Electronic Supplementary Information

Site-Selectivity and Mechanism of Pd-Catalyzed C(sp^2)–H Arylation of Simple Arenes

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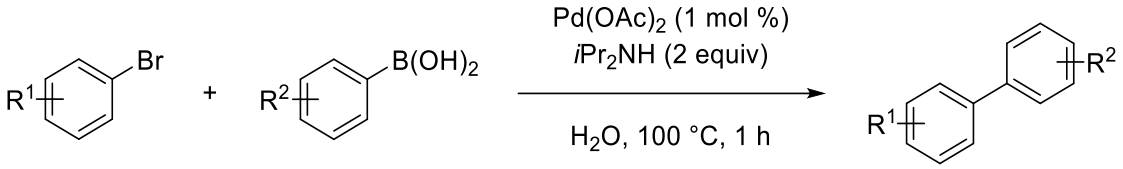
1. General Information

Unless otherwise noted, all reactions were performed under inert conditions. Benzene, ether, pentane and diethyl ether were dried using a PureSolv solvent purification system. All chemicals were purchased from commercial sources (Sigma-Aldrich, Alfa Aesar, TCI, or Strem) and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) on EMD Silica Gel 60 F254 plates, and visualized either using UV light (254 nm) or by staining with potassium permanganate and heating. Nuclear magnetic resonance (NMR) spectra were recorded in $CDCl_3$ and CD_3OD on a Bruker DPX-300 (300 MHz) spectrometer, Varian 400 and 500 NMR (400 and 500 MHz), Bruker AVANCE 300 (300 MHz), Bruker AVANCE 400 (400 MHz), or Bruker AVANCE III HD (400 MHz), and the residual solvent signal was used as a reference. Chemical shifts are reported in ppm and coupling constants are given in Hz. Gas chromatography (GC) was carried out using a 7890A or 7890B GC system (Agilent Technologies) equipped with an HP-5 column and a flame ionization detector (FID). Gas chromatography–mass spectrometry (GC-MS) was carried out using 5977B GC/MSD system (Agilent Technologies) equipped with an HP-5MS column. Elemental analysis was conducted at KAIST Analysis Center for Research Advancement (KARA) using a Flash 1112 elemental analyzer. High-resolution mass spectrometry (HRMS) was performed at the Organic Chemistry Research Center in Sogang University using the ESI method and Korea Basic Science Institute (KBSI) for EI method. X-ray diffraction data of **4b** was collected on a Bruker D8 QUEST coated with Paraton-*N* oil under a stream of N_2 (g) at 173 K by using APEX III software.

2. Preparation of Biaryl Authentic Samples (3aa–3am, 3bb–3fb, 3hb–3ob, 3ij, 3kj)

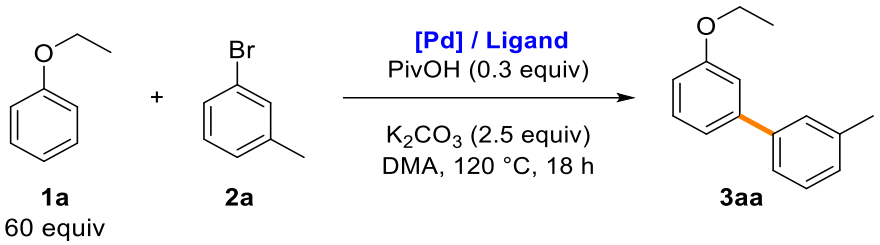


Authentic samples were prepared following slightly modified literature procedure.[1] To a stirred solution of arylboronic acid (0.75 mmol, 1.5 equiv), *i*Pr_2NH (140 μL, 1.0 mmol, 2.0 equiv), $Pd(OAc)_2$ (1.1 mg, 0.0050 mmol, 1.0 mol %) and H_2O (1.0 mL) was added aryl bromide (0.50 mmol, 1.0 equiv) under air. The reaction was vigorously stirred at 100 ℃ for 1 h. The reaction mixture was then cooled and diluted with EtOAc (10 mL), washed with water (3 x 10 mL), dried (anhydrous Na_2SO_4), filtered, and concentrated under reduced pressure. The resulting residue was purified by flash column chromatography (silica gel, hexanes/EtOAc gradient elution) to afford the authentic samples of biaryls.

Biaryls **3kj** were synthesized by literature procedures.[2]

3. Optimization of Reaction Conditions

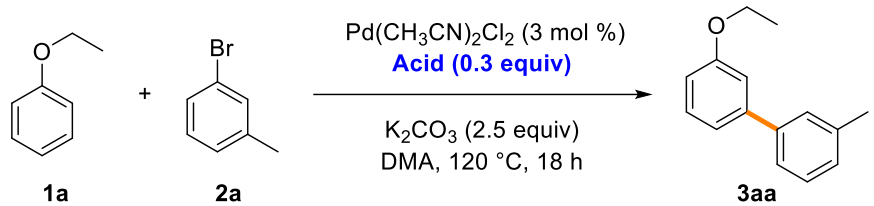
Table S1. Evaluation of Catalytic Condition for the Direct C–H Arylation of Ethoxybenzene[a]

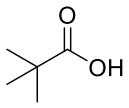
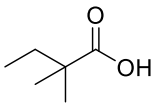
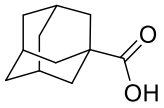
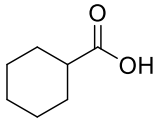
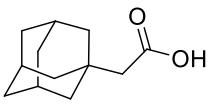
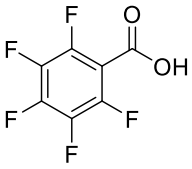
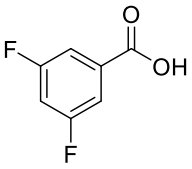
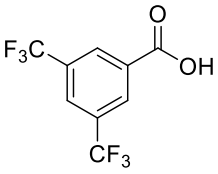
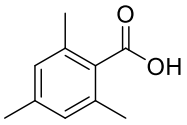
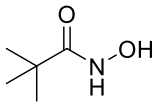


Entry	[Pd] (mol %)	Ligand (mol %)	Temperature (°C)	Yield (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	$Pd(OAc)_2$ (3)	PCy_3 (3)	120	71	1 / 8.2 / 2.9	8 / 68 / 24
2	$Pd(OAc)_2$ (3)	PPh_3 (3)	120	48	1 / 8.5 / 2.8	8 / 69 / 23
3	$Pd(OAc)_2$ (3)	$P(C_6F_5)_3$ (3)	120	14	1 / 6.0 / 2.0	11 / 67 / 22
4	$Pd(OAc)_2$ (3)	1,10-phen (3)	120	0	-	-
5	$Pd(PPh_3)_4$ (3)	-	120	54	1 / 5.3 / 1.9	12 / 65 / 23
6	$Pd(CO_2CF_3)_2$ (3)	-	120	68	1 / 10.0 / 3.1	7 / 71 / 22
7	$Pd(PhCN)_2Cl_2$ (3)	-	120	70	1 / 10.7 / 3.1	7 / 72 / 21
8	$Pd(CH_3CN)_4(BF_4)_2$ (3)	-	120	17	1 / 8.9 / 2.8	8 / 70 / 22
9	$Pd(CH_3CN)_2Cl_2$ (3)	-	120	79	1 / 10.2 / 3.2	7 / 71 / 22
10	$Pd(CH_3CN)_2Cl_2$ (3)	-	100	35	1 / 10.7 / 3.1	7 / 72 / 21
11	$Pd(CH_3CN)_2Cl_2$ (3)	-	140	44	1 / 6.8 / 2.4	8 / 71 / 21
12	$Pd(CH_3CN)_2Cl_2$ (1)	-	120	79	1 / 10.2 / 3.1	7 / 71 / 22
13	$Pd(CH_3CN)_2Cl_2$ (10)	-	120	15	1 / 10.3 / 3.0	7 / 72 / 21
14[b]	$Pd(CH_3CN)_2Cl_2$ (3)	-	120	56	1 / 9.3 / 2.7	8 / 71 / 21

[a]The total yield and regioselectivity (*ortho* / *meta* / *para*) were determined by GC analysis of the reaction mixture using dodecane as an internal standard. [b]With H_2O (2 equiv)

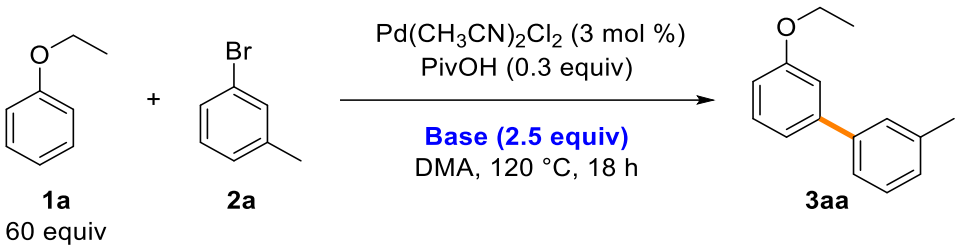
Table S2. Acid Screening[a]



				
79% (7 / 72 / 22)	22% (8 / 72 / 21)	3% (16 / 48 / 36)	9% (22 / 41 / 37)	11% (21 / 46 / 33)
				
0%	0%	0%	26% (15 / 50 / 35)	2% (38 / 36 / 26)

[a]The total yield and regioselectivity (*ortho* / *meta* / *para*) were determined by GC analysis of the reaction mixture using dodecane as an internal standard.

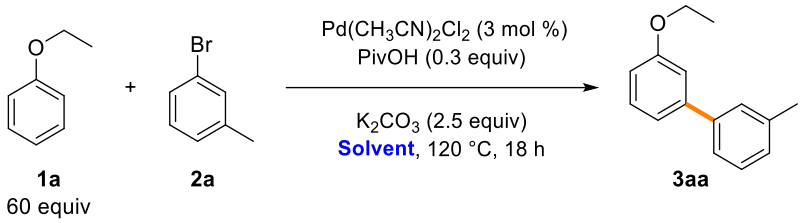
Table S3. Base Screening[a]



Entry	Base	Yield (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	K_2CO_3	79	1 / 10.2 / 3.2	7 / 71 / 22
2	Na_2CO_3	0	-	-
3	Rb_2CO_3	75	1 / 5.7 / 2.9	10 / 59 / 31
4	Cs_2CO_3	0	-	-
5	K_3PO_4	1.3	1 / 0.7 / 0.8	40 / 30 / 30
6[b]	NaOPiv	1.3	1 / 1.6 / 1.2	26 / 43 / 31
7	KOPiv	25	1 / 5.2 / 1.8	13 / 65 / 22
8[b]	KOPiv	32	1 / 6.2 / 2.0	11 / 68 / 21
9[b]	CsOPiv	4.3	1 / 1.4 / 1.8	31 / 45 /24
10	DABCO	0	-	-
11	Quinuclidine	0	-	-
12	TEA	0	-	-

[a]The total yield and regioselectivity (*ortho* / *meta* / *para*) were determined by GC analysis of the reaction mixture using dodecane as an internal standard. [b]Without PivOH.

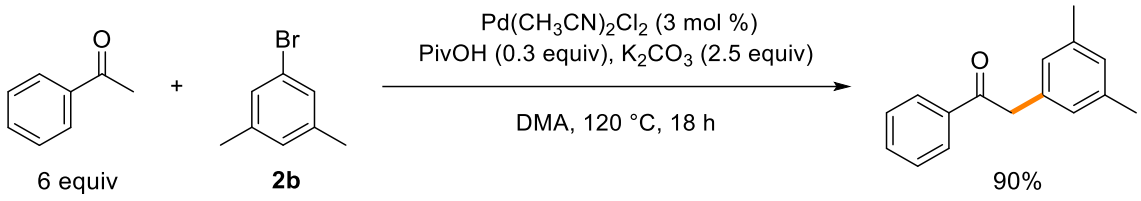
Table S4. Solvent Screening[a]



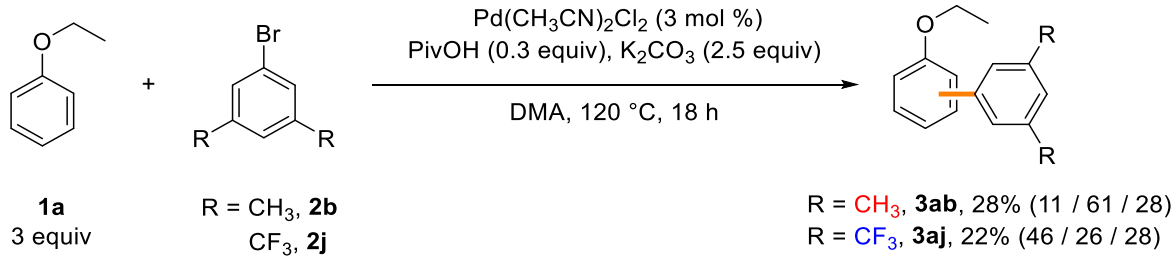
Entry	Solvent	Yield (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	DMA	79	1 / 10.2 / 3.2	7 / 71 / 22
2	DMF	7.3	1 / 3.3 / 1.8	17 / 54 / 30
3	DMSO	3.7	1 / 0.3 / 0.6	51 / 17 / 32
4	CH_3CN	0	-	-
5	Cyclohexane	0	-	-
6	Hexane	0	-	-
7	1,4-Dioxane	0	-	-
8	DCE	0	-	-
9	Mesitylene	0	-	-

[a]The total yield and regioselectivity (*ortho* / *meta* / *para*) were determined by GC analysis of the reaction mixture using dodecane as an internal standard.

Scheme S1. Reaction with Acetophenone



Scheme S2. Reactions of Ethoxybenzene under the Stoichiometric Conditions



4. General Procedure for the C–H Arylation Reaction

K_2CO_3 was dried at 120 ℃ in an oven overnight. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), and pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol). Aryl halide (1.0 equiv, 0.20 mmol) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and arene (60 equiv). The Schlenk tube was sealed and heated to 120 ℃ for 18 h. Upon completion of the reaction, the mixture was cooled down to room temperature. The crude mixture was filtered through Celite® and then analyzed by GC using dodecane as an internal standard and isolated by silica gel flash chromatography using hexane and EtOAc as eluent.

5. Mechanistic Studies

5.1. Comparison of the Reaction Rates

Reaction rates of various arenes are compared by obtaining the initial rates of the C–H arylation. Initial rates were analyzed by total yields combining all regioisomers. For accurate comparison of the reaction rates, all arene compounds (99+% purity) were purified by passing through a short pad of activated neutral alumina, and used in a glove box.

All reactions were conducted using the above general procedure with the following modification. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA). $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol, stock solution in DMA) was then added to the Schlenk tube as a solution in DMA, followed by **2b** (28 μL, 0.2 mmol, 1.0 equiv), arene (6.0 equiv) and dodecane (0.044 mmol, 10 μL) as an internal standard. The amount of DMA was varied to maintain the concentration of [Pd] (4.6 mM) and substrate (154 mM). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken as indicated times and analyzed by GC. The same experiment was repeated two more times in each substrates and the average rate values were used to compare the reaction rates.

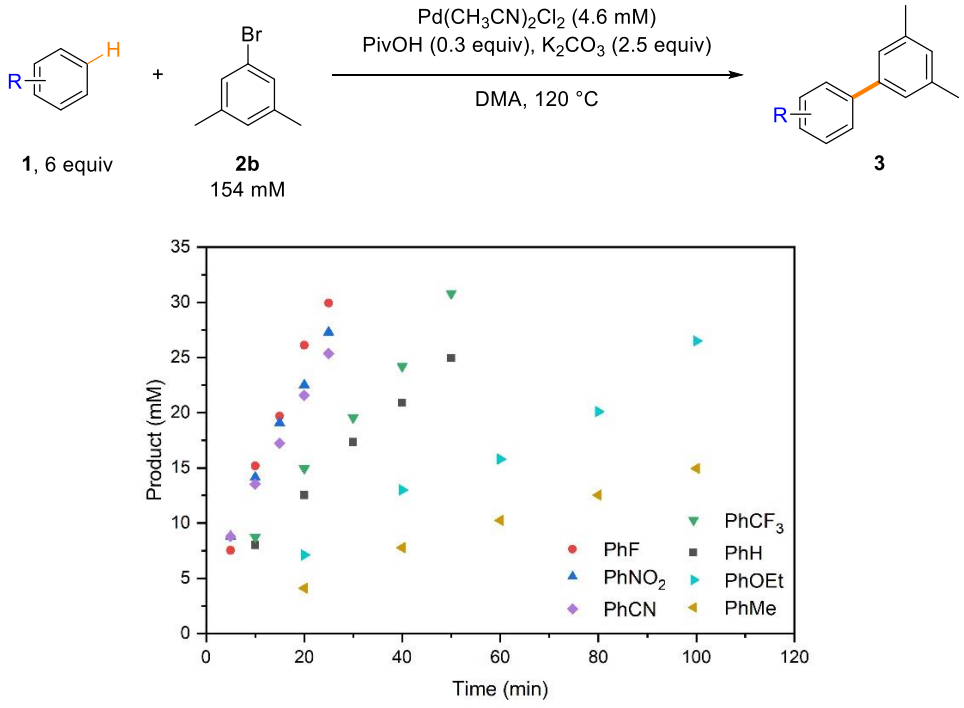


Table S5. Summary of the Comparison of the Reaction Rates of Various Arenes

R	F	NO_2	CN	CF_3	H	Me	OEt
Reaction rate (mM/min)	1.1147	0.9066	0.8245	0.2329	0.4223	0.2295	0.1324
k_{rel}[a]	2.6	2.2	1.9	1.3	1	0.54	0.31

[a] k_{rel} = relative reaction rate vs $k_{(R=H)}$

5.2. Kinetic Isotope Effect (KIE) Experiments

The KIE was determined by comparing the initial reaction rates of the C–H arylation with benzene and benzene-d_6. Both reactions were conducted using the above general procedure with the following modification. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), and pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol). **2b** (28 μL, 0.2 mmol, 1.0 equiv, 91 mM) and dodecane (0.044 mmol, 10 μL) as an internal standard were then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene or benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 5 min and analyzed by GC. The observed large primary KIE value (4.43) suggested that the C–H bond cleavage step of the arene is involved in the rate-limiting step.

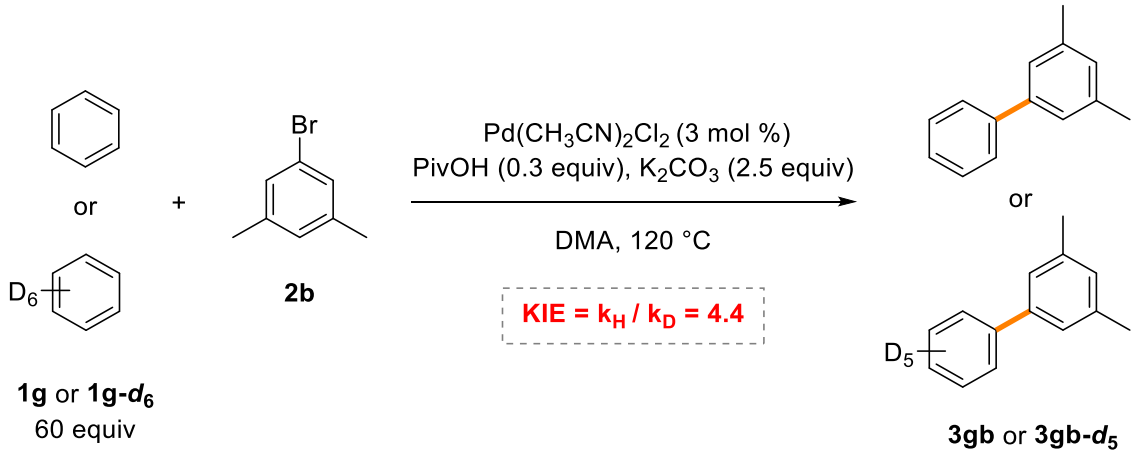
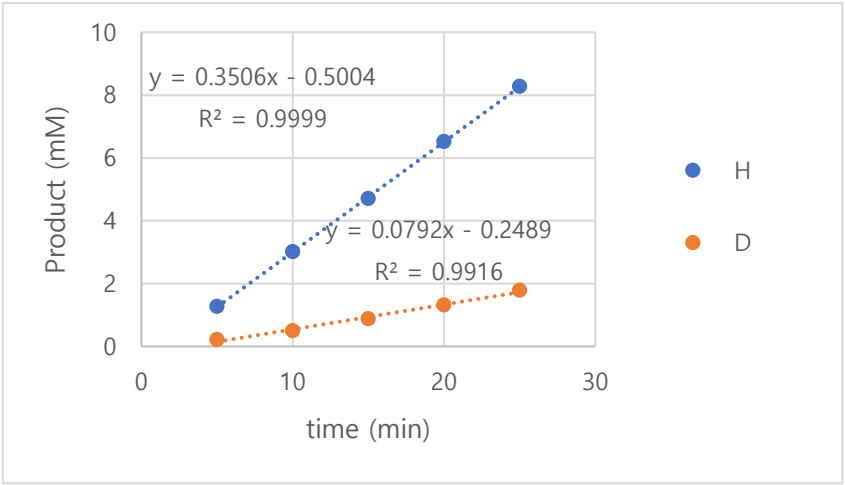


Figure S1. Initial Rates of the C–H Arylation of Benzene and Benzene-d_6



KIE = k_H/k_D = 0.3506/0.0792 = 4.43

5.3. Kinetic Data

As shown in Scheme 3b, to obtain more information about mechanism of the reaction, kinetic studies were conducted such as the order of [Pd], [ArBr], KOPiv and K_2CO_3. Each kinetic experiment was conducted using the general procedure with the following modification.

5.3.1. Order in [Pd]

The order in [Pd] was determined by obtaining the initial rates of the C–H arylation with benzene at differing concentrations of $Pd(CH_3CN)_2Cl_2$ precatalyst. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), **2b** (28 µL, 0.2 mmol, 1.0 equiv, 94 mM), and dodecane (0.044 mmol, 10 µL) as an internal standard. Different amount of $Pd(CH_3CN)_2Cl_2$ (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 5 min and analyzed by GC. The same experiment was repeated two more times in each [Pd] concentrations and the average rate values were used.

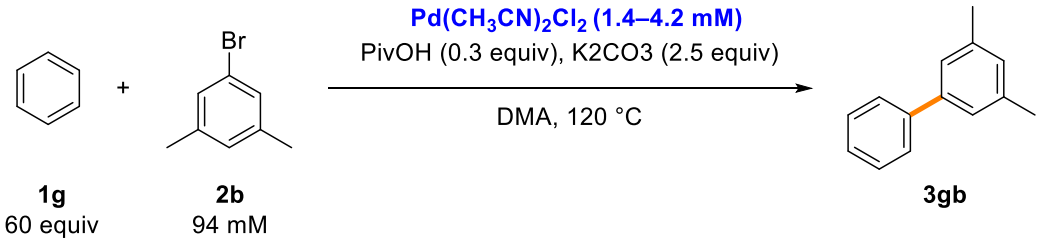


Table S6. Results to Determine the Order of $Pd(CH_3CN)_2Cl_2$

Entry	Amount of **$Pd(CH_3CN)_2Cl_2$**			Rate (mM/min)
	mg	mmol	mM	
1	0.80	0.00308	1.402	0.1500
2	0.96	0.00370	1.682	0.1796
3	1.28	0.00493	2.243	0.2595
4	1.60	0.00617	2.803	0.3506
5	2.40	0.00925	4.205	0.4699

Figure S2. Initial Rates with Different Concentrations of $Pd(CH_3CN)_2Cl_2$

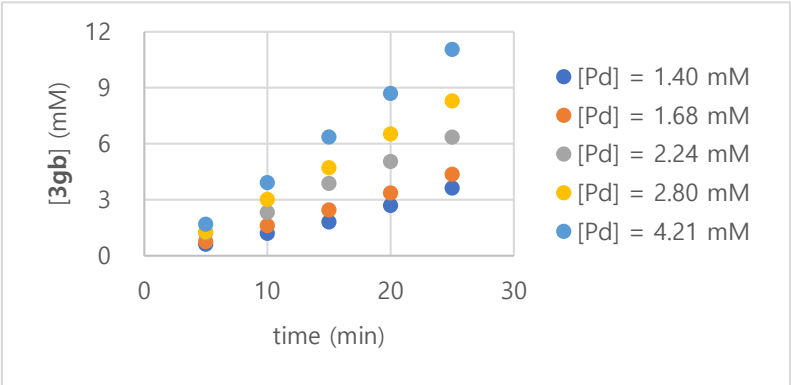
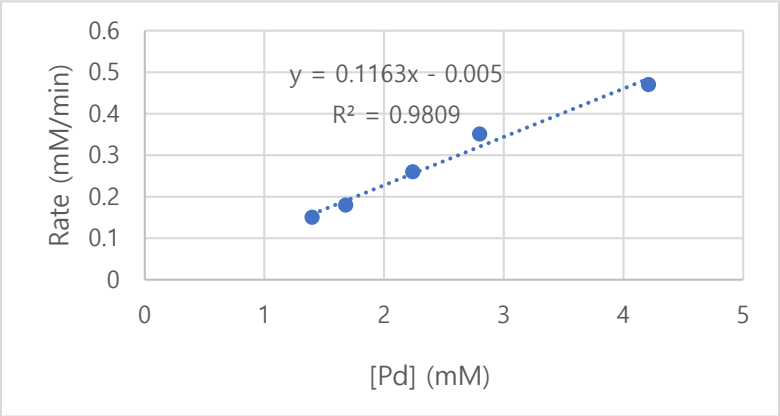


Figure S3. Plot of Initial Rates with Different Concentrations of $Pd(CH_3CN)_2Cl_2$



5.3.2. Order in [ArBr]

The order in [ArBr] was determined by obtaining the initial rate of the C–H arylation with benzene at differing concentrations of 1-bromo-3,5-dimethylbenzene **2b**. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), and dodecane (0.044 mmol, 10 μL) as an internal standard. Different amount of **2b** was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 5 min and analyzed by GC. The same experiment was repeated two more times in each [ArBr] concentrations and the average rate values were used.

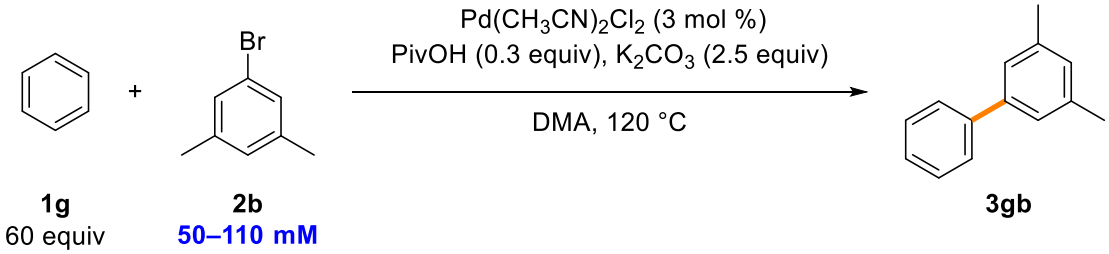


Table S7. Results to Determine the Order of **2b**

Entry	Amount of **2b**			Rate (mM/min)
	μL	mmol	mM	
1	15	0.110	50.2	0.3495
2	20	0.147	66.9	0.3696
3	25	0.184	83.6	0.3354
4	28	0.206	93.7	0.3506
5	33	0.243	110	0.3283

Figure S4. Initial Rates of the C–H Arylation with Different Concentrations of **2b**

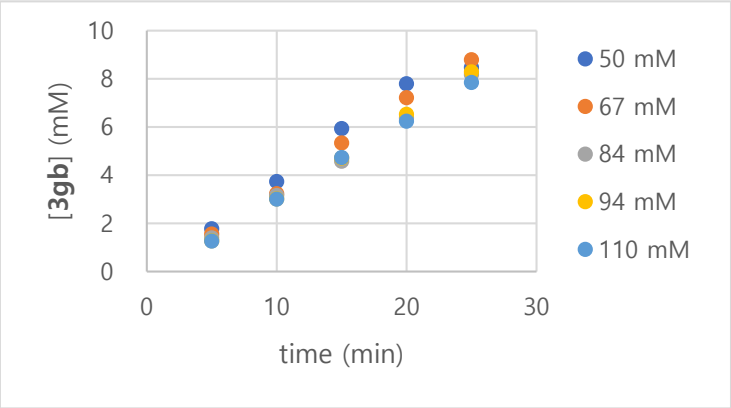
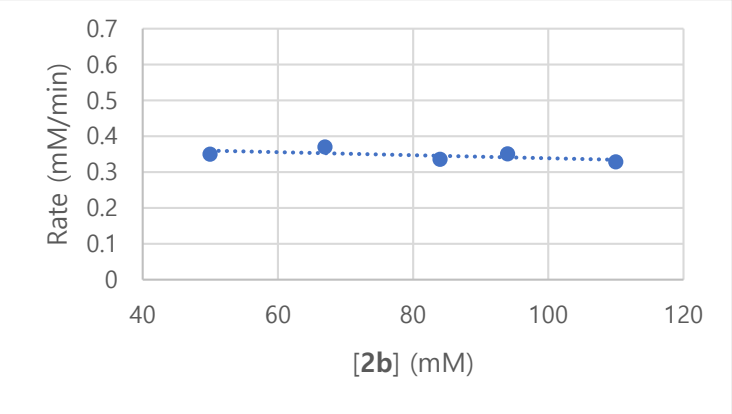


Figure S5. Plot of Initial Rates with Different Concentrations of **2b**



5.3.3. Dependence on KOPiv

The dependence on KOPiv was determined by obtaining the initial rate of the C–H arylation with benzene at differing amount of KOPiv. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol, 1.0 equiv, 94 mM), and dodecane (0.044 mmol, 10 μL) as an internal standard. Different amount of KOPiv was the Schlenk tube in, followed by DMA (1.2 mL) and benzene (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 5 min and analyzed by GC. The same experiment was repeated in each KOPiv equivalence and the average rate values were used.

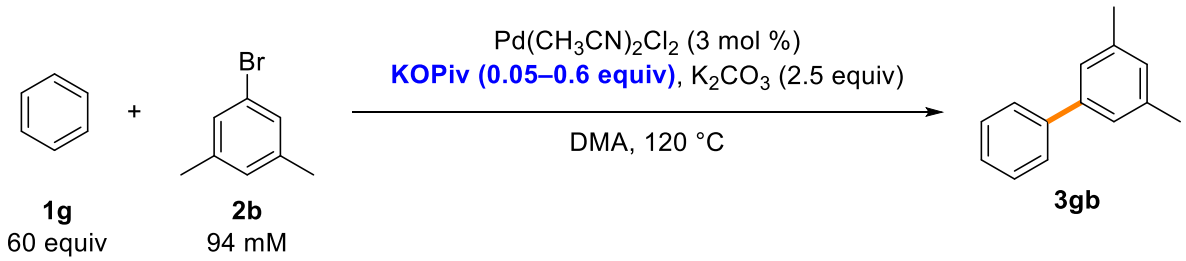


Table S8. Results to Determine the Dependence of KOPiv

Entry	Amount of **KOPiv**			**Rate (mM/min)**
	mg	mmol	equiv	
1	1.40	0.010	0.050	0.0587
2	2.80	0.020	0.10	0.3435
3	2.61	0.040	0.20	0.3551
4	11.2	0.080	0.40	0.2610
5	16.8	0.120	0.60	0.1027

Figure S6. Initial Rates of the C–H Arylation with Different Equivalences of KOPiv

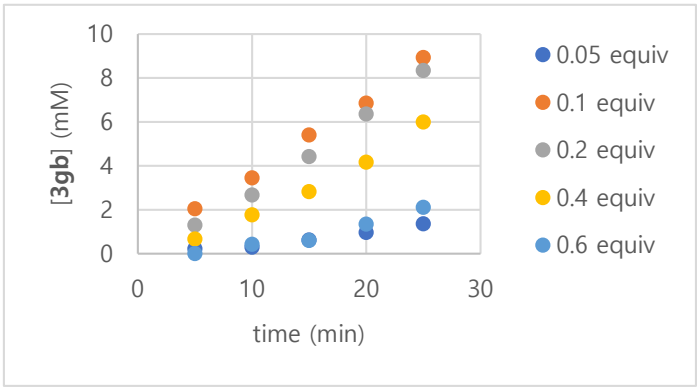
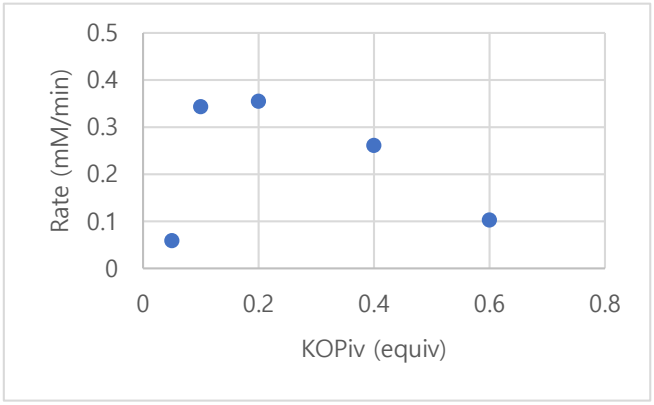


Figure S7. Plot of Initial Rates with Different Concentration of KOPiv



5.3.4. Dependence on K_2CO_3

The dependence on K_2CO_3 was determined by obtaining the initial rate of the C–H arylation with benzene at differing amount of K_2CO_3. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with KOPiv (0.30 equiv, 8.4 mg, 0.060 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.044 mmol, 10 μL) as an internal standard. Different amount of K_2CO_3 was the Schlenk tube in, followed by DMA (1.2 mL) and benzene (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 5 min and analyzed by GC. The same experiment was repeated two more times in each equivalence of K_2CO_3 and the average rate values were used.

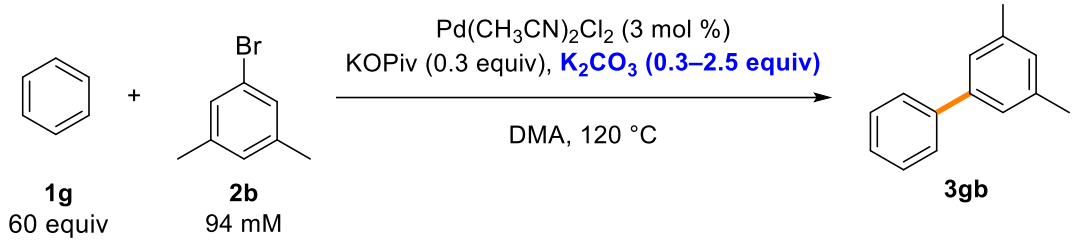


Table S9. Results to Determine the Dependence of K_2CO_3

Entry	Amount of **K_2CO_3**			Rate (mM/min)
	mg	mmol	equiv	
1	8.29	0.060	0.30	0.3262
2	13.8	0.10	0.50	0.3676
3	19.4	0.14	0.70	0.3244
4	41.5	0.30	1.50	0.3325
5	69.1	0.50	2.50	0.3278

Figure S8. Initial Rates of the C–H Arylation with Different Equivalences of K_2CO_3

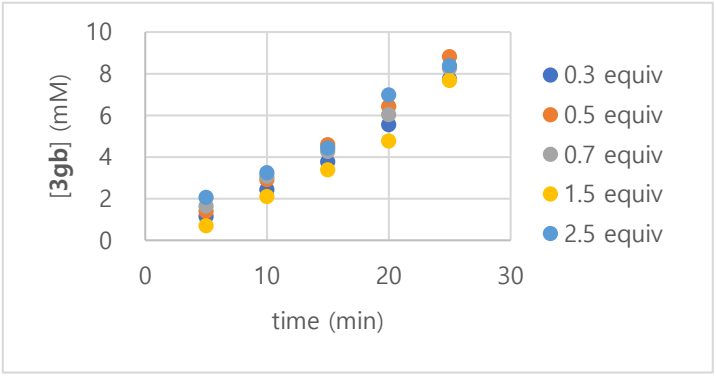
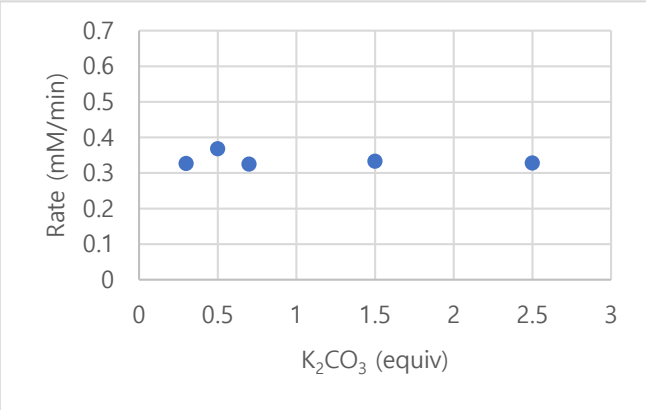


Figure S9. Plot of Initial Rates with Different Concentration of K_2CO_3



5.4. Kinetic Data in [Pd] at Low Concentrations in C_6D_6

To distinguish between monometallic and bimetallic processes, the order in [Pd] was determined by obtaining the initial rate of the C–H arylation at low concentration of [Pd] in C_6D_6. Each kinetic experiment was conducted using the general procedure with the following modification.

5.4.1. Order in $Pd(CH_3CN)_2Cl_2$ at Low Concentrations

The order in $Pd(CH_3CN)_2Cl_2$ was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(CH_3CN)_2Cl_2$ in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 μL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.044 mmol, 10 μL) as an internal standard. Different amount of $Pd(CH_3CN)_2Cl_2$ (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated in each [Pd] concentrations and the average rate values were used.

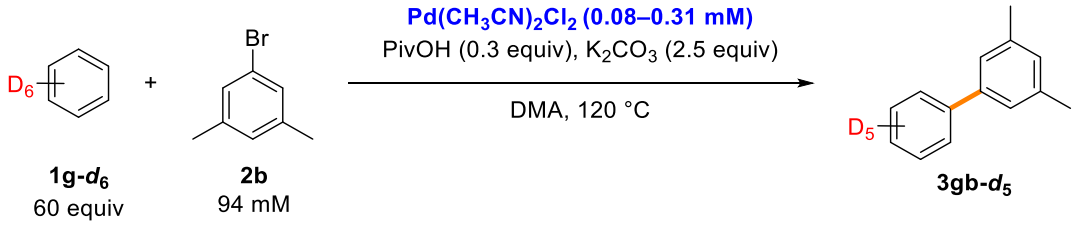


Table S10. Results to Determine the Order of $Pd(CH_3CN)_2Cl_2$ at Low Concentrations

Entry	Amount of **$Pd(CH_3CN)_2Cl_2$**			Rate (mM/h)
	mg	mmol	mM	
1	0.048	0.0001850	0.0841	0.1198
2	0.072	0.0002775	0.1262	0.2621
3	0.088	0.0003392	0.1542	0.5334
4	0.14	0.0005551	0.2523	0.8665
5	0.18	0.0006784	0.3084	1.6128

Figure S10. Initial Rates of the C–H Arylation with Different Concentrations of $Pd(CH_3CN)_2Cl_2$

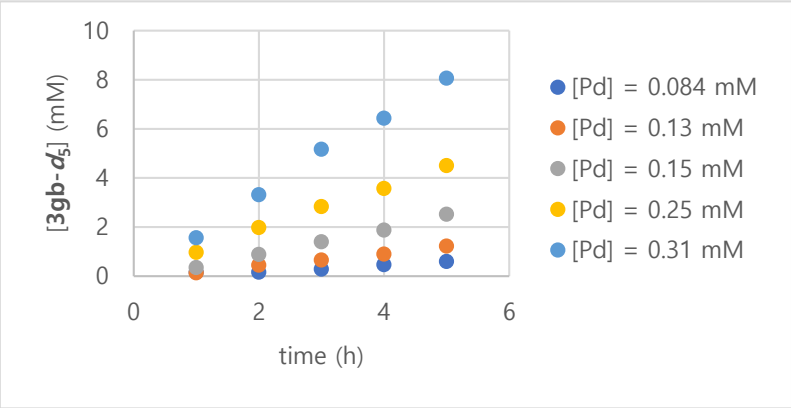
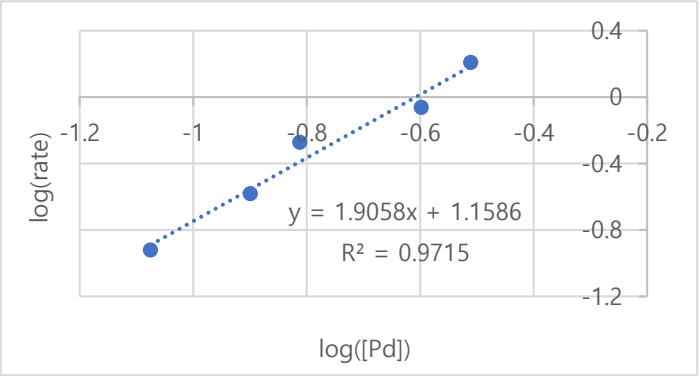


Figure S11. Plot of Initial Rates with Different Concentration of $Pd(CH_3CN)_2Cl_2$



5.4.2. Order in $Pd(OAc)_2$ at Low Concentrations

The order in $Pd(OAc)_2$ was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(OAc)_2$ in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 µL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.066 mmol, 15 µL) as an internal standard. Different amount of $Pd(OAc)_2$ (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 °C. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated two more times in each [Pd] concentrations and the average rate values were used.

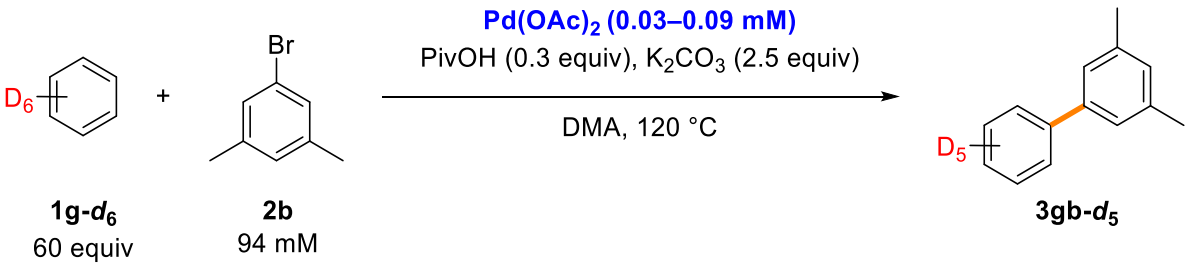


Table S11. Results to Determine the Order of $Pd(OAc)_2$ at Low Concentrations

Entry	Amount of **$Pd(OAc)_2$**			Rate (mM/h)
	mg	mmol	mM	
1	0.016	0.0000715	0.0325	0.0299
2	0.022	0.0000990	0.0450	0.0423
3	0.030	0.0001320	0.0600	0.1133
4	0.037	0.0001650	0.0750	0.1522
5	0.044	0.0001980	0.0900	0.2876

Figure S12. Plot of Initial Rates of the C–H Arylation with Different Concentration of $Pd(OAc)_2$ at Low Concentrations

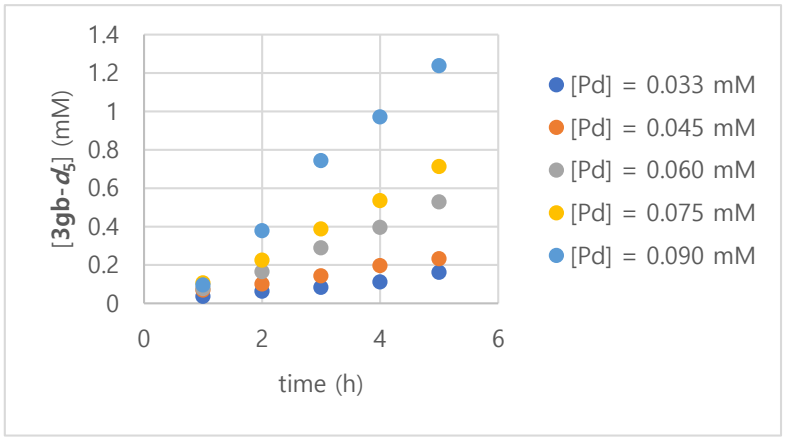
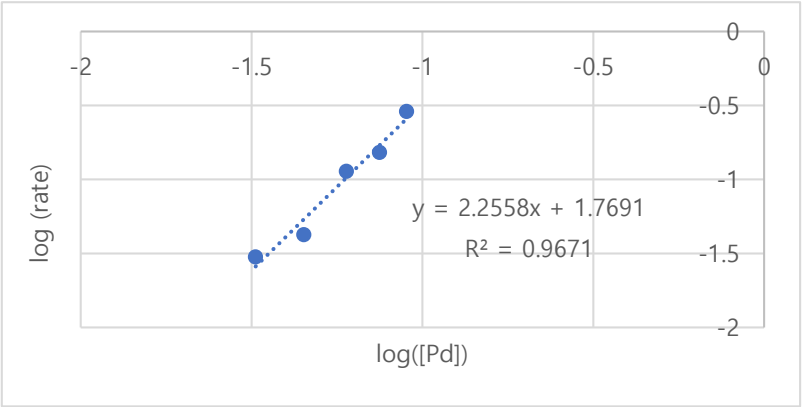


Figure S13. Plot of Initial Rates with Different Concentration of $Pd(OAc)_2$



5.4.3. Order in $Pd(OAc)_2$ with DavePhos at Low Concentrations

The order in [Pd] was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(OAc)_2$ and Davephos (1:1 ratio) in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 μL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.044 mmol, 10 μL) as an internal standard. Different amount of $Pd(OAc)_2$ (stock solution in DMA) and DavePhos (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 °C. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated in each [Pd] concentrations and the average rate values were used.

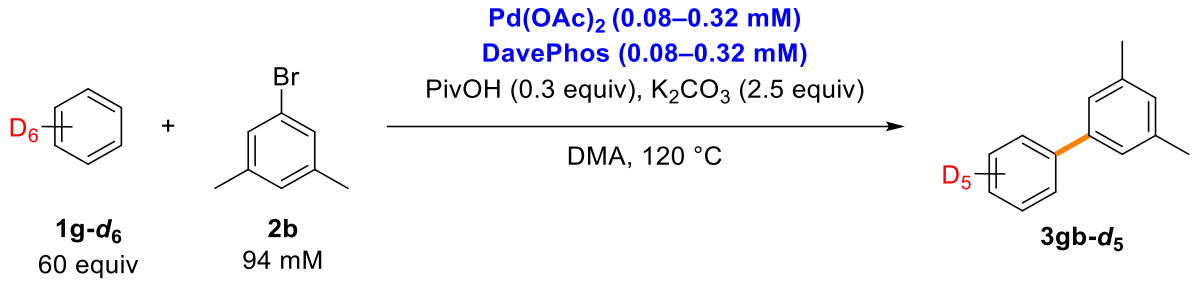


Table S12. Results to Determine the Order of $Pd(OAc)_2$ with DavePhos at Low Concentrations

Entry	Amount of **$Pd(OAc)_2$**			Amount of **DavePhos**	Rate (mM/h)
	mg	mmol	mM	mg	
1	0.040	0.000178	0.0810	0.070	0.0553
2	0.070	0.000312	0.1417	0.123	0.1867
3	0.100	0.000445	0.2025	0.175	0.4475
4	0.130	0.000579	0.2632	0.228	0.6459
5	0.160	0.000713	0.3239	0.280	0.7159

Figure S14. Plot of Initial Rates of the C–H Arylation with Different Concentration of $Pd(OAc)_2$/DavePhos at Low Concentrations

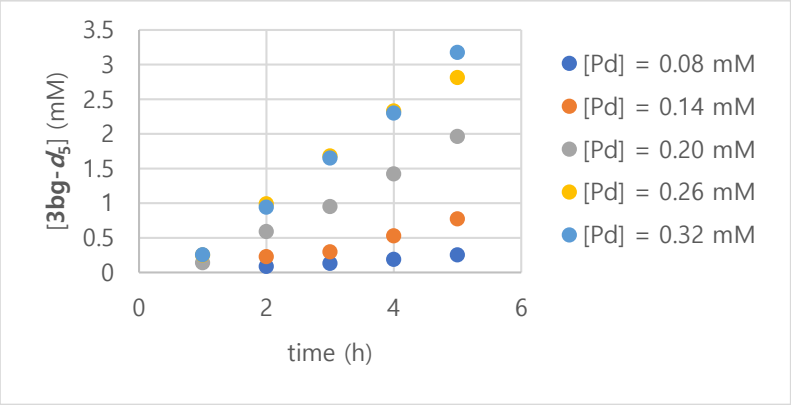
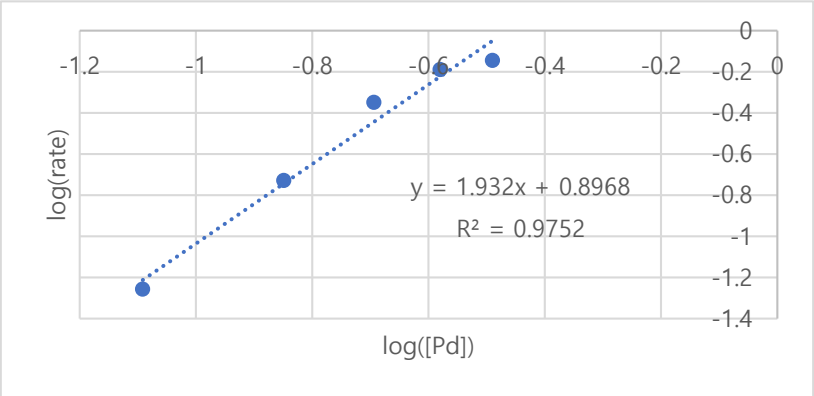


Figure S15. Plot of Initial Rates with Different Concentration of $Pd(OAc)_2$/DavePhos



5.4.4. Order in $Pd(OAc)_2$ with PCy_3 at Low Concentrations

The order in [Pd] was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(OAc)_2$ and PCy_3 (1:1 ratio) in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 μL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.066 mmol, 15 μL) as an internal standard. Different amount of $Pd(OAc)_2$ (stock solution in DMA) and PCy_3 (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 °C. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated two more times in each [Pd] concentrations and the average rate values were used.

