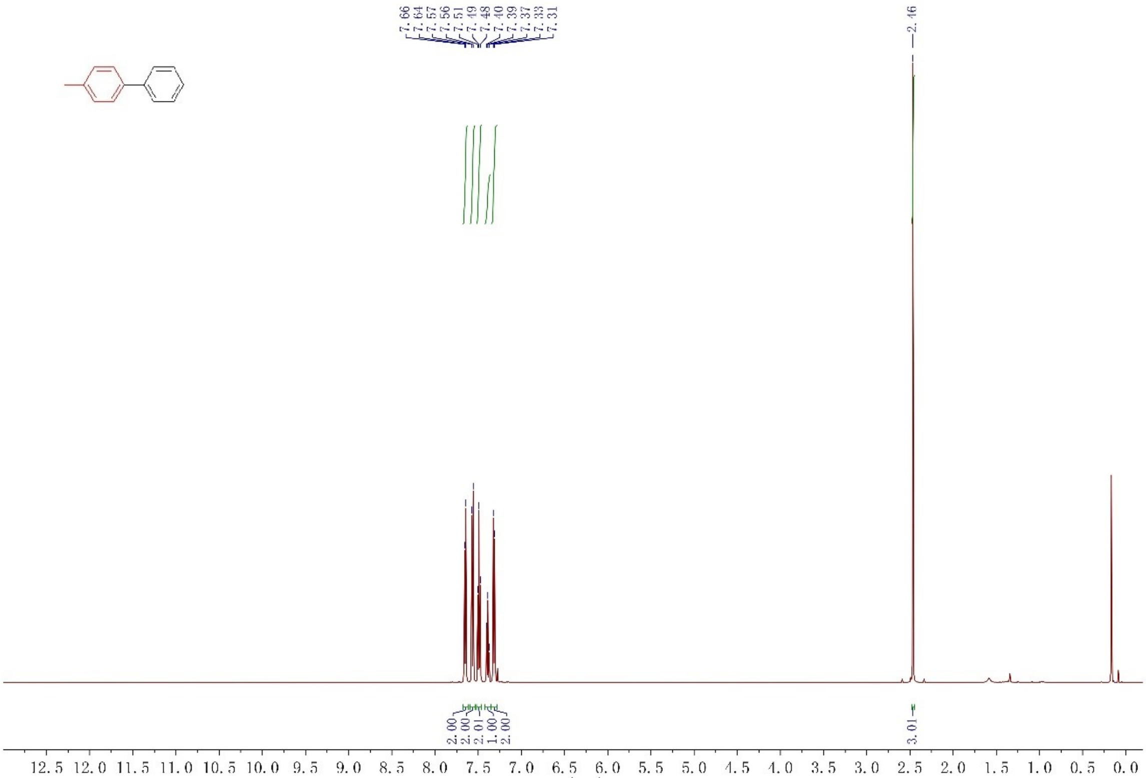
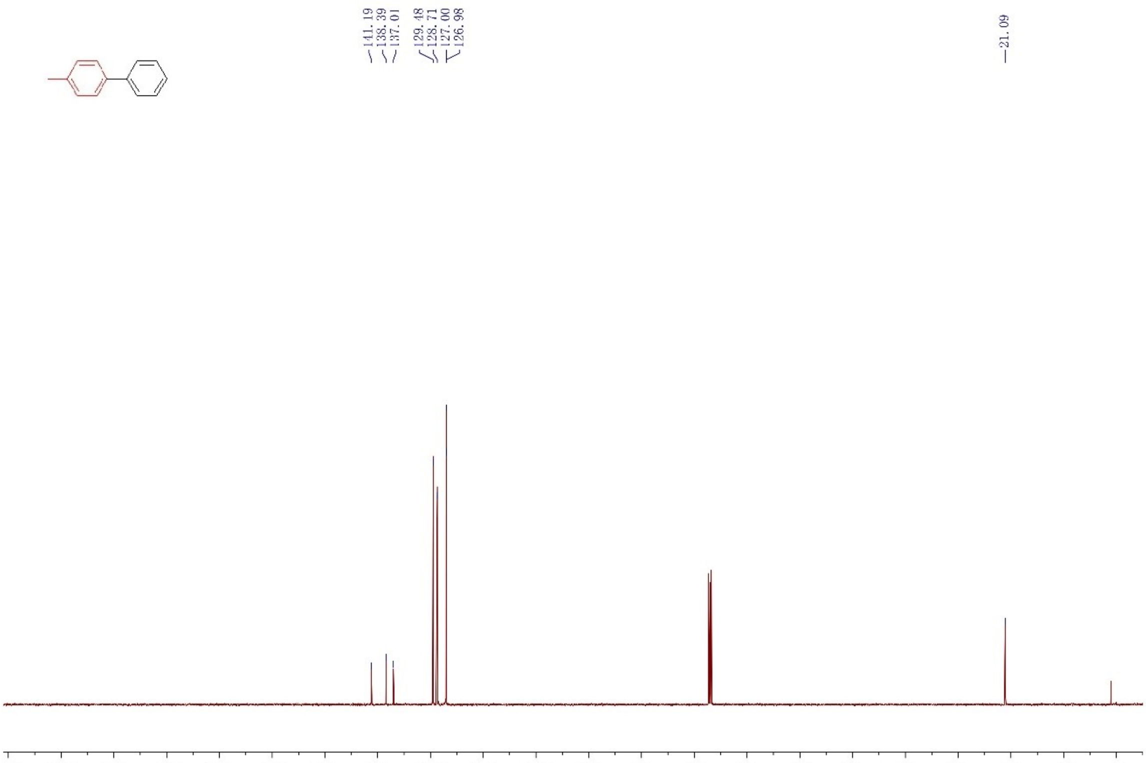
8: Copies of ^{1}H and ^{13}C spectra for coupling products.

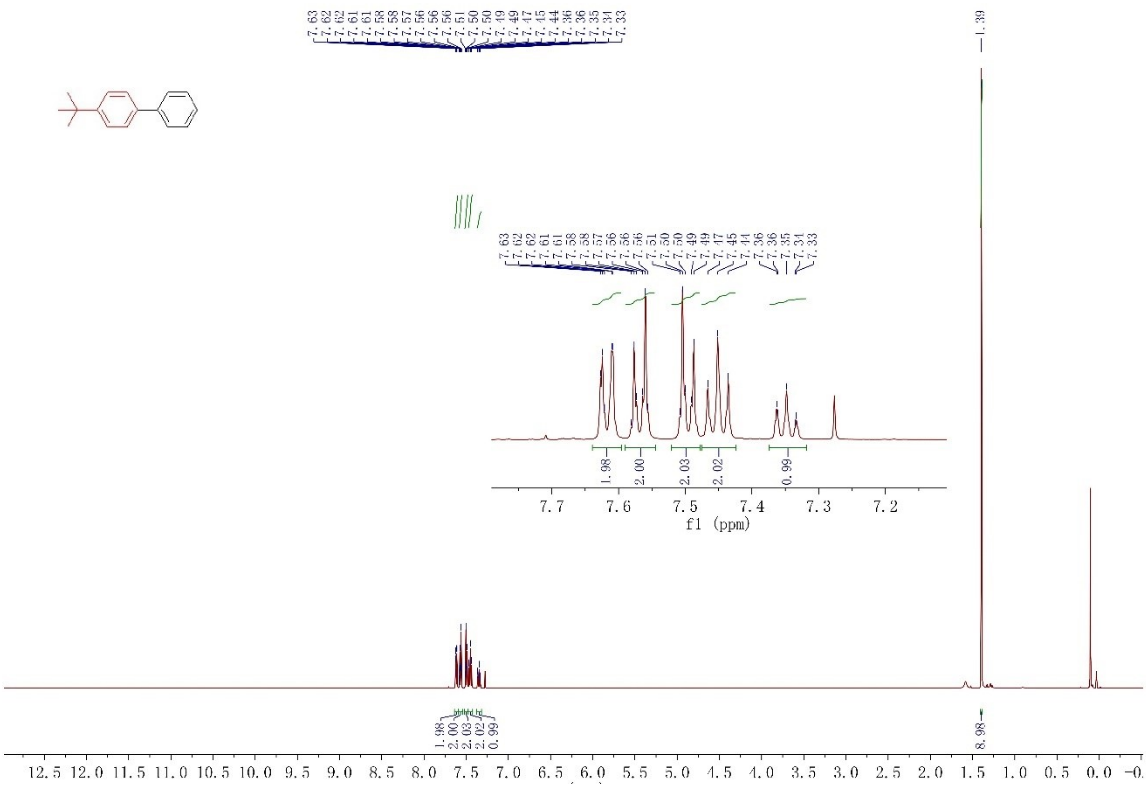
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



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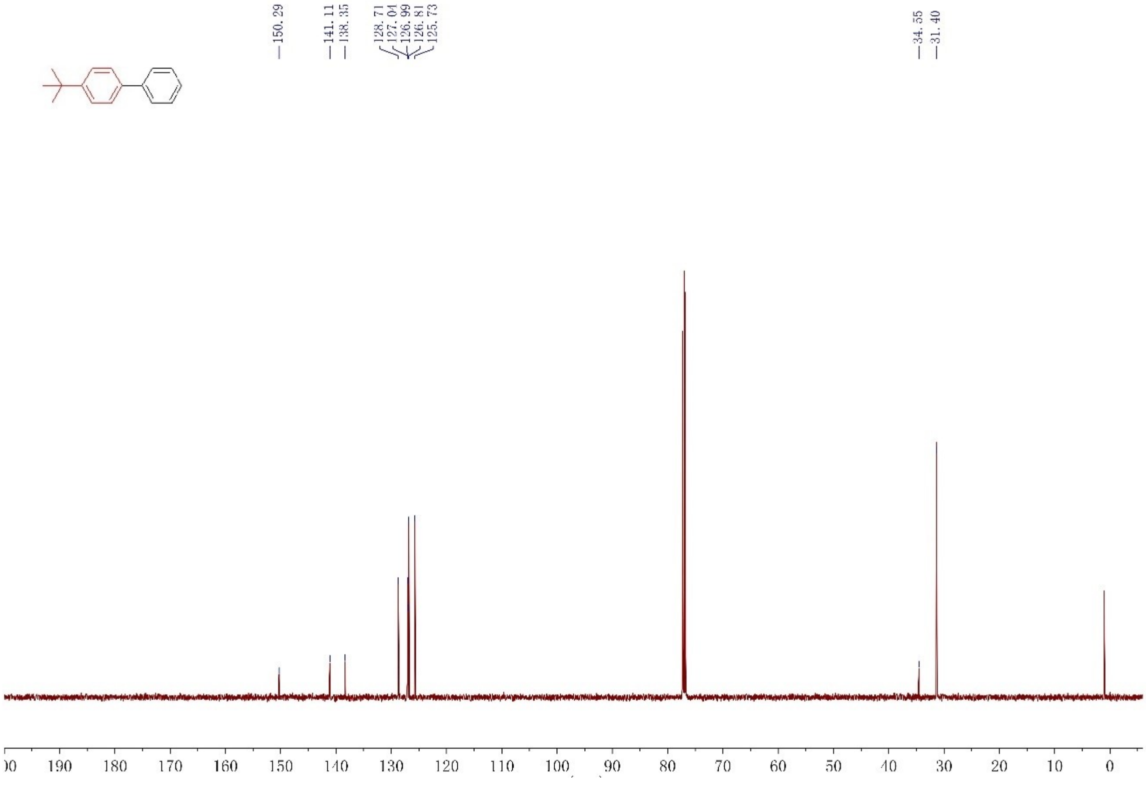
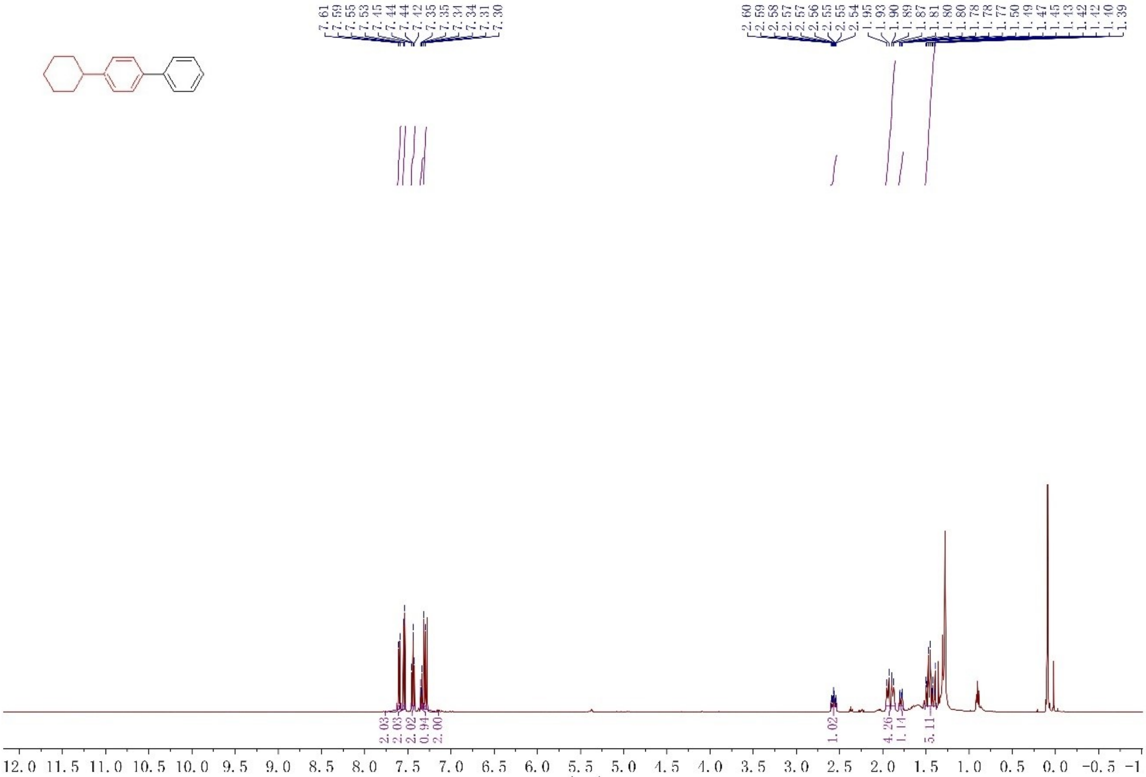


^{1}H NMR (500 MHz, $CDCl_3$)



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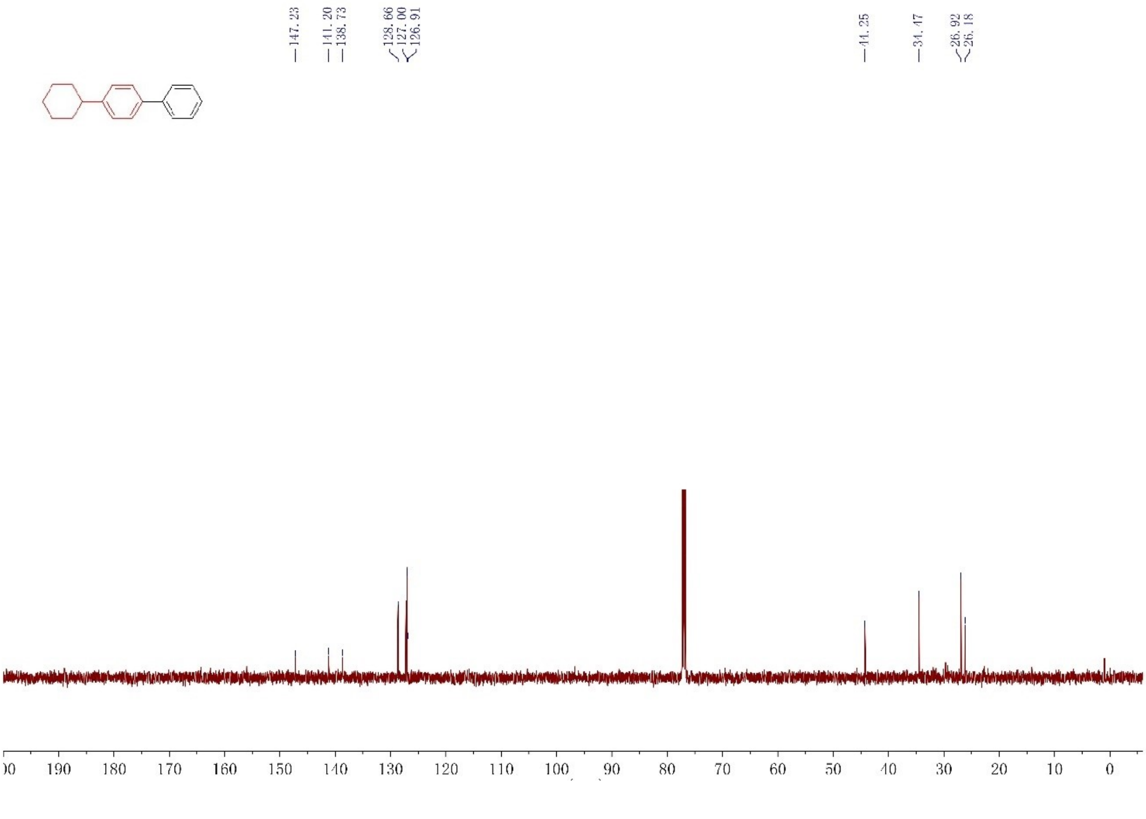

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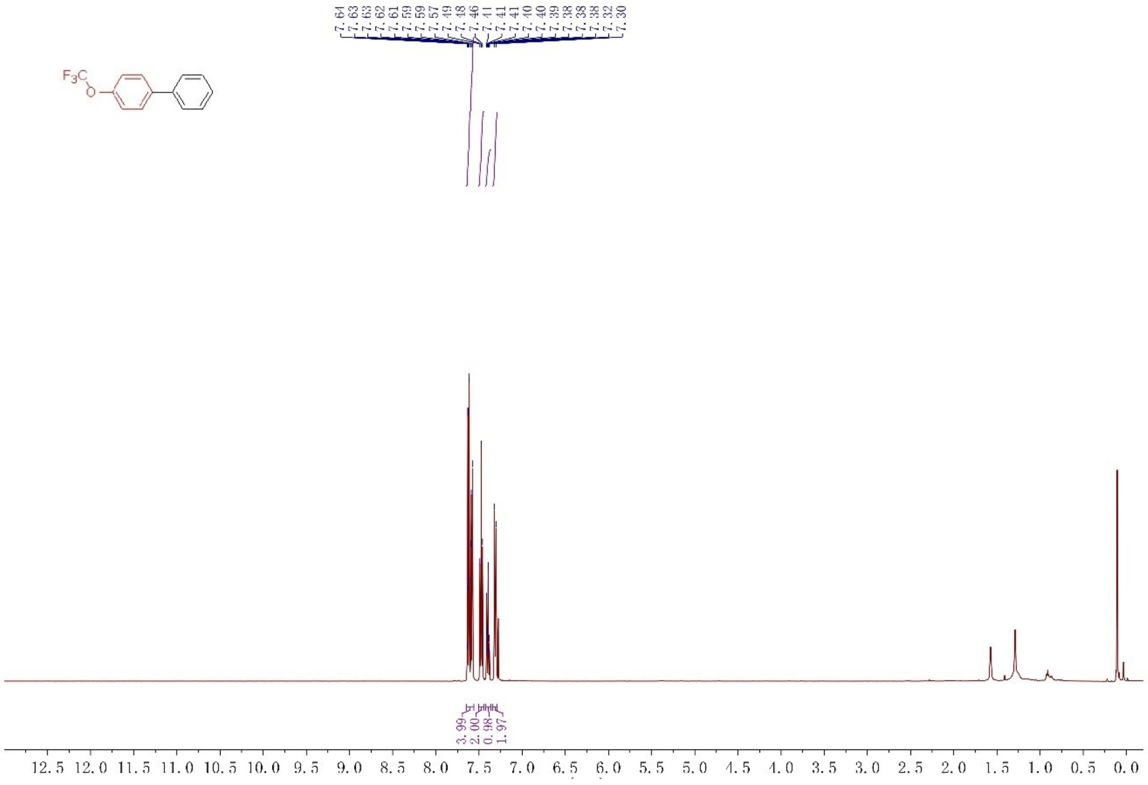

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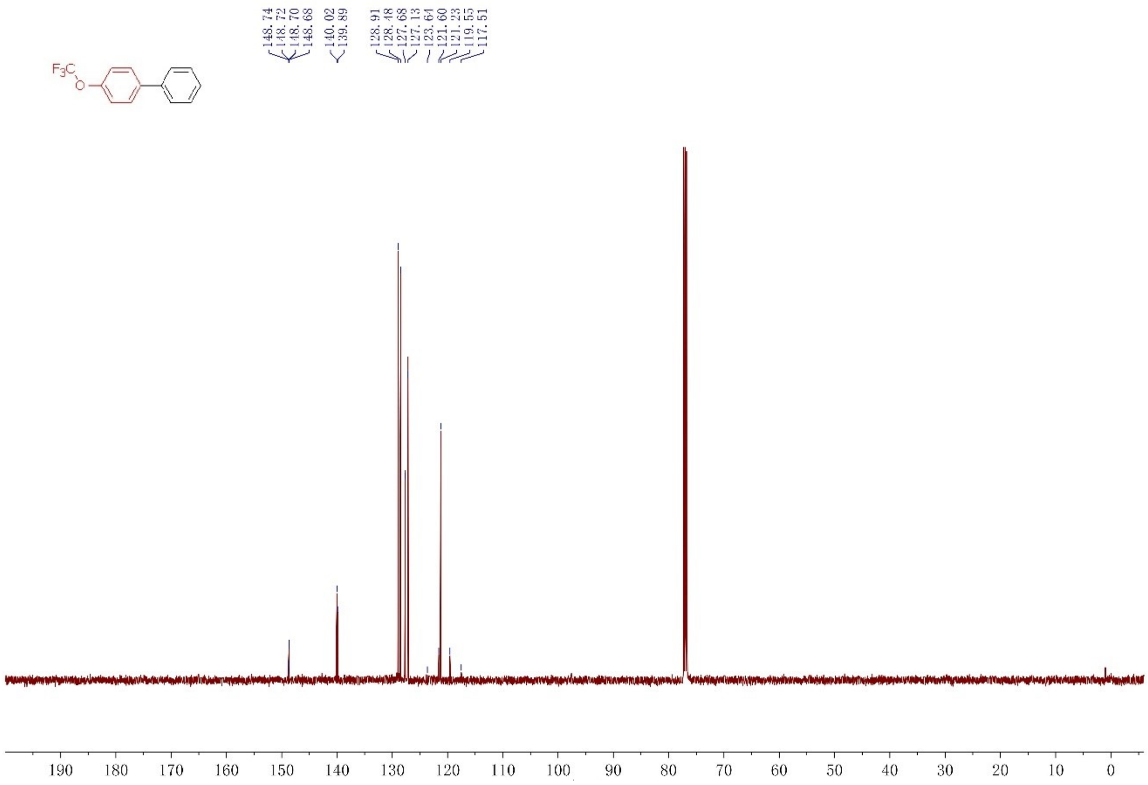
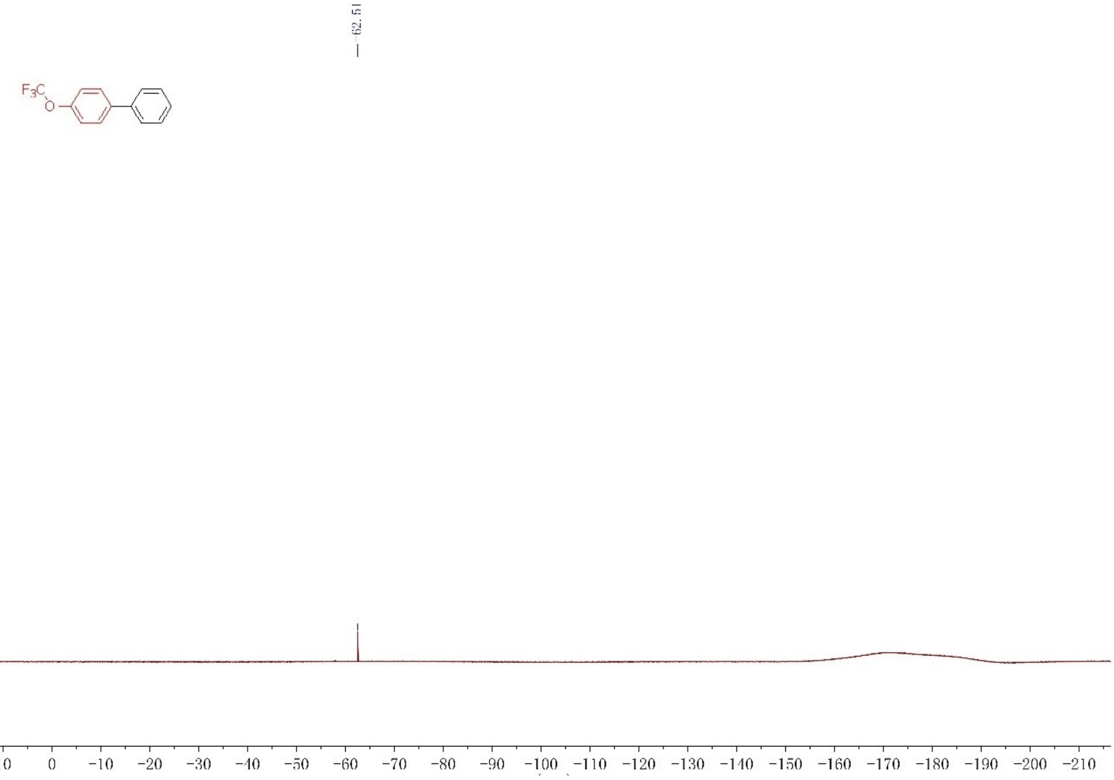


^{19}F NMR (565 MHz, $CDCl_3$)



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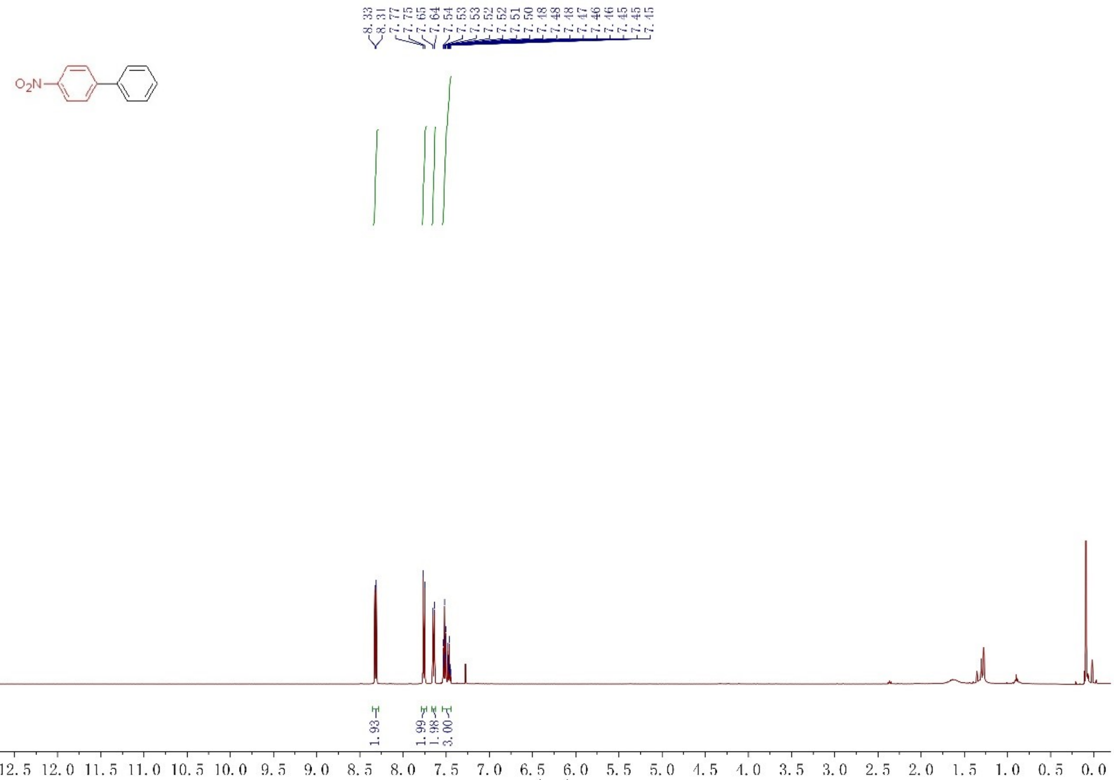

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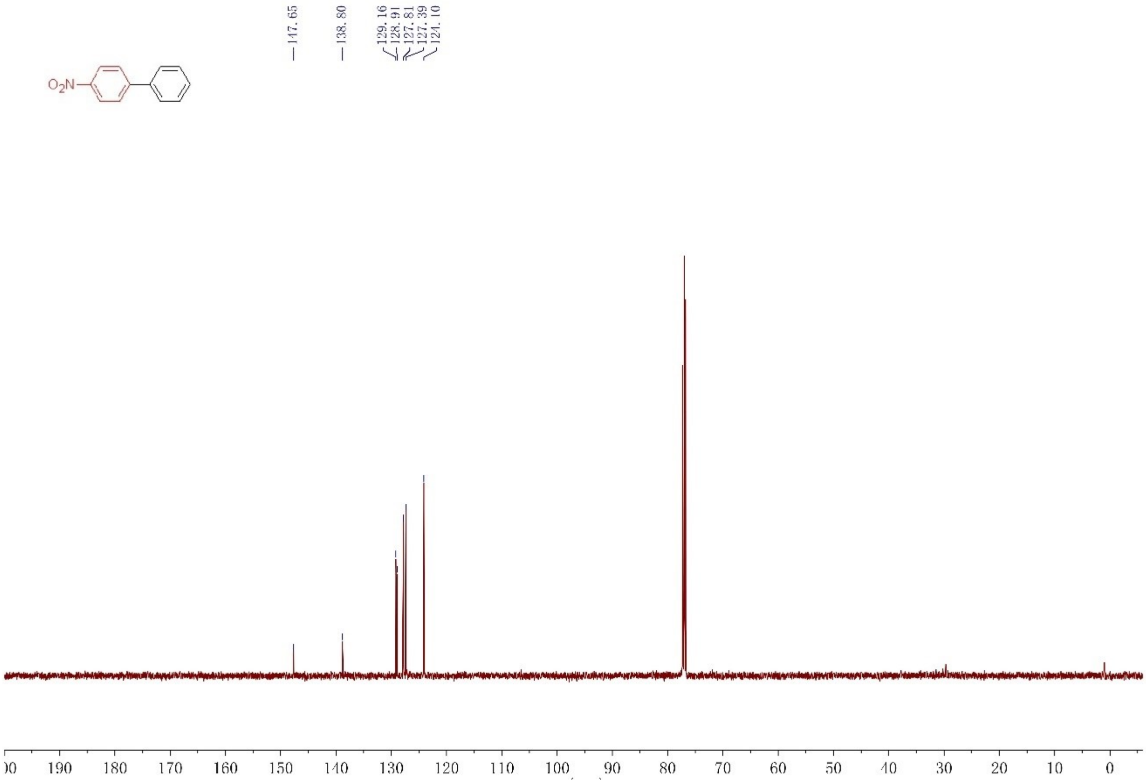

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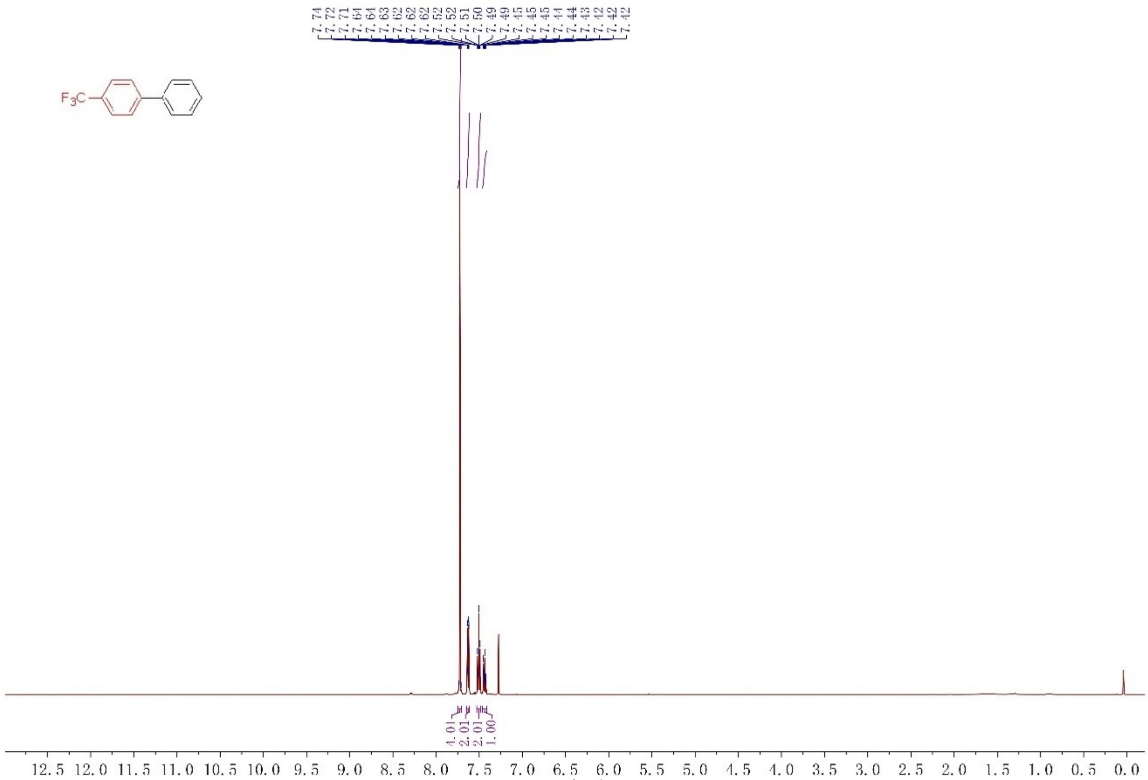

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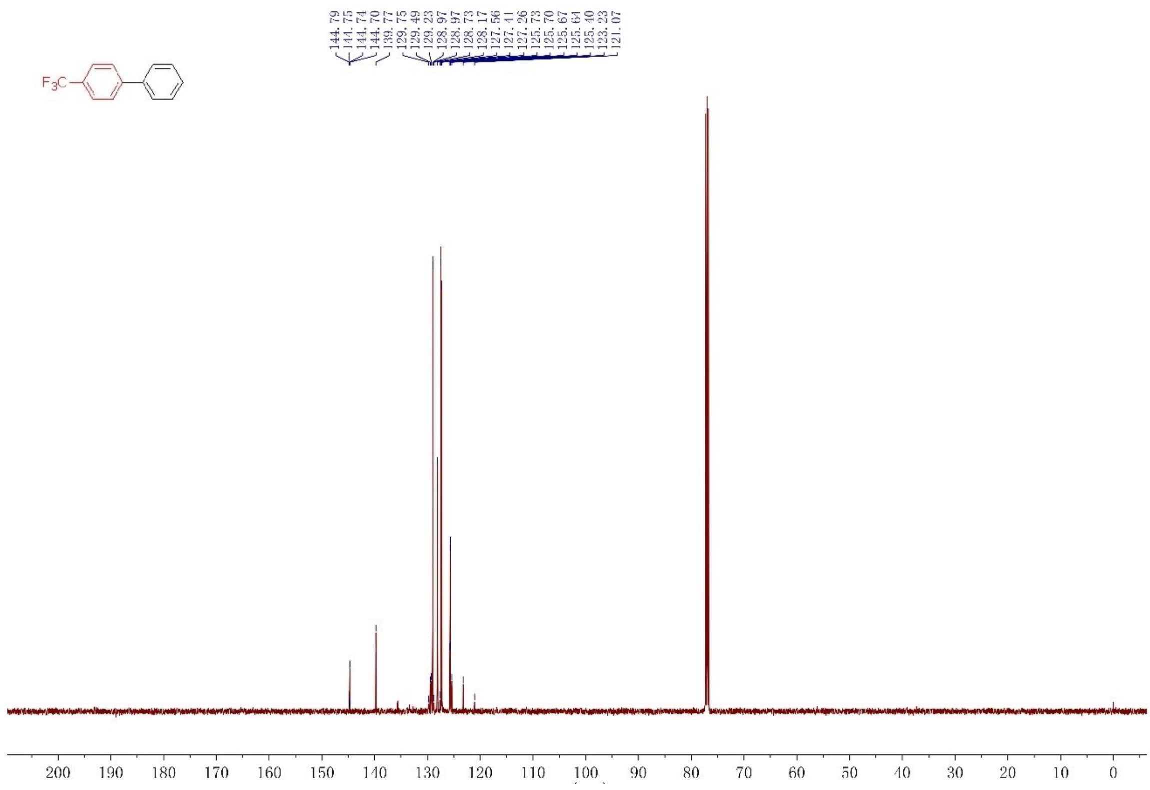

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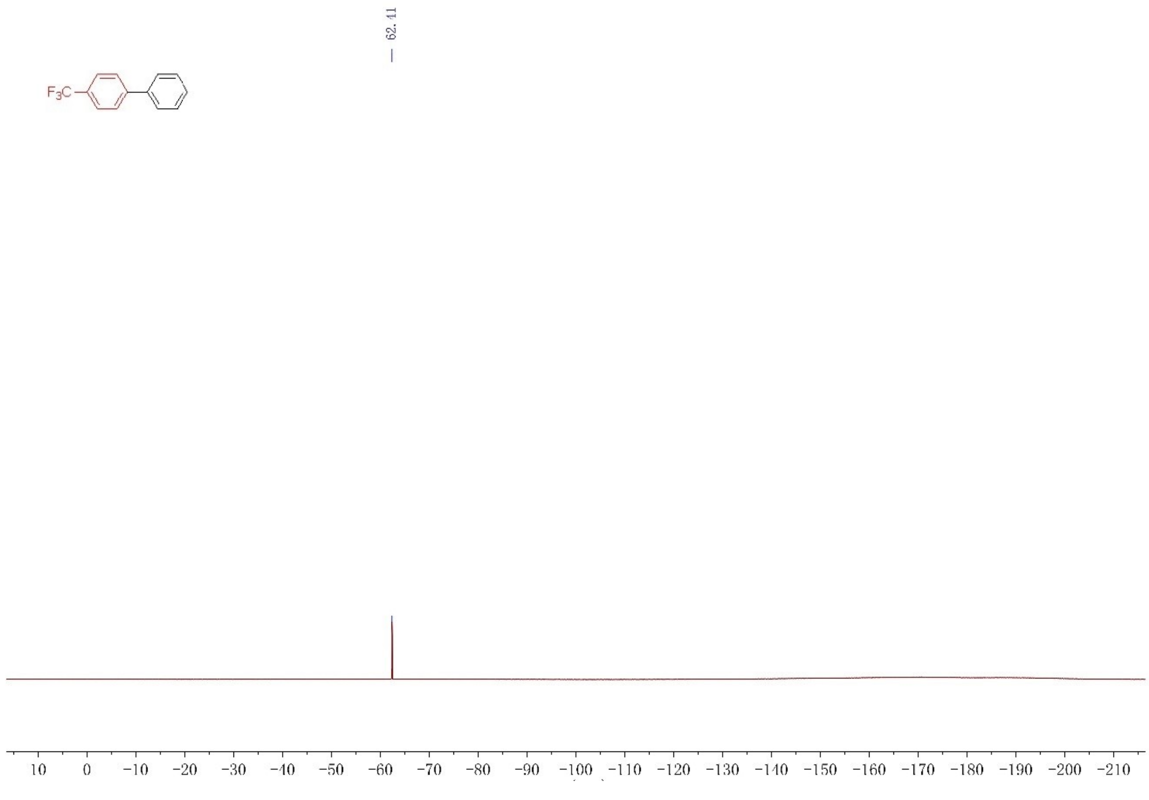

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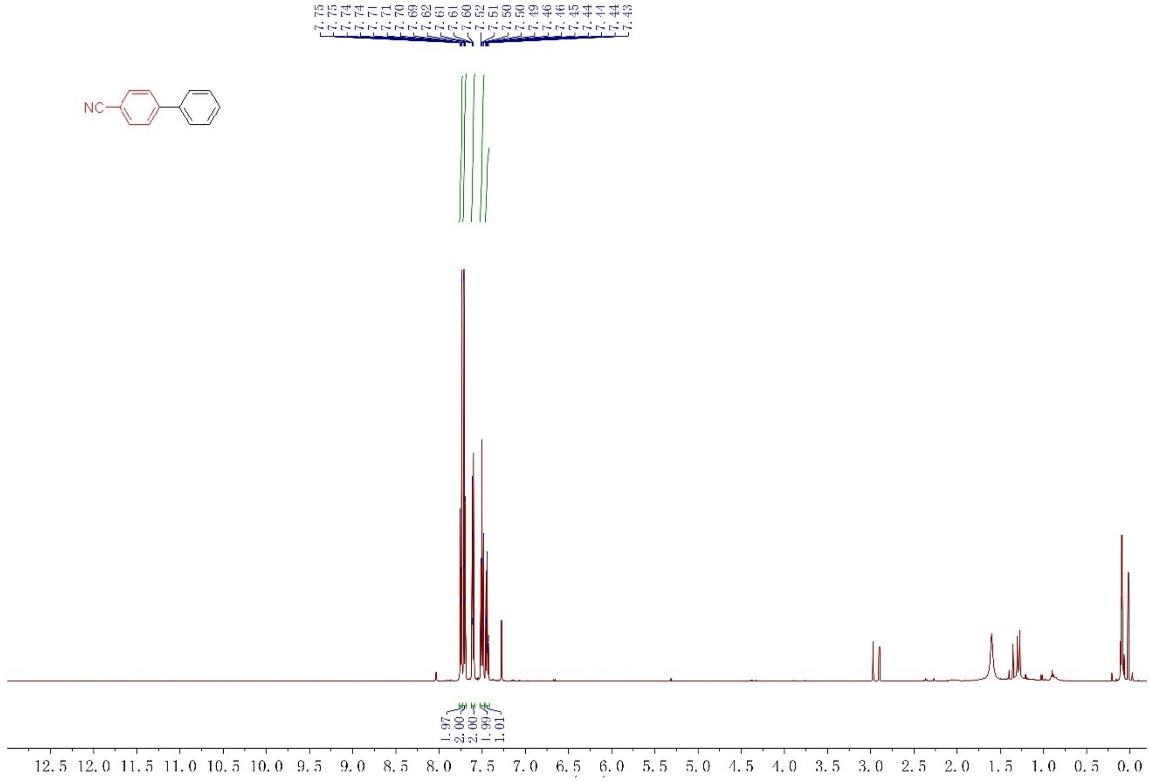
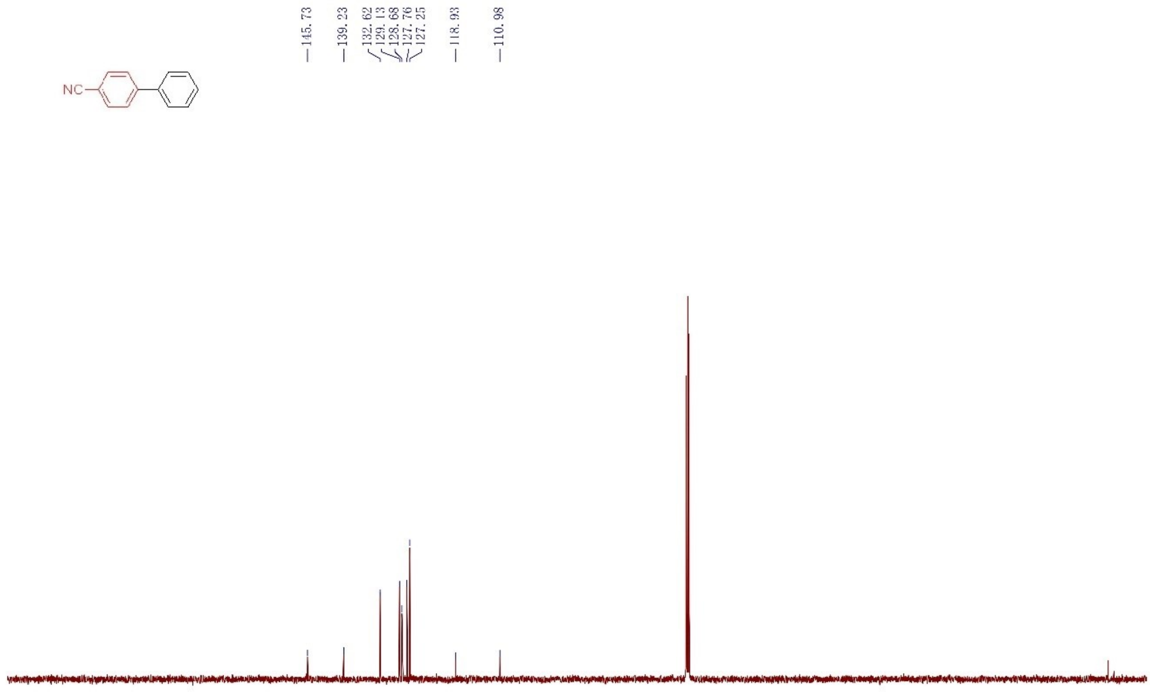
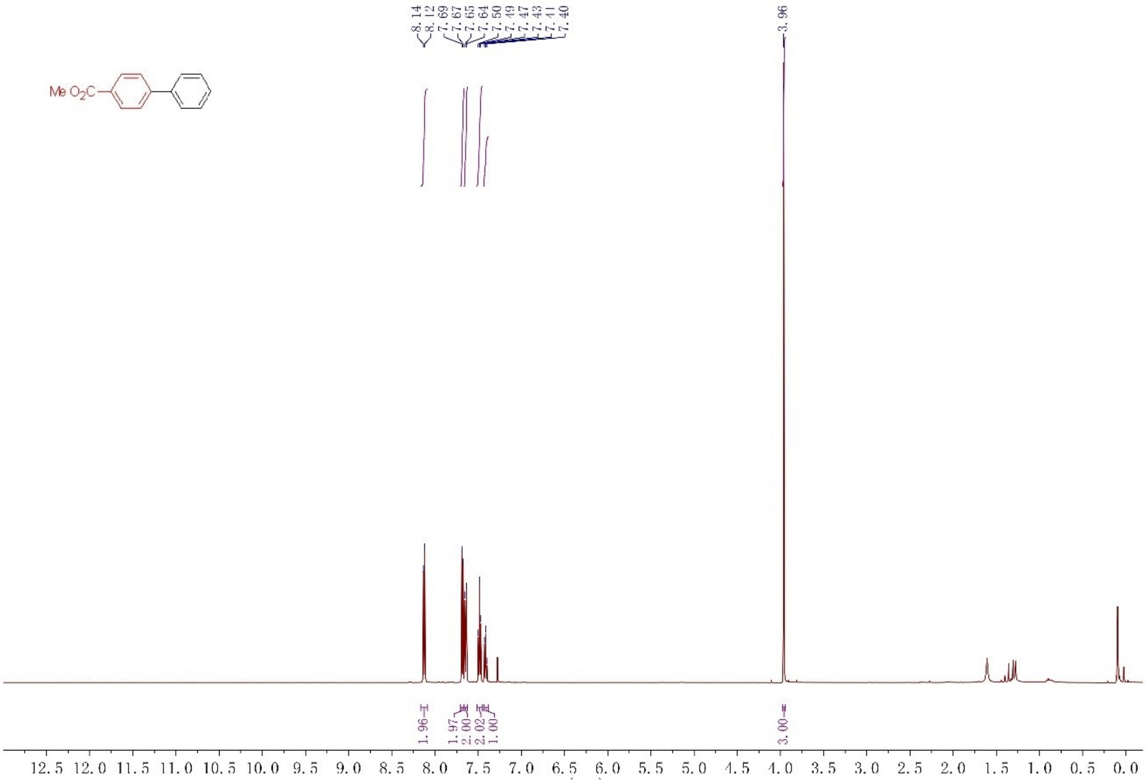