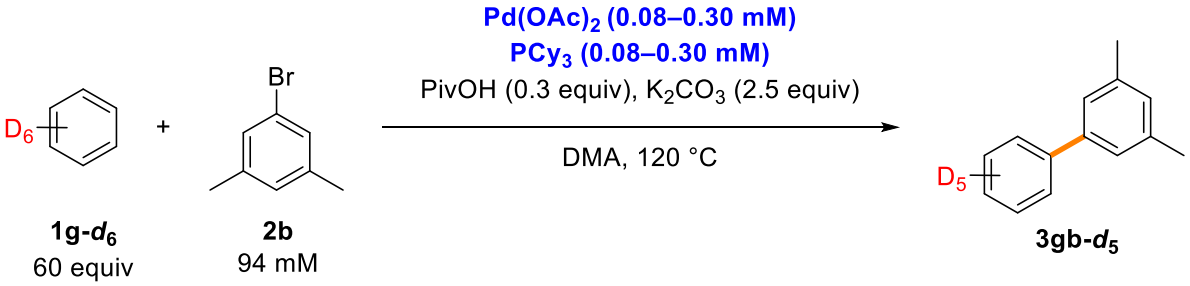


Table S13. Results to Determine the Order of $Pd(OAc)_2$ with PCy_3 at Low Concentrations

Entry	Amount of **$Pd(OAc)_2$**			Amount of **PCy_3**	Rate (mM/h)
	mg	mmol	mM	mg	
1	0.040	0.0001782	0.0810	0.050	0.0502
2	0.065	0.0002895	0.1316	0.081	0.0955
3	0.090	0.0004009	0.1822	0.11	0.2478
4	0.12	0.0005345	0.2430	0.14	0.6518
5	0.15	0.0006682	0.3037	0.19	0.8386

Figure S16. Plot of Initial Rates of the C–H Arylation with Different Concentration of $Pd(OAc)_2/PCy_3$ at Low Concentrations

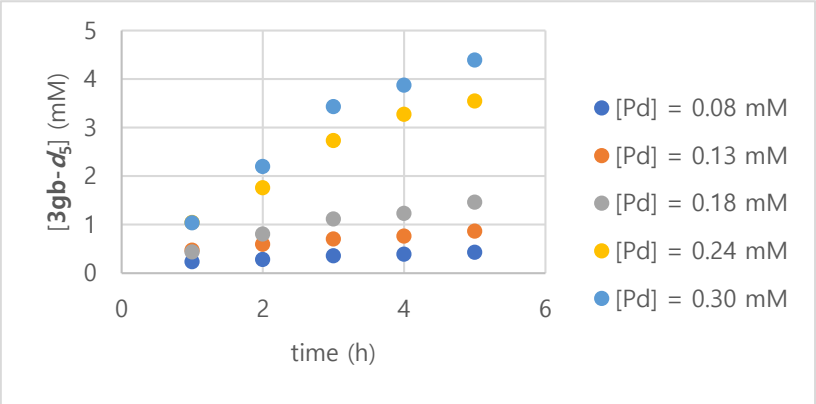
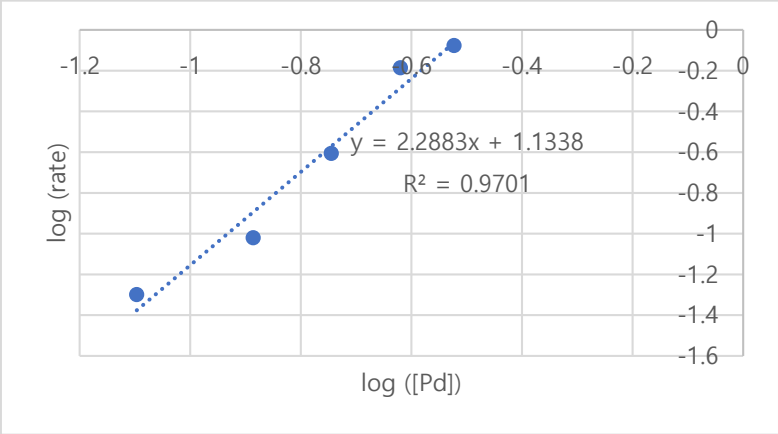


Figure S17. Plot of Initial Rates with Different Concentration of $Pd(OAc)_2/PCy_3$



5.4.5. Order in $Pd(OAc)_2$ with PPh_3 at Low Concentrations

The order in [Pd] was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(OAc)_2$ and PPh_3 (1:1 ratio) in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 μL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.066 mmol, 15 μL) as an internal standard. Different amount of $Pd(OAc)_2$ (stock solution in DMA) and PPh_3 (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 ℃. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated two more times in each [Pd] concentrations and the average rate values were used.

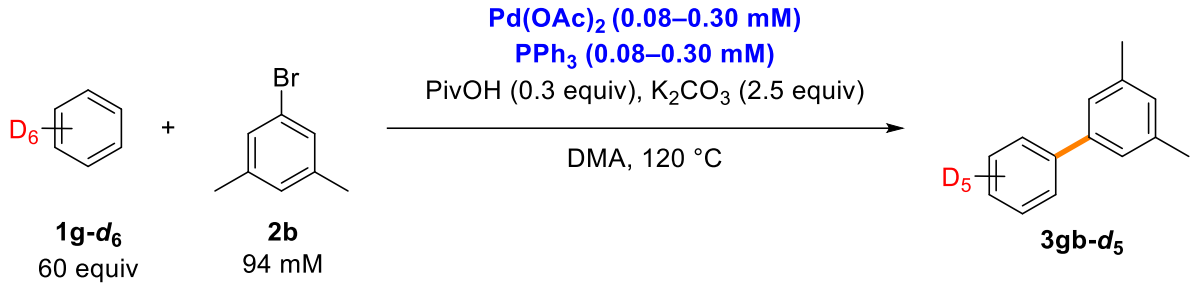


Table S14. Results to Determine the Order of $Pd(OAc)_2$ with PPh_3 at Low Concentrations

Entry	Amount of **$Pd(OAc)_2$**			Amount of **PPh_3**	Rate (mM/h)
	mg	mmol	mM	mg	
1	0.040	0.0001782	0.0810	0.047	0.0214
2	0.065	0.0002895	0.1316	0.076	0.0719
3	0.090	0.0004009	0.1822	0.11	0.1526
4	0.12	0.0005345	0.2430	0.14	0.2602
5	0.15	0.0006682	0.3037	0.18	0.4070

Figure S18. Plot of Initial Rates of the C–H Arylation with Different Concentration of $Pd(OAc)_2/PPh_3$ at Low Concentrations

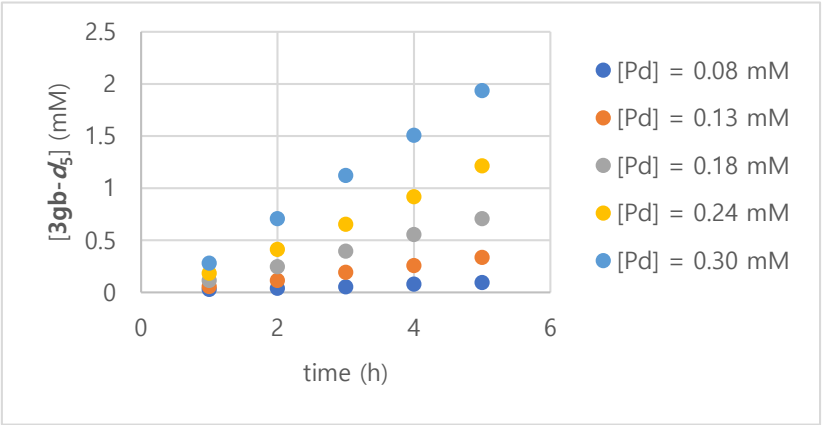
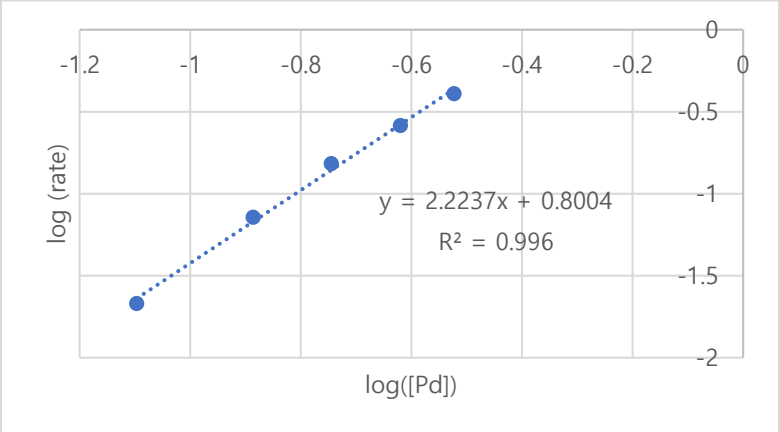


Figure S19. Plot of Initial Rates with Different Concentration of $Pd(OAc)_2/PPh_3$



5.4.6. Order in $Pd(OAc)_2$ with $P(C_6F_5)_3$ at Low Concentrations

The order in [Pd] was determined by obtaining the initial rate of the C–H arylation at low concentration of $Pd(OAc)_2$ and $P(C_6F_5)_3$ (1:1 ratio) in benzene-d_6. Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol, stock solution in DMA), 1-bromo-3,5-dimethylbenzene (**2b**, 28 μL, 0.20 mmol, 1.0 equiv, 94 mM), and dodecane (0.066 mmol, 15 μL) as an internal standard. Different amount of $Pd(OAc)_2$ (stock solution in DMA) and $P(C_6F_5)_3$ (stock solution in DMA) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and benzene-d_6 (60 equiv, 1.0 mL, 12 mmol). Each tube was sealed and heated to 120 °C. Aliquots of the reaction mixture were taken every 1 h and analyzed by GC. The same experiment was repeated two more times in each [Pd] concentrations and the average rate values were used.

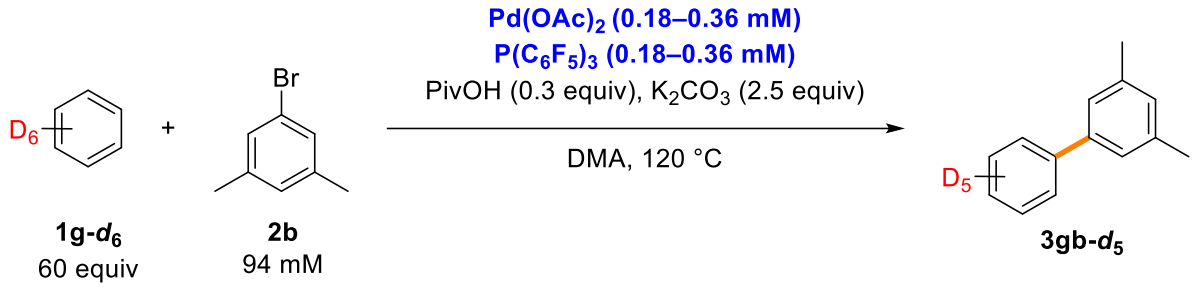


Table S15. Results to Determine the Order of $Pd(OAc)_2$ with $P(C_6F_5)_3$ at Low Concentrations

Entry	Amount of **$Pd(OAc)_2$**			Amount of **$P(C_6F_5)_3$**	Rate (mM/h)
	mg	mmol	mM	mg	
1	0.090	0.0004009	0.1822	0.21	0.0345
2	0.12	0.0005345	0.2430	0.28	0.0590
3	0.15	0.0006682	0.3037	0.36	0.1081
4	0.18	0.0008018	0.3644	0.43	0.1320

Figure S20. Plot of Initial Rates of the C–H Arylation with Different Concentration of $Pd(OAc)_2/P(C_6F_5)_3$ at Low Concentrations

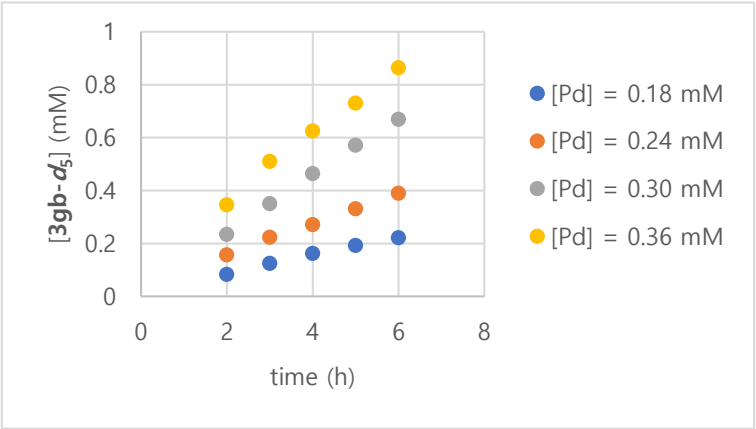
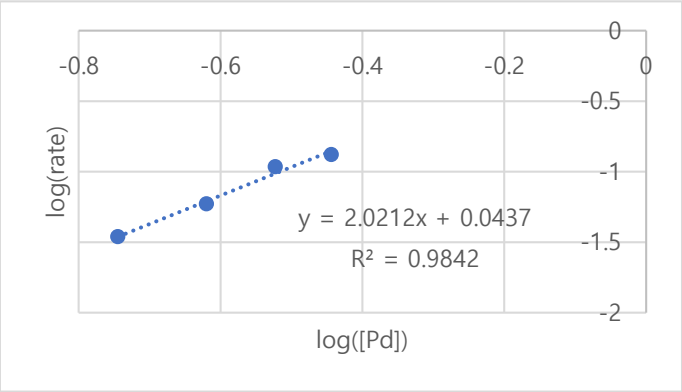
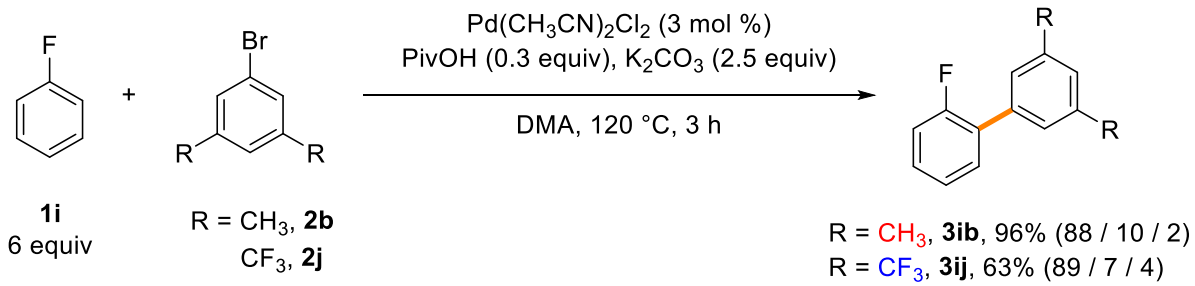


Figure S21. Plot of Initial Rates with Different Concentration of $Pd(OAc)_2/P(C_6F_5)_3$



5.5. Reaction of Electron-poor Arenes with Two Different Aryl Bromides

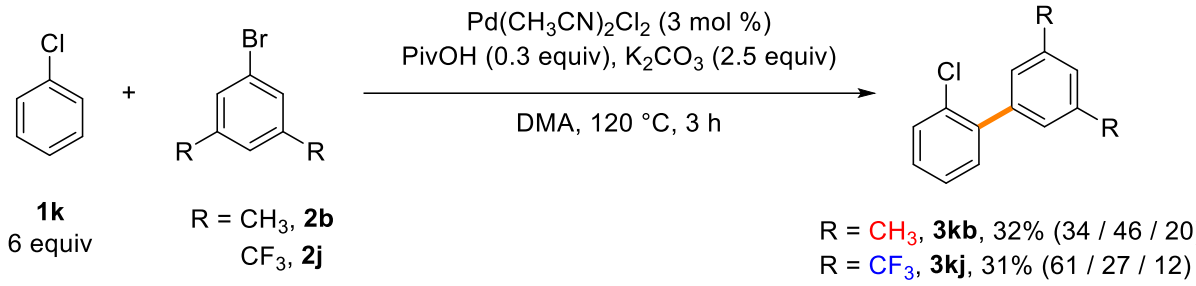
Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), and pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol). Aryl bromide (**2b** or **2j**, 1.0 equiv, 0.20 mmol) was then added to the Schlenk tube in, followed by DMA (1.2 mL) and arenes (**1i** or **1k**, 6.0 equiv, 1.2 mmol). The Schlenk tube was sealed and heated to 120 ℃ for 3 h. Upon completion of the reaction, the mixture was cooled to room temperature. The crude mixture was filtered through Celite® and then the yield and selectivity of the products **3ib** and **3ij** were analyzed by GC for the yield and ^{19}F-NMR measurement for the selectivity. For **3kb** and **3kj**, the yield and selectivity of the products were analyzed by GC using dodecane as an internal standard.



1i
6 equiv

R = CH_3, **2b**
CF_3, **2j**

R = CH_3, **3ib**, 96% (88 / 10 / 2)
R = CF_3, **3ij**, 63% (89 / 7 / 4)



1k
6 equiv

R = CH_3, **2b**
CF_3, **2j**

R = CH_3, **3kb**, 32% (34 / 46 / 20)
R = CF_3, **3kj**, 31% (61 / 27 / 12)

5.6. Competition Experiments

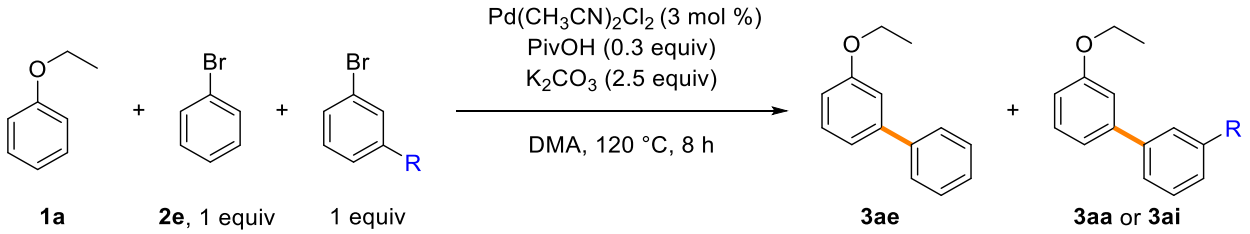
5.6.1. Competition between Two Different Aryl Bromides

Experiment A: bromobenzene (**2e**) vs 3-bromotoluene (**2a**)

To a 10 mL Schlenk tube equipped with a magnetic stirring bar were added K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol), DMA (1.2 mL) and ethoxybenzene (60 equiv, 1.52 mL, 12 mmol) followed by **2e** (22 μL, 0.20 mmol, 1.0 equiv) and **2a** (25 μL, 0.20 mmol, 1.0 equiv). The Schlenk tube was sealed and heated to 120 ℃ for 6 h. Upon completion of the reaction, the mixture was cooled to room temperature. The crude mixture was filtered through Celite® and then analyzed by GC using dodecane as an internal standard.

Experiment B: bromobenzene (**2e**) vs 3-bromobenzotrifluoride (**2i**)

The reaction was conducted using **2e** (22 μL, 0.20 mmol, 1.0 equiv) and **2i** (28 μL, 0.20 mmol, 1.0 equiv) as competing substrates followed by the above procedure.

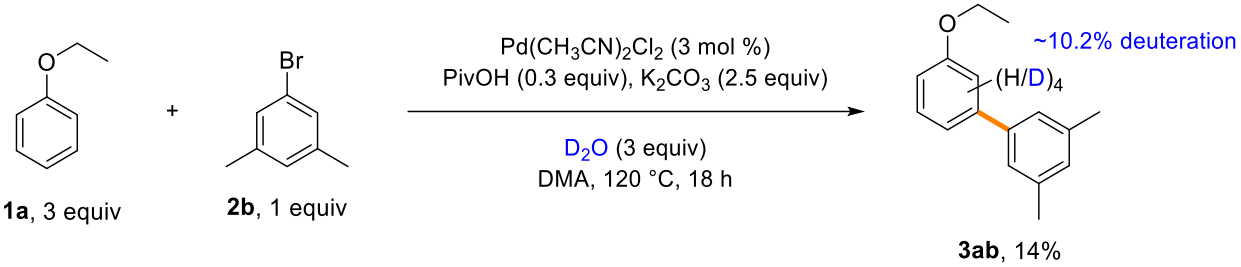


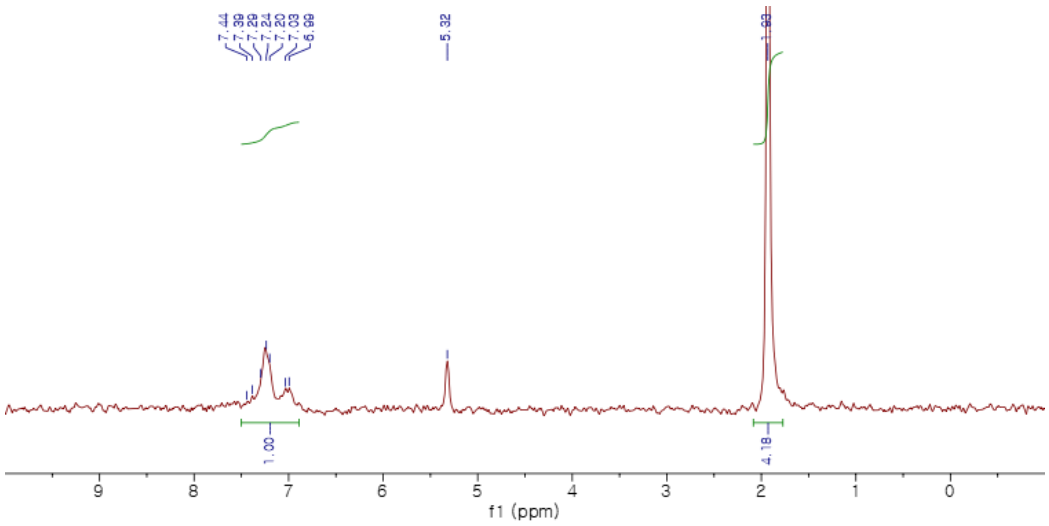
1a **2e**, 1 equiv 1 equiv R = CH_3, **2a** CF_3, **2i** **3ae** **3aa** or **3ai**

	yield of **3ae** (%)	yield (%)
R = CH_3	30 (12 / 65 / 23)	**3aa**, 24 (8 / 68 / 24)
R = CF_3	trace	**3ai**, 10 (18 / 51 / 31)

5.6.2. H/D scrambling Experiment with D_2O

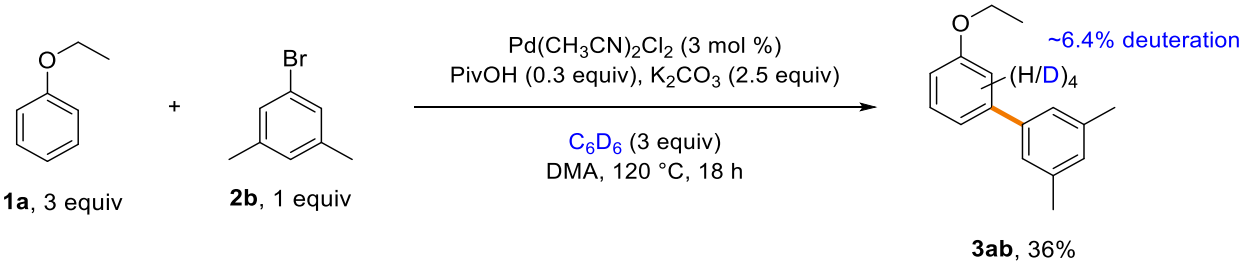
H/D scrambling between with D_2O was determined by ^2H NMR analysis of the product **3ab**. The reactions were conducted using the above general procedure with the following modification. To a 4 mL vial equipped with a magnetic stirring bar were added K_2CO_3 (2.5 equiv, 138 mg, 1.0 mmol), $Pd(CH_3CN)_2Cl_2$ (0.030 equiv, 3.1 mg, 0.012 mmol), pivalic acid (0.30 equiv, 12.3 mg, 0.12 mmol). 1-bromo-3,5-dimethylbenzene (**2b,** 1.0 equiv, 56 μL, 0.40 mmol) and ethoxybenzene (3.0 equiv, 152 μL, 1.2 mmol) were then added to the vial in, followed by DMA (1.2 mL) and D_2O (3.0 equiv, 22 μL, 1.2 mmol). The reaction vial was sealed and heated to 120 ℃ for 18 h. Upon completion of the reaction, the mixture was cooled down to room temperature. The crude mixture was filtered through Celite® and then the yield was analyzed by GC using dodecane as internal standard. The product was isolated by flash column chromatography and preparative TLC (PTLC) using hexane/ether eluent. The isolated product **3ab** was further analyzed by ^2H NMR spectroscopy in CH_2Cl_2 solvent with CD_3CN (1.93 ppm) as an internal standard.

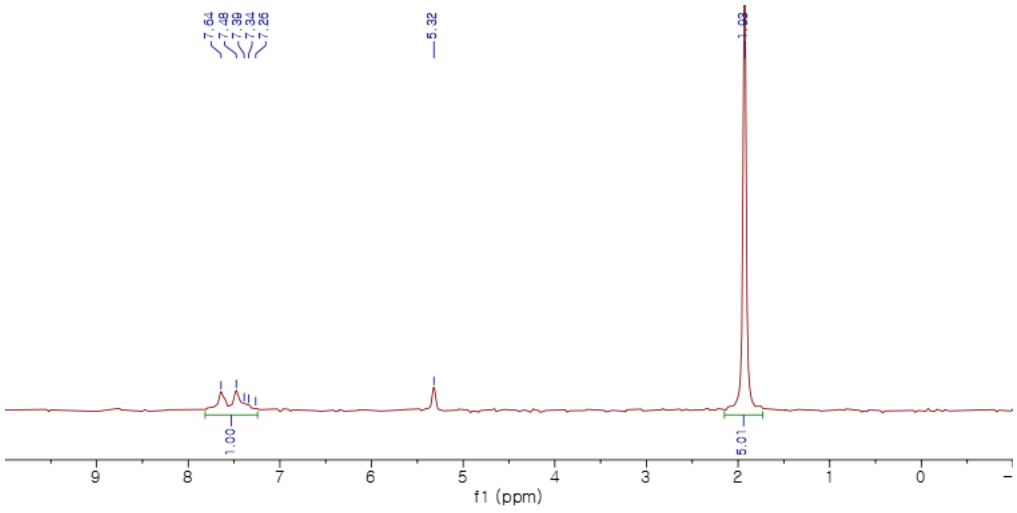




5.6.3. H/D Scrambling Experiment between Ethoxybenzene and Benzene-d_6

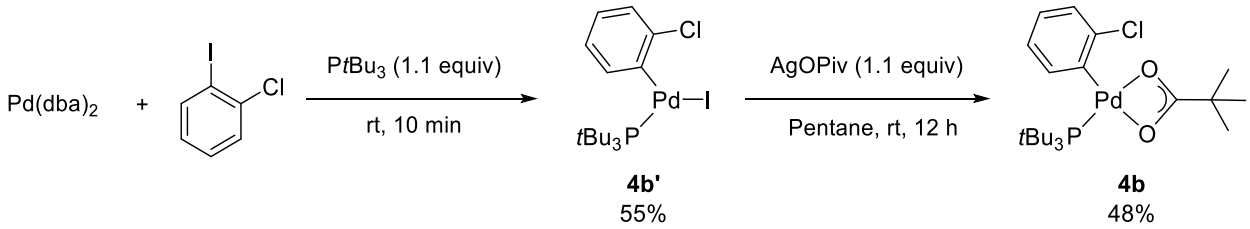
H/D scrambling between two arene substrates was determined by ^{2}H NMR analysis of the product **3ab**. The reactions were conducted using the above general procedure with the following modification. To a 4 mL vial equipped with a magnetic stirring bar were added K_2CO_3 (2.5 equiv, 138 mg, 1.0 mmol), $Pd(CH_3CN)_2Cl_2$ (0.030 equiv, 3.1 mg, 0.012 mmol), pivalic acid (0.30 equiv, 12.3 mg, 0.12 mmol), DMA (1.2 mL), ethoxybenzene (3.0 equiv, 152 µL, 1.2 mmol) and benzene-d_6 (3.0 equiv, 107 µL, 1.2 mmol) followed by **2b** (56 µL, 0.40 mmol, 1.0 equiv). The reaction vial was sealed and heated to 120 ℃ for 18 h. Upon completion of the reaction, the mixture was cooled down to room temperature. The crude mixture was filtered through Celite® and then the yield was analyzed by gas chromatography using dodecane as internal standard. The product was isolated by flash column chromatography and preparative TLC (PTLC) using hexane/ether eluent. The isolated product **3ab** was further analyzed by ^{2}H NMR spectroscopy in CH_2Cl_2 solvent with CD_3CN (1.93 ppm) as an internal standard. H/D scrambling on the aryl group was clearly detected suggesting that the C–H bond cleavage facilitated by CMD process is reversible.





5.7. Synthesis of Pd Complex 4a and 4b

AgOPiv and Pd complex **4a** were synthesized by literature procedures.[3]



5.7.1. Synthesis of Intermediate Pd Complex 4b'

Inside a glove box, to a stirred solution of P*t*Bu$_3$ (45 mg, 1.1 equiv, 0.22 mmol) and 1-chloro-2-iodobenzene (1.0 mL) was added Pd(dba)$_2$ (115 mg, 1.0 equiv, 0.2 mmol). The reaction mixture was stirred at room temperature for 10 min. Pentane (20 mL) was added and the resulting mixture was stirred for 1 min and then cooled at -20 ℃ for 1 h. The solid was filtered, washed with ether until the filtrate contained no free dba, as judged by ^{1}H NMR spectroscopy. The solid was dried under reduced pressure to obtain the title compound as an orange color solid (60 mg, 55%).

^{1}H NMR (400 MHz, C_6D_6) δ 7.21 (d, J = 7.5 Hz, 1H), 6.98 – 6.95 (m, 1H), 6.61 (t, *J* = 7.4 Hz, 1H), 6.53 (t, *J* = 7.2 Hz, 1H), 1.03 (d, *J* = 12.6 Hz, 27H); ^{13}C NMR (151 MHz, CD_2Cl_2) δ 138.02 (d, *J* = 5.0 Hz), 137.66 (d, *J* = 2.0 Hz), 129.34, 128.73, 125.67, 125.27 (d, *J* = 2.3 Hz), 41.50 (d, *J* = 8.1 Hz), 31.88 (d, *J* = 2.8 Hz); ^{31}P NMR (162 MHz, C_6D_6) δ 53.9; Anal. calc'd for $C_{18}H_{31}ClIPPd$: C, 39.51; H, 5.71. Found: C, 38.3; H, 5.49.

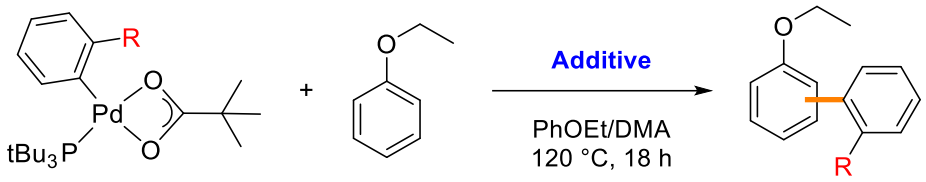
5.7.2. Synthesis of Pd Complex 4b

Inside a glove box, to a stirred solution of **4b'** (60 mg, 0.11 mmol, 1.0 equiv) and AgOPiv (25 mg, 0.12 mmol, 1.1 equiv) was added pentane (5 mL). The reaction mixture was stirred at room temperature for 12 h. The resulting mixture was filtered through Celite® and concentrated under reduced pressure. Recrystallization from pentane at -20 ℃ produced the Pd complex **4b** as yellow crystals which is suitable for X-ray diffraction analysis. Further filtration and drying afforded the title compound as a yellow solid (30 mg, 48%).

^{1}H NMR (400 MHz, C_6D_6) δ 7.42 (dt, *J* = 7.3, 2.1 Hz, 1H), 7.07 – 7.03 (m, 1H), 6.71 – 6.60 (m, 2H), 1.32 (d, *J* = 12.7 Hz, 27H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, C_6D_6) δ 194.8, 141.1 (d, *J* = 3.0 Hz), 140.5, 138.6 (d, *J* = 3.2 Hz), 128.7, 125.4, 124.6 (d, *J* = 1.5 Hz), 40.6 (d, *J* = 11.8 Hz), 40.4, 32.2 (d, *J* = 3.2 Hz), 27.5; ^{31}P NMR (162 MHz, C_6D_6) δ 76.1; Anal. calc'd for $C_{23}H_{40}ClO_2PPd$: C, 52.98; H, 7.73. Found: C, 52.7; H, 7.82.

5.8. Stoichiometric Reaction of Pd Complex

Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with Pd complex (0.0060 mmol, 1.0 equiv) and the corresponding additives (see table below) followed by DMA (1.2 mL) and ethoxybenzene (1.5 mL). The Schlenk tube was sealed and heated to 120 ℃ for 18 h. Upon the completion of the reaction, the mixture was cooled down to room temperature. The crude mixture was filtered through Celite® and then analyzed by gas chromatography for **3ac** or GC-MS for **3am** using dodecane (3.0 μL) as an internal standard.



2.1 mM
R = Me, **4a**
= Cl, **4b**

R = Me, **3ac**
= Cl, **3am**

Entry	Pd complex	Additive (equiv)	Yield of 3ac or 3am (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	**4a**	None	0	-	-
2	**4a**	PivOH (20), K_2CO_3 (160)	0.6	1 / 0.7 / 0.7	42 / 30 / 28
3	**4a**	PivOH (20), K_2CO_3 (160), *n*Bu_4NBr (10)	21	1 / 1.3 / 1.4	27 / 35 / 38
4	**4a**	*n*Bu_4NBr (10), $Pd(OPiv)_2$ (5)	22	1 / 3.9 / 2.2	14 / 55 / 31
4	**4a**	PivOH (20), K_2CO_3 (160), $Pd(CH_3CN)_2Cl_2$ (5)	26	1 / 0.8 / 1.6	29 / 24 / 47
5	**4a**	PivOH (20), K_2CO_3 (160), *n*Bu_4NBr (10), $Pd(CH_3CN)_2Cl_2$ (5)	65	1 / 6.2 / 2.6	10 / 64 / 26
6	**4b**	PivOH (20), K_2CO_3 (160), *n*Bu_4NBr (10)	7	1 / 0.1 / 0.1	84 / 8 / 8.0
7	**4b**	PivOH (20), K_2CO_3 (160), *n*Bu_4NBr (10), $Pd(CH_3CN)_2Cl_2$ (5)	65	1 / 0.7 / 0.4	48 / 33 / 19

5.9. Effect of Crown Ethers

Inside a glove box, a 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with K_2CO_3 (2.5 equiv, 69 mg, 0.50 mmol), $Pd(CH_3CN)_2Cl_2$ (3.0 mol %, 1.6 mg, 0.0060 mmol), and pivalic acid (0.30 equiv, 6.1 mg, 0.060 mmol). Aryl bromide (1.0 equiv, 0.20 mmol) and crown ether additive were then added to the Schlenk tube, followed by DMA (1.2 mL) and arene (60 equiv, 12 mmol). The Schlenk tube was sealed and heated to 120 ℃ for 18 h. Upon completion of the reaction, the mixture was cooled down to room temperature. The crude mixture was filtered through Celite® and then analyzed by gas chromatography using dodecane as an internal standard.

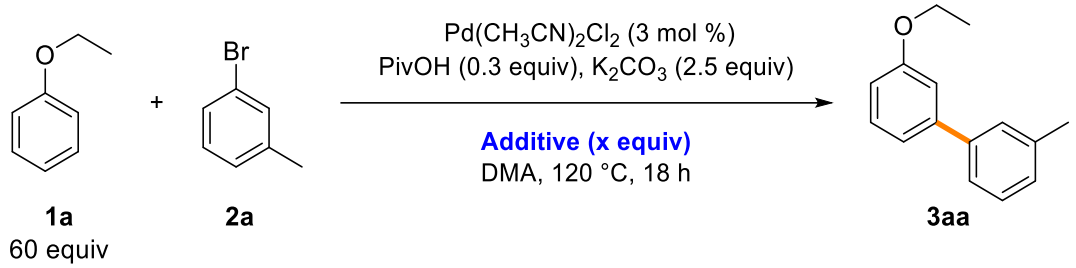


Table S16. Impact of Crown Ether Additives in the C–H Arylation of Ethoxybenzene

Entry	Additive (x equiv)	Yield (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	-	79	1 / 10.2 / 3.2	7 / 71 / 22
2	18-Crown-6 (0.3)	91	1 / 8.0 / 2.6	9 / 69 / 22
3	18-Crown-6 (1)	90	1 / 4.4 / 1.9	14 / 60 / 26
4	18-Crown-6 (2.5)	85	1 / 2.8 / 1.5	19 / 53 / 28
5	18-Crown-6 (5)	80	1 / 2.0 / 1.4	23 / 47 / 30
6	18-Crown-6 (10)	59	1 / 1.4 / 1.2	29 / 39 / 32
7	15-Crown-5 (1)	0	-	-
8	12-Crown-4 (1)	0	-	-
9	diethyl ether (5)	55	1 / 10.2 / 3.0	7 / 72 / 21

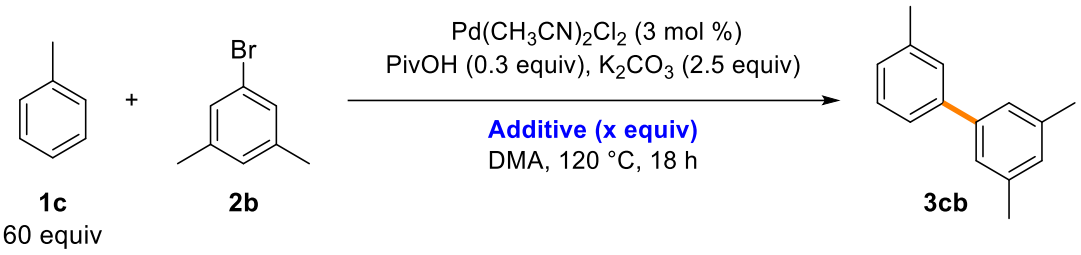
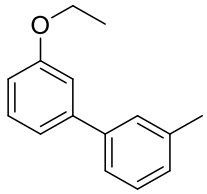


Table S17. Impact of Crown Ether Additives in the C–H Arylation of Toluene[a]

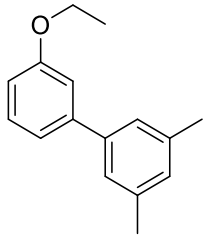
Entry	Additive (x equiv)	Yield (%)	Selectivity (o / m / p)	% Selectivity (o / m / p)
1	-	87	1 / 13.0 / 6.1	5 / 64 / 31
2	18-Crown-6 (0.3)	91	1 / 10.1 / 4.9	6 / 63 / 31
3	18-Crown-6 (1)	90	1 / 5.5 / 2.9	11 / 58 / 31
4	18-Crown-6 (2.5)	85	1 / 3.0 / 1.9	17 / 51 / 32
5	18-Crown-6 (5)	80	1 / 2.1 / 1.5	22 / 46 / 32

6. Characterization Data



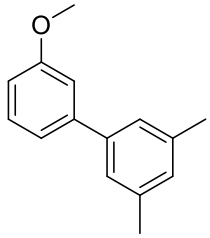
3-Ehoxy-3'-methyl-1,1'-biphenyl (3aa)

A modification of general procedure was employed for the reaction of 3-bromotoluene (**2a**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale yellow oil (76% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.37 (m, 2H), 7.37 – 7.30 (m, 2H), 7.17 (dd, *J* = 7.6, 1.3 Hz, 2H), 7.13 (t, *J* = 2.1 Hz, 1H), 6.89 (dd, *J* = 8.2, 2.6 Hz, 1H), 4.11 (q, *J* = 6.9 Hz, 2H), 2.42 (s, 3H), 1.45 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 143.0, 141.3, 138.4, 129.8, 128.8, 128.2, 128.1, 124.4, 119.7, 113.6, 113.3, 63.6, 21.7, 15.1; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1200. The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 2H), 7.35 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.34 – 7.28 (m, 2H), 7.15 (d, *J* = 7.3 Hz, 1H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 4.06 (q, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.37 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.0, 138.7, 137.5, 131.1, 131.0, 130.4, 128.5, 127.9, 127.6, 126.9, 120.9, 112.8, 64.2, 21.7, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1199. The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.7 Hz, 2H), 7.38 (d, *J* = 10.8 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.14 (d, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 2.43 (s, 3H), 1.46 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.6, 141.0, 138.4, 133.9, 128.8, 128.3, 127.7, 127.5, 124.0, 114.8, 77.4, 77.2, 76.9, 63.7, 21.7, 15.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1203.



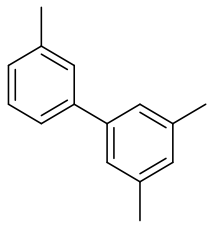
3'-Ethoxy-3,5-dimethyl-1,1'-biphenyl (3ab)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale yellow oil (81% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 1H), 7.35 (s, 2H), 7.32 – 7.25 (m, 2H), 7.11 (s, 1H), 6.99 (dd, *J* = 7.7, 2.1 Hz, 1H), 4.18 (q, *J* = 7.0 Hz, 2H), 2.50 (s, 6H), 1.55 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 143.0, 141.2, 138.2, 129.7, 129.1, 125.2, 119.6, 113.5, 113.1, 63.4, 21.4, 15.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{18}O$, 226.1358; found, 226.1361. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.38 (ddd, *J* = 8.1, 7.5, 1.8 Hz, 1H), 7.32 (s, 2H), 7.15 – 7.03 (m, 3H), 4.13 (q, *J* = 7.0 Hz, 2H), 2.48 (s, 6H), 1.46 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.0, 138.6, 137.3, 131.2, 131.0, 128.5, 128.4, 127.5, 120.9, 112.8, 64.1, 21.5, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{18}O$, 226.1358; found, 226.1360. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.30 (s, 2H), 7.12 – 7.01 (m, 3H), 4.18 (q, *J* = 7.0 Hz, 2H), 2.49 (s, 6H), 1.55 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.5, 141.0, 138.3, 134.0, 128.4, 128.3, 124.8, 114.8, 63.6, 21.5, 15.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{18}O$, 226.1358; found, 226.1359.



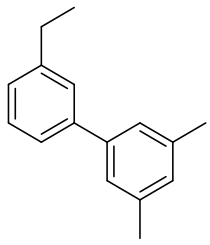
3'-Methoxy-3,5-dimethyl-1,1'-biphenyl (3bb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and anisole (**1b**, 60 equiv). The isomeric mixture of compound was obtained as a colorless oil (58% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.9 Hz, 1H), 7.20 (s, 2H), 7.16 (d, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 2.3 Hz, 1H), 7.00 (s, 1H), 6.88 (dd, *J* = 7.9, 2.2 Hz, 1H), 3.87 (s, 3H), 2.38 (s, 6H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.4 Hz, 2H), 7.14 (s, 2H), 7.04 – 6.97 (m, 3H), 3.82 (s, 3H), 2.37 (s, 6H). The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 2H), 7.18 (s, 2H), 6.98 – 6.95 (m, 3H), 3.85 (s, 3H), 2.38 (s, 6H). Their identity was confirmed by comparison with reported data.[4]



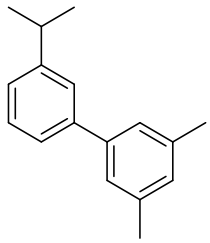
3,3',5-Trimethyl-1,1'-biphenyl (3cb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and toluene (**1c**, 60 equiv). The isomeric mixture of compound was obtained as a colorless oil (87% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.26 (s, 2H), 7.17 (d, *J* = 7.5 Hz, 1H), 7.01 (s, 1H), 2.44 (s, 3H), 2.41 (s, 6H). The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 4H), 7.16 (s, 1H), 7.13 (s, 2H), 2.54 (s, 6H), 2.46 (s, 3H). The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.26 (s, 2H), 7.25 (s, 2H), 7.01 (s, 1H), 2.41 (d, *J* = 4.0 Hz, 9H). Their identity was confirmed by comparison with reported data.[4b, 5]



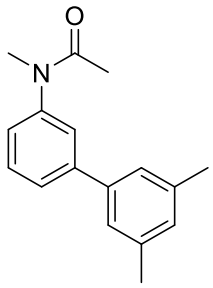
3'-Ethyl-3,5-dimethyl-1,1'-biphenyl (3db)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and ethylbenzene (**1d**, 60 equiv). The isomeric mixture of compound was obtained as a colorless oil (77% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, *J* = 9.2 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.35 (s, 2H), 7.30 (d, *J* = 7.3 Hz, 1H), 7.12 (s, 1H), 2.84 (q, *J* = 7.6 Hz, 2H), 2.51 (s, 6H), 1.42 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.7, 141.7, 138.3, 138.2, 128.9, 128.7, 127.0, 126.8, 125.3, 124.7, 29.1, 21.5, 15.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{16}H_{18}$, 210.1409; found, 210.1410. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 2H), 7.33 – 7.26 (m, 2H), 7.09 (s, 1H), 7.04 (s, 2H), 2.71 (q, *J* = 7.6 Hz, 2H), 2.46 (s, 6H), 1.22 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.0, 142.0, 141.7, 137.5, 130.0, 128.52, 128.4, 127.4, 127.2, 125.5, 26.3, 21.5, 15.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{16}H_{18}$, 210.1409; found, 210.1407. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.38 (s, 2H), 7.14 (s, 1H), 2.85 (q, *J* = 7.6 Hz, 2H), 2.54 (s, 6H), 1.45 (t, *J* = 7.6 Hz, 3H). Identity of the *para*-isomer was confirmed by comparison with reported data.[6]



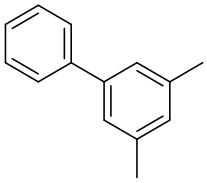
3'-Isopropyl-3,5-dimethyl-1,1'-biphenyl (3eb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and cumene (**1e**, 60 equiv). The isomeric mixture of compound was obtained as a colorless oil (79% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 3H), 7.24 – 7.22 (m, 3H), 7.02 (s, 1H), 3.00 (hept, *J* = 6.9 Hz, 1H), 2.42 (s, 6H), 1.34 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.4, 141.8, 141.7, 138.3, 128.9, 128.7, 125.6, 125.3, 125.3, 124.9, 77.6, 77.2, 76.7, 34.4, 24.2, 21.6.; HRMS-EI (m/z) $[M]^+$ calcd for $C_{17}H_{20}$, 224.1565; found, 224.1564. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 – 7.31 (m, 2H), 7.24 – 7.17 (m, 2H), 7.02 (s, 1H), 6.94 (s, 2H), 3.10 (hept, *J* = 6.9 Hz, 1H), 2.39 (s, 6H), 1.20 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.5, 142.2, 141.5, 137.5, 130.0, 128.4, 127.6, 127.3, 125.6, 125.3, 77.6, 77.2, 76.8, 29.5, 24.5, 21.5; found, 224.1565. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.24 (s, 2H), 7.01 (s, 1H), 2.98 (hept, *J* = 6.9 Hz, 1H), 2.41 (s, 6H), 1.33 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.9, 141.4, 139.1, 138.3, 128.8, 127.2, 126.9, 125.1, 77.6, 77.2, 76.7, 33.9, 24.2, 21.6; HRMS-EI (m/z) $[M]^+$ calcd for $C_{17}H_{20}$, 224.1565; found, 224.1563.



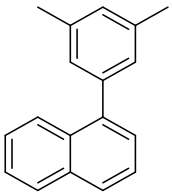
***N*-(3',5'-Dimethyl-[1,1'-biphenyl]-3-yl)-*N*-methylacetamide (3fb)**

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and *N*-methylacetanilide (**1f**, 60 equiv). The isomeric mixture of compound was obtained and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (400 MHz, CD_3OD) δ 7.15 – 6.93 (m, 3H), 6.75 (s, 2H), 6.71 (d, *J* = 7.6 Hz, 1H), 6.57 (s, 1H), 2.81 (s, 3H), 1.92 (s, 6H), 1.42 (s, 3H); ^{13}C NMR (75 MHz, CD_3OD) δ 172.9, 146.0, 144.8, 141.0, 139.6, 132.1, 131.3, 130.5, 127.7, 126.6, 125.9, 37.6, 22.4, 21.5; HRMS-ESI (m/z) $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO$, 276.1359; found, 276.1367. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 3H), 7.23 – 7.19 (m, 1H), 6.99 (s, 1H), 6.88 (s, 2H), 3.02 (s, 3H), 2.33 (s, 6H), 1.80 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 142.1, 140.3, 138.8, 138.2, 131.6, 129.5, 128.7, 128.5, 128.3, 126.3, 37.2, 22.4, 21.5; HRMS-ESI (m/z) $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO$, 276.1359; found, 276.1368. The *para*-isomer; ^{1}H NMR (300 MHz, CD_3OD) δ 7.65 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.22 (s, 2H), 7.00 (s, 1H), 3.25 (s, 3H), 2.35 (s, 6H), 1.88 (s, 3H); ^{13}C NMR (75 MHz, CD_3OD) δ 173.0, 144.5, 142.6, 141.1, 139.6, 130.31, 129.4, 128.4, 125.9, 37.6, 22.4, 21.5; HRMS-ESI (m/z) $[M+Na]^+$ calcd for $C_{17}H_{19}NNaO$, 276.1359; found, 276.1362.



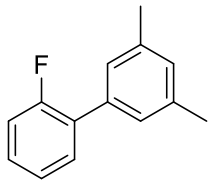
3,5-Dimethyl-1,1'-biphenyl (3gb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and benzene (**1g**, 60 equiv). The title compound was obtained as a white solid (>99% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.0 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 2H), 7.51 – 7.46 (m, 1H), 7.40 (s, 2H), 7.16 (s, 1H), 2.55 (s, 6H). Its identity was confirmed by comparison with reported data.[7]



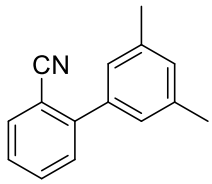
1-(3,5-Dimethylphenyl)naphthalene (3hb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and naphthalene (**1h**, 60 equiv). The isomeric mixture of compound was obtained and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (t, *J* = 9.2 Hz, 2H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.57 – 7.40 (m, 4H), 7.14 (s, 2H), 7.10 (s, 1H), 2.43 (s, 6H). The β isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (s, 1H), 8.04 – 7.90 (m, 3H), 7.84 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.63 – 7.51 (m, 2H), 7.45 (s, 2H), 7.13 (s, 1H), 2.52 (s, 6H). Their identity was confirmed by comparison with reported data.[4b, 8]



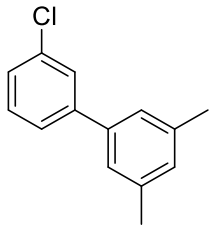
3'-Fluoro-3,5-dimethyl-1,1'-biphenyl (3ib)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and fluorobenzene (**1i**, 6 equiv) for 3 h. The isomeric mixture of compound was obtained as a colorless oil (96% yield) and its identity was confirmed by comparison with ^{1}H and ^{19}F NMR spectra. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (td, *J* = 7.7, 1.8 Hz, 1H), 7.34 – 7.10 (m, 5H), 7.04 (s, 1H), 2.40 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.8. The *meta*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 2H), 7.31 – 7.25 (m, 1H), 7.19 (s, 2H), 7.07 – 6.96 (m, 2H), 2.39 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.4. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (ddt, *J* = 8.4, 5.2, 3.0 Hz, 2H), 7.18 (s, 2H), 7.11 (t, *J* = 8.7 Hz, 2H), 7.02 (s, 1H), 2.40 (s, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.0. Their identity was confirmed by comparison with reported data.[4b, 9]



3',5'-Dimethyl-[1,1'-biphenyl]-2-carbonitrile (3jb)

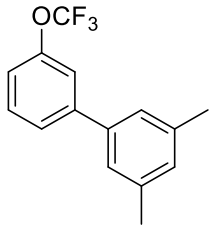
A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and benzonitrile (**1j**, 60 equiv). The isomeric mixture of compound was obtained and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.62 (td, *J* = 7.8, 1.4 Hz, 1H), 7.51 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.42 (td, *J* = 7.6, 1.3 Hz, 1H), 7.19 (s, 2H), 7.10 (s, 1H), 2.41 (d, *J* = 0.5 Hz, 6H). The *meta*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (t, *J* = 1.5 Hz, 1H), 7.79 (dt, *J* = 7.8, 1.6 Hz, 1H), 7.61 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.17 (s, 2H), 7.06 (s, 1H), 2.40 (s, 6H). The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 4H), 7.20 (s, 2H), 7.07 (s, 1H), 2.40 (s, 6H). Their identity was confirmed by comparison with reported data.[10]



3'-Chloro-3,5-dimethyl-1,1'-biphenyl (3kb)

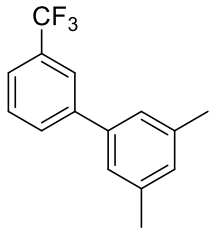
A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and chlorobenzene (**1k**, 60 equiv). The isomeric mixture of compound was obtained and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR

(300 MHz, $CDCl_3$) δ 7.56 (t, *J* = 1.8 Hz, 1H), 7.45 (dt, *J* = 7.4, 1.6 Hz, 1H), 7.37 – 7.28 (m, 2H), 7.18 (s, 2H), 7.02 (s, 1H), 2.39 (s, 6H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 6.8, 1.3 Hz, 1H), 7.42 – 7.28 (m, 3H), 7.14 (s, 2H), 7.11 (s, 1H), 2.46 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.9, 139.5, 137.6, 132.6, 131.5, 130.0, 129.4, 128.4, 127.3, 126.8, 21.5; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_{13}Cl$, 216.0706; found, 216.0707. The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.21 (s, 2H), 7.05 (s, 1H), 2.42 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.1, 140.0, 138.5, 133.3, 129.4, 128.9, 128.5, 125.0, 21.50; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_{13}Cl$, 216.0706; found, 216.0703. Identity of the *meta*-isomer was confirmed by comparison with reported data.[4b]



3,5-Dimethyl-3'-(trifluoromethoxy)-1,1'-biphenyl (3lb)

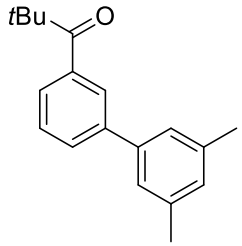
A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and (trifluoromethoxy)benzene (**1l**, 60 equiv). The isomeric mixture of compound was obtained as a colorless oil (64% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 – 7.45 (m, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.21 (s, 3H), 7.05 (s, 1H), 2.40 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.0, 144.0, 139.9, 138.7, 130.1, 129.9, 125.7, 125.3, 121.1 (q, *J* = 257.7 Hz), 120.0, 119.5, 21.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.7; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}F_3O$, 266.0918; found, 266.0920. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 – 7.40 (m, 1H), 7.38 – 7.26 (m, 3H), 7.13 (s, 2H), 7.04 (s, 1H), 2.38 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.5, 137.9, 137.0, 135.8, 131.7, 129.5, 128.5, 127.2, 127.0, 121.3, 120.8 (q, *J* = 259.2 Hz), 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}F_3O$, 266.0918; found, 266.0918. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (dt, *J* = 8.7, 2.6 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.18 (s, 2H), 7.04 (s, 1H), 2.40 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.8, 140.6, 140.1, 138.7, 129.6, 128.6, 125.3, 121.1 (q, *J* = 257.0 Hz), 121.3, 21.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}F_3O$, 266.0918; found, 266.0915.



3,5-Dimethyl-3'-(trifluoromethyl)-1,1'-biphenyl (3mb)

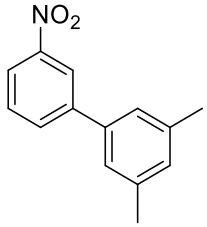
A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and benzotrifluoride (**1m**, 6 equiv). The isomeric mixture of compound was obtained as a colorless oil (86% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (s, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.63 – 7.49

(m, 2H), 7.22 (s, 2H), 7.06 (s, 1H), 2.41 (s, 6H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.03 (s, 1H), 6.95 (s, 2H), 2.36 (s, 6H). The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (m, 4H), 7.31 (s, 2H), 7.16 (s, 1H), 2.50 (s, 6H). Their identity was confirmed by comparison with reported data.[4b, 11]



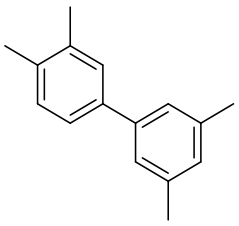
1-(3',5'-Dimethyl-[1,1'-biphenyl]-3-yl)-2,2-dimethylpropan-1-one (3nb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and pivalophenone (**1n**, 6 equiv). The isomeric mixture of compound was obtained and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (t, *J* = 1.6 Hz, 1H), 7.64 (t, *J* = 8.6 Hz, 2H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.21 (s, 2H), 7.02 (s, 1H), 2.39 (s, 6H), 1.38 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.7, 141.6, 140.6, 139.3, 138.6, 129.6, 129.4, 128.4, 126.8, 126.4, 125.2, 44.5, 28.2, 21.5; HRMS-EI (m/z) $[M]^+$ calcd for $C_{19}H_{22}O$, 266.1671; found, 266.1672. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.42 (m, 2H), 7.39 – 7.34 (m, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 7.03 (s, 2H), 7.01 (s, 1H), 2.37 (s, 6H), 0.94 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 217.0, 141.2, 141.0, 138.3, 138.1, 129.6, 129.3, 128.8, 127.4, 126.7, 125.9, 45.0, 27.5, 21.4; HRMS-EI (m/z) $[M]^+$ calcd for $C_{19}H_{22}O$, 266.1671; found, 266.1673. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.27 (s, 2H), 7.07 (s, 1H), 2.43 (s, 6H), 1.44 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 208.5, 144.1, 140.2, 138.5, 136.8, 129.7, 128.8, 126.8, 125.2, 44.3, 28.3, 21.5; HRMS-EI (m/z) $[M]^+$ calcd for $C_{19}H_{22}O$, 266.1671; found, 266.1673.



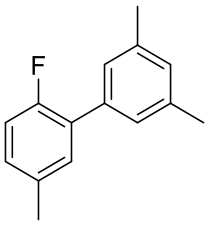
3,5-Dimethyl-3'-nitro-1,1'-biphenyl (3ob)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and nitrobenzene (**1o**, 6 equiv). The isomeric mixture of compound was obtained as a pail yellow oil (95% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.44 (t, *J* = 1.9 Hz, 1H), 8.18 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.24 (s, 2H), 7.08 (s, 1H), 2.41 (s, 6H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.60 (td, *J* = 7.6, 1.3 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.05 (s, 1H), 6.95 (s, 2H), 2.36 (s, 6H). The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.9 Hz, 2H), 7.24 (s, 2H), 7.09 (s, 1H), 2.41 (s, 6H). Their identity was confirmed by comparison with reported data.[12]



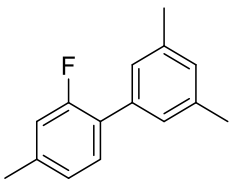
3,3',4,5'-Tetramethyl-1,1'-biphenyl (3pb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and 4-fluorotoluene (**1p**, 60 equiv). The title compound was obtained as a colorless oil (53% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 (s, 1H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.23 (m, 3H), 7.01 (s, 1H), 2.42 (s, 6H), 2.37 (s, 3H), 2.34 (s, 3H). Its identity was confirmed by comparison with reported data.[13]



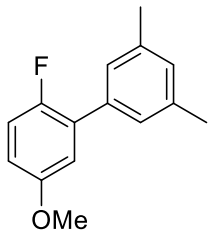
2-Fluoro-3',5,5'-trimethyl-1,1'-biphenyl (3qb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and 4-fluorotoluene (**1q**, 6 equiv). The title compound was obtained as a colorless oil (93% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.30 (s, 2H), 7.21 – 7.10 (m, 3H), 2.51 (s, 4H), 2.48 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.1 (d, *J* = 244.7 Hz), 137.94, 136.0 (d, *J* = 1.0 Hz), 133.6 (d, *J* = 3.7 Hz), 131.3 (d, *J* = 3.4 Hz), 129.3, 129.2 (d, *J* = 8.0 Hz), 129.0 (d, *J* = 13.8 Hz), 127.0 (d, *J* = 2.7 Hz), 115.8 (d, *J* = 23.0 Hz), 21.5, 20.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.1; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{15}F$, 214.1158; found, 214.1156.



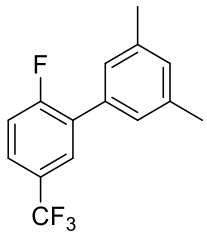
2-Fluoro-3',4,5'-trimethyl-1,1'-biphenyl (3rb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and 3-fluorotoluene (**1r**, 60 equiv). The title compound was obtained as a colorless oil (92% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (t, *J* = 8.2 Hz, 1H), 7.40 – 7.35 (m, 2H), 7.17 – 7.10 (m, 3H), 2.55 (s, 6H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7 (d, *J* = 247.2 Hz), 139.3 (d, *J* = 8.0 Hz), 137.9, 135.9, 130.5 (d, *J* = 4.1 Hz), 129.2, 126.9 (d, *J* = 2.8 Hz), 126.4 (d, *J* = 13.6 Hz), 125.1 (d, *J* = 3.2 Hz), 116.6 (d, *J* = 22.7 Hz), 21.4, 21.0 (d, *J* = 1.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{15}F$, 214.1158; found, 214.1158.



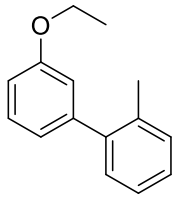
2-Fluoro-5-methoxy-3',5'-dimethyl-1,1'-biphenyl (3sb)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and 4-fluoroanisole (**1s**, 6 equiv) for 3 h. The title compound was obtained as a pale-yellow oil (87% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.19 (s, 2H), 7.07 (t, *J* = 9.4 Hz, 1H), 7.05 (s, 1H), 6.98 – 6.93 (m, 1H), 6.86 – 6.81 (m, 1H), 3.84 (s, 3H), 2.40 (s, 6H). Its identity was confirmed by comparison with reported data.[4b]



2-Fluoro-3',5'-dimethyl-5-(trifluoromethyl)-1,1'-biphenyl (3tb)

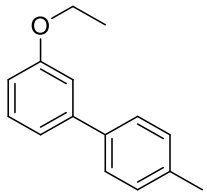
A modification of general procedure was employed for the reaction of 1-bromo-3,5-dimethylbenzene (**2b**, 0.2 mmol) and 4-fluorobenzotrifluoride (**1t**, 6 equiv) for 3 h. The title compound was obtained as a colorless oil (94% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 6.9, 2.2 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.25 (t, *J* = 9.2 Hz, 1H), 7.17 (s, 2H), 7.08 (s, 1H), 2.40 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.49 (d, *J* = 251.2 Hz), 138.4, 134.3, 130.4, 130.2, 128.7 – 128.3 (m), 126.9 (d, *J* = 2.6 Hz), 126.2 – 125.9 (m), 125.3, 122.6, 116.80 (d, *J* = 24.4 Hz), 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.9, -112.2; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{12}F_4$, 268.0875; found, 268.0873.



3'-Ethoxy-2-methyl-1,1'-biphenyl (3ac)

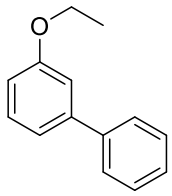
A modification of general procedure was employed for the reaction of 2-bromotoluene (**2c**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow oil (78% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.8 Hz, 1H), 7.32 – 7.26 (m, 4H), 6.95 – 6.88 (m, 3H), 4.10 (q, *J* = 7.0 Hz, 2H), 2.32 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8, 143.5, 142.0, 135.5, 130.4, 129.8,

129.2, 127.4, 125.8, 121.7, 115.5, 113.1, 77.4, 77.2, 76.9, 63.6, 20.6, 15.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1198. The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (t, *J* = 7.8 Hz, 1H), 7.27 – 7.18 (m, 5H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 4.04 (q, *J* = 7.0 Hz, 2H), 2.20 (s, 3H), 1.29 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 139.0, 136.9, 131.6, 131.3, 130.2, 129.6, 128.6, 127.2, 125.4, 120.6, 112.3, 64.0, 20.1, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1201. The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 6H), 6.97 (d, *J* = 8.6 Hz, 2H), 4.11 (q, *J* = 7.0 Hz, 2H), 2.31 (s, 3H), 1.48 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 141.7, 135.6, 134.3, 130.4, 130.4, 130.0, 127.1, 125.9, 114.1, 63.6, 20.7, 15.1; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1202.



3-Ethoxy-4'-methyl-1,1'-biphenyl (3ad)

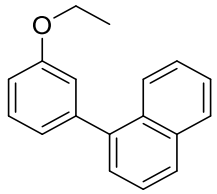
A modification of general procedure was employed for the reaction of 4-bromotoluene (**2d**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow solid (83% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.9 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.16 (s, 1H), 6.91 (dd, *J* = 8.3, 2.6 Hz, 1H), 4.14 (q, *J* = 7.0 Hz, 2H), 2.44 (s, 3H), 1.49 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 142.8, 138.4, 137.3, 129.8, 129.6, 127.2, 119.5, 113.5, 113.1, 63.6, 21.3, 15.1; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1198. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.0 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.25 (t, *J* = 7.9 Hz, 2H), 7.08 – 6.96 (m, 2H), 4.07 (q, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.38 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.0, 147.4, 136.5, 135.8, 131.0, 129.5, 128.8, 128.4, 120.9, 112.8, 64.1, 21.4, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O$, 212.1201; found, 212.1202. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 2.43 (s, 3H), 1.48 (t, *J* = 7.0 Hz, 3H); Identity of the *para*-isomer was confirmed by comparison with reported data.[14]



3-Ethoxy-1,1'-biphenyl (3ae)

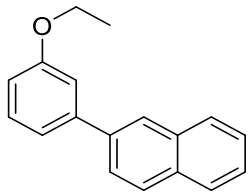
A modification of general procedure was employed for the reaction of bromobenzene (**2e**, 0.2 mmol). The isomeric mixture of compound was obtained as a colorless oil (81% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.1 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 2H), 7.23 – 7.13 (m, 2H), 6.98 – 6.85 (m, 1H), 4.12 (q, *J* = 7.0 Hz, 2H), 1.47 (t, *J* = 7.0 Hz, 3H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 (dt, *J* = 8.2, 1.8 Hz, 2H), 7.43 – 7.37 (m, 2H), 7.36 – 7.27 (m, 3H), 7.05 – 6.97 (m, 2H), 4.05 (q, *J* = 7.0 Hz, 2H), 1.35 (t, *J* = 7.0 Hz, 3H). The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$)

δ 7.61 – 7.51 (m, 4H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.36 – 7.29 (m, 1H), 7.04 – 6.94 (m, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H). Their identity was confirmed by comparison with reported data.[14-15]



1-(3-Ethoxyphenyl)naphthalene (3af)

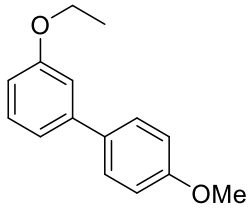
A modification of general procedure was employed for the reaction of 1-bromonaphthalene (**2f**, 0.2 mmol). The isomeric mixture of compound was obtained as a yellow oil (73% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.62 – 7.44 (m, 5H), 7.20 (d, *J* = 7.3 Hz, 2H), 7.07 (dd, *J* = 7.6, 1.9 Hz, 1H), 4.10 (q, *J* = 7.0 Hz, 2H), 1.50 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.9, 142.2, 140.3, 133.9, 131.7, 129.3, 128.3, 127.7, 126.8, 126.1, 126.1, 125.8, 125.4, 122.5, 116.2, 113.5, 63.4, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{16}O$, 248.1201; found, 248.1198. The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.46 – 7.40 (m, 2H), 7.37 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.11 (dt, *J* = 7.4, 1.0 Hz, 1H), 7.05 (d, *J* = 8.3 Hz, 1H), 4.03 – 3.90 (m, 2H), 1.10 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.6, 137.3, 133.5, 132.2, 132.1, 130.1, 129.0, 128.1, 127.6, 127.4, 126.7, 125.5, 125.5, 125.4, 120.6, 112.5, 63.9, 14.6; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{16}O$, 248.1201; found, 248.1199. The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.42 (m, 6H), 7.07 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.0 Hz, 2H), 1.52 (t, *J* = 7.0 Hz, 3H). Identity of the *para*-isomer was confirmed by comparison with reported data.[16]



2-(3-Ethoxyphenyl)naphthalene (3ag)

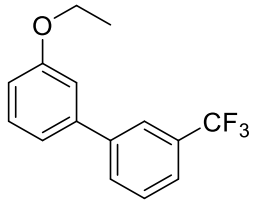
A modification of general procedure was employed for the reaction of 2-bromonaphthalene (**2g**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow solid (82% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.95 – 7.87 (m, 3H), 7.77 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.34 – 7.28 (m, 2H), 6.95 (ddd, *J* = 8.1, 2.5, 1.0 Hz, 1H), 4.16 (q, *J* = 7.0 Hz, 2H), 1.50 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 142.7, 138.6, 133.8, 132.8, 130.0, 128.5, 128.3, 127.8, 126.4, 126.1, 126.0, 125.7, 120.0, 113.9, 113.4, 63.7, 15.1; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{16}O$, 248.1201; found, 248.1199. The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.93 – 7.86 (m, 3H), 7.78 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.54 – 7.46 (m, 3H), 7.36 (td, *J* = 8.2, 1.7 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.37 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 136.5, 133.6, 132.5, 131.3, 131.0, 128.8, 128.4, 128.3, 128.2,

127.7, 127.1, 126.0, 125.8, 121.1, 112.9, 64.2, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{16}O$, 248.1201; found, 248.1198. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.91 – 7.84 (m, 3H), 7.73 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.48 (pd, *J* = 6.8, 3.4 Hz, 2H), 7.02 (d, *J* = 8.7 Hz, 2H), 4.11 (q, *J* = 7.0 Hz, 2H), 1.47 (t, *J* = 7.0 Hz, 3H). Identity of the *para*-isomer was confirmed by comparison with reported data.[17]



3-Ethoxy-4'-methoxy-1,1'-biphenyl (3ah)

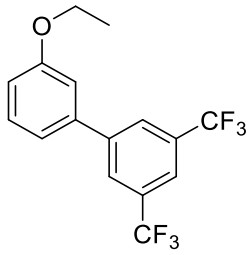
A modification of general procedure was employed for the reaction of 4-bromoanisole (**2h**, 0.2 mmol). The isomeric mixture of compound was obtained as a white solid (61% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.3 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.14 – 7.09 (m, 2H), 6.97 (d, *J* = 8.3 Hz, 2H), 6.85 (dd, *J* = 8.2, 2.5 Hz, 1H), 4.10 (q, *J* = 7.0 Hz, 2H), 3.85 (s, 3H), 1.45 (t, *J* = 7.0 Hz, 3H). The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.8 Hz, 2H), 7.32 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.03 – 6.93 (m, 4H), 4.04 (q, *J* = 7.0 Hz, 2H), 3.85 (s, 3H), 1.36 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 155.8, 140.0, 130.8, 130.6, 128.8, 128.7, 122.0, 120.8, 115.1, 112.6, 112.6, 63.9, 55.1, 14.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{16}O_2$, 228.1150; found, 228.1147. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 3.7 Hz, 2H), 7.46 (d, *J* = 3.7 Hz, 2H), 6.97 (d, *J* = 2.9 Hz, 2H), 6.94 (d, *J* = 2.7 Hz, 2H), 4.07 (q, *J* = 7.0 Hz, 2H), 3.84 (s, 3H), 1.44 (t, *J* = 7.0 Hz, 3H). Identity of the meta and *para*-isomers was confirmed by comparison with reported data.[18]



3-Ethoxy-3'-(trifluoromethyl)-1,1'-biphenyl (3ai)

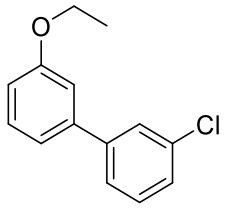
A modification of general procedure was employed for the reaction of 3-bromobenzotrifluoride (**2i**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow oil (54% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.20 – 7.12 (m, 2H), 6.98 – 6.90 (m, 1H), 4.10 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 142.1, 141.3, 131.2 (q, *J* = 32.4 Hz), 130.6, 130.1, 129.3, 124.4 (q, *J* = 272.4 Hz), 124.1 (m), 119.6, 113.9, 113.8, 63.7, 14.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}F_3O$, 266.0918; found, 266.0917. The *ortho*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.41 – 7.28 (m, 2H), 7.04 (td, *J* = 7.5, 1.0 Hz, 1H), 6.99 (d, *J* = 8.1 Hz, 1H), 4.05 (q, *J* = 7.0 Hz, 2H), 1.36 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.0, 139.5, 132.9, 130.8, 130.3 (q, *J* = 31.9 Hz), 129.5, 129.2, 128.4, 126.7 (q, *J* = 3.9 Hz), 124.6 (q, *J* = 271.79 Hz), 123.5 (q, *J* = 3.8 Hz), 121.1, 112.6, 64.1, 14.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.5; HRMS-EI (m/z) $[M]^+$ calcd for

$C_{15}H_{13}F_3O$, 266.0918; found, 266.0917. The *para*-isomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.60 – 7.45 (m, 4H), 6.99 (d, *J* = 8.7 Hz, 2H), 4.06 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl) δ 159.1, 141.6, 132.0, 131.1 (q, *J* = 31.5 Hz), 129.9, 129.2, 128.2, 124.3 (q, *J* = 217.6 Hz), 123.3 (q, *J* = 3.8 Hz), 123.2 (q, *J* = 3.8 Hz), 115.0, 63.5, 14.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.6; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}F_3O$, 266.0918; found, 266.0917.



3'-Ethoxy-3,5-bis(trifluoromethyl)-1,1'-biphenyl (3aj)

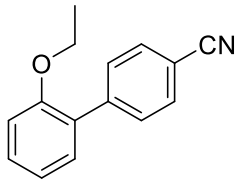
A modification of general procedure was employed for the reaction of 1-bromo-3,5-bis(trifluoromethyl)benzene (**2j**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow oil (69% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (s, 2H), 7.86 (s, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.12 (t, *J* = 2.1 Hz, 1H), 6.98 (dd, *J* = 8.3, 2.4 Hz, 1H), 4.12 (q, *J* = 7.0 Hz, 2H), 1.47 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.8, 143.4, 139.8, 132.2 (q, *J* = 33.2 Hz), 130.5, 127.4 (m), 123.6 (q, *J* = 272.2 Hz), 121.2 (m), 119.6, 114.6, 114.0, 63.9, 15.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{16}H_{12}F_6O$, 334.0792; found, 334.0789. The *ortho*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 2H), 7.81 (s, 1H), 7.39 – 7.35 (m, 2H), 7.07 (td, *J* = 7.6, 0.8 Hz, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 4.08 (q, *J* = 7.0 Hz, 2H), 1.37 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.9, 140.6, 131.2 (q, *J* = 33.0 Hz), 130.6, 130.4, 129.9 (m), 127.5, 123.7(d, *J* = 272.7 Hz), 121.2, 120.5 (q, *J* = 4.1 Hz), 112.6, 64.2, 14.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{16}H_{12}F_6O$, 334.0792; found, 334.0795. The *para*-isomer; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (s, 2H), 7.79 (s, 1H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H). Identity of the *para*-isomer was confirmed by comparison with reported data.[19]



3-Chloro-3'-ethoxy-1,1'-biphenyl (3ak)

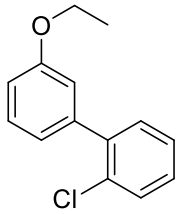
A modification of general procedure was employed for the reaction of 1-bromo-3-chlorobenzene (**2k**, 0.2 mmol). The isomeric mixture of compound was obtained as a pale-yellow oil (49% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 – 7.63 (m, 1H), 7.52 – 7.49 (m, 1H), 7.41 – 7.36 (m, 3H), 7.20 – 7.15 (m, 2H), 6.96 (ddd, *J* = 8.3, 2.4, 0.8 Hz, 1H), 4.12 (q, *J* = 7.0 Hz, 2H), 1.50 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 143.1, 141.3, 134.7, 130.0, 129.9, 127.4, 127.4, 125.4, 119.5, 113.9, 113.5, 63.6,

14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_{13}ClO$, 232.0655; found, 232.0658. The *ortho*-isomer ^1H NMR (300 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.63 – 7.49 (m, 1H), 7.47 – 7.33 (m, 4H), 7.12 (t, *J* = 7.1 Hz, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 4.12 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.8, 140.5, 133.7, 130.8, 129.8, 129.4, 129.2, 129.2, 127.8, 126.8, 120.9, 112.6, 64.1, 14.7; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_{13}ClO$, 232.0655; found, 232.0656. The *para*-isomer; ^1H NMR (300 MHz, $CDCl_3$) δ 7.60 (t, *J* = 1.6 Hz, 1H), 7.52 (dt, *J* = 8.8, 3.0 Hz, 2H), 7.46 (dt, *J* = 7.3, 1.7 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.00 (dt, *J* = 8.8, 2.7 Hz, 2H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.49 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 142.8, 134.7, 132.1, 130.0, 128.2, 126.8, 126.6, 124.8, 114.9, 63.6, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_{13}ClO$, 232.0655; found, 232.0655.



2'-Ethoxy-[1,1'-biphenyl]-4-carbonitrile (3al)

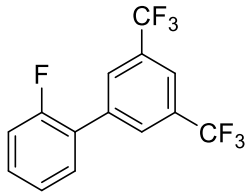
A modification of general procedure was employed for the reaction of 4-bromobenzonitrile (**2l**, 0.2 mmol). The isomeric mixture of compound was obtained as a colorless oil (44% yield) and its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 4H), 7.37 (ddd, *J* = 8.2, 7.4, 1.8 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.05 (td, *J* = 7.5, 1.1 Hz, 1H), 7.00 (dd, *J* = 8.3, 1.1 Hz, 1H), 4.07 (q, *J* = 7.0 Hz, 2H), 1.37 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 143.6, 131.7, 130.7, 130.3, 130.0, 128.7, 121.0, 119.3, 112.5, 110.3, 64.0, 14.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}NO$, 223.0997; found, 223.0999. The *meta*-isomer; ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.63 (m, 4H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.15 (ddd, *J* = 7.7, 1.7, 0.9 Hz, 1H), 7.11 – 7.09 (m, 1H), 6.95 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.45 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 145.6, 140.6, 132.6, 130.2, 127.8, 119.6, 119.0, 114.5, 113.8, 111.1, 63.7, 14.9; ; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}NO$, 223.0997; found, 223.0998. The *para*-isomer; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 4H), 7.53 (d, *J* = 8.9 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.45 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 145.3, 132.7, 131.4, 128.4, 127.2, 119.3, 115.1, 110.1, 63.7, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}NO$, 223.0997; found, 223.0998.



2-Chloro-3'-ethoxy-1,1'-biphenyl (3am)

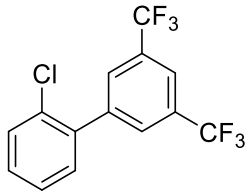
^1H NMR (300 MHz, $CDCl_3$) δ 7.47 – 7.42 (m, 1H), 7.35 – 7.23 (m, 4H), 7.02 – 6.95 (m, 2H), 6.90 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 4.05 (q, *J* = 7.0 Hz, 2H), 1.41 (t, *J* = 7.0 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 140.7, 140.5, 131.3, 129.9, 129.1, 128.6, 126.8, 121.7, 115.6, 113.8, 63.5, 14.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}ClO$, 232.0652; found, 232.0656. The *ortho*-isomer; ^1H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 1H), 7.36 – 7.29 (m, 1H), 7.28 – 7.20 (m, 3H), 7.19 – 7.13 (m, 1H), 6.99 (dt, *J* = 7.4, 1.0 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 1H), 4.00 (q, *J* = 6.9 Hz, 2H), 1.24 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101

MHz, $CDCl_3$) δ k 131.9, 131.1, 129.4, 129.3, 129.0, 128.5, 126.4, 120.4, 112.3, 64.1, 14.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}ClO$, 232.0655; found, 232.0656. The *para*-isomer; ^1H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.31 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.25 – 7.20 (m, 1H), 6.94 (d, *J* = 8.2 Hz, 2H), 4.07 (q, *J* = 7.0 Hz, 2H), 1.43 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.6, 140.3, 132.7, 131.8, 131.5, 130.7, 130.1, 128.3, 126.9, 114.1, 63.6, 15.0; HRMS-EI (m/z) $[M]^+$ calcd for $C_{15}H_{13}ClO$, 232.0655; found, 232.0654.



2-Fluoro-3',5'-bis(trifluoromethyl)-1,1'-biphenyl (3ij)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-trifluoromethylbenzene (**2j**, 0.2 mmol) and fluorobenzene (**1i**, 6 equiv) for 3 h. The isomeric mixture was analyzed by ^{19}F NMR and GC. Its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^1H NMR (600 MHz, $CDCl_3$) δ 8.00 (s, 2H), 7.89 (s, 1H), 7.47 (td, *J* = 7.7, 1.7 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.29 (td, *J* = 7.6, 1.2 Hz, 1H), 7.22 (ddd, *J* = 10.7, 8.3, 1.2 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9, -118.0. The *meta*-isomer; ^1H NMR (400 MHz, $CDCl_3$ δ 8.00 (s, 2H), 7.90 (s, 1H), 7.49 (td, *J* = 8.0, 5.8 Hz, 1H), 7.40 (ddd, *J* = 7.7, 1.8, 1.0 Hz, 1H), 7.31 (ddd, *J* = 9.7, 2.5, 1.7 Hz, 1H), 7.16 (tdd, *J* = 8.3, 2.5, 1.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5 (d, *J* = 247.5 Hz), 142.2 (d, *J* = 2.3 Hz), 140.6 (d, *J* = 7.7 Hz), 132.5 (q, *J* = 33.4 Hz), 131.1 (d, *J* = 8.4 Hz), 127.4 (d, *J* = 2.4 Hz), 123.5 (q, *J* = 273.1 Hz), 123.1 (d, *J* = 3.0 Hz), 121.7 (m), 116.0 (d, *J* = 21.1 Hz), 114.5 (d, *J* = 22.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.0, -111.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_7F_7$, 308.0436; found, 308.0433. The *para*-isomer; ^1H NMR (600 MHz, $CDCl_3$) δ 7.98 (s, 2H), 7.87 (s, 1H), 7.62 – 7.56 (m, 2H), 7.23 – 7.17 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9, -112.8. Identity of the ortho and *para*-isomers were confirmed by comparison with reported data.[20]



2-Chloro-3',5'-bis(trifluoromethyl)-1,1'-biphenyl (3kj)

A modification of general procedure was employed for the reaction of 1-bromo-3,5-trifluoromethylbenzene (**2j**, 0.2 mmol) and chlorobenzene (**1k**, 60 equiv) for 3 h. The isomeric mixture was analyzed by GC. Its identity was confirmed by comparison with NMR and GC spectra of authentic samples. ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 3H), 7.58 – 7.53 (m, 1H), 7.44 – 7.37 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 137.7, 132.5, 131.7 (q, *J* = 33.9 Hz), 131.3, 130.5, 130.2, 129.9 (m), 127.5, 123.5 (q, *J* = 273.7 Hz), 121.7 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_7ClF_6$, 324.0140; found, 324.0142. The *meta*-isomer; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 2H), 7.90 (s, 1H), 7.60 – 7.58 (m, 1H), 7.51 – 7.46 (m, 1H), 7.46 – 7.43 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 140.2, 135.5, 132.5 (q, *J* = 37.4 Hz), 130.7, 129.1, 127.6, 127.4 (m), 125.6, 123.4 (q, *J* = 276.0 Hz), 121.7 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9; HRMS-EI (m/z) $[M]^+$ calcd for

$C_{14}H_7ClF_6$, 324.0140; found, 324.0142.. The *para*-isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 2H), 7.88 (s, 1H), 7.55 (dt, *J* = 8.7, 2.3 Hz, 2H), 7.48 (dt, *J* = 8.7, 2.3 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.1, 136.6, 135.3, 132.3 (q, *J* = 32.7 Hz), 129.5, 128.5, 127.0 (m), 123.3 (q, *J* = 273.5 Hz), 121.2 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{14}H_7ClF_6$, 324.0140; found, 324.0140.

7. Calculation of Proton Affinities of Arenes

7.1. General Methods

The calculations were performed using the Gaussian 09[21] (DFT) and Gaussian 16[22] (G3MP2 and G4MP2) program packages. The gas-phase geometries of thirteen aromatic compounds (Figure S22) and their deprotonated counterparts have been fully optimized using a spin-restricted formalism at the density functional theory (DFT) using the B3LYP hybrid functional and the 6-31++G(d,p) basis sets.[23] Single point frequency calculations were then performed to characterize the minimum-energy stationary points. Thermodynamic parameters that include the zero-point energies (ZPE) and thermal corrections at 298.15K were obtained from frequency calculations. G3MP2[24] and G4MP2[25] calculations were followed with the geometries obtained from the DFT calculations. Proton affinities (PAs) were calculated by the following relation.

$AH(g) \rightarrow A^-(g) + H^+(g)$ $\qquad PA(A^-) = \Delta H°(A^-) + \Delta H°(H^+) - \Delta H°(AH)$

The value of $\Delta H°(H^+)$ was calculated as $5/2RT$ according to an ideal gas expression. The calculated PAs are listed in Table S18.

7.2. Calculational results of Proton Affinities

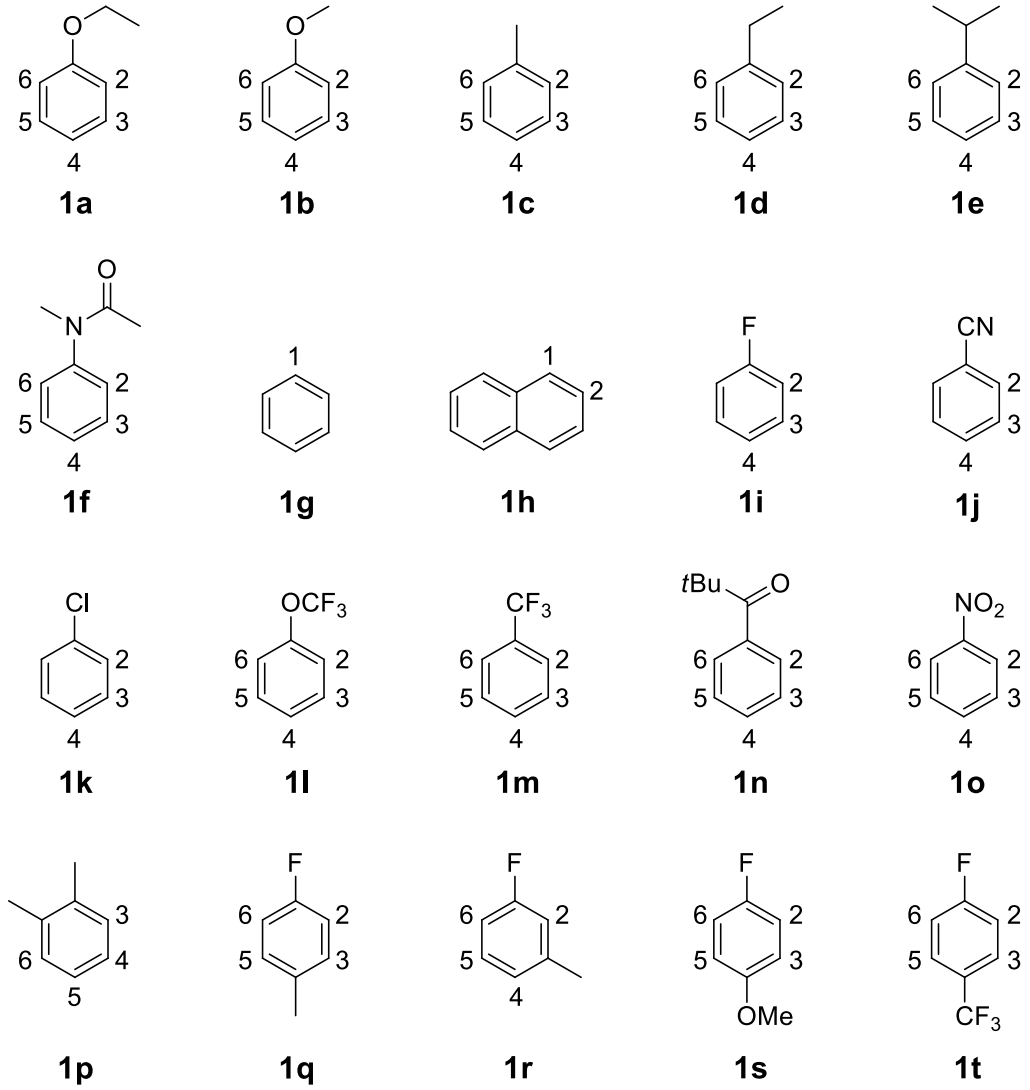


Figure S22. Schematic representation of substituted benzenes and naphthalene with the numbering of deprotonation position.

Table S18. The Calculated Proton Affinities of Arenes with the Numbering of Deprotonation Position

Compound		DFT[a]	G3MP2	G4MP2
Ethoxybenzene	**1a**			
	1a$_2$	391.9138	391.5291	390.2271
	1a$_3$	399.6899	399.1603	398.2309
	1a$_4$	401.7651	401.2260	400.3268
	1a$_5$	400.5596	399.9823	399.0480
	1a$_6$	397.5783	396.9841	396.0748
Anisole	**1b**			
	1b$_2$	391.7519	391.3861	390.2710
	1b$_3$	399.6253	399.0486	398.2040
	1b$_4$	401.6327	401.0710	400.2352
	1b$_5$	400.4297	399.8549	398.9733
	1b$_6$	397.4930	396.9458	396.0861
Toluene	**1c**			
	1c$_2$	400.1906	400.0507	400.1555
	1c$_3$	401.3214	400.8150	400.1254
	1c$_4$	401.4043	400.9838	400.6098
	1c$_5$	401.3214	400.8200	400.1254
	1c$_6$	400.1906	400.0507	400.1555
Ethylbenzene	**1d**			
	1d$_2$	399.0392	397.7402	398.1054
	1d$_3$	400.7981	399.6491	399.5895
	1d$_4$	400.7654	399.8411	399.8505
	1d$_5$	400.7981	399.6378	399.5895
	1d$_6$	400.8671	400.0049	398.1048
Isopropylbenzene	**1e**			
	1e$_2$	397.7070	397.0575	396.6371
	1e$_3$	400.6098	399.8650	399.3761
	1e$_4$	400.5395	399.9961	399.5707
	1e$_5$	400.3268	399.7081	399.1371
	1e$_6$	398.7869	397.8990	396.9395
N-Methylacetanilide	**1f**			
	1f$_2$	384.9930	385.1254	385.4009
	1f$_3$	389.5060	389.6887	389.6485
	1f$_4$	390.1499	389.9020	390.4925
	1f$_5$	389.5060	389.6887	389.6485
	1f$_6$	384.9930	385.1248	385.1863
Benzene	**1g**			
	1g$_1$	400.8031	400.4486	398.3464
Naphthalene	**1h**			
	1h$_1$	394.1251	393.4656	392.7076
	1h$_2$	395.4429	395.0614	394.3109
Fluorobenzene	**1i**			
	1i$_2$	387.8544	388.3891	387.1999
	1i$_3$	393.9074	394.2149	393.1977

	1i$_4$	395.8822	396.1934	395.5941
Benzonitrile	**1j**			
	1j$_2$	382.9624	382.8017	382.2665
	1j$_3$	384.8349	385.2741	384.7577
	1j$_4$	384.4427	385.0018	385.0702
Chlorobenzene	**1k**			
	1k$_2$	386.2411	387.3010	387.2263
	1k$_3$	390.6713	391.1658	390.6600
	1k$_4$	393.1186	393.1098	392.7013
Trifluoromethoxybenzene	**1l**			
	1l$_2$	381.6936	383.4951	380.7052
	1l$_3$	388.4437	389.3197	389.6014
	1l$_4$	389.9679	390.7931	391.4858
	1l$_5$	388.4437	389.3165	389.5293
	1l$_6$	381.9615	383.5133	383.3853
Trifluoromethylbenzene	**1m**			
	1m$_2$	386.1332	387.4309	385.0627
	1m$_3$	388.9614	390.3218	389.0637
	1m$_4$	388.3935	389.3046	388.8522
	1m$_5$	388.9614	389.7232	389.2387
	1m$_6$	386.1351	386.7563	386.6113
Pivalophenone	**1n**			
	1n$_2$	383.9250	385.3218	385.1737
	1n$_3$	393.1952	393.3646	393.2755
	1n$_4$	390.1323	391.5825	391.1966
	1n$_5$	390.7328	391.4664	391.4720
	1n$_6$	383.9250	385.3287	385.1725
Nitrobenzene	**1o**			
	1o$_2$	380.1913	380.1631	379.6397
	1o$_3$	382.5382	384.6636	384.2714
	1o$_4$	381.0654	383.4970	383.2404
1,2-Dimethylbenzene	**1p**			
	1p$_3$	400.7849	400.2622	399.5795
	1p$_4$	401.9966	401.4752	400.9104
	1p$_5$	401.9966	401.4758	400.9104
	1p$_6$	400.7849	400.1831	399.5795
1-Fluoro-4-methylbenzene	**1q**			
	1q$_2$	388.4907	389.5186	389.3034
	1q$_3$	393.5516	394.0975	392.9429
	1q$_5$	393.5516	393.6796	392.9103
	1q$_6$	388.4907	388.9200	387.3763
1-Fluoro-3-methylbenzene	**1r**			
	1r$_2$	387.5865	388.3226	387.5488
	1r$_4$	395.5389	395.7391	395.5753

	1r$_5$	394.6585	395.4341	394.8901
	1r$_6$	388.8139	389.7815	390.0206
1-Fluoro-4-anisole	**1s**			
	1s$_2$	387.5702	387.9034	386.8027
	1s$_3$	390.8332	390.8922	389.9861
	1s$_5$	385.2992	385.5691	384.4314
	1s$_6$	386.9847	387.3267	386.2204
1-Fluoro-4-trifluoromethylbenzene	**1t**			
	1t$_2$	375.4009	378.2837	378.1964
	1t$_3$	379.3322	381.3240	380.2151
	1t$_5$	379.3322	380.6331	380.2158
	1t$_6$	375.4009	377.6894	376.9559

[a]B3LYP/6-31++G(d,p).