¹³C NMR (126 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



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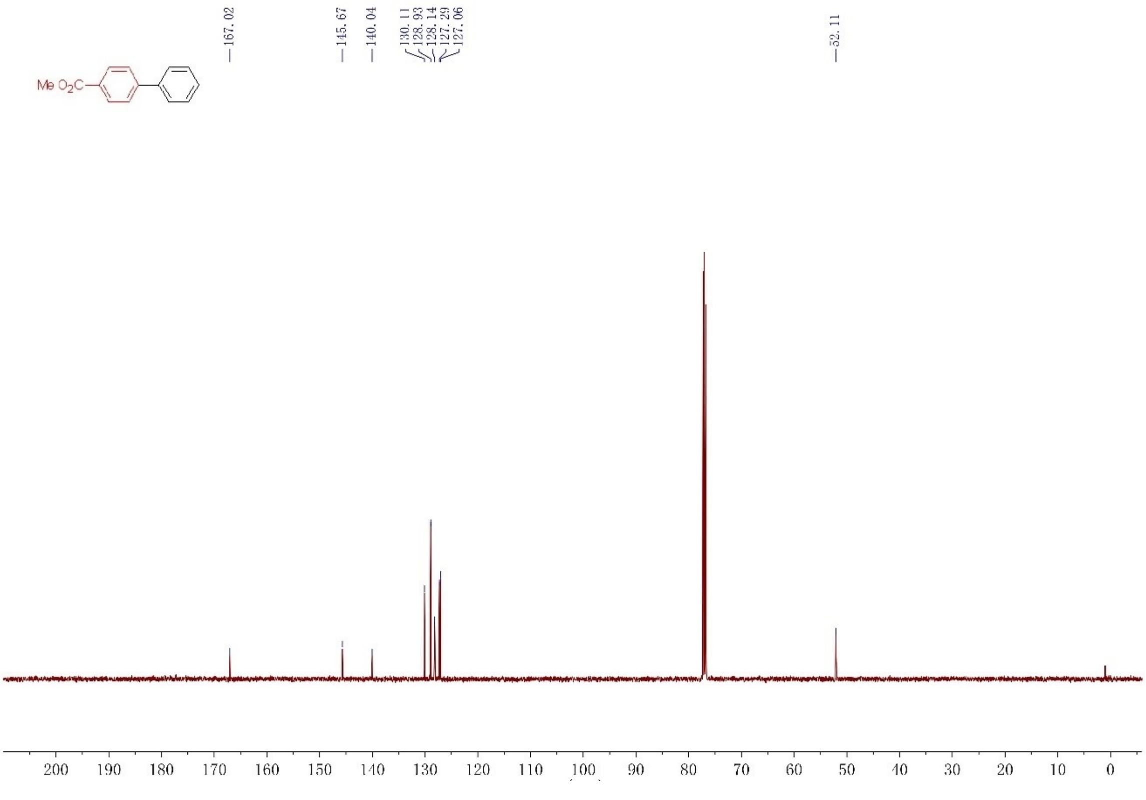

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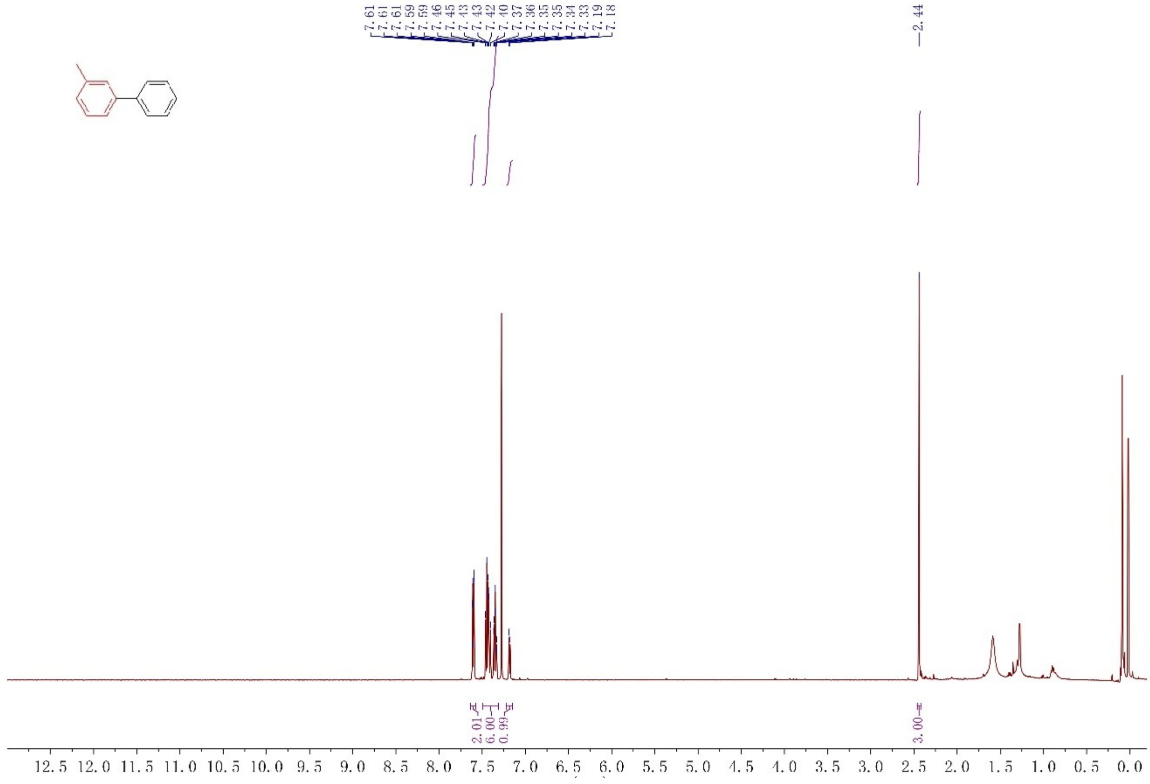

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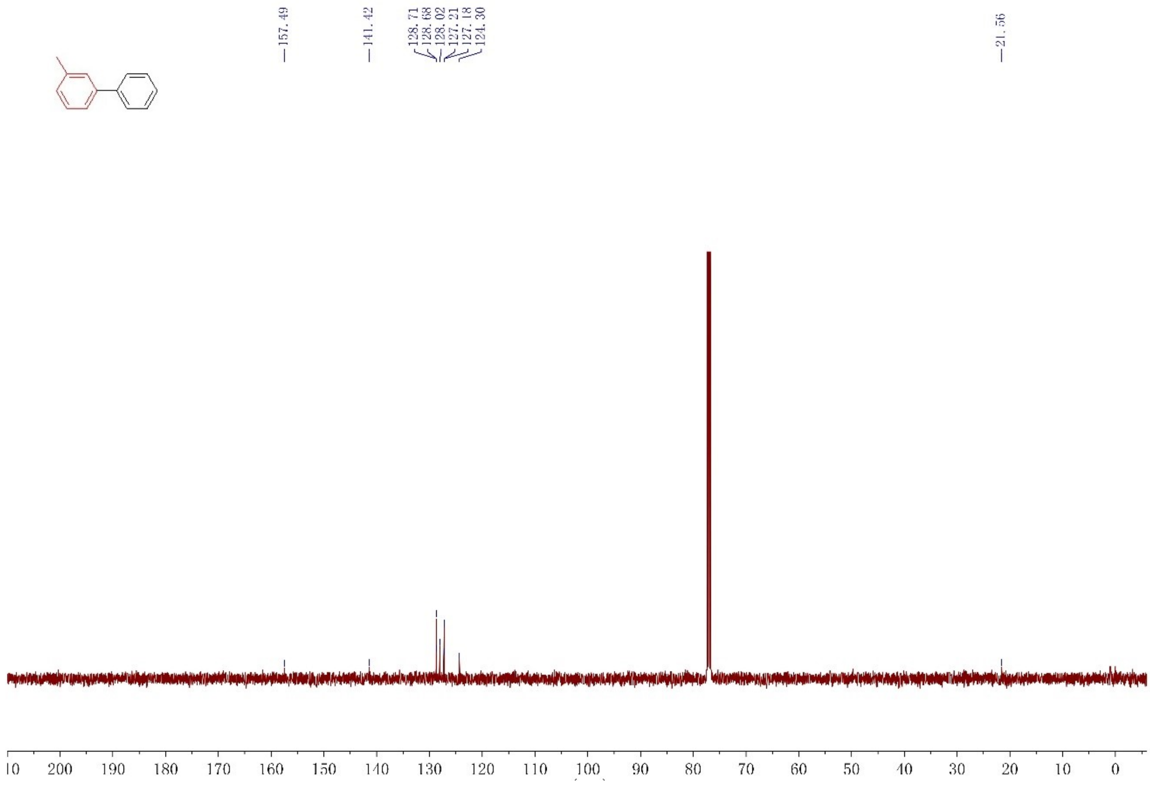

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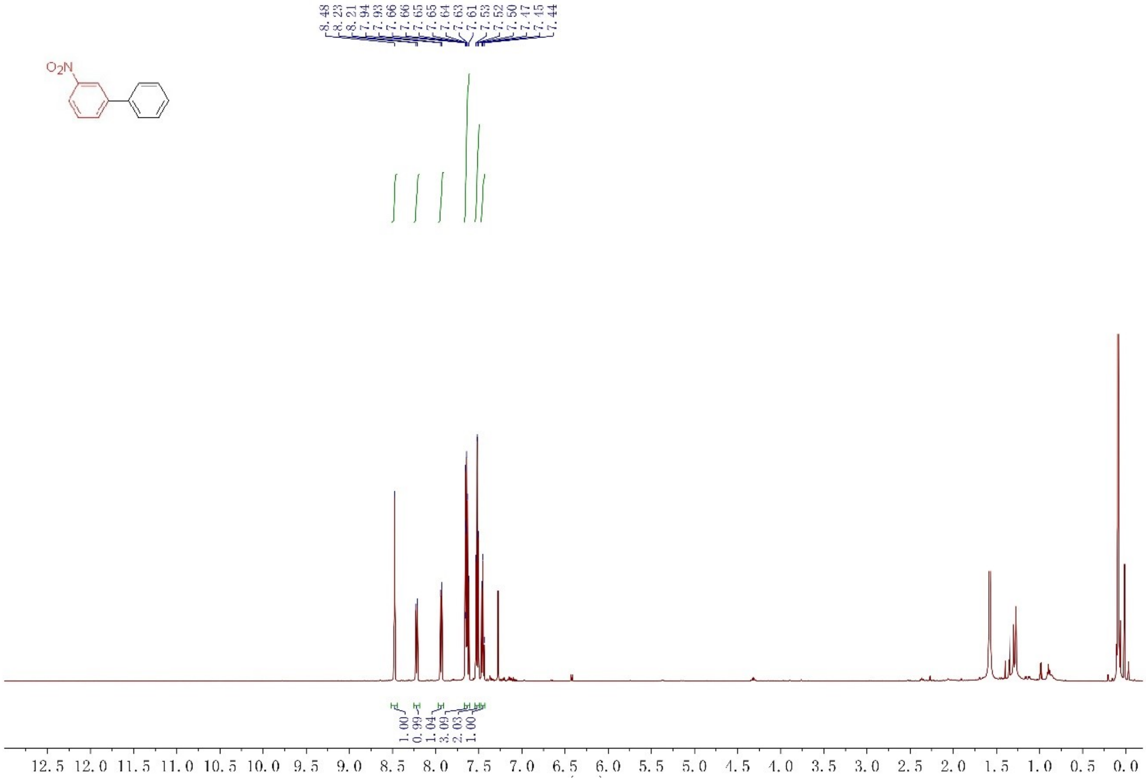
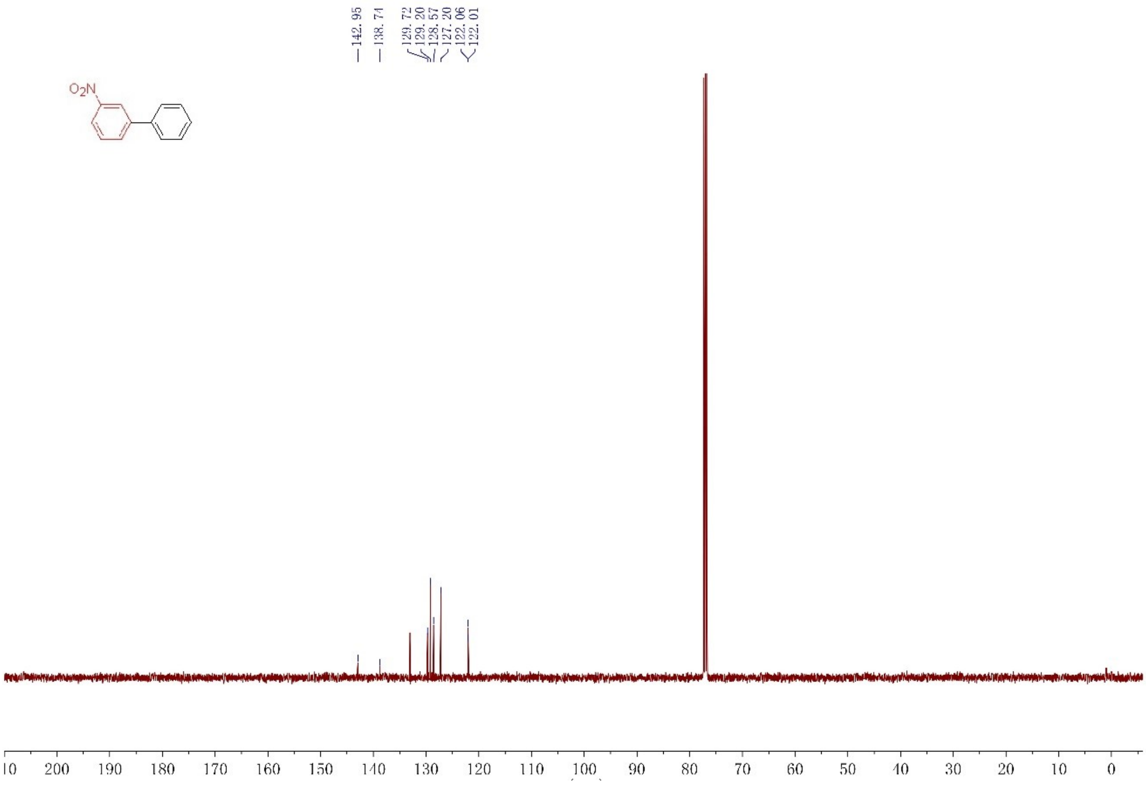
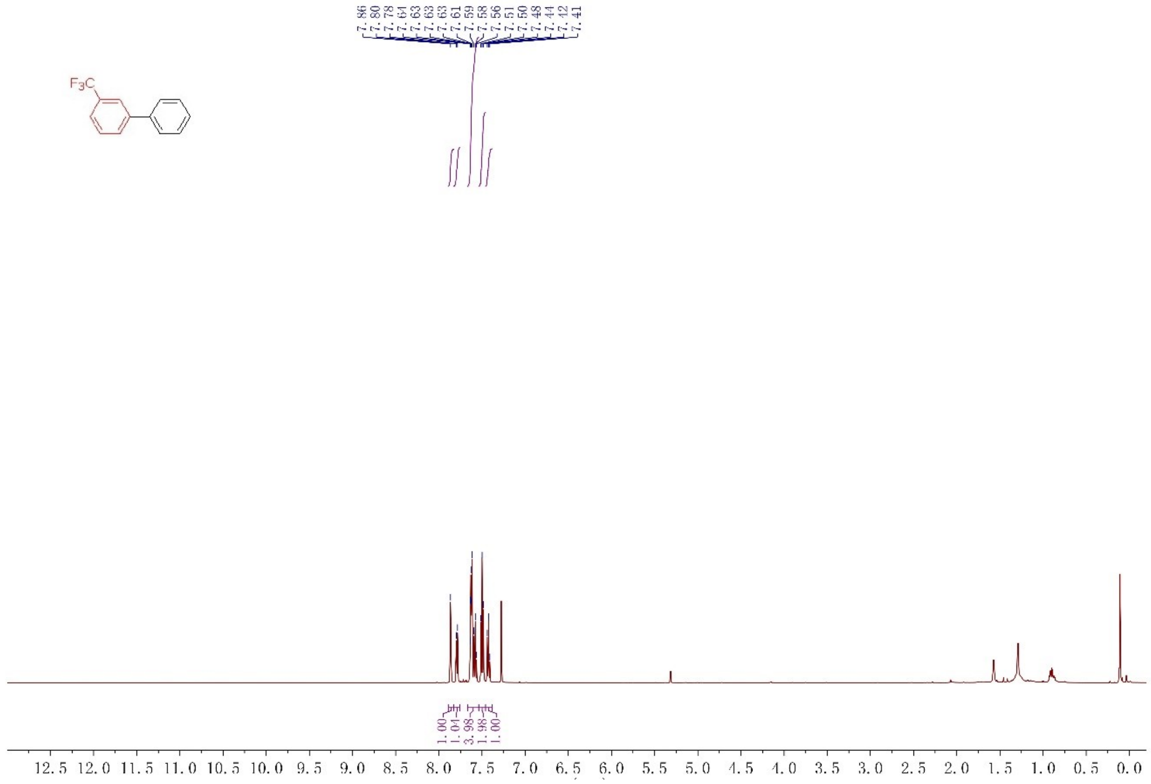


^{13}**C NMR** (126 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



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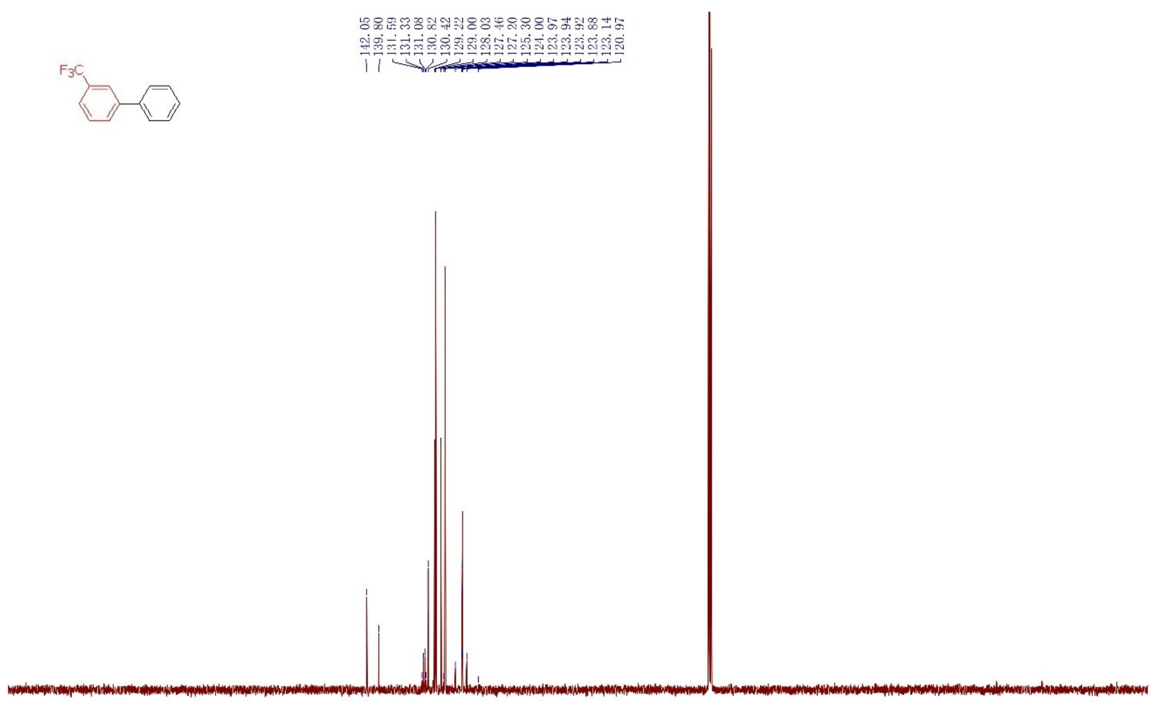

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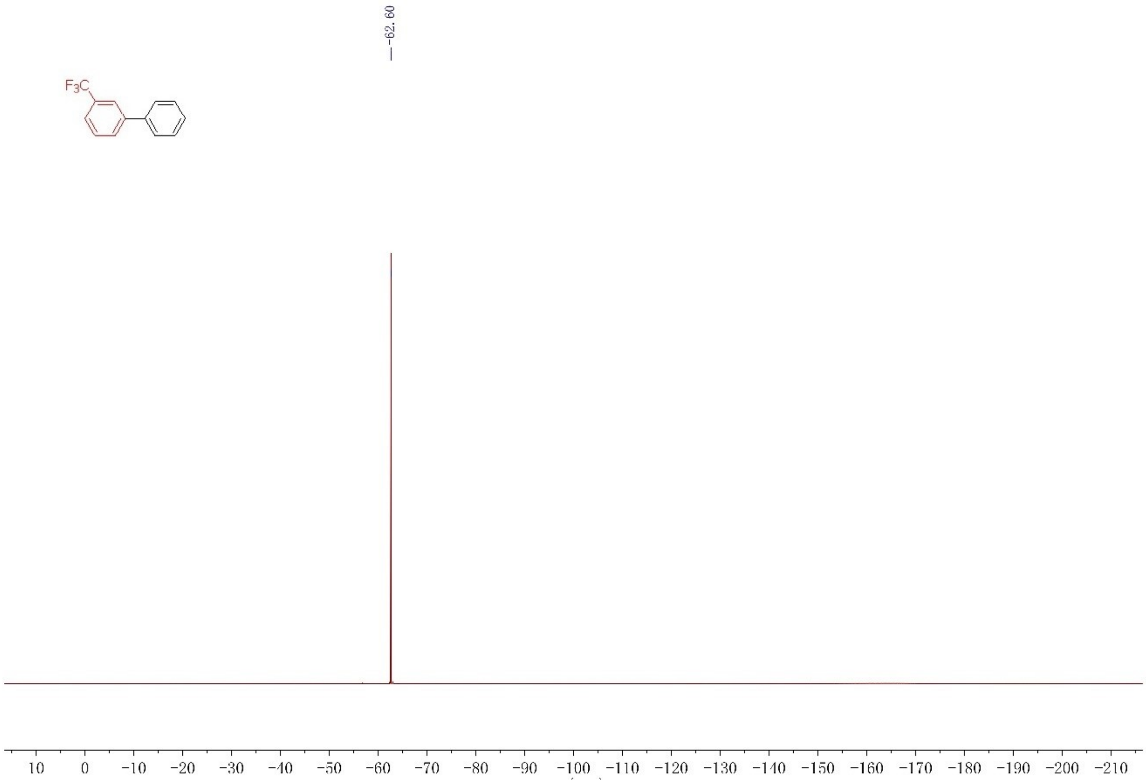

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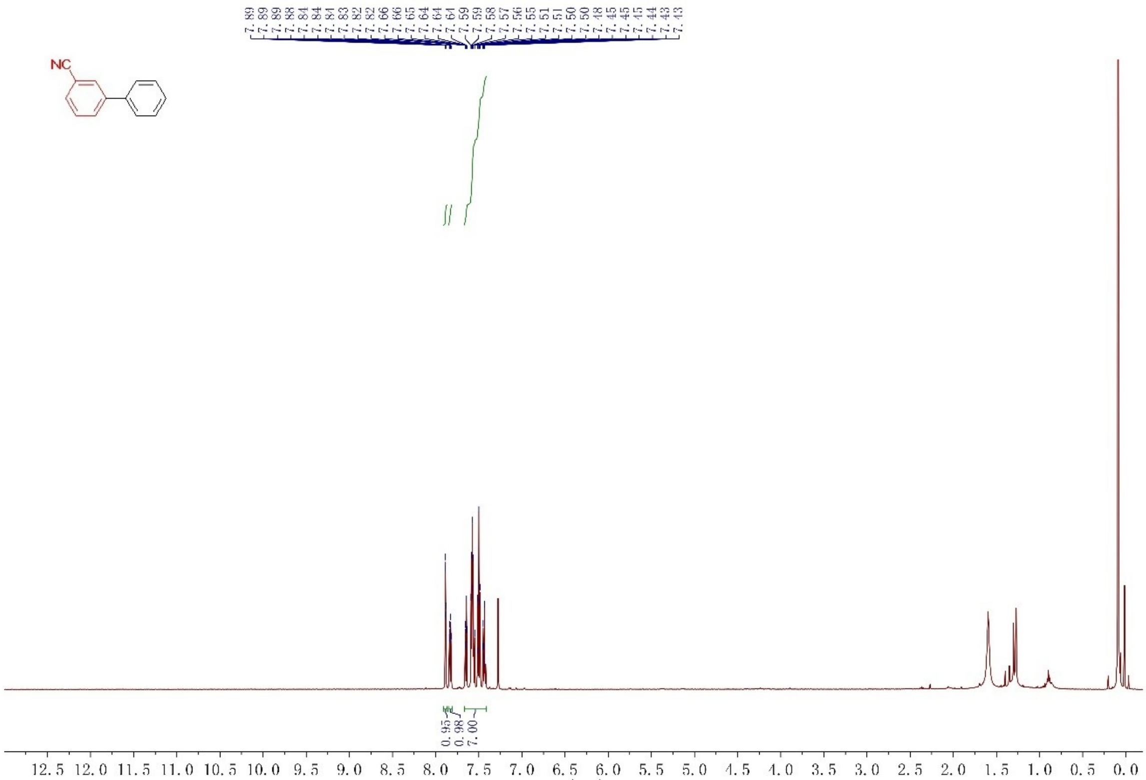

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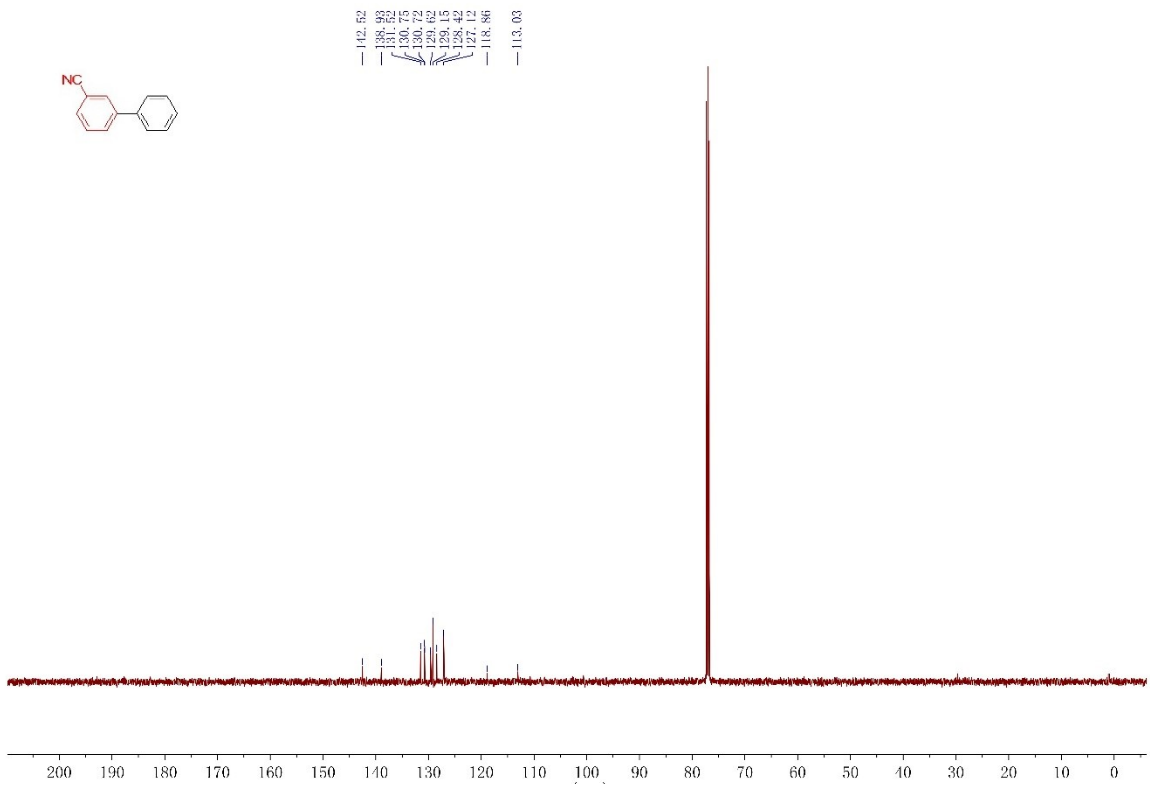

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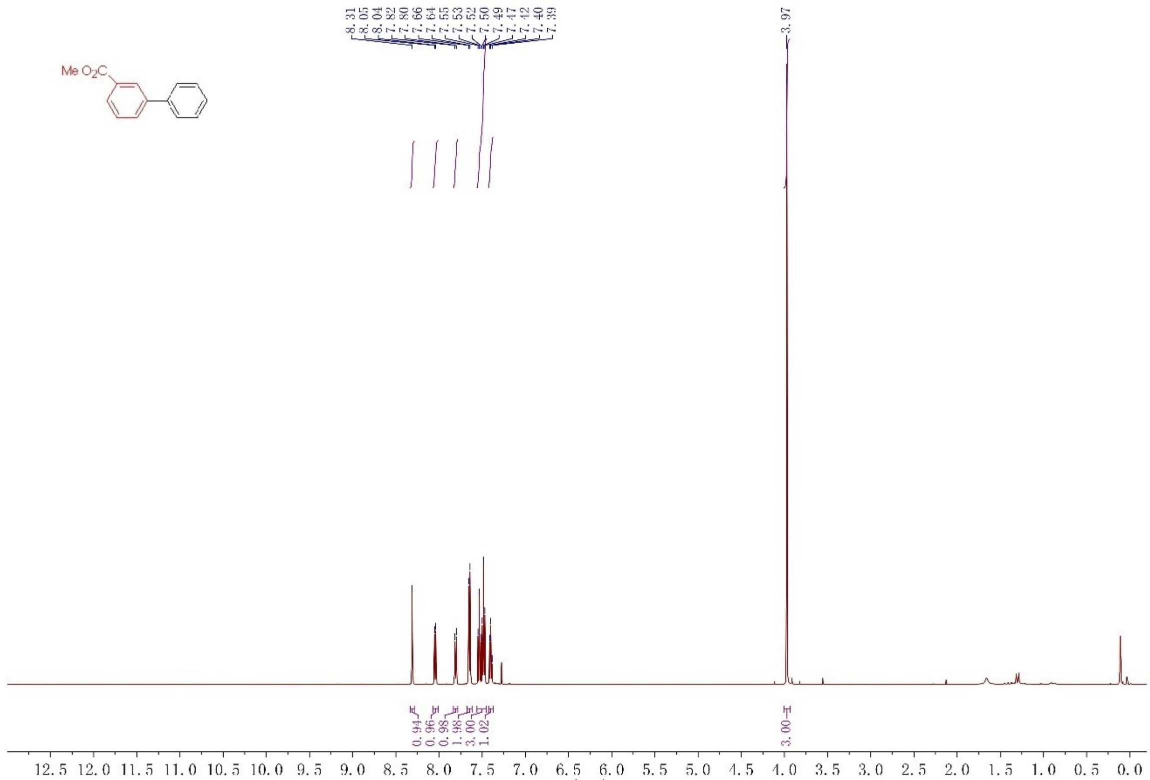
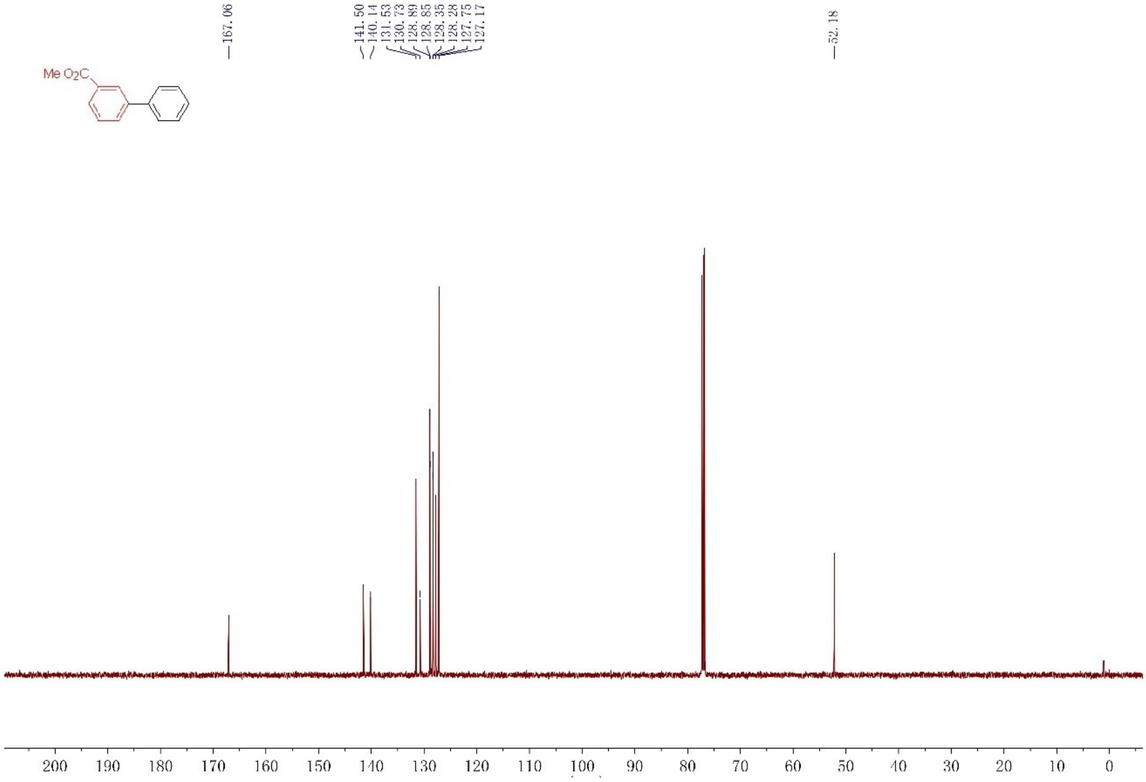
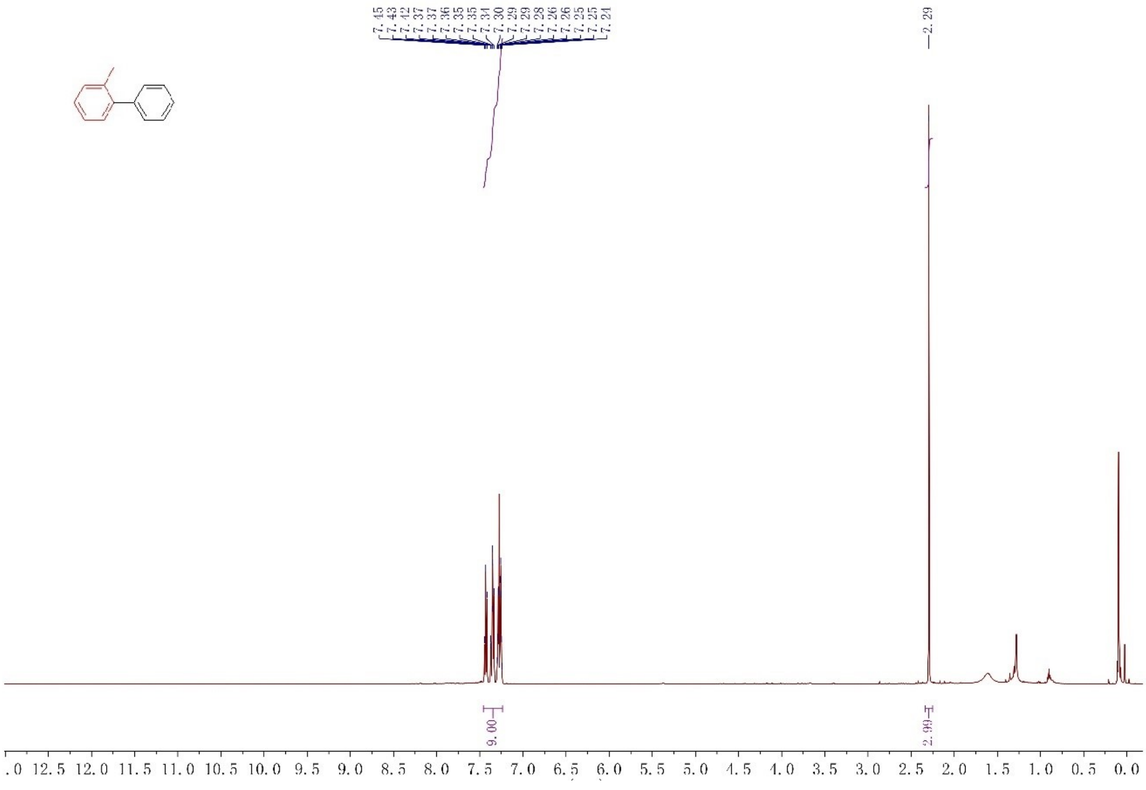


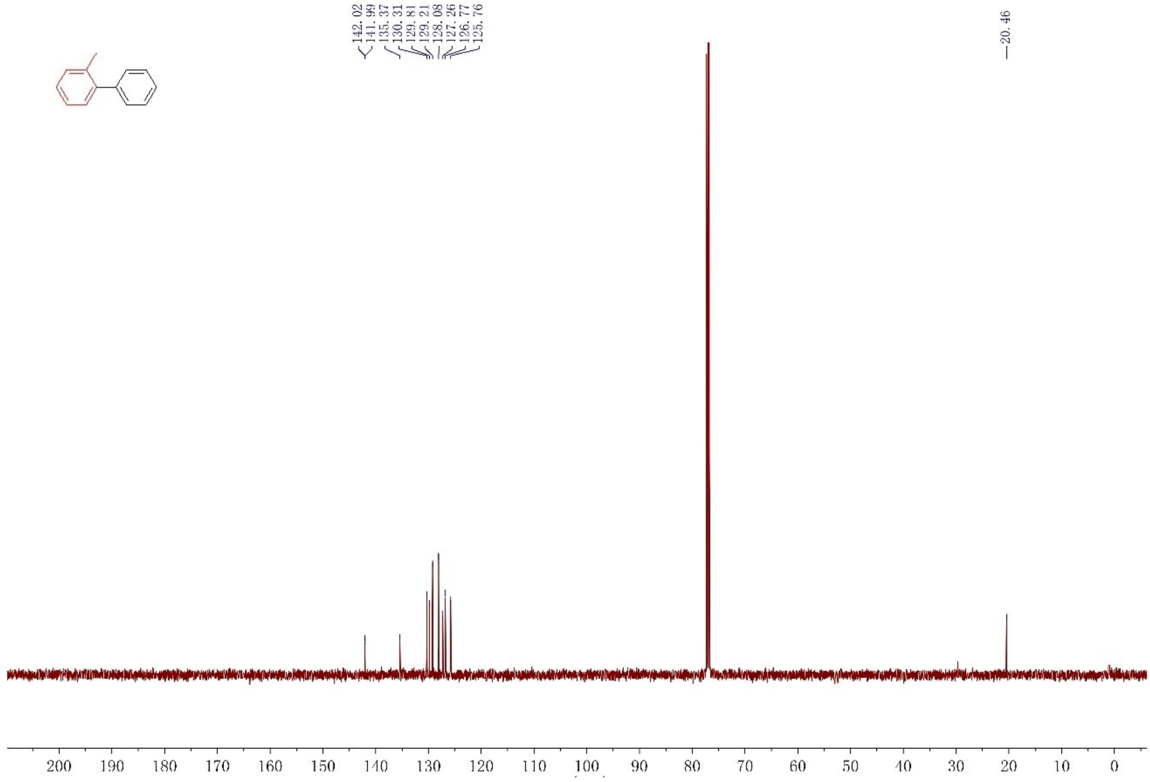
^{13}C NMR (126 MHz, $CDCl_3$)



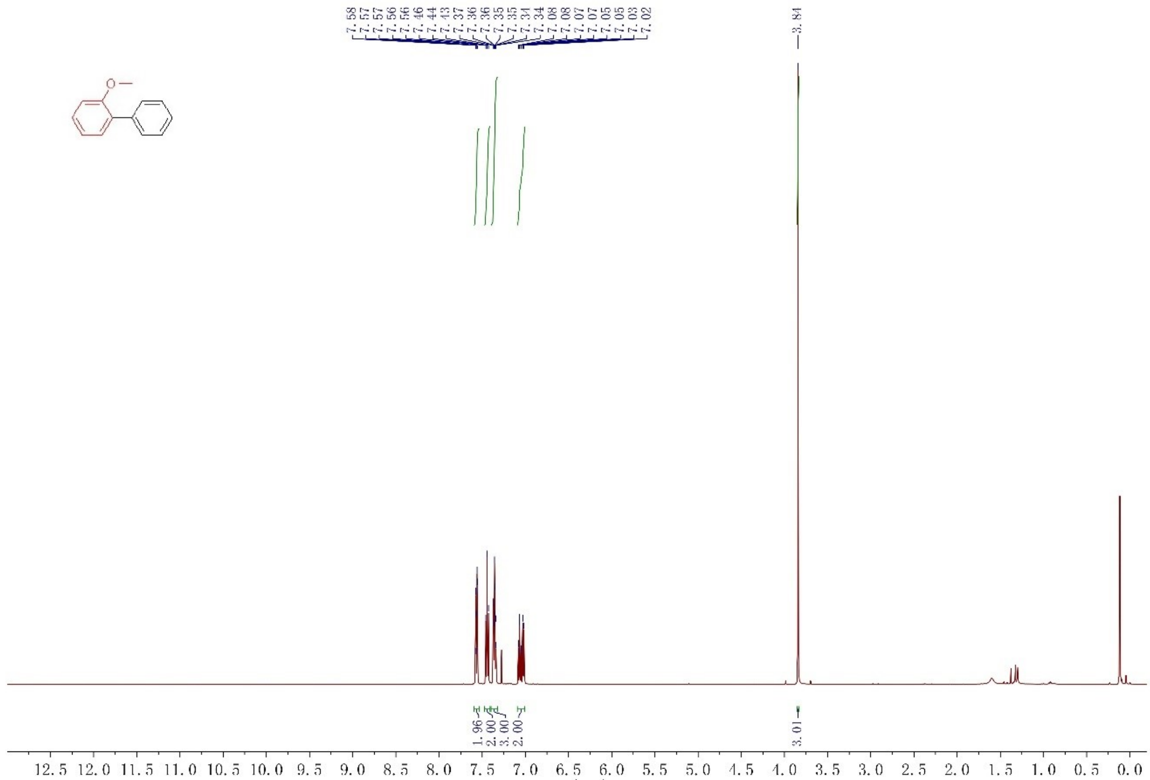
^{1}H NMR (500 MHz, $CDCl_3$)