8. Calculation of Reductive Elimination Process

8.1. General Methods

All calculations were carried out using DFT[26] as implemented in the Gaussian 09[21] program packages. Gas phase geometry optimizations were conducted with the B3LYP hybrid functional[27] including Grimme's D3 dispersion correction[28] and the 6-31G**/LanL2DZ(Pd)[29] basis set. The energies of the optimized structures were reevaluated by additional single point calculations using the B3LYP hybrid functional including Grimme's D3 dispersion correction and the 6-311++G**/SDD(Pd) basis set. The integral equation formalism variant of the Polarizable Continuum Model (IEFPCM) was employed as implemented to account for the solvation effects for *N*,*N*-dimethylacetamide (ε=37.781). Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LanL2DZ(Pd) basis set to confirm proper convergence to well-defined minima (no imaginary frequency) or saddle points (one and only one imaginary frequency) on the potential energy surface. All thermal corrections from the vibrational frequency calculations were performed at 120 ℃ (393.15 K).

8.2. Comparison of the Reductive Elimination Processes

Figure S23. DFT Computed Energy Profiles for Reductive Elimination Processes

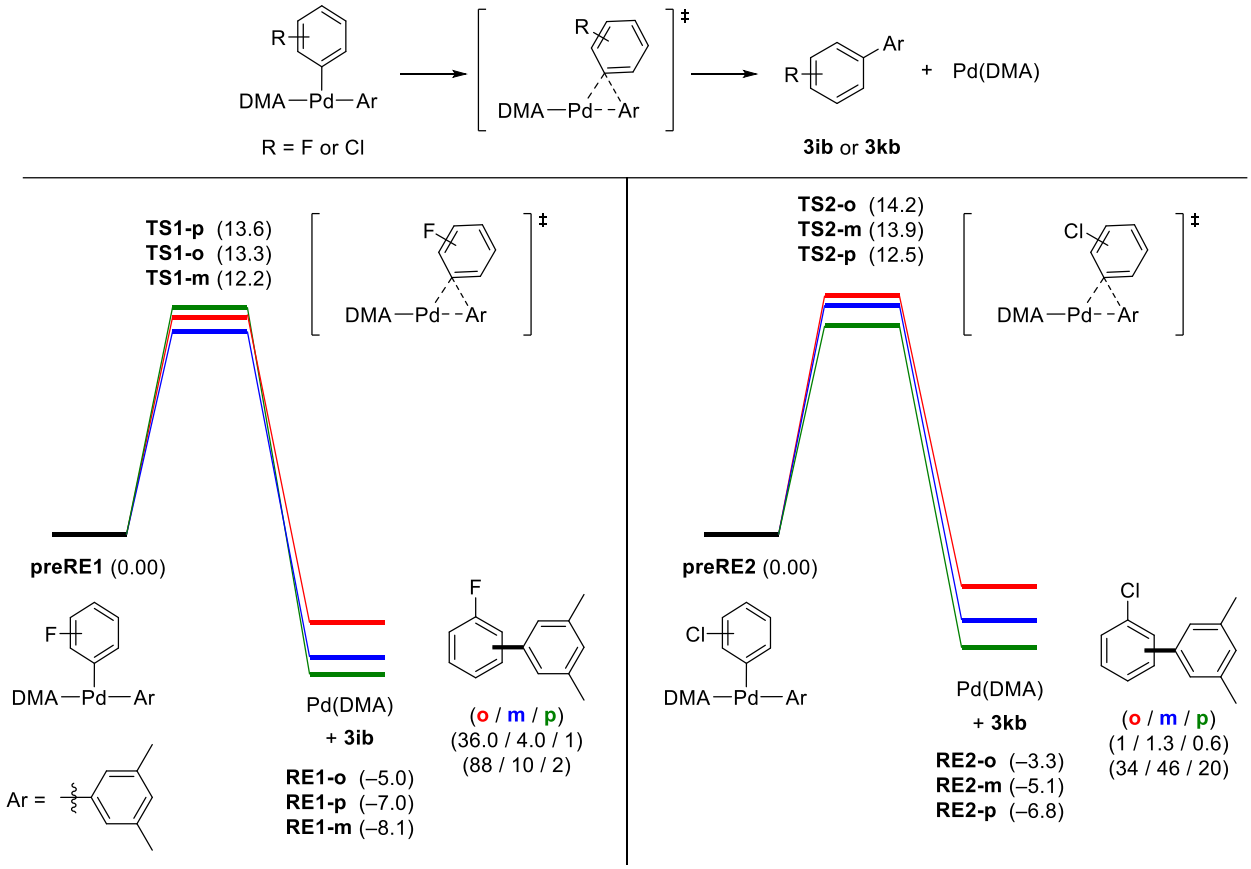


Table S19. Investigation of Theoretical Selectivity in Reductive Elimination Processes

Arylation site	DFT calculated				Experimental	
	ΔG	ΔG‡	ΔΔG‡[b]	%Selectivity (o / m / p)	ΔΔG‡[b]	%Selectivity (o / m / p)
Fluorobenzene						
ortho	−5.04	13.27	0		0	
meta	−8.08	12.20	−1.07	(17.8 / 69.9 / 12.3)	1.71	(87.8 / 9.8 / 2.4)
para	−6.97	13.56	0.29		2.81	
Chlorobenzene						
ortho	−3.32	14.20	0		0	
meta	−5.10	13.89	−0.31	(9.1 / 13.6 / 77.3)	-0.23	(34.2 / 45.7 / 20.2)
para	−6.80	12.53	−1.67		-0.41	

$$\frac{[\mathbf{A}]}{[\mathbf{B}]} = e^{-\frac{\Delta\Delta G^{\ddagger}}{RT}} \qquad (\Delta\Delta G^{\ddagger} = \Delta G_A^{\ddagger} - \Delta G_B^{\ddagger})$$

8.3. DFT-optimized structures' energy components

	E(SCF)/(Hartree)	Thermal correction to G /(Hartree)	G(sol)/(kcal/mol)
	6-311++G**/SDD	6-31G**/LanL2DZ	
Pd(DMA)	-415.8457	0.076136	-260899.1356
3ib-o	-641.3715	0.167356	-402361.3459
3ib-m	-641.3735	0.167588	-402362.4893
3ib-p	-641.3731	0.167591	-402362.2454
preRE1-o	-1057.2379	0.272236	-663255.4423
preRE1-m	-1057.2353	0.272717	-663253.5480
preRE1-p	-1057.2338	0.269789	-663254.4133
TS1-o	-1057.2183	0.273792	-663242.1698
TS1-m	-1057.2170	0.273833	-663241.3466
TS1-p	-1057.2151	0.272729	-663240.8479
3kb-o	-1001.7259	0.165703	-628488.0099
3kb-m	-1001.7288	0.165247	-628490.1478
3kb-p	-1001.7286	0.164811	-628490.3188
preRE2-o	-1417.5943	0.269898	-889383.8271
preRE2-m	-1417.5929	0.267948	-889384.1840
preRE2-p	-1417.5906	0.268002	-889382.6549
TS2-o	-1417.5718	0.269988	-889369.6284
TS2-m	-1417.5737	0.270864	-889370.2970
TS2-p	-1417.5723	0.269735	-889370.1230

9. Cartesian Coordinates of Optimized Geometry

1a. Ethoxybenzene

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.05595	-0.21587	0.00000	-0.05216	-0.21646	0.00000	-0.05272	-0.21546	0.00000
6	-0.94827	-1.30006	0.00000	-0.94384	-1.29664	0.00000	-0.94506	-1.29490	0.00000
6	-2.32111	-1.07202	0.00000	-2.31363	-1.06817	0.00000	-2.31316	-1.06828	0.00000
6	-2.82705	0.23477	0.00000	-2.81299	0.23787	0.00000	-2.81683	0.23397	0.00000
6	-1.93644	1.30726	0.00000	-1.92267	1.30667	0.00000	-1.92867	1.30240	0.00000
6	-0.55171	1.09486	0.00000	-0.54063	1.09259	0.00000	-0.54881	1.09101	0.00000
8	1.27238	-0.54208	0.00000	1.27515	-0.55753	0.00000	1.26818	-0.54182	0.00000
6	2.24444	0.50624	0.00000	2.22550	0.50815	0.00000	2.23101	0.50414	0.00000
6	3.61935	-0.13871	0.00000	3.59469	-0.13197	0.00000	3.60739	-0.13740	0.00000
1	-0.54201	-2.30645	0.00000	-0.53385	-2.30265	0.00000	-0.53641	-2.29902	0.00000
1	-3.00145	-1.91901	0.00000	-2.99626	-1.91440	0.00000	-2.99246	-1.91470	0.00000
1	-3.89837	0.40966	0.00000	-3.88465	0.41630	0.00000	-3.88681	0.40889	0.00000
1	-2.31221	2.32671	-0.00001	-2.29763	2.32739	-0.00001	-2.30375	2.32094	-0.00001
1	0.11783	1.94659	0.00000	0.12933	1.94517	0.00000	0.12111	1.94077	0.00000
1	2.10794	1.13659	-0.88988	2.08303	1.13643	-0.88878	2.09574	1.13890	-0.88731
1	2.10794	1.13660	0.88987	2.08302	1.13644	0.88878	2.09574	1.13890	0.88731
1	4.39406	0.63521	0.00000	4.37223	0.63671	0.00000	4.38269	0.63433	0.00000
1	3.75383	-0.76409	0.88751	3.71898	-0.75667	0.88643	3.73990	-0.76368	0.88644
1	3.75383	-0.76409	-0.88751	3.71898	-0.75668	-0.88642	3.73990	-0.76369	-0.88643

$1a_2$.

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.18176	0.00000	0.00000	0.18788	0.00000	0.00000	0.18674	0.00000
6	-0.19003	1.57430	0.00000	-0.20978	1.57574	0.00000	-0.21495	1.57017	0.00000
6	-1.49538	2.07794	0.00000	-1.52269	2.04648	0.00000	-1.52490	2.04701	0.00000
6	-2.56968	1.17894	0.00000	-2.57073	1.12280	0.00000	-2.57393	1.12782	0.00000
6	-2.30719	-0.20444	0.00000	-2.27036	-0.25110	0.00000	-2.28170	-0.24403	0.00000
6	-1.01684	-0.78450	0.00000	-0.97466	-0.81933	0.00000	-0.98646	-0.80814	0.00000
8	1.36704	-0.17660	0.00000	1.37987	-0.13250	0.00000	1.37032	-0.14427	0.00000
6	1.66909	-1.56115	0.00000	1.65963	-1.52037	0.00000	1.67177	-1.51901	0.00000
6	3.18836	-1.69415	0.00000	3.17252	-1.64688	0.00000	3.19182	-1.64731	0.00000
1	0.66969	2.24601	0.00000	0.63860	2.26269	0.00000	0.62998	2.25958	0.00000
1	-1.66592	3.15403	0.00000	-1.72096	3.11962	0.00000	-1.71814	3.11867	0.00000
1	-3.59623	1.55291	0.00000	-3.60667	1.47289	0.00000	-3.60685	1.48246	0.00000
1	-3.18289	-0.86528	0.00000	-3.13916	-0.92655	0.00000	-3.15034	-0.91738	0.00000
1	1.22144	-2.04983	0.87598	1.20930	-2.00848	0.87288	1.22493	-2.01839	0.87125
1	1.22144	-2.04983	-0.87598	1.20930	-2.00848	-0.87288	1.22493	-2.01839	-0.87125
1	3.47906	-2.75314	0.00000	3.47797	-2.69963	0.00000	3.49472	-2.70178	0.00000
1	3.62356	-1.21713	-0.88644	3.59454	-1.16173	-0.88462	3.62415	-1.16513	-0.88431
1	3.62356	-1.21713	0.88644	3.59454	-1.16173	0.88462	3.62415	-1.16513	0.88431

$1a_3$.

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.22133	0.00000	0.00000	0.22197	0.00000	0.00000	0.21888	0.00000
6	-0.21850	1.60394	0.00000	-0.23935	1.59589	0.00000	-0.21019	1.59854	0.00000
6	-1.54176	2.05770	0.00000	-1.56520	2.02605	0.00000	-1.52754	2.05343	0.00000
6	-2.60774	1.14207	0.00000	-2.60522	1.08208	0.00000	-2.58832	1.14210	0.00000
6	-2.44665	-0.26776	0.00000	-2.44635	-0.32782	0.00000	-2.45327	-0.27142	0.00000
6	-1.08157	-0.67443	0.00000	-1.06819	-0.68746	0.00000	-1.08396	-0.66480	0.00000
8	1.35388	-0.15643	0.00000	1.36948	-0.12003	0.00000	1.35038	-0.15934	0.00000
6	1.65835	-1.53567	0.00000	1.66606	-1.49905	0.00000	1.64414	-1.52951	0.00000
6	3.17508	-1.67912	0.00000	3.17730	-1.61999	0.00000	3.16098	-1.67772	0.00000

1	0.63033	2.28387	0.00000	0.60346	2.28569	0.00000	0.64435	2.26973	0.00000
1	-1.73254	3.13533	0.00000	-1.77614	3.10065	0.00000	-1.71051	3.13234	0.00000
1	-3.61849	1.56574	0.00000	-3.62285	1.49890	0.00000	-3.59492	1.58174	0.00000
1	-0.85974	-1.74329	0.00000	-0.81934	-1.75440	0.00000	-0.85264	-1.73469	0.00000
1	1.22615	-2.02680	0.88589	1.23764	-1.99343	0.88395	1.21236	-2.02887	0.88260
1	1.22615	-2.02680	-0.88589	1.23764	-1.99343	-0.88395	1.21236	-2.02887	-0.88260
1	3.45854	-2.73895	0.00000	3.48608	-2.67076	0.00000	3.44872	-2.73522	0.00000
1	3.60764	-1.20302	-0.88673	3.59170	-1.13153	-0.88522	3.59314	-1.19926	-0.88503
1	3.60764	-1.20302	0.88673	3.59170	-1.13153	0.88522	3.59314	-1.19926	0.88503

1a$_4$.

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.11061	-0.21841	0.00000	-0.10375	-0.22102	0.00000	-0.10572	-0.21810	0.00000
6	-1.01646	-1.28345	0.00000	-1.00950	-1.28170	0.00000	-1.01176	-1.27758	0.00000
6	-2.39661	-1.01803	-0.00001	-2.38497	-1.00430	-0.00001	-2.38506	-1.00965	-0.00001
6	-2.98634	0.27656	-0.00001	-2.99247	0.28368	-0.00001	-2.99249	0.27696	-0.00001
6	-2.00271	1.29372	-0.00001	-1.98726	1.28248	-0.00001	-1.99489	1.28162	-0.00001
6	-0.60273	1.08912	-0.00001	-0.58830	1.08610	-0.00001	-0.60030	1.08389	-0.00001
8	1.25103	-0.55973	0.00001	1.25601	-0.57688	0.00001	1.25088	-0.56008	0.00001
6	2.19391	0.48909	0.00001	2.17496	0.49210	0.00001	2.17993	0.48696	0.00001
6	3.58548	-0.13016	0.00001	3.56121	-0.12034	0.00001	3.57449	-0.12629	0.00001
1	-0.62555	-2.30256	0.00001	-0.61495	-2.30037	0.00001	-0.61424	-2.29386	0.00001
1	-3.04748	-1.90054	0.00000	-3.03231	-1.89441	0.00000	-3.02735	-1.90205	0.00000
1	-2.31855	2.34417	-0.00001	-2.29239	2.34028	-0.00001	-2.30024	2.33812	-0.00001
1	0.07050	1.94578	-0.00001	0.08646	1.94251	-0.00001	0.07634	1.93734	-0.00001
1	2.06020	1.13051	-0.88657	2.03379	1.13088	-0.88493	2.04864	1.13473	-0.88346
1	2.06019	1.13051	0.88657	2.03379	1.13089	0.88493	2.04863	1.13473	0.88347
1	4.35288	0.65370	0.00001	4.33247	0.65705	0.00001	4.34352	0.65440	0.00001
1	3.72798	-0.75721	0.88662	3.69275	-0.74689	0.88523	3.71623	-0.75483	0.88504
1	3.72799	-0.75722	-0.88659	3.69276	-0.74690	-0.88521	3.71624	-0.75483	-0.88501

1a$_5$.

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.11436	-0.24018	0.00000	0.11149	-0.23650	0.00000	0.11376	-0.23692	0.00000
6	1.00337	-1.32830	0.00001	1.01094	-1.31476	0.00001	1.00451	-1.31642	0.00001
6	2.41430	-1.20772	0.00000	2.42287	-1.21513	0.00000	2.41684	-1.21476	0.00000
6	2.84970	0.14990	-0.00001	2.82408	0.15242	-0.00001	2.83128	0.14991	-0.00001
6	1.98918	1.25318	-0.00001	1.96760	1.25912	-0.00001	1.97763	1.25063	-0.00001
6	0.59363	1.07483	-0.00001	0.57730	1.07736	-0.00001	0.58687	1.07538	-0.00001
6	-2.18629	0.50468	0.00000	-2.16773	0.50215	0.00000	-2.17146	0.49949	0.00000
1	0.53235	-2.31666	0.00001	0.52779	-2.30161	0.00001	0.51806	-2.30057	0.00001
1	3.92410	0.36736	-0.00001	3.89846	0.38816	-0.00001	3.90553	0.38086	-0.00001
1	2.38747	2.27263	-0.00002	2.36357	2.28012	-0.00002	2.37166	2.27150	-0.00002
1	-0.06882	1.93486	-0.00001	-0.08914	1.93623	-0.00001	-0.07874	1.93168	-0.00001
6	-3.58444	-0.09992	0.00001	-3.55938	-0.09854	0.00001	-3.57131	-0.10186	0.00001
1	-2.04778	1.14488	-0.88721	-2.02417	1.14118	-0.88535	-2.03660	1.14636	-0.88404
1	-2.04778	1.14489	0.88721	-2.02417	1.14119	0.88534	-2.03659	1.14637	0.88404
1	-3.73220	-0.72597	0.88636	-3.69475	-0.72452	0.88499	-3.71703	-0.72968	0.88478
1	-4.34487	0.69104	0.00001	-4.32542	0.68430	0.00001	-4.33513	0.68429	0.00001
1	-3.73221	-0.72598	-0.88634	-3.69475	-0.72453	-0.88497	-3.71703	-0.72969	-0.88476
8	-1.25414	-0.55324	0.00001	-1.25755	-0.57216	0.00001	-1.25036	-0.55422	0.00001

1a$_6$.

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.10677	-0.30039	0.00000	-0.11317	-0.30565	0.00000	-0.11222	-0.29987	0.00000
6	-0.94615	-1.42899	0.00000	-0.93216	-1.44845	0.00000	-0.93530	-1.43956	0.00000

6	-2.31440	-1.09082	0.00000	-2.29539	-1.08170	0.00000	-2.29918	-1.08457	0.00000
6	-2.82089	0.22736	-0.00001	-2.80392	0.23253	-0.00001	-2.80731	0.22630	-0.00001
6	-1.92614	1.29664	-0.00001	-1.90948	1.29809	-0.00001	-1.91949	1.29435	-0.00001
6	-0.54371	1.03576	-0.00001	-0.53273	1.03648	-0.00001	-0.54264	1.03287	-0.00001
6	2.19886	0.47415	0.00000	2.17648	0.48033	0.00000	2.18243	0.47300	0.00000
1	-3.05854	-1.89696	0.00000	-3.05186	-1.88113	0.00000	-3.05252	-1.88520	0.00000
1	-3.89772	0.41421	-0.00001	-3.88099	0.42343	-0.00001	-3.88345	0.41499	-0.00001
1	-2.28080	2.32670	-0.00002	-2.26388	2.33026	-0.00002	-2.27391	2.32395	-0.00002
1	0.14214	1.88253	-0.00001	0.15564	1.88107	-0.00001	0.14372	1.87820	-0.00001
6	3.60372	-0.11912	0.00001	3.57363	-0.11117	0.00001	3.58968	-0.11564	0.00001
1	2.06272	1.11872	0.88692	2.03701	1.12400	0.88490	2.05068	1.12506	0.88357
1	2.06272	1.11871	-0.88692	2.03702	1.12399	-0.88489	2.05068	1.12506	-0.88357
1	3.75333	-0.74592	-0.88547	3.71019	-0.73794	-0.88419	3.73855	-0.74384	-0.88409
1	4.36042	0.67644	0.00001	4.33790	0.67430	0.00001	4.34915	0.67562	0.00001
1	3.75332	-0.74591	0.88549	3.71018	-0.73794	0.88422	3.73854	-0.74384	0.88411
8	1.27941	-0.58952	0.00001	1.27866	-0.60036	0.00001	1.27535	-0.58642	0.00001

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Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.45351	-0.27167	0.00000	-0.45451	-0.27129	0.00000	-0.45501	-0.27171	0.00000
6	0.49627	-1.30545	-0.00001	0.49389	-1.30182	-0.00001	0.49498	-1.30034	-0.00001
6	1.85428	-1.00144	-0.00001	1.84913	-0.99909	-0.00001	1.84826	-0.99737	-0.00001
6	2.28695	0.33150	-0.00001	2.27680	0.33221	-0.00001	2.27828	0.33108	-0.00001
6	1.33866	1.35325	0.00000	1.32998	1.35115	0.00000	1.33218	1.34851	0.00000
6	-0.03225	1.06424	0.00000	-0.03844	1.06219	0.00000	-0.03373	1.06013	0.00000
8	-1.76263	-0.67058	0.00000	-1.76126	-0.68417	0.00000	-1.75670	-0.67128	0.00001
1	0.14608	-2.33264	-0.00001	0.13894	-2.32850	-0.00001	0.14277	-2.32558	-0.00001
1	2.58061	-1.80930	-0.00001	2.57679	-1.80689	-0.00001	2.57390	-1.80437	-0.00001
1	3.34696	0.56524	-0.00001	3.33720	0.56848	-0.00001	3.33683	0.56534	-0.00001
1	1.65751	2.39188	0.00000	1.64900	2.39068	0.00000	1.64990	2.38634	0.00000
6	-2.77696	0.32523	0.00001	-2.75428	0.33330	0.00001	-2.76124	0.32388	0.00001
1	-3.72441	-0.21523	0.00001	-3.70864	-0.19182	0.00001	-3.71492	-0.20669	0.00001
1	-2.71892	0.95673	0.89567	-2.68258	0.96201	0.89413	-2.70336	0.95964	0.89308
1	-2.71893	0.95674	-0.89564	-2.68259	0.96201	-0.89410	-2.70336	0.95964	-0.89306
1	-0.74846	1.87726	0.00001	-0.75338	1.87750	0.00001	-0.75053	1.87089	0.00001

$1b_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.48074	0.00000	0.00000	0.47764	0.00000	0.00000	0.48074	0.00000
6	-1.36004	0.12532	0.00000	-1.36214	0.13798	0.00000	-1.35692	0.13508	0.00000
6	-1.70308	-1.23122	0.00000	-1.70768	-1.21335	0.00000	-1.70689	-1.21442	0.00000
6	-0.68201	-2.19032	0.00000	-0.69009	-2.17047	0.00000	-0.69241	-2.17166	0.00000
6	0.66016	-1.76401	0.00000	0.64964	-1.74252	0.00000	0.64563	-1.75042	0.00000
6	1.07993	-0.41324	0.00000	1.09327	-0.39935	0.00000	1.08325	-0.40745	0.00000
8	0.19461	1.87935	0.00000	0.19070	1.87935	0.00000	0.20136	1.87457	0.00000
1	-2.13052	0.89765	0.00000	-2.12604	0.91785	0.00000	-2.12405	0.91021	0.00000
1	-2.75098	-1.52970	0.00000	-2.75759	-1.51131	0.00000	-2.75539	-1.50871	0.00000
1	-0.93052	-3.25425	0.00000	-0.94175	-3.23467	0.00000	-0.94757	-3.23358	0.00000
1	1.42127	-2.55421	0.00000	1.40359	-2.54433	0.00000	1.39843	-2.55134	0.00000
6	1.53612	2.33060	0.00000	1.54922	2.27277	0.00000	1.54508	2.28846	0.00000
1	1.47609	3.42698	0.00000	1.53231	3.36992	0.00000	1.52269	3.38813	0.00000
1	2.08565	1.97570	0.88107	2.08530	1.89575	0.87709	2.09426	1.91840	0.87584
1	2.08565	1.97570	-0.88107	2.08530	1.89575	-0.87709	2.09426	1.91840	-0.87584

$1b_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z

6	0.00000	0.47460	0.00000	0.00000	0.47542	0.00000	0.00000	0.47331	0.00000
6	-1.37412	0.20698	0.00000	-1.37018	0.21451	0.00000	-1.37049	0.20884	0.00000
6	-1.78010	-1.13163	0.00000	-1.77997	-1.11771	0.00000	-1.77271	-1.12549	0.00000
6	-0.82690	-2.16431	0.00000	-0.82036	-2.14335	0.00000	-0.82016	-2.14958	0.00000
6	0.57639	-1.95350	0.00000	0.58688	-1.96296	0.00000	0.58696	-1.95902	0.00000
6	0.93372	-0.57397	0.00000	0.92515	-0.57919	0.00000	0.92548	-0.57485	0.00000
8	0.32893	1.84083	0.00000	0.32012	1.84895	0.00000	0.32464	1.83723	0.00000
1	-2.08391	1.03098	0.00000	-2.07294	1.04655	0.00000	-2.07499	1.03616	0.00000
1	-2.85025	-1.36092	0.00000	-2.85125	-1.34504	0.00000	-2.84356	-1.35107	0.00000
1	-1.21445	-3.18950	0.00000	-1.22172	-3.16723	0.00000	-1.21993	-3.17271	0.00000
1	1.99403	-0.31443	0.00000	1.98831	-0.31502	0.00000	1.98542	-0.30139	0.00000
6	1.69593	2.18093	0.00000	1.69510	2.15169	0.00000	1.68287	2.16896	0.00000
1	1.74069	3.27525	0.00000	1.76496	3.24375	0.00000	1.74142	3.26446	0.00000
1	2.21644	1.79871	0.89079	2.20598	1.75749	0.88820	2.21141	1.78682	0.88723
1	2.21644	1.79871	-0.89079	2.20598	1.75749	-0.88820	2.21141	1.78682	-0.88723

$1b_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.40425	-0.27146	0.00000	0.40879	-0.27239	0.00000	0.40799	-0.27090	0.00000
6	-0.55925	-1.28475	0.00000	-0.55258	-1.28313	0.00000	-0.55479	-1.27906	0.00000
6	-1.92246	-0.94296	-0.00001	-1.91129	-0.93290	-0.00001	-1.91138	-0.93586	-0.00001
6	-2.43918	0.38252	-0.00001	-2.44956	0.38557	-0.00002	-2.44725	0.38208	-0.00001
6	-1.40091	1.34353	-0.00001	-1.39262	1.32921	-0.00001	-1.39617	1.33035	-0.00001
6	-0.01421	1.06121	0.00000	-0.00599	1.05850	0.00000	-0.01440	1.05606	0.00000
8	1.74448	-0.68735	0.00001	1.74653	-0.70039	0.00001	1.74360	-0.68683	0.00001
1	-0.22551	-2.32398	0.00000	-0.21291	-2.32137	0.00000	-0.21378	-2.31567	0.00000
1	-2.62146	-1.78783	-0.00001	-2.60510	-1.78733	-0.00002	-2.60203	-1.79117	-0.00001
1	-1.65791	2.40989	-0.00001	-1.64080	2.40187	-0.00001	-1.64352	2.40177	-0.00001
1	0.70587	1.87891	0.00000	0.71267	1.87839	0.00001	0.70808	1.87104	0.00000
6	2.73257	0.31374	0.00001	2.70840	0.32637	0.00001	2.71641	0.31489	0.00001
1	3.69734	-0.20389	0.00002	3.68322	-0.16933	0.00002	3.69126	-0.18675	0.00002
1	2.67050	0.95735	-0.89154	2.62988	0.96675	-0.88921	2.65438	0.96502	-0.88808
1	2.67049	0.95735	0.89157	2.62988	0.96676	0.88923	2.65436	0.96501	0.88811

$1b_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.40244	-0.28477	0.00000	0.40243	-0.28125	0.00000	0.40118	-0.28265	0.00000
6	-0.53522	-1.33148	-0.00001	-0.54634	-1.31669	-0.00001	-0.53966	-1.31903	-0.00001
6	-1.93904	-1.14600	-0.00001	-1.95214	-1.15230	-0.00001	-1.94564	-1.15067	-0.00001
6	-2.31219	0.23012	-0.00001	-2.29008	0.23230	-0.00001	-2.29517	0.23213	-0.00001
6	-1.40233	1.29290	0.00000	-1.38353	1.29821	0.00000	-1.39054	1.29127	0.00000
6	-0.01630	1.05058	0.00000	-0.00300	1.05255	0.00000	-0.00957	1.05034	0.00000
8	1.75488	-0.65919	0.00000	1.75316	-0.68020	0.00000	1.74844	-0.66412	0.00001
1	-0.11012	-2.34037	-0.00001	-0.10914	-2.32472	-0.00001	-0.10019	-2.32504	-0.00001
1	-3.37562	0.49610	-0.00001	-3.35251	0.51726	-0.00001	-3.35736	0.51354	-0.00001
1	-1.75354	2.32955	0.00000	-1.73201	2.33642	0.00000	-1.73591	2.32964	0.00000
1	0.68489	1.87933	0.00001	0.70140	1.88056	0.00001	0.69577	1.87423	0.00001
6	2.72250	0.36140	0.00001	2.69900	0.35928	0.00001	2.70505	0.35309	0.00001
1	3.69865	-0.13480	0.00001	3.68241	-0.11967	0.00001	3.68915	-0.13034	0.00001
1	2.64884	1.00361	-0.89214	2.61326	0.99958	-0.88956	2.63354	1.00204	-0.88860
1	2.64883	1.00360	0.89217	2.61325	0.99958	0.88958	2.63354	1.00203	0.88862

$1b_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.53772	0.00000	0.00000	0.53313	0.00000	0.00000	0.53195	0.00000
6	-1.40615	0.56157	0.00000	-1.40457	0.60693	0.00000	-1.40502	0.58607	0.00000

6	-1.97448	-0.72782	0.00000	-1.97064	-0.68601	0.00000	-1.96673	-0.70621	0.00000
6	-1.23971	-1.93404	0.00000	-1.26289	-1.90475	0.00000	-1.24795	-1.91474	0.00000
6	0.15331	-1.87838	0.00000	0.12773	-1.87248	0.00000	0.14023	-1.87422	0.00000
6	0.79145	-0.62428	0.00000	0.78434	-0.63422	0.00000	0.78352	-0.62892	0.00000
8	0.61540	1.81220	0.00000	0.63749	1.80294	0.00000	0.62817	1.80113	0.00000
1	-3.06731	-0.82478	0.00000	-3.06760	-0.77666	0.00000	-3.06162	-0.80568	0.00000
1	-1.74942	-2.90085	0.00000	-1.78723	-2.86478	0.00000	-1.76297	-2.87833	0.00000
1	0.75229	-2.78839	0.00000	0.71193	-2.79433	0.00000	0.73223	-2.78820	0.00000
1	1.88088	-0.59931	0.00000	1.87387	-0.62699	0.00000	1.87230	-0.61066	0.00000
6	2.01745	1.87672	0.00000	2.04057	1.81195	0.00000	2.02000	1.84576	0.00000
1	2.28183	2.94026	0.00000	2.34152	2.86474	0.00000	2.31077	2.90434	0.00000
1	2.46364	1.40331	0.89164	2.47019	1.32362	0.88874	2.46984	1.36563	0.88779
1	2.46364	1.40331	-0.89164	2.47019	1.32362	-0.88874	2.46984	1.36563	-0.88779

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Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.91577	0.00000	-0.01178	0.91266	-0.00005	0.01633	0.91139	0.00001	-0.01043
6	0.19500	-1.20354	-0.00913	0.19591	-1.20157	0.00831	0.19373	-1.19974	-0.00840
6	-1.20234	-1.20660	0.00212	-1.19839	-1.20494	-0.00201	-1.19859	-1.20268	0.00204
6	-1.90737	0.00000	0.00868	-1.90063	0.00003	-0.00913	-1.90098	0.00000	0.00808
6	-1.20235	1.20659	0.00212	-1.19831	1.20498	-0.00202	-1.19860	1.20268	0.00204
6	0.19499	1.20354	-0.00913	0.19595	1.20154	0.00832	0.19372	1.19974	-0.00840
6	2.42751	0.00000	0.00966	2.41785	-0.00001	-0.01170	2.42081	0.00000	0.00847
1	0.73393	-2.14812	-0.01810	0.73683	-2.14634	0.01803	0.73336	-2.14256	-0.01708
1	-1.73938	-2.15117	0.00177	-1.73678	-2.14962	-0.00300	-1.73502	-2.14620	0.00111
1	-2.99349	-0.00001	0.01433	-2.98760	0.00006	-0.01451	-2.98586	-0.00001	0.01299
1	-1.73939	2.15116	0.00177	-1.73667	2.14969	-0.00302	-1.73504	2.14619	0.00111
1	0.73392	2.14813	-0.01810	0.73693	2.14628	0.01806	0.73335	2.14256	-0.01708
1	2.83477	0.88580	-0.48777	2.82137	0.88506	0.48771	2.82742	0.88571	-0.48846
1	2.80760	-0.00032	1.03926	2.82144	-0.88468	0.48835	2.80550	-0.00032	1.03598
1	2.83477	-0.88549	-0.48832	2.79423	-0.00035	-1.04020	2.82743	-0.88540	-0.48900

$1c_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.90103	0.06941	0.00000	0.88710	0.06613	0.00000	0.88896	0.06803	0.00000
6	0.21767	-1.16063	0.00000	0.20895	-1.16503	0.00000	0.21079	-1.15754	0.00000
6	-1.18520	-1.19962	0.00000	-1.18854	-1.19460	0.00000	-1.18589	-1.19548	0.00000
6	-1.88615	0.00979	0.00000	-1.87714	0.01767	0.00000	-1.87697	0.01337	0.00000
6	-1.17279	1.22417	0.00000	-1.14963	1.22187	0.00000	-1.15999	1.21833	0.00000
6	0.23835	1.33037	0.00000	0.26172	1.34790	0.00000	0.25007	1.34284	0.00000
6	2.42447	0.04786	0.00000	2.40478	0.03355	0.00000	2.41272	0.03726	0.00000
1	0.77379	-2.10317	0.00000	0.76334	-2.11015	0.00000	0.76434	-2.10175	0.00000
1	-1.71165	-2.15376	0.00000	-1.72472	-2.14557	0.00000	-1.71521	-2.14741	0.00000
1	-2.97995	0.00601	0.00000	-2.97199	0.02143	0.00000	-2.97080	0.01030	0.00000
1	-1.77426	2.14157	0.00000	-1.75879	2.13923	0.00000	-1.77190	2.13213	0.00000
1	2.81709	0.57771	0.87795	2.79904	0.55949	0.87711	2.81570	0.56474	0.87517
1	2.83366	-0.97408	0.00001	2.81068	-0.98888	0.00001	2.82405	-0.98357	0.00001
1	2.81709	0.57769	-0.87796	2.79904	0.55946	-0.87712	2.81570	0.56472	-0.87518

$1c_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.87538	-0.00210	0.01015	0.87226	-0.00193	0.01807	0.86959	-0.00054	0.00007
6	0.13422	-1.19461	0.00945	0.14334	-1.19543	0.01117	0.13938	-1.19467	0.00007
6	-1.26444	-1.12492	-0.00049	-1.25087	-1.13353	-0.00127	-1.25309	-1.12633	0.00000
6	-1.90936	0.12400	-0.01078	-1.89077	0.11705	-0.01386	-1.89568	0.11754	-0.00009
6	-1.23563	1.37440	-0.00224	-1.24866	1.38529	-0.00320	-1.24554	1.38069	-0.00002

6	0.17715	1.22291	0.01092	0.16094	1.21452	0.01266	0.16546	1.21362	0.00009
6	2.39203	-0.04353	-0.01144	2.38149	-0.03108	-0.01649	2.38423	-0.03376	-0.00008
1	0.64289	-2.16025	0.01813	0.66099	-2.15836	0.02286	0.65347	-2.15637	0.00013
1	-1.84795	-2.05082	0.00269	-1.83124	-2.06232	0.00242	-1.83083	-2.05572	0.00006
1	-3.00603	0.10603	-0.02229	-2.99102	0.08172	-0.02718	-2.99468	0.08204	-0.00019
1	0.80389	2.12491	0.02562	0.79681	2.11593	0.03231	0.80314	2.11204	0.00022
1	2.81325	0.93103	0.26442	2.79793	0.87814	0.43268	2.79467	0.98307	0.00180
1	2.79342	-0.79208	0.68666	2.78367	-0.89102	0.53456	2.79410	-0.55388	0.87881
1	2.78440	-0.29569	-1.00867	2.77644	-0.09348	-1.04015	2.79403	-0.55050	-0.88102

1c$_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.87700	-0.00001	0.01392	0.87726	-0.00009	0.02007	0.87496	0.00000	0.01240
6	0.14181	-1.19494	0.01010	0.14589	-1.19236	0.00954	0.14093	-1.18994	0.00885
6	-1.26507	-1.17559	-0.00365	-1.25857	-1.16211	-0.00387	-1.25863	-1.16529	-0.00347
6	-2.06169	0.00000	-0.01156	-2.07778	0.00008	-0.01236	-2.07210	0.00000	-0.01031
6	-1.26506	1.17560	-0.00365	-1.25841	1.16220	-0.00386	-1.25862	1.16530	-0.00347
6	0.14181	1.19494	0.01010	0.14602	1.19231	0.00952	0.14093	1.18994	0.00885
6	2.39168	0.00000	-0.01198	2.38420	-0.00004	-0.01453	2.38648	0.00000	-0.01044
1	0.67908	-2.15003	0.02149	0.68594	-2.14700	0.02217	0.68335	-2.14189	0.01944
1	-1.75893	-2.15526	-0.00224	-1.74531	-2.14985	-0.00331	-1.74326	-2.15249	-0.00143
1	-1.75891	2.15526	-0.00224	-1.74505	2.14999	-0.00332	-1.74325	2.15249	-0.00143
1	0.67909	2.15003	0.02149	0.68615	2.14691	0.02224	0.68335	2.14189	0.01944
1	2.80187	0.88622	0.49036	2.79270	0.88513	0.48783	2.79821	0.88550	0.49137
1	2.80181	-0.88693	0.48916	2.79278	-0.88588	0.48657	2.79814	-0.88618	0.49022
1	2.79308	0.00068	-1.03771	2.78105	0.00074	-1.03923	2.79977	0.00066	-1.03201

1c$_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.87538	0.00210	0.01015	0.87224	0.00186	0.01810	0.86959	0.00054	0.00007
6	0.17715	-1.22291	0.01092	0.16090	-1.21454	0.01266	0.16546	-1.21362	0.00009
6	-1.23563	-1.37440	-0.00224	-1.24869	-1.38522	-0.00320	-1.24554	-1.38069	-0.00002
6	-1.90936	-0.12400	-0.01078	-1.89078	-0.11698	-0.01388	-1.89568	-0.11754	-0.00009
6	-1.26444	1.12492	-0.00049	-1.25081	1.13351	-0.00129	-1.25309	1.12633	0.00000
6	0.13422	1.19461	0.00945	0.14339	1.19538	0.01120	0.13938	1.19467	0.00007
6	2.39203	0.04353	-0.01144	2.38148	0.03108	-0.01652	2.38423	0.03376	-0.00008
1	0.80389	-2.12491	0.02562	0.79669	-2.11598	0.03231	0.80314	-2.11204	0.00022
1	-3.00603	-0.10603	-0.02229	-2.99101	-0.08162	-0.02712	-2.99468	-0.08204	-0.00019
1	-1.84795	2.05082	0.00269	-1.83113	2.06231	0.00233	-1.83083	2.05572	0.00006
1	0.64289	2.16025	0.01813	0.66103	2.15828	0.02294	0.65347	2.15637	0.00013
1	2.79342	0.79208	0.68666	2.78351	0.89116	0.53441	2.79410	0.55388	0.87881
1	2.81325	-0.93103	0.26442	2.79798	-0.87801	0.43282	2.79467	-0.98307	0.00180
1	2.78440	0.29569	-1.00867	2.77653	0.09338	-1.04013	2.79403	0.55050	-0.88102

1c$_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.90100	-0.06963	0.00000	0.88710	-0.06612	0.00000	0.88896	-0.06803	0.00000
6	0.23822	-1.33049	0.00000	0.26171	-1.34791	0.00000	0.25007	-1.34284	0.00000
6	-1.17291	-1.22409	-0.00001	-1.14962	-1.22189	-0.00001	-1.15999	-1.21833	-0.00001
6	-1.88612	-0.00962	-0.00001	-1.87715	-0.01766	-0.00001	-1.87697	-0.01337	-0.00001
6	-1.18504	1.19970	-0.00001	-1.18855	1.19459	0.00000	-1.18589	1.19548	0.00000
6	0.21778	1.16052	0.00000	0.20897	1.16503	0.00000	0.21079	1.15754	0.00000
6	2.42445	-0.04786	0.00001	2.40477	-0.03355	0.00001	2.41272	-0.03726	0.00001
1	-1.77454	-2.14138	-0.00001	-1.75878	-2.13924	-0.00001	-1.77190	-2.13213	-0.00001
1	-2.97992	-0.00567	-0.00001	-2.97199	-0.02142	-0.00001	-2.97080	-0.01031	-0.00001
1	-1.71140	2.15390	-0.00001	-1.72474	2.14557	0.00000	-1.71521	2.14741	-0.00001

1	0.77432	2.10284	0.00000	0.76336	2.11016	0.00001	0.76434	2.10175	0.00001
1	2.83300	0.97427	-0.00001	2.81069	0.98888	-0.00002	2.82406	0.98357	-0.00001
1	2.81711	-0.57758	0.87802	2.79902	-0.55945	0.87715	2.81569	-0.56470	0.87520
1	2.81712	-0.57762	-0.87797	2.79902	-0.55952	-0.87708	2.81570	-0.56476	-0.87514

1d. Ethylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.435834	-0.000017	-0.327316	-0.439665	0.000000	-0.343636	-0.433717	0.000000	-0.326775
6	0.270804	-1.203720	-0.184750	0.260245	-1.202342	-0.191883	0.269649	-1.200017	-0.184359
6	1.639636	-1.207054	0.095929	1.624656	-1.205744	0.095359	1.633547	-1.203193	0.095754
6	2.329552	0.000017	0.238530	2.310798	0.000000	0.241757	2.320937	0.000000	0.237434
6	1.639610	1.207072	0.095914	1.624656	1.205744	0.095359	1.633547	1.203192	0.095754
6	0.270779	1.203703	-0.184765	0.260245	1.202342	-0.191882	0.269649	1.200017	-0.184359
6	-1.927478	-0.000021	-0.591338	-1.924486	0.000000	-0.592125	-1.922276	0.000000	-0.592817
1	-0.256243	-2.148359	-0.299572	-0.269176	-2.146741	-0.310389	-0.258466	-2.142691	-0.299116
1	2.167408	-2.151304	0.198351	2.153185	-2.149998	0.202731	2.160818	-2.146331	0.198176
1	3.394303	0.000035	0.453204	3.375117	0.000000	0.462913	3.384404	0.000000	0.452155
1	2.167367	2.151331	0.198323	2.153186	2.149998	0.202732	2.160818	2.146331	0.198176
1	-0.256291	2.148329	-0.299600	-0.269176	2.146741	-0.310388	-0.258466	2.142691	-0.299115
6	-2.768626	0.000015	0.699261	-2.717832	0.000000	0.716329	-2.756955	0.000000	0.699926
1	-2.191194	0.878888	-1.192213	-2.196242	0.879228	-1.187562	-2.187293	0.878560	-1.192337
1	-2.191199	-0.878958	-1.192172	-2.196242	-0.879227	-1.187563	-2.187293	-0.878559	-1.192338
1	-3.839480	0.000015	0.467218	-3.795595	0.000000	0.527477	-3.828437	0.000000	0.475481
1	-2.552670	-0.883967	1.308864	-2.473380	-0.883612	1.312193	-2.536187	-0.883201	1.307788
1	-2.552660	0.884029	1.308813	-2.473380	0.883611	1.312194	-2.536187	0.883200	1.307789

$1d_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.41710	-0.05043	-0.30841	-0.41321	-0.12860	-0.28514	-0.39455	-0.23044	0.00000
6	0.34603	-1.21412	-0.09637	0.40541	-1.24609	-0.04901	0.55870	-1.26156	0.00000
6	1.72088	-1.12880	0.16640	1.77099	-1.07170	0.18933	1.92097	-0.97052	0.00000
6	2.31319	0.13743	0.21488	2.28524	0.22514	0.18878	2.31027	0.37031	0.00000
6	1.52299	1.28232	0.00030	1.42200	1.30946	-0.05022	1.33105	1.36870	0.00000
6	0.13430	1.26281	-0.27523	0.03134	1.22461	-0.30388	-0.07130	1.15177	0.00000
6	-1.91276	-0.20513	-0.56515	-1.89746	-0.36270	-0.50714	-1.86455	-0.67402	0.00000
1	-0.12658	-2.20053	-0.13874	-0.01507	-2.25783	-0.05244	0.24143	-2.31000	-0.00001
1	2.31136	-2.03084	0.32463	2.41830	-1.93153	0.37142	2.66023	-1.77047	0.00000
1	3.38479	0.22965	0.41353	3.35220	0.38622	0.37267	3.37398	0.62381	0.00000
1	2.04195	2.24758	0.04653	1.89663	2.30249	-0.03935	1.70491	2.40261	0.00001
6	-2.76649	0.19197	0.65197	-2.71272	0.29234	0.60498	-2.87543	0.47346	0.00000
1	-2.18765	0.44627	-1.40536	-2.18726	0.09260	-1.46315	-2.06033	-1.32108	-0.87245
1	-2.15339	-1.24054	-0.85676	-2.12983	-1.43752	-0.57298	-2.06033	-1.32109	0.87243
1	-3.84384	0.14315	0.43243	-3.79556	0.24951	0.42361	-3.90832	0.09291	0.00000
1	-2.56188	-0.46665	1.50661	-2.50529	-0.19145	1.56616	-2.72126	1.11855	0.86902
1	-2.51099	1.21559	0.94679	-2.38363	1.33280	0.66786	-2.72126	1.11857	-0.86900

$1d_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.39140	-0.01356	-0.32807	0.39540	-0.00092	-0.34613	0.36408	0.26326	-0.00001
6	-0.32242	1.18792	-0.19455	-0.31304	1.19553	-0.19285	-0.61068	1.26985	0.00001
6	-1.69174	1.13566	0.09568	-1.67545	1.13643	0.10361	-1.95525	0.90947	0.00001
6	-2.33233	-0.10547	0.25069	-2.30048	-0.11341	0.25060	-2.31784	-0.44318	0.00000
6	-1.68779	-1.36569	0.12058	-1.67749	-1.38440	0.11351	-1.41232	-1.53508	-0.00002
6	-0.30615	-1.23105	-0.17700	-0.30094	-1.21696	-0.19058	-0.06377	-1.07326	-0.00002
6	1.88635	0.00593	-0.58979	1.88320	0.02164	-0.59158	1.82800	0.69240	-0.00002
1	0.18424	2.14658	-0.31985	0.19465	2.15641	-0.31456	-0.31308	2.31947	0.00002

1	-2.25598	2.06797	0.19479	-2.24388	2.06568	0.21520	-2.71644	1.69587	0.00002
1	-3.40426	-0.07431	0.48102	-3.37469	-0.07533	0.48777	-3.39870	-0.64424	0.00000
1	0.29529	-2.14087	-0.31192	0.31718	-2.11947	-0.33818	0.73057	-1.82927	-0.00003
6	2.73478	0.03352	0.69704	2.68211	0.01069	0.71400	2.87328	-0.42780	0.00004
1	2.16508	-0.88312	-1.17328	2.16968	-0.85184	-1.19314	2.01834	1.33898	-0.87178
1	2.15015	0.87998	-1.20467	2.16038	0.91110	-1.17611	2.01832	1.33905	0.87169
1	3.81184	0.03434	0.47415	3.76671	0.01603	0.54176	3.89005	-0.01381	0.00004
1	2.50796	0.92604	1.29216	2.42369	0.88549	1.31842	2.76896	-1.06999	0.88034
1	2.51314	-0.84018	1.32010	2.42645	-0.87963	1.29532	2.76899	-1.07005	-0.88023

1d$_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.39124	-0.00003	-0.32727	-0.39867	-0.00005	-0.34736	-0.36781	-0.28523	0.00000
6	0.32883	-1.19575	-0.17687	0.31395	-1.19372	-0.18607	0.63079	-1.26801	-0.00001
6	1.70406	-1.17649	0.11634	1.68557	-1.16331	0.11432	1.98317	-0.91882	-0.00001
6	2.48312	0.00004	0.27954	2.48468	0.00005	0.28977	2.50353	0.40615	-0.00001
6	1.70402	1.17652	0.11630	1.68548	1.16337	0.11426	1.43929	1.34332	0.00000
6	0.32878	1.19572	-0.17691	0.31389	1.19370	-0.18615	0.06874	1.04192	0.00000
6	-1.88260	-0.00006	-0.59506	-1.88367	-0.00012	-0.59619	-1.83013	-0.70086	0.00000
1	-0.19569	-2.15064	-0.29714	-0.21361	-2.14770	-0.31042	0.32801	-2.32140	-0.00001
1	2.18945	-2.15554	0.21252	2.16333	-2.15023	0.21333	2.68478	-1.76569	-0.00001
1	2.18937	2.15560	0.21245	2.16319	2.15031	0.21322	1.67586	2.41740	0.00000
1	-0.19577	2.15059	-0.29721	-0.21370	2.14766	-0.31056	-0.66382	1.85215	0.00001
6	-2.74405	0.00004	0.68414	-2.68931	0.00009	0.70567	-2.85904	0.43459	0.00001
1	-2.15082	0.88084	-1.19695	-2.16296	0.88073	-1.19097	-2.03112	-1.34424	-0.87145
1	-2.15081	-0.88106	-1.19680	-2.16298	-0.88118	-1.19067	-2.03112	-1.34424	0.87145
1	-3.81884	0.00002	0.45032	-3.77261	0.00013	0.52623	-3.88207	0.03780	0.00001
1	-2.52620	-0.88309	1.29584	-2.43613	-0.88234	1.30027	-2.74591	1.07493	0.88131
1	-2.52621	0.88327	1.29570	-2.43599	0.88261	1.30008	-2.74591	1.07493	-0.88129

1d$_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.39140	-0.01356	0.32807	0.39541	-0.00157	0.34613	0.36168	-0.29121	0.00001
6	-0.30615	-1.23105	0.17700	-0.30145	-1.21722	0.19010	-0.61562	-1.30392	-0.00001
6	-1.68779	-1.36569	-0.12058	-1.67809	-1.38399	-0.11410	-2.02249	-1.13443	-0.00003
6	-2.33233	-0.10547	-0.25069	-2.30055	-0.11274	-0.25067	-2.35413	0.25094	-0.00001
6	-1.69174	1.13566	-0.09568	-1.67499	1.13680	-0.10316	-1.43638	1.30285	0.00001
6	-0.32242	1.18792	0.19455	-0.31259	1.19526	0.19336	-0.06300	1.03963	0.00002
6	1.88635	0.00593	0.58979	1.88322	0.02019	0.59158	1.83501	-0.67919	0.00003
1	0.29529	-2.14087	0.31192	0.31631	-2.12003	0.33732	-0.20997	-2.32903	-0.00003
1	-3.40426	-0.07431	-0.48102	-3.37474	-0.07410	-0.48780	-3.41359	0.54520	-0.00002
1	-2.25598	2.06797	-0.19479	-2.24304	2.06633	-0.21435	-1.77455	2.34347	0.00002
1	0.18424	2.14658	0.31985	0.19540	2.15590	0.31550	0.65064	1.86051	0.00004
6	2.73478	0.03352	-0.69704	2.68218	0.01177	-0.71400	2.85012	0.46846	-0.00002
1	2.15015	0.87998	1.20467	2.16062	0.90839	1.17793	2.03845	-1.32087	0.87102
1	2.16508	-0.88312	1.17328	2.16953	-0.85458	1.19134	2.03845	-1.32094	-0.87091
1	3.81184	0.03434	-0.47415	3.76676	0.01694	-0.54168	3.87925	0.08729	-0.00002
1	2.51315	-0.84018	-1.32010	2.42672	-0.87751	-1.29698	2.73009	1.10779	-0.88184
1	2.50796	0.92604	-1.29216	2.42366	0.88764	-1.31683	2.73011	1.10785	0.88176

1d$_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.417099	0.050423	-0.308429	-0.413196	0.128491	-0.285059	-0.409496	0.127075	-0.271861
6	0.134301	-1.262816	-0.275222	0.031419	-1.224707	-0.303735	0.050304	-1.221304	-0.293852
6	1.522992	-1.282311	0.000311	1.422124	-1.309445	-0.050152	1.440669	-1.308221	-0.047277
6	2.313190	-0.137424	0.214882	2.285341	-0.225056	0.188685	2.295729	-0.221563	0.184077

6	1.720872	1.128800	0.166397	1.770987	1.071761	0.189276	1.779082	1.072150	0.187554
6	0.346024	1.214112	-0.096366	0.405363	1.246051	-0.048925	0.411023	1.237979	-0.042233
6	-1.912756	0.205117	-0.565157	-1.897435	0.362670	-0.507147	-1.899331	0.363040	-0.505203
1	2.041951	-2.247573	0.046547	1.896808	-2.302459	-0.039204	1.917090	-2.298774	-0.037866
1	3.384795	-0.229633	0.413518	3.352357	-0.386057	0.372434	3.363769	-0.376444	0.360297
1	2.311353	2.030847	0.324624	2.418255	1.931643	0.371315	2.421137	1.933953	0.363708
1	-0.126594	2.200520	-0.138727	-0.015182	2.257778	-0.052286	-0.008613	2.248615	-0.042007
6	-2.766487	-0.191958	0.651968	-2.712936	-0.292315	0.604838	-2.755023	-0.292916	0.588305
1	-2.153384	1.240526	-0.856774	-2.129693	1.437523	-0.572913	-2.129829	1.438151	-0.571598
1	-2.187656	-0.446288	-1.405360	-2.187203	-0.092488	-1.463252	-2.184233	-0.085020	-1.468060
1	-3.843830	-0.143141	0.432448	-3.795759	-0.249014	0.423450	-3.831193	-0.251886	0.365758
1	-2.510993	-1.215580	0.946806	-2.384244	-1.332897	0.667672	-2.435203	-1.337011	0.672925
1	-2.561865	0.466660	1.506613	-2.505341	0.191275	1.566099	-2.590666	0.190988	1.559778

1e. Isopropylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.13843	-0.19461	0.00000	-0.14386	-0.20375	0.00000	-0.13711	-0.19586	0.00000
6	0.75153	-1.27800	0.00000	0.74868	-1.28058	0.00000	0.75085	-1.27453	0.00000
6	2.13589	-1.07996	0.00000	2.12849	-1.07310	0.00000	2.12987	-1.07514	0.00000
6	2.65779	0.21508	0.00000	2.63884	0.22387	0.00000	2.64829	0.21618	0.00000
6	1.78359	1.30656	0.00000	1.76022	1.30838	0.00000	1.77595	1.30292	0.00000
6	0.40240	1.10173	0.00000	0.38331	1.09475	0.00000	0.39982	1.09715	0.00000
6	-1.64419	-0.42791	0.00000	-1.63708	-0.43555	0.00000	-1.63961	-0.42941	0.00000
1	0.35541	-2.29098	0.00000	0.35645	-2.29632	0.00000	0.35545	-2.28650	0.00000
1	2.80339	-1.93734	0.00000	2.80381	-1.92544	0.00000	2.79756	-1.93084	0.00000
1	3.73230	0.37393	0.00000	3.71310	0.39014	0.00000	3.72139	0.37593	0.00000
1	2.17804	2.31906	0.00000	2.14936	2.32388	0.00000	2.16868	2.31479	0.00000
1	-0.25987	1.96361	0.00000	-0.28712	1.95193	0.00000	-0.26446	1.95602	0.00000
6	-2.31451	0.13155	1.27016	-2.28941	0.13296	1.26126	-2.30658	0.13172	1.26887
6	-2.31451	0.13155	-1.27016	-2.28941	0.13296	-1.26126	-2.30658	0.13172	-1.26887
1	-1.79788	-1.51526	0.00000	-1.79755	-1.52218	0.00000	-1.79467	-1.51568	0.00000
1	-3.38417	-0.10719	1.27821	-3.35919	-0.09939	1.28265	-3.37739	-0.09829	1.27674
1	-1.86344	-0.28911	2.17473	-1.82773	-0.28272	2.16121	-1.85886	-0.29318	2.17221
1	-2.21673	1.22182	1.32408	-2.18144	1.22128	1.29770	-2.20038	1.22035	1.32481
1	-3.38417	-0.10719	-1.27821	-3.35919	-0.09939	-1.28265	-3.37739	-0.09829	-1.27674
1	-2.21673	1.22182	-1.32408	-2.18144	1.22128	-1.29770	-2.20038	1.22035	-1.32481
1	-1.86344	-0.28912	-2.17473	-1.82773	-0.28272	-2.16121	-1.85886	-0.29318	-2.17221

$1e_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.12058	0.14314	0.00000	0.12370	0.16839	0.00000	0.11851	0.16301	-0.00002
6	-0.74844	1.24932	-0.00002	-0.75577	1.26354	-0.00003	-0.75748	1.25414	-0.00007
6	-2.13885	1.06723	-0.00003	-2.13577	1.04726	-0.00003	-2.13951	1.05151	-0.00007
6	-2.63947	-0.23872	-0.00001	-2.60363	-0.26748	-0.00001	-2.61500	-0.25813	0.00001
6	-1.74418	-1.32474	0.00001	-1.68065	-1.32847	0.00002	-1.70577	-1.32496	0.00007
6	-0.33393	-1.20600	0.00001	-0.27183	-1.19801	0.00002	-0.29821	-1.19690	0.00007
6	1.63228	0.42038	0.00000	1.62232	0.45000	0.00000	1.62782	0.44189	0.00000
1	-0.34482	2.26715	-0.00003	-0.36919	2.28877	-0.00005	-0.36894	2.27713	-0.00012
1	-2.80976	1.92580	-0.00004	-2.83065	1.88895	-0.00005	-2.82447	1.89803	-0.00011
1	-3.72007	-0.40785	-0.00002	-3.68099	-0.46038	-0.00001	-3.69287	-0.44080	0.00001
1	-2.19390	-2.32537	0.00002	-2.11871	-2.33791	0.00003	-2.14867	-2.33061	0.00013
6	2.30277	-0.15224	1.26253	2.25469	-0.15430	1.25209	2.27665	-0.15422	1.26054
6	2.30277	-0.15230	-1.26250	2.25470	-0.15435	-1.25206	2.27669	-0.15419	-1.26052
1	1.78456	1.51272	-0.00002	1.79405	1.53950	-0.00002	1.79671	1.53089	0.00002
1	3.39166	0.00851	1.25140	3.35005	-0.06194	1.25285	3.37301	-0.06753	1.24634
1	1.89484	0.31375	2.16845	1.86518	0.33131	2.15419	1.90619	0.34346	2.16518
1	2.09491	-1.22656	1.31735	1.96414	-1.20844	1.28112	1.98873	-1.20975	1.31709
1	3.39167	0.00845	-1.25137	3.35007	-0.06198	-1.25281	3.37305	-0.06752	-1.24629
1	2.09491	-1.22662	-1.31726	1.96415	-1.20849	-1.28105	1.98874	-1.20971	-1.31712
1	1.89485	0.31365	-2.16845	1.86520	0.33123	-2.15418	1.90627	0.34352	-2.16516

$1e_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.09350	0.17217	-0.00002	0.09978	0.18471	-0.00002	0.09131	0.17553	-0.00002
6	-0.79749	1.25590	-0.00013	-0.79016	1.26326	-0.00013	-0.79355	1.25740	-0.00013
6	-2.17672	1.00806	-0.00011	-2.16254	1.00849	-0.00011	-2.16598	1.00601	-0.00010
6	-2.65269	-0.31282	0.00002	-2.62034	-0.31890	0.00002	-2.63421	-0.31128	0.00003
6	-1.82236	-1.46720	0.00014	-1.80728	-1.48621	0.00015	-1.82010	-1.47762	0.00014
6	-0.44132	-1.13494	0.00011	-0.43449	-1.12179	0.00011	-0.44447	-1.12502	0.00010
6	1.59900	0.43089	-0.00004	1.59298	0.43731	-0.00004	1.59414	0.43208	-0.00004
1	-0.41559	2.27840	-0.00024	-0.40872	2.28788	-0.00024	-0.40973	2.27811	-0.00023
1	-2.87417	1.85114	-0.00020	-2.86671	1.84703	-0.00020	-2.86149	1.85051	-0.00018
1	-3.74218	-0.43867	0.00003	-3.71444	-0.43882	0.00003	-3.72749	-0.42518	0.00004
1	0.28527	-1.95672	0.00020	0.30960	-1.93489	0.00020	0.29631	-1.93889	0.00018
6	2.28702	-0.11750	1.26673	2.26064	-0.12284	1.25768	2.27689	-0.12015	1.26550
6	2.28703	-0.11776	-1.26668	2.26065	-0.12310	-1.25764	2.27691	-0.12042	-1.26546
1	1.74274	1.52327	-0.00015	1.74898	1.52811	-0.00015	1.74457	1.52269	-0.00016
1	3.36042	0.12202	1.27391	3.33629	0.09972	1.27992	3.35358	0.10170	1.27569
1	1.83239	0.30596	2.16913	1.79824	0.30168	2.15382	1.82851	0.31188	2.16609
1	2.18123	-1.20656	1.32595	2.13337	-1.20836	1.30044	2.15397	-1.20626	1.32790
1	3.36043	0.12175	-1.27391	3.33630	0.09946	-1.27991	3.35360	0.10143	-1.27568
1	2.18124	-1.20684	-1.32569	2.13338	-1.20863	-1.30018	2.15400	-1.20655	-1.32762
1	1.83241	0.30551	-2.16918	1.79826	0.30124	-2.15387	1.82854	0.31141	-2.16615

$1e_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.09424	-0.18683	0.00000	-0.10359	-0.19694	0.00000	-0.09581	-0.18967	0.00000
6	0.81084	-1.25920	0.00000	0.80338	-1.26229	0.00000	0.80924	-1.25564	0.00000
6	2.19987	-1.03659	0.00000	2.18688	-1.01937	0.00000	2.18999	-1.02636	0.00000
6	2.81626	0.24219	0.00000	2.81832	0.25405	0.00000	2.82244	0.24569	0.00000
6	1.85414	1.28808	0.00000	1.83004	1.27755	0.00000	1.84424	1.27782	0.00000
6	0.46025	1.10424	0.00000	0.43760	1.09579	0.00000	0.45669	1.09758	0.00000
6	-1.59892	-0.42766	0.00000	-1.59538	-0.43628	0.00000	-1.59619	-0.42987	0.00000
1	0.41786	-2.28224	0.00000	0.41319	-2.28738	0.00000	0.41332	-2.27720	0.00000
1	2.83063	-1.93419	0.00000	2.81825	-1.92129	0.00000	2.81466	-1.93116	0.00000
1	2.19964	2.32927	0.00000	2.16075	2.32765	0.00000	2.17846	2.32521	0.00000
1	-0.20006	1.97758	0.00000	-0.23127	1.96431	0.00000	-0.20963	1.96640	0.00000
6	-2.28677	0.12344	1.26652	-2.26102	0.12682	1.25767	-2.27877	0.12475	1.26523
6	-2.28677	0.12344	-1.26652	-2.26102	0.12682	-1.25767	-2.27877	0.12475	-1.26523
1	-1.74670	-1.51813	0.00000	-1.75256	-1.52558	0.00000	-1.74889	-1.51907	0.00000
1	-3.36164	-0.10898	1.27242	-3.33678	-0.09392	1.28134	-3.35664	-0.09090	1.27439
1	-1.83558	-0.30330	2.16888	-1.79779	-0.29649	2.15365	-1.83273	-0.30975	2.16557
1	-2.17744	1.21279	1.32772	-2.13520	1.21312	1.29930	-2.15375	1.21140	1.32985
1	-3.36164	-0.10898	-1.27242	-3.33678	-0.09392	-1.28134	-3.35664	-0.09090	-1.27439
1	-2.17744	1.21279	-1.32772	-2.13520	1.21312	-1.29930	-2.15375	1.21140	-1.32985
1	-1.83558	-0.30330	-2.16888	-1.79779	-0.29649	-2.15365	-1.83273	-0.30975	-2.16557

$1e_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.09363	-0.19846	0.00000	-0.09958	-0.20564	0.00000	-0.09103	-0.19883	0.00000
6	0.78822	-1.29987	-0.00002	0.79867	-1.29241	-0.00002	0.79400	-1.28977	-0.00001
6	2.20658	-1.23410	-0.00002	2.21733	-1.23724	-0.00002	2.21225	-1.23847	-0.00001
6	2.67993	0.10475	0.00000	2.64888	0.11637	0.00000	2.66125	0.10933	0.00000
6	1.84979	1.23883	0.00001	1.81678	1.24892	0.00001	1.83545	1.23900	0.00001
6	0.45715	1.09432	0.00001	0.43078	1.09102	0.00001	0.44858	1.09342	0.00001
6	-1.60429	-0.41343	0.00000	-1.59630	-0.42546	0.00000	-1.59789	-0.41801	-0.00001
1	0.30665	-2.28782	-0.00003	0.31281	-2.28310	-0.00003	0.30168	-2.27555	-0.00003
1	3.76066	0.29203	0.00000	3.72914	0.32769	0.00000	3.74148	0.31320	0.00000
1	2.28355	2.24348	0.00002	2.24220	2.25802	0.00003	2.26271	2.24621	0.00002

1	-0.18411	1.97638	0.00002	-0.22402	1.96586	0.00002	-0.19904	1.96999	0.00002
6	-2.28244	0.14732	1.26637	-2.25717	0.14317	1.25736	-2.27307	0.14379	1.26515
6	-2.28244	0.14735	-1.26636	-2.25717	0.14320	-1.25735	-2.27307	0.14382	-1.26514
1	-1.76524	-1.50183	-0.00002	-1.76104	-1.51344	-0.00002	-1.75906	-1.50573	-0.00002
1	-3.35868	-0.07958	1.27828	-3.33437	-0.07111	1.28398	-3.35176	-0.06805	1.27935
1	-1.82984	-0.27864	2.16832	-1.79476	-0.28193	2.15296	-1.82575	-0.28971	2.16525
1	-2.16886	1.23695	1.32365	-2.12712	1.22966	1.29874	-2.14580	1.23078	1.32704
1	-3.35868	-0.07955	-1.27827	-3.33437	-0.07108	-1.28398	-3.35176	-0.06802	-1.27935
1	-2.16887	1.23698	-1.32362	-2.12713	1.22969	-1.29871	-2.14581	1.23081	-1.32701
1	-1.82984	-0.27859	-2.16833	-1.79476	-0.28188	-2.15296	-1.82576	-0.28965	-2.16525

1e$_6$

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.10566	-0.25185	-0.00001	-0.10340	-0.25933	-0.00001	-0.09848	-0.24999	-0.00001
6	0.72445	-1.40837	-0.00004	0.70433	-1.43403	-0.00004	0.71216	-1.42152	-0.00003
6	2.11150	-1.11200	-0.00003	2.08561	-1.10391	-0.00003	2.09586	-1.10613	-0.00003
6	2.65138	0.18515	0.00000	2.62734	0.19161	0.00000	2.63795	0.18348	0.00001
6	1.78952	1.28866	0.00003	1.76638	1.29096	0.00003	1.78440	1.28689	0.00003
6	0.40794	1.06084	0.00003	0.39031	1.06014	0.00003	0.40854	1.05914	0.00002
6	-1.62707	-0.44540	-0.00001	-1.61324	-0.44793	-0.00001	-1.61883	-0.44243	-0.00001
1	2.82947	-1.94087	-0.00005	2.81968	-1.92385	-0.00005	2.82374	-1.92961	-0.00004
1	3.73404	0.34037	0.00001	3.71039	0.35047	0.00001	3.72020	0.34003	0.00001
1	2.18175	2.30526	0.00005	2.15844	2.30975	0.00006	2.17828	2.30220	0.00005
1	-0.26253	1.92586	0.00005	-0.28771	1.92083	0.00005	-0.26255	1.92349	0.00004
6	-2.30055	0.11846	1.26667	-2.26832	0.12258	1.25823	-2.29035	0.11997	1.26555
6	-2.30055	0.11853	-1.26665	-2.26832	0.12264	-1.25822	-2.29036	0.12005	-1.26554
1	-1.76508	-1.53394	-0.00004	-1.74743	-1.53680	-0.00004	-1.75312	-1.53120	-0.00004
1	-3.37901	-0.10023	1.27995	-3.34620	-0.09045	1.29160	-3.36993	-0.09058	1.28577
1	-1.85094	-0.31876	2.16546	-1.80230	-0.30814	2.14987	-1.84006	-0.31877	2.16243
1	-2.18177	1.20843	1.33249	-2.14020	1.21009	1.30579	-2.16597	1.20835	1.33452
1	-3.37901	-0.10016	-1.27995	-3.34621	-0.09038	-1.29160	-3.36993	-0.09051	-1.28576
1	-2.18177	1.20851	-1.33242	-2.14021	1.21016	-1.30572	-2.16598	1.20843	-1.33445
1	-1.85094	-0.31864	-2.16547	-1.80230	-0.30803	-2.14988	-1.84008	-0.31864	-2.16245

1f. *N*-Methylacetanilide

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.33608	0.24961	0.02387	-0.32758	0.24898	-0.00027	-0.33406	0.25147	0.00014
6	-1.05159	0.34705	-1.17604	-1.01723	0.14043	-1.21140	-1.02830	0.14092	-1.20657
6	-2.42814	0.11007	-1.19258	-2.39103	-0.09641	-1.20863	-2.40066	-0.09467	-1.20572
6	-3.09768	-0.21943	-0.01038	-3.07950	-0.21086	0.00007	-3.08847	-0.21488	-0.00006
6	-2.38693	-0.30754	1.18992	-2.39168	-0.09068	1.20858	-2.40043	-0.09707	1.20571
6	-1.01043	-0.06851	1.20902	-1.01788	0.14614	1.21098	-1.02807	0.13852	1.20677
7	1.07309	0.52298	0.04471	1.07076	0.52318	-0.00052	1.07016	0.52204	0.00023
1	-2.97620	0.18170	-2.12752	-2.92564	-0.18758	-2.15067	-2.93213	-0.18429	-2.14726
1	-4.16761	-0.40470	-0.02428	-4.15052	-0.39528	0.00021	-4.15752	-0.39855	-0.00014
1	-2.90287	-0.55983	2.11175	-2.92680	-0.17740	2.15075	-2.93170	-0.18857	2.14717
1	-0.45073	-0.13041	2.13794	-0.46757	0.24369	2.14406	-0.48247	0.23339	2.13976
6	2.04022	-0.45850	-0.06032	2.02937	-0.46762	0.00085	2.04019	-0.46139	-0.00034
8	3.23950	-0.19239	-0.01151	3.23543	-0.21391	0.00014	3.22889	-0.19483	-0.00006
6	1.55381	-1.88785	-0.23897	1.50469	-1.88735	0.00334	1.54157	-1.89796	-0.00139
1	2.42865	-2.51498	-0.40952	2.36590	-2.55458	0.00515	2.41391	-2.55039	-0.00221
1	1.02876	-2.23964	0.65493	0.88739	-2.08101	0.88413	0.92682	-2.10913	0.87816
1	0.86163	-1.98299	-1.08052	0.88850	-2.08447	-0.87747	0.92624	-2.10766	-0.88088
6	1.47349	1.92081	0.22289	-0.32758	0.24898	-0.00027	1.47397	1.92479	0.00130
1	2.56099	1.96919	0.17458	-1.01723	0.14043	-1.21140	2.56288	1.95443	0.00142
1	1.03962	2.54416	-0.56639	-2.39103	-0.09641	-1.20863	1.09015	2.44017	-0.88648
1	1.13272	2.29936	1.19359	-3.07950	-0.21086	0.00007	1.08999	2.43887	0.88976
1	-0.52263	0.60215	-2.08988	-2.39168	-0.09068	1.20858	-0.48289	0.23765	-2.13947

$1f_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.37391	0.26006	0.00705	0.36578	0.21141	-0.04967	0.37574	0.19372	-0.09246
6	1.02630	-0.17500	1.17343	1.14241	0.69722	1.01453	1.12901	0.76617	0.94094
6	2.40322	-0.41910	1.13621	2.51679	0.46062	1.00041	2.50474	0.55064	0.98076
6	3.08663	-0.20571	-0.06822	3.05809	-0.25259	-0.07149	3.07871	-0.24041	-0.01600
6	2.38636	0.24779	-1.19802	2.21607	-0.70976	-1.09855	2.27322	-0.79096	-1.01754
6	0.99203	0.51210	-1.23235	0.81412	-0.50835	-1.17469	0.87174	-0.60855	-1.13644
7	-1.06864	0.50776	0.14033	-1.05240	0.55406	0.02969	-1.05536	0.51947	-0.07226
1	2.92779	-0.76345	2.02585	3.14999	0.82079	1.81174	3.11059	0.98390	1.77358
1	4.16228	-0.39083	-0.11935	4.13294	-0.45081	-0.10051	4.15528	-0.42361	-0.00150
1	2.97619	0.40118	-2.10877	2.71075	-1.26538	-1.90714	2.79033	-1.40393	-1.76624
6	-2.01571	-0.44298	-0.06818	-2.01230	-0.40083	0.17035	-2.03150	-0.39693	0.16691
8	-3.23888	-0.21454	-0.01058	-3.22534	-0.18717	-0.01067	-3.23421	-0.15548	0.04482
6	-1.51072	-1.84378	-0.38826	-1.50424	-1.76243	0.59099	-1.54827	-1.76815	0.61482
1	-2.37967	-2.47943	-0.56840	-2.36697	-2.40055	0.79081	-2.42405	-2.38953	0.81134
1	-0.86295	-1.81847	-1.27005	-0.88881	-2.16066	-0.22011	-0.91828	-2.19444	-0.17226
1	-0.91561	-2.25461	0.43334	-0.86618	-1.69311	1.47593	-0.92706	-1.69823	1.51319
6	-1.46203	1.90470	0.26183	-1.41175	1.79839	-0.62301	-1.42432	1.79491	-0.65655
1	-2.54953	1.97449	0.20750	-2.48797	1.94621	-0.53029	-2.51031	1.89322	-0.62158
1	-1.11366	2.31881	1.21791	-0.87191	2.62561	-0.15202	-0.95623	2.62092	-0.10668
1	-0.99900	2.47161	-0.55433	-1.12906	1.75058	-1.68156	-1.08030	1.84492	-1.69875
1	0.46576	-0.32583	2.09775	0.67689	1.24410	1.83748	0.64686	1.37171	1.70948

$1f_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.38437	0.24437	-0.01807	0.37613	0.24210	-0.00378	0.38373	0.24454	-0.01458
6	1.09479	0.22713	1.18782	1.07787	0.17656	1.20157	1.08405	0.19669	1.19170
6	2.47250	-0.01590	1.13220	2.45108	-0.06136	1.13580	2.45743	-0.04161	1.13284
6	3.10028	-0.22726	-0.10714	3.07121	-0.21326	-0.11611	3.08418	-0.21855	-0.10532
6	2.43973	-0.21341	-1.36580	2.43579	-0.15093	-1.38759	2.44553	-0.17926	-1.37542
6	1.04847	0.03926	-1.23925	1.04716	0.09452	-1.22972	1.05516	0.06813	-1.23107
7	-1.04288	0.52162	0.00816	-1.03980	0.51921	0.02957	-1.04017	0.51858	0.01068
1	3.04970	-0.03994	2.06038	3.03039	-0.12472	2.06161	3.02838	-0.08783	2.06358
1	4.18001	-0.41316	-0.07688	4.15428	-0.39827	-0.08115	4.16601	-0.40179	-0.06380
1	0.41876	0.07714	-2.13600	0.40327	0.17289	-2.11899	0.41695	0.13015	-2.12303
6	-2.00022	-0.45058	0.03721	-1.99128	-0.45407	0.02092	-2.00060	-0.44853	0.02548
8	-3.21707	-0.19998	0.01715	-3.21273	-0.21944	0.00132	-3.20648	-0.20393	0.01022
6	-1.50526	-1.88839	0.10167	-1.45968	-1.87307	0.04797	-1.49085	-1.88335	0.07107
1	-2.37874	-2.53940	0.16322	-2.31621	-2.54857	0.03885	-2.35707	-2.54654	0.06299
1	-0.91225	-2.13767	-0.78324	-0.81394	-2.06152	-0.81254	-0.83865	-2.09534	-0.77978
1	-0.85481	-2.04737	0.96680	-0.85196	-2.04445	0.93965	-0.89203	-2.05807	0.96927
6	-1.44057	1.92246	-0.09080	-1.43761	1.91276	-0.03974	-1.44075	1.91401	-0.05945
1	-2.52950	1.98146	-0.06460	-2.52635	1.96093	-0.01331	-2.53039	1.96091	-0.05329
1	-1.01473	2.49352	0.74289	-1.01407	2.46251	0.80726	-1.03807	2.47155	0.79537
1	-1.06559	2.35515	-1.02609	-1.06230	2.36325	-0.96454	-1.05112	2.37711	-0.97405
1	0.57938	0.39270	2.13222	0.55327	0.29952	2.14967	0.56166	0.33887	2.13469

$1f_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.38081	0.24696	-0.00007	-0.37128	0.24141	0.00011	-0.37747	0.24482	0.00000
6	-1.08468	0.13265	-1.20464	-1.06957	0.13332	-1.20433	-1.08259	0.13013	-1.19972
6	-2.46849	-0.11077	-1.17951	-2.45290	-0.10516	-1.16739	-2.46091	-0.10759	-1.16968
6	-3.25064	-0.24960	-0.00042	-3.25446	-0.24348	-0.00014	-3.25805	-0.24546	0.00001
6	-2.46887	-0.11023	1.17887	-2.45301	-0.10573	1.16724	-2.46089	-0.10762	1.16969
6	-1.08506	0.13320	1.20432	-1.06968	0.13274	1.20443	-1.08257	0.13010	1.19972
7	1.04148	0.52307	0.00009	1.03964	0.52003	0.00024	1.03999	0.51981	-0.00001
1	-2.95822	-0.19582	-2.15618	-2.93761	-0.18682	-2.15070	-2.94253	-0.19015	-2.15296

1	-2.95891	-0.19483	2.15542	-2.93781	-0.18788	2.15047	-2.94250	-0.19020	2.15297
1	-0.54222	0.22985	2.14812	-0.52021	0.22773	2.14589	-0.53480	0.22650	2.14008
6	1.99839	-0.45131	0.00035	1.99296	-0.45308	-0.00006	2.00160	-0.44743	-0.00001
8	3.21453	-0.20094	0.00040	3.21313	-0.21522	-0.00015	3.20636	-0.20129	0.00001
6	1.50258	-1.89040	0.00062	1.46376	-1.87313	-0.00027	1.49418	-1.88381	-0.00001
1	2.37644	-2.54371	0.00094	2.32196	-2.54646	-0.00040	2.36245	-2.54429	-0.00002
1	0.88037	-2.09424	0.87694	0.83718	-2.05550	0.87567	0.86877	-2.08051	0.87465
1	0.88072	-2.09467	-0.87586	0.83713	-2.05522	-0.87622	0.86874	-2.08050	-0.87464
6	1.44351	1.92687	-0.00019	1.43691	1.91627	0.00032	1.44296	1.91733	0.00000
1	2.53295	1.98184	0.00026	2.52596	1.96277	0.00065	2.53260	1.96383	-0.00002
1	1.04448	2.43195	-0.88799	1.03759	2.41760	-0.88731	1.04686	2.42879	-0.88579
1	1.04369	2.43249	0.88694	1.03701	2.41760	0.88769	1.04690	2.42877	0.88582
1	-0.54154	0.22887	-2.14831	-0.52001	0.22875	-2.14570	-0.53482	0.22655	-2.14008

$1f_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.38437	0.24437	-0.01807	-0.37613	0.24210	-0.00378	-0.38373	0.24454	-0.01458
6	-1.04847	0.03926	-1.23925	-1.04716	0.09452	-1.22972	-1.05516	0.06813	-1.23107
6	-2.43973	-0.21341	-1.36580	-2.43579	-0.15093	-1.38759	-2.44553	-0.17925	-1.37542
6	-3.10028	-0.22726	-0.10714	-3.07121	-0.21326	-0.11611	-3.08418	-0.21855	-0.10532
6	-2.47250	-0.01590	1.13220	-2.45108	-0.06136	1.13579	-2.45743	-0.04162	1.13285
6	-1.09479	0.22713	1.18782	-1.07787	0.17656	1.20157	-1.08405	0.19669	1.19170
7	1.04288	0.52162	0.00816	1.03980	0.51921	0.02957	1.04017	0.51858	0.01068
1	-4.18001	-0.41316	-0.07688	-4.15428	-0.39827	-0.08115	-4.16601	-0.40179	-0.06380
1	-3.04970	-0.03994	2.06038	-3.03039	-0.12472	2.06160	-3.02838	-0.08783	2.06358
1	-0.57938	0.39270	2.13222	-0.55327	0.29952	2.14967	-0.56166	0.33886	2.13469
6	2.00022	-0.45058	0.03721	1.99128	-0.45407	0.02092	2.00060	-0.44854	0.02548
8	3.21707	-0.19998	0.01715	3.21273	-0.21944	0.00131	3.20648	-0.20393	0.01022
6	1.50526	-1.88839	0.10167	1.45968	-1.87307	0.04797	1.49085	-1.88335	0.07107
1	2.37874	-2.53940	0.16322	2.31621	-2.54857	0.03885	2.35706	-2.54654	0.06298
1	0.85481	-2.04737	0.96680	0.85196	-2.04444	0.93966	0.89202	-2.05807	0.96927
1	0.91225	-2.13767	-0.78324	0.81394	-2.06152	-0.81254	0.83865	-2.09534	-0.77978
6	1.44057	1.92246	-0.09080	1.43761	1.91276	-0.03974	1.44075	1.91401	-0.05945
1	2.52950	1.98146	-0.06460	2.52634	1.96093	-0.01329	2.53039	1.96091	-0.05329
1	1.06559	2.35515	-1.02609	1.06231	2.36324	-0.96455	1.05112	2.37711	-0.97404
1	1.01473	2.49352	0.74289	1.01405	2.46252	0.80724	1.03807	2.47154	0.79537
1	-0.41876	0.07714	-2.13600	-0.40326	0.17289	-2.11898	-0.41695	0.13016	-2.12303

$1f_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.37391	0.26006	0.00705	-0.36578	0.21141	-0.04966	-0.38875	0.26800	0.06018
6	-0.99203	0.51210	-1.23235	-0.81412	-0.50834	-1.17470	-1.09260	1.07572	-0.85210
6	-2.38636	0.24779	-1.19802	-2.21607	-0.70975	-1.09855	-2.47233	0.75562	-0.86252
6	-3.08663	-0.20571	-0.06822	-3.05809	-0.25259	-0.07149	-3.08130	-0.22455	-0.07103
6	-2.40322	-0.41910	1.13621	-2.51679	0.46062	1.00042	-2.31327	-0.96226	0.83020
6	-1.02630	-0.17500	1.17343	-1.14241	0.69722	1.01453	-0.94630	-0.70059	0.90426
7	1.06864	0.50776	0.14033	1.05240	0.55406	0.02969	1.05402	0.49256	0.19791
1	-2.97619	0.40118	-2.10877	-2.71075	-1.26537	-1.90715	-3.13653	1.30579	-1.54087
1	-4.16228	-0.39083	-0.11935	-4.13294	-0.45081	-0.10051	-4.15473	-0.41267	-0.14171
1	-2.92779	-0.76345	2.02585	-3.14999	0.82078	1.81174	-2.76647	-1.71545	1.47094
1	-0.46576	-0.32583	2.09775	-0.67689	1.24409	1.83749	-0.32446	-1.24360	1.61666
6	2.01571	-0.44298	-0.06818	2.01230	-0.40083	0.17035	2.01729	-0.39733	-0.14695
8	3.23888	-0.21454	-0.01058	3.22534	-0.18717	-0.01067	3.22411	-0.18347	-0.00313
6	1.51072	-1.84378	-0.38826	1.50424	-1.76243	0.59098	1.54646	-1.71045	-0.76895
1	2.37967	-2.47943	-0.56840	2.36697	-2.40055	0.79080	2.40694	-2.15392	-1.27427
1	0.91561	-2.25461	0.43334	0.86618	-1.69312	1.47592	1.19001	-2.40849	-0.00581
1	0.86295	-1.81847	-1.27005	0.88881	-2.16066	-0.22011	0.72383	-1.55192	-1.46964
6	1.46203	1.90470	0.26183	1.41175	1.79839	-0.62301	1.44524	1.84102	0.57254
1	2.54953	1.97449	0.20750	2.48797	1.94621	-0.53028	2.49289	1.99523	0.31053
1	0.99900	2.47161	-0.55433	1.12906	1.75058	-1.68156	0.78767	2.52566	0.02663
1	1.11366	2.31881	1.21791	0.87191	2.62561	-0.15202	1.32322	2.00807	1.65332

1g. Benzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	1.39834	0.00000	0.00000	1.39524	0.00000	0.000000	1.393362	0.000000
6	1.21100	0.69917	0.00000	1.20831	0.69762	0.00000	1.206687	0.696681	0.000000
6	1.21100	-0.69917	0.00000	1.20831	-0.69762	0.00000	1.206687	-0.696681	0.000000
6	0.00000	-1.39834	0.00000	0.00000	-1.39524	0.00000	0.000000	-1.393362	0.000000
6	-1.21100	-0.69917	0.00000	-1.20831	-0.69762	0.00000	-1.206687	-0.696681	0.000000
6	-1.21100	0.69917	0.00000	-1.20831	0.69762	0.00000	-1.206687	0.696681	0.000000
1	0.00000	2.48475	0.00000	0.00000	2.48238	0.00000	0.000000	2.478476	0.000000
1	2.15185	1.24237	0.00000	2.14980	1.24119	0.00000	2.146423	1.239238	0.000000
1	2.15185	-1.24237	0.00000	2.14980	-1.24119	0.00000	2.146423	-1.239238	0.000000
1	0.00000	-2.48475	0.00000	0.00000	-2.48238	0.00000	0.000000	-2.478476	0.000000
1	-2.15185	-1.24237	0.00000	-2.14980	-1.24119	0.00000	-2.146423	-1.239238	0.000000
1	-2.15185	1.24237	0.00000	-2.14980	1.24119	0.00000	-2.146423	1.239238	0.000000

$1g_1$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.20545	0.65238	0.00000	0.00000	0.00000	1.37124	-1.36981	0.00000	0.00000
6	0.00000	1.36732	0.00000	0.00000	-1.19789	0.65332	-0.64972	1.19588	0.00000
6	1.22583	0.67785	0.00000	0.00000	-1.16448	-0.75169	0.75037	1.16812	0.00000
6	1.36276	-0.73752	0.00000	0.00000	0.00000	-1.56816	1.56187	0.00000	0.00000
6	0.10296	-1.39697	0.00000	0.00000	1.16448	-0.75169	0.75037	-1.16812	0.00000
6	-1.14470	-0.74782	0.00000	0.00000	1.19789	0.65332	-0.64972	-1.19588	0.00000
1	-2.16393	1.17110	0.00000	0.00000	0.00000	2.46299	-2.45922	0.00000	0.00000
1	-0.02028	2.46173	0.00000	0.00000	-2.15155	1.19197	-1.19017	2.14744	0.00000
1	2.13027	1.29910	0.00000	0.00000	-2.15029	-1.24249	1.23972	2.15340	0.00000
1	0.07753	-2.49393	0.00000	0.00000	2.15029	-1.24249	1.23972	-2.15340	0.00000
1	-2.07200	-1.32941	0.00000	0.00000	2.15155	1.19197	-1.19017	-2.14744	0.00000

1h. Naphthalene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	2.43628	-0.70914	0.00000	0.70656	-2.42974	-2.42843	0.70703	0.00000
6	0.00000	1.24589	-1.40386	0.00000	1.40188	-1.24016	-1.24254	1.39923	0.00000
6	0.00000	2.43628	0.70914	0.00000	-0.70656	-2.42974	-2.42843	-0.70703	0.00000
6	0.00000	1.24589	1.40386	0.00000	-1.40188	-1.24016	-1.24254	-1.39923	0.00000
6	0.00000	0.00000	0.71725	0.00000	-0.71550	0.00000	0.00000	-0.71553	0.00000
6	0.00000	0.00000	-0.71725	0.00000	0.71550	0.00000	0.00000	0.71553	0.00000
1	0.00000	1.24424	2.49098	0.00000	-2.49076	-1.23898	-1.23903	-2.48526	0.00000
6	0.00000	-1.24589	1.40386	0.00000	-1.40188	1.24016	1.24254	-1.39923	0.00000
6	0.00000	-1.24589	-1.40386	0.00000	1.40188	1.24016	1.24254	1.39923	0.00000
6	0.00000	-2.43628	-0.70914	0.00000	0.70656	2.42974	2.42843	0.70703	0.00000
6	0.00000	-2.43628	0.70914	0.00000	-0.70656	2.42974	2.42843	-0.70703	0.00000
1	0.00000	-1.24424	2.49098	0.00000	-2.49076	1.23898	1.23903	-2.48526	0.00000
1	0.00000	-1.24424	-2.49098	0.00000	2.49076	1.23898	1.23903	2.48526	0.00000
1	0.00000	-3.38028	-1.24635	0.00000	1.24532	3.37422	3.37186	1.24297	0.00000
1	0.00000	-3.38028	1.24635	0.00000	-1.24532	3.37422	3.37186	-1.24297	0.00000
1	0.00000	1.24424	-2.49098	0.00000	2.49076	-1.23898	-1.23902	2.48526	0.00000
1	0.00000	3.38028	-1.24635	0.00000	1.24532	-3.37422	-3.37186	1.24297	0.00000
1	0.00000	3.38028	1.24635	0.00000	-1.24532	-3.37422	-3.37186	-1.24297	0.00000

$1h_1$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	2.44827	-0.67611	0.00000	2.42734	-0.67341	0.00000	2.43463	-0.67115	0.00000
6	1.31499	-1.50033	0.00000	1.30880	-1.52082	0.00000	1.31307	-1.51129	0.00000
6	2.41729	0.74634	0.00000	2.40656	0.74701	0.00000	2.40539	0.74521	0.00000
6	1.21499	1.42981	0.00000	1.20738	1.43034	0.00000	1.20982	1.42996	0.00000
6	0.00000	0.69283	0.00000	0.00000	0.69370	0.00000	0.00000	0.69440	0.00000
6	0.07460	-0.75425	0.00000	0.08558	-0.74997	0.00000	0.07997	-0.74937	0.00000
1	1.18174	2.51942	0.00000	1.17317	2.52225	0.00000	1.17391	2.51861	0.00000
6	-1.27161	1.33630	0.00000	-1.26674	1.33447	0.00000	-1.27023	1.33088	0.00000
6	-1.16858	-1.45537	0.00000	-1.15843	-1.44796	0.00000	-1.16071	-1.44704	0.00000
6	-2.39291	-0.81158	0.00000	-2.38066	-0.80824	0.00000	-2.38318	-0.81137	0.00000
6	-2.44431	0.60678	0.00000	-2.43814	0.60609	0.00000	-2.43699	0.60218	0.00000
1	-1.30699	2.42706	0.00000	-1.30393	2.42716	0.00000	-1.30782	2.42090	0.00000
1	-1.10463	-2.54141	0.00000	-1.08666	-2.53539	0.00000	-1.08847	-2.53238	0.00000
1	-3.31813	-1.38570	0.00000	-3.30610	-1.38527	0.00000	-3.30703	-1.38631	0.00000
1	-3.40625	1.11744	0.00000	-3.40218	1.11576	0.00000	-3.39951	1.11016	0.00000
1	3.44394	-1.13422	0.00000	3.43087	-1.12328	0.00000	3.43783	-1.11767	0.00000
1	3.35389	1.31088	0.00000	3.34474	1.31155	0.00000	3.34050	1.31212	0.00000

$1h_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	2.44827	-0.67611	0.00000	-2.61962	-0.66464	0.00000	-2.61292	-0.66384	0.00000
6	1.31499	-1.50033	0.00000	-1.37920	-1.32090	0.00000	-1.37848	-1.32299	0.00000
6	2.41729	0.74634	0.00000	-2.42576	0.76238	0.00000	-2.42626	0.76864	0.00000
6	1.21499	1.42981	0.00000	-1.21338	1.44185	0.00000	-1.21898	1.43727	0.00000
6	0.00000	0.69283	0.00000	0.00000	0.71821	0.00000	0.00000	0.71563	0.00000
6	0.07460	-0.75425	0.00000	-0.08991	-0.71548	0.00000	-0.09047	-0.71822	0.00000
1	1.18174	2.51942	0.00000	-1.17141	2.53635	0.00000	-1.16998	2.52967	0.00000
6	-1.27161	1.33630	0.00000	1.27965	1.32924	0.00000	1.27786	1.32581	0.00000
6	-1.16858	-1.45537	0.00000	1.12007	-1.45638	0.00000	1.12444	-1.45502	0.00000
6	-2.39291	-0.81158	0.00000	2.35537	-0.83820	0.00000	2.35360	-0.83534	0.00000
6	-2.44431	0.60678	0.00000	2.43542	0.57392	0.00000	2.43446	0.57737	0.00000
1	-1.30699	2.42706	0.00000	1.33823	2.41965	0.00000	1.33080	2.41387	0.00000
1	-1.10463	-2.54141	0.00000	1.05533	-2.54642	0.00000	1.06047	-2.54234	0.00000
1	-3.31813	-1.38570	0.00000	3.26853	-1.43353	0.00000	3.26678	-1.42705	0.00000
1	-3.40625	1.11744	0.00000	3.40937	1.06296	0.00000	3.40592	1.06577	0.00000

1	3.44394	-1.13422	0.00000	-1.35650	-2.42302	0.00000	-1.35337	-2.42277	0.00000
1	3.35389	1.31088	0.00000	-3.31943	1.40395	0.00000	-3.32006	1.40699	0.00000

1i. Fluorobenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.00000	0.92683	0.00000	0.00000	-0.92761	0.00000	0.00000	0.93354
6	0.00000	-1.21992	0.26109	0.00000	-1.21665	-0.25946	0.00000	-1.21406	0.26064
6	0.00000	-1.21024	-1.13697	0.00000	-1.20787	1.13518	0.00000	-1.20551	-1.13224
6	0.00000	0.00000	-1.83751	0.00000	0.00000	1.83412	0.00000	0.00000	-1.83125
6	0.00000	1.21024	-1.13697	0.00000	1.20787	1.13518	0.00000	1.20551	-1.13224
6	0.00000	1.21992	0.26109	0.00000	1.21665	-0.25946	0.00000	1.21406	0.26064
9	0.00000	0.00000	2.28820	0.00000	0.00000	-2.28453	0.00000	0.00000	2.27189
1	0.00000	-2.14428	0.82855	0.00000	-2.14080	-0.82877	0.00000	-2.13732	0.82781
1	0.00000	-2.15254	-1.67664	0.00000	-2.15094	1.67512	0.00000	-2.14715	-1.67084
1	0.00000	0.00000	-2.92300	0.00000	0.00000	2.92040	0.00000	0.00000	-2.91546
1	0.00000	2.15254	-1.67664	0.00000	2.15094	1.67512	0.00000	2.14715	-1.67084
1	0.00000	2.14428	0.82855	0.00000	2.14080	-0.82877	0.00000	2.13732	0.82781