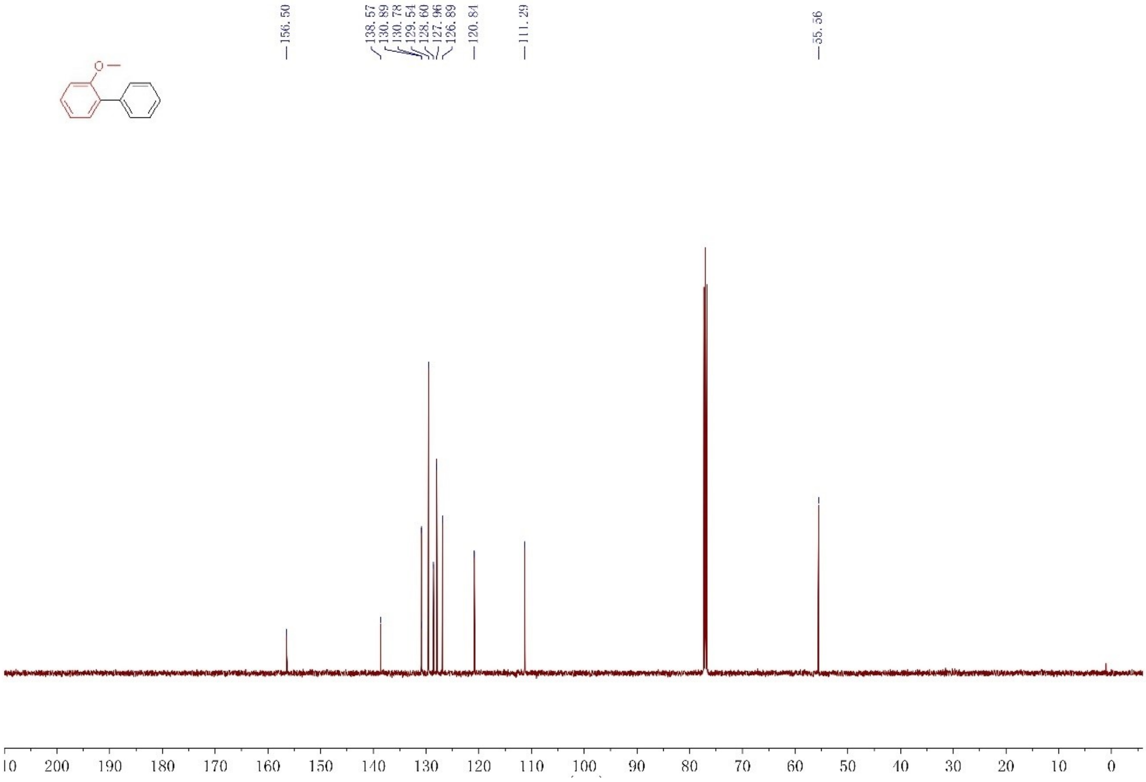
^{13}C NMR (126 MHz, $CDCl_3$)



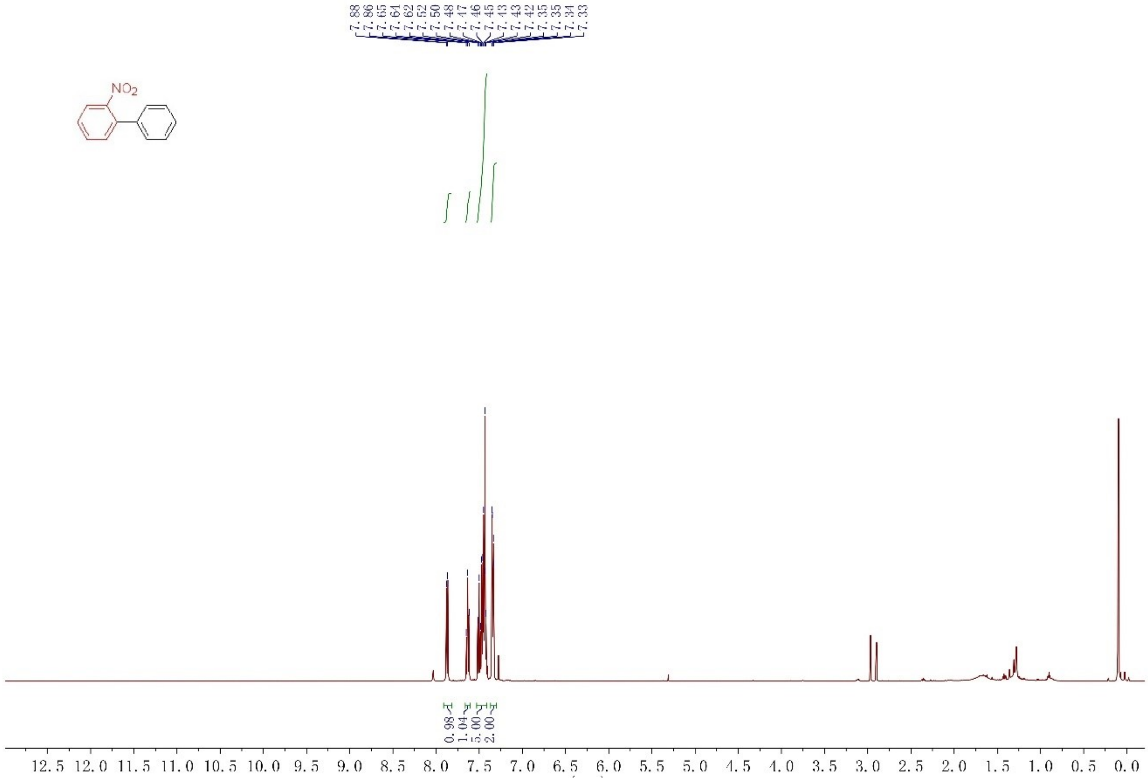
^{1}H NMR (500 MHz, $CDCl_3$)



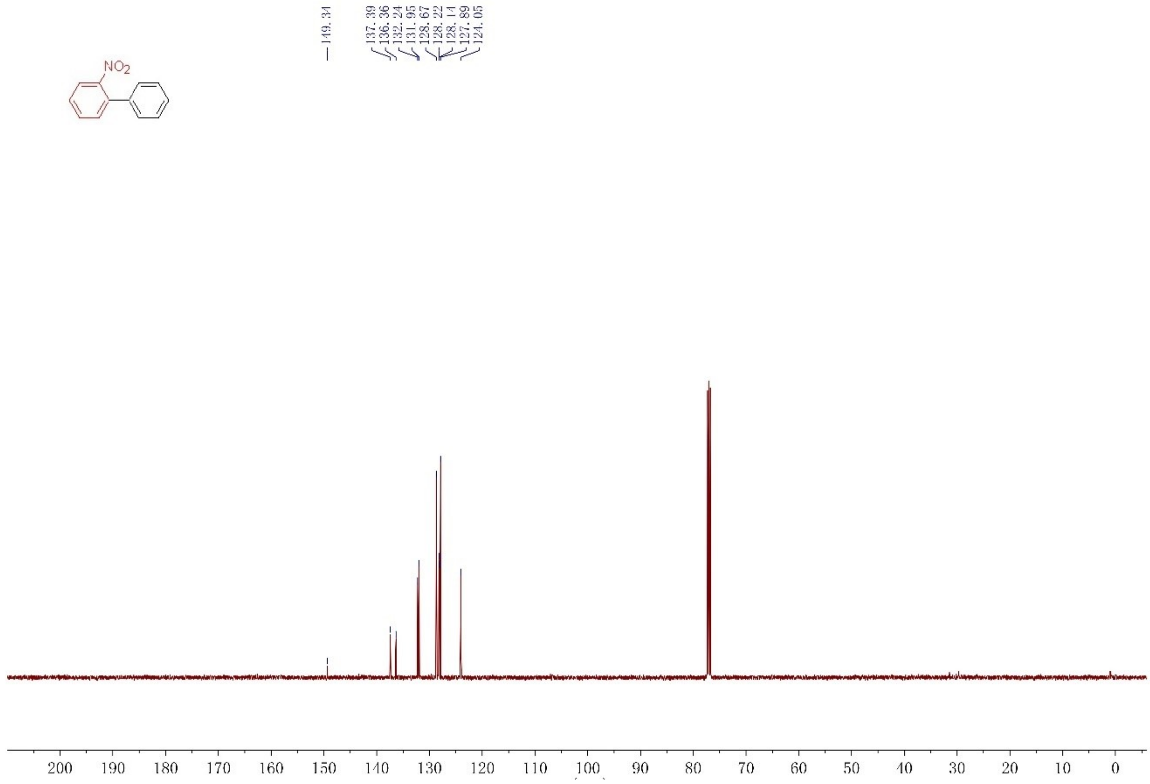
^{13}**C NMR** (126 MHz, $CDCl_3$)



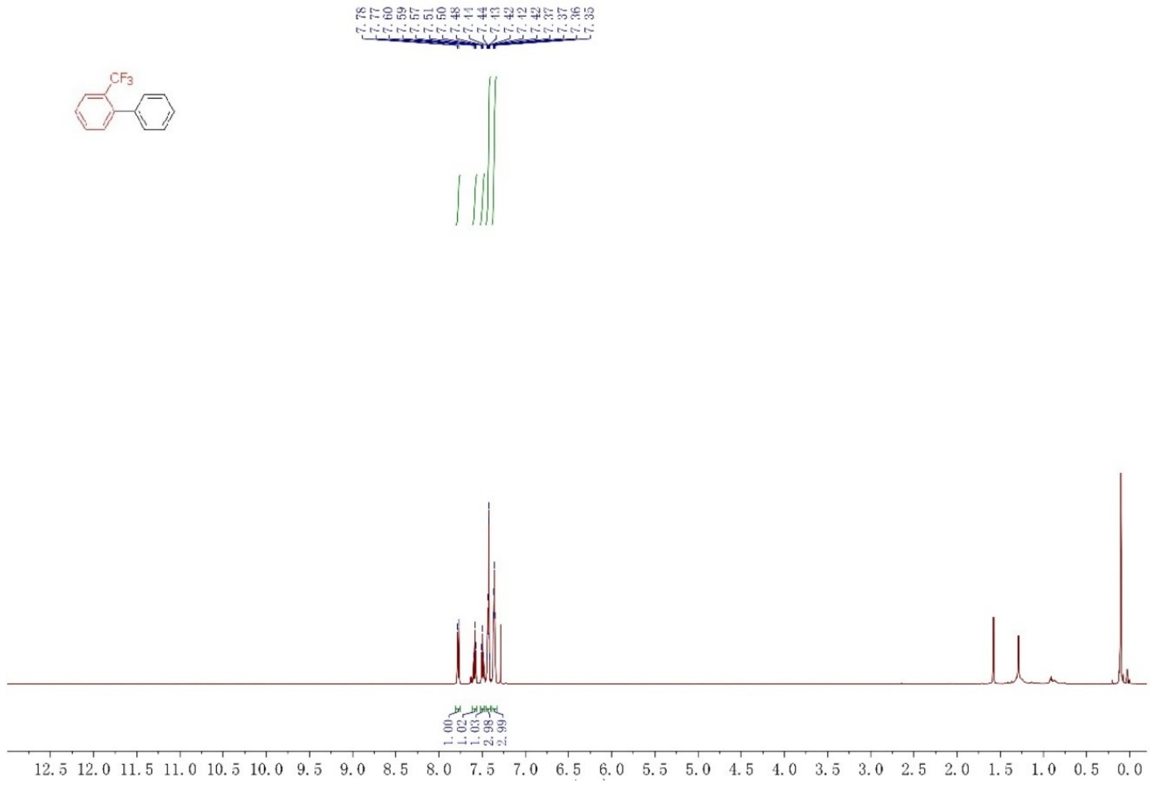
^{1}**H NMR** (500 MHz, $CDCl_3$)



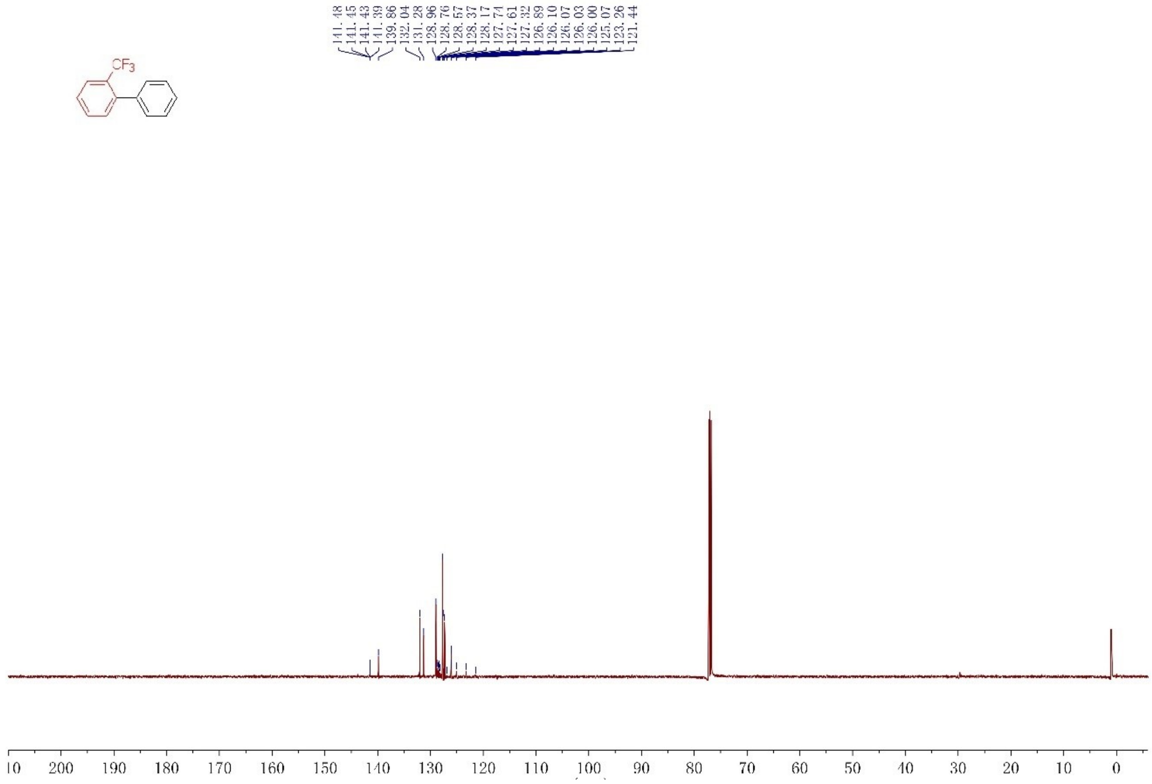
^{13}C NMR (126 MHz, $CDCl_3$)



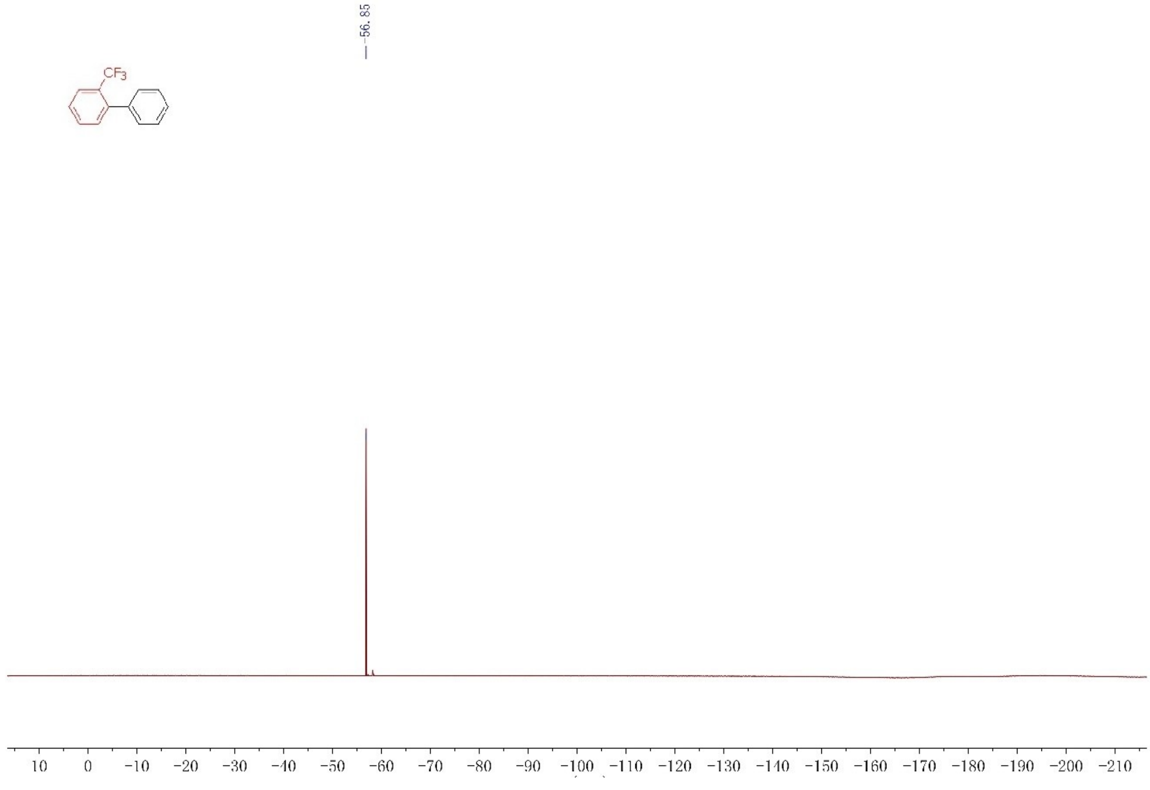
^{1}H NMR (600 MHz, $CDCl_3$)



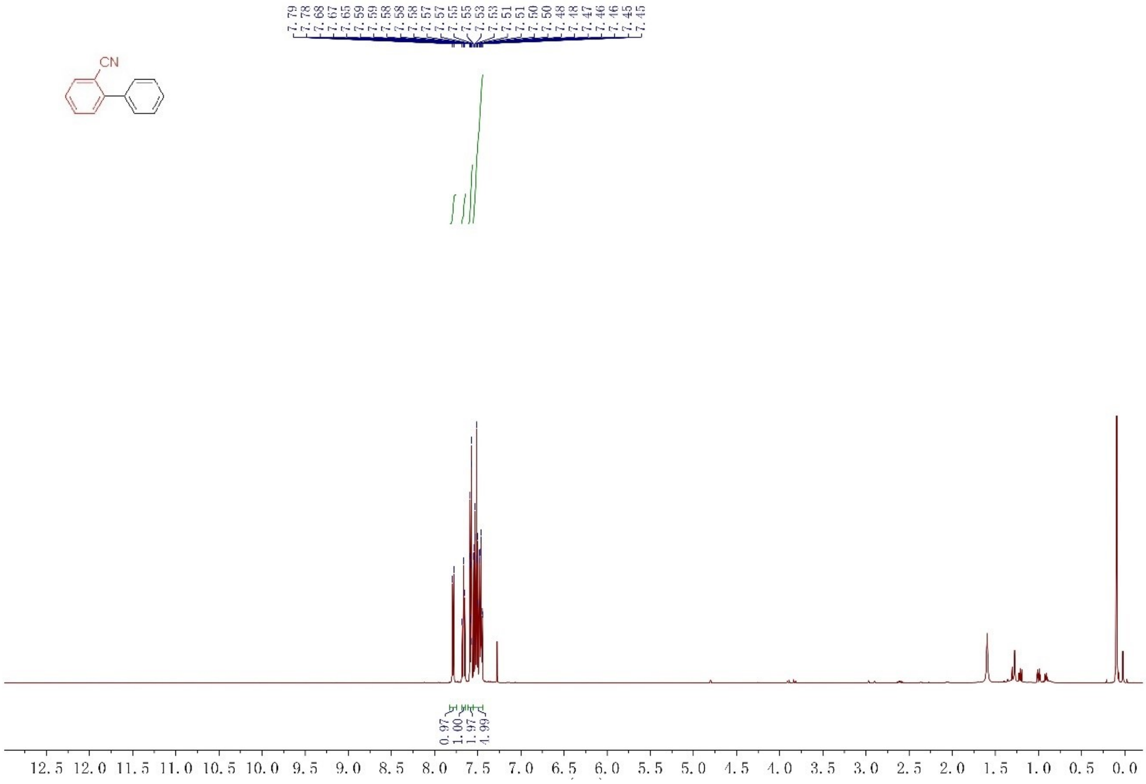
^{13}C NMR (151 MHz, $CDCl_3$)



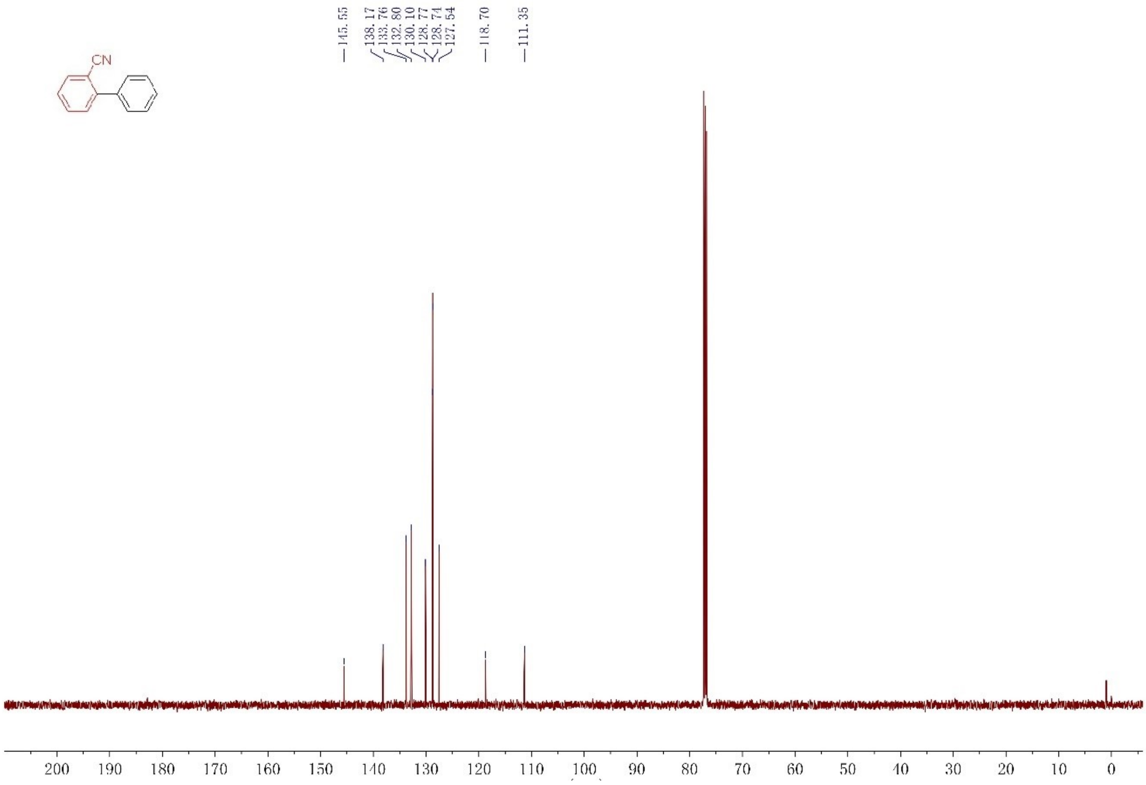
^{19}F NMR (565 MHz, $CDCl_3$)



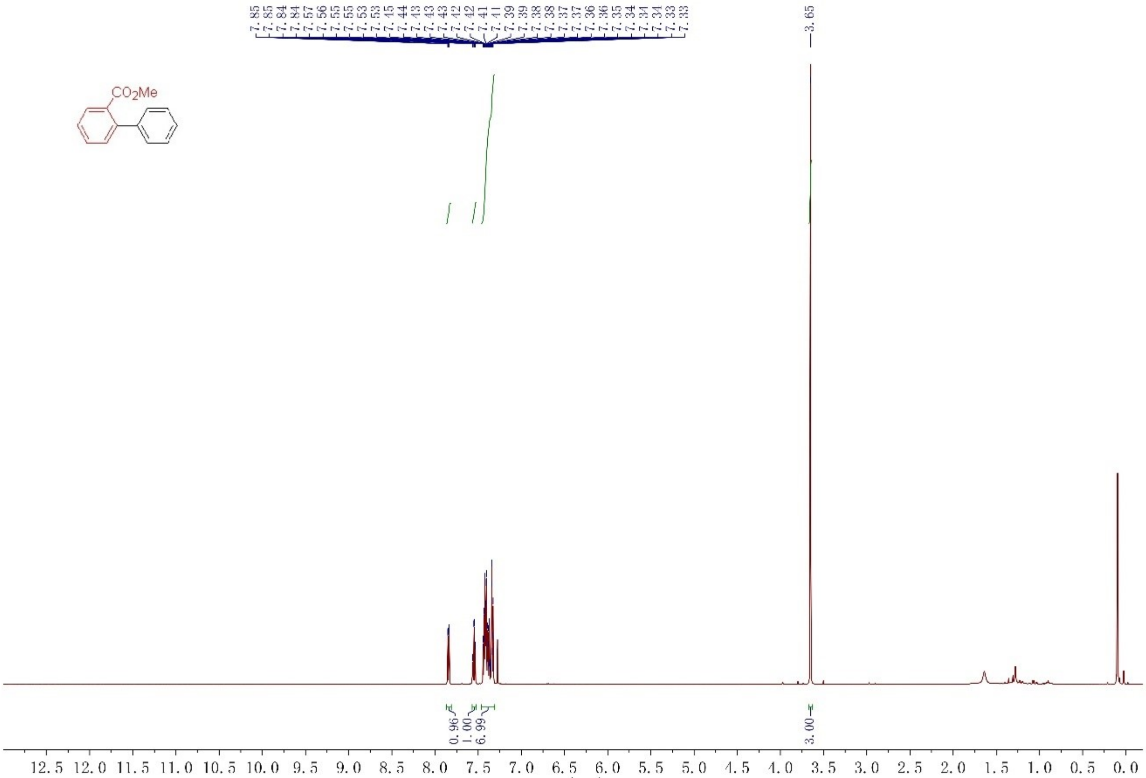
^{1}H NMR (500 MHz, $CDCl_3$)



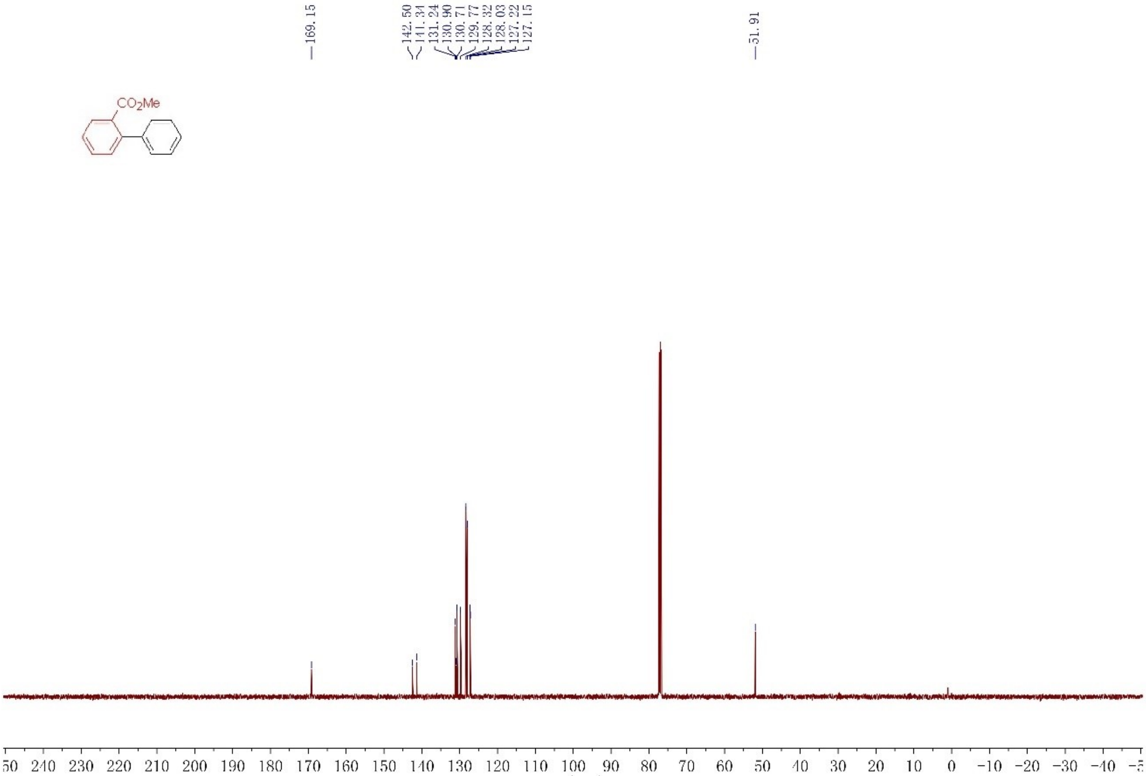
^{13}C NMR (126 MHz, $CDCl_3$)



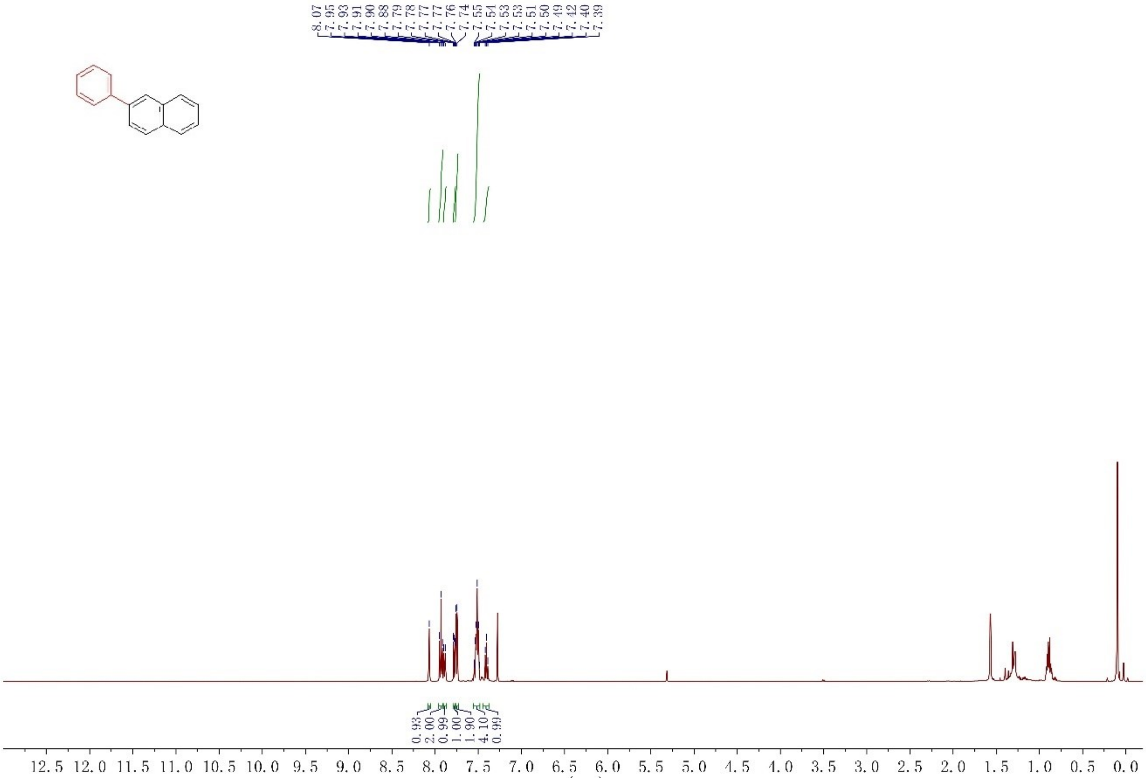
^{1}H NMR (500 MHz, $CDCl_3$)



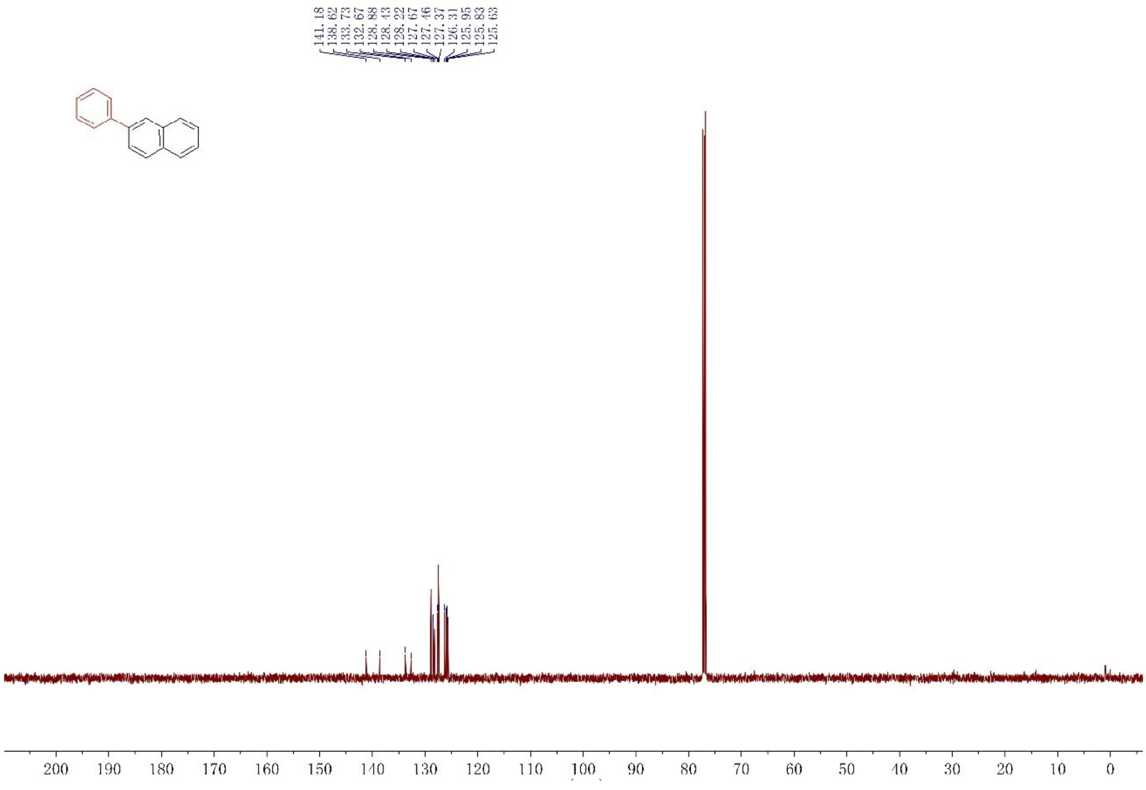
^{13}C NMR (126 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (126 MHz, $CDCl_3$)



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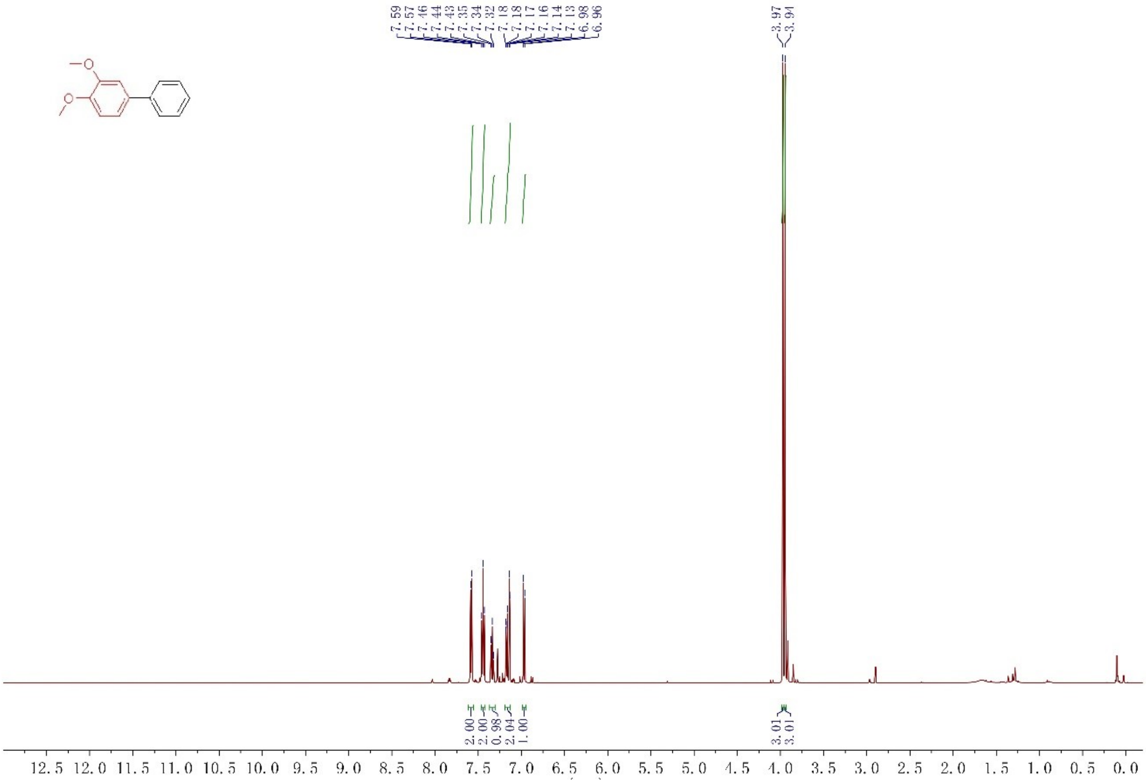
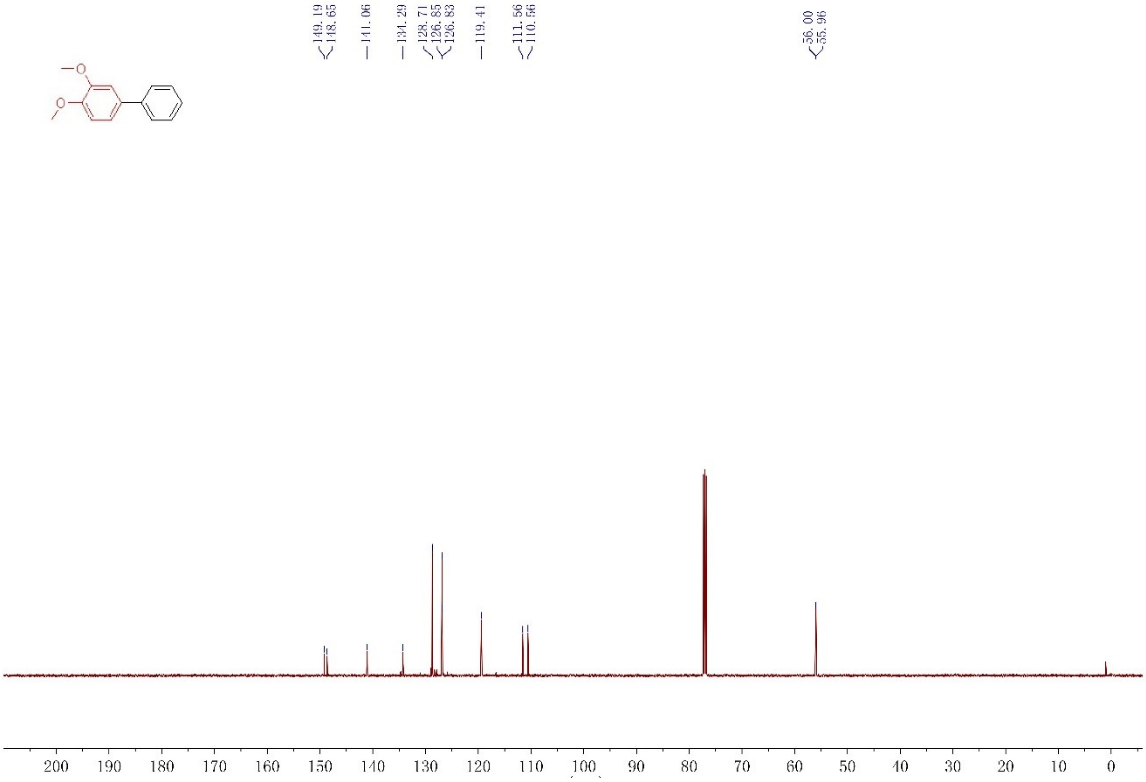


[13]C NMR (126 MHz, $CDCl_3$)



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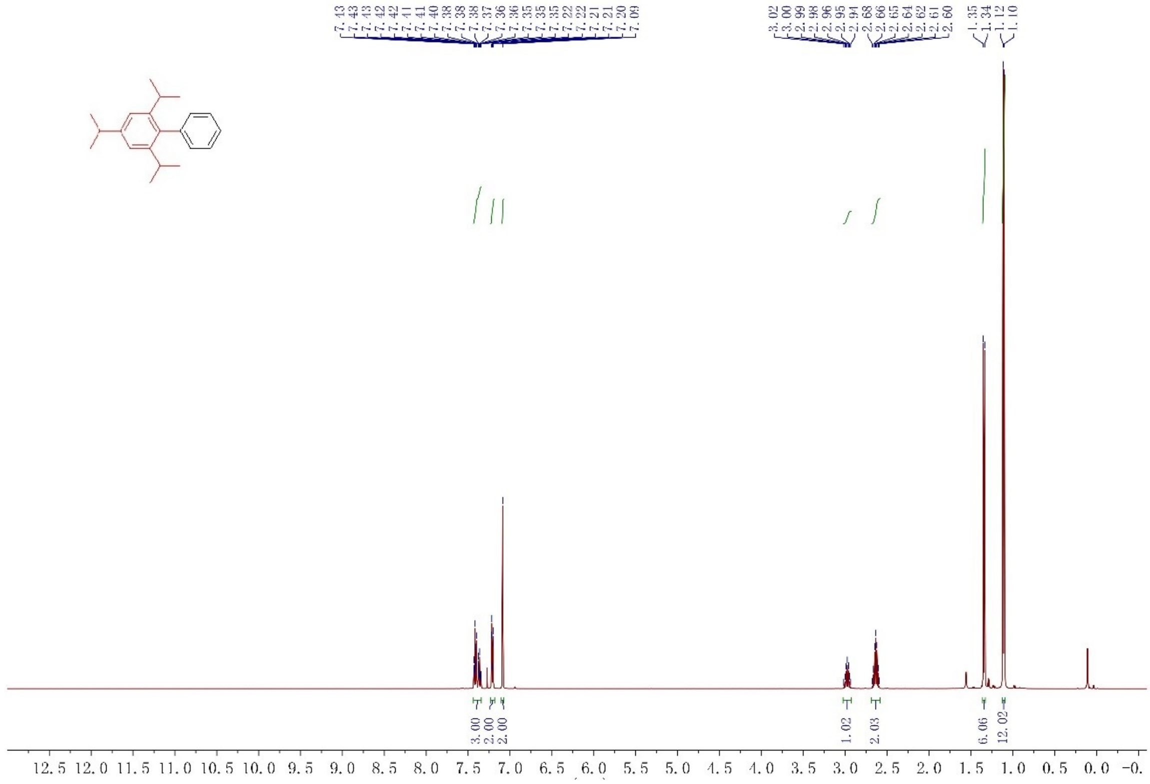
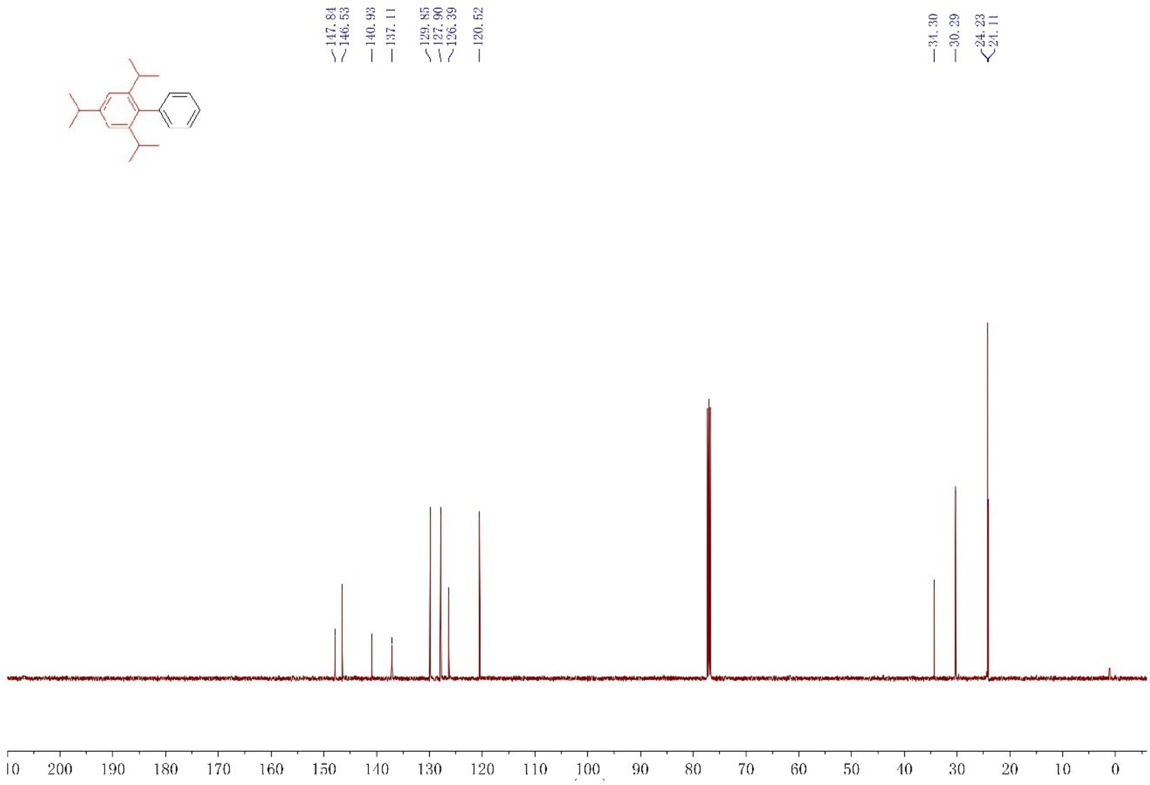


[13]C NMR (126 MHz, $CDCl_3$)



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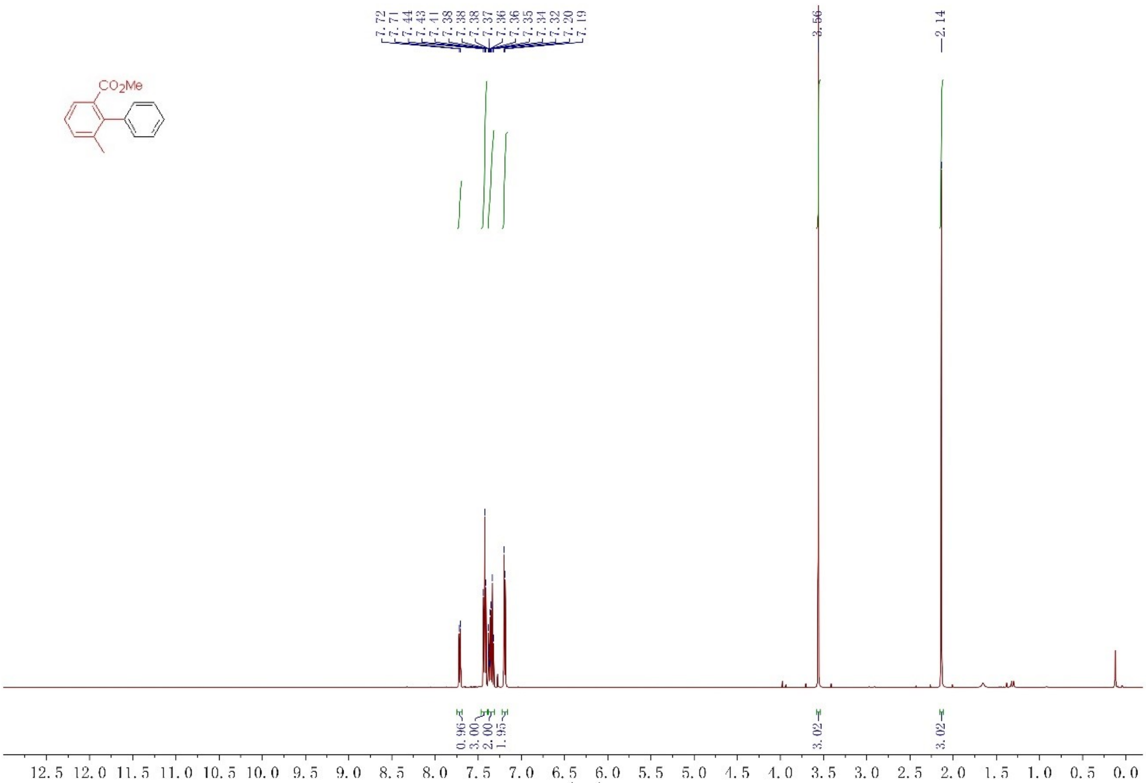
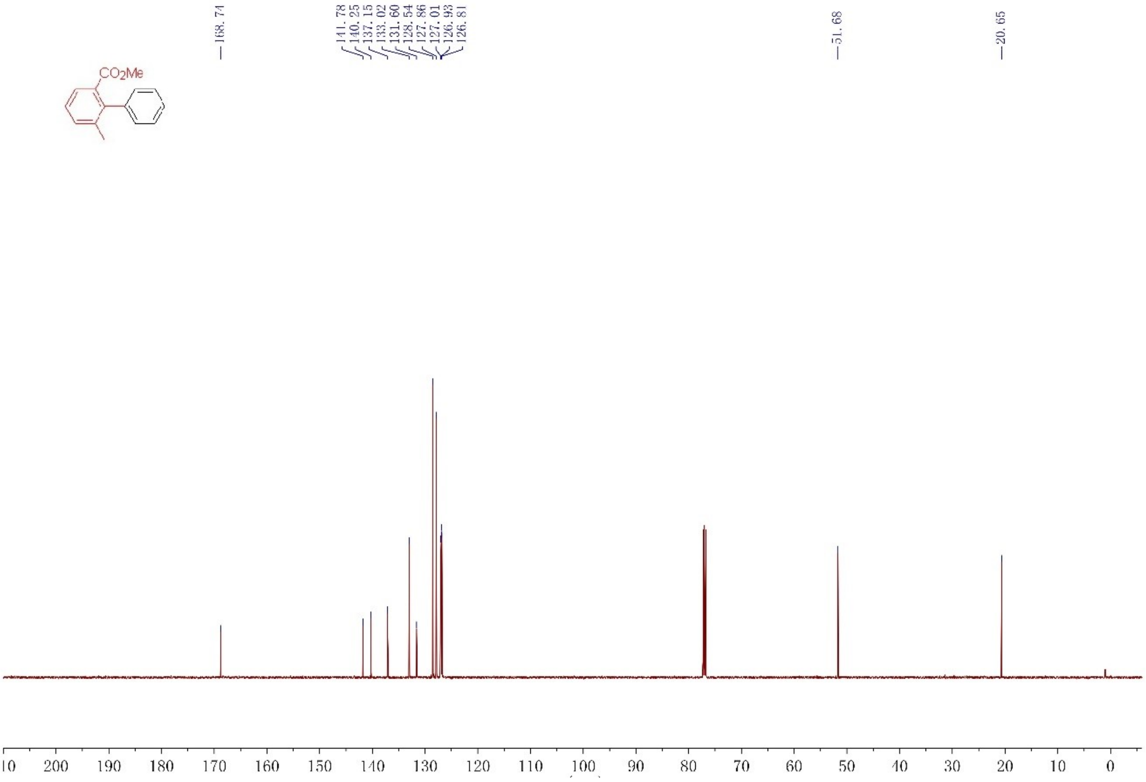


[13]C NMR (126 MHz, $CDCl_3$)



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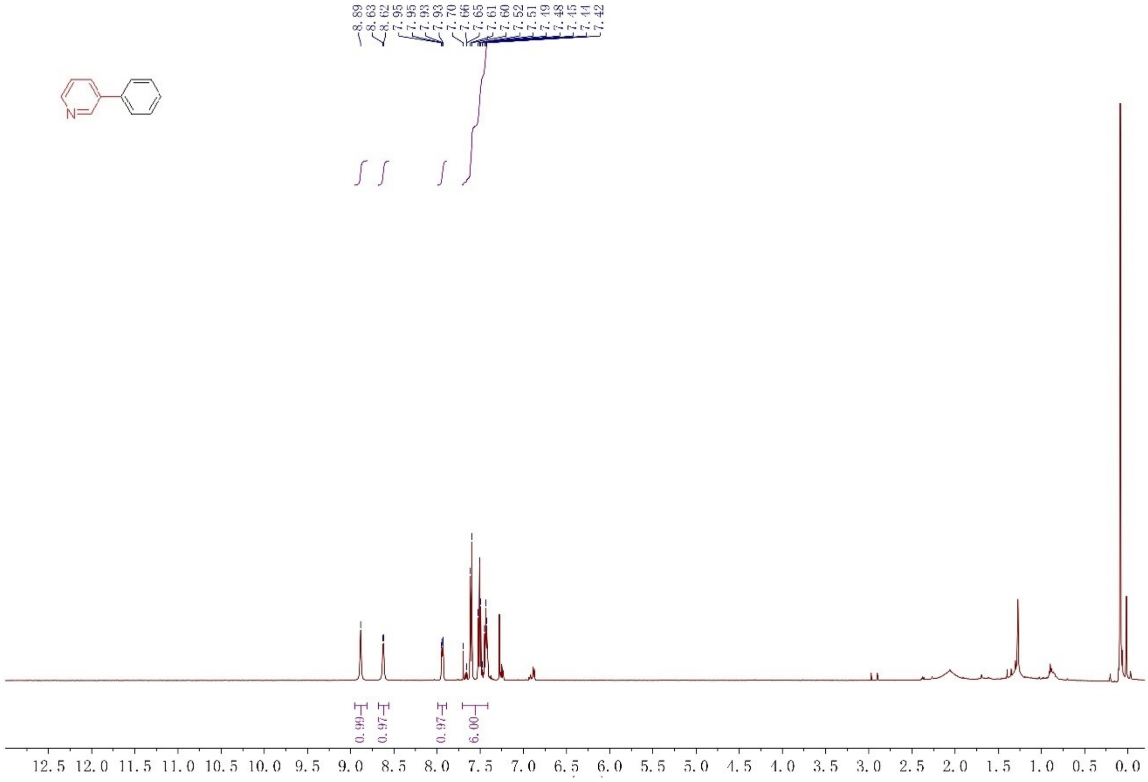

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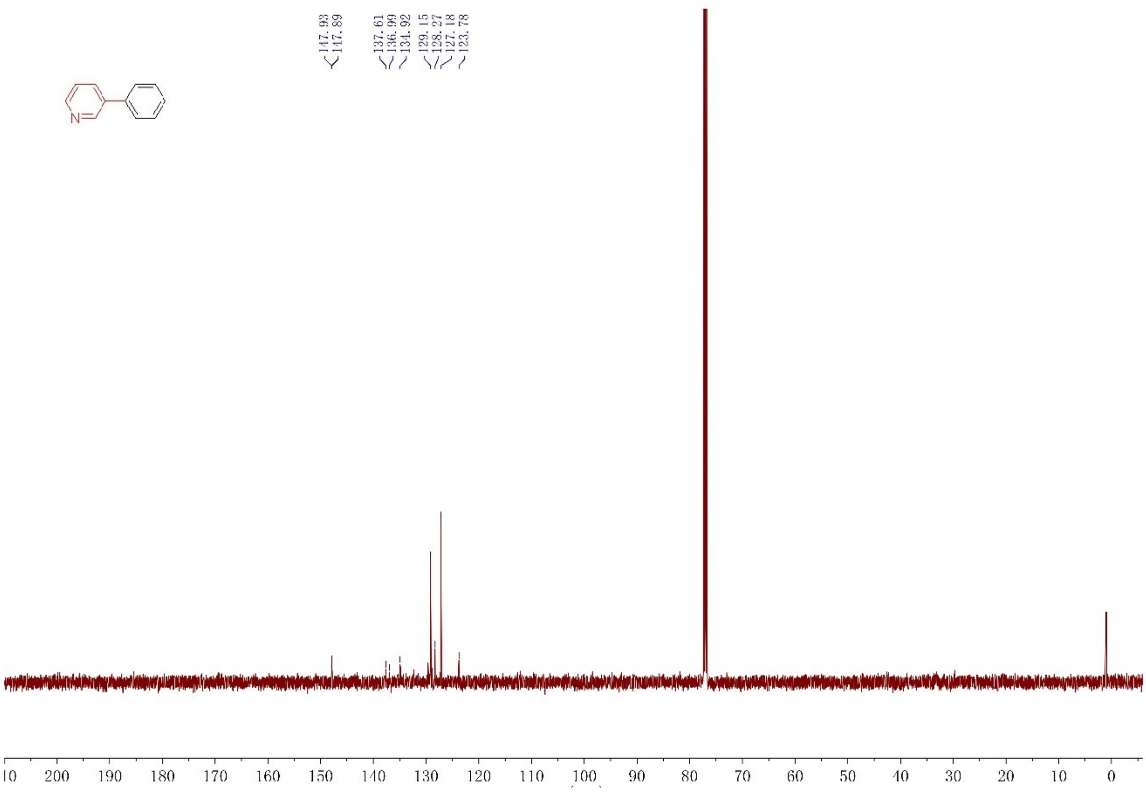

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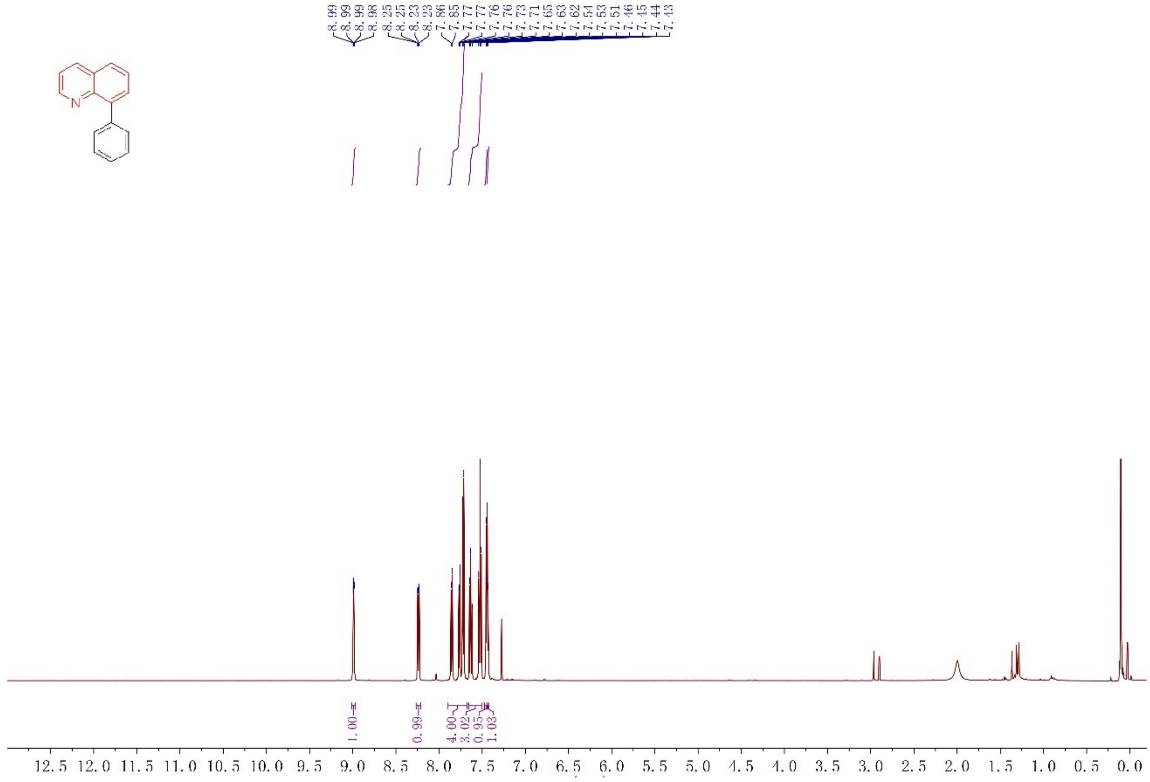

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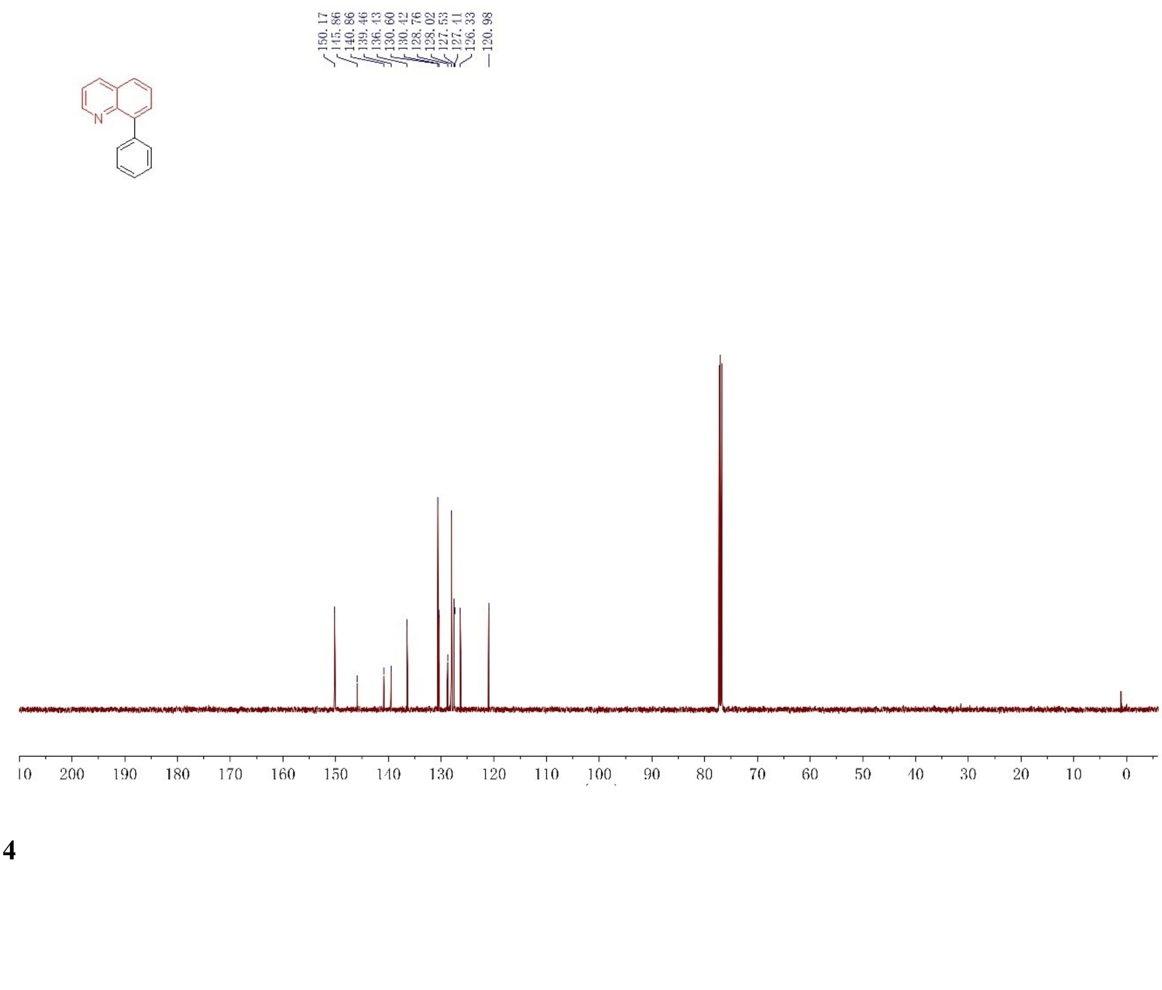

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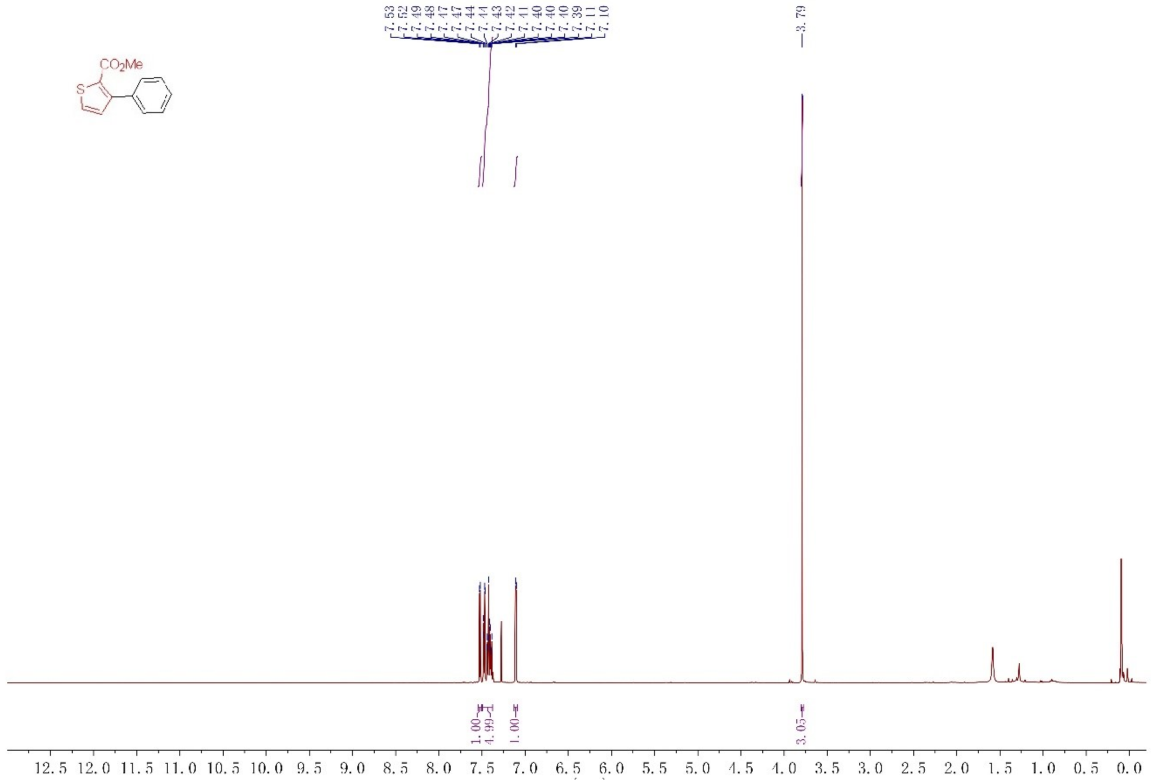

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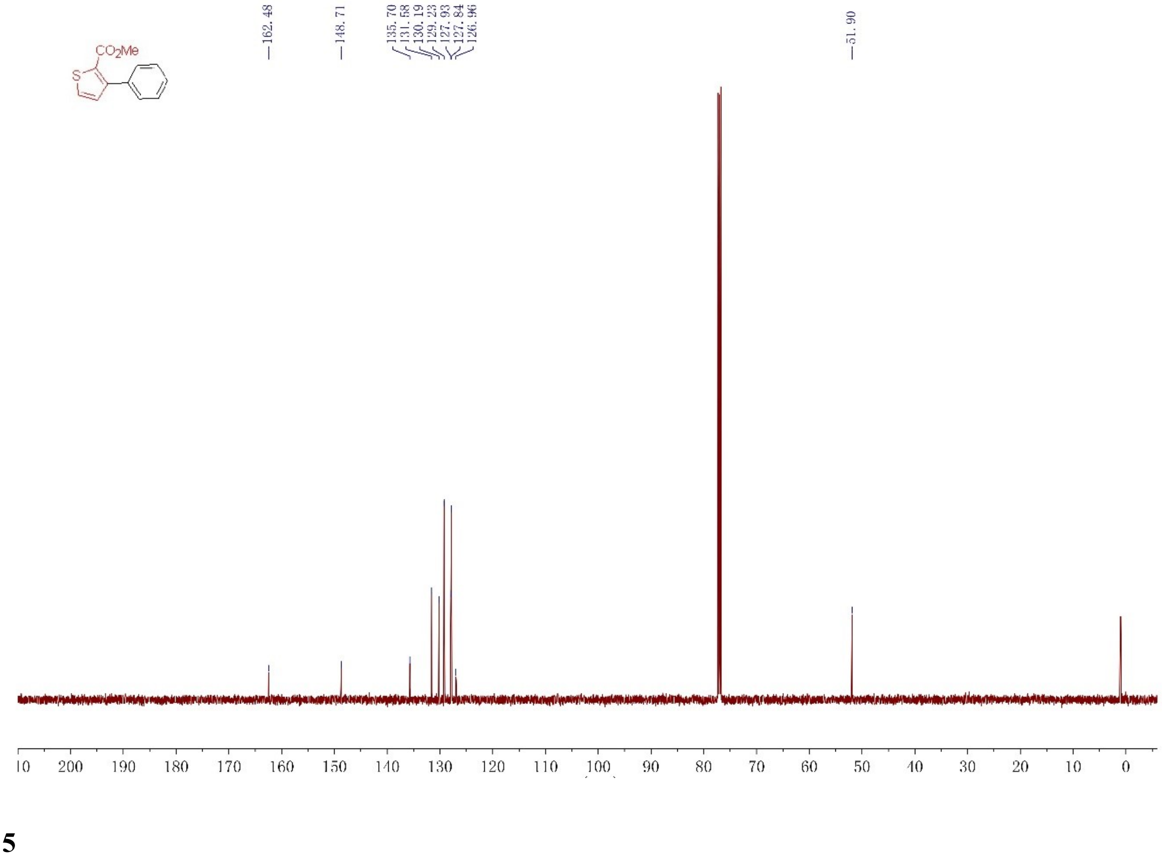

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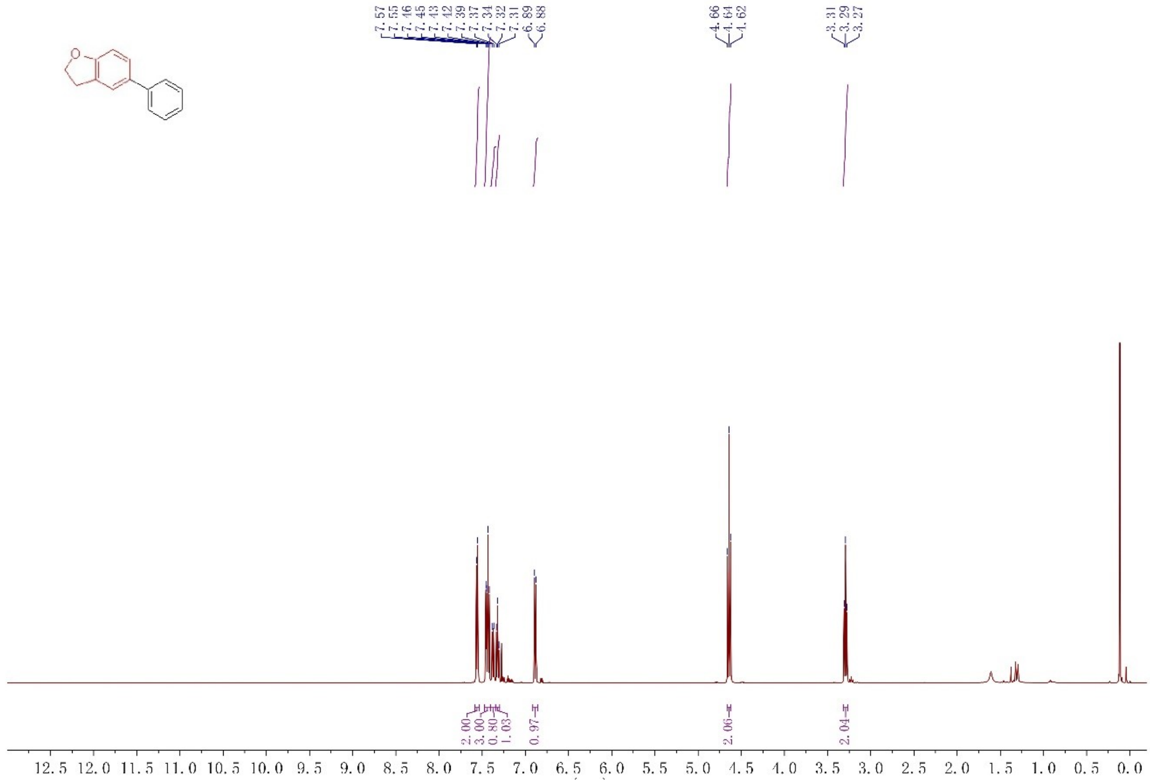

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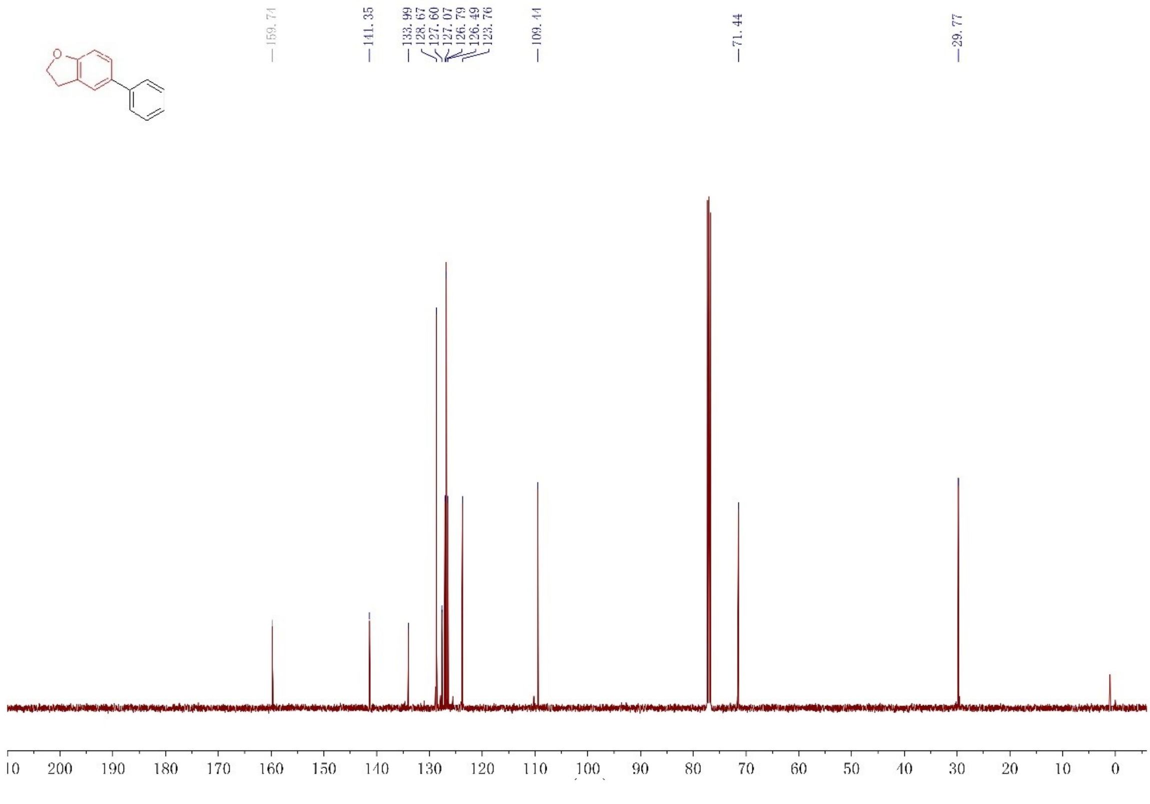

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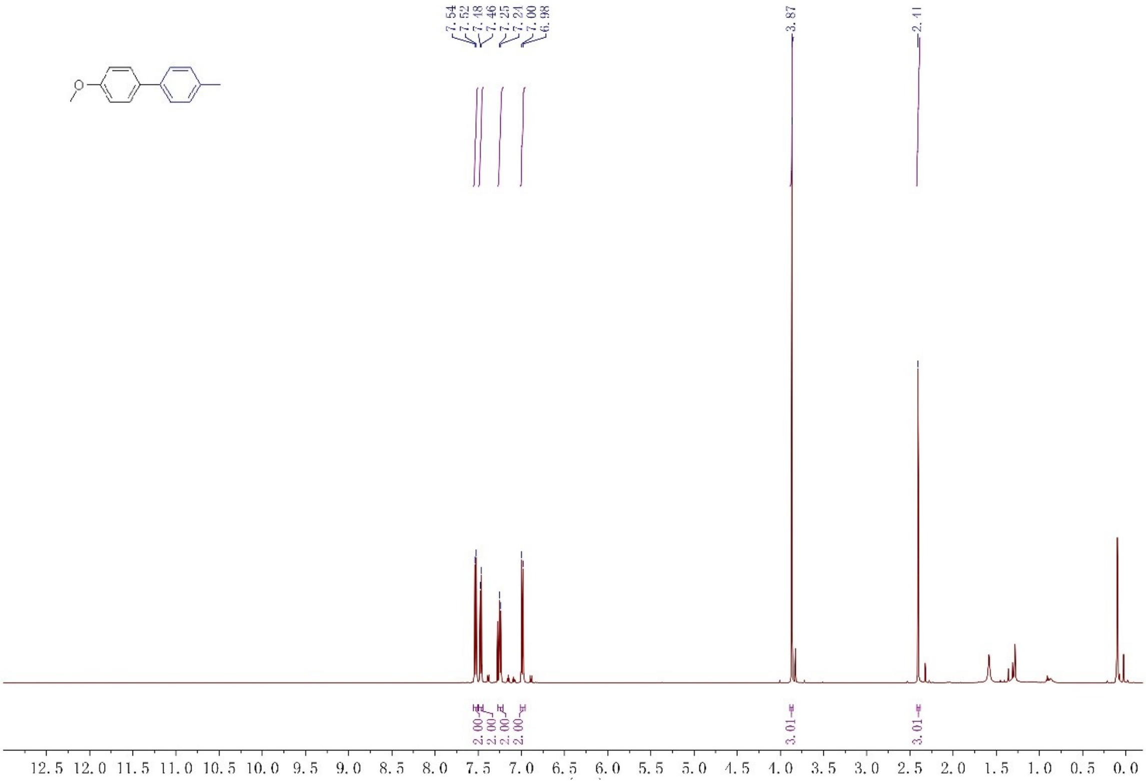
[1]H NMR (500 MHz, $CDCl_3$)



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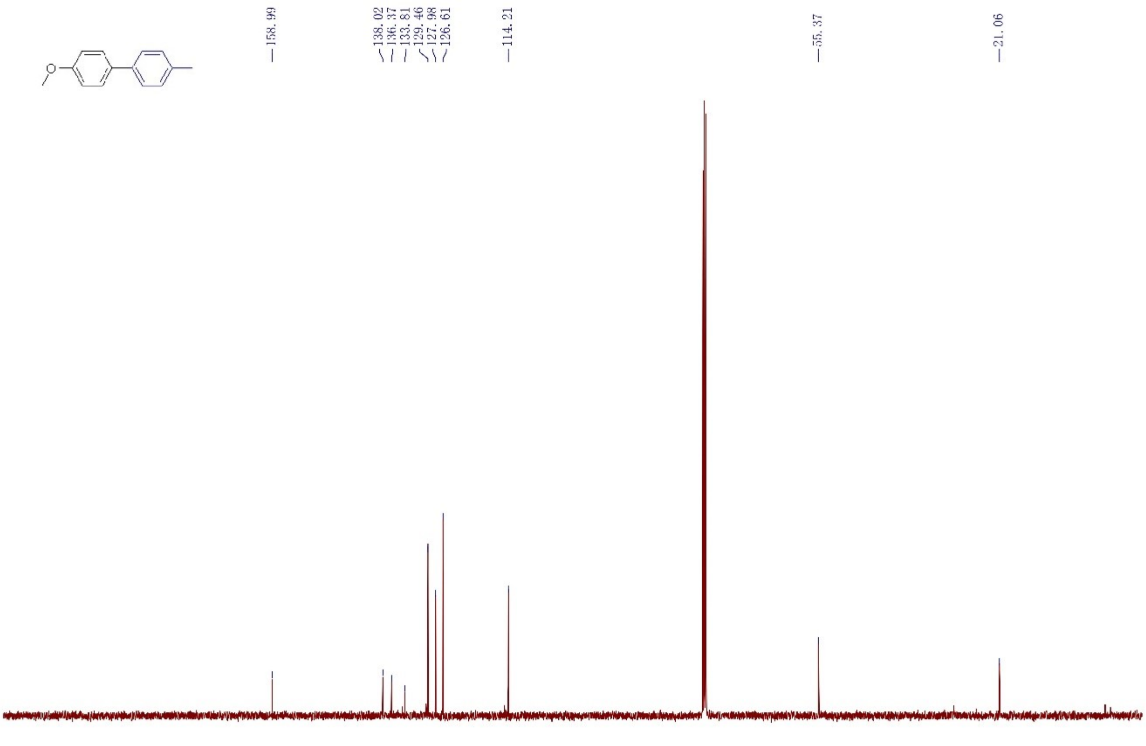

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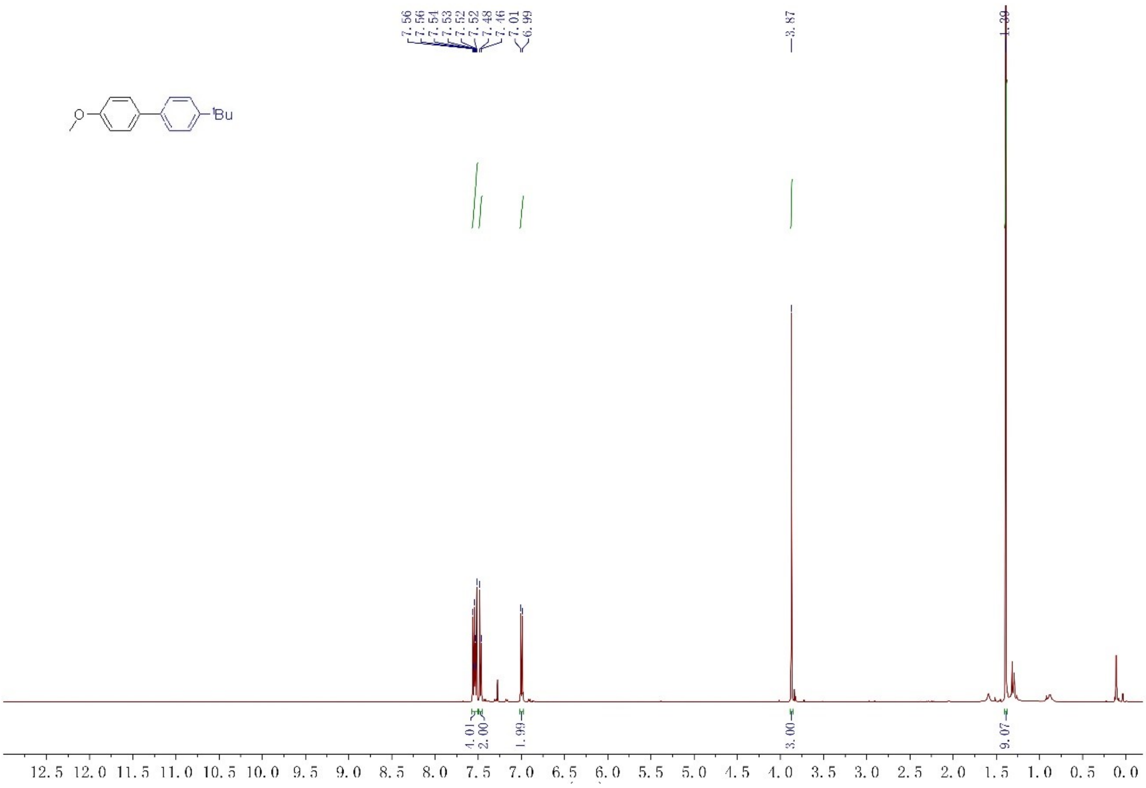

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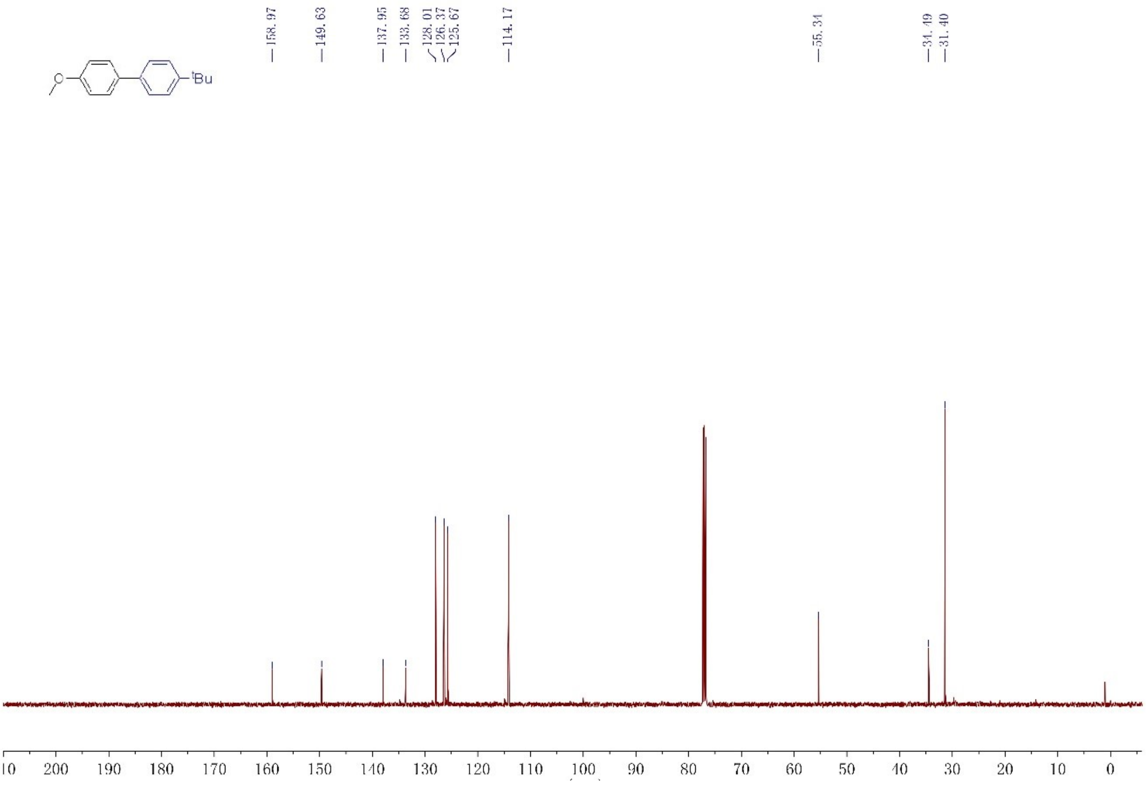

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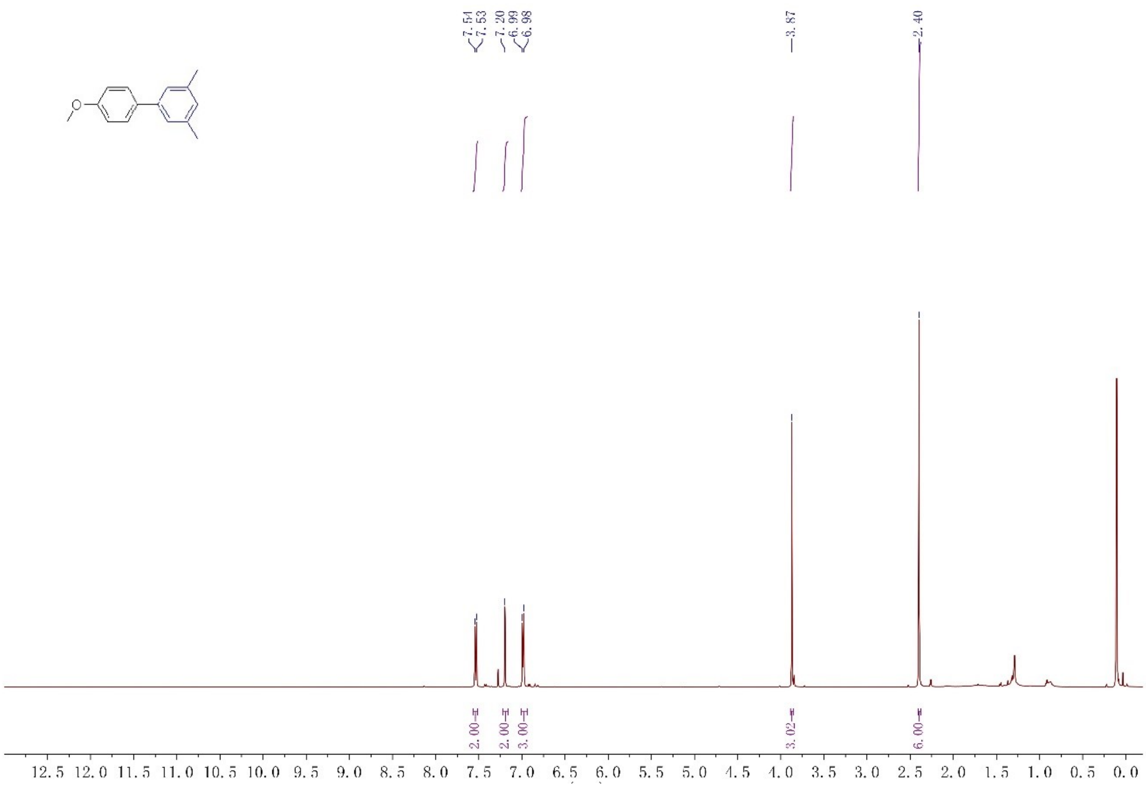