$1i_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.90296	0.00000	0.00000	0.89735	0.00000	0.00000	0.90582	0.00000
6	1.30250	0.43618	0.00000	1.31797	0.45770	0.00000	1.31143	0.44772	0.00000
6	1.33734	-0.98041	0.00000	1.33370	-0.95874	0.00000	1.32750	-0.96847	0.00000
6	0.19974	-1.81138	0.00000	0.20789	-1.80476	0.00000	0.19858	-1.80177	0.00000
6	-1.07649	-1.23562	0.00000	-1.06806	-1.24066	0.00000	-1.07413	-1.23272	0.00000
6	-1.18400	0.16282	0.00000	-1.18221	0.15240	0.00000	-1.17790	0.16019	0.00000
9	-0.21788	2.30434	0.00000	-0.24094	2.28502	0.00000	-0.22160	2.27896	0.00000
1	2.30968	-1.48759	0.00000	2.30726	-1.47128	0.00000	2.29755	-1.48533	0.00000
1	0.30586	-2.89866	0.00000	0.32242	-2.89217	0.00000	0.30416	-2.88893	0.00000
1	-1.97242	-1.85473	0.00000	-1.96156	-1.86649	0.00000	-1.96906	-1.85252	0.00000
1	-2.15672	0.65455	0.00000	-2.15537	0.64502	0.00000	-2.15114	0.65147	0.00000

$1i_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.87832	0.00000	0.00000	0.88019	0.00000	0.00000	0.88477	0.00000
6	1.20669	0.18955	0.00000	1.20640	0.19750	0.00000	1.20453	0.19607	0.00000
6	1.12272	-1.21169	0.00000	1.13021	-1.19917	0.00000	1.12244	-1.19989	0.00000
6	-0.13155	-1.84250	0.00000	-0.12448	-1.82767	0.00000	-0.12562	-1.82851	0.00000
6	-1.38218	-1.16389	0.00000	-1.39151	-1.17920	0.00000	-1.38811	-1.17066	0.00000
6	-1.24205	0.25209	0.00000	-1.23264	0.23275	0.00000	-1.23040	0.24256	0.00000
9	0.06726	2.27773	0.00000	0.05277	2.27219	0.00000	0.05710	2.25802	0.00000
1	2.15239	0.72440	0.00000	2.14902	0.74091	0.00000	2.14686	0.73569	0.00000
1	2.04514	-1.79987	0.00000	2.05598	-1.78319	0.00000	2.04830	-1.78254	0.00000
1	-0.12351	-2.93830	0.00000	-0.09816	-2.92678	0.00000	-0.10150	-2.92666	0.00000
1	-2.12113	0.90289	0.00000	-2.10964	0.89287	0.00000	-2.10460	0.90534	0.00000

$1i_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	0.00000	0.88306	0.00000	0.00000	0.88752	0.00000	0.00000	0.89358
6	0.00000	1.21117	0.20734	0.00000	1.20760	0.20890	0.00000	1.20331	0.20764

6	0.00000	1.17772	-1.20397	0.00000	1.16502	-1.19951	0.00000	1.16658	-1.19684
6	0.00000	0.00000	-1.99671	0.00000	0.00000	-2.01323	0.00000	0.00000	-2.00655
6	0.00000	-1.17772	-1.20397	0.00000	-1.16502	-1.19951	0.00000	-1.16658	-1.19684
6	0.00000	-1.21117	0.20734	0.00000	-1.20760	0.20890	0.00000	-1.20331	0.20764
9	0.00000	0.00000	2.27770	0.00000	0.00000	2.27403	0.00000	0.00000	2.26261
1	0.00000	2.14534	0.76994	0.00000	2.14084	0.77466	0.00000	2.13519	0.77437
1	0.00000	2.15558	-1.69886	0.00000	2.15096	-1.68704	0.00000	2.15254	-1.68204
1	0.00000	-2.15558	-1.69886	0.00000	-2.15096	-1.68704	0.00000	-2.15254	-1.68204
1	0.00000	-2.14534	0.76994	0.00000	-2.14084	0.77466	0.00000	-2.13519	0.77437

1j. Benzonitrile

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.21193	-1.48513	0.00000	0.00000	1.20918	-1.48366	1.20804	-1.48020	0.00000
6	1.21852	-0.09110	0.00000	0.00000	1.21744	-0.09142	1.21416	-0.09077	0.00000
6	0.00000	0.61062	0.00000	0.00000	0.00000	0.60335	0.00000	0.60959	0.00000
6	-1.21853	-0.09110	0.00000	0.00000	-1.21744	-0.09142	-1.21416	-0.09077	0.00000
6	-1.21194	-1.48513	0.00000	0.00000	-1.20918	-1.48366	-1.20804	-1.48020	0.00000
6	-0.00001	-2.18275	0.00000	0.00000	0.00000	-2.18078	0.00000	-2.17557	0.00000
1	2.15276	-2.02672	0.00000	0.00000	2.15074	-2.02621	2.14792	-2.02110	0.00000
1	2.15377	0.45867	0.00000	0.00000	2.15298	0.46129	2.14747	0.45969	0.00000
6	0.00000	2.04651	0.00000	0.00000	0.00000	2.03749	0.00000	2.04049	0.00000
1	-2.15377	0.45868	0.00000	0.00000	-2.15298	0.46129	-2.14747	0.45969	0.00000
1	-2.15277	-2.02671	0.00000	0.00000	-2.15074	-2.02621	-2.14792	-2.02110	0.00000
1	-0.00001	-3.26861	0.00000	0.00000	0.00000	-3.26763	0.00000	-3.26027	0.00000
7	0.00002	3.21046	0.00000	0.00000	0.00000	3.21971	0.00000	3.19823	0.00000

1j$_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.44227	-1.26481	0.00000	1.43545	-1.24668	0.00000	1.43132	-1.25843	0.00000
6	1.35620	0.15555	0.00000	1.36466	0.17213	0.00000	1.35969	0.16233	0.00000
6	0.00000	0.59686	0.00000	0.00000	0.58016	0.00000	0.00000	0.59166	0.00000
6	-1.13862	-0.24735	0.00000	-1.13989	-0.25289	0.00000	-1.13576	-0.24755	0.00000
6	-0.96242	-1.62843	0.00000	-0.95731	-1.63214	0.00000	-0.96407	-1.62337	0.00000
6	0.34684	-2.13756	0.00000	0.34708	-2.13267	0.00000	0.34165	-2.12862	0.00000
1	2.43524	-1.72701	0.00000	2.42877	-1.71573	0.00000	2.42150	-1.73009	0.00000
6	-0.26660	2.01766	0.00000	-0.27236	2.00198	0.00000	-0.26622	2.00859	0.00000
1	-2.14251	0.17851	0.00000	-2.14523	0.17373	0.00000	-2.13842	0.17982	0.00000
1	-1.82218	-2.29565	0.00000	-1.81603	-2.30374	0.00000	-1.82337	-2.28973	0.00000
1	0.50131	-3.21953	0.00000	0.50894	-3.21439	0.00000	0.49313	-3.21073	0.00000
7	-0.51970	3.15889	0.00000	-0.52033	3.16011	0.00000	-0.50750	3.14615	0.00000

1j$_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.38629	-1.51912	0.00000	1.40040	-1.52835	0.00000	1.39006	-1.52546	0.00000
6	1.24510	-0.10983	0.00000	1.23936	-0.12030	0.00000	1.23577	-0.11796	0.00000
6	0.00000	0.57237	0.00000	0.00000	0.56564	0.00000	0.00000	0.57105	0.00000
6	-1.20545	-0.15889	0.00000	-1.20577	-0.15528	0.00000	-1.20484	-0.15272	0.00000
6	-1.12391	-1.55047	0.00000	-1.12470	-1.54406	0.00000	-1.12542	-1.53885	0.00000
6	0.13217	-2.18596	0.00000	0.13258	-2.17338	0.00000	0.12557	-2.17230	0.00000
1	2.13585	0.52400	0.00000	2.12789	0.52465	0.00000	2.12300	0.52349	0.00000
6	-0.04390	2.00496	0.00000	-0.04135	1.99608	0.00000	-0.03778	1.99813	0.00000
1	-2.16194	0.35725	0.00000	-2.16184	0.36683	0.00000	-2.15735	0.36849	0.00000
1	-2.04390	-2.13912	0.00000	-2.04610	-2.13251	0.00000	-2.04808	-2.12252	0.00000
1	0.11699	-3.28176	0.00000	0.10508	-3.27242	0.00000	0.09561	-3.26984	0.00000
7	-0.05555	3.17446	0.00000	-0.06117	3.18162	0.00000	-0.04476	3.16129	0.00000

1j$_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.18256	-1.54570	0.00000	0.00000	1.16776	-1.54431	0.00000	1.17382	-1.53861
6	1.21247	-0.14856	0.00000	0.00000	1.20889	-0.14490	0.00000	1.20657	-0.14835
6	0.00000	0.57518	0.00000	0.00000	0.00000	0.56903	0.00000	0.00000	0.57742
6	-1.21247	-0.14856	0.00000	0.00000	-1.20889	-0.14490	0.00000	-1.20657	-0.14835
6	-1.18256	-1.54570	0.00000	0.00000	-1.16776	-1.54431	0.00000	-1.17382	-1.53861
6	0.00000	-2.34141	0.00000	0.00000	0.00000	-2.35794	0.00000	0.00000	-2.34787
1	2.15647	-2.04661	0.00000	0.00000	2.14966	-2.03719	0.00000	2.15384	-2.03151
1	2.15583	0.39906	0.00000	0.00000	2.15305	0.40467	0.00000	2.14760	0.40245
6	0.00000	2.00262	0.00000	0.00000	0.00000	1.99820	0.00000	0.00000	1.99844
1	-2.15583	0.39906	0.00000	0.00000	-2.15305	0.40467	0.00000	-2.14760	0.40245
1	-2.15647	-2.04661	0.00000	0.00000	-2.14966	-2.03719	0.00000	-2.15384	-2.03151
7	0.00000	3.17255	0.00000	0.00000	0.00000	3.18283	0.00000	0.00000	3.16195

1k. Chlorobenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.20860	-1.57552	0.00000	0.00000	-1.20625	-1.56794	0.00000	-1.20494	-1.56957
6	1.21686	-0.17800	0.00000	0.00000	-1.21391	-0.17376	0.00000	-1.21348	-0.17700
6	0.00000	0.50498	0.00000	0.00000	0.00000	0.51013	0.00000	0.00000	0.50378
6	-1.21686	-0.17800	0.00000	0.00000	1.21391	-0.17376	0.00000	1.21348	-0.17700
6	-1.20860	-1.57552	0.00000	0.00000	1.20625	-1.56794	0.00000	1.20494	-1.56957
6	0.00000	-2.27711	0.00000	0.00000	0.00000	-2.26827	0.00000	0.00000	-2.26839
1	2.15228	-2.11302	0.00000	0.00000	-2.15051	-2.10608	0.00000	-2.14747	-2.10640
1	2.15034	0.37407	0.00000	0.00000	-2.14781	0.38035	0.00000	-2.14418	0.37676
17	0.00000	2.26563	0.00000	0.00000	0.00000	2.25032	0.00000	0.00000	2.25638
1	-2.15034	0.37407	0.00000	0.00000	2.14781	0.38035	0.00000	2.14418	0.37676
1	-2.15228	-2.11302	0.00000	0.00000	2.15051	-2.10608	0.00000	2.14747	-2.10640
1	0.00000	-3.36275	0.00000	0.00000	0.00000	-3.35474	0.00000	0.00000	-3.35266

1k$_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.58377	-1.23930	0.00000	1.56418	-1.21523	0.00000	1.61008	-1.19860	0.00000
6	1.34180	0.15924	0.00000	1.35627	0.18790	0.00000	1.34350	0.19411	0.00000
6	0.00000	0.43996	0.00000	0.00000	0.45072	0.00000	0.00000	0.42486	0.00000
6	-1.07711	-0.45048	0.00000	-1.07990	-0.43919	0.00000	-1.05761	-0.47752	0.00000
6	-0.77256	-1.81794	0.00000	-0.77897	-1.80234	0.00000	-0.72369	-1.83306	0.00000
6	0.57209	-2.21375	0.00000	0.55978	-2.19737	0.00000	0.62604	-2.19243	0.00000
1	2.61803	-1.60177	0.00000	2.59742	-1.59037	0.00000	2.65146	-1.54386	0.00000
17	-0.56745	2.25146	0.00000	-0.55549	2.21040	0.00000	-0.63174	2.23727	0.00000
1	-2.10999	-0.10840	0.00000	-2.11327	-0.09398	0.00000	-2.09596	-0.15664	0.00000
1	-1.57427	-2.55468	0.00000	-1.58317	-2.53885	0.00000	-1.50652	-2.58825	0.00000
1	0.82488	-3.27633	0.00000	0.81424	-3.26050	0.00000	0.90069	-3.24909	0.00000

1k$_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.46269	-1.54584	0.00000	1.45129	-1.57151	0.00000	1.47529	-1.54202	0.00000
6	1.27256	-0.13744	0.00000	1.25601	-0.16527	0.00000	1.26868	-0.13736	0.00000
6	0.00000	0.43376	0.00000	0.00000	0.44699	0.00000	0.00000	0.42712	0.00000

6	-1.17428	-0.31579	0.00000	-1.18362	-0.28292	0.00000	-1.17141	-0.31826	0.00000
6	-1.03055	-1.71069	0.00000	-1.06298	-1.67466	0.00000	-1.02180	-1.70734	0.00000
6	0.25030	-2.28355	0.00000	0.21031	-2.26314	0.00000	0.25689	-2.26926	0.00000
1	2.12961	0.53975	0.00000	2.12058	0.50946	0.00000	2.11655	0.55333	0.00000
17	-0.17850	2.25699	0.00000	-0.13222	2.23451	0.00000	-0.18813	2.25095	0.00000
1	-2.14794	0.16374	0.00000	-2.15049	0.21512	0.00000	-2.14259	0.16227	0.00000
1	-1.92778	-2.33674	0.00000	-1.97075	-2.28591	0.00000	-1.91893	-2.33324	0.00000
1	0.29636	-3.37817	0.00000	0.22241	-3.36219	0.00000	0.29731	-3.36580	0.00000

1k$_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.17583	-1.64753	0.00000	0.00000	-1.16287	-1.63642	0.00000	-1.16697	-1.63978
6	1.21042	-0.23823	0.00000	0.00000	-1.20710	-0.22972	0.00000	-1.20642	-0.23745
6	0.00000	0.44914	0.00000	0.00000	0.00000	0.45849	0.00000	0.00000	0.44865
6	-1.21042	-0.23823	0.00000	0.00000	1.20710	-0.22972	0.00000	1.20642	-0.23745
6	-1.17583	-1.64753	0.00000	0.00000	1.16287	-1.63642	0.00000	1.16697	-1.63978
6	0.00000	-2.44281	0.00000	0.00000	0.00000	-2.45208	0.00000	0.00000	-2.44916
1	2.15521	-2.13949	0.00000	0.00000	-2.14960	-2.12179	0.00000	-2.15278	-2.12372
1	2.15224	0.30965	0.00000	0.00000	-2.14870	0.32145	0.00000	-2.14413	0.31589
17	0.00000	2.25005	0.00000	0.00000	0.00000	2.23270	0.00000	0.00000	2.24385
1	-2.15224	0.30965	0.00000	0.00000	2.14870	0.32145	0.00000	2.14413	0.31589
1	-2.15521	-2.13949	0.00000	0.00000	2.14960	-2.12179	0.00000	2.15278	-2.12372

1l. Trifluoromethoxybenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.49039	-0.00004	-0.44491	0.46629	-0.00006	-0.47525	0.51127	0.36790	-0.00010
6	1.14272	1.21811	-0.27683	1.11082	1.21766	-0.29247	1.49455	1.35316	-0.00007
6	2.49173	1.21081	0.08735	2.45161	1.20912	0.08979	2.83396	0.98346	-0.00001
6	3.16581	0.00004	0.27113	3.12132	0.00006	0.28331	3.19144	-0.36361	0.00001
6	2.49178	-1.21078	0.08737	2.45172	-1.20905	0.08980	2.19604	-1.33514	-0.00003
6	1.14278	-1.21814	-0.27681	1.11090	-1.21773	-0.29241	0.84668	-0.98309	-0.00008
8	-0.85117	-0.00008	-0.88749	-0.86780	-0.00009	-0.92885	-0.79029	0.86410	-0.00017
1	0.60197	2.14524	-0.43089	0.56791	2.14304	-0.45610	1.19166	2.39347	-0.00008
1	3.01418	2.15268	0.22380	2.97287	2.15113	0.23644	3.59837	1.75296	0.00001
1	3.01428	-2.15262	0.22384	2.97305	-2.15102	0.23650	2.46192	-2.38684	-0.00001
1	0.60207	-2.14530	-0.43085	0.56810	-2.14316	-0.45604	0.08695	-1.75108	-0.00012
6	-1.82909	-0.00001	0.04424	-1.80145	-0.00001	0.05280	-1.85800	0.03282	0.00004
9	-3.00609	-0.00013	-0.59389	-3.00159	-0.00020	-0.52777	-2.94452	0.78740	0.00002
9	-1.78660	-1.08592	0.85336	-1.70874	-1.08282	0.85056	-1.89165	-0.76062	-1.07882
9	-1.78669	1.08612	0.85308	-1.70895	1.08309	0.85021	-1.89146	-0.76031	1.07913
1	4.21452	0.00006	0.55194	4.16662	0.00011	0.57952	4.23638	-0.65250	0.00005

1l$_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.60344	0.25609	0.00015	-0.550426	-0.105311	-0.448239	-0.55043	-0.10531	-0.44824
6	1.51018	1.31958	0.00006	-1.116474	1.161194	-0.283733	-1.11647	1.16119	-0.28373
6	2.87279	1.00286	-0.00006	-2.460344	1.207870	0.088613	-2.46034	1.20787	0.08861
6	3.25084	-0.34669	-0.00008	-3.145442	0.004509	0.269824	-3.14544	0.00451	0.26982
6	2.26215	-1.34548	0.00001	-2.471783	-1.212966	0.074451	-2.47178	-1.21297	0.07445
6	0.86550	-1.09975	0.00014	-1.113636	-1.361629	-0.310510	-1.11364	-1.36163	-0.31051
8	-0.77820	0.78941	0.00032	0.857543	-0.021772	-0.920855	0.85754	-0.02177	-0.92086
1	1.16922	2.35399	0.00008	-0.535837	2.068927	-0.440886	-0.53584	2.06893	-0.44089
1	3.61864	1.79551	-0.00013	-2.958516	2.166768	0.231020	-2.95852	2.16677	0.23102
1	4.30967	-0.61341	-0.00018	-4.199033	0.019635	0.559982	-4.19903	0.01964	0.55998
1	2.61530	-2.38292	-0.00002	-3.072998	-2.118936	0.232194	-3.07300	-2.11894	0.23219
6	-1.84976	0.02035	-0.00001	1.774627	-0.019190	0.023960	1.77463	-0.01919	0.02396

9	-2.95251	0.85071	0.00003	3.004465	0.022349	-0.556559	3.00447	0.02235	-0.55656
9	-2.00014	-0.77567	-1.09214	1.715125	1.070178	0.854251	1.71513	1.07018	0.85425
9	-2.00047	-0.77617	1.09171	1.770067	-1.093536	0.846566	1.77007	-1.09354	0.84657

$1l_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.56631	-0.05354	-0.41879	-0.53762	-0.05077	-0.44890	-0.58948	0.31221	-0.00013
6	-1.18803	1.18243	-0.27695	-1.14857	1.18571	-0.29326	-1.54041	1.32399	-0.00005
6	-2.54277	1.15873	0.08012	-2.49269	1.16399	0.08519	-2.87873	0.93130	0.00003
6	-3.19942	-0.06881	0.26711	-3.14197	-0.06611	0.27818	-3.20561	-0.42696	0.00005
6	-2.59713	-1.34745	0.11814	-2.56782	-1.35846	0.12451	-2.27474	-1.49922	-0.00003
6	-1.22379	-1.26823	-0.24264	-1.20314	-1.26010	-0.25808	-0.92782	-1.03667	-0.00012
8	0.82151	-0.05343	-0.87265	0.83739	-0.05778	-0.91842	0.76195	0.83669	-0.00024
1	-0.64108	2.10585	-0.43891	-0.59670	2.10594	-0.46686	-1.22857	2.36312	-0.00006
1	-3.07656	2.10442	0.20542	-3.02278	2.11076	0.22256	-3.65341	1.70258	0.00009
1	-4.25836	-0.01316	0.54272	-4.19855	0.00389	0.57170	-4.27848	-0.65868	0.00012
1	-0.63481	-2.17569	-0.39801	-0.60629	-2.16412	-0.42761	-0.11538	-1.76440	-0.00019
6	1.78927	0.00230	0.02724	1.76046	0.00025	0.03445	1.81994	0.04507	0.00003
9	2.98699	-0.05182	-0.61777	2.98078	-0.05860	-0.54878	2.92059	0.82150	-0.00002
9	1.80480	1.15260	0.76874	1.73151	1.14872	0.76224	1.91522	-0.75690	1.08046
9	1.78686	-1.01484	0.93177	1.70030	-1.01026	0.93266	1.91545	-0.75732	-1.08008

$1l_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.55604	-0.00002	-0.42110	0.52884	0.00002	-0.45304	0.57769	0.35126	-0.00037
6	1.21501	1.21225	-0.25527	1.18034	1.21083	-0.27294	1.56134	1.32887	-0.00012
6	2.57525	1.17933	0.10628	2.53337	1.16702	0.10971	2.90372	0.92958	0.00009
6	3.34158	0.00003	0.30939	3.31462	0.00003	0.32992	3.37786	-0.40969	0.00011
6	2.57529	-1.17930	0.10630	2.53333	-1.16703	0.10970	2.28801	-1.31784	-0.00015
6	1.21505	-1.21227	-0.25525	1.18038	-1.21086	-0.27290	0.92041	-0.99340	-0.00040
8	-0.81730	-0.00006	-0.87811	-0.83489	-0.00002	-0.92144	-0.76674	0.85715	-0.00064
1	0.67714	2.14745	-0.40801	0.64027	2.14418	-0.43546	1.25870	2.37573	-0.00010
1	3.05609	2.15582	0.22904	3.00572	2.15066	0.23984	3.62906	1.75401	0.00027
1	3.05616	-2.15578	0.22907	3.00572	-2.15065	0.23985	2.49400	-2.39647	-0.00017
1	0.67721	-2.14749	-0.40798	0.64028	-2.14420	-0.43543	0.15919	-1.76750	-0.00062
6	-1.78715	-0.00001	0.02640	-1.76106	0.00000	0.03436	-1.81171	0.04864	0.00011
9	-2.98105	-0.00014	-0.62367	-2.97751	-0.00041	-0.55624	-2.92352	0.80226	-0.00004
9	-1.79134	-1.08655	0.84987	-1.71499	-1.08265	0.84805	-1.88915	-0.75994	-1.07906
9	-1.79146	1.08674	0.84961	-1.71549	1.08307	0.84750	-1.88854	-0.75871	1.08022

$1l_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.56631	0.05354	-0.41879	0.53757	0.05065	-0.44906	0.59072	0.37641	-0.00050
6	1.22379	1.26823	-0.24264	1.20293	1.26000	-0.25818	1.55834	1.37407	-0.00010
6	2.59713	1.34745	0.11814	2.56763	1.35853	0.12449	2.95551	1.12738	0.00023
6	3.19942	0.06881	0.26711	3.14187	0.06630	0.27827	3.22941	-0.26871	0.00011
6	2.54277	-1.15873	0.08012	2.49271	-1.16391	0.08520	2.27167	-1.28322	-0.00030
6	1.18803	-1.18243	-0.27695	1.14867	-1.18581	-0.29328	0.90662	-0.97604	-0.00064
8	-0.82151	0.05343	-0.87265	-0.83747	0.05751	-0.91855	-0.77339	0.85784	-0.00086
1	0.63481	2.17569	-0.39801	0.60601	2.16397	-0.42779	1.17124	2.39911	-0.00004
1	4.25836	0.01317	0.54272	4.19842	-0.00361	0.57194	4.27478	-0.60326	0.00035
1	3.07656	-2.10442	0.20542	3.02290	-2.11063	0.22265	2.56428	-2.33642	-0.00039
1	0.64108	-2.10585	-0.43891	0.59690	-2.10611	-0.46690	0.15247	-1.75100	-0.00102
6	-1.78927	-0.00230	0.02724	-1.76041	-0.00024	0.03448	-1.80838	0.04043	0.00016
9	-2.98699	0.05182	-0.61777	-2.98078	0.05843	-0.54865	-2.93341	0.77613	-0.00001
9	-1.80480	-1.15260	0.76874	-1.73133	-1.14856	0.76257	-1.87810	-0.77296	-1.07876

9	-1.78687	1.01484	0.93177	-1.70015	1.01048	0.93240	-1.87726	-0.77129	1.08036

1l$_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.576271	-0.127356	-0.414684	-0.550384	-0.105166	-0.448346	-0.56019	-0.13317	-0.42985
6	-1.186800	-1.357980	-0.279086	-1.113520	-1.361558	-0.310633	-1.10762	1.13893	-0.28203
6	-2.553284	-1.206332	0.079150	-2.471651	-1.213010	0.074396	-2.45210	1.22119	0.07657
6	-3.198420	0.028490	0.254589	-3.145373	0.004382	0.269964	-3.16329	0.03331	0.26060
6	-2.483653	1.221427	0.076628	-2.460421	1.207810	0.088697	-2.52285	-1.19718	0.08218
6	-1.130565	1.146729	-0.271979	-1.116602	1.161266	-0.283819	-1.16208	-1.36785	-0.28599
8	0.848724	-0.095693	-0.873102	0.857459	-0.021483	-0.920762	0.85477	-0.10054	-0.89174
1	-3.164755	-2.103462	0.226534	-3.072808	-2.119042	0.232042	-0.51119	2.03470	-0.43835
1	-4.256068	0.067703	0.524122	-4.198919	0.019408	0.560316	-2.92931	2.18985	0.20597
1	-2.965132	2.189231	0.202523	-2.958685	2.166659	0.23116	-4.21812	0.07764	0.53898
1	-0.538283	2.046903	-0.423883	-0.536098	2.069066	-0.441142	-3.14310	-2.08844	0.24040
6	1.808391	-0.027781	0.016736	1.774622	-0.019162	0.024008	1.79168	-0.02424	0.02314
9	3.018602	-0.092363	-0.619417	3.004374	0.023324	-0.556532	3.00132	-0.10810	-0.57510
9	1.836754	1.154898	0.734949	1.714736	1.069521	0.855056	1.79981	1.15498	0.71147
9	1.817761	-1.006758	0.960846	1.770536	-1.094133	0.845711	1.75690	-0.98413	0.96576

1m. Trifluoromethylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.05300	0.00012	-0.03264	-0.04793	0.00017	-0.04247	-0.00021	0.05463	0.00000
6	-0.74812	-1.21404	-0.01986	-0.73712	-1.21330	-0.02539	-1.39105	0.17614	0.00000
6	-2.14376	-1.21050	0.00178	-2.13001	-1.20850	0.00131	-1.97312	1.43803	0.00000
6	-2.84236	-0.00008	0.01299	-2.82737	-0.00009	0.01678	-1.16902	2.57767	0.00000
6	-2.14393	1.21043	0.00178	-2.13025	1.20841	0.00131	0.21711	2.45265	0.00000
6	-0.74827	1.21416	-0.01986	-0.73732	1.21347	-0.02538	0.80526	1.18972	0.00000
6	1.45237	0.00006	-0.00423	1.44590	0.00006	-0.00145	0.60415	-1.32451	0.00000
1	-0.20254	-2.15141	-0.03333	-0.18802	-2.14982	-0.04414	-2.00985	-0.71438	0.00000
1	-2.68384	-2.15229	0.00739	-2.67188	-2.15038	0.00896	-3.05346	1.53390	0.00000
1	-3.92823	-0.00015	0.02795	-3.91403	-0.00020	0.03654	-1.62492	3.56210	0.00000
1	-2.68413	2.15214	0.00739	-2.67228	2.15019	0.00896	0.84452	3.33737	0.00000
1	-0.20282	2.15160	-0.03332	-0.18840	2.15009	-0.04411	1.88280	1.08360	0.00000
9	1.98024	1.09220	-0.61172	1.96902	1.09094	-0.60670	1.94380	-1.29454	0.00000
9	1.93562	-0.00220	1.26987	1.90877	-0.00231	1.27126	0.21711	-2.02987	1.07800
9	1.98013	-1.09009	-0.61547	1.96879	-1.08876	-0.61061	0.21711	-2.02987	-1.07800

1m$_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.063753	0.082692	0.000000	-0.05806	0.08433	0.00000	-0.06093	0.08231	0.00000
6	-1.407036	0.535507	0.000000	-1.41291	0.50281	0.00000	-1.41057	0.51894	0.00000
6	-1.489819	1.952842	0.000000	-1.48233	1.91933	0.00000	-1.48130	1.93653	0.00000
6	-0.385861	2.817405	0.000000	-0.38739	2.79743	0.00000	-0.38439	2.80134	0.00000
6	0.914660	2.293839	0.000000	0.91125	2.28445	0.00000	0.91357	2.28530	0.00000
6	1.078697	0.906821	0.000000	1.08498	0.90202	0.00000	1.07583	0.90321	0.00000
6	0.147236	-1.409530	0.000000	0.15086	-1.39520	0.00000	0.15274	-1.40754	0.00000
1	-2.479478	2.423434	0.000000	-2.47296	2.39555	0.00000	-2.46896	2.41574	0.00000
1	-0.530335	3.901008	0.000000	-0.54003	3.88078	0.00000	-0.52827	3.88488	0.00000
1	1.782675	2.950682	0.000000	1.77570	2.94912	0.00000	1.77926	2.94424	0.00000
1	2.081047	0.482230	0.000000	2.08894	0.47917	0.00000	2.07713	0.47767	0.00000
9	1.480759	-1.780753	0.000000	1.47590	-1.77363	0.00000	1.47003	-1.77402	0.00000
9	-0.385861	-2.044891	1.087266	-0.38739	-2.01738	1.08516	-0.38439	-2.02650	1.07699
9	-0.385861	-2.044891	-1.087266	-0.38739	-2.01738	-1.08516	-0.38439	-2.02650	-1.07699

1m$_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.09804	-0.01044	-0.03273	-0.00182	0.09336	0.00000	-0.00798	0.09557	0.00000
6	0.78754	-1.24169	-0.02055	-1.29944	0.64452	0.00000	-1.30039	0.64914	0.00000
6	2.20093	-1.37258	0.00323	-1.61208	2.02853	0.00000	-1.60523	2.03471	0.00000
6	2.85393	-0.11094	0.01482	-0.41599	2.79941	0.00000	-0.41113	2.80695	0.00000
6	2.20332	1.13540	0.00204	0.89797	2.30221	0.00000	0.89488	2.30346	0.00000
6	0.80813	1.19946	-0.01883	1.12010	0.92673	0.00000	1.11350	0.92814	0.00000
6	-1.39381	0.00887	-0.00507	0.15867	-1.37717	0.00000	0.15971	-1.38643	0.00000
1	0.17135	-2.14437	-0.03566	-2.12099	-0.08460	0.00000	-2.12282	-0.07601	0.00000
1	3.94955	-0.08285	0.03439	-0.50047	3.89594	0.00000	-0.49213	3.90256	0.00000
1	2.77953	2.06371	0.00700	1.75497	2.98150	0.00000	1.75550	2.97630	0.00000
1	0.28670	2.15193	-0.03039	2.12501	0.51110	0.00000	2.11418	0.50970	0.00000
9	-1.94266	1.20848	-0.38521	1.46052	-1.79423	0.00000	1.45394	-1.79186	0.00000
9	-1.97064	-0.92967	-0.81732	-0.41599	-1.98119	1.08330	-0.41113	-1.98750	1.07588
9	-1.92400	-0.23846	1.24332	-0.41599	-1.98119	-1.08330	-0.41113	-1.98750	-1.07588

1m$_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.09357	0.00003	0.04110	-0.08769	0.00003	0.05368	-0.00606	0.09115	0.00000
6	-0.81091	-1.20770	0.02153	-0.79742	-1.20467	0.02801	-1.37577	0.38684	0.00000
6	-2.21109	-1.17959	-0.00604	-2.19797	-1.16589	-0.00560	-1.79429	1.71594	0.00000
6	-3.00771	-0.00003	-0.02115	-3.01292	-0.00003	-0.02600	-0.94462	2.86007	0.00000
6	-2.21114	1.17956	-0.00604	-2.19802	1.16586	-0.00560	0.42237	2.46736	0.00000
6	-0.81095	1.20773	0.02153	-0.79746	1.20470	0.02801	0.90025	1.15549	0.00000
6	1.39025	0.00002	0.00808	1.38734	0.00001	0.00405	0.44126	-1.32325	0.00000
1	-0.27074	-2.15457	0.03481	-0.25415	-2.15102	0.04747	-2.09528	-0.43373	0.00000
1	-2.70889	-2.15542	-0.01310	-2.68882	-2.14915	-0.01407	-2.88182	1.86550	0.00000
1	-2.70897	2.15538	-0.01310	-2.68890	2.14911	-0.01409	1.19632	3.24605	0.00000
1	-0.27082	2.15461	0.03481	-0.25423	2.15107	0.04745	1.96827	0.94238	0.00000
9	1.95423	1.09301	0.61174	1.94807	1.08976	0.60512	1.78474	-1.46640	0.00000
9	1.95423	-1.09251	0.61260	1.94806	-1.08917	0.60614	-0.00606	-2.03023	1.07500
9	1.92376	-0.00051	-1.26850	1.89397	-0.00060	-1.26970	-0.00606	-2.03023	-1.07500

1m$_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.09804	0.01044	-0.03273	-0.09253	0.00508	-0.04468	0.00041	0.10562	0.00000
6	-0.80813	-1.19946	-0.01883	-0.79466	-1.20424	-0.02428	-1.39805	0.18258	0.00000
6	-2.20332	-1.13540	0.00204	-2.18559	-1.14005	0.00129	-1.97573	1.44629	0.00000
6	-2.85393	0.11094	0.01481	-2.82885	0.10908	0.01883	-1.16409	2.58975	0.00000
6	-2.20093	1.37258	0.00323	-2.19833	1.38394	0.00397	0.25468	2.60432	0.00000
6	-0.78754	1.24169	-0.02055	-0.78723	1.23145	-0.02626	0.77019	1.27834	0.00000
6	1.39381	-0.00887	-0.00507	1.38624	-0.00698	-0.00252	0.61872	-1.25129	0.00000
1	-0.28670	-2.15193	-0.03039	-0.26806	-2.15581	-0.03990	-2.00265	-0.72045	0.00000
1	-2.77953	-2.06371	0.00701	-2.76306	-2.06858	0.00840	-3.06481	1.53213	0.00000
1	-3.94955	0.08285	0.03439	-3.92744	0.06882	0.04437	-1.70266	3.54727	0.00000
1	-0.17135	2.14437	-0.03565	-0.15854	2.13057	-0.04773	1.85360	1.13164	0.00000
9	1.97064	0.92966	-0.81733	1.95741	0.92837	-0.81481	1.96616	-1.24096	0.00000
9	1.92400	0.23848	1.24331	1.89686	0.24724	1.24251	0.25468	-2.00309	1.07713
9	1.94266	-1.20848	-0.38519	1.93714	-1.20280	-0.37474	0.25468	-2.00309	-1.07713

1m$_6$

Atomic Number	Atomic Coordinate		
	DFT	G3MP2	G4MP2

	x	y	z	x	y	z	x	y	z
6	-0.08990	0.05307	0.00002	-0.09079	0.04718	-0.00007	-0.00353	0.14547	0.00000
6	-0.76719	-1.18211	0.00001	-0.76160	-1.18729	0.00000	-1.25496	-0.49755	0.00000
6	-2.16386	-1.19000	0.00000	-2.15520	-1.18501	0.00001	-2.41445	0.26519	0.00000
6	-2.84349	0.03622	0.00000	-2.82373	0.04033	0.00003	-2.28926	1.65913	0.00000
6	-2.12134	1.23817	0.00000	-2.08697	1.23529	0.00000	-1.02402	2.24438	0.00000
6	-0.70459	1.33042	0.00001	-0.67306	1.34054	-0.00007	0.21490	1.54310	0.00000
6	1.41693	0.02735	0.00001	1.40322	0.02174	-0.00002	1.17517	-0.79067	0.00000
1	-0.22250	-2.12460	0.00001	-0.21851	-2.13150	-0.00004	-1.32484	-1.58593	0.00000
1	-2.70890	-2.13224	-0.00001	-2.70836	-2.12459	0.00001	-3.39288	-0.21036	0.00000
1	-3.93663	0.04625	-0.00001	-3.91752	0.05861	0.00003	-3.19157	2.27594	0.00000
1	-2.71013	2.16240	0.00000	-2.68138	2.15969	0.00005	-1.00438	3.34196	0.00000
9	1.98183	0.63444	-1.08736	1.95447	0.63184	-1.08542	2.37083	-0.19741	0.00000
9	1.98187	0.63474	1.08717	1.95443	0.63285	1.08491	1.17517	-1.63662	1.07827
9	1.94950	-1.25034	0.00017	1.94160	-1.24678	0.00058	1.17517	-1.63662	-1.07827

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Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.714236	0.254431	0.077599	-0.69753	0.24411	-0.11474	-0.71647	0.25320	0.00010
6	-1.682167	1.257118	-0.120639	-1.63389	1.25098	0.16501	-1.69893	1.25667	-0.00014
6	-3.036923	0.942405	-0.197972	-2.98727	0.94999	0.27857	-3.04992	0.94069	-0.00024
6	-3.457113	-0.384450	-0.060144	-3.43185	-0.35965	0.09075	-3.45474	-0.39357	-0.00008
6	-2.510633	-1.389292	0.150238	-2.51151	-1.36290	-0.20981	-2.49594	-1.40169	0.00019
6	-1.151008	-1.074806	0.210263	-1.15176	-1.06897	-0.30353	-1.14045	-1.08269	0.00027
6	0.724065	0.716633	0.161807	0.73269	0.68855	-0.23453	0.71916	0.73260	0.00022
6	1.932739	-0.228530	-0.075976	1.91008	-0.23118	0.10906	1.93399	-0.23076	-0.00008
6	3.195150	0.639096	-0.253229	3.13622	0.64696	0.36538	3.21747	0.62030	-0.00035
6	2.142252	-1.128665	1.169155	1.62598	-1.05907	1.36607	1.93902	-1.10251	1.27718
6	1.745555	-1.082205	-1.351727	2.21420	-1.13901	-1.09260	1.93842	-1.10241	-1.27743
8	0.930170	1.898138	0.410223	0.94826	1.84842	-0.59464	0.92070	1.93188	0.00053
1	-1.345777	2.284231	-0.210218	-1.27721	2.26954	0.28686	-1.36638	2.28727	-0.00024
1	-3.765654	1.730908	-0.362063	-3.69860	1.73911	0.50909	-3.78978	1.73435	-0.00046
1	-4.513252	-0.632505	-0.114405	-4.48973	-0.59601	0.17313	-4.51034	-0.64487	-0.00015
1	-2.827714	-2.421410	0.267910	-2.85204	-2.38245	-0.37248	-2.80021	-2.44306	0.00034
1	-0.444677	-1.876509	0.379929	-0.46188	-1.86709	-0.55081	-0.42547	-1.89238	0.00049
1	4.062718	-0.010330	-0.413478	3.99307	0.01228	0.61271	4.09292	-0.03736	-0.00038
1	3.100680	1.307339	-1.114379	3.38099	1.24729	-0.51192	3.26641	1.26540	-0.88038
1	3.379832	1.260931	0.625365	2.95948	1.33170	1.19944	3.26662	1.26562	0.87950
1	3.048681	-1.728950	1.031307	2.52238	-1.62777	1.63445	2.84261	-1.72138	1.29063
1	2.277576	-0.519646	2.069106	1.37696	-0.40772	2.21023	1.95465	-0.47411	2.17365
1	1.314827	-1.818057	1.351497	0.80531	-1.76500	1.23428	1.07936	-1.76919	1.35590
1	2.657570	-1.660631	-1.536830	3.11149	-1.72997	-0.88019	2.84236	-1.72075	-1.29168
1	0.913552	-1.785423	-1.285022	1.40445	-1.83488	-1.32074	1.07909	-1.76960	-1.35545
1	1.574195	-0.445462	-2.226750	2.40702	-0.53537	-1.98473	1.95293	-0.47395	-2.17387

$1n_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.72455	-0.23307	0.00000	-0.71517	-0.23491	-0.00001	-0.71932	-0.23874	-0.00026
6	-1.03573	1.16048	-0.00001	-0.99930	1.16066	-0.00002	-1.01727	1.15486	-0.00029
6	-2.43264	1.42460	-0.00001	-2.39260	1.41387	-0.00002	-2.41111	1.41745	-0.00008
6	-3.42652	0.44135	0.00000	-3.39689	0.43779	0.00001	-3.40450	0.44161	0.00015
6	-3.06472	-0.91754	0.00001	-3.03968	-0.91475	0.00002	-3.05125	-0.91463	0.00015
6	-1.71519	-1.25050	0.00000	-1.69384	-1.25515	0.00001	-1.70827	-1.25032	-0.00006
6	0.69078	-0.73640	-0.00001	0.69692	-0.73621	-0.00001	0.69050	-0.74489	-0.00055
6	1.91230	0.23506	0.00000	1.89078	0.23815	0.00001	1.90208	0.23692	0.00005
6	1.88336	1.12739	1.26287	1.83692	1.12295	1.25073	1.85795	1.12870	1.26013
6	3.21335	-0.59003	0.00000	3.18912	-0.56571	0.00002	3.20405	-0.58174	-0.00067
6	1.88337	1.12741	-1.26285	1.83696	1.12296	-1.25071	1.85766	1.13047	-1.25877
8	0.93163	-1.95102	-0.00001	0.94798	-1.95363	-0.00004	0.93913	-1.94792	-0.00021
1	-2.77155	2.46667	-0.00001	-2.73668	2.45675	-0.00003	-2.75170	2.45969	-0.00008
1	-4.48382	0.71917	0.00000	-4.45355	0.72033	0.00001	-4.46094	0.71988	0.00032
1	-3.82661	-1.69576	0.00001	-3.80549	-1.69145	0.00004	-3.81691	-1.68796	0.00031

1	-1.40508	-2.29333	0.00001	-1.38230	-2.29872	0.00002	-1.39576	-2.29139	-0.00008
1	2.77836	1.76738	1.28240	2.71683	1.78098	1.27657	2.73677	1.78931	1.28199
1	0.98246	1.74653	1.25054	0.91606	1.71080	1.21538	0.93798	1.72024	1.23780
1	1.88816	0.51589	2.17501	1.84719	0.50791	2.15943	1.87712	0.52021	2.17343
1	4.07432	0.09159	0.00001	4.04306	0.12289	0.00004	4.06742	0.09610	-0.00027
1	3.27939	-1.23616	0.88139	3.25578	-1.20903	0.88170	3.26963	-1.22925	0.87868
1	3.27940	-1.23614	-0.88139	3.25581	-1.20902	-0.88166	3.26946	-1.22799	-0.88097
1	2.77837	1.76740	-1.28237	2.71686	1.78099	-1.27653	2.73651	1.79107	-1.27992
1	1.88817	0.51592	-2.17500	1.84725	0.50792	-2.15942	1.87656	0.52328	-2.17293
1	0.98246	1.74655	-1.25052	0.91610	1.71081	-1.21539	0.93773	1.72204	-1.23536

$\mathbf{1n_3}$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.75853	0.29912	0.00000	-0.72883	0.27981	0.16247	-0.74160	0.28454	0.13584
6	-1.77559	1.29342	-0.00001	-1.67362	1.26782	-0.22276	-1.70323	1.26824	-0.21483
6	-3.17644	1.05860	-0.00001	-3.06810	1.08309	-0.40357	-3.09828	1.07154	-0.33313
6	-3.48233	-0.32629	0.00000	-3.42535	-0.26527	-0.13363	-3.45101	-0.27830	-0.09269
6	-2.52498	-1.35872	0.00001	-2.54518	-1.29525	0.24213	-2.54604	-1.31247	0.18737
6	-1.16523	-1.05676	0.00001	-1.18625	-1.03299	0.38623	-1.19088	-1.03914	0.31703
6	0.66327	0.75185	0.00000	0.68230	0.69052	0.29157	0.66955	0.71366	0.25312
6	1.88322	-0.24276	0.00000	1.84490	-0.24431	-0.13158	1.86257	-0.24271	-0.10858
6	3.18684	0.58157	0.00000	3.05285	0.62587	-0.48236	3.10070	0.62502	-0.40217
6	1.88679	-1.11655	1.27713	2.22786	-1.13350	1.05853	2.18267	-1.12854	1.11716
6	1.88678	-1.11655	-1.27714	1.48474	-1.09421	-1.35107	1.57282	-1.11083	-1.34768
8	0.94106	1.95393	0.00000	0.98718	1.82197	0.70070	0.95979	1.85833	0.58372
1	-1.41227	2.32048	-0.00002	-1.23730	2.25655	-0.40746	-1.27862	2.25424	-0.42021
1	-4.53281	-0.64146	0.00000	-4.48348	-0.55617	-0.20818	-4.51118	-0.56457	-0.10285
1	-2.83706	-2.40651	0.00002	-2.91630	-2.30528	0.43902	-2.89621	-2.33490	0.34665
1	-0.45225	-1.87172	0.00002	-0.51725	-1.82166	0.72304	-0.51073	-1.83434	0.60252
1	4.04932	-0.09812	-0.00001	3.89805	-0.01002	-0.77275	3.97068	-0.01351	-0.60215
1	3.24899	1.22816	-0.87965	2.81801	1.29406	-1.31636	2.93461	1.26181	-1.27687
1	3.24900	1.22816	0.87964	3.34381	1.24698	0.36578	3.32377	1.28369	0.43852
1	2.78958	-1.74241	1.29557	3.11047	-1.73572	0.80770	3.06401	-1.75203	0.91636
1	1.90109	-0.48338	2.17194	2.47158	-0.51142	1.92605	2.40331	-0.50516	1.99041
1	1.01726	-1.77024	1.35242	1.42317	-1.81439	1.34305	1.35654	-1.79177	1.38210
1	2.78958	-1.74240	-1.29557	2.35846	-1.67866	-1.66750	2.45570	-1.71377	-1.60028
1	1.01725	-1.77024	-1.35242	0.65953	-1.77640	-1.14854	0.72647	-1.78142	-1.19951
1	1.90108	-0.48338	-2.17194	1.18190	-0.45306	-2.18530	1.33987	-0.48098	-2.21318

$\mathbf{1n_4}$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.74709	0.26797	0.00000	-0.73323	0.25984	0.00001	-0.74118	0.26560	-0.00036
6	-1.77491	1.24402	0.00000	-1.74396	1.24243	-0.00001	-1.76651	1.23955	-0.00017
6	-3.11971	0.87691	0.00000	-3.09085	0.87736	-0.00003	-3.10466	0.87522	0.00011
6	-3.60691	-0.46517	0.00000	-3.61193	-0.44973	-0.00002	-3.61124	-0.46049	0.00024
6	-2.53611	-1.40522	0.00001	-2.53541	-1.37956	0.00000	-2.53199	-1.39194	0.00004
6	-1.17644	-1.08227	0.00001	-1.16715	-1.08251	0.00001	-1.17679	-1.07897	-0.00024
6	0.65345	0.74523	0.00000	0.66531	0.73509	0.00002	0.65254	0.74545	-0.00067
6	1.88493	-0.22787	0.00000	1.87244	-0.23410	0.00000	1.88022	-0.23083	0.00003
6	3.17716	0.61375	-0.00001	3.15996	0.59071	-0.00002	3.16873	0.61291	-0.00018
6	1.89728	-1.10308	1.27613	1.86905	-1.09668	1.26816	1.88956	-1.10244	1.27509
6	1.89727	-1.10308	-1.27612	1.86901	-1.09668	-1.26816	1.88995	-1.10368	-1.27418
8	0.90721	1.95742	0.00000	0.92562	1.95090	0.00005	0.91220	1.94725	-0.00008
1	-1.47815	2.29103	-0.00001	-1.43603	2.28774	-0.00002	-1.46007	2.28324	-0.00026
1	-3.84374	1.69898	-0.00001	-3.80094	1.71606	-0.00004	-3.82115	1.70643	0.00023
1	-2.77198	-2.47535	0.00001	-2.77162	-2.45315	0.00001	-2.76273	-2.46499	0.00009
1	-0.45569	-1.89539	0.00001	-0.45665	-1.90580	0.00003	-0.45572	-1.89211	-0.00038
1	4.04846	-0.05438	-0.00001	4.02623	-0.08227	-0.00003	4.04591	-0.04682	0.00030
1	3.23064	1.26105	-0.87977	3.21213	1.23522	-0.88025	3.21676	1.26048	-0.87885
1	3.23065	1.26105	0.87976	3.21216	1.23522	0.88021	3.21647	1.26136	0.87786
1	2.80608	-1.72003	1.29421	2.75636	-1.74258	1.28101	2.78121	-1.74337	1.28733
1	1.90424	-0.47121	2.17200	1.90710	-0.45367	2.15430	1.92434	-0.46886	2.16856