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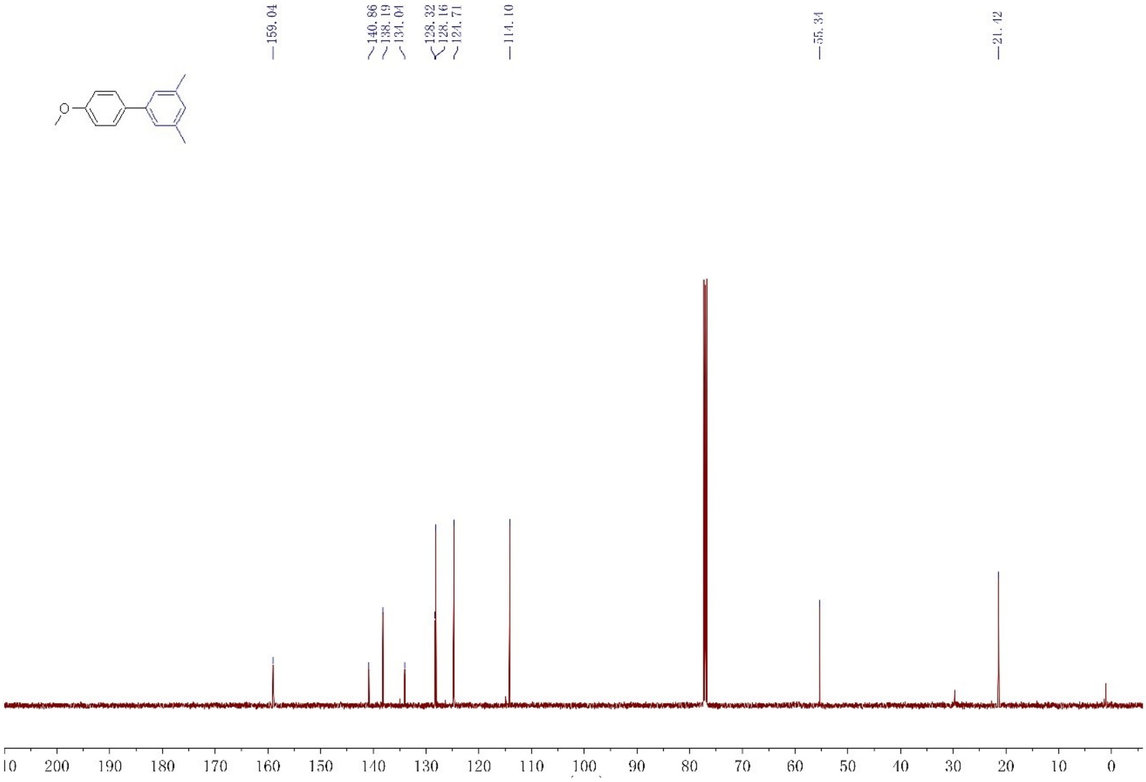

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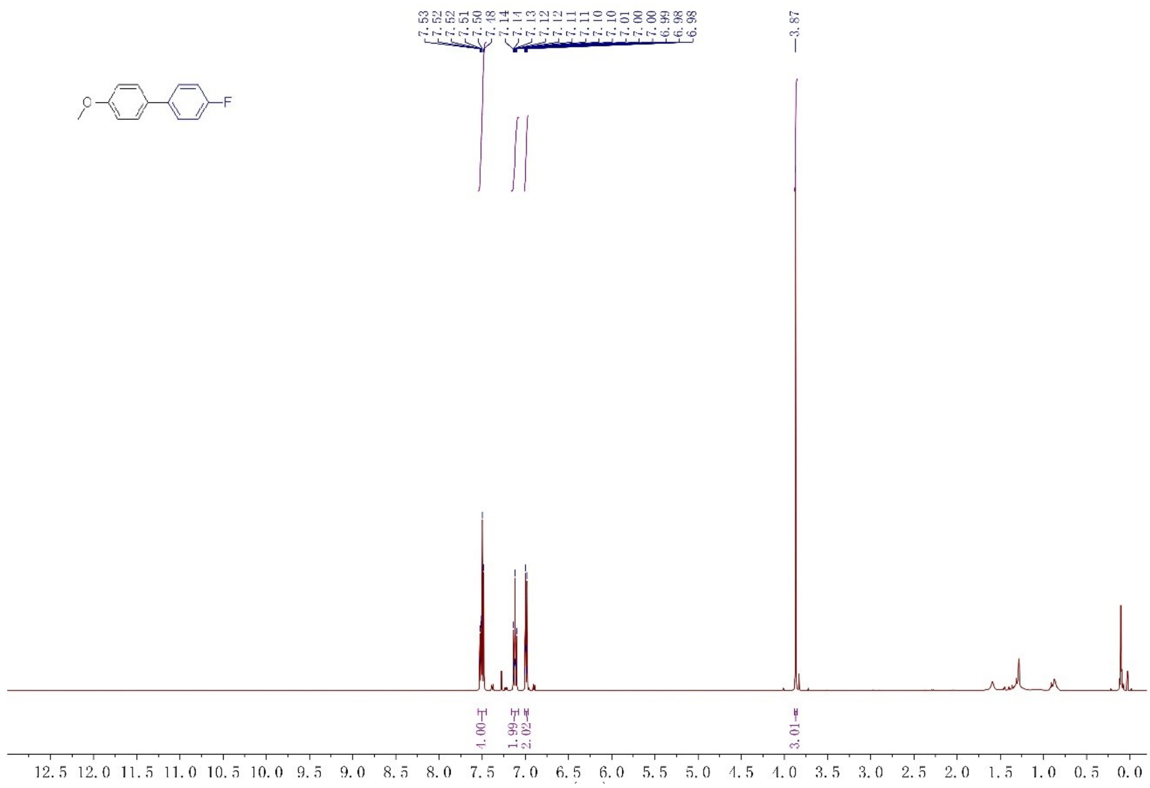

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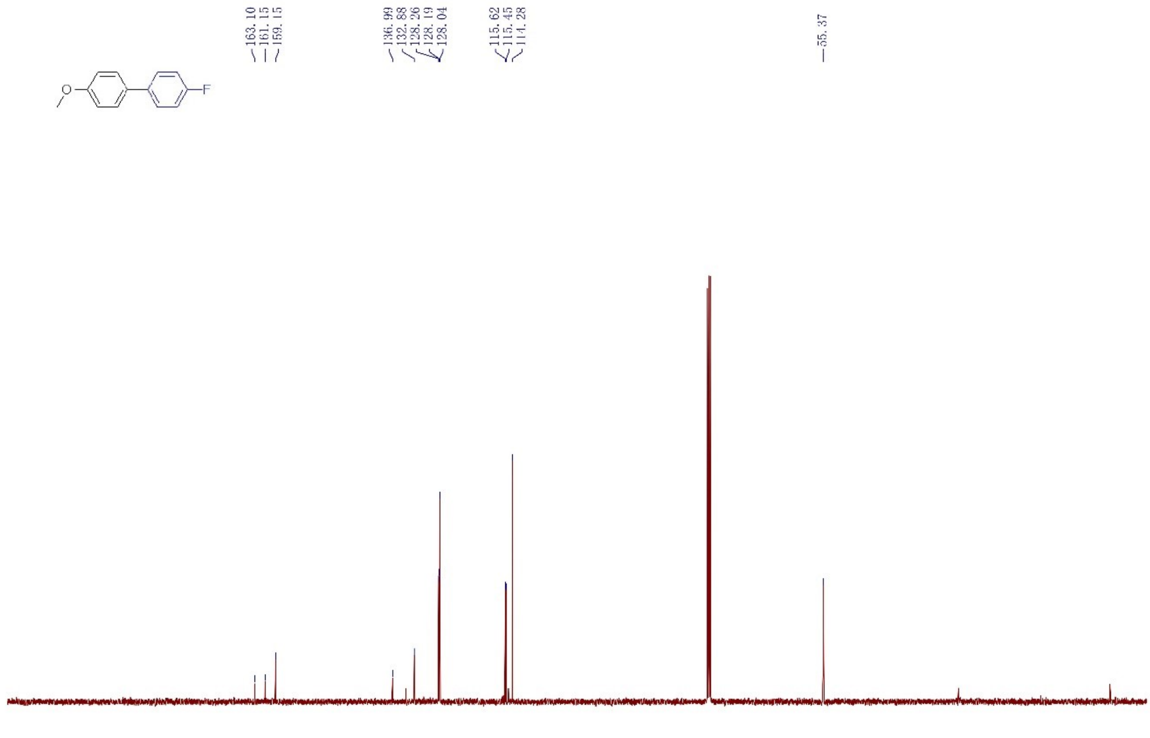
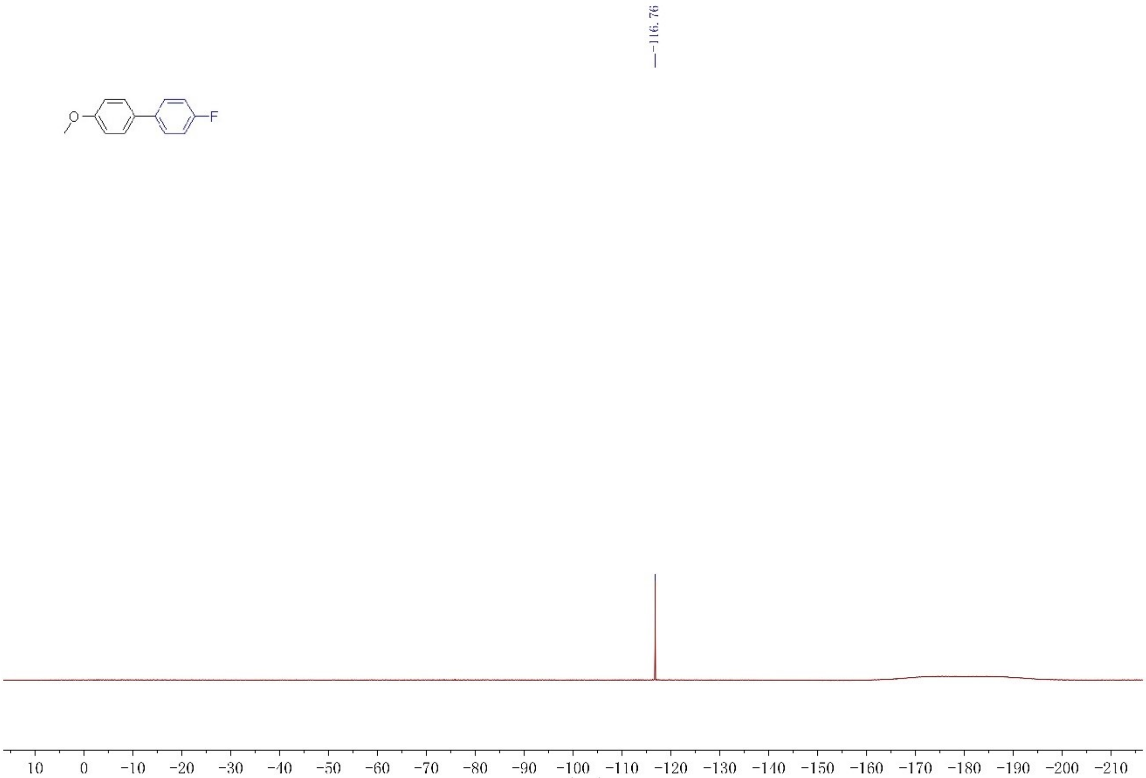
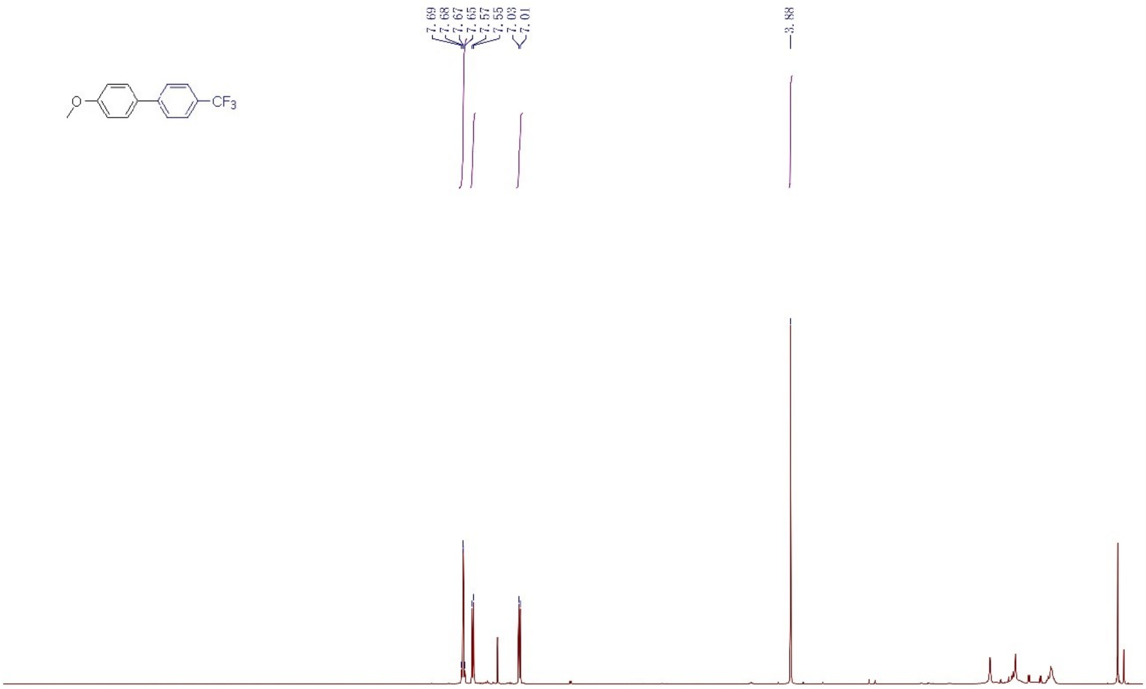


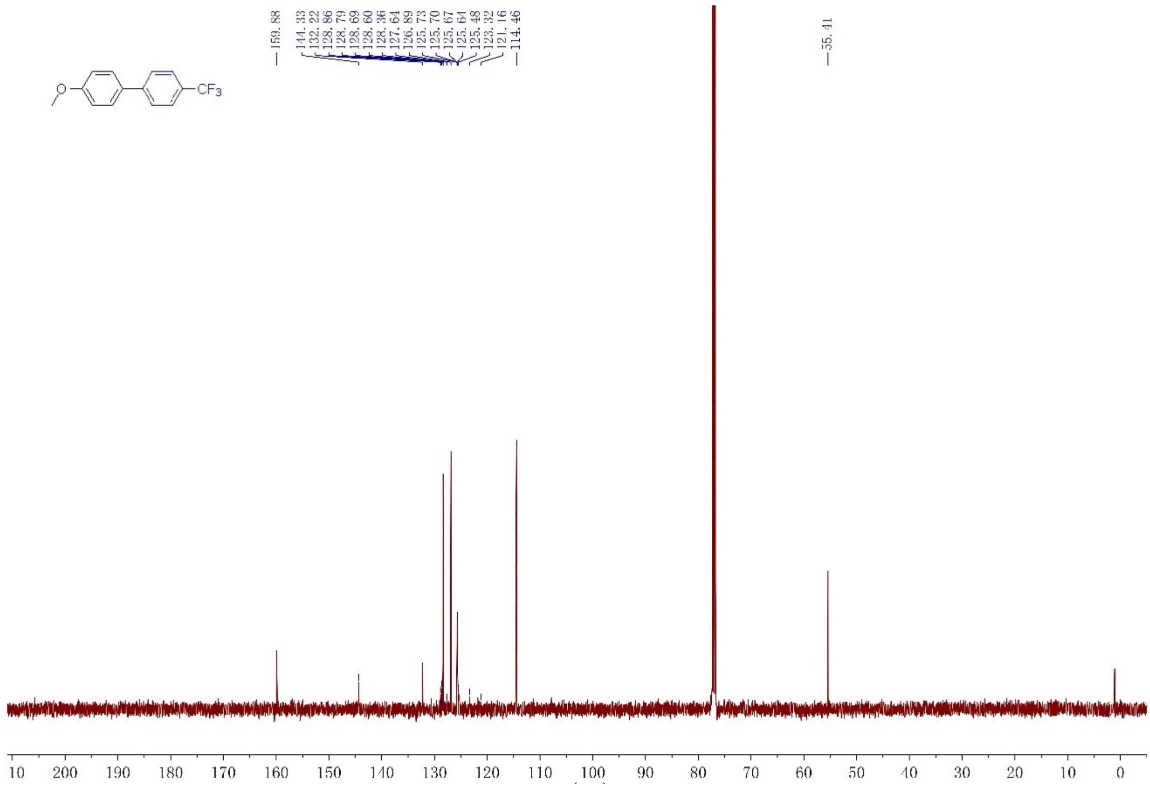
[19]F NMR (565 MHz, $CDCl_3$)



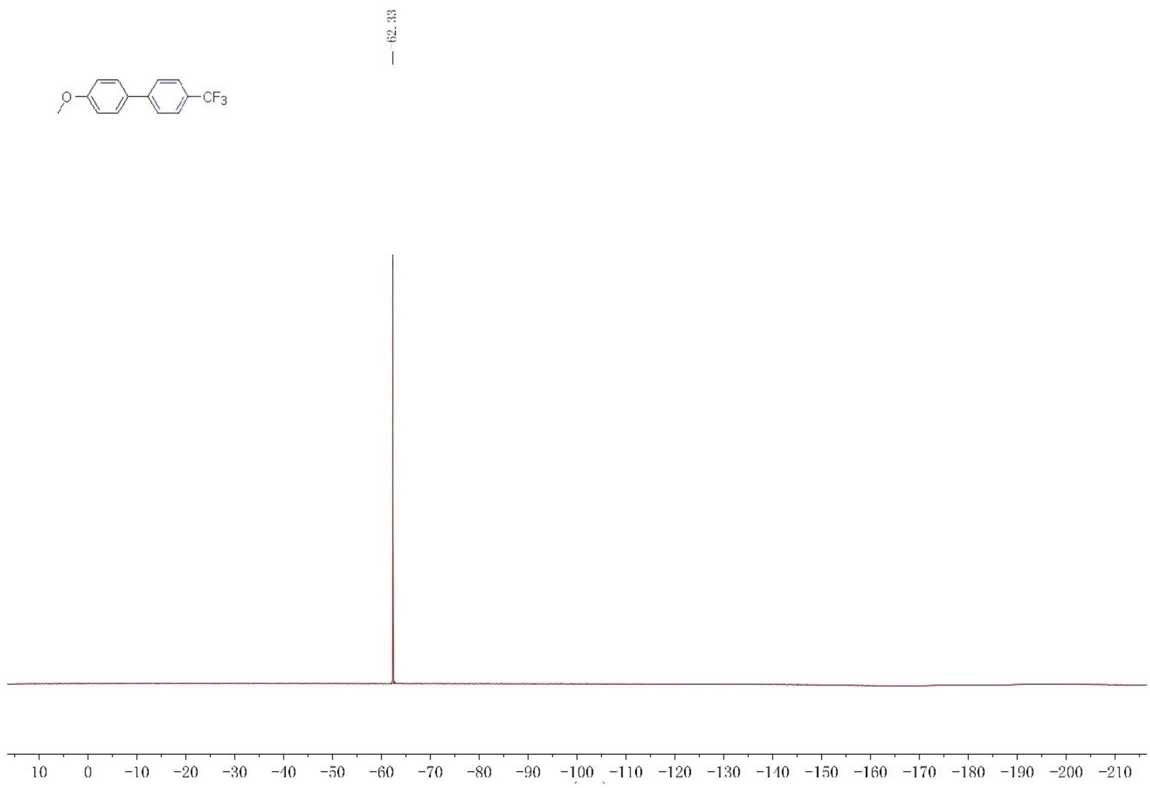
[1]H NMR (500 MHz, $CDCl_3$)



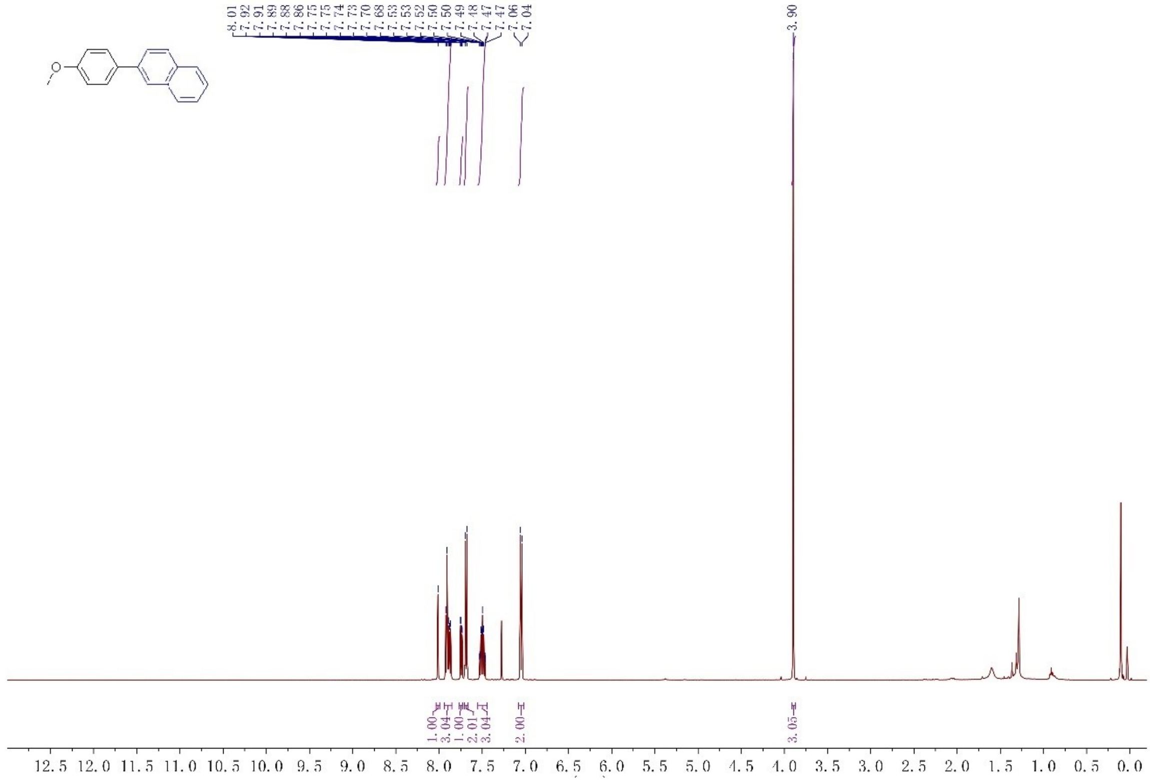
^{13}C NMR (126 MHz, $CDCl_3$)



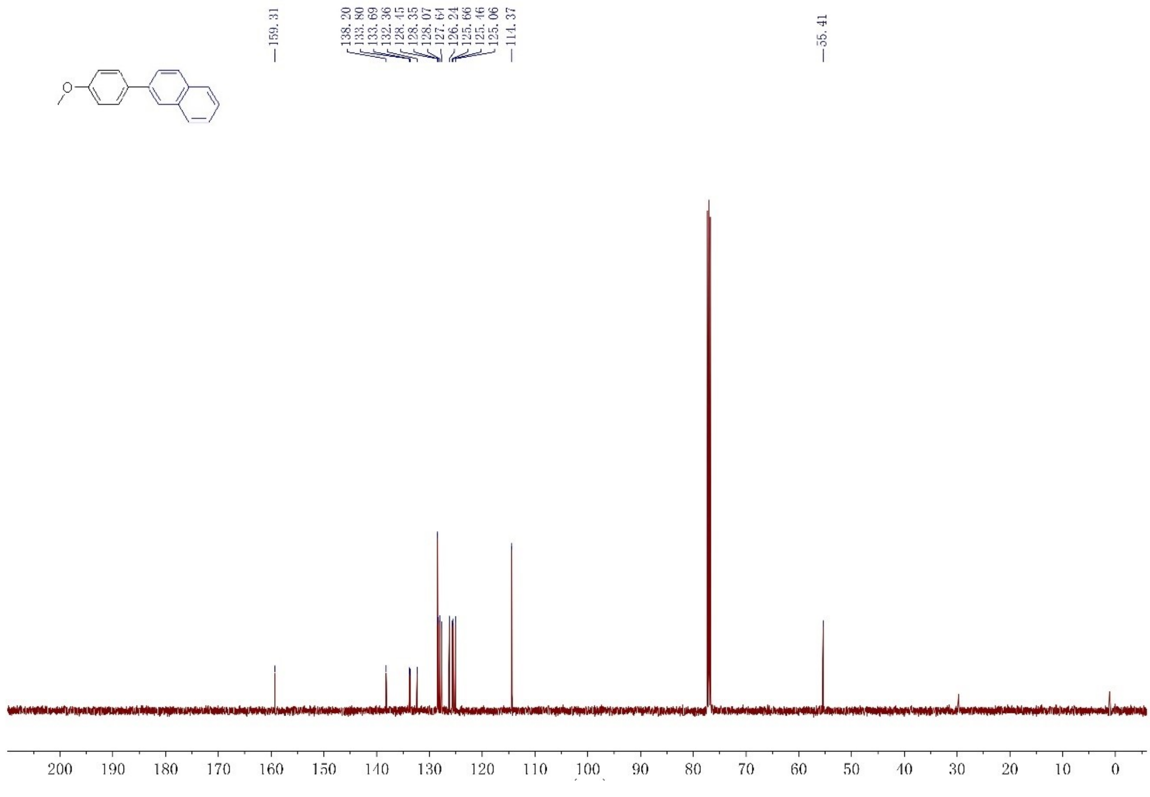
^{19}F NMR (565 MHz, $CDCl_3$)



[1]H NMR (500 MHz, $CDCl_3$)



[13]C NMR (126 MHz, $CDCl_3$)



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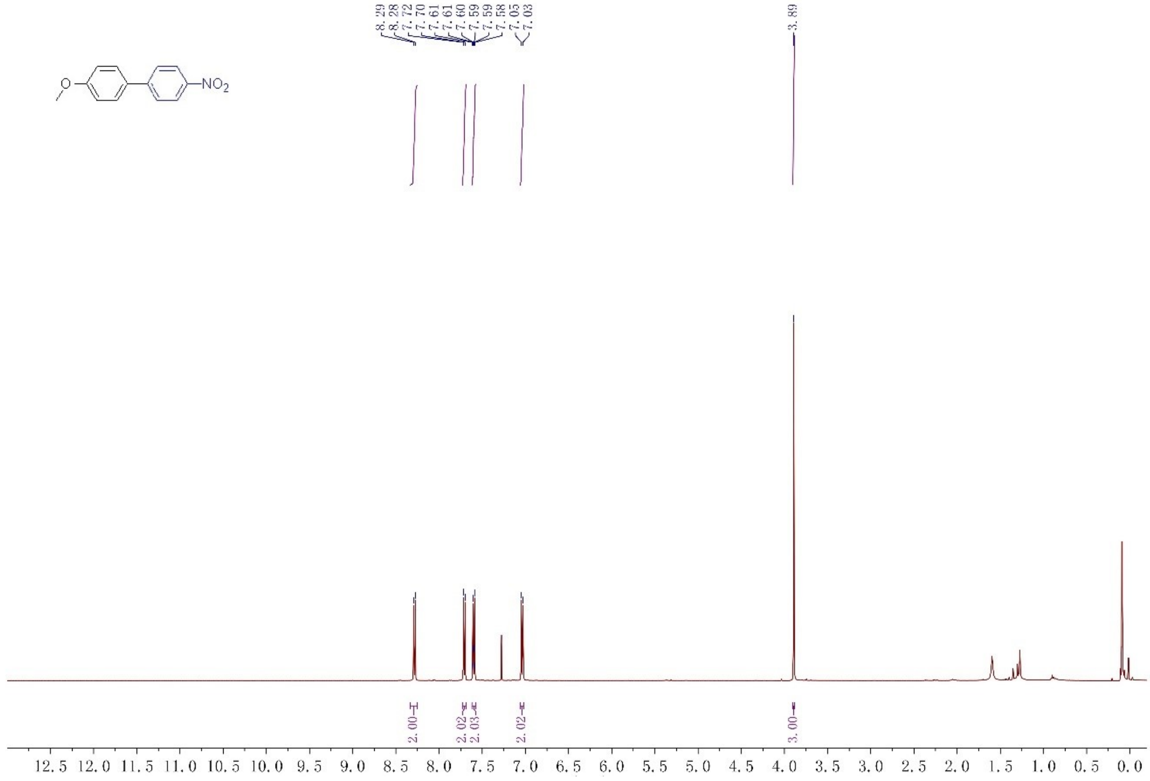
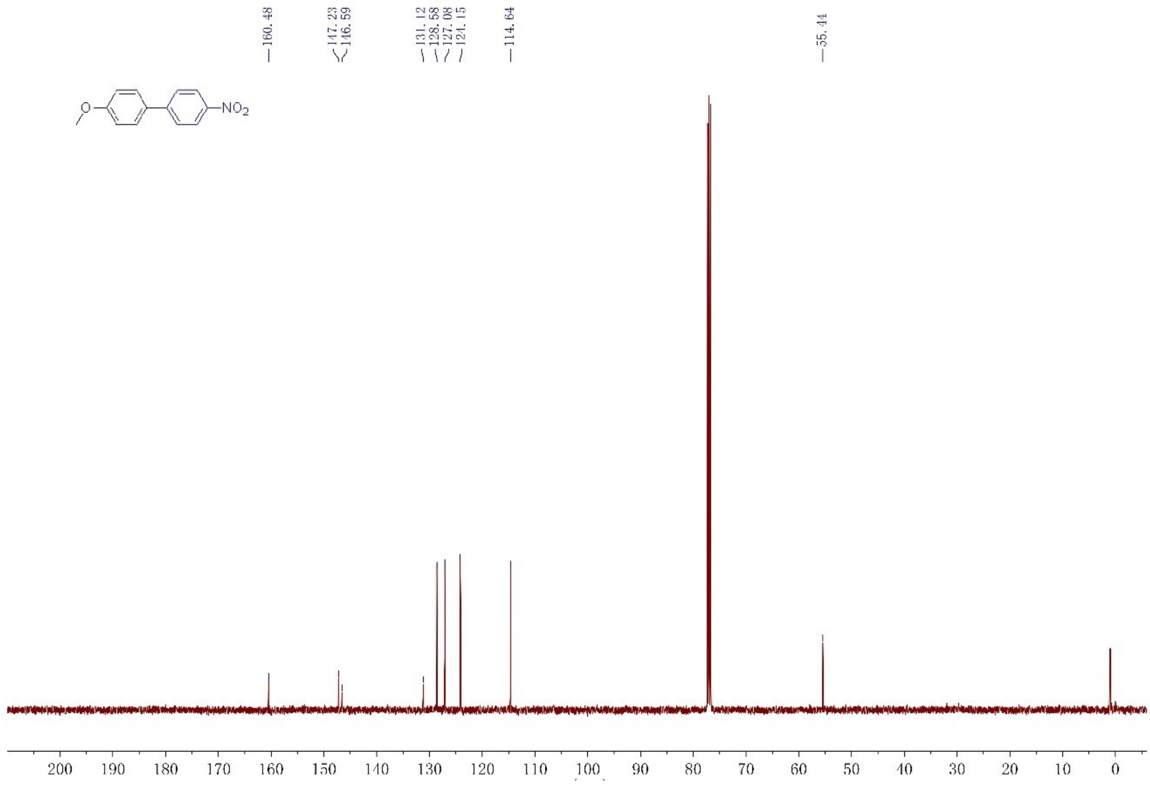
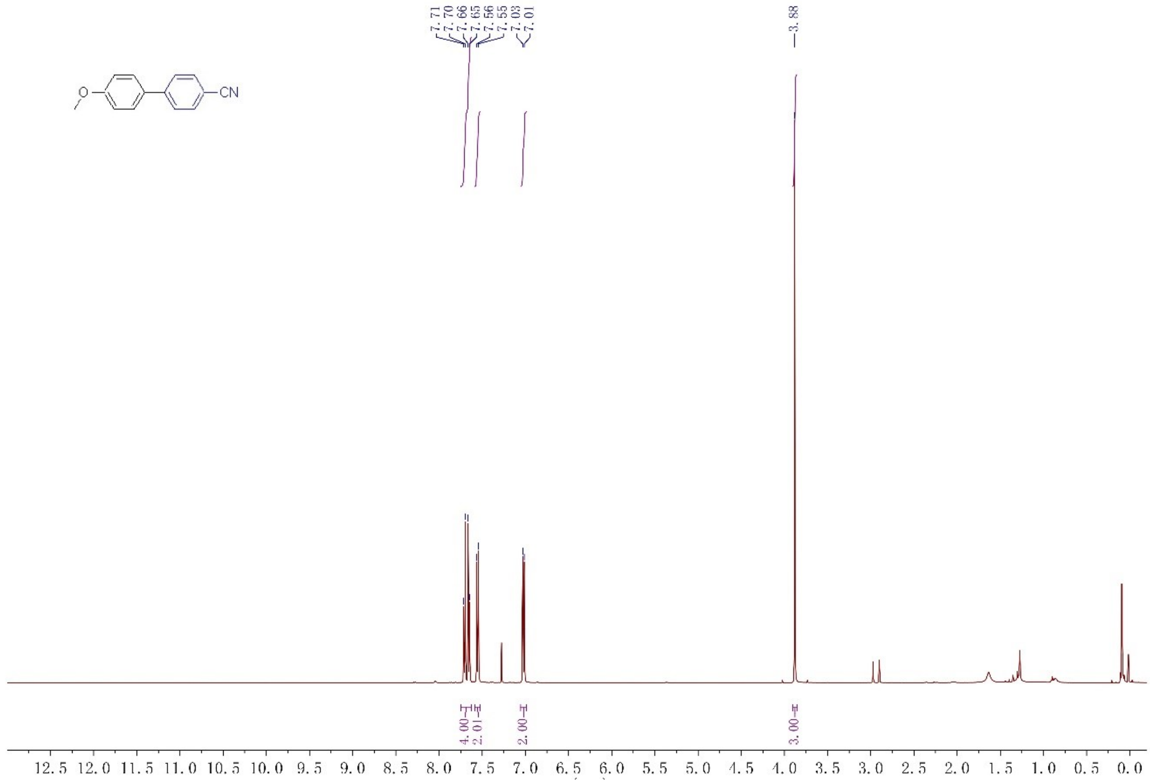


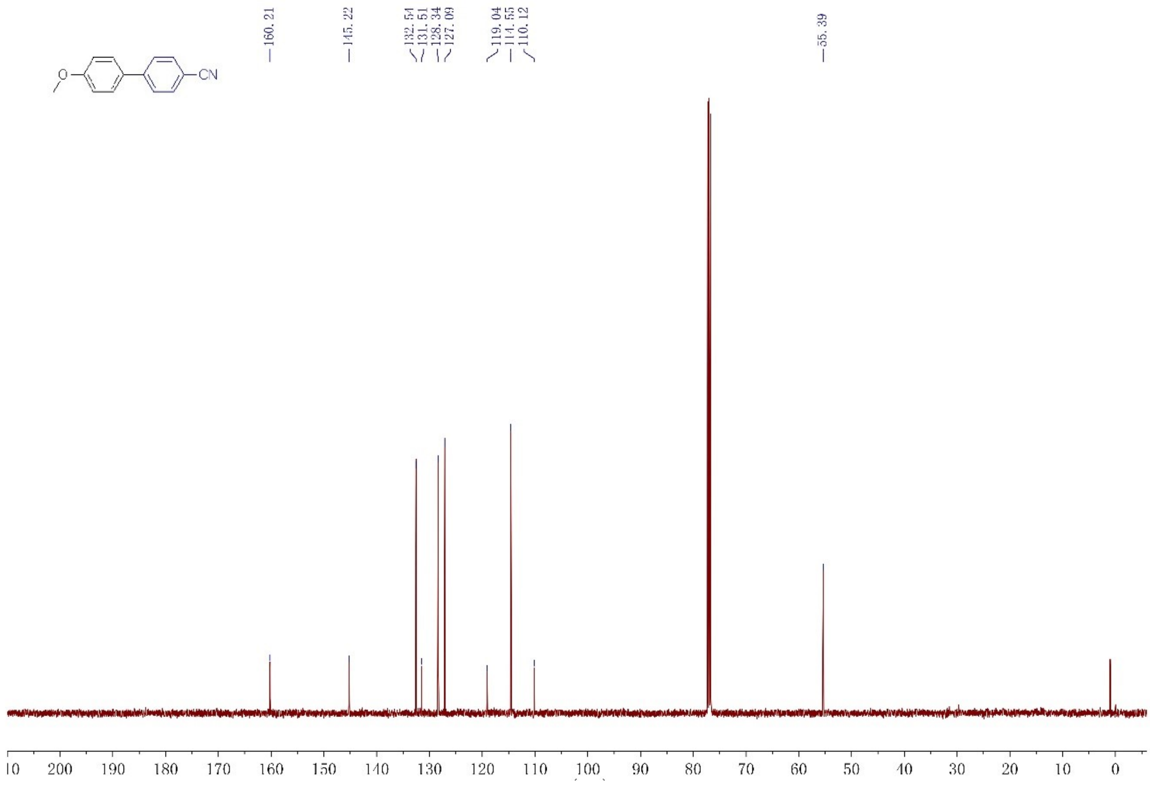
^{13}C NMR (126 MHz, $CDCl_3$)



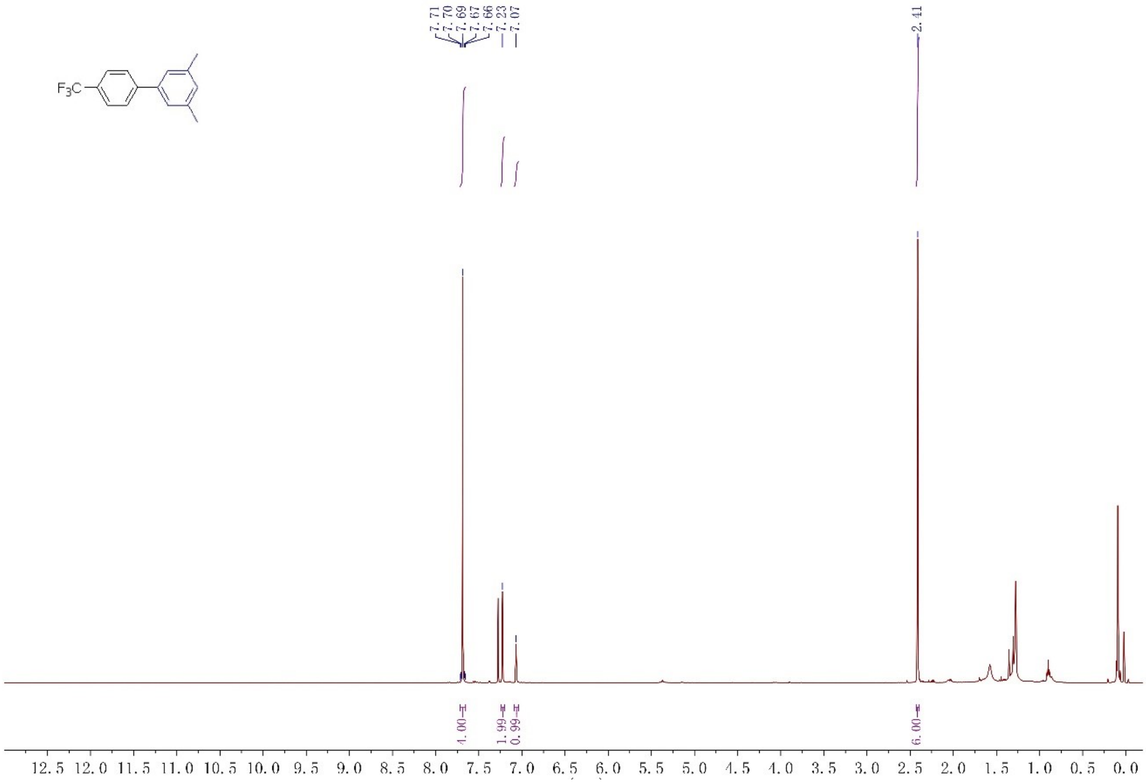
^{1}H NMR (500 MHz, $CDCl_3$)



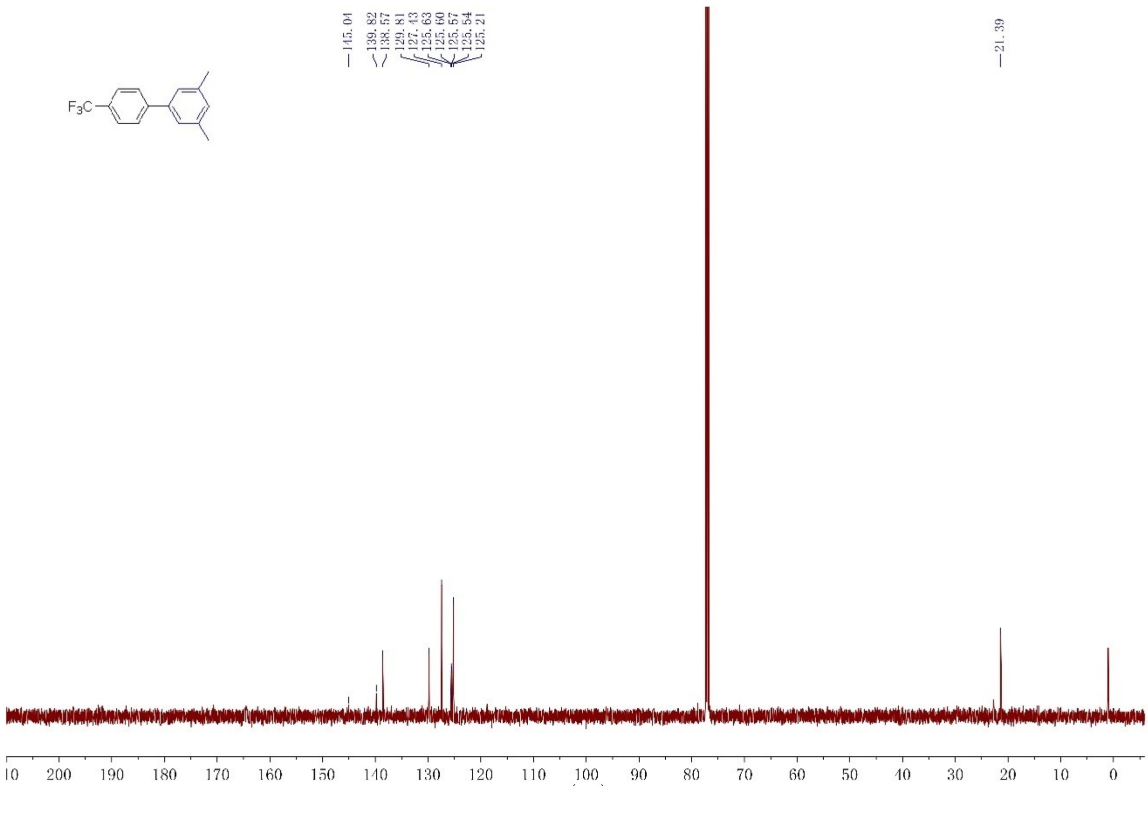
^{13}C NMR (126 MHz, $CDCl_3$)



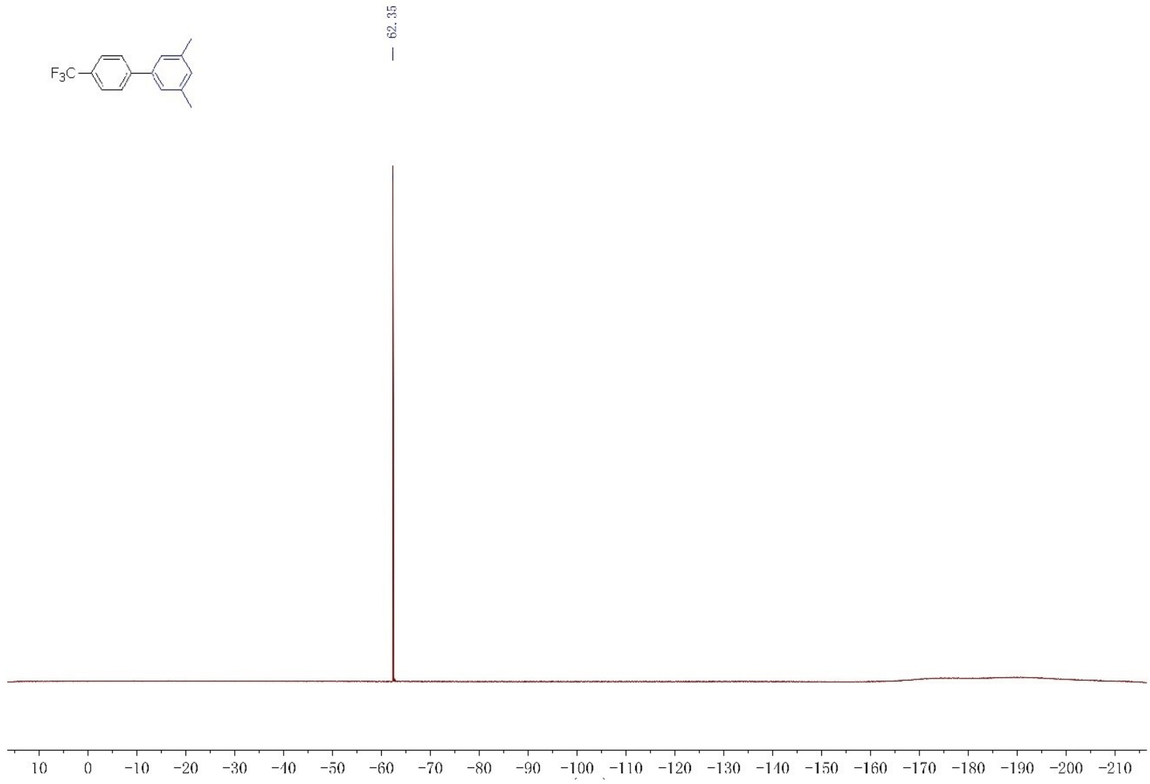
¹H NMR (500 MHz, $CDCl_3$)



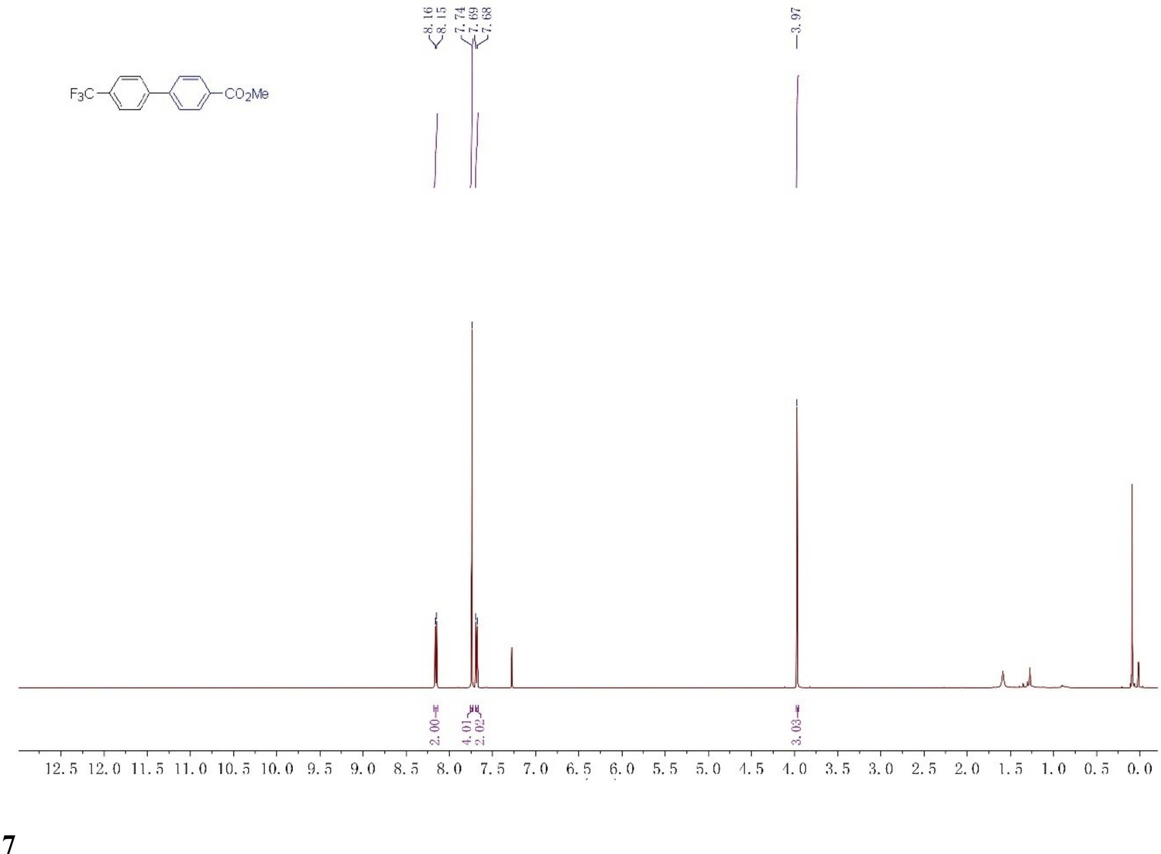
¹³C NMR (126 MHz, $CDCl_3$)



[19]F NMR (565 MHz, $CDCl_3$)



[1]H NMR (500 MHz, $CDCl_3$)



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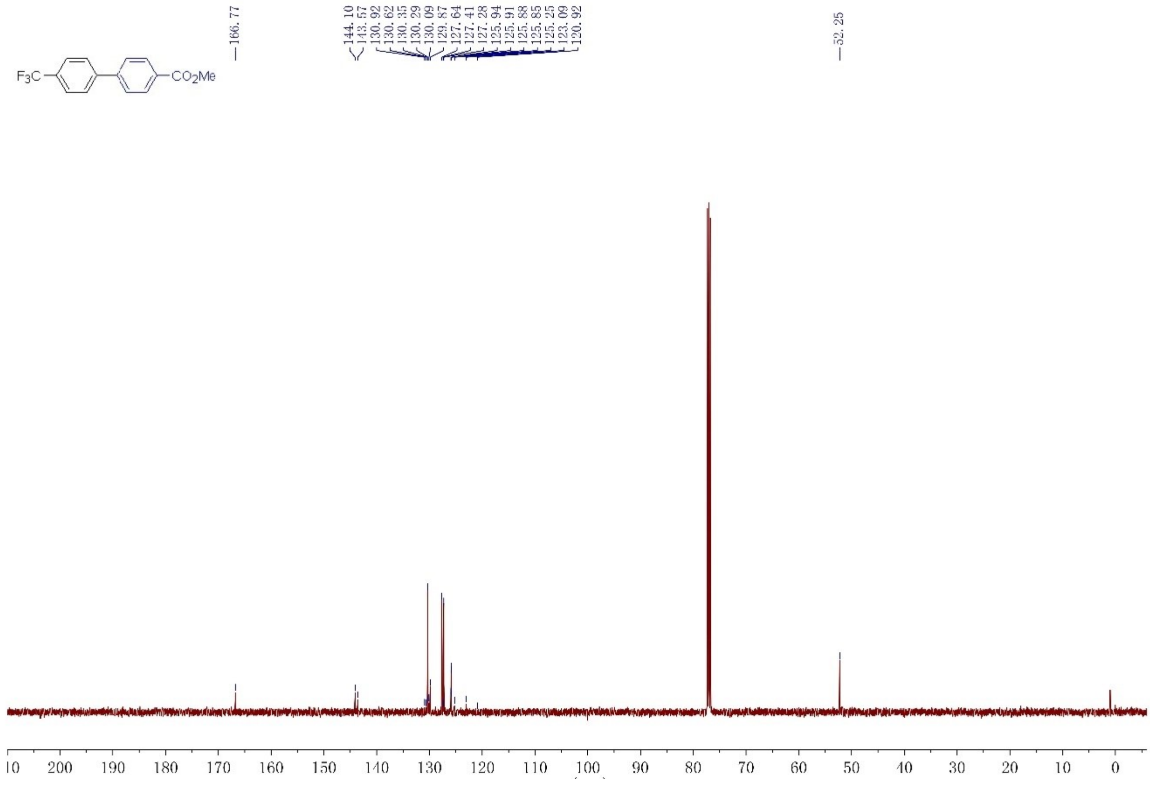

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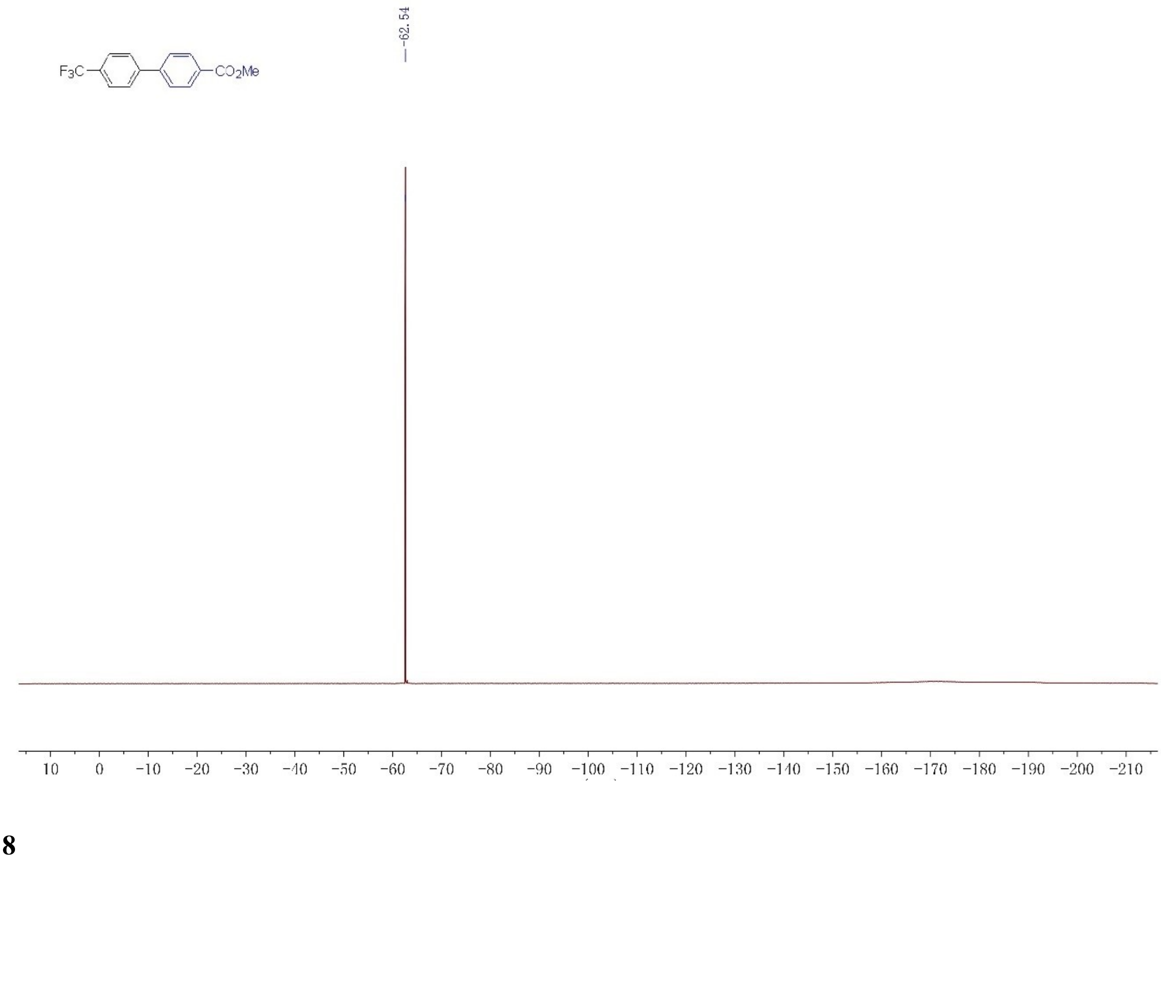

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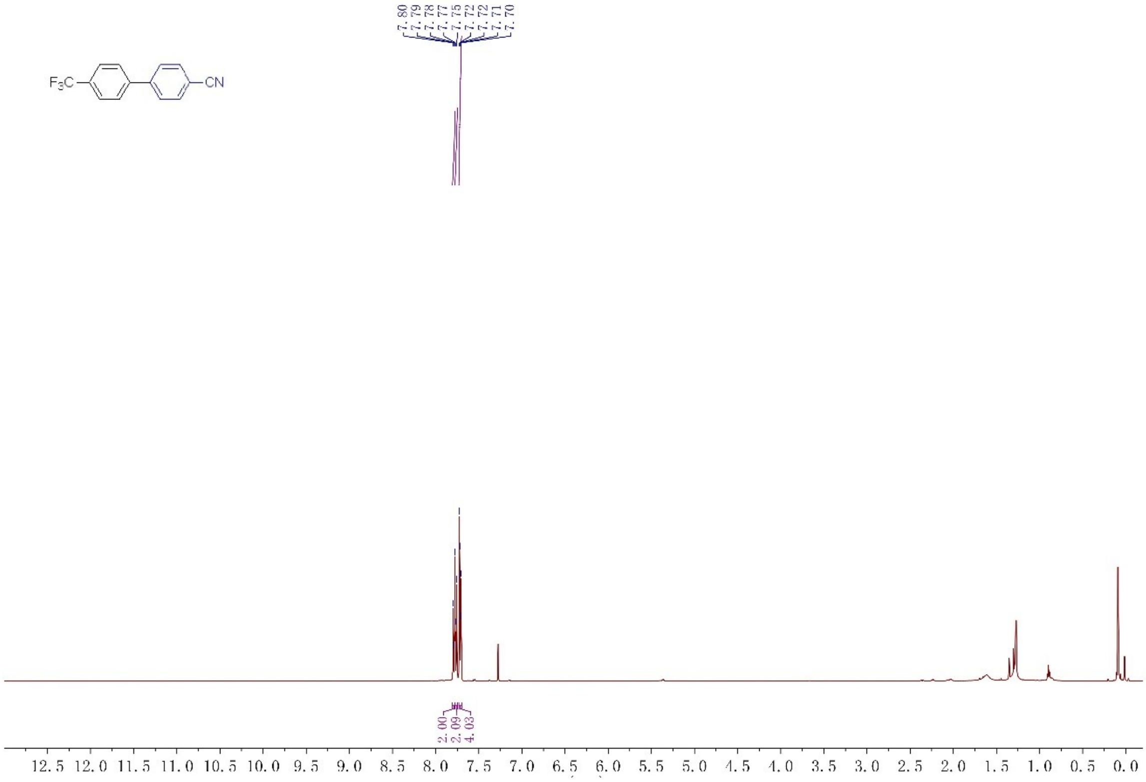

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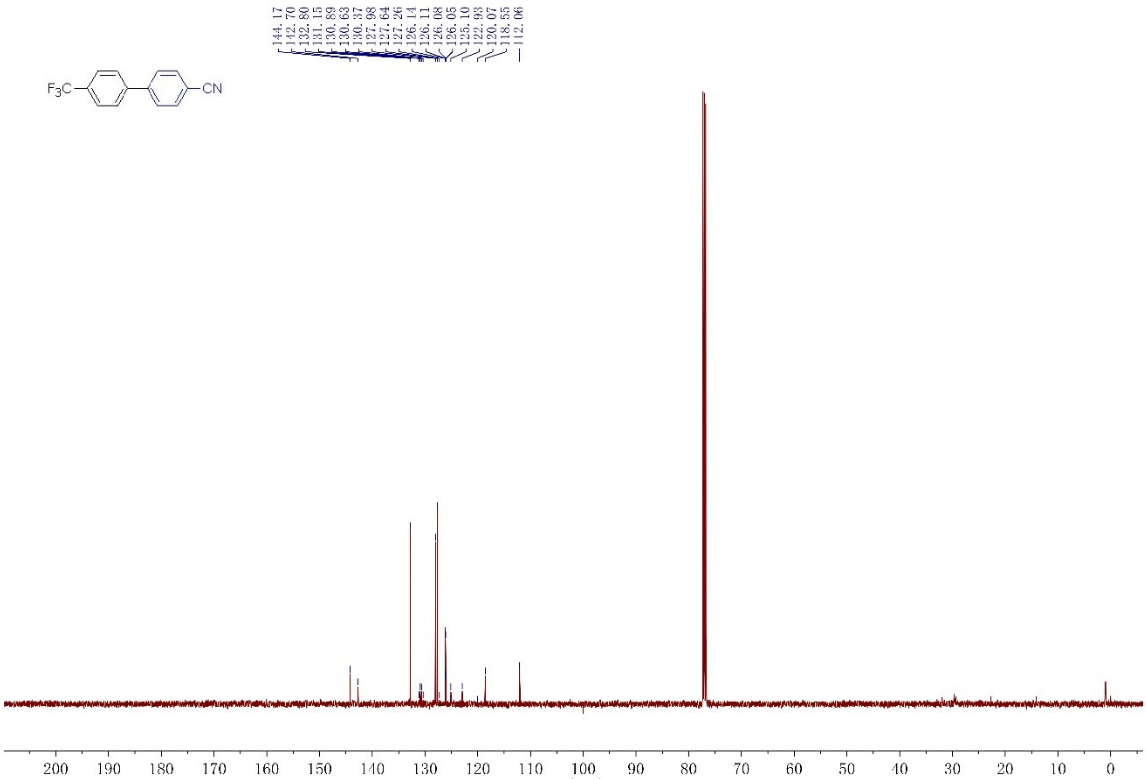
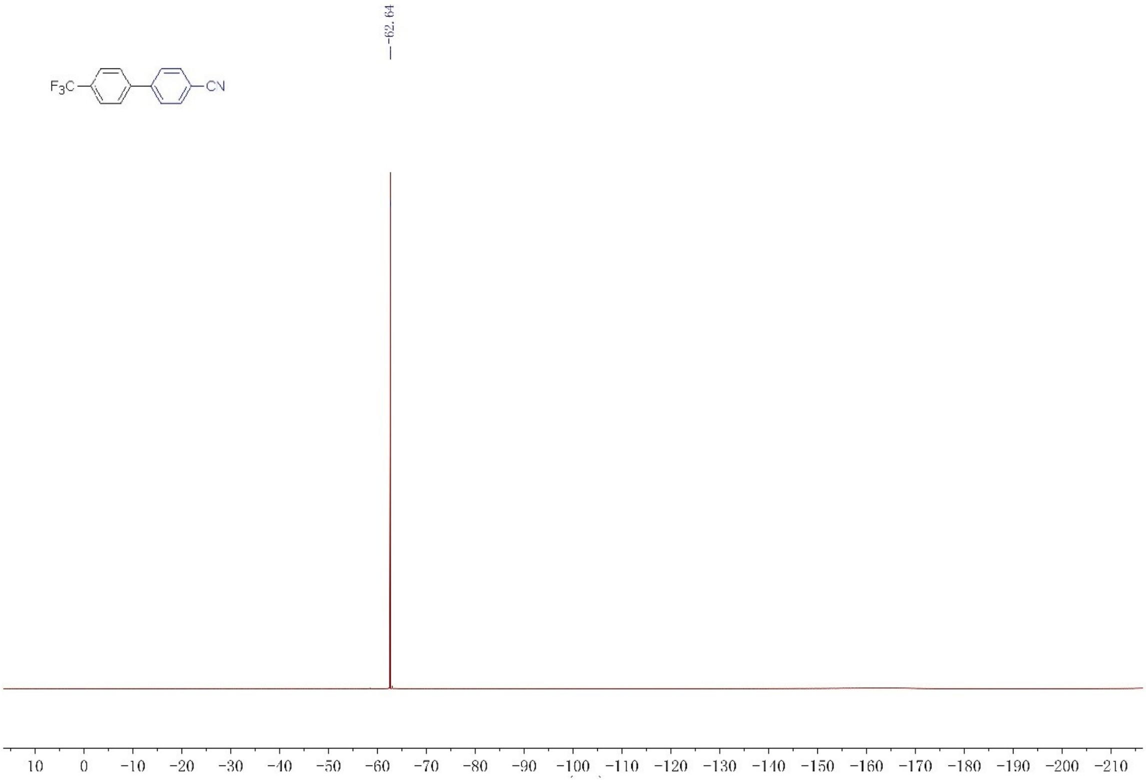
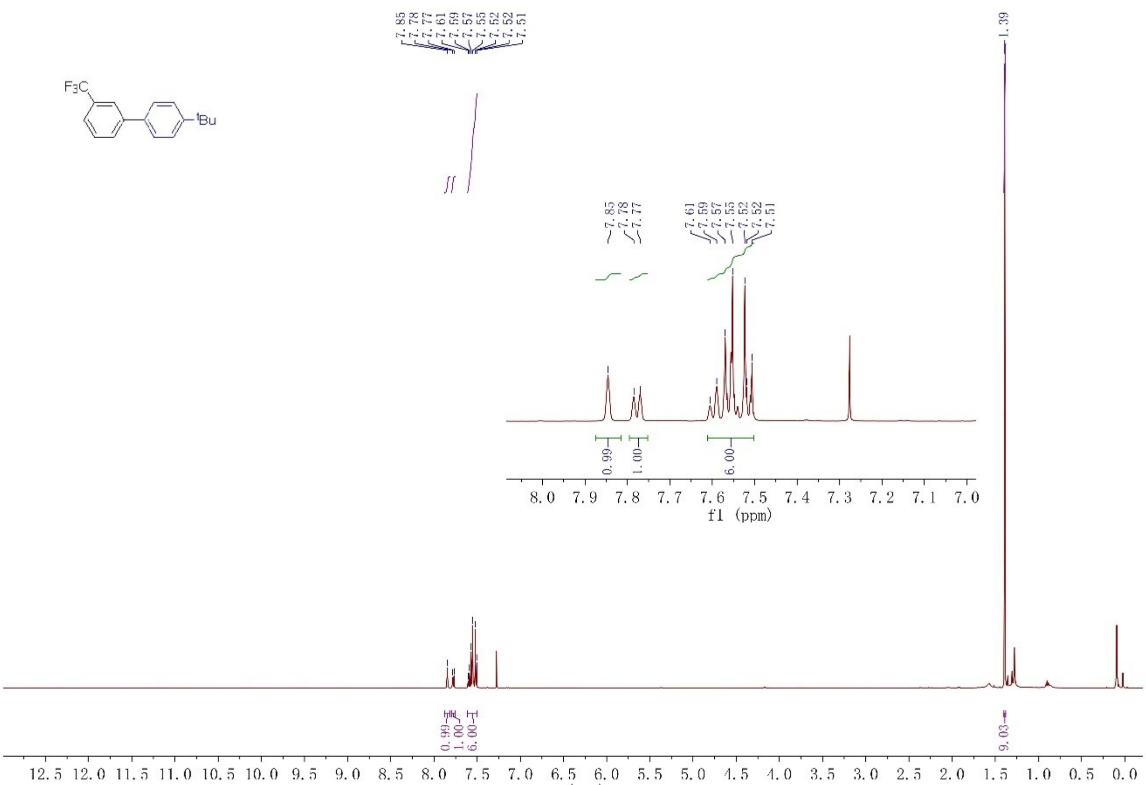


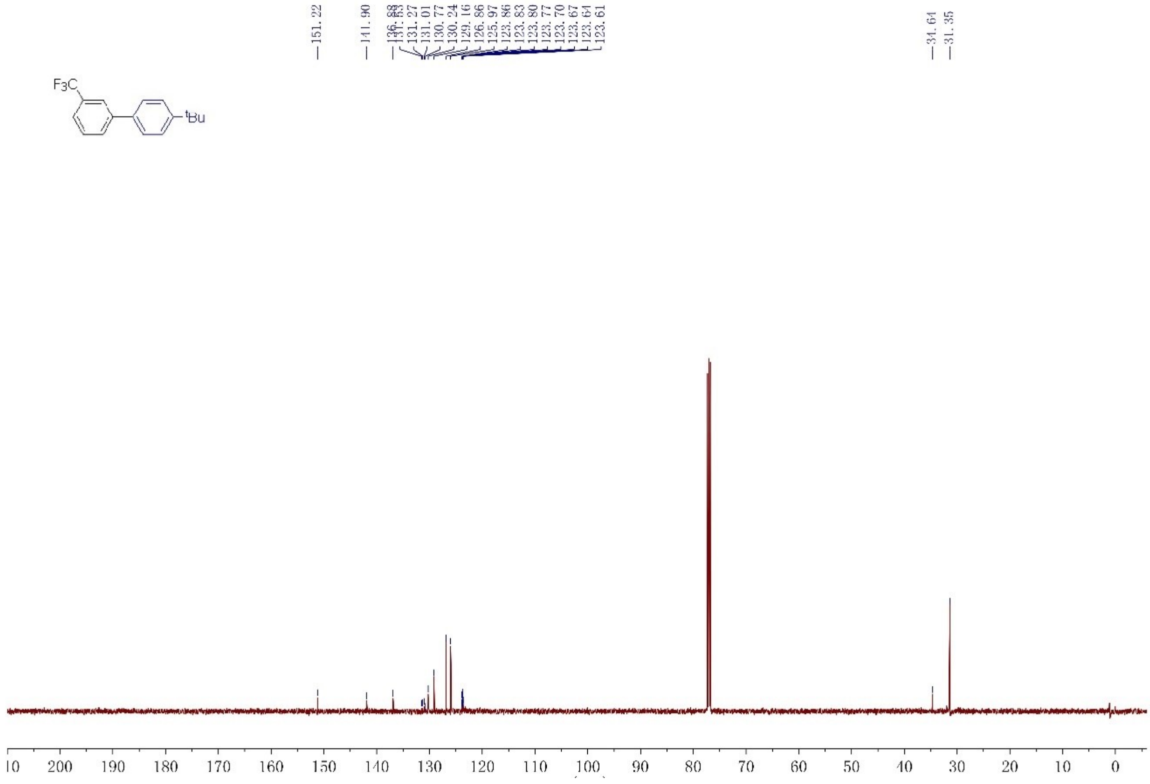
^{19}F NMR (565 MHz, $CDCl_3$)



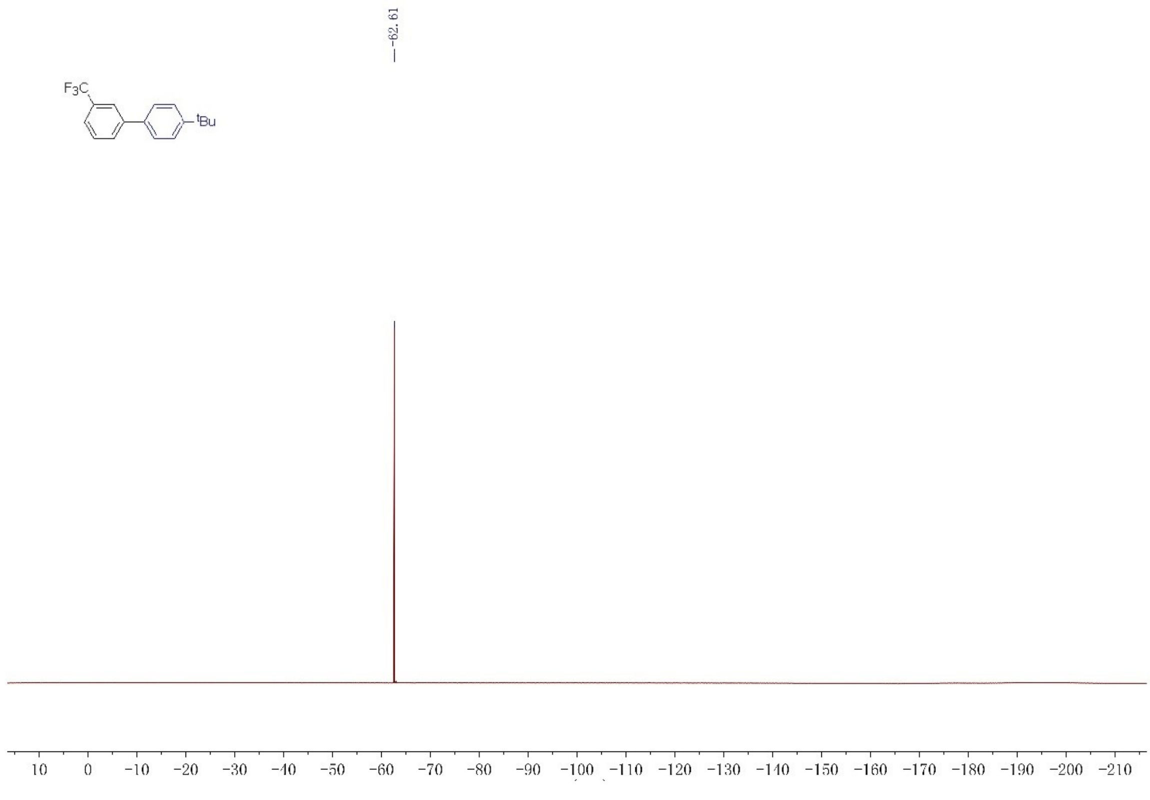
^{1}H NMR (500 MHz, $CDCl_3$)



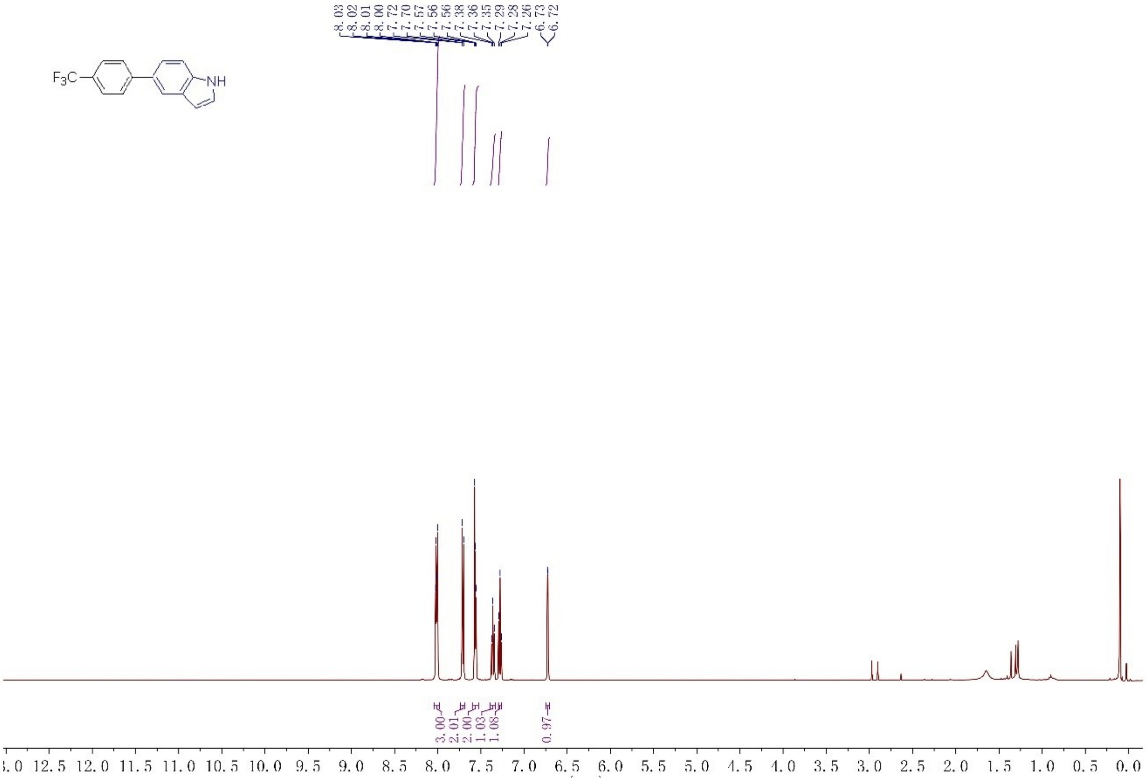
¹³C NMR (126 MHz, $CDCl_3$)



¹⁹F NMR (565 MHz, $CDCl_3$)



[1]H NMR (500 MHz, $CDCl_3$)



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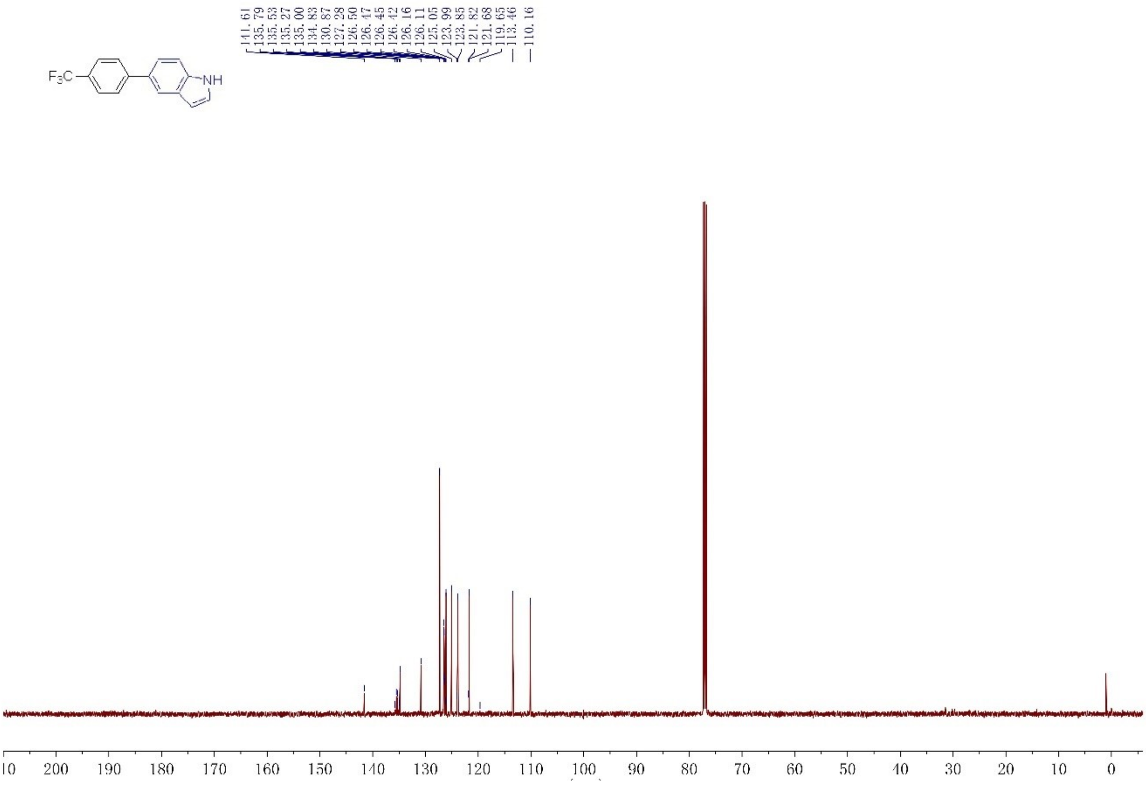

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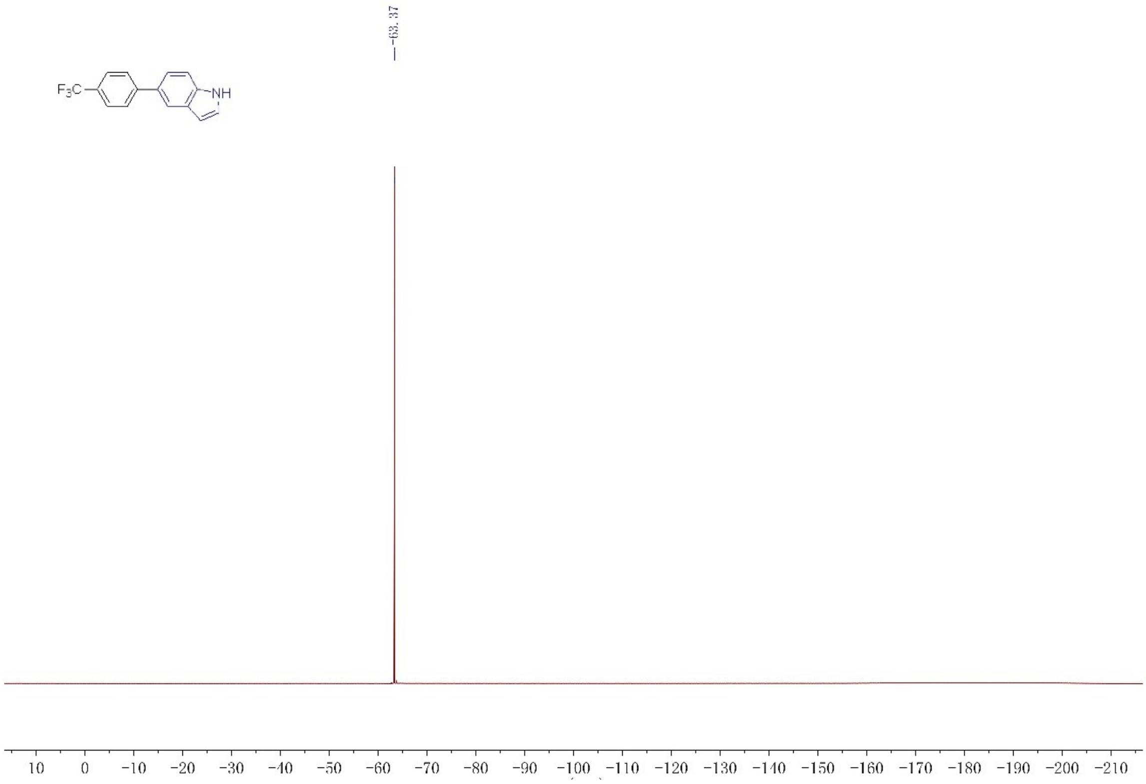

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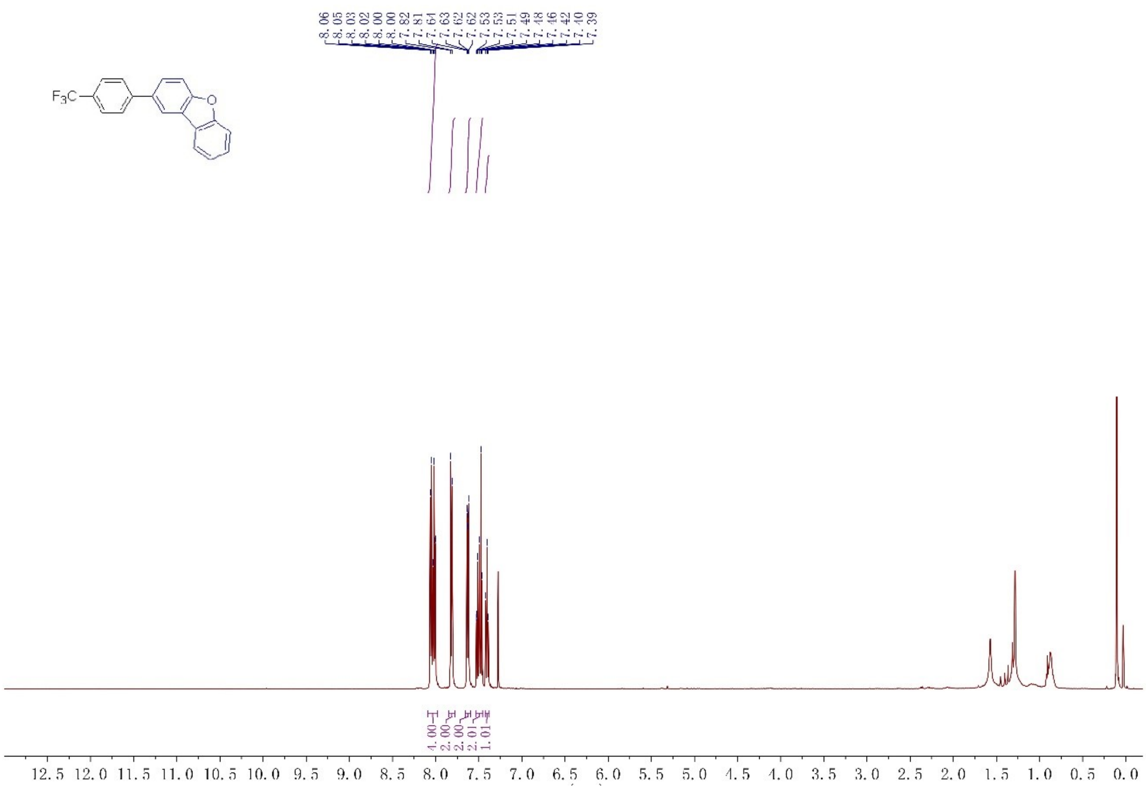

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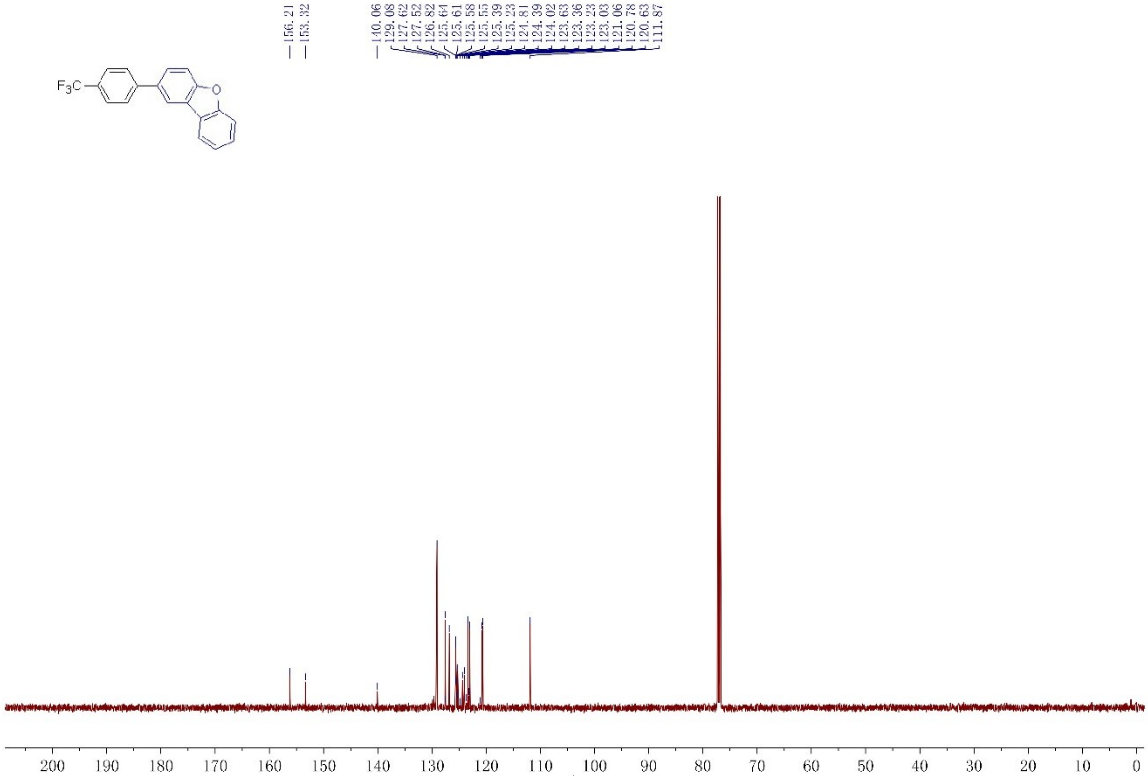