1	1.03397	-1.76551	1.34749	0.98178	-1.72240	1.35039	1.00931	-1.73935	1.35925
1	2.80607	-1.72003	-1.29421	2.75633	-1.74257	-1.28105	2.78160	-1.74462	-1.28552
1	1.03396	-1.76552	-1.34748	0.98175	-1.72240	-1.35036	1.00972	-1.74068	-1.35797
1	1.90422	-0.47122	-2.17200	1.90703	-0.45367	-2.15430	1.92500	-0.47098	-2.16825

$1n_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.75266	0.24603	0.00000	-0.73070	0.24179	-0.12320	-0.74273	0.24697	-0.10191
6	-1.75697	1.24211	0.00000	-1.68915	1.24130	0.13637	-1.72300	1.23902	0.10574
6	-3.09392	0.86147	0.00000	-3.02477	0.87864	0.24268	-3.05427	0.86648	0.18846
6	-3.44293	-0.50472	0.00000	-3.39840	-0.46980	0.09144	-3.41139	-0.48877	0.09407
6	-2.51340	-1.57412	0.00001	-2.52798	-1.54628	-0.22463	-2.51890	-1.55293	-0.17876
6	-1.17065	-1.11288	0.00001	-1.18755	-1.08901	-0.31687	-1.18531	-1.08886	-0.28018
6	0.65788	0.73437	0.00000	0.67151	0.70282	-0.20423	0.66092	0.72361	-0.15892
6	1.89481	-0.22716	0.00000	1.86328	-0.23468	0.09979	1.87730	-0.23225	0.08401
6	3.18102	0.62400	-0.00001	3.08693	0.62898	0.41057	3.12102	0.63322	0.36160
6	1.91088	-1.10216	1.27665	1.58221	-1.13055	1.30866	1.65329	-1.16100	1.29398
6	1.91087	-1.10217	-1.27665	2.18049	-1.07421	-1.14506	2.14736	-1.05284	-1.19815
8	0.89923	1.94731	0.00000	0.93984	1.88164	-0.49687	0.92102	1.90222	-0.38651
1	-1.46260	2.28669	-0.00001	-1.35899	2.27063	0.26088	-1.40562	2.27086	0.21113
1	-3.87020	1.63114	-0.00001	-3.77361	1.64585	0.46002	-3.81324	1.63400	0.35761
1	-4.51566	-0.73146	0.00000	-4.46837	-0.68165	0.23261	-4.47458	-0.71220	0.25437
1	-0.39445	-1.87519	0.00001	-0.43073	-1.82708	-0.59925	-0.42292	-1.82185	-0.55439
1	4.05622	-0.03878	-0.00001	3.94657	-0.01563	0.63043	3.99951	-0.00908	0.50245
1	3.23139	1.27127	-0.88023	3.33196	1.27855	-0.43114	3.31189	1.32374	-0.46172
1	3.23139	1.27128	0.88021	2.90081	1.26896	1.27816	2.98795	1.23631	1.26525
1	2.82239	-1.71499	1.29175	2.46931	-1.73639	1.53429	2.54564	-1.77868	1.46276
1	1.91879	-0.46990	2.17255	1.35783	-0.51820	2.18890	1.48058	-0.57272	2.20257
1	1.04906	-1.76615	1.34611	0.73362	-1.79255	1.14193	0.79394	-1.81726	1.16100
1	2.82238	-1.71499	-1.29175	3.07853	-1.67909	-0.96557	3.04387	-1.67286	-1.06625
1	1.04905	-1.76616	-1.34610	1.36238	-1.74447	-1.41114	1.31477	-1.70971	-1.45427
1	1.91878	-0.46991	-2.17256	2.37670	-0.41598	-1.99830	2.32425	-0.38427	-2.04803

$1n_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.72455	0.23306	0.00000	-0.71517	0.23491	0.00000	-0.71938	0.23873	0.00005
6	-1.71519	1.25050	0.00000	-1.69384	1.25515	-0.00001	-1.70834	1.25023	0.00003
6	-3.06471	0.91754	0.00001	-3.03969	0.91475	0.00001	-3.05136	0.91452	0.00001
6	-3.42652	-0.44135	0.00001	-3.39689	-0.43779	0.00002	-3.40464	-0.44164	0.00000
6	-2.43264	-1.42461	0.00001	-2.39260	-1.41387	0.00002	-2.41121	-1.41748	0.00001
6	-1.03572	-1.16048	0.00000	-0.99930	-1.16066	0.00001	-1.01742	-1.15487	0.00004
6	0.69078	0.73640	-0.00001	0.69692	0.73621	-0.00002	0.69042	0.74482	0.00004
6	1.91230	-0.23506	0.00000	1.89078	-0.23815	0.00000	1.90213	-0.23673	0.00000
6	3.21334	0.59004	0.00000	3.18912	0.56571	0.00001	3.20423	0.58174	-0.00001
6	1.88337	-1.12739	1.26286	1.83693	-1.12295	1.25072	1.85808	-1.12953	1.25940
6	1.88338	-1.12740	-1.26286	1.83695	-1.12295	-1.25072	1.85803	-1.12948	-1.25944
8	0.93160	1.95102	-0.00002	0.94798	1.95363	-0.00005	0.93888	1.94798	-0.00008
1	-1.40507	2.29332	0.00000	-1.38231	2.29872	-0.00002	-1.39602	2.29135	0.00003
1	-3.82662	1.69575	0.00001	-3.80549	1.69145	0.00001	-3.81694	1.68792	0.00000
1	-4.48381	-0.71916	0.00001	-4.45355	-0.72034	0.00003	-4.46106	-0.72001	-0.00002
1	-2.77154	-2.46668	0.00001	-2.73668	-2.45675	0.00003	-2.75186	-2.45968	0.00000
1	4.07431	-0.09158	0.00000	4.04306	-0.12289	0.00002	4.06751	-0.09624	-0.00004
1	3.27939	1.23615	-0.88139	3.25580	1.20903	-0.88167	3.26973	1.22860	-0.87981
1	3.27938	1.23616	0.88139	3.25578	1.20903	0.88169	3.26977	1.22856	0.87983
1	2.77836	-1.76740	1.28238	2.71684	-1.78097	1.27657	2.73677	-1.79034	1.28052
1	1.88819	-0.51590	2.17501	1.84719	-0.50791	2.15942	1.87748	-0.52179	2.17314
1	0.98246	-1.74653	1.25054	0.91608	-1.71081	1.21538	0.93812	-1.72105	1.23662
1	2.77837	-1.76740	-1.28237	2.71685	-1.78099	-1.27654	2.73668	-1.79034	-1.28059
1	0.98247	-1.74654	-1.25053	0.91609	-1.71081	-1.21539	0.93802	-1.72093	-1.23669
1	1.88819	-0.51591	-2.17501	1.84724	-0.50792	-2.15942	1.87748	-0.52170	-2.17316

1o. Nitrobenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.00000	-2.51966	0.00000	0.00000	-2.51570	0.00000	0.00000	-2.51127	0.00000
6	0.00000	-1.82337	1.21328	0.00000	-1.81762	1.20897	0.00000	-1.81784	1.20987
6	0.00000	-0.42862	1.22209	0.00000	-0.42427	1.22149	0.00001	-0.42734	1.21790
6	0.00000	0.24434	0.00000	0.00000	0.24157	0.00000	0.00001	0.24338	0.00000
6	0.00000	-0.42862	-1.22209	0.00000	-0.42427	-1.22149	0.00001	-0.42734	-1.21790
6	0.00000	-1.82337	-1.21328	0.00000	-1.81762	-1.20897	0.00000	-1.81784	-1.20987
1	0.00000	-3.60551	0.00000	0.00000	-3.60286	0.00000	0.00000	-3.59606	0.00000
1	0.00000	-2.36519	2.15370	0.00000	-2.35957	2.15122	0.00000	-2.35959	2.14907
1	0.00000	0.13679	2.14566	0.00000	0.14226	2.14613	0.00001	0.14303	2.13664
7	0.00000	1.71956	0.00000	0.00000	1.71163	0.00000	0.00001	1.71762	0.00000
1	0.00000	0.13679	-2.14566	0.00000	0.14226	-2.14613	0.00001	0.14303	-2.13664
1	0.00000	-2.36519	-2.15370	0.00000	-2.35957	-2.15122	0.00000	-2.35959	-2.14907
8	0.00000	2.29382	1.09004	0.00000	2.28773	1.09934	-0.00001	2.28470	1.08503
8	0.00000	2.29382	-1.09004	0.00000	2.28773	-1.09934	-0.00001	2.28470	-1.08503

$1o_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.52048	-0.00785	-0.00059				-2.51193	-0.01039	-0.00001
6	-1.83002	-1.22108	-0.08915				-1.82078	-1.21962	0.00000
6	-0.41259	-1.34844	-0.09569				-0.40471	-1.35600	0.00001
6	0.20823	-0.09732	-0.00337				0.20274	-0.09676	0.00001
6	-0.41689	1.16247	0.08571				-0.42043	1.16191	0.00000
6	-1.80781	1.20118	0.09264				-1.80597	1.20072	0.00000
1	-3.61289	0.01081	-0.00217				-3.60401	0.00955	-0.00002
1	-2.43939	-2.12870	-0.15851				-2.43607	-2.12759	0.00000
7	1.70800	-0.03989	-0.00585				1.70494	-0.03562	0.00002
1	0.16888	2.07410	0.15368				0.16810	2.07217	0.00001
1	-2.32960	2.15277	0.17112				-2.32975	2.15366	0.00000
8	2.36155	-1.05844	0.21546				2.35502	-1.07252	0.00012
8	2.25525	1.06300	-0.22302				2.24917	1.08032	-0.00014

$1o_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.52798	-0.11397	-0.03111				-2.51423	-0.10640	0.03302
6	-1.87023	-1.35658	0.11279				-1.88008	-1.36464	-0.09164
6	-0.46305	-1.25111	0.15076				-0.47209	-1.24483	-0.12815
6	0.21265	-0.02256	-0.00640				0.20885	-0.02355	0.00220
6	-0.48350	1.19451	-0.08326				-0.47657	1.19500	0.06291
6	-1.87313	1.13677	-0.06901				-1.86159	1.13925	0.05464
1	-3.61668	-0.09599	-0.14774				-3.60575	-0.06980	0.13715
1	0.15876	-2.12603	0.33762				0.15887	-2.11989	-0.28626
7	1.66196	0.01403	-0.02244				1.66142	0.01043	0.01927
1	0.06163	2.12717	-0.16972				0.07831	2.12125	0.13323
1	-2.44672	2.06282	-0.14129				-2.42993	2.06953	0.10924
8	2.28545	-1.03370	-0.27325				2.27851	-1.04084	0.22379
8	2.24464	1.08513	0.25269				2.23934	1.08546	-0.20205

$1o_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.68015	0.00000	-0.00011				-2.68582	0.00000	-0.00008

6	-1.88079	1.18483	-0.00009				-1.87422	1.17637	-0.00001
6	-0.48633	1.21748	-0.00003				-0.48565	1.21179	0.00012
6	0.21708	0.00000	0.00001				0.21814	0.00000	0.00020
6	-0.48633	-1.21748	-0.00002				-0.48565	-1.21179	0.00013
6	-1.88079	-1.18483	-0.00008				-1.87422	-1.17637	0.00000
1	-2.38276	2.15708	-0.00011				-2.36897	2.15456	-0.00005
1	0.07138	2.14964	-0.00001				0.07856	2.13906	0.00017
7	1.65633	0.00000	0.00007				1.65627	0.00000	0.00034
1	0.07138	-2.14964	0.00001				0.07856	-2.13906	0.00019
1	-2.38276	-2.15708	-0.00009				-2.36897	-2.15456	-0.00004
8	2.26327	1.08981	0.00009				2.25697	1.08379	-0.00031
8	2.26327	-1.08981	0.00010				2.25697	-1.08379	-0.00030

1p. 1,2-Dimethylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.74662	-1.38550	0.00000	-0.74426	-1.38432	0.00026	-0.74493	-1.38104	0.00003
6	-1.96282	-0.69742	0.00000	-1.95688	-0.69638	-0.00019	-1.95680	-0.69506	-0.00001
6	-1.96282	0.69742	0.00000	-1.95687	0.69640	0.00015	-1.95680	0.69506	0.00000
6	-0.74662	1.38550	0.00000	-0.74424	1.38432	-0.00021	-0.74493	1.38104	-0.00002
6	0.47912	0.70674	0.00000	0.47694	0.70404	0.00013	0.47593	0.70433	0.00001
6	0.47912	-0.70674	0.00000	0.47694	-0.70407	-0.00011	0.47593	-0.70433	0.00001
1	-0.74637	-2.47297	0.00000	-0.74374	-2.47300	-0.00002	-0.74322	-2.46736	0.00004
1	-2.89902	-1.24838	0.00000	-2.89471	-1.24636	0.00020	-2.89206	-1.24512	0.00002
1	-2.89902	1.24838	0.00000	-2.89470	1.24638	-0.00022	-2.89206	1.24512	-0.00004
1	-0.74637	2.47297	0.00000	-0.74370	2.47299	0.00004	-0.74322	2.46735	-0.00002
6	1.77665	1.48152	0.00000	1.77293	1.46862	0.00006	1.77209	1.47694	0.00001
6	1.77665	-1.48152	0.00000	1.77295	-1.46861	-0.00008	1.77209	-1.47694	-0.00002
1	1.59070	2.55906	0.00000	1.58685	2.54556	-0.00008	1.58790	2.55424	-0.00010
1	2.38840	1.24817	-0.88031	2.37957	1.23200	-0.88066	2.38489	1.24261	-0.87881
1	2.38840	1.24817	0.88031	2.37945	1.23222	0.88091	2.38479	1.24278	0.87895
1	2.38840	-1.24817	0.88031	2.37986	-1.23150	0.88031	2.38505	-1.24239	0.87863
1	2.38840	-1.24817	-0.88031	2.37920	-1.23269	-0.88125	2.38463	-1.24300	-0.87913
1	1.59070	-2.55906	0.00000	1.58687	-2.54555	0.00070	1.58791	-2.55424	0.00039

$1p_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.79033	1.34713	0.00000	0.77757	1.35475	-0.00004	0.78435	1.34922	-0.00002
6	1.98176	0.61375	0.00000	1.96782	0.62827	-0.00017	1.97028	0.61770	-0.00001
6	1.92782	-0.78914	0.00000	1.91264	-0.77423	0.00017	1.91563	-0.77891	0.00003
6	0.72607	-1.53855	0.00000	0.73135	-1.55974	0.00012	0.72754	-1.55303	0.00000
6	-0.45195	-0.74402	0.00000	-0.43493	-0.74143	-0.00003	-0.44064	-0.73937	0.00001
6	-0.44152	0.67466	0.00000	-0.44416	0.67405	-0.00018	-0.43906	0.67313	-0.00003
1	0.81029	2.43804	0.00000	0.79067	2.44779	-0.00022	0.79886	2.43950	-0.00006
1	2.94131	1.13886	0.00000	2.92586	1.15809	-0.00018	2.92714	1.14693	-0.00003
1	2.88750	-1.31927	0.00000	2.88602	-1.28776	0.00036	2.88549	-1.29580	0.00009
6	-1.80211	-1.45155	0.00000	-1.77879	-1.44643	-0.00014	-1.78888	-1.45019	-0.00003
6	-1.72580	1.48356	0.00000	-1.73210	1.46202	0.00018	-1.72391	1.47661	0.00003
1	-1.62385	-2.53022	0.00000	-1.57845	-2.52051	-0.00076	-1.60011	-2.52733	-0.00025
1	-2.41442	-1.19948	-0.88250	-2.39265	-1.20143	-0.88076	-2.40977	-1.20581	-0.87889
1	-2.41442	-1.19948	0.88250	-2.39209	-1.20234	0.88113	-2.40957	-1.20619	0.87909
1	-2.34994	1.26760	0.87925	-2.35214	1.24149	0.87936	-2.35166	1.26134	0.87713
1	-2.34994	1.26760	-0.87925	-2.35321	1.24046	-0.87795	-2.35208	1.26082	-0.87663
1	-1.51409	2.56132	0.00000	-1.53038	2.54063	-0.00056	-1.52016	2.55549	-0.00032

$1p_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z

6	0.84264	1.32586	0.00000	0.82121	1.33553	0.00012	0.82731	1.32754	0.00000
6	2.02316	0.56403	0.00000	2.00258	0.57744	0.00001	2.00612	0.57498	0.00000
6	2.06033	-0.85435	0.00000	2.08330	-0.84051	-0.00004	2.07602	-0.84274	0.00002
6	0.75640	-1.41307	0.00000	0.77545	-1.39177	-0.00007	0.76880	-1.39457	-0.00003
6	-0.45884	-0.69587	0.00000	-0.45023	-0.69637	0.00001	-0.44927	-0.69614	-0.00001
6	-0.41992	0.71456	0.00000	-0.42858	0.70874	-0.00008	-0.42605	0.71021	-0.00002
1	0.89431	2.42037	0.00000	0.85922	2.43163	-0.00004	0.86461	2.42226	0.00000
1	2.96399	1.12814	0.00000	2.93496	1.16291	0.00014	2.93791	1.15864	0.00003
1	0.65166	-2.50671	0.00000	0.67114	-2.49010	-0.00005	0.65959	-2.49093	-0.00002
6	-1.78555	-1.42988	0.00000	-1.76526	-1.43609	0.00006	-1.76670	-1.44193	0.00001
6	-1.68603	1.54453	0.00000	-1.70252	1.51295	-0.00005	-1.69677	1.52791	0.00000
1	-1.62012	-2.51373	0.00000	-1.58568	-2.51705	0.00003	-1.59059	-2.52392	-0.00001
1	-2.40044	-1.18896	-0.88102	-2.38145	-1.20305	-0.88000	-2.38900	-1.21029	-0.87833
1	-2.40044	-1.18896	0.88103	-2.38125	-1.20303	0.88025	-2.38895	-1.21032	0.87840
1	-2.31804	1.35015	0.88037	-2.32758	1.30707	0.87979	-2.33152	1.33158	0.87811
1	-2.31804	1.35015	-0.88037	-2.32789	1.30664	-0.87956	-2.33174	1.33127	-0.87788
1	-1.44604	2.61476	0.00000	-1.47725	2.58548	-0.00035	-1.46715	2.60019	-0.00021

$1p_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.75640	-1.41307	0.00000	-0.77545	-1.39178	-0.00005	-0.76881	-1.39457	-0.00001
6	-2.06033	-0.85435	0.00000	-2.08329	-0.84050	-0.00004	-2.07602	-0.84274	0.00000
6	-2.02316	0.56403	0.00000	-2.00257	0.57744	0.00001	-2.00612	0.57498	0.00000
6	-0.84264	1.32586	0.00000	-0.82119	1.33551	0.00006	-0.82731	1.32754	0.00001
6	0.41992	0.71456	0.00000	0.42859	0.70871	0.00001	0.42605	0.71021	0.00001
6	0.45884	-0.69587	0.00000	0.45025	-0.69641	0.00008	0.44927	-0.69614	0.00001
1	-0.65166	-2.50671	0.00000	-0.67116	-2.49010	-0.00004	-0.65959	-2.49093	0.00001
1	-2.96399	1.12814	0.00000	-2.93494	1.16292	0.00001	-2.93791	1.15864	-0.00002
1	-0.89431	2.42037	0.00000	-0.85919	2.43161	0.00002	-0.86460	2.42226	0.00001
6	1.68603	1.54453	0.00000	1.70247	1.51304	-0.00005	1.69677	1.52792	-0.00001
6	1.78555	-1.42988	0.00000	1.76527	-1.43614	0.00002	1.76670	-1.44193	0.00000
1	2.31804	1.35015	0.88037	2.32775	1.30709	0.87961	2.33162	1.33144	0.87799
1	1.44604	2.61476	0.00000	1.47709	2.58555	-0.00010	1.46715	2.60019	-0.00003
1	2.31804	1.35015	-0.88037	2.32763	1.30697	-0.87976	2.33163	1.33141	-0.87800
1	2.40044	-1.18896	0.88102	2.38150	-1.20299	0.88002	2.38902	-1.21022	0.87831
1	2.40044	-1.18897	-0.88103	2.38125	-1.20324	-0.88022	2.38892	-1.21039	-0.87842
1	1.62012	-2.51373	0.00000	1.58566	-2.51710	0.00020	1.59060	-2.52392	0.00011

$1p_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-0.72607	-1.53855	0.00000	-0.73135	-1.55975	0.00005	-0.72754	-1.55303	0.00004
6	-1.92782	-0.78914	0.00000	-1.91264	-0.77423	-0.00009	-1.91563	-0.77891	-0.00003
6	-1.98176	0.61375	0.00000	-1.96781	0.62826	0.00004	-1.97028	0.61770	-0.00002
6	-0.79033	1.34713	0.00000	-0.77755	1.35472	-0.00002	-0.78434	1.34922	-0.00001
6	0.44152	0.67466	0.00000	0.44416	0.67403	0.00011	0.43906	0.67313	0.00004
6	0.45195	-0.74402	0.00000	0.43495	-0.74147	0.00009	0.44064	-0.73937	0.00007
1	-2.88750	-1.31927	0.00000	-2.88602	-1.28777	-0.00016	-2.88549	-1.29580	-0.00002
1	-2.94131	1.13886	0.00000	-2.92586	1.15809	-0.00009	-2.92714	1.14694	-0.00004
1	-0.81029	2.43804	0.00000	-0.79063	2.44777	0.00012	-0.79886	2.43950	-0.00002
6	1.72580	1.48356	0.00000	1.73204	1.46211	-0.00005	1.72391	1.47661	0.00000
6	1.80211	-1.45155	0.00000	1.77881	-1.44647	-0.00003	1.78888	-1.45018	-0.00004
1	1.51409	2.56132	0.00000	1.53014	2.54069	0.00016	1.52015	2.55549	0.00012
1	2.34995	1.26760	-0.87925	2.35248	1.24133	-0.87888	2.35179	1.26117	-0.87696
1	2.34994	1.26760	0.87926	2.35278	1.24103	0.87847	2.35195	1.26100	0.87680
1	2.41442	-1.19948	0.88250	2.39238	-1.20203	0.88096	2.40969	-1.20607	0.87895
1	2.41441	-1.19948	-0.88250	2.39236	-1.20169	-0.88092	2.40965	-1.20593	-0.87903
1	1.62385	-2.53022	0.00000	1.57865	-2.52059	-0.00025	1.60012	-2.52733	-0.00012

1q. 1-Fluoro-4-methylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.42574	0.00000	-0.00365	1.423716	-0.000010	-0.004016	1.43027	0.00000	-0.00325
6	0.75477	-1.21567	0.00157	0.751081	-1.213501	0.001826	0.75324	-1.21017	0.00133
6	-0.64259	-1.20289	0.01003	-0.642794	-1.201277	0.009448	-0.63880	-1.19858	0.00907
6	-1.36458	0.00000	0.01127	-1.360878	0.000011	0.016141	-1.35822	-0.00002	0.01039
6	-0.64259	1.20289	0.01003	-0.642768	1.201303	0.009441	-0.63881	1.19856	0.00907
6	0.75477	1.21567	0.00157	0.751090	1.213505	0.001830	0.75322	1.21016	0.00133
9	2.78824	0.00000	-0.00851	2.781042	-0.000013	-0.008902	2.76970	0.00002	-0.00787
1	1.31630	-2.14380	0.00327	1.315488	-2.140869	0.002344	1.31444	-2.13690	0.00349
1	-1.17802	-2.14881	0.01763	-1.180319	-2.147412	0.017439	-1.17493	-2.14271	0.01613
6	-2.87645	0.00000	-0.01309	-2.865906	-0.000007	-0.015388	-2.86794	0.00001	-0.01162
1	-1.17801	2.14881	0.01763	-1.180290	2.147440	0.017423	-1.17496	2.14268	0.01614
1	1.31630	2.14380	0.00327	1.315520	2.140859	0.002351	1.31442	2.13690	0.00349
1	-3.28408	-0.88482	0.48548	-3.269937	-0.884322	0.484628	-3.27522	-0.88544	0.48521
1	-3.25696	-0.00015	-1.04236	-3.241148	-0.000191	-1.044120	-3.25361	0.00120	-1.03885
1	-3.28408	0.88497	0.48521	-3.269942	0.884471	0.484351	-3.27522	0.88432	0.48724

$1q_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.40251	-0.10265	0.00181	1.392663	-0.106314	0.003477	1.40314	-0.10039	0.00000
6	0.79059	-1.34224	-0.00492	0.799867	-1.362039	-0.005266	0.79756	-1.35225	0.00015
6	-0.61964	-1.21717	-0.01348	-0.606429	-1.210129	-0.014567	-0.60781	-1.20943	0.00016
6	-1.33840	-0.00141	-0.01016	-1.332487	0.000749	-0.017786	-1.32823	0.00107	0.00003
6	-0.60933	1.19674	-0.01163	-0.610258	1.196989	-0.012939	-0.60792	1.19563	-0.00009
6	0.79183	1.15166	-0.00604	0.785544	1.151788	-0.006364	0.78890	1.14780	-0.00011
9	2.81932	-0.03952	0.01496	2.797884	-0.027392	0.016885	2.79138	-0.03425	-0.00004
1	-1.23011	-2.12979	-0.02693	-1.228974	-2.119498	-0.031672	-1.22815	-2.11842	0.00029
6	-2.85443	0.01630	0.01813	-2.840697	0.013165	0.023231	-2.84281	0.01271	-0.00003
1	-1.12340	2.15830	-0.01856	-1.128842	2.158222	-0.022283	-1.12685	2.15340	-0.00018
1	1.38252	2.06767	-0.01185	1.383568	2.063890	-0.012510	1.37874	2.06461	-0.00019
1	-3.24971	0.21894	1.02534	-3.233231	0.039430	1.049116	-3.26133	-0.49930	0.87851
1	-3.26176	-0.95217	-0.29733	-3.249728	-0.885493	-0.452812	-3.26129	-0.49814	-0.87927
1	-3.27023	0.78534	-0.64769	-3.252974	0.884723	-0.500515	-3.24054	1.03543	0.00061

$1q_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	1.38714	-0.01595	0.00000	1.38377	-0.01561	0.00000	1.39111	-0.01491	0.00000
6	0.71872	-1.23813	0.00000	0.69996	-1.23045	0.00000	0.71099	-1.22731	0.00000
6	-0.69442	-1.32885	0.00000	-0.71084	-1.34522	0.00000	-0.69956	-1.34025	0.00000
6	-1.35822	-0.06648	0.00000	-1.34314	-0.06504	0.00000	-1.34430	-0.06572	0.00000
6	-0.67514	1.16096	0.00000	-0.66920	1.16647	0.00000	-0.66790	1.15748	0.00000
6	0.72997	1.20393	0.00000	0.73030	1.20419	0.00000	0.73135	1.20181	0.00000
9	2.78682	0.00626	0.00000	2.77585	-0.00215	-0.00001	2.76417	0.00175	0.00000
1	1.33847	-2.13934	0.00000	1.33253	-2.12764	0.00000	1.34486	-2.12237	0.00000
6	-2.88133	-0.04656	0.00000	-2.86001	-0.03934	0.00000	-2.86720	-0.04032	0.00000
1	-1.22499	2.10652	0.00000	-1.22082	2.11243	0.00000	-1.21735	2.10336	0.00000
1	1.28566	2.13753	0.00000	1.29466	2.13448	0.00000	1.28905	2.13338	0.00000
1	-3.27532	-0.57482	0.87810	-3.25271	-0.56574	0.87730	-3.27043	-0.56719	0.87545
1	-3.27532	-0.57480	-0.87811	-3.25271	-0.56571	-0.87731	-3.27043	-0.56716	-0.87546
1	-3.29029	0.97503	0.00002	-3.26868	0.98154	0.00002	-3.28012	0.97956	0.00002

$1q_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.38714	-0.01595	0.00000	-1.38455	-0.01521	-0.00437	-1.39123	-0.01475	0.00001

6	-0.72997	1.20393	0.00000	-0.72558	1.20364	-0.00022	-0.73129	1.20177	0.00000
6	0.67514	1.16096	0.00000	0.67163	1.16102	0.00825	0.66790	1.15755	-0.00001
6	1.35822	-0.06648	-0.00001	1.34446	-0.07309	0.01298	1.34437	-0.06572	0.00000
6	0.69442	-1.32885	-0.00001	0.70780	-1.34991	0.01204	0.69962	-1.34039	-0.00002
6	-0.71872	-1.23813	0.00000	-0.70531	-1.23028	0.00049	-0.71076	-1.22717	-0.00001
9	-2.78682	0.00626	0.00000	-2.77651	0.00552	-0.00676	-2.76430	0.00159	0.00001
1	-1.28566	2.13753	0.00000	-1.28686	2.13575	0.00464	-1.28877	2.13361	-0.00002
1	1.22499	2.10652	-0.00001	1.22625	2.10565	0.01471	1.21724	2.10345	-0.00003
6	2.88133	-0.04656	0.00001	2.86153	-0.03671	-0.01095	2.86717	-0.04034	0.00001
1	-1.33847	-2.13934	0.00000	-1.33932	-2.12613	0.00089	-1.34492	-2.12219	-0.00001
1	3.29029	0.97503	-0.00017	3.27706	0.79380	0.57769	3.28013	0.97951	-0.00022
1	3.27532	-0.57497	-0.87800	3.25355	0.06703	-1.03296	3.27024	-0.56742	-0.87532
1	3.27531	-0.57466	0.87821	3.23807	-0.98256	0.38655	3.27024	-0.56697	0.87562

$1q_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.40251	-0.10265	-0.00181	-1.39265	-0.10634	-0.00348	-1.40390	-0.10231	-0.00047
6	-0.79183	1.15166	0.00604	-0.78556	1.15180	0.00642	-0.78638	1.14698	0.00114
6	0.60933	1.19674	0.01163	0.61022	1.19703	0.01301	0.60787	1.19563	0.00222
6	1.33840	-0.00141	0.01016	1.33248	0.00080	0.01790	1.32975	-0.00126	0.00180
6	0.61964	-1.21717	0.01348	0.60647	-1.21009	0.01465	0.60741	-1.20846	0.00256
6	-0.79059	-1.34224	0.00492	-0.79983	-1.36204	0.00532	-0.79965	-1.35151	0.00100
9	-2.81932	-0.03952	-0.01497	-2.79788	-0.02744	-0.01701	-2.79243	-0.03157	-0.00286
1	-1.38252	2.06767	0.01185	-1.38362	2.06388	0.01261	-1.37608	2.06404	0.00264
1	1.12340	2.15830	0.01856	1.12881	2.15826	0.02240	1.12450	2.15497	0.00355
6	2.85443	0.01630	-0.01813	2.84068	0.01314	-0.02337	2.84349	0.01210	-0.00338
1	1.23011	-2.12979	0.02693	1.22902	-2.11946	0.03185	1.22881	-2.11690	0.00529
1	3.27023	0.78534	0.64768	3.25305	0.88532	0.49927	3.26376	0.57350	0.84415
1	3.24971	0.21893	-1.02535	3.23298	0.03818	-1.04937	3.26019	0.47044	-0.91302
1	3.26176	-0.95216	0.29733	3.24985	-0.88495	0.45362	3.23908	-1.00892	0.05392

1r. 1-Fluoro-3-methylbenzene

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.20126	-0.37357	0.00110	-1.201812	-0.371724	0.000568	-1.20311	-0.38090	-0.00004
6	0.04178	-0.99171	-0.00915	0.039758	-0.989771	-0.009265	0.04238	-0.98679	-0.00006
6	1.20160	-0.20181	-0.01085	1.197393	-0.205341	-0.016427	1.19661	-0.19596	0.00000
6	1.06235	1.19399	-0.00774	1.065873	1.187820	-0.007702	1.05525	1.19356	0.00007
6	-0.20207	1.78995	0.00208	-0.193286	1.787325	0.002287	-0.20731	1.78343	0.00008
6	-1.35877	1.00681	0.00707	-1.349057	1.007865	0.008348	-1.35616	0.99892	0.00003
9	-2.31505	-1.15798	0.00127	-2.315337	-1.148967	0.001734	-2.29658	-1.15470	-0.00011
1	0.09653	-2.07600	-0.01665	0.091122	-2.075370	-0.018815	0.10137	-2.06970	-0.00012
6	2.56613	-0.85135	0.00876	2.554610	-0.855280	0.011793	2.55954	-0.84428	0.00003
1	1.95085	1.81922	-0.01476	1.958489	1.809352	-0.016712	1.94166	1.81938	0.00011
1	-0.28954	2.87244	0.00257	-0.278382	2.870847	0.004184	-0.29754	2.86447	0.00013
1	-2.35206	1.44173	0.01126	-2.342170	1.445403	0.012568	-2.34988	1.42952	0.00003
1	2.59343	-1.74432	-0.62382	2.548293	-1.805797	-0.528274	2.69704	-1.48193	-0.88046
1	2.83811	-1.16280	1.02498	2.871536	-1.059778	1.039802	2.69733	-1.48121	0.88100
1	3.33950	-0.16237	-0.34259	3.308286	-0.209319	-0.445973	3.35606	-0.09608	-0.00039

$1r_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.14549	-0.41318	0.00000	-1.134413	-0.416827	-0.000003	-1.14460	-0.42074	0.00000
6	0.04242	-1.11204	0.00000	0.047752	-1.138057	0.000003	0.04476	-1.12710	0.00000
6	1.17335	-0.25416	0.00001	1.158338	-0.253389	0.000005	1.16024	-0.24904	0.00001
6	1.07351	1.15225	0.00000	1.070951	1.152644	0.000000	1.06254	1.15155	0.00000
6	-0.18424	1.77133	-0.00001	-0.181628	1.769552	-0.000006	-0.18997	1.76687	-0.00001

6	-1.33282	0.97229	-0.00001	-1.324359	0.968787	-0.000008	-1.32816	0.96277	-0.00001
9	-2.36195	-1.14209	0.00000	-2.351015	-1.126319	-0.000005	-2.33928	-1.13306	0.00000
6	2.56203	-0.88023	0.00001	2.544030	-0.872648	0.000013	2.55368	-0.86552	0.00001
1	1.97294	1.77213	0.00000	1.973547	1.770484	0.000001	1.96044	1.77350	0.00000
1	-0.26883	2.85703	-0.00001	-0.269427	2.856843	-0.000010	-0.27818	2.85161	-0.00001
1	-2.33041	1.40998	-0.00001	-2.326027	1.399673	-0.000013	-2.32763	1.39708	-0.00001
1	2.69349	-1.52514	-0.87854	2.675751	-1.515186	-0.877779	2.69611	-1.51234	-0.87589
1	2.69349	-1.52512	0.87858	2.675755	-1.515157	0.877825	2.69611	-1.51231	0.87593
1	3.36438	-0.12764	0.00001	3.345518	-0.120162	0.000000	3.35578	-0.11283	0.00000

$1r_4$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.17284	-0.36229	0.00001	-1.171744	-0.362458	0.000010	-1.17583	-0.37177	0.00000
6	0.08295	-0.95631	0.00001	0.079138	-0.954679	-0.000022	0.08199	-0.94818	0.00000
6	1.22325	-0.12394	0.00001	1.215762	-0.118356	-0.000041	1.21521	-0.11291	-0.00001
6	1.16062	1.29713	0.00002	1.186315	1.305408	-0.000037	1.16904	1.30867	0.00000
6	-0.15940	1.80059	-0.00001	-0.147744	1.790685	0.000009	-0.16455	1.78966	0.00000
6	-1.33300	1.01175	0.00000	-1.322335	1.014658	0.000027	-1.32813	1.00449	0.00000
9	-2.30069	-1.18168	-0.00001	-2.299354	-1.168291	-0.000002	-2.28232	-1.17648	0.00000
1	0.15352	-2.04462	0.00003	0.146729	-2.045117	-0.000055	0.15420	-2.03718	0.00000
6	2.58904	-0.79759	-0.00001	2.565483	-0.812180	0.000029	2.57651	-0.79764	0.00000
1	-0.31767	2.88485	0.00000	-0.312522	2.877799	-0.000002	-0.33619	2.87428	0.00000
1	-2.33258	1.44601	-0.00002	-2.323714	1.447375	0.000038	-2.33202	1.42930	0.00000
1	2.52098	-1.89573	0.00006	2.708244	-1.453116	-0.882154	2.72862	-1.44279	-0.88052
1	3.16916	-0.48566	0.87793	2.708701	-1.451975	0.882966	2.72868	-1.44265	0.88062
1	3.16905	-0.48576	-0.87806	3.337502	-0.038822	-0.000631	3.35210	-0.02664	-0.00008

$1r_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.19423	-0.30588	-0.00001	-1.191357	-0.312207	-0.000010	-1.19622	-0.31585	-0.00001
6	0.02589	-0.96828	-0.00001	0.026622	-0.970561	-0.000009	0.02575	-0.96967	0.00000
6	1.18727	-0.17444	0.00000	1.182495	-0.178044	0.000004	1.17891	-0.17234	0.00001
6	1.04505	1.22573	0.00001	1.032726	1.220373	0.000013	1.03073	1.22053	0.00000
6	-0.18746	1.93583	0.00001	-0.185779	1.953685	0.000012	-0.19365	1.94432	0.00000
6	-1.32082	1.07903	0.00000	-1.300636	1.076059	0.000001	-1.31036	1.06743	-0.00001
9	-2.34524	-1.10417	-0.00002	-2.340709	-1.098940	-0.000024	-2.32619	-1.09765	-0.00001
1	0.06228	-2.05547	-0.00002	0.062802	-2.059531	-0.000018	0.06641	-2.05577	0.00000
6	2.55279	-0.83549	0.00002	2.541257	-0.836024	0.000016	2.54579	-0.82551	0.00002
1	1.98077	1.79800	0.00002	1.979472	1.782855	0.000020	1.97508	1.78416	0.00001
1	-2.33656	1.48393	0.00000	-2.325204	1.469245	-0.000002	-2.33567	1.45615	-0.00001
1	2.70125	-1.47388	-0.88310	2.693114	-1.472569	-0.881800	2.70383	-1.46622	-0.88004
1	2.70129	-1.47376	0.88321	2.693161	-1.472441	0.881917	2.70385	-1.46616	0.88011
1	3.34720	-0.08022	-0.00005	3.331080	-0.076783	-0.000058	3.33659	-0.06682	-0.00002

$1r_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-1.23984	-0.24967	0.00214	-1.234636	-0.249201	0.001975	-1.23909	-0.26189	-0.00003
6	-0.03150	-0.94974	-0.01174	-0.025340	-0.948214	-0.011064	-0.02637	-0.94572	-0.00004
6	1.16720	-0.21783	-0.01362	1.165836	-0.213533	-0.019499	1.16468	-0.20931	0.00000
6	1.06502	1.18007	-0.00839	1.059593	1.179932	-0.008244	1.04957	1.18132	0.00005
6	-0.19936	1.80310	0.00367	-0.209610	1.788046	0.004213	-0.21639	1.78834	0.00006
6	-1.43839	1.11908	0.00907	-1.459362	1.121505	0.010120	-1.45727	1.11074	0.00002
9	-2.37331	-1.10082	0.00248	-2.349136	-1.109873	0.002526	-2.34222	-1.10750	-0.00008
1	-0.01731	-2.04083	-0.02309	-0.010894	-2.040300	-0.023579	-0.00155	-2.03688	-0.00009
6	2.50877	-0.92013	0.01170	2.503469	-0.906819	0.014264	2.50942	-0.89892	0.00003
1	1.97705	1.78333	-0.01705	1.971335	1.785989	-0.018695	1.95988	1.78684	0.00008

1	-0.19616	2.89969	0.00296	-0.201725	2.888136	0.004398	-0.21204	2.88696	0.00009
1	2.48816	-1.85062	-0.57074	2.476307	-1.851179	-0.541975	2.64982	-1.54470	-0.87931
1	2.81731	-1.19007	1.03326	2.823678	-1.145147	1.037383	2.65006	-1.54421	0.87970
1	3.29934	-0.28336	-0.40462	3.283825	-0.278940	-0.430849	3.32649	-0.16790	-0.00028

1s. 1-Fluoro-4-anisole

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.91318	0.28117	0.00000	0.9137	0.2807	0.0000	0.91300	0.28147	0.00000
6	0.03940	1.38026	0.00000	0.0415	1.3776	0.0000	0.03834	1.37481	0.00000
6	-1.33851	1.18447	-0.00001	-1.3331	1.1832	0.0000	-1.33432	1.17839	-0.00001
6	-1.83100	-0.11771	-0.00001	-1.8265	-0.1176	0.0000	-1.83401	-0.11909	-0.00001
6	-0.99171	-1.21928	0.00000	-0.9848	-1.2158	0.0000	-0.98732	-1.21300	0.00000
6	0.39557	-1.02023	0.00000	0.3999	-1.0187	0.0000	0.39487	-1.01530	0.00000
8	2.24770	0.58570	0.00001	2.2465	0.5975	0.0000	2.24091	0.58649	0.00001
1	0.45985	2.38030	-0.00001	0.4676	2.3765	0.0000	0.46004	2.37312	-0.00001
1	-2.02671	2.02285	-0.00001	-2.0232	2.0212	0.0000	-2.02171	2.01618	-0.00001
9	-3.18104	-0.31141	-0.00001	-3.1705	-0.3117	0.0000	-3.16109	-0.31039	-0.00001
1	-1.41176	-2.21933	0.00000	-1.4078	-2.2157	0.0000	-1.40594	-2.21259	0.00000
6	3.18664	-0.48154	0.00001	3.1617	-0.4909	0.0000	3.16862	-0.47998	0.00001
1	4.17097	-0.01191	0.00001	4.1521	-0.0378	0.0000	4.15912	-0.02202	0.00001
1	3.08250	-1.10678	0.89600	3.0433	-1.1121	0.8945	3.06376	-1.10979	0.89331
1	3.08251	-1.10678	-0.89597	3.0433	-1.1121	-0.8944	3.06376	-1.10979	-0.89329
1	1.04903	-1.88403	0.00001	1.0511	-1.8854	0.0000	1.04853	-1.87742	0.00001

$1s_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.87587	0.29394	0.00000	0.8739	0.2910	0.0000	0.87169	0.29220	0.00000
6	0.00805	1.40253	0.00000	-0.0023	1.3921	0.0000	0.00036	1.39202	0.00000
6	-1.39972	1.30721	-0.00001	-1.4111	1.3242	0.0000	-1.40696	1.31364	-0.00001
6	-1.82493	-0.01362	-0.00001	-1.8133	-0.0085	0.0000	-1.82351	-0.01596	-0.00001
6	-1.03789	-1.15849	0.00000	-1.0263	-1.1576	0.0000	-1.03054	-1.15395	0.00000
6	0.36205	-1.00636	0.00000	0.3680	-1.0078	0.0000	0.36423	-1.00510	0.00000
8	2.24809	0.57808	0.00001	2.2464	0.5941	0.0000	2.23958	0.58142	0.00001
1	0.49778	2.38133	-0.00001	0.5016	2.3676	0.0000	0.50195	2.36733	-0.00001
9	-3.21700	-0.27939	-0.00001	-3.1906	-0.2916	0.0000	-3.18702	-0.28401	-0.00001
1	-1.48257	-2.15366	0.00000	-1.4786	-2.1500	0.0000	-1.47274	-2.15059	0.00000
6	3.14256	-0.50680	0.00001	3.1149	-0.5115	0.0000	3.12230	-0.49979	0.00001
1	4.15072	-0.08001	0.00001	4.1300	-0.1048	0.0000	4.13795	-0.08732	0.00001
1	3.02350	-1.14181	0.89241	2.9818	-1.1428	0.8899	3.00445	-1.14180	0.88891
1	3.02351	-1.14182	-0.89239	2.9818	-1.1428	-0.8899	3.00446	-1.14180	-0.88888
1	0.99932	-1.88458	0.00001	1.0053	-1.8876	0.0000	1.00497	-1.87951	0.00001

$1s_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.88254	0.35936	0.00000	0.8730	0.3639	0.0000	0.87366	0.35922	0.00000
6	0.06611	1.50725	0.00000	0.0775	1.5267	0.0000	0.07057	1.51607	0.00000
6	-1.31262	1.21495	-0.00001	-1.2959	1.2087	0.0000	-1.30245	1.20456	-0.00001
6	-1.80218	-0.09356	-0.00001	-1.7963	-0.0953	0.0000	-1.80358	-0.09656	-0.00001
6	-0.97328	-1.19956	0.00000	-0.9647	-1.1982	0.0000	-0.97035	-1.19723	0.00000
6	0.41641	-0.96482	0.00000	0.4192	-0.9663	0.0000	0.41353	-0.96103	0.00000
8	2.27195	0.62255	0.00001	2.2658	0.6291	0.0000	2.26385	0.62063	0.00001
1	-2.05533	2.01819	-0.00001	-2.0508	2.0053	0.0000	-2.05690	2.00036	-0.00001
9	-3.18340	-0.31466	-0.00001	-3.1695	-0.3144	0.0000	-3.15901	-0.31051	-0.00001
1	-1.38308	-2.20552	0.00000	-1.3787	-2.2042	0.0000	-1.37955	-2.20283	0.00000
6	3.15498	-0.46790	0.00001	3.1233	-0.4817	0.0000	3.13357	-0.46665	0.00001
1	4.16816	-0.05085	0.00001	4.1427	-0.0832	0.0000	4.15526	-0.06581	0.00001

1	3.03737	-1.10749	0.89189	2.9937	-1.1185	0.8891	3.01748	-1.11403	0.88802
1	3.03738	-1.10750	-0.89186	2.9937	-1.1185	-0.8890	3.01748	-1.11404	-0.88799
1	1.07880	-1.82972	0.00001	1.0816	-1.8308	0.0000	1.07686	-1.82438	0.00001

$1s_5$

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.89537	0.22692	0.00000	0.8892	0.2298	0.0000	0.89074	0.23085	0.00000
6	0.06254	1.35681	0.00000	0.0606	1.3626	0.0000	0.05930	1.35439	0.00000
6	-1.32762	1.17790	-0.00001	-1.3229	1.1768	0.0000	-1.32538	1.17348	-0.00001
6	-1.79605	-0.12908	-0.00001	-1.7870	-0.1308	0.0000	-1.79508	-0.13072	-0.00001
6	-0.94732	-1.23340	0.00000	-0.9233	-1.2242	0.0000	-0.93431	-1.22274	0.00000
6	0.46221	-1.10802	0.00000	0.4861	-1.1138	0.0000	0.47306	-1.10768	0.00000
8	2.26719	0.56110	0.00001	2.2583	0.5794	0.0000	2.25827	0.56775	0.00001
1	0.48944	2.36030	-0.00001	0.4901	2.3656	0.0000	0.48289	2.35895	-0.00001
1	-2.01815	2.01656	-0.00001	-2.0220	2.0103	0.0000	-2.01958	2.00816	-0.00001
9	-3.18241	-0.32069	-0.00001	-3.1634	-0.3306	0.0000	-3.15368	-0.32644	-0.00001
1	-1.42150	-2.21923	0.00000	-1.4055	-2.2099	0.0000	-1.41583	-2.20750	0.00000
6	3.17970	-0.52032	0.00001	3.1345	-0.5312	0.0000	3.14649	-0.52075	0.00001
1	4.17713	-0.06203	0.00001	4.1439	-0.1021	0.0000	4.15689	-0.08692	0.00001
1	3.05221	-1.16152	0.88149	2.9873	-1.1690	0.8776	3.01180	-1.16890	0.87641
1	3.05222	-1.16153	-0.88146	2.9873	-1.1690	-0.8776	3.01180	-1.16890	-0.87638