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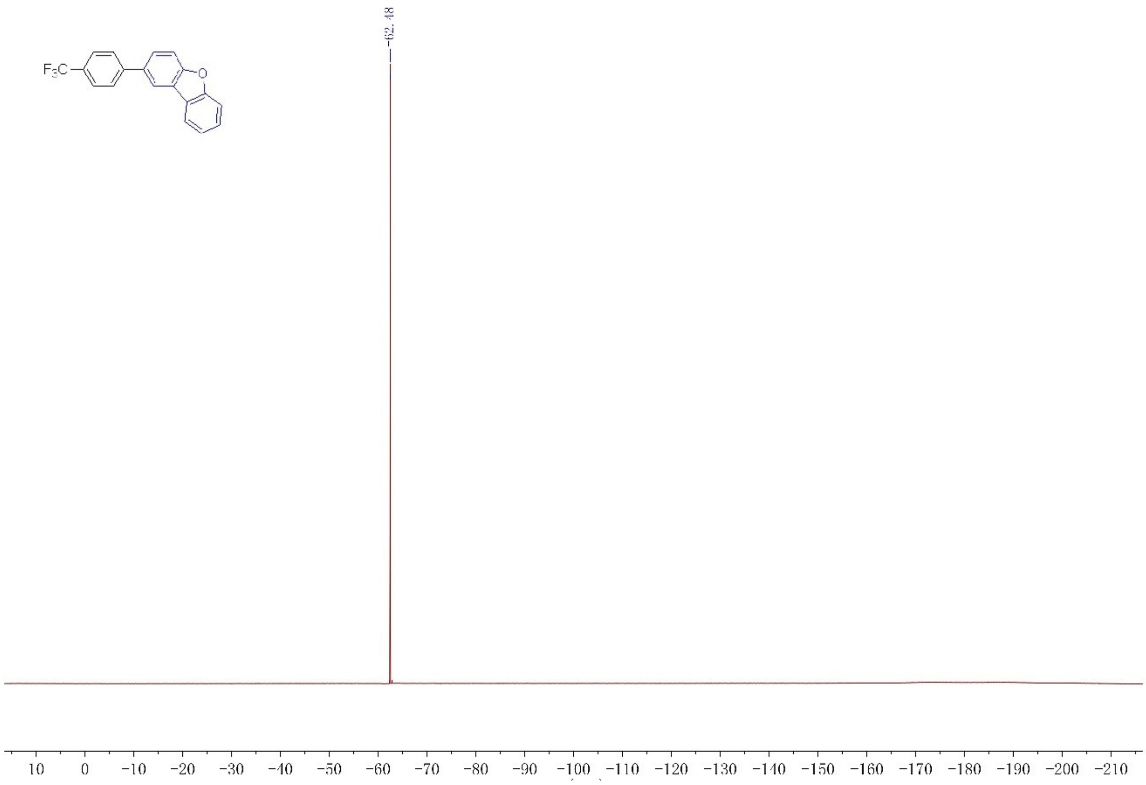
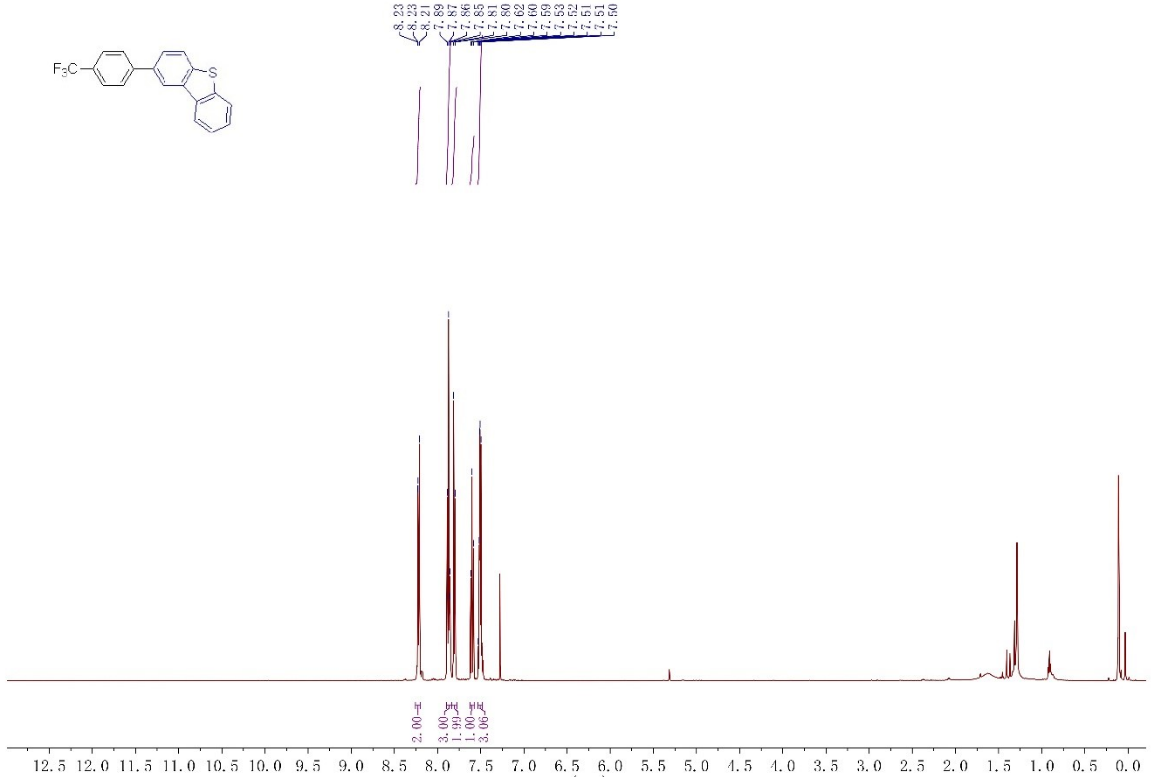
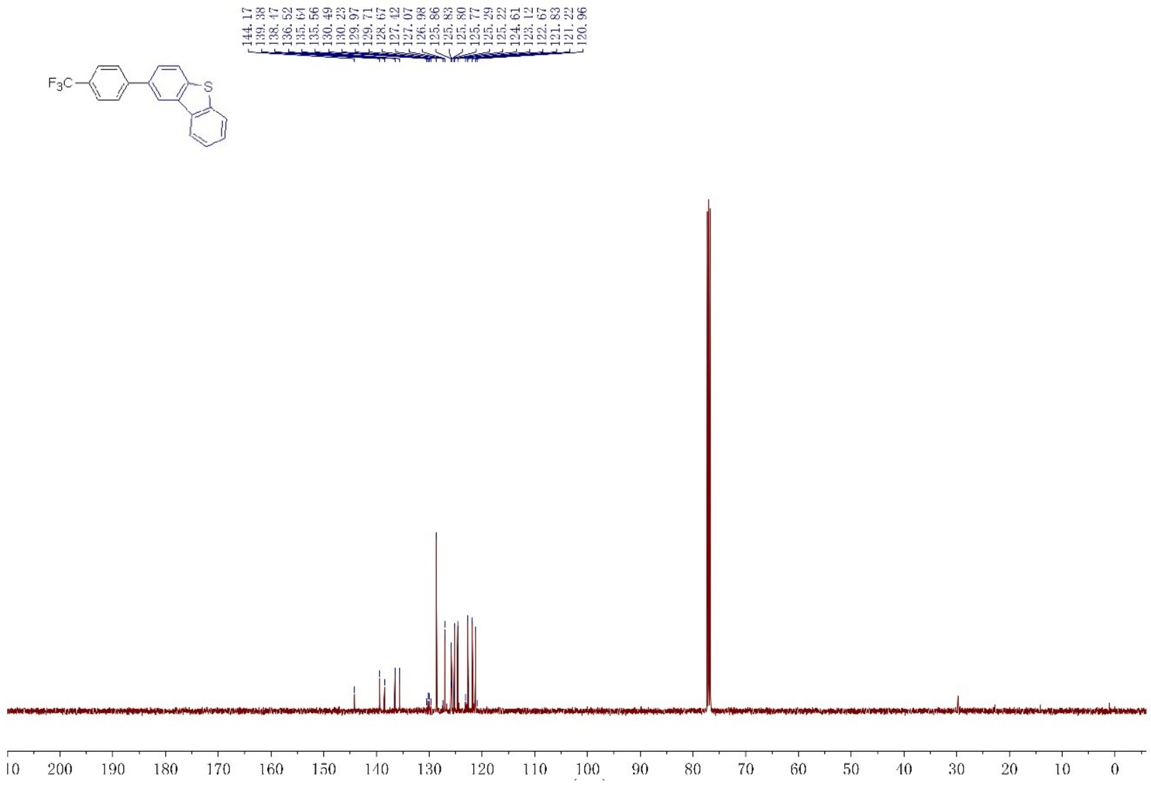


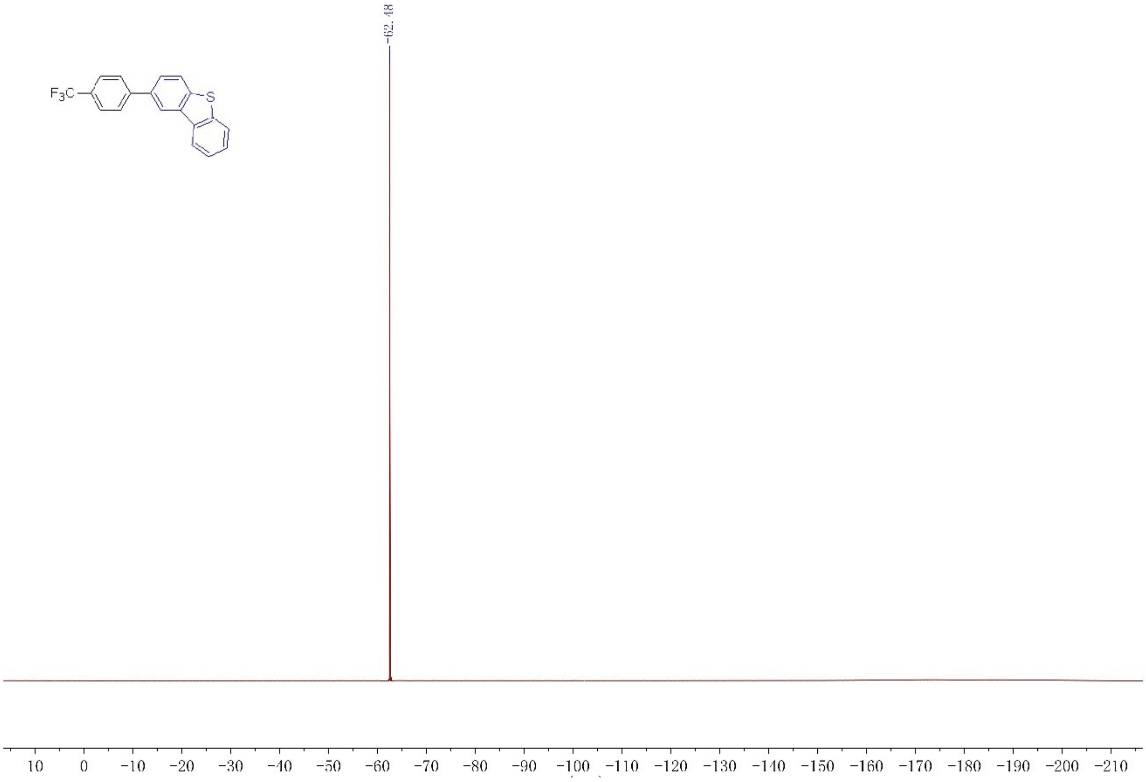
^{1}H NMR (500 MHz, $CDCl_3$)



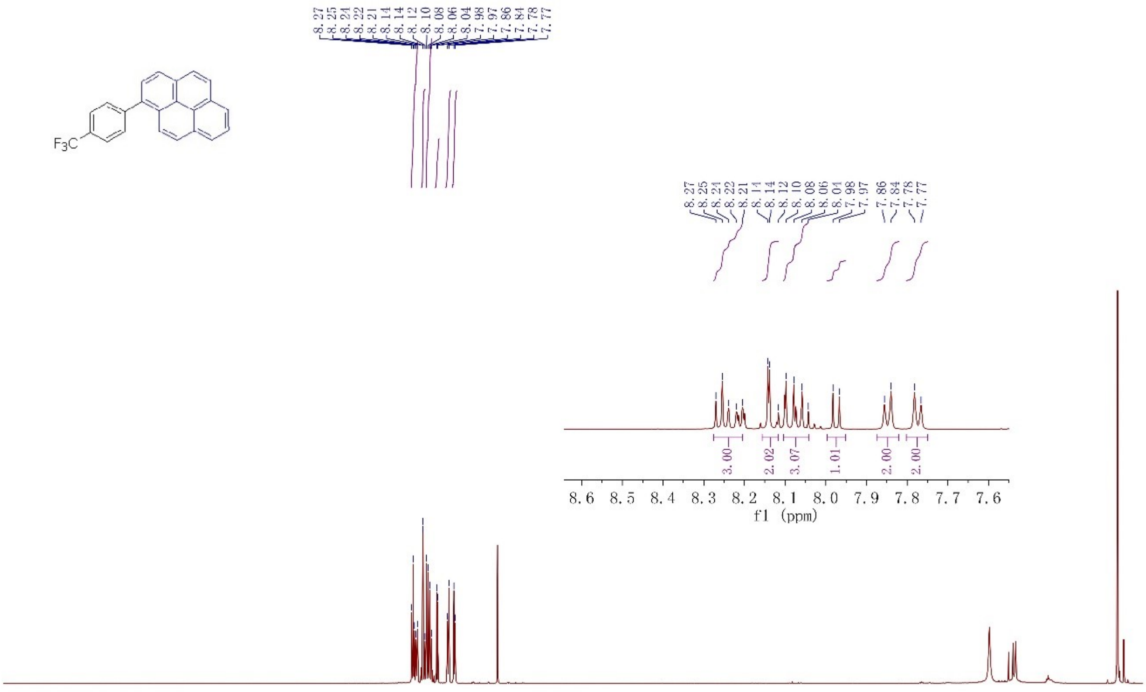
^{13}C NMR (126 MHz, $CDCl_3$)



[19]F NMR (565 MHz, $CDCl_3$)



[1]H NMR (500 MHz, $CDCl_3$)



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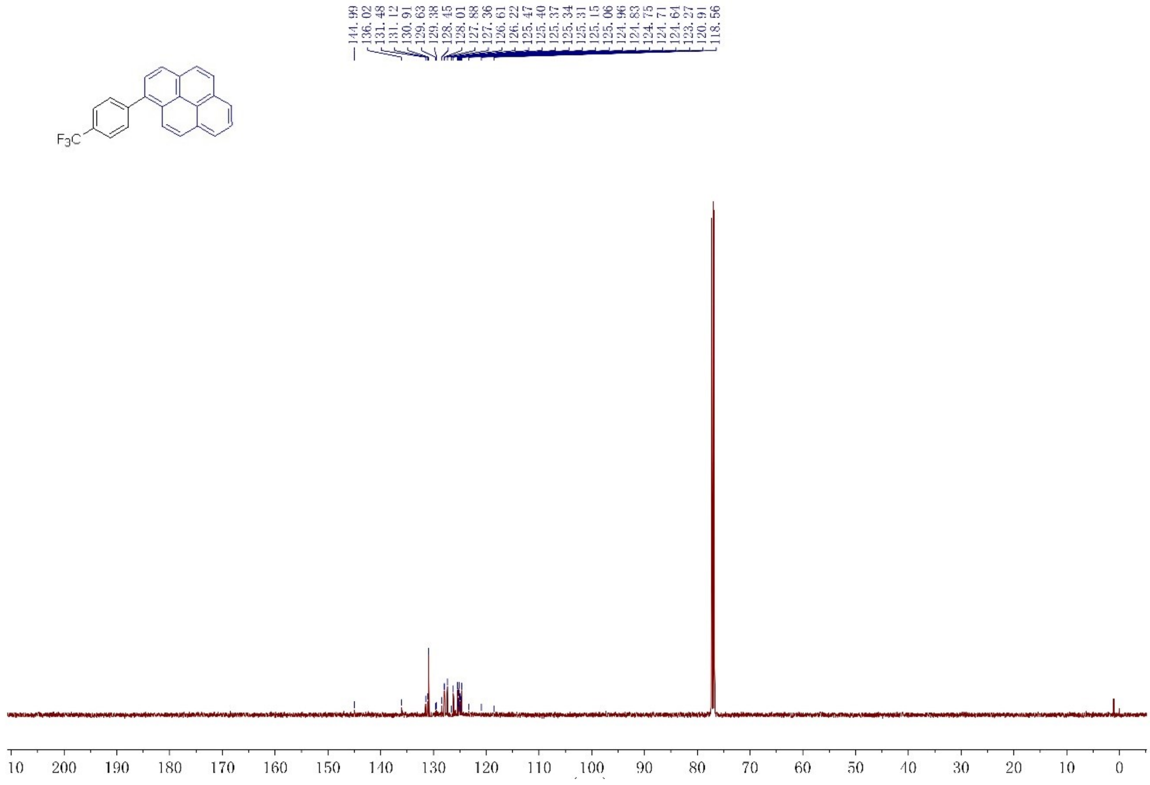
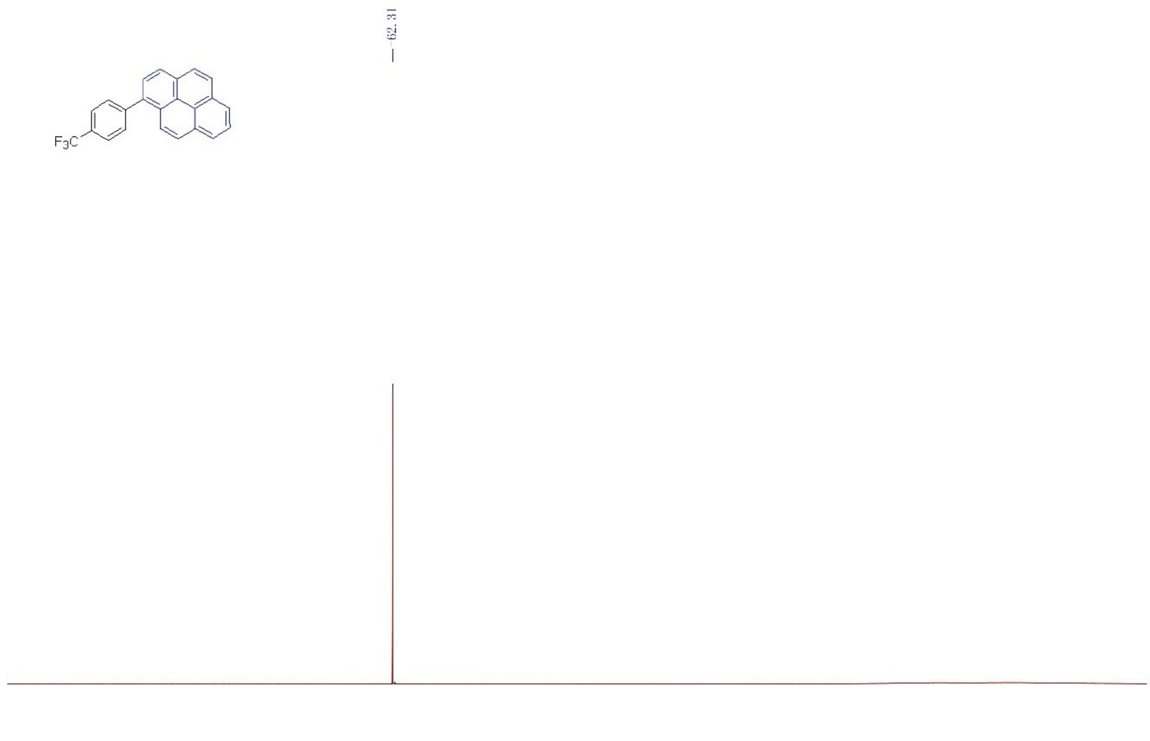
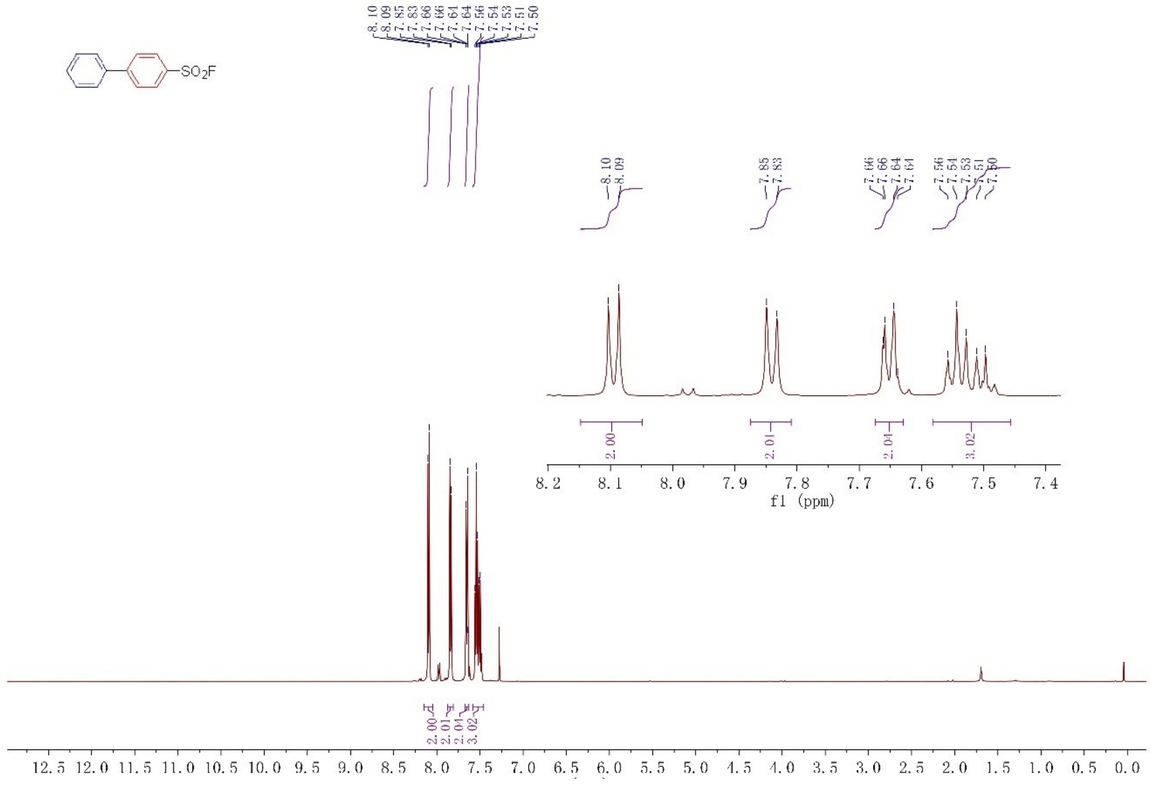
[13]C NMR (126 MHz, $CDCl_3$)



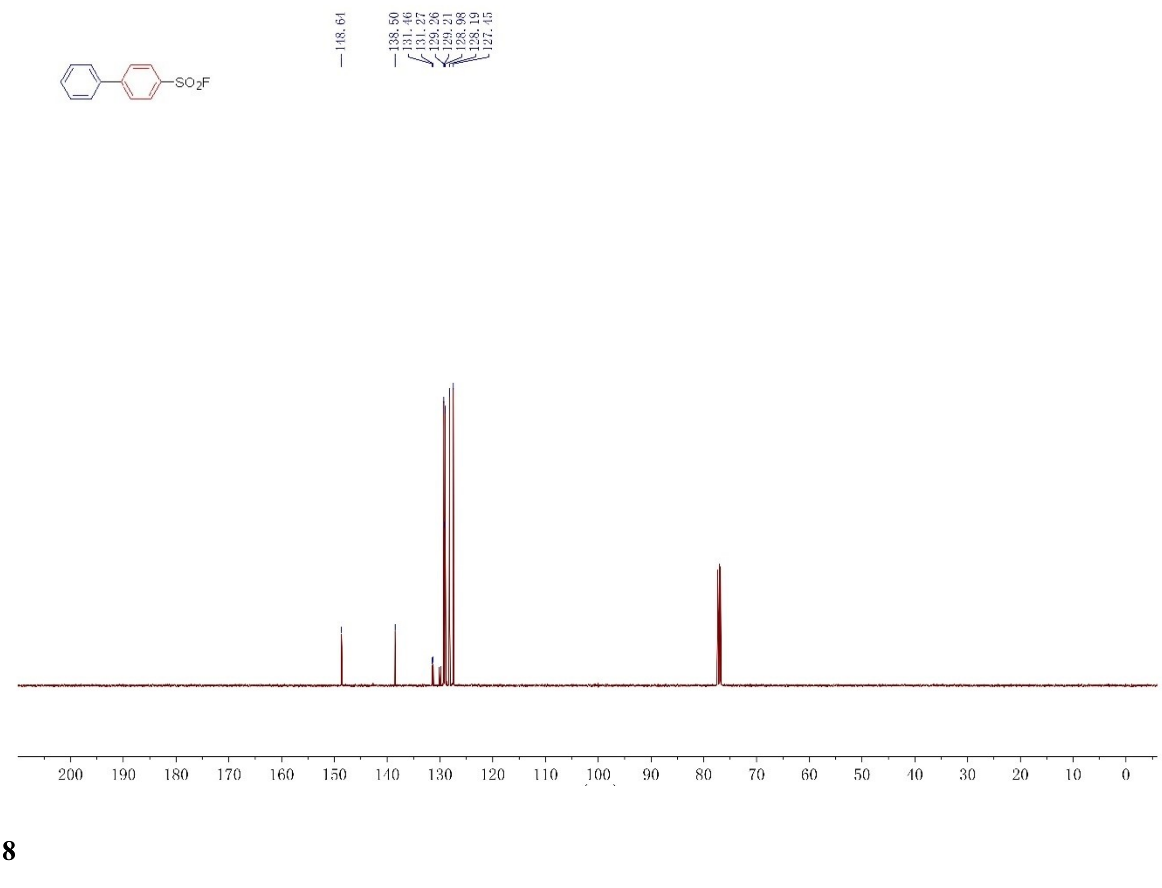
[19]F NMR (565 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)

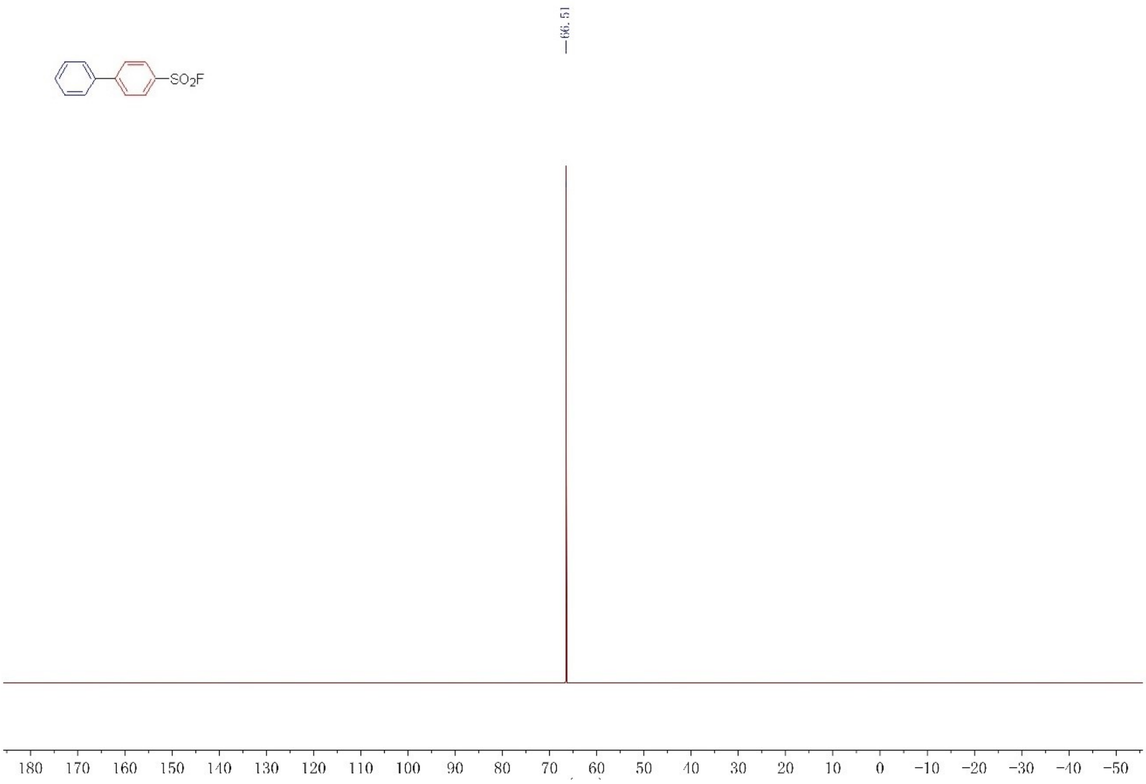


^{13}C NMR (126 MHz, $CDCl_3$)

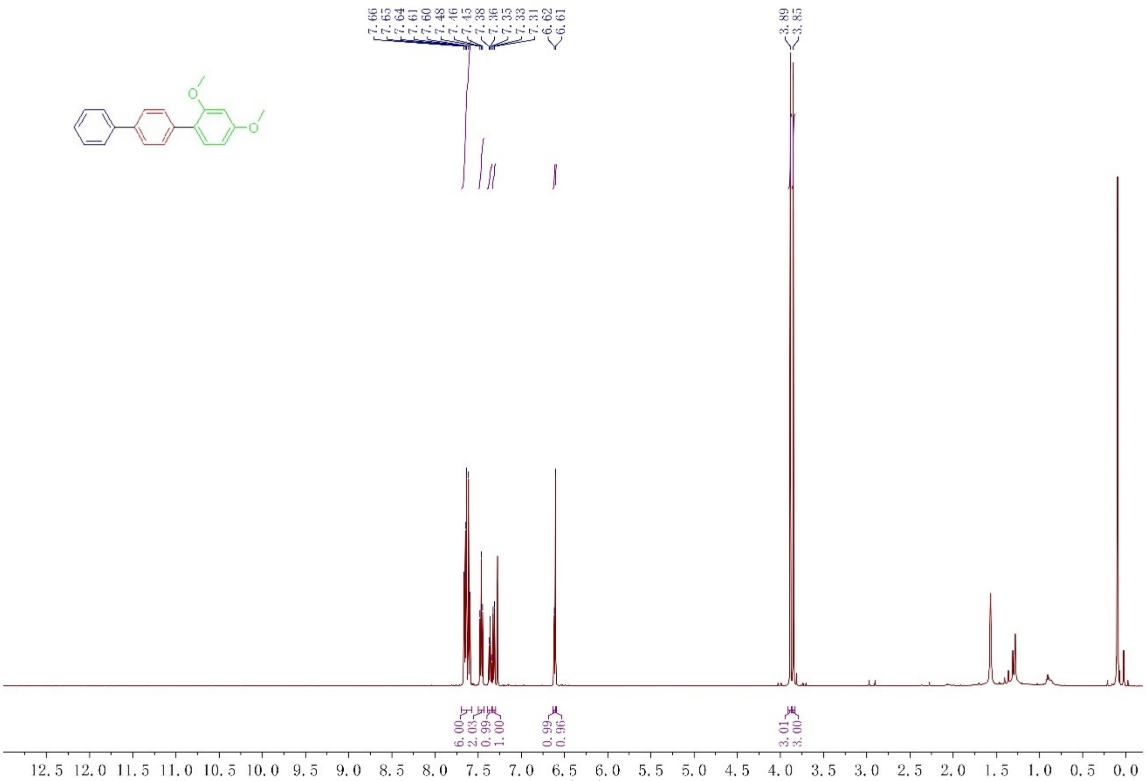


8

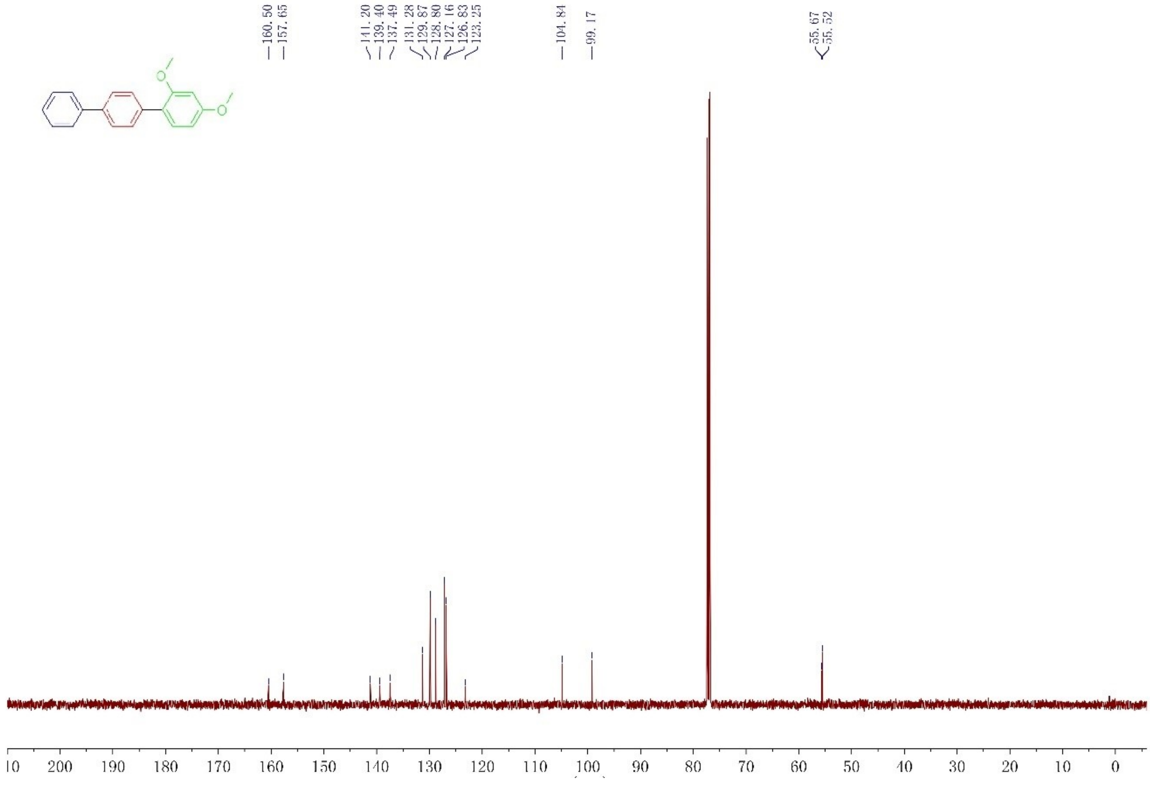
^{19}F NMR (565 MHz, $CDCl_3$)



^{1}H NMR (500 MHz, $CDCl_3$)



[13]C NMR (126 MHz, $CDCl_3$)



9. Table of Energies

Zero-point correction (ZPE), thermal correction to enthalpy (TCH), thermal correction to Gibbs free energy (TCG), energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree) of the structures calculated at the PBE0-D3BJ/6-311+G(d,p)/def2-TZVP//PBE0-D3BJ/6-31G(d)/def2-SVP/SMD (N,N-Dimethylformamide) level of theory.

Table S11. Energies for all calculated species.

Structures	ZPE	tcH	tcG	E	H	G	Imaginary Frequency
ArPh	0.216580	0.228929	0.178610	-576.947854	-576.946910	-576.997229	
$ArSO_2F$	0.137999	0.149736	0.100385	-993.660753	-993.659808	-993.709159	
$B(OH)_2F$	0.037103	0.042084	0.010799	-276.169507	-276.168563	-276.199848	
$PhB(OH)_2$	0.126277	0.135089	0.092818	-407.667587	-407.666643	-407.708914	
BSO_2F	0.046692	0.055178	0.013485	-824.433963	-824.433019	-824.474713	
LPd	0.679528	0.715931	0.611707	-1785.329850	-1785.328906	-1785.433129	
SO_2	0.007028	0.011044	-0.017171	-548.266346	-548.265402	-548.293617	
Int1	0.818640	0.867524	0.733815	-2779.038108	-2779.037164	-2779.170874	
Ts1	0.818200	0.866489	0.735508	-2779.003322	-2779.002378	-2779.133359	51.21i
Int2	0.818392	0.867829	0.732860	-2779.036416	-2779.035472	-2779.170441	
Ts2	0.947492	1.004156	0.857498	-3186.708198	-3186.707254	-3186.853912	241.83i
Int3	0.896467	0.945201	0.814389	-2362.266610	-2362.265666	-2362.396477	
Ts3	0.895410	0.944661	0.809758	-2362.258645	-2362.257701	-2362.392603	298.14i

Ts4	0.817763	0.866641	0.731075	-2778.990619	-2778.989674	-2779.125240	106.01i
Int4	0.819982	0.868667	0.737361	-2779.046586	-2779.045642	-2779.176948	
Ts5	0.818203	0.866852	0.735731	-2779.003357	-2779.002412	-2779.133532	48.79i
Int5	0.808477	0.853966	0.729878	-2230.737494	-2230.736550	-2230.860638	
Ts6	0.937677	0.990946	0.852133	-2638.423963	-2638.423019	-2638.561832	74.24i

10. Cartesian Coordinates of the Structures

ArPh

C	0.14887	0.0862	-0.02947
C	-0.5041	1.27327	-0.39519
C	-0.64621	-1.00947	0.31264
C	-1.88456	1.35892	-0.41741
H	0.08567	2.13609	-0.69286
C	-2.03648	-0.94106	0.29548
H	-0.1708	-1.93458	0.62775
C	-2.66415	0.25026	-0.07144
H	-2.38861	2.27445	-0.71102
H	-2.61398	-1.81365	0.58001
O	-4.00664	0.43117	-0.12302
C	-4.82576	-0.66273	0.21355
H	-4.66025	-0.98787	1.24927
H	-5.85428	-0.31426	0.10684
H	-4.6608	-1.51376	-0.46057
C	1.62267	0.00108	-0.00533
C	2.28345	-1.16483	-0.41281
C	2.39833	1.0846	0.4265
C	3.67086	-1.24656	-0.38565
H	1.7004	-2.00525	-0.7802
C	3.78601	1.00578	0.44914
H	1.90349	1.98811	0.77298
C	4.42919	-0.16092	0.04445
H	4.16247	-2.15882	-0.71311
H	4.3674	1.85645	0.79479
H	5.51367	-0.22338	0.0635

$ArSO_2F$

C	-0.51707	0.05795	0.08122
C	0.06451	1.32861	0.05627
C	0.26325	-1.09302	0.07533
C	1.44023	1.4375	0.01785
H	-0.56449	2.21237	0.08014
C	1.64724	-0.9834	0.03755
H	-0.21231	-2.06766	0.11258
C	2.24032	0.28448	0.00526
H	1.9295	2.40562	0.00239
H	2.25029	-1.88365	0.03884
S	-2.25975	-0.08951	0.12433

O	-2.63912	-1.4012	0.59312
O	-2.85069	1.12301	0.63838
F	-2.58284	-0.08767	-1.45181
O	3.56691	0.50044	-0.03186
C	4.4258	-0.62068	-0.04273
H	4.25299	-1.24718	-0.9265
H	5.43912	-0.2195	-0.07633
H	4.30394	-1.22551	0.86433

$B(OH)_2F$

B	0.01519	0.02077	0.00001
O	-0.69434	-1.14387	0.00003
H	-1.64444	-0.97737	-0.00026
O	1.36956	0.0168	-0.00005
H	1.70574	-0.88744	0.00025
F	-0.61545	1.1975	0.00002

$PhB(OH)_2$

B	-1.74292	-0.00196	-0.00596
O	-2.51699	1.11899	0.14791
H	-1.99052	1.91009	0.30682
O	-2.38281	-1.19715	-0.15668
H	-3.33973	-1.07116	-0.11257
C	-0.17762	0.01166	-0.00936
C	0.56151	1.19913	-0.08555
C	0.53118	-1.19519	0.07033
C	1.9523	1.19089	-0.07824
H	0.05158	2.15901	-0.16985
C	1.92152	-1.21453	0.08229
H	-0.02592	-2.12657	0.12358
C	2.63443	-0.01998	0.00889
H	2.50426	2.12479	-0.14241
H	2.45228	-2.16073	0.14736
H	3.72121	-0.0322	0.01692

BSO_2F

B	1.46039	0.09407	0.0565
O	2.56658	0.763	-0.35705
H	2.34563	1.63258	-0.71352
O	1.5304	-1.15523	0.58074
H	2.43833	-1.48278	0.58994

S	-1.15616	-0.08803	0.35938
O	-2.21078	0.88971	0.20182
O	0.2194	0.72402	-0.04841
F	-1.15912	-0.99819	-0.99176

LPd

C	1.01485	0.26738	1.52404
C	1.56278	0.39557	2.80067
C	0.77826	0.27555	3.94302
C	-0.58363	0.03518	3.8105
C	-1.14585	-0.08102	2.54286
C	-0.37525	0.03296	1.38064
C	1.87491	0.43117	0.32235
C	1.86823	1.71342	-0.31672
C	2.41926	1.85539	-1.62127
C	3.04244	0.73239	-2.21409
C	3.13424	-0.47891	-1.55239
C	2.53131	-0.62891	-0.2895
H	2.62315	0.61434	2.89058
H	1.22832	0.37855	4.92654
H	-1.21427	-0.06149	4.69021
H	-2.20937	-0.26592	2.46485
H	2.54338	2.83803	-2.06471
H	3.49501	0.8471	-3.19536
H	3.6131	-1.3388	-2.00844
O	2.46085	-1.88039	0.26819
C	3.39502	-2.16398	1.3195
C	4.70438	-2.65465	0.72624
C	2.72903	-3.17761	2.22602
H	3.57321	-1.2369	1.87925
H	5.1349	-1.89761	0.0626
H	5.43212	-2.87223	1.51593
H	4.5356	-3.56882	0.14634
H	1.81311	-2.7573	2.65202
H	2.46925	-4.07893	1.65999
H	3.39899	-3.46353	3.04374
O	1.54585	2.74655	0.50328
C	1.04013	3.96111	-0.05722
C	2.15042	4.99532	-0.12857
C	-0.11078	4.38999	0.83208
H	0.65058	3.73675	-1.06217
H	2.98351	4.64734	-0.74701
H	1.77511	5.93388	-0.55083

H	2.53708	5.19897	0.87607
H	-0.88007	3.61264	0.84546
H	0.24156	4.54726	1.85725
H	-0.55413	5.3228	0.4676
P	-1.10212	-0.10179	-0.31849
Pd	0.1718	1.23759	-1.6681
C	-2.95709	0.07221	-0.18339
C	-3.83049	-1.00432	0.47252
C	-3.29859	1.47862	0.32722
H	-3.21646	0.0638	-1.25497
C	-5.3137	-0.67118	0.30048
H	-3.61303	-1.10088	1.54244
H	-3.62092	-1.98216	0.02798
C	-4.78645	1.78319	0.17255
H	-3.01633	1.56992	1.38481
H	-2.69616	2.21466	-0.22089
C	-5.64569	0.71545	0.84403
H	-5.92572	-1.43587	0.795
H	-5.56799	-0.70891	-0.7692
H	-5.01033	2.77399	0.58712
H	-5.03549	1.82572	-0.89796
H	-6.71097	0.9357	0.70247
H	-5.46247	0.73228	1.92888
C	-0.72811	-1.87427	-0.75695
C	-0.85972	-2.92336	0.34761
C	-1.45579	-2.29606	-2.03611
H	0.34052	-1.8142	-1.00326
C	-0.33951	-4.27061	-0.15137
H	-1.90615	-3.0289	0.66221
H	-0.2905	-2.60613	1.22677
C	-0.94626	-3.65371	-2.51756
H	-2.53793	-2.36284	-1.85232
H	-1.3104	-1.53399	-2.81313
C	-1.06027	-4.71265	-1.4231
H	-0.44674	-5.0301	0.63376
H	0.73602	-4.17157	-0.35575
H	-1.49677	-3.96636	-3.41387
H	0.10807	-3.55116	-2.81258
H	-0.65944	-5.6704	-1.77816
H	-2.12364	-4.88233	-1.19543

SO_2

S	0.	0.	0.36915

O	0.	-1.25299	-0.36915
O	0.	1.25299	-0.36915

Int1

C	-0.90733	0.76585	2.32827
C	-1.08732	1.27217	3.62161
C	-1.99311	2.29227	3.88025
C	-2.74462	2.8263	2.8375
C	-2.56552	2.34327	1.54693
C	-1.64666	1.32201	1.26603
C	0.04458	-0.37317	2.18166
C	1.42365	-0.1763	2.41295
C	2.2905	-1.27031	2.48081
C	1.79906	-2.55589	2.27041
C	0.45695	-2.77309	1.99251
C	-0.41922	-1.68377	1.96318
H	-0.49953	0.84824	4.43127
H	-2.11471	2.66574	4.89328
H	-3.46388	3.61861	3.02603
H	-3.15283	2.76729	0.74056
H	3.34667	-1.12701	2.67279
H	2.48287	-3.39906	2.30755
H	0.0699	-3.76413	1.78677
O	-1.75278	-1.88467	1.72496
C	-2.57675	-1.99407	2.90134
C	-2.52552	-3.40782	3.45179
C	-3.96836	-1.56821	2.48502
H	-2.19363	-1.29026	3.65253
H	-1.50454	-3.68237	3.73433
H	-3.1591	-3.4941	4.3414
H	-2.88196	-4.11954	2.69912
H	-3.95866	-0.53089	2.13932
H	-4.3318	-2.20669	1.67195
H	-4.66341	-1.65156	3.32667
O	1.79831	1.11522	2.55253
C	3.18382	1.46306	2.49597
C	3.79836	1.39357	3.88449
C	3.23312	2.85859	1.90671
H	3.69156	0.77288	1.81073
H	3.71354	0.39102	4.3149
H	4.85935	1.66313	3.84861
H	3.28553	2.09397	4.55252
H	2.75934	2.86523	0.92172

H	2.70015	3.56426	2.55286
H	4.27072	3.18997	1.79964
P	-1.30656	0.73367	-0.43581
Pd	0.49561	-0.68596	-0.54039
C	-1.01307	2.25995	-1.46792
C	-2.16567	3.18047	-1.87393
C	0.125	3.05641	-0.8169
H	-0.61187	1.81649	-2.3936
C	-1.66536	4.29669	-2.79237
H	-2.62184	3.6349	-0.98538
H	-2.94963	2.6119	-2.38439
C	0.6085	4.18289	-1.72593
H	-0.22902	3.47854	0.13373
H	0.94852	2.37494	-0.56895
C	-0.54092	5.09694	-2.14114
H	-2.49834	4.95678	-3.06432
H	-1.29835	3.85229	-3.72939
H	1.3924	4.76184	-1.2199
H	1.06746	3.74971	-2.62803
H	-0.18352	5.87881	-2.82248
H	-0.93185	5.60925	-1.24981
C	-2.84907	-0.12817	-1.00449
C	-4.21024	0.52975	-0.7696
C	-2.67625	-0.55647	-2.46733
H	-2.81017	-1.03866	-0.38763
C	-5.33739	-0.40526	-1.20994
H	-4.2869	1.46778	-1.33361
H	-4.33122	0.78594	0.28839
C	-3.81594	-1.47319	-2.9056
H	-2.65855	0.33349	-3.11478
H	-1.71116	-1.06408	-2.59235
C	-5.17734	-0.82522	-2.66864
H	-6.30841	0.0812	-1.05308
H	-5.32761	-1.30148	-0.57251
H	-3.69391	-1.74114	-3.96204
H	-3.75441	-2.41047	-2.33431
H	-5.98325	-1.51065	-2.9586
H	-5.27295	0.06234	-3.31218
C	2.14944	-1.72871	-1.5061
C	3.35055	-1.7772	-0.73696
C	1.78881	-0.52711	-2.21576
C	4.12129	-0.65765	-0.60579
H	3.64245	-2.71275	-0.27338
C	2.65484	0.60208	-2.08844