$1s_6$

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	0.87643	0.26585	0.00000	0.8745	0.2669	0.0000	0.87279	0.26509	0.00000
6	0.00949	1.36363	0.00000	0.0126	1.3623	0.0000	0.01057	1.36062	0.00000
6	-1.36927	1.12129	-0.00001	-1.3614	1.1219	0.0000	-1.36233	1.11631	-0.00001
6	-1.80287	-0.20458	-0.00001	-1.7900	-0.2077	0.0000	-1.80190	-0.20476	-0.00001
6	-1.02368	-1.34570	0.00000	-1.0258	-1.3657	0.0000	-1.02700	-1.35569	0.00000
6	0.36344	-1.04373	0.00000	0.3545	-1.0401	0.0000	0.35490	-1.03716	0.00000
8	2.24158	0.59183	0.00001	2.2409	0.6055	0.0000	2.23426	0.59171	0.00001
1	0.41323	2.37272	-0.00001	0.4244	2.3699	0.0000	0.41976	2.36654	-0.00001
1	-2.07812	1.94934	-0.00001	-2.0765	1.9456	0.0000	-2.06977	1.94617	-0.00001
9	-3.21457	-0.33967	-0.00001	-3.1914	-0.3277	0.0000	-3.18669	-0.33119	-0.00001
6	3.16454	-0.47236	0.00001	3.1359	-0.4819	0.0000	3.14429	-0.46968	0.00001
1	4.15987	-0.01592	0.00001	4.1398	-0.0471	0.0000	4.14763	-0.02672	0.00001
1	3.06014	-1.10929	0.89111	3.0170	-1.1154	0.8887	3.04246	-1.11362	0.88755
1	3.06015	-1.10929	-0.89108	3.0170	-1.1154	-0.8886	3.04246	-1.11363	-0.88752
1	1.07478	-1.87160	0.00001	1.0724	-1.8668	0.0000	1.07561	-1.85999	0.00001

1t. 1-Fluoro-4-trifluoromethylbenzene

Atomic Number	Atomic Coordinate DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.40213	0.00000	0.00345	-2.39178	0.00001	0.00432	-2.40228	0.00000	0.00469
6	-1.73548	-1.21991	-0.00574	-1.72273	-1.21691	-0.00917	-1.72891	-1.21449	-0.00554
6	-0.34093	-1.21369	-0.02381	-0.33107	-1.21294	-0.03041	-0.33905	-1.20847	-0.02307
6	0.35603	-0.00003	-0.03521	0.35983	0.00004	-0.04613	0.35703	0.00002	-0.02890
6	-0.34091	1.21365	-0.02381	-0.33108	1.21297	-0.03041	-0.33907	1.20850	-0.02307
6	-1.73545	1.21990	-0.00574	-1.72277	1.21691	-0.00917	-1.72893	1.21449	-0.00554
9	-3.75742	0.00002	0.01879	-3.74441	-0.00002	0.02470	-3.73626	-0.00002	0.01959
1	-2.30035	-2.14533	-0.00161	-2.29060	-2.14165	-0.00323	-2.29348	-2.13885	-0.00431
1	0.20195	-2.15233	-0.03570	0.21525	-2.15077	-0.04752	0.20674	-2.14401	-0.03986
6	1.86020	-0.00001	-0.00219	1.85288	0.00001	0.00120	1.86181	0.00001	-0.00037
1	0.20200	2.15228	-0.03570	0.21521	2.15082	-0.04752	0.20671	2.14405	-0.03985
1	-2.30030	2.14534	-0.00161	-2.29065	2.14164	-0.00323	-2.29351	2.13885	-0.00431
9	2.38758	-1.09184	-0.61004	2.37607	-1.09003	-0.60466	2.37087	-1.08365	-0.60714
9	2.34104	0.00050	1.27247	2.31123	-0.00043	1.27501	2.33781	-0.00037	1.25841

9	2.38755	1.09138	-0.61089	2.37612	1.09042	-0.60394	2.37090	1.08400	-0.60651

$1t_2$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.39095	-0.10293	0.00001	-2.37366	-0.10657	0.00002	-2.38682	-0.10196	0.00001
6	-1.78155	-1.34653	0.00000	-1.77788	-1.36412	0.00001	-1.78324	-1.35427	0.00001
6	-0.37500	-1.22473	-0.00002	-0.37385	-1.21483	0.00000	-0.37925	-1.21569	0.00000
6	0.32100	0.00687	-0.00002	0.32376	0.01400	-0.00001	0.32077	0.00785	-0.00001
6	-0.39120	1.21336	0.00000	-0.38247	1.21834	-0.00001	-0.38595	1.21076	0.00000
6	-1.78754	1.15671	0.00002	-1.77474	1.15621	0.00001	-1.77706	1.15222	0.00001
9	-3.79736	-0.04497	0.00003	-3.77170	-0.03634	0.00003	-3.76734	-0.03821	0.00003
1	0.23786	-2.13027	-0.00003	0.25415	-2.11512	-0.00001	0.24341	-2.11712	-0.00001
6	1.81060	0.00912	-0.00001	1.80145	0.00805	-0.00001	1.81014	0.00868	-0.00001
1	0.12482	2.16787	0.00000	0.13663	2.17324	-0.00001	0.13540	2.16122	-0.00001
1	-2.38308	2.06798	0.00003	-2.37959	2.06250	0.00001	-2.37152	2.06440	0.00001
9	2.35938	-0.62954	-1.08610	2.33613	-0.63113	-1.08317	2.34441	-0.62570	-1.07546
9	2.35937	-0.62934	1.08621	2.33614	-0.63101	1.08322	2.34442	-0.62556	1.07552
9	2.36619	1.26199	-0.00012	2.35867	1.25546	-0.00008	2.35421	1.25013	-0.00009

$1t_3$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.38606	-0.02853	0.00001	-2.37240	-0.02569	0.00001	-2.38306	-0.02694	0.00001
6	-1.71226	-1.24241	0.00002	-1.68144	-1.23349	0.00002	-1.69838	-1.23221	0.00002
6	-0.29568	-1.32336	0.00002	-0.26907	-1.33150	0.00002	-0.28464	-1.32800	0.00002
6	0.32668	-0.04810	0.00000	0.32370	-0.04166	0.00000	0.32509	-0.04509	0.00000
6	-0.34536	1.18781	-0.00001	-0.33933	1.19538	-0.00001	-0.34461	1.18408	-0.00001
6	-1.74283	1.20500	0.00000	-1.73367	1.20514	0.00000	-1.73734	1.20284	0.00000
9	-3.77813	-0.01457	0.00002	-3.75848	-0.02440	0.00002	-3.75008	-0.01866	0.00002
1	-2.32376	-2.14828	0.00004	-2.30255	-2.13667	0.00004	-2.32086	-2.13316	0.00004
6	1.83166	-0.02978	-0.00001	1.81656	-0.02597	-0.00001	1.82837	-0.02455	-0.00001
1	0.19793	2.13084	-0.00002	0.20484	2.13863	-0.00002	0.19993	2.12570	-0.00002
1	-2.31325	2.12861	-0.00001	-2.31195	2.12578	-0.00001	-2.30962	2.12445	-0.00001
9	2.39340	-0.63981	-1.08704	2.36305	-0.63995	-1.08498	2.37391	-0.63607	-1.07654
9	2.39341	-0.63979	1.08703	2.36306	-0.63992	1.08497	2.37392	-0.63605	1.07653
9	2.36712	1.24584	-0.00003	2.35944	1.23971	-0.00003	2.35759	1.23546	-0.00003

$1t_5$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.38606	0.02853	0.00000	-2.37246	0.02562	0.00006	-2.38305	0.02694	0.00001
6	-1.74283	-1.20500	0.00000	-1.73350	-1.20499	0.00003	-1.73732	-1.20283	0.00000
6	-0.34536	-1.18781	0.00000	-0.33923	-1.19476	0.00011	-0.34460	-1.18408	-0.00006
6	0.32668	0.04810	0.00000	0.32381	0.04206	-0.00023	0.32509	0.04509	-0.00011
6	-0.29568	1.32336	0.00000	-0.26955	1.33167	0.00008	-0.28464	1.32801	-0.00008
6	-1.71226	1.24241	0.00000	-1.68184	1.23355	0.00014	-1.69838	1.23221	-0.00002
9	-3.77813	0.01457	0.00000	-3.75827	0.02396	-0.00014	-3.75008	0.01866	0.00004
1	-2.31325	-2.12861	0.00000	-2.31139	-2.12567	0.00020	-2.30959	-2.12446	0.00002
1	0.19793	-2.13084	0.00000	0.20510	-2.13776	0.00010	0.19994	-2.12570	-0.00006
6	1.83166	0.02978	0.00000	1.81668	0.02604	-0.00014	1.82836	0.02455	-0.00003
1	-2.32376	2.14828	0.00000	-2.30286	2.13656	0.00048	-2.32087	2.13315	0.00002
9	2.36712	-1.24584	0.00002	2.35887	-1.23979	-0.00143	2.35757	-1.23547	-0.00105
9	2.39341	0.63981	1.08703	2.36340	0.63838	1.08558	2.37381	0.63512	1.07715
9	2.39340	0.63979	-1.08704	2.36329	0.64098	-1.08413	2.37400	0.63701	-1.07594

$1t_6$

Atomic Number	Atomic Coordinate								
	DFT			G3MP2			G4MP2		
	x	y	z	x	y	z	x	y	z
6	-2.39096	0.10294	0.00001	-2.37447	0.10495	0.00259	-2.38765	0.09950	0.00321
6	-1.78754	-1.15672	-0.00002	-1.76847	-1.15498	-0.01124	-1.76996	-1.15111	-0.01034
6	-0.39120	-1.21335	-0.00007	-0.37702	-1.20926	-0.02944	-0.37936	-1.20077	-0.02699
6	0.32101	-0.00686	-0.00011	0.32435	-0.00079	-0.04802	0.32147	0.00677	-0.03428
6	-0.37500	1.22473	-0.00008	-0.37962	1.22361	-0.03156	-0.38616	1.22548	-0.02920
6	-1.78155	1.34652	-0.00002	-1.78529	1.36431	-0.00950	-1.79169	1.35502	-0.00866
9	-3.79736	0.04497	0.00007	-3.77192	0.02670	0.02890	-3.76709	0.02692	0.02899
1	-2.38304	-2.06801	-0.00001	-2.36826	-2.06448	-0.00607	-2.35889	-2.06686	-0.01115
1	0.12483	-2.16786	-0.00009	0.14691	-2.16160	-0.04258	0.14731	-2.14867	-0.04051
6	1.81060	-0.00910	-0.00001	1.80142	-0.00454	0.00036	1.80956	-0.00337	-0.00059
1	0.23787	2.13027	-0.00011	0.24137	2.12734	-0.05007	0.23011	2.12976	-0.05087
9	2.36618	-1.26199	-0.00095	2.35713	-1.20300	-0.35232	2.35004	-1.17180	-0.43098
9	2.35931	0.62857	1.08672	2.30561	0.27147	1.24277	2.32669	0.18705	1.24541
9	2.35944	0.63030	-1.08561	2.36857	0.92249	-0.82384	2.36639	0.96857	-0.76080

Pd(DMA)

	Atomic Coordinate		
Atom	x	y	z
Pd	1.98009	0.07404	0.00004
O	0.17923	0.50299	0.00011
C	1.14556	0.27789	0.00013
N	2.41968	0.21019	0.00025
C	3.62443	0.60374	0.00025
H	4.23152	0.38543	-0.8883
H	-4.2326	0.38475	0.88689
H	3.39086	1.66598	0.00032
C	2.64566	1.65117	0.00001
H	3.21711	1.94436	0.88912
H	3.21528	1.94447	0.89025
H	1.68441	2.16064	0.00099
C	0.93844	1.78056	0.00011
H	-1.3781	2.24743	0.88725
H	1.37825	2.24745	0.88739
H	0.13997	1.9534	0.0002

3ib-o

	Atomic Coordinate		
Atom	x	y	z
C	-1.01695	1.267764	0.241775
C	-0.26346	0.123494	-0.0585
C	-0.9401	-1.07347	-0.33965
C	-2.33542	-1.13359	-0.33024
C	-3.05809	0.02852	-0.03544

C	-2.41451	1.235941	0.253099
H	-0.50472	2.193247	0.490691
H	-0.36943	-1.96618	-0.56981
H	-4.14555	-0.00981	-0.02599
C	1.218313	0.202966	-0.10037
C	2.044056	-0.81236	0.402196
C	1.87412	1.322245	-0.64314
C	3.430801	-0.74316	0.382349
C	3.264061	1.418053	-0.67581
H	1.2698	2.118621	-1.06606
C	4.047186	0.383258	-0.16144
H	3.999415	-1.56757	0.798398
H	3.733856	2.294945	-1.11014
H	5.130595	0.446983	-0.18495
C	-3.05185	-2.43577	-0.60182
H	-3.28038	-2.96	0.334384
H	-4.00077	-2.27085	-1.12165
H	-2.44271	-3.10909	-1.21186
C	-3.20991	2.486762	0.545638
H	-2.67594	3.149204	1.233761
H	-3.40014	3.056149	-0.37273
H	-4.18182	2.249761	0.988722
F	1.482033	-1.91659	0.94948

3ib-m

	Atomic Coordinate		
Atom	x	y	z
C	1.299128	-1.19942	-0.23768
C	0.467724	-0.11035	0.059915
C	1.057504	1.140142	0.299556
C	2.442776	1.311954	0.243531
C	3.244245	0.203032	-0.05272
C	2.688994	-1.05781	-0.29423
H	0.853374	-2.16652	-0.45373
H	0.425893	1.985924	0.557268
H	4.324629	0.325245	-0.09664
C	-1.00631	-0.27711	0.120692
C	-1.85686	0.721026	-0.38087
C	-1.58247	-1.43056	0.680608
C	-3.23171	0.545778	-0.31086
C	-2.96732	-1.58215	0.736216
H	-0.93908	-2.1979	1.098125
C	-3.81373	-0.59056	0.238189
H	-3.39441	-2.47653	1.179788

H	-4.8936	-0.68113	0.267892
H	-1.46236	1.616573	-0.84721
C	3.572615	-2.24791	-0.58652
H	3.853019	-2.76559	0.339233
H	3.064923	-2.97656	-1.22566
H	4.499391	-1.94716	-1.08433
C	3.064684	2.669243	0.474494
H	3.272073	3.173092	-0.47768
H	2.403272	3.321151	1.052392
H	4.015112	2.588258	1.011234
F	-4.0331	1.514361	-0.80695

3ib-p

	Atomic Coordinate		
Atom	x	y	z
C	1.270515	-1.19192	-0.18255
C	0.553455	0.000001	0.000007
C	1.270516	1.191919	0.18255
C	2.668082	1.207462	0.180289
C	3.351811	0.000002	-1.4E-05
C	2.668079	-1.20746	-0.18031
H	0.728853	-2.11831	-0.35384
H	0.72886	2.118312	0.353836
H	4.439945	-2E-06	-0.00002
C	-0.93095	0.000002	0.000004
C	-1.65422	1.038972	-0.61046
C	-1.65422	-1.03897	0.610466
C	-3.04745	1.047879	-0.61388
C	-3.04745	-1.04788	0.613873
H	-1.11763	-1.83902	1.110576
C	-3.72313	0	-5E-06
H	-3.61223	-1.84137	1.090739
H	-1.11763	1.839028	-1.11056
H	-3.61222	1.84137	-1.09075
C	3.426151	-2.5037	-0.34701
H	3.67554	-2.94107	0.627759
H	2.838012	-3.2448	-0.8963
H	4.367272	-2.35154	-0.88433
C	3.426154	2.503695	0.34703
H	3.675644	2.941026	-0.62773
H	2.837974	3.244817	0.89624
H	4.367225	2.351535	0.884431
F	-5.07375	0	-1E-06

preRE1-o

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.00199	-1.0595	-0.34797
C	-1.85401	-0.38911	-0.14642
C	-2.7229	-1.1031	0.691367
C	-2.3562	0.673946	-0.91056
C	-4.09303	-0.8039	0.729252
C	-3.72024	0.99093	-0.88595
C	-4.57261	0.2449	-0.06247
H	-5.63157	0.495618	-0.02736
C	0.577416	0.569702	0.646388
C	0.875448	1.750516	-0.03026
C	0.830083	0.560402	2.027248
C	1.442812	2.864866	0.579161
C	1.401631	1.664611	2.672572
C	1.712568	2.817127	1.949147
H	1.651845	3.746667	-0.01842
H	1.591349	1.624146	3.741652
H	2.150601	3.678781	2.443897
O	2.007136	-2.09696	-0.68336
C	2.943009	-1.4434	-0.16404
N	3.568727	-0.45923	-0.8448
C	4.439643	0.530944	-0.21996
H	5.275308	0.757301	-0.88929
H	3.880549	1.454018	-0.02301
H	4.844587	0.165851	0.721527
C	3.119065	-0.13669	-2.20022
H	2.376079	0.665441	-2.18132
H	3.983047	0.177775	-2.79267
H	2.667534	-1.02135	-2.64483
C	3.383246	-1.75785	1.249993
H	4.464283	-1.90158	1.331103
H	3.084372	-0.94383	1.918323
H	2.870617	-2.66867	1.557127
H	-1.68134	1.267629	-1.51847
H	-2.34283	-1.89899	1.328853
H	0.580737	-0.32223	2.608276
C	-4.26473	2.107641	-1.74717
H	-5.11403	2.607195	-1.26951
H	-3.49924	2.861955	-1.9542
H	-4.6151	1.725482	-2.71455
C	-5.03169	-1.60941	1.598363
H	-5.90242	-1.02006	1.902982
H	-5.40616	-2.49211	1.064358

H	-4.53133	-1.96718	2.504095
F	0.633281	1.838043	-1.37335

preRE1-m

	Atomic Coordinate		
Atom	x	y	z
Pd	0.26119	-1.12938	-0.0943
C	2.114512	-0.44194	0.066941
C	2.892371	-0.24225	-1.0839
C	2.704222	-0.23926	1.323776
C	4.24515	0.113906	-0.99383
C	4.054573	0.118362	1.441073
C	4.808337	0.293266	0.274629
H	5.853632	0.587003	0.355526
C	-0.40412	0.745688	-0.09975
C	-1.4468	1.036724	0.793081
C	-0.06733	1.690448	-1.08105
C	-2.16906	2.213257	0.632982
C	-0.80154	2.874675	-1.20276
C	-1.87872	3.146037	-0.35348
H	-0.53908	3.59278	-1.97522
H	-2.47291	4.049109	-0.43844
O	-1.83466	-2.03519	-0.19871
C	-2.77868	-1.32972	-0.61973
N	-3.85933	-1.08497	0.158072
C	-4.89427	-0.10652	-0.16339
H	-5.87214	-0.50437	0.126268
H	-4.71263	0.824064	0.387131
H	-4.91828	0.114592	-1.22796
C	-3.88905	-1.57035	1.535175
H	-3.81505	-0.72595	2.231182
H	-4.83216	-2.09471	1.721776
H	-3.0529	-2.24755	1.693538
C	-2.73129	-0.7282	-2.00924
H	-3.62883	-0.96105	-2.58941
H	-2.61992	0.358645	-1.94651
H	-1.85701	-1.13458	-2.5154
H	2.109461	-0.34619	2.227584
H	2.447283	-0.35831	-2.0705
H	0.76211	1.501529	-1.75284
C	4.688049	0.300282	2.801616
H	5.48583	1.049663	2.776561
H	3.951062	0.61492	3.547163
H	5.133475	-0.63694	3.159197

C	5.0824	0.282147	-2.24118
H	5.892532	1.002299	-2.08735
H	5.544041	-0.66784	-2.53949
H	4.477963	0.627657	-3.08615
H	-1.73649	0.352738	1.581956
F	-3.23275	2.432322	1.457407

preRE1-p

	Atomic Coordinate		
Atom	x	y	z
Pd	0.16498	-1.23886	-0.18611
C	1.974037	-0.43862	-0.06342
C	2.710636	-0.13793	-1.21772
C	2.583711	-0.27891	1.190426
C	4.049894	0.269291	-1.13522
C	3.921051	0.12472	1.299786
C	4.63764	0.396528	0.128164
H	5.672613	0.726048	0.202406
C	-0.54534	0.622552	-0.16525
C	-0.55273	1.408804	0.996732
C	-1.20139	1.111357	-1.30649
C	-1.25459	2.618339	1.046258
C	-1.90388	2.321964	-1.27402
C	-1.92679	3.050945	-0.09095
H	-2.41717	2.70739	-2.14935
O	-1.80153	-2.4051	-0.34291
C	-2.83811	-1.70286	-0.35984
N	-3.32875	-1.13357	0.763719
C	-4.30211	-0.04519	0.759409
H	-4.99697	-0.17245	1.595224
H	-3.78844	0.917793	0.866996
H	-4.87803	-0.02967	-0.16327
C	-2.64341	-1.34635	2.036633
H	-1.96282	-0.51554	2.249453
H	-3.39072	-1.41584	2.832851
H	-2.06931	-2.26934	1.98614
C	-3.57142	-1.48998	-1.66858
H	-4.64008	-1.70915	-1.58991
H	-3.45365	-0.45297	-1.99841
H	-3.11791	-2.14772	-2.40915
H	2.018566	-0.46675	2.101648
H	2.242201	-0.20944	-2.19635
H	-1.17417	0.550023	-2.23565
C	4.582771	0.245448	2.653489

H	5.355068	1.021395	2.655361
H	3.855803	0.489337	3.434858
H	5.067308	-0.69595	2.942675
C	4.84461	0.550199	-2.39012
H	5.67168	1.240699	-2.19702
H	5.277605	-0.37197	-2.79835
H	4.215142	0.985838	-3.17286
H	-0.00124	1.085491	1.873546
H	-1.2728	3.230217	1.942491
F	-2.60843	4.22043	-0.0501

TS1-o

	Atomic Coordinate		
Atom	x	y	z
Pd	0.184513	-1.14446	-0.09542
C	-1.5881	-0.14364	0.027739
C	-2.37403	-0.41638	1.163553
C	-2.22948	0.199469	-1.17581
C	-3.76935	-0.39459	1.098078
C	-3.62693	0.230269	-1.26072
C	-4.38058	-0.06423	-0.11959
H	-5.46701	-0.02611	-0.1746
C	0.119747	0.839675	0.402733
C	0.567753	1.755672	-0.5589
C	0.315827	1.227244	1.74515
C	1.176314	2.965473	-0.25364
C	0.940086	2.429372	2.085099
C	1.369695	3.308019	1.087533
H	1.494317	3.612705	-1.0649
H	1.07943	2.683529	3.132157
H	1.843008	4.250672	1.344106
O	2.117856	-2.30349	-0.2296
C	2.886781	-1.42307	0.23234
N	3.540468	-0.56136	-0.58567
C	4.20876	0.638274	-0.08807
H	4.988643	0.929729	-0.79663
H	3.499779	1.469132	0.018644
H	4.683753	0.454871	0.874941
C	3.20323	-0.55967	-2.00974
H	2.375599	0.130491	-2.21047
H	4.082177	-0.25414	-2.58386
H	2.900048	-1.56271	-2.30367
C	3.134613	-1.33353	1.726185
H	4.198813	-1.41369	1.969749

H	2.757114	-0.38337	2.116983
H	2.591613	-2.15156	2.197965
H	-1.63561	0.463721	-2.04269
H	-1.8948	-0.64208	2.112339
H	-0.03742	0.573591	2.536282
C	-4.30504	0.554945	-2.57211
H	-5.28919	1.007381	-2.41475
H	-3.70468	1.24581	-3.17228
H	-4.45431	-0.35142	-3.17236
C	-4.60763	-0.73583	2.308538
H	-4.96276	-1.77293	2.26314
H	-4.03749	-0.62526	3.235948
H	-5.49236	-0.09402	2.375929
F	0.446401	1.443685	-1.88293

TS1-m

	Atomic Coordinate		
Atom	x	y	z
Pd	0.089859	-1.16985	-0.40801
C	-1.65571	-0.18138	-0.03651
C	-2.40838	-0.58527	1.079615
C	-2.32788	0.369564	-1.14115
C	-3.80385	-0.48735	1.085147
C	-3.72265	0.477301	-1.15972
C	-4.4445	0.04965	-0.0385
H	-5.52838	0.148825	-0.03522
C	0.128634	0.69683	0.412692
C	0.490886	1.770163	-0.42309
C	0.455045	0.781742	1.782845
C	1.191836	2.84663	0.105829
C	1.161439	1.875917	2.284918
C	1.54708	2.928036	1.448725
H	1.41228	1.914652	3.341791
H	2.085504	3.79499	1.814416
O	1.95849	-2.37224	-0.78948
C	2.743973	-1.71468	-0.06048
N	3.488765	-0.69918	-0.56339
C	4.18136	0.269957	0.281435
H	5.05326	0.652589	-0.25656
H	3.522404	1.111232	0.531086
H	4.531292	-0.18881	1.204795
C	3.255108	-0.26972	-1.94061
H	2.542428	0.563444	-1.9613
H	4.201913	0.05347	-2.38272

H	2.843442	-1.10115	-2.50876
C	2.911331	-2.08084	1.402298
H	3.955442	-2.29322	1.653012
H	2.55803	-1.26518	2.040657
H	2.305345	-2.96638	1.589656
H	-1.76204	0.730756	-1.99602
H	-1.90442	-0.97075	1.961848
H	0.152551	-0.01085	2.459387
C	-4.43741	1.027889	-2.37226
H	-3.80149	1.720789	-2.93196
H	-4.72622	0.222394	-3.05913
H	-5.35268	1.558659	-2.09142
C	-4.6063	-0.96896	2.272016
H	-5.51466	-0.37383	2.409785
H	-4.91814	-2.01259	2.139341
H	-4.02368	-0.91832	3.19713
H	0.235513	1.784348	-1.47628
F	1.549934	3.855234	-0.72385

TS1-p

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.01547	-1.28376	0.056019
C	1.68401	-0.15772	0.022724
C	2.397411	-0.10685	-1.18858
C	2.392097	-0.01209	1.22766
C	3.787177	0.044083	-1.20531
C	3.783574	0.1406	1.23676
C	4.464779	0.171986	0.014515
H	5.544229	0.311474	0.010747
C	-0.13441	0.756571	-0.02038
C	-0.49863	1.441195	1.155757
C	-0.51095	1.326154	-1.25326
C	-1.24518	2.620419	1.110942
C	-1.25945	2.503619	-1.3138
C	-1.61982	3.13257	-0.12698
H	-1.55627	2.94109	-2.26162
O	-1.83029	-2.62997	-0.00083
C	-2.65841	-1.77645	-0.40729
N	-3.41488	-1.05937	0.461533
C	-4.15044	0.138338	0.06419
H	-4.99871	0.275617	0.740374
H	-3.50767	1.025998	0.118303
H	-4.54095	0.045906	-0.94818

C	-3.14066	-1.17698	1.891897
H	-2.43131	-0.40191	2.207237
H	-4.07523	-1.05944	2.447771
H	-2.70866	-2.15478	2.094534
C	-2.86808	-1.56527	-1.89463
H	-3.91369	-1.71151	-2.18371
H	-2.56528	-0.55374	-2.18167
H	-2.24134	-2.28557	-2.41886
H	1.8569	-0.00388	2.173633
H	1.864695	-0.17409	-2.13337
H	-0.21303	0.848987	-2.18145
C	4.536993	0.252064	2.54236
H	3.921515	0.711174	3.322473
H	4.841701	-0.73678	2.907477
H	5.445772	0.851798	2.4305
C	4.54966	0.05475	-2.51027
H	5.004933	-0.92349	-2.70912
H	3.895591	0.289432	-3.35551
H	5.36004	0.791069	-2.49412
H	-0.19317	1.052849	2.121721
H	-1.53182	3.147143	2.015448
F	-2.33982	4.277663	-0.17794

3kb-o

	Atomic Coordinate		
Atom	x	y	z
C	1.156175	-1.28311	0.416904
C	0.378218	-0.25772	-0.13808
C	1.017823	0.871441	-0.66393
C	2.410053	0.990918	-0.63191
C	3.159949	-0.04697	-0.06764
C	2.550377	-1.19084	0.459394
H	0.661761	-2.15653	0.833844
H	0.421947	1.663113	-1.10704
H	4.244428	0.037802	-0.03771
C	-1.0996	-0.41368	-0.20778
C	-2.02044	0.530707	0.280535
C	-1.63435	-1.57778	-0.78861
C	-3.39851	0.332141	0.18452
C	-3.00624	-1.79085	-0.88954
H	-0.94029	-2.31498	-1.18021
C	-3.89304	-0.82956	-0.40453
H	-4.07154	1.084283	0.580601
H	-3.38012	-2.69984	-1.35054

H	-4.96577	-0.97931	-0.47838
C	3.085462	2.231123	-1.16841
H	3.160302	3.002439	-0.39198
H	4.100585	2.018068	-1.51666
H	2.523632	2.663806	-2.00168
C	3.382806	-2.31261	1.034759
H	2.816777	-2.89884	1.76465
H	3.713778	-3.00128	0.247408
H	4.281	-1.93094	1.52995
Cl	-1.47639	1.999576	1.09492

3kb-m

	Atomic Coordinate		
Atom	x	y	z
C	1.739586	-1.16546	-0.3012
C	0.815634	-0.18724	0.0953
C	1.284893	1.100135	0.39412
C	2.642934	1.417422	0.299487
C	3.538363	0.417743	-0.09605
C	3.103641	-0.87784	-0.39806
H	1.384905	-2.15877	-0.56226
H	0.583274	1.859209	0.729401
H	4.598111	0.652985	-0.17049
C	-0.62997	-0.51002	0.197516
C	-1.5968	0.422596	-0.21168
C	-1.06282	-1.74676	0.70342
C	-2.94935	0.11183	-0.10686
C	-2.42113	-2.04215	0.797523
H	-0.32839	-2.46787	1.047168
C	-3.3824	-1.1149	0.393716
H	-2.73966	-2.99978	1.198364
H	-4.44173	-1.33304	0.46399
H	-1.29535	1.374887	-0.63221
C	4.092466	-1.94813	-0.7968
H	4.522027	-2.43461	0.087721
H	3.618585	-2.72771	-1.40045
H	4.923911	-1.53108	-1.37325
C	3.130119	2.816581	0.59486
H	3.149206	3.425947	-0.31719
H	2.479128	3.324621	1.312471
H	4.145485	2.810136	1.002623
Cl	-4.14297	1.296596	-0.63398

3kb-p

	Atomic Coordinate		
Atom	x	y	z
C	1.689262	-1.19261	-0.18094
C	0.973051	0.000014	0.000011
C	1.689262	1.192596	0.180973
C	3.086796	1.207858	0.179762
C	3.770025	-4E-06	0.000019
C	3.08676	-1.20789	-0.17971
H	1.147552	-2.11914	-0.35097
H	1.147596	2.119152	0.350987
H	4.858141	-3.6E-05	0.00001
C	-0.51084	0.000003	0.000009
C	-1.23493	1.039213	-0.60718
C	-1.23492	-1.03921	0.607182
C	-2.62779	1.04768	-0.61087
C	-2.62779	-1.04768	0.610868
H	-0.70062	-1.84144	1.106377
C	-3.31521	-4E-06	-1E-06
H	-3.17675	-1.85037	1.090362
H	-0.70062	1.841439	-1.10637
H	-3.17676	1.850364	-1.09037
C	3.845363	-2.50373	-0.34643
H	4.101702	-2.93675	0.628431
H	3.25472	-3.24766	-0.88905
H	4.78271	-2.35223	-0.89042
C	3.845338	2.503754	0.346362
H	4.100588	2.937323	-0.62854
H	3.255098	3.247298	0.889952
H	4.783267	2.352163	0.889319
Cl	-5.07547	-4E-06	-9E-06

preRE2-o

	Atomic Coordinate		
Atom	x	y	z
Pd	0.038694	0.664184	-0.9765
C	1.894206	0.356209	-0.34789
C	2.529101	1.292503	0.480666
C	2.623598	-0.74196	-0.82375
C	3.890006	1.17342	0.791793
C	3.986843	-0.88159	-0.5265
C	4.60197	0.081339	0.281308
H	5.655719	-0.02927	0.531936
C	-0.52051	-0.21387	0.723639
C	-0.85057	-1.57201	0.808812

C	-0.76137	0.570252	1.865074
C	-1.45839	-2.12262	1.941639
C	-1.37049	0.040375	3.005972
C	-1.72937	-1.30829	3.04165
H	-1.70488	-3.17928	1.958024
H	-1.55256	0.678162	3.866789
H	-2.19754	-1.73395	3.924307
O	-2.01413	1.165553	-1.83702
C	-2.85224	1.284607	-0.91133
N	-3.67773	0.271984	-0.57586
C	-4.53356	0.273825	0.606274
H	-5.46505	-0.25117	0.374185
H	-4.03287	-0.24131	1.435331
H	-4.78505	1.285503	0.919002
C	-3.57108	-1.01851	-1.25461
H	-3.34354	-1.79959	-0.52451
H	-4.51868	-1.25433	-1.75181
H	-2.76804	-0.97433	-1.98547
C	-2.94565	2.586084	-0.13991
H	-3.95579	3.006052	-0.15867
H	-2.65424	2.426989	0.902654
H	-2.25401	3.291305	-0.59884
H	2.130187	-1.50797	-1.41545
H	1.964763	2.122005	0.901588
H	-0.46699	1.615687	1.859589
C	4.776116	-2.04689	-1.07801
H	5.610425	-2.31455	-0.42166
H	4.144854	-2.93235	-1.20308
H	5.199403	-1.80764	-2.06197
C	4.579291	2.209681	1.649846
H	5.388425	1.76786	2.240435
H	5.022376	3.003146	1.034419
H	3.878003	2.688158	2.341021
Cl	-0.52619	-2.67148	-0.54173

preRE2-m

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.4679	-1.17957	-0.28847
C	-2.27923	-0.37583	-0.21233
C	-3.0737	-0.52753	0.935171
C	-2.82768	0.26474	-1.33293
C	-4.4035	-0.087	0.961346
C	-4.15602	0.714626	-1.33247

C	-4.92692	0.534339	-0.17898
H	-5.95387	0.895788	-0.16354
C	0.291879	0.536525	0.373731
C	1.36158	1.064705	-0.36614
C	-0.03557	1.118383	1.606523
C	2.112203	2.113284	0.165132
C	0.726591	2.17543	2.112668
C	1.818142	2.681466	1.402241
H	0.470357	2.612729	3.074244
H	2.418257	3.496664	1.790397
O	1.57203	-2.16162	-0.50061
C	2.515869	-1.78431	0.230609
N	3.680297	-1.36082	-0.31053
C	4.772163	-0.75907	0.447902
H	5.725757	-1.17992	0.11181
H	4.789318	0.324649	0.283547
H	4.671347	-0.94839	1.513816
C	3.81648	-1.25714	-1.76205
H	3.87612	-0.20269	-2.05561
H	4.73225	-1.76467	-2.08322
H	2.953964	-1.72073	-2.23524
C	2.365858	-1.78149	1.7383
H	3.186576	-2.3025	2.239068
H	2.318138	-0.75258	2.10829
H	1.424907	-2.27488	1.977337
H	-2.21798	0.431924	-2.21753
H	-2.65899	-0.99009	1.829074
H	-0.88354	0.748107	2.171307
C	-4.7457	1.37011	-2.56047
H	-5.53594	2.080407	-2.29703
H	-3.98278	1.908104	-3.13204
H	-5.18903	0.623813	-3.23211
C	-5.2633	-0.29324	2.187411
H	-5.96502	0.535368	2.329336
H	-5.85898	-1.21119	2.103735
H	-4.65571	-0.38119	3.093636
H	1.634473	0.652592	-1.33009
Cl	3.498274	2.720555	-0.76031

preRE2-p

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.4727	-1.40127	0.120772
C	-2.1642	-0.36794	0.035849

C	-2.87001	-0.0519	1.205893
C	-2.72744	-0.03994	-1.20568
C	-4.13969	0.538789	1.146203
C	-3.99592	0.550265	-1.29248
C	-4.68558	0.834483	-0.1085
H	-5.66415	1.308415	-0.16426
C	0.453546	0.359815	0.148821
C	0.627776	1.123736	-1.01426
C	1.100279	0.778598	1.322063
C	1.487352	2.226875	-1.03335
C	1.96088	1.88191	1.320203
C	2.158402	2.587662	0.13448
H	2.466294	2.193285	2.228722
O	1.333515	-2.80186	0.209524
C	2.431812	-2.21237	0.336965
N	3.070985	-1.67295	-0.72352
C	4.171547	-0.71981	-0.60997
H	4.913415	-0.92361	-1.38824
H	3.797278	0.303233	-0.73461
H	4.663099	-0.79355	0.357598
C	2.468426	-1.77251	-2.05117
H	1.919892	-0.85604	-2.29099
H	3.260856	-1.92373	-2.79032
H	1.778267	-2.61342	-2.06942
C	3.069274	-2.10988	1.707383
H	4.104387	-2.46303	1.711626
H	3.055511	-1.07108	2.051452
H	2.475347	-2.71552	2.390804
H	-2.1793	-0.23872	-2.12465
H	-2.4301	-0.25459	2.179424
H	0.945984	0.242716	2.253854
C	-4.61227	0.857207	-2.63815
H	-5.30083	1.706228	-2.5804
H	-3.84716	1.092197	-3.38519
H	-5.18338	-3.8E-05	-3.01696
C	-4.91057	0.838591	2.411463
H	-5.54547	1.722891	2.29523
H	-5.56615	0.001229	2.682716
H	-4.23862	1.012774	3.257706
H	0.090611	0.865303	-1.92135
Cl	3.264265	3.962554	0.113925
H	1.629035	2.804198	-1.94114

TS2-o

	Atomic Coordinate		
Atom	x	y	z
Pd	0.148984	-0.86614	-0.77773
C	-1.62163	-0.1631	-0.02145
C	-2.34816	-1.07366	0.773859
C	-2.33835	0.754794	-0.80829
C	-3.74348	-1.09137	0.771309
C	-3.74024	0.760274	-0.81897
C	-4.42719	-0.15911	-0.02264
H	-5.51557	-0.15018	-0.01382
C	0.094756	0.435918	0.808982
C	0.573118	1.75575	0.664709
C	0.326215	-0.15075	2.077528
C	1.227142	2.441384	1.692039
C	0.995696	0.508764	3.104219
C	1.446437	1.817851	2.91898
H	1.569051	3.456234	1.517131
H	1.156804	0.001838	4.05172
H	1.954265	2.351973	3.716077
O	2.041083	-1.82473	-1.55016
C	2.804943	-1.4948	-0.60808
N	3.583172	-0.38782	-0.69237
C	4.218441	0.21757	0.474904
H	5.104889	0.770437	0.152285
H	3.531886	0.910965	0.978335
H	4.53669	-0.54053	1.189155
C	3.430142	0.485725	-1.85514
H	2.672741	1.254974	-1.66778
H	4.389439	0.965767	-2.06771
H	3.116835	-0.1105	-2.70987
C	2.914174	-2.36595	0.629354
H	3.948275	-2.66842	0.822668
H	2.53542	-1.83294	1.506557
H	2.301331	-3.25086	0.461659
H	-1.80856	1.474668	-1.41776
H	-1.82386	-1.77973	1.410699
H	-0.03236	-1.15827	2.25736
C	-4.48709	1.734191	-1.70148
H	-3.96743	2.69567	-1.76275
H	-4.57758	1.348412	-2.72461
H	-5.50005	1.917763	-1.33022
C	-4.50909	-2.10088	1.595388
H	-3.87153	-2.56993	2.350682
H	-5.35671	-1.63551	2.109965
H	-4.91489	-2.90046	0.963335

Cl	0.434805	2.631068	-0.87182

TS2-m

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.13211	-1.30633	-0.48572
C	-1.77704	-0.17966	-0.04542
C	-2.61697	-0.63688	0.984959
C	-2.33611	0.582282	-1.08531
C	-3.99234	-0.38314	0.962946
C	-3.7092	0.847905	-1.13053
C	-4.52111	0.36363	-0.09769
H	-5.58691	0.583867	-0.11247
C	0.071423	0.429484	0.560609
C	0.607982	1.525233	-0.14326
C	0.334839	0.332057	1.941837
C	1.423209	2.442172	0.515856
C	1.148466	1.267106	2.582544
C	1.711815	2.334007	1.876902
H	1.347953	1.16845	3.646501
H	2.341668	3.068379	2.365402
O	1.656341	-2.59542	-0.96782
C	2.503973	-2.06251	-0.20783
N	3.324066	-1.0765	-0.64507
C	4.132314	-0.25957	0.25706
H	4.99312	0.128882	-0.29339
H	3.552539	0.58641	0.646047
H	4.506903	-0.84701	1.094326
C	3.115855	-0.51927	-1.98005
H	2.529944	0.405083	-1.91726
H	4.08566	-0.29934	-2.43587
H	2.575271	-1.24264	-2.58649
C	2.65261	-2.54387	1.222641
H	3.6737	-2.87346	1.438717
H	2.389287	-1.74328	1.920991
H	1.965909	-3.37789	1.361658
H	-1.6975	0.985485	-1.86693
H	-2.19674	-1.18905	1.821409
H	-0.09865	-0.47995	2.516342
C	-4.30617	1.625662	-2.28065
H	-3.57815	2.315148	-2.71924
H	-4.6401	0.951857	-3.07967
H	-5.17639	2.208299	-1.96219
C	-4.89498	-0.9178	2.050943

H	-5.71553	-0.22577	2.266002
H	-5.34525	-1.87358	1.754936
H	-4.34418	-1.09056	2.980657
H	0.400038	1.662451	-1.19771
Cl	2.134348	3.769848	-0.40905

TS2-p

	Atomic Coordinate		
Atom	x	y	z
Pd	-0.34177	-1.45848	0.015627
C	-1.85139	-0.08302	-0.00568
C	-2.54931	0.150097	1.192328
C	-2.52389	0.108397	-1.22532
C	-3.89611	0.527173	1.184787
C	-3.87152	0.483005	-1.25924
C	-4.54059	0.694702	-0.0476
H	-5.58246	1.009304	-0.06371
C	0.088345	0.534425	0.016685
C	0.547205	1.118319	-1.18054
C	0.563479	1.074945	1.228854
C	1.484216	2.152148	-1.17578
C	1.503445	2.106417	1.248783
C	1.965857	2.633131	0.042544
H	1.872915	2.500664	2.189825
O	1.308297	-2.99655	0.0807
C	2.263905	-2.26238	0.436778
N	3.084568	-1.68706	-0.47493
C	4.016822	-0.61183	-0.14662
H	4.889874	-0.68076	-0.80202
H	3.544004	0.367375	-0.28917
H	4.361951	-0.68743	0.882795
C	2.7624	-1.8254	-1.89342
H	2.145622	-0.98244	-2.22671
H	3.690419	-1.84554	-2.47166
H	2.208275	-2.74925	-2.04606
C	2.547247	-2.04419	1.910857
H	3.571779	-2.32426	2.175035
H	2.393934	-0.99414	2.178208
H	1.846169	-2.65942	2.473525
H	-1.99279	-0.02484	-2.1642
H	-2.03652	0.050578	2.145301
H	0.199775	0.685146	2.17445
C	-4.59575	0.64042	-2.57644
H	-3.90295	0.881135	-3.38876

H	-5.11517	-0.28547	-2.85357
H	-5.34933	1.432939	-2.52739
C	-4.64802	0.735929	2.479144
H	-3.96804	0.962056	3.306168
H	-5.36669	1.557803	2.396733
H	-5.21332	-0.16274	2.756018
H	0.172538	0.761316	-2.13437
Cl	3.167994	3.922612	0.057397
H	1.839057	2.581817	-2.10683

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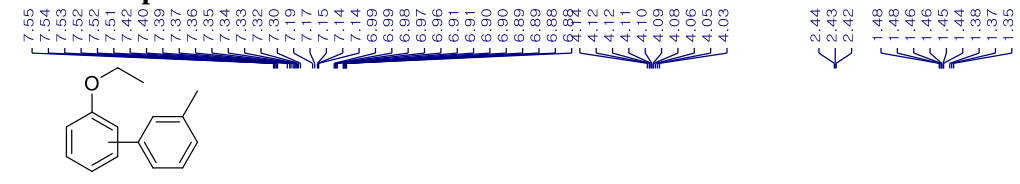
11. NMR Spectra



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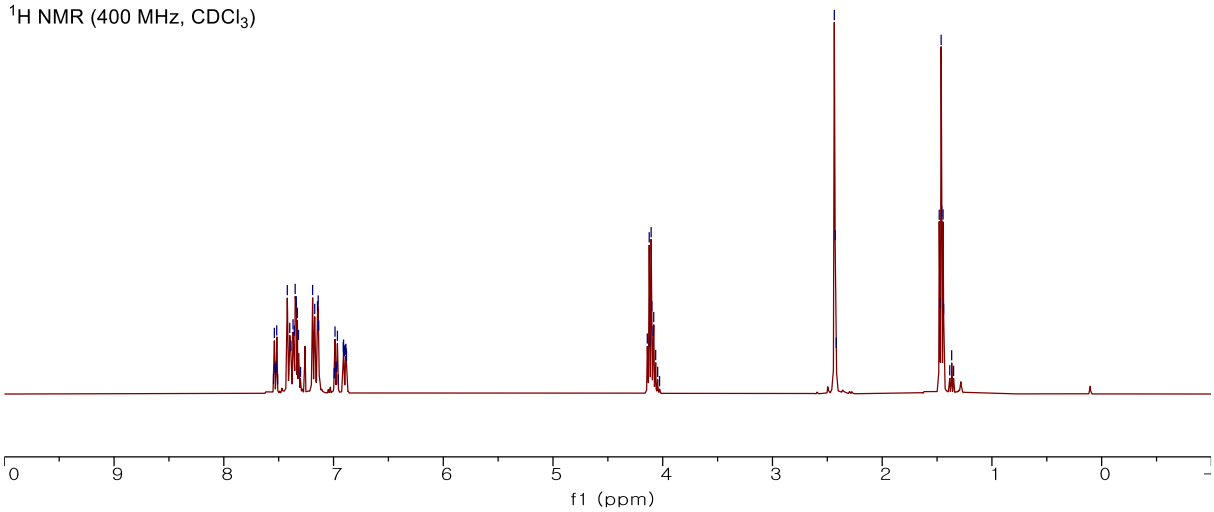

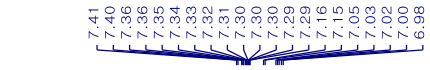

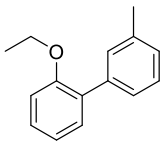

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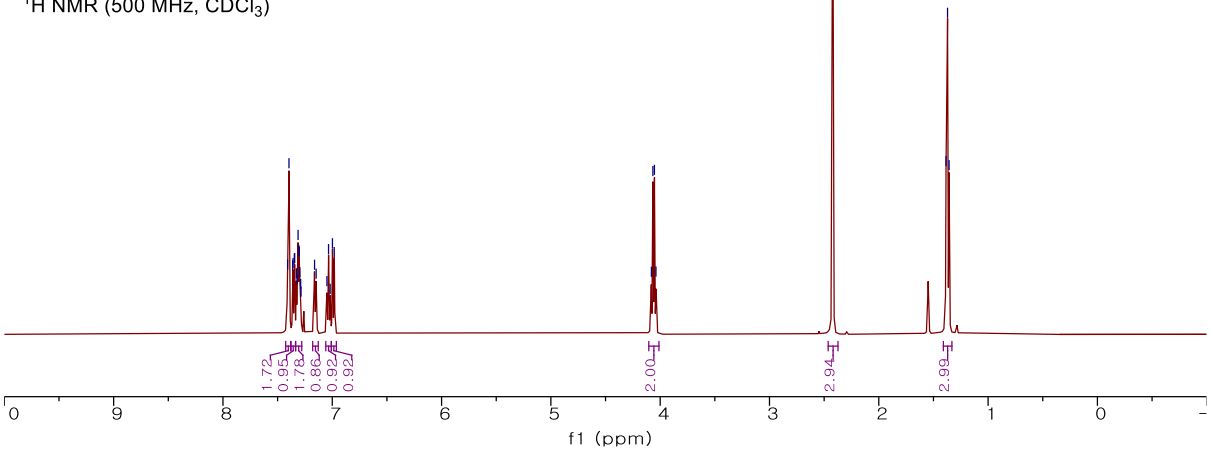