H	1.14846	-0.59576	-3.09098
C	3.76681	0.54521	-1.27698
H	5.03458	-0.6663	-0.01948
H	2.41822	1.49221	-2.66047
S	1.50407	-3.25088	-2.09977
O	0.76953	-3.04926	-3.33009
O	2.4781	-4.31085	-1.9487
F	0.36439	-3.61063	-1.00503
O	4.62433	1.57405	-1.06108
C	4.37375	2.77955	-1.74321
H	3.39567	3.19838	-1.47356
H	5.15998	3.47135	-1.43682
H	4.41539	2.63906	-2.83136

Ts1

C	0.64456	2.46889	0.29373
C	0.60955	3.83024	0.62347
C	1.55022	4.39309	1.47564
C	2.55841	3.59591	2.00942
C	2.58618	2.23779	1.71664
C	1.62982	1.64832	0.87658
C	-0.32088	2.01722	-0.74975
C	-1.71468	2.0724	-0.52771
C	-2.60413	1.93176	-1.59791
C	-2.11507	1.66845	-2.873
C	-0.75279	1.53218	-3.10422
C	0.13966	1.72608	-2.04934
H	-0.16506	4.45095	0.18145
H	1.50417	5.45295	1.71028
H	3.31431	4.02576	2.6608
H	3.36577	1.62325	2.15101
H	-3.67344	2.00286	-1.4434
H	-2.81618	1.54486	-3.69363
H	-0.3599	1.27931	-4.08265
O	1.48257	1.60845	-2.26641
C	2.18493	2.83455	-2.54321
C	1.92966	3.29427	-3.96776
C	3.64479	2.54188	-2.27236
H	1.82993	3.59927	-1.83881
H	0.86595	3.48746	-4.13755
H	2.47833	4.22069	-4.17001
H	2.26316	2.52969	-4.67804
H	3.78549	2.26559	-1.2244

H	3.98614	1.71316	-2.90237
H	4.25958	3.42143	-2.48874
O	-2.08564	2.26826	0.75963
C	-3.46296	2.15193	1.12235
C	-4.16527	3.48637	0.93371
C	-3.47469	1.6834	2.56437
H	-3.93003	1.37962	0.49784
H	-4.09231	3.83386	-0.10138
H	-5.22595	3.40384	1.19374
H	-3.70699	4.24251	1.58021
H	-3.00728	0.69824	2.64903
H	-2.92054	2.38499	3.19669
H	-4.50366	1.62046	2.93459
P	1.50178	-0.16533	0.6575
Pd	-0.36646	-0.77171	-0.59612
C	1.15955	-0.78283	2.38375
C	2.19891	-0.55916	3.48261
C	-0.20757	-0.24872	2.82799
H	1.0561	-1.86801	2.22772
C	1.75506	-1.22721	4.78528
H	2.31214	0.51731	3.66295
H	3.17917	-0.94349	3.17844
C	-0.65357	-0.89077	4.13905
H	-0.15035	0.84236	2.94706
H	-0.94871	-0.43493	2.03885
C	0.39274	-0.70699	5.23515
H	2.50618	-1.05757	5.56677
H	1.69882	-2.31497	4.63309
H	-1.61615	-0.46813	4.45544
H	-0.81973	-1.9658	3.97345
H	0.07596	-1.21114	6.15645
H	0.4786	0.36336	5.47358
C	3.11608	-0.86943	0.0854
C	4.43842	-0.22577	0.50044
C	3.12948	-2.37324	0.39462
H	3.0176	-0.76264	-1.00394
C	5.59336	-0.90038	-0.24251
H	4.59325	-0.33371	1.58346
H	4.43684	0.84685	0.28143
C	4.27721	-3.05148	-0.34696
H	3.26159	-2.51894	1.4767
H	2.17976	-2.83539	0.10993
C	5.61766	-2.40824	-0.00114
H	6.54649	-0.44775	0.05894

H	5.47811	-0.7065	-1.31881
H	4.29307	-4.12166	-0.10804
H	4.08595	-2.97336	-1.4257
H	6.42688	-2.87042	-0.57996
H	5.84367	-2.59667	1.05933
C	-1.95725	-2.04422	-1.13051
C	-2.85645	-1.42839	-2.00877
C	-2.34159	-2.36734	0.17739
C	-4.12515	-1.10735	-1.56674
H	-2.53448	-1.2082	-3.02062
C	-3.61709	-2.03288	0.62776
H	-1.65224	-2.91511	0.8126
C	-4.50182	-1.3887	-0.24351
H	-4.84636	-0.6199	-2.21538
H	-3.90975	-2.28625	1.64039
S	-0.29581	-2.80292	-1.80509
O	-0.09902	-3.97953	-0.95934
O	-0.65536	-2.90005	-3.21877
F	1.3323	-2.34491	-2.05158
O	-5.74611	-0.98884	0.09997
C	-6.18413	-1.25103	1.41458
H	-5.54571	-0.75392	2.15647
H	-7.19598	-0.84867	1.47979
H	-6.20796	-2.32815	1.6219

Int2

C	-2.28827	-0.64709	1.62408
C	-3.21789	-1.0627	2.58266
C	-3.37334	-0.37374	3.7779
C	-2.58752	0.74648	4.03444
C	-1.64745	1.15784	3.09727
C	-1.48033	0.47461	1.8842
C	-2.18121	-1.39391	0.35003
C	-1.63073	-2.68413	0.32128
C	-1.48046	-3.35824	-0.89929
C	-1.81896	-2.72467	-2.08563
C	-2.33521	-1.42638	-2.08706
C	-2.53596	-0.77715	-0.86548
H	-3.82161	-1.94121	2.37335
H	-4.1043	-0.71004	4.50783
H	-2.69868	1.29539	4.96525
H	-1.02841	2.02038	3.31781
H	-1.06164	-4.35662	-0.93622

H	-1.63936	-3.2206	-3.03173
H	-2.58244	-0.9159	-3.00958
O	-3.05295	0.49013	-0.84625
C	-4.44415	0.58668	-0.48195
C	-5.31483	0.27622	-1.68489
C	-4.64118	1.98591	0.05951
H	-4.63691	-0.14253	0.31662
H	-5.11503	-0.73136	-2.0633
H	-6.37496	0.33444	-1.41532
H	-5.11819	0.99285	-2.48944
H	-4.01446	2.14265	0.94227
H	-4.3707	2.72721	-0.70076
H	-5.68748	2.14467	0.33896
O	-1.22495	-3.15978	1.51974
C	-0.49534	-4.38685	1.59659
C	-1.45165	-5.56757	1.60988
C	0.3316	-4.2892	2.86361
H	0.17965	-4.44993	0.73205
H	-2.07992	-5.58783	0.71432
H	-0.8965	-6.51003	1.66081
H	-2.10731	-5.5039	2.48494
H	1.01207	-3.43359	2.8141
H	-0.32232	-4.15908	3.73216
H	0.92282	-5.19954	3.00408
P	-0.16892	0.97746	0.70402
Pd	0.10228	-0.24944	-1.2997
C	1.37584	1.13421	1.72716
C	1.66683	2.42931	2.48905
C	1.49406	-0.0814	2.65666
H	2.15858	1.03354	0.96394
C	3.06625	2.35705	3.10385
H	0.93361	2.58635	3.29128
H	1.60471	3.29546	1.82262
C	2.88287	-0.14624	3.2857
H	0.73396	-0.01196	3.44571
H	1.28282	-1.00296	2.10179
C	3.21469	1.14798	4.02361
H	3.28004	3.28462	3.64925
H	3.8047	2.28771	2.29192
H	2.93973	-1.00194	3.97038
H	3.62448	-0.32235	2.49494
H	4.23155	1.10494	4.4322
H	2.53486	1.26245	4.88102
C	-0.70142	2.62286	0.02119

C	-1.2173	3.67371	1.0076
C	0.38431	3.18672	-0.9059
H	-1.55006	2.32324	-0.61152
C	-1.70385	4.91414	0.25779
H	-0.42434	3.96596	1.70685
H	-2.0348	3.25931	1.60629
C	-0.10733	4.44238	-1.62219
H	1.29013	3.42276	-0.32978
H	0.66665	2.42698	-1.64429
C	-0.61134	5.49188	-0.63681
H	-2.0547	5.66567	0.97585
H	-2.57063	4.64034	-0.36131
H	0.69755	4.84941	-2.2456
H	-0.92203	4.1626	-2.30513
H	-0.98461	6.37227	-1.17378
H	0.22537	5.83631	-0.01071
C	2.04314	-0.40241	-0.98047
C	2.46793	-1.51734	-0.25252
C	2.9793	0.52311	-1.42071
C	3.81093	-1.67961	0.06262
H	1.74904	-2.26168	0.07933
C	4.32986	0.37582	-1.09204
H	2.67657	1.35733	-2.04356
C	4.74851	-0.72387	-0.34221
H	4.15665	-2.54058	0.62731
H	5.03959	1.1154	-1.44667
S	0.55148	-0.63891	-3.57439
O	1.66941	0.11637	-4.13642
O	0.2576	-1.95083	-4.15657
F	-0.7813	0.2928	-4.0306
O	6.03147	-0.95546	0.04082
C	7.00571	-0.02662	-0.36568
H	6.80244	0.97538	0.03711
H	7.95486	-0.38793	0.03408
H	7.07445	0.03564	-1.4599

Ts2

C	-0.98909	-2.57617	-0.48002
C	-1.41257	-3.89914	-0.67345
C	-1.6708	-4.42178	-1.93113
C	-1.54594	-3.59679	-3.04147
C	-1.12603	-2.2848	-2.87246
C	-0.80396	-1.75375	-1.61213

C	-0.89977	-2.16473	0.95053
C	-2.10807	-1.99484	1.66419
C	-2.09572	-1.73291	3.03521
C	-0.87922	-1.65628	3.70798
C	0.31707	-1.86402	3.03941
C	0.29732	-2.14886	1.67145
H	-1.55421	-4.51929	0.20759
H	-1.98886	-5.45489	-2.03816
H	-1.775	-3.9646	-4.03741
H	-1.06379	-1.65588	-3.74804
H	-3.02071	-1.58589	3.57987
H	-0.87144	-1.44432	4.77327
H	1.27037	-1.83807	3.55572
O	1.48817	-2.4464	1.06151
C	1.7684	-3.85917	0.81534
C	1.33421	-4.73153	1.97933
C	3.25713	-3.9597	0.55873
H	1.21026	-4.13698	-0.08619
H	0.25838	-4.67151	2.17205
H	1.5795	-5.77322	1.74783
H	1.86575	-4.45071	2.8952
H	3.54254	-3.38307	-0.32189
H	3.82086	-3.58161	1.41761
H	3.52369	-5.00893	0.39278
O	-3.23567	-2.11937	0.9255
C	-4.5076	-2.25034	1.56108
C	-4.62899	-3.6056	2.23998
C	-5.52991	-2.07429	0.45551
H	-4.62836	-1.43945	2.29287
H	-3.8511	-3.75425	2.99437
H	-5.60371	-3.70032	2.72969
H	-4.53872	-4.40053	1.49169
H	-5.43581	-1.08911	-0.00899
H	-5.38009	-2.83631	-0.3166
H	-6.54319	-2.17662	0.85619
P	-0.29679	0.01797	-1.57259
Pd	1.10532	0.6929	0.15014
C	-1.89359	0.93715	-1.80695
C	-2.52094	0.84058	-3.20081
C	-2.92273	0.52748	-0.75346
H	-1.6175	1.9827	-1.62279
C	-3.76165	1.73297	-3.28575
H	-2.80824	-0.19992	-3.40315
H	-1.81137	1.1396	-3.97741

C	-4.1461	1.43683	-0.82311
H	-3.21882	-0.51304	-0.93064
H	-2.48797	0.56838	0.24638
C	-4.78506	1.39183	-2.20685
H	-4.20883	1.64533	-4.28367
H	-3.45139	2.78199	-3.17092
H	-4.87023	1.14505	-0.05204
H	-3.83928	2.46465	-0.58375
H	-5.64006	2.07669	-2.2648
H	-5.17741	0.38019	-2.38981
C	0.79318	0.45737	-3.04419
C	0.63499	-0.1462	-4.44516
C	0.86517	1.99383	-3.08197
H	1.77325	0.10651	-2.72032
C	1.74239	0.37602	-5.36521
H	-0.34216	0.08547	-4.88672
H	0.73081	-1.2335	-4.38875
C	1.96219	2.47569	-4.02713
H	-0.09983	2.41258	-3.39911
H	1.06821	2.37294	-2.07198
C	1.77773	1.89821	-5.42467
H	1.60513	-0.04939	-6.36686
H	2.70861	0.00684	-4.99432
H	1.96413	3.57232	-4.05539
H	2.93352	2.16214	-3.62386
H	2.58454	2.23352	-6.08725
H	0.8372	2.2725	-5.85659
C	-0.36068	1.84858	0.84989
C	-1.04905	1.43892	1.99367
C	-0.62518	3.11103	0.33056
C	-1.97971	2.2706	2.60096
H	-0.85818	0.4625	2.42122
C	-1.55878	3.96122	0.93293
H	-0.09707	3.46933	-0.54959
C	-2.24353	3.53772	2.07235
H	-2.51723	1.95429	3.49049
H	-1.73313	4.94305	0.50542
S	3.04794	-0.48677	-0.69396
O	4.13905	-0.66748	0.33639
O	2.99068	-1.58868	-1.65103
F	3.71993	0.73787	-1.60275
O	-3.17496	4.27519	2.73267
C	-3.47848	5.54694	2.21728
H	-3.87576	5.48522	1.19455

H	-4.24216	5.96729	2.87404
H	-2.59973	6.20636	2.21843
B	3.9487	-0.09934	1.88238
O	3.52187	-1.22461	2.63693
H	2.81399	-1.67028	2.14867
O	5.25866	0.36449	2.16892
H	5.22773	0.95116	2.93144
C	2.88171	1.17069	1.89459
C	2.11294	1.33941	3.0706
C	3.00225	2.31501	1.05985
C	1.55788	2.56163	3.42407
H	2.01029	0.48281	3.73077
C	2.43609	3.54605	1.4099
H	3.62682	2.25724	0.17204
C	1.7277	3.67358	2.597
H	0.98692	2.65583	4.34396
H	2.56325	4.40365	0.75384
H	1.28934	4.62883	2.87201

Int3

C	-0.86212	-2.42769	0.54293
C	-0.95402	-3.74102	1.02168
C	-2.12657	-4.21978	1.59064
C	-3.23839	-3.3869	1.68655
C	-3.1557	-2.07714	1.23002
C	-1.97393	-1.57744	0.6649
C	0.41227	-2.05555	-0.1453
C	1.6406	-2.10215	0.56653
C	2.85355	-2.18783	-0.12148
C	2.86061	-2.16316	-1.51
C	1.68104	-2.06217	-2.23802
C	0.46467	-2.02895	-1.56059
H	-0.08633	-4.38959	0.9357
H	-2.1743	-5.24294	1.95316
H	-4.16394	-3.75286	2.12214
H	-4.02289	-1.43237	1.31415
H	3.79518	-2.21464	0.41179
H	3.81307	-2.18547	-2.02967
H	1.68499	-1.99646	-3.32009
O	-0.71581	-1.99787	-2.25186
C	-1.2472	-3.29232	-2.60517
C	-0.67317	-3.75908	-3.93108
C	-2.75341	-3.14435	-2.63492

H	-0.97083	-4.00069	-1.81272
H	0.41251	-3.87863	-3.8723
H	-1.1051	-4.72602	-4.21161
H	-0.90406	-3.03337	-4.71858
H	-3.12626	-2.88443	-1.64124
H	-3.0421	-2.355	-3.33819
H	-3.22443	-4.08008	-2.95319
O	1.51393	-2.08651	1.90857
C	2.67658	-1.95455	2.73458
C	3.27853	-3.32365	3.00256
C	2.20143	-1.26563	3.9985
H	3.39607	-1.30451	2.22254
H	3.56297	-3.82486	2.07222
H	4.17133	-3.23333	3.63001
H	2.5507	-3.95553	3.52324
H	1.78078	-0.2835	3.76248
H	1.42656	-1.86374	4.48983
H	3.03492	-1.13231	4.69544
P	-1.75033	0.16678	0.16426
Pd	0.54673	0.50448	-0.30893
C	-2.1442	1.16488	1.67685
C	-3.56885	1.21386	2.23018
C	-1.15514	0.75736	2.77739
H	-1.8705	2.18105	1.35238
C	-3.64555	2.18062	3.41349
H	-3.86962	0.21605	2.57464
H	-4.28012	1.51897	1.45513
C	-1.23905	1.70321	3.97213
H	-1.3758	-0.27005	3.10001
H	-0.1364	0.73794	2.36662
C	-2.66338	1.78991	4.51446
H	-4.66978	2.20902	3.80609
H	-3.41339	3.19646	3.06189
H	-0.54796	1.3746	4.75875
H	-0.91016	2.70497	3.65967
H	-2.71513	2.50635	5.34357
H	-2.95393	0.81123	4.92451
C	-2.98177	0.5557	-1.16804
C	-4.38329	-0.05428	-1.10085
C	-3.06025	2.07704	-1.35359
H	-2.48002	0.1352	-2.0529
C	-5.17351	0.29792	-2.36191
H	-4.92086	0.32685	-0.22205
H	-4.32667	-1.14176	-0.99284

C	-3.85163	2.42643	-2.61096
H	-3.55816	2.52588	-0.48205
H	-2.05759	2.51316	-1.4038
C	-5.2461	1.80742	-2.58047
H	-6.18167	-0.13118	-2.30206
H	-4.68405	-0.17046	-3.22881
H	-3.91574	3.51612	-2.71786
H	-3.30556	2.05552	-3.49074
H	-5.78832	2.03181	-3.50736
H	-5.82294	2.2615	-1.76094
C	2.51913	0.92632	-0.44709
C	3.27387	1.06912	0.72645
C	3.21895	0.93386	-1.65256
C	4.66204	1.12906	0.70419
H	2.76822	1.12559	1.68985
C	4.61533	1.00659	-1.70271
H	2.67584	0.86745	-2.59327
C	5.34292	1.08832	-0.51639
H	5.24325	1.22601	1.61779
H	5.11565	1.00566	-2.66638
O	6.70406	1.14849	-0.44201
C	7.41269	1.15465	-1.65302
H	7.14687	2.01978	-2.27628
H	8.47047	1.21528	-1.3886
H	7.23862	0.23635	-2.23219
C	0.46704	2.4922	-0.43046
C	0.42103	3.30727	0.70502
C	0.35516	3.10392	-1.68549
C	0.21958	4.6835	0.59433
H	0.55178	2.87062	1.69228
C	0.15495	4.47913	-1.79757
H	0.41909	2.50058	-2.58799
C	0.07674	5.27562	-0.65714
H	0.18168	5.29442	1.49397
H	0.06244	4.92955	-2.78366
H	-0.07912	6.3476	-0.74447

Ts3

C	-0.84139	-2.31731	0.98688
C	-0.92827	-3.50632	1.7213
C	-2.05703	-3.81153	2.47088
C	-3.12865	-2.92336	2.49726
C	-3.05051	-1.73396	1.78236

C	-1.91551	-1.4082	1.02726
C	0.3846	-2.12647	0.15467
C	1.65069	-1.98038	0.76959
C	2.82059	-2.07696	0.00913
C	2.73512	-2.27609	-1.3632
C	1.50471	-2.39391	-1.99937
C	0.33967	-2.33678	-1.23803
H	-0.08943	-4.19686	1.69552
H	-2.10037	-4.74141	3.03134
H	-4.01945	-3.15226	3.07587
H	-3.88674	-1.0443	1.81086
H	3.79389	-1.95053	0.46643
H	3.65052	-2.31499	-1.94516
H	1.42748	-2.52222	-3.07355
O	-0.8836	-2.48212	-1.83624
C	-1.38757	-3.83236	-1.85869
C	-0.89255	-4.55202	-3.10058
C	-2.89681	-3.73704	-1.78864
H	-1.01883	-4.34816	-0.96212
H	0.20031	-4.60527	-3.11181
H	-1.28329	-5.57513	-3.13228
H	-1.22576	-4.02379	-4.00067
H	-3.20349	-3.27861	-0.84479
H	-3.27698	-3.12799	-2.61653
H	-3.34753	-4.73251	-1.85772
O	1.60946	-1.76555	2.10221
C	2.81163	-1.47394	2.81871
C	3.50012	-2.76691	3.2225
C	2.38079	-0.6393	4.00835
H	3.46585	-0.87049	2.17832
H	3.74814	-3.37495	2.34699
H	4.42643	-2.55574	3.76746
H	2.84117	-3.35367	3.87177
H	1.88564	0.27563	3.6689
H	1.67606	-1.20017	4.63137
H	3.24758	-0.36593	4.6189
P	-1.71489	0.18595	0.14968
Pd	0.53406	0.53165	-0.38191
C	-2.15992	1.5216	1.36594
C	-3.60996	1.78693	1.77294
C	-1.27096	1.35536	2.60512
H	-1.79602	2.41531	0.83285
C	-3.69149	3.02019	2.67445
H	-4.0172	0.92422	2.31635

H	-4.24048	1.93976	0.89108
C	-1.35933	2.58082	3.50995
H	-1.58424	0.45963	3.16018
H	-0.23468	1.17691	2.28675
C	-2.80393	2.87374	3.90733
H	-4.7331	3.19831	2.97024
H	-3.37114	3.90164	2.0998
H	-0.73838	2.43453	4.403
H	-0.94825	3.4487	2.97426
H	-2.85615	3.77935	4.52442
H	-3.18197	2.04727	4.52749
C	-2.94508	0.18901	-1.23914
C	-4.36202	-0.32206	-0.97444
C	-2.96345	1.57701	-1.89234
H	-2.47175	-0.50729	-1.94724
C	-5.17176	-0.33825	-2.27089
H	-4.87106	0.31866	-0.24312
H	-4.32948	-1.32894	-0.54565
C	-3.78536	1.55741	-3.17925
H	-3.40167	2.30851	-1.19796
H	-1.93929	1.91415	-2.09122
C	-5.19961	1.03796	-2.93109
H	-6.19187	-0.69008	-2.07157
H	-4.71959	-1.06219	-2.96502
H	-3.81656	2.5625	-3.61786
H	-3.28447	0.90817	-3.91237
H	-5.76421	0.99938	-3.87103
H	-5.73166	1.7416	-2.27343
C	2.44672	1.23159	-0.6311
C	3.23305	1.36072	0.52644
C	3.10925	0.93428	-1.82544
C	4.60175	1.14205	0.50266
H	2.76361	1.63345	1.4691
C	4.4874	0.71887	-1.87103
H	2.54374	0.85847	-2.75109
C	5.23902	0.80941	-0.69875
H	5.20692	1.23314	1.40089
H	4.9579	0.4842	-2.82058
O	6.58257	0.60969	-0.62161
C	7.25601	0.28214	-1.81013
H	7.16604	1.07902	-2.56089
H	8.30687	0.15952	-1.54121
H	6.88242	-0.65675	-2.24263
C	0.87352	2.50587	-0.7274

C	0.77486	3.40611	0.3474
C	0.60929	3.00076	-2.01651
C	0.38993	4.72874	0.14652
H	1.00044	3.0682	1.35573
C	0.2231	4.32311	-2.21412
H	0.70182	2.33954	-2.87458
C	0.10517	5.19735	-1.13465
H	0.31396	5.39815	1.00102
H	0.01367	4.67291	-3.22273
H	-0.19155	6.23066	-1.29121

Ts4

C	-2.88789	-1.09065	1.07532
C	-3.85549	-1.66612	1.90151
C	-4.53088	-0.91262	2.85546
C	-4.24205	0.44138	2.98694
C	-3.26296	1.01924	2.1851
C	-2.55784	0.2714	1.23453
C	-2.26332	-1.92638	0.01404
C	-1.15747	-2.75935	0.29862
C	-0.55646	-3.49822	-0.73332
C	-1.05926	-3.41016	-2.03068
C	-2.16379	-2.61977	-2.31954
C	-2.76233	-1.88844	-1.29393
H	-4.07578	-2.72418	1.78632
H	-5.28052	-1.38049	3.4876
H	-4.77068	1.04863	3.71674
H	-3.04303	2.07383	2.30466
H	0.28766	-4.14605	-0.52751
H	-0.58042	-3.98059	-2.82143
H	-2.55867	-2.53647	-3.32638
O	-3.80221	-1.04596	-1.58286
C	-5.11827	-1.55346	-1.30204
C	-5.64064	-2.31549	-2.50733
C	-5.97277	-0.36142	-0.92675
H	-5.04751	-2.23189	-0.4422
H	-4.97921	-3.1528	-2.75262
H	-6.64013	-2.71742	-2.30743
H	-5.69963	-1.6525	-3.37755
H	-5.5841	0.11126	-0.01994
H	-5.96904	0.37607	-1.73691
H	-7.00716	-0.67193	-0.74554
O	-0.788	-2.81713	1.59731

C	0.53171	-3.2613	1.93437
C	0.49882	-4.74168	2.27427
C	0.98857	-2.39479	3.09043
H	1.19245	-3.07599	1.07635
H	0.11957	-5.33756	1.43812
H	1.50239	-5.10063	2.52686
H	-0.15623	-4.91093	3.13569
H	1.04402	-1.35027	2.77265
H	0.28705	-2.47695	3.9274
H	1.98039	-2.70969	3.43227
P	-1.17551	0.97764	0.24442
Pd	0.29911	-0.61431	-0.34437
C	-0.39636	2.34164	1.2463
C	-1.04227	3.72569	1.36591
C	0.0088	1.79908	2.62207
H	0.53627	2.47593	0.67726
C	-0.08934	4.68843	2.07803
H	-1.98278	3.67591	1.93044
H	-1.2907	4.12364	0.37729
C	0.9475	2.7691	3.33318
H	-0.88772	1.6374	3.23538
H	0.49571	0.82683	2.49829
C	0.32815	4.15945	3.44725
H	-0.55925	5.67564	2.17295
H	0.80665	4.82403	1.45474
H	1.20101	2.38097	4.32779
H	1.88822	2.82607	2.7677
H	1.02834	4.85555	3.92592
H	-0.5579	4.10758	4.09786
C	-2.01596	1.71086	-1.24046
C	-3.30433	2.49928	-1.00479
C	-1.01366	2.48807	-2.09975
H	-2.2973	0.80994	-1.80289
C	-3.92861	2.88862	-2.34449
H	-3.10237	3.40685	-0.42187
H	-4.00922	1.89671	-0.42305
C	-1.65238	2.89491	-3.42631
H	-0.68229	3.3911	-1.56779
H	-0.11764	1.87909	-2.26651
C	-2.94665	3.67597	-3.20949
H	-4.84564	3.46873	-2.17916
H	-4.22334	1.97089	-2.87437
H	-0.9426	3.48597	-4.0186
H	-1.87073	1.98768	-4.00868

H	-3.40544	3.93096	-4.17316
H	-2.71291	4.62865	-2.71074
C	4.4497	0.20272	-0.57551
C	4.98846	0.5394	-1.8181
C	5.26529	-0.26214	0.44754
C	6.34898	0.40995	-2.0283
H	4.34	0.91533	-2.60216
C	6.63474	-0.39351	0.24018
H	4.83086	-0.50388	1.41175
C	7.18062	-0.0586	-1.00241
H	6.79971	0.67099	-2.9803
H	7.26164	-0.74908	1.04978
S	2.69617	0.36002	-0.30027
O	2.5789	0.44731	1.15727
O	2.28102	1.36748	-1.27726
F	2.47746	-1.26074	-0.85867
O	8.49311	-0.14525	-1.30809
C	9.3745	-0.60423	-0.3087
H	9.12795	-1.62639	0.00636
H	10.36853	-0.59585	-0.75791
H	9.36733	0.05645	0.56786

Int4

C	-2.26893	-1.71894	0.47082
C	-3.17273	-2.69162	0.90902
C	-4.42497	-2.33761	1.39676
C	-4.79625	-0.99655	1.44432
C	-3.89967	-0.0192	1.02766
C	-2.63	-0.36499	0.55054
C	-0.99551	-2.18546	-0.15533
C	-0.04511	-2.93426	0.59148
C	0.94615	-3.66237	-0.07625
C	1.031	-3.62054	-1.45595
C	0.12242	-2.8876	-2.21874
C	-0.90742	-2.21738	-1.57677
H	-2.88016	-3.73694	0.86122
H	-5.11131	-3.10836	1.7359
H	-5.77582	-0.71031	1.81634
H	-4.18779	1.02471	1.08212
H	1.68137	-4.21677	0.49284
H	1.8328	-4.15897	-1.95241
H	0.19456	-2.84084	-3.29942
O	-1.87999	-1.58396	-2.29718

C	-3.00431	-2.42394	-2.64921
C	-2.76238	-3.07004	-4.00083
C	-4.23927	-1.54918	-2.62321
H	-3.09764	-3.20057	-1.8787
H	-1.87831	-3.71382	-3.97739
H	-3.62194	-3.68536	-4.28815
H	-2.61437	-2.29995	-4.76557
H	-4.40934	-1.15595	-1.61747
H	-4.12491	-0.70996	-3.31776
H	-5.11858	-2.12733	-2.92557
O	-0.16102	-2.88717	1.92769
C	1.06052	-2.93885	2.71214
C	1.18646	-4.31905	3.32754
C	0.95485	-1.83243	3.74153
H	1.88758	-2.70106	2.0357
H	1.21625	-5.1021	2.56259
H	2.10313	-4.38724	3.92296
H	0.33309	-4.51983	3.98489
H	1.00168	-0.85278	3.25729
H	0.02094	-1.91874	4.3078
H	1.79392	-1.8955	4.44317
P	-1.372	0.88546	0.11529
Pd	0.5776	-0.29141	0.13854
C	-1.40436	2.18109	1.43069
C	-2.49132	3.25922	1.43368
C	-1.29417	1.49313	2.79804
H	-0.45365	2.6968	1.23624
C	-2.18898	4.28134	2.53221
H	-3.48296	2.82384	1.61464
H	-2.5337	3.77049	0.46671
C	-1.00371	2.51987	3.88748
H	-2.23129	0.96459	3.02175
H	-0.49865	0.74072	2.77499
C	-2.06039	3.62124	3.90226
H	-2.97245	5.04941	2.54657
H	-1.24729	4.79197	2.28642
H	-0.95688	2.02022	4.86275
H	-0.01069	2.95166	3.70509
H	-1.81921	4.3747	4.66204
H	-3.03143	3.18764	4.18585
C	-1.82624	1.56707	-1.53958
C	-3.29112	1.97082	-1.72956
C	-0.86646	2.68848	-1.95042
H	-1.64166	0.70292	-2.19368

C	-3.53338	2.38661	-3.18059
H	-3.5471	2.81009	-1.0719
H	-3.95172	1.14021	-1.4606
C	-1.13242	3.11055	-3.39367
H	-0.99167	3.55406	-1.28595
H	0.17014	2.36198	-1.82405
C	-2.59054	3.51041	-3.60285
H	-4.57963	2.68977	-3.31149
H	-3.37163	1.51661	-3.83418
H	-0.46496	3.93688	-3.6665
H	-0.88719	2.27235	-4.06239
H	-2.76698	3.78132	-4.65104
H	-2.80906	4.40759	-3.00488
C	3.45315	1.1757	-0.03753
C	3.69835	1.80977	-1.25404
C	4.39192	0.3283	0.53527
C	4.90674	1.60175	-1.89546
H	2.95199	2.47669	-1.67297
C	5.6107	0.12672	-0.1017
H	4.16235	-0.16447	1.47109
C	5.86739	0.75886	-1.3226
H	5.13976	2.08798	-2.83737
H	6.3442	-0.52886	0.35372
S	1.89889	1.44555	0.7806
O	2.11448	1.28337	2.23559
O	1.43293	2.77038	0.29864
F	2.25593	-1.35793	0.33057
O	7.0172	0.62343	-2.02394
C	8.01644	-0.21257	-1.49082
H	7.66471	-1.24766	-1.38989
H	8.84538	-0.18134	-2.19988
H	8.36333	0.14629	-0.51287

Ts5

C	-1.28364	-1.36777	1.75412
C	-1.52619	-2.03608	2.95664
C	-2.37377	-1.50879	3.92338
C	-3.00133	-0.2892	3.69454
C	-2.73888	0.40663	2.51998
C	-1.87453	-0.10324	1.54355
C	-0.48969	-2.05114	0.70431
C	0.90005	-2.25996	0.82492
C	1.60434	-2.80299	-0.2579

C	0.93049	-3.18008	-1.41401
C	-0.45286	-3.08081	-1.50458
C	-1.15121	-2.53999	-0.42951
H	-1.03973	-2.99339	3.11959
H	-2.54843	-2.05248	4.84763
H	-3.67887	0.13142	4.43212
H	-3.21107	1.36937	2.36663
H	2.67959	-2.91831	-0.20675
H	1.49641	-3.58538	-2.24824
H	-0.99607	-3.41124	-2.38329
O	-2.52194	-2.45918	-0.47516
C	-3.20531	-3.51693	0.22456
C	-3.34547	-4.7272	-0.68091
C	-4.53541	-2.95723	0.68237
H	-2.60546	-3.7835	1.10456
H	-2.36327	-5.08884	-1.00079
H	-3.85562	-5.5428	-0.15682
H	-3.9283	-4.46757	-1.57178
H	-4.38197	-2.11392	1.36252
H	-5.12219	-2.61619	-0.17826
H	-5.11169	-3.72759	1.20531
O	1.44757	-1.93942	2.00533
C	2.86828	-1.75882	2.10493
C	3.53458	-3.08516	2.43558
C	3.08655	-0.71556	3.1807
H	3.23227	-1.36188	1.15017
H	3.33002	-3.85054	1.68073
H	4.62004	-2.95523	2.50559
H	3.16929	-3.45528	3.40002
H	2.57309	0.19994	2.88417
H	2.68884	-1.06622	4.13981
H	4.15792	-0.51862	3.29819
P	-1.42651	0.95498	0.11425
Pd	0.80023	0.66371	-0.61984
C	-1.42905	2.73754	0.69008
C	-2.75052	3.51303	0.76949
C	-0.60188	2.93757	1.96555
H	-0.85711	3.193	-0.13654
C	-2.46267	5.00001	0.9905
H	-3.36418	3.14986	1.60397
H	-3.34734	3.38954	-0.1406
C	-0.3267	4.42195	2.19041
H	-1.16084	2.53752	2.82239
H	0.32332	2.35772	1.89966

C	-1.61877	5.23146	2.24132
H	-3.40819	5.55275	1.05484
H	-1.92811	5.39217	0.11284
H	0.24453	4.55525	3.11721
H	0.30788	4.79894	1.37432
H	-1.40278	6.30058	2.35864
H	-2.19838	4.9289	3.12619
C	-2.77046	0.94223	-1.17579
C	-2.51224	0.03002	-2.37745
C	-4.1596	0.66928	-0.59148
H	-2.74017	1.97898	-1.54932
C	-3.58686	0.23422	-3.44261
H	-2.52406	-1.01292	-2.05281
H	-1.52221	0.21841	-2.80362
C	-5.24518	0.83894	-1.65334
H	-4.17071	-0.35682	-0.20904
H	-4.36484	1.3266	0.26027
C	-4.97655	-0.03744	-2.8729
H	-3.38682	-0.423	-4.29737
H	-3.54168	1.26655	-3.82075
H	-6.22488	0.60406	-1.2187
H	-5.28526	1.8933	-1.96564
H	-5.74565	0.1263	-3.63761
H	-5.04056	-1.09505	-2.57781
C	2.84683	0.56139	-1.00676
C	3.48446	-0.49387	-1.65864
C	3.59326	1.43169	-0.21722
C	4.84462	-0.71048	-1.47805
H	2.92246	-1.16382	-2.30184
C	4.95744	1.22308	-0.02876
H	3.10644	2.24306	0.31403
C	5.58631	0.14157	-0.65461
H	5.3562	-1.53264	-1.96979
H	5.51221	1.89774	0.61438
S	0.99091	0.97802	-2.75248
O	1.02157	2.34658	-3.2506
O	1.15935	-0.11069	-3.70407
F	1.25127	0.71789	1.3007
O	6.90216	-0.15609	-0.52833
C	7.68431	0.67353	0.297
H	7.32375	0.66629	1.33437
H	8.69543	0.26438	0.26498
H	7.70134	1.70835	-0.06956

Int5

C	2.40002	0.35066	1.10038
C	3.48225	0.61911	1.94329
C	3.70347	-0.13396	3.0902
C	2.84306	-1.18214	3.40387
C	1.75081	-1.44555	2.58444
C	1.50383	-0.67845	1.43951
C	2.30181	1.10882	-0.17927
C	1.99978	2.48993	-0.20748
C	2.10389	3.19852	-1.41555
C	2.49661	2.54865	-2.57034
C	2.81721	1.19013	-2.56479
C	2.74653	0.48712	-1.37327
H	4.15615	1.43049	1.68284
H	4.54943	0.09243	3.73309
H	3.01377	-1.78802	4.28929
H	1.08103	-2.25772	2.84397
H	1.83577	4.24579	-1.45118
H	2.54261	3.10657	-3.50072
H	3.11774	0.6728	-3.4693
O	3.10137	-0.83452	-1.32387
C	4.48757	-1.06996	-0.99616
C	5.31618	-1.12481	-2.26668
C	4.54582	-2.35296	-0.19457
H	4.83153	-0.23791	-0.36742
H	5.25955	-0.17815	-2.81214
H	6.36807	-1.31829	-2.0295
H	4.95344	-1.92662	-2.9191
H	3.983	-2.24783	0.73714
H	4.12309	-3.18233	-0.77233
H	5.5839	-2.60015	0.05116
O	1.64856	3.05481	0.96505
C	0.70803	4.15705	0.93338
C	1.46249	5.46408	1.09102
C	-0.25941	3.90269	2.07118
H	0.16119	4.09131	-0.01533
H	2.18656	5.61527	0.28424
H	0.76416	6.30792	1.08357
H	2.00785	5.47537	2.04168
H	-0.78579	2.95822	1.90457
H	0.26961	3.84748	3.02933
H	-1.0012	4.70651	2.12415
P	0.00429	-0.8937	0.40845

Pd	-0.30022	1.08505	-0.67162
C	-1.40167	-1.26453	1.56113
C	-1.59473	-2.66365	2.15394
C	-1.44247	-0.19939	2.66428
H	-2.26151	-1.07361	0.9018
C	-2.92041	-2.72378	2.91632
H	-0.77949	-2.91299	2.84547
H	-1.5912	-3.42671	1.37019
C	-2.76379	-0.26347	3.4252
H	-0.60839	-0.35878	3.36048
H	-1.28845	0.79478	2.22796
C	-2.99521	-1.65662	4.00455
H	-3.05338	-3.72322	3.34876
H	-3.74519	-2.57542	2.20436
H	-2.77437	0.49052	4.2218
H	-3.58456	-0.01454	2.73745
H	-3.9646	-1.70337	4.51556
H	-2.2279	-1.86267	4.76562
C	0.31132	-2.35493	-0.68668
C	0.99104	-3.56062	-0.0334
C	-0.96557	-2.76225	-1.42976
H	1.01885	-1.94802	-1.42275
C	1.2934	-4.62473	-1.08842
H	0.34454	-3.99291	0.74068
H	1.91532	-3.24826	0.46121
C	-0.65695	-3.83588	-2.47133
H	-1.70519	-3.1535	-0.71803
H	-1.42828	-1.89196	-1.90385
C	0.03258	-5.04294	-1.84142
H	1.76678	-5.49503	-0.61685
H	2.02227	-4.21623	-1.80405
H	-1.5819	-4.14066	-2.97581
H	-0.00267	-3.4058	-3.2436
H	0.27661	-5.78775	-2.60884
H	-0.66181	-5.52968	-1.14043
C	-2.21627	0.76218	-0.96711
C	-2.64352	0.28577	-2.21029
C	-3.17749	1.12626	-0.03133
C	-3.9956	0.12527	-2.48433
H	-1.91681	0.05092	-2.98311
C	-4.54245	0.97224	-0.29537
H	-2.88155	1.55365	0.92201
C	-4.95463	0.45803	-1.52393
H	-4.33342	-0.24817	-3.44683

H	-5.26265	1.26951	0.46008
F	-0.61578	2.86671	-1.49302
O	-6.25225	0.25436	-1.88214
C	-7.2402	0.61433	-0.95159
H	-7.20335	1.68648	-0.7141
H	-8.19904	0.38364	-1.41981
H	-7.14785	0.04092	-0.01836

TS6

C	-0.08592	-2.14964	1.80576
C	-0.34425	-3.22832	2.66606
C	-0.05942	-4.53844	2.31557
C	0.49845	-4.80046	1.06955
C	0.74776	-3.74796	0.19978
C	0.47038	-2.41228	0.5392
C	-0.39225	-0.81276	2.37204
C	-1.70449	-0.49644	2.77578
C	-1.95076	0.66495	3.51319
C	-0.90366	1.54353	3.78483
C	0.38691	1.28014	3.34799
C	0.63428	0.09047	2.66108
H	-0.77673	-3.01035	3.63805
H	-0.26862	-5.34636	3.01105
H	0.73402	-5.81711	0.76789
H	1.15997	-3.97589	-0.77335
H	-2.95038	0.90754	3.85339
H	-1.10941	2.45457	4.34016
H	1.20901	1.96805	3.51055
O	1.88678	-0.18186	2.19547
C	2.75334	-0.98844	3.01777
C	3.29451	-0.17789	4.1815
C	3.83481	-1.47592	2.07549
H	2.16689	-1.84017	3.39041
H	2.48416	0.16247	4.83429
H	3.97747	-0.79019	4.78067
H	3.83195	0.70033	3.8101
H	3.40416	-2.13576	1.3167
H	4.28919	-0.62114	1.56521
H	4.60653	-2.0251	2.62405
O	-2.65808	-1.36826	2.37384
C	-4.03765	-1.05548	2.56883
C	-4.48319	-1.51141	3.94832
C	-4.78192	-1.7497	1.446

H	-4.17224	0.02847	2.45965
H	-3.88852	-1.03971	4.73687
H	-5.5365	-1.26239	4.11549
H	-4.36574	-2.59693	4.03608
H	-4.45943	-1.35178	0.48001
H	-4.58161	-2.8262	1.46728
H	-5.86041	-1.59146	1.54802
P	0.67133	-1.18162	-0.81392
Pd	0.8464	1.08172	-0.46235
C	-0.67276	-1.71184	-1.98807
C	-0.43972	-2.99016	-2.79927
C	-2.02452	-1.79856	-1.26799
H	-0.7217	-0.87556	-2.69736
C	-1.55577	-3.15954	-3.83138
H	-0.44937	-3.8597	-2.13088
H	0.53368	-2.97371	-3.29961
C	-3.15306	-1.98412	-2.28028
H	-2.0052	-2.6486	-0.57261
H	-2.20187	-0.90287	-0.66659
C	-2.92557	-3.20998	-3.16017
H	-1.3824	-4.0695	-4.41942
H	-1.52391	-2.31663	-4.53736
H	-4.11311	-2.06601	-1.75543
H	-3.21463	-1.08267	-2.90528
H	-3.71709	-3.29447	-3.91534
H	-2.98484	-4.11607	-2.53925
C	2.33348	-1.39147	-1.61925
C	3.05376	-2.73368	-1.74637
C	2.29308	-0.65705	-2.96993
H	2.92501	-0.74384	-0.9514
C	4.46948	-2.50265	-2.28218
H	2.51816	-3.41416	-2.42408
H	3.12248	-3.22951	-0.77299
C	3.71042	-0.43111	-3.48699
H	1.71989	-1.23728	-3.70734
H	1.78518	0.30993	-2.85388
C	4.46478	-1.751	-3.60977
H	4.98401	-3.46607	-2.38732
H	5.03264	-1.9205	-1.53938
H	3.6791	0.08479	-4.45503
H	4.22979	0.23181	-2.78188
H	5.4931	-1.57582	-3.94903
H	3.98162	-2.37423	-4.37754
B	2.86836	3.3163	1.01079

O	3.09823	2.38578	1.96767
H	2.79401	1.5268	1.60252
O	3.7746	4.33955	0.89897
H	3.46762	5.00052	0.2679
C	1.53124	3.47243	0.14388
C	0.37251	3.98305	0.76999
C	1.54614	3.46065	-1.27251
C	-0.6835	4.50067	0.03177
H	0.31937	3.98599	1.85599
C	0.48323	3.99124	-2.01291
H	2.43188	3.08852	-1.78276
C	-0.62201	4.52177	-1.36241
H	-1.56421	4.88376	0.5392
H	0.5235	3.97662	-3.09889
H	-1.45303	4.92109	-1.93627
F	2.8996	0.97996	-0.16692
C	-1.0737	1.33383	-0.85937
C	-1.97916	1.5718	0.17956
C	-1.54721	1.43754	-2.16611
C	-3.31026	1.87687	-0.07597
H	-1.64102	1.53033	1.20766
C	-2.88165	1.7502	-2.44416
H	-0.87033	1.28968	-3.0057
C	-3.77422	1.95774	-1.39202
H	-4.0106	2.06308	0.73448
H	-3.20564	1.82524	-3.47733
O	-5.09633	2.24655	-1.54351
C	-5.59548	2.30717	-2.85482
H	-5.46739	1.35126	-3.38185
H	-6.66081	2.52847	-2.76633
H	-5.1105	3.10175	-3.43892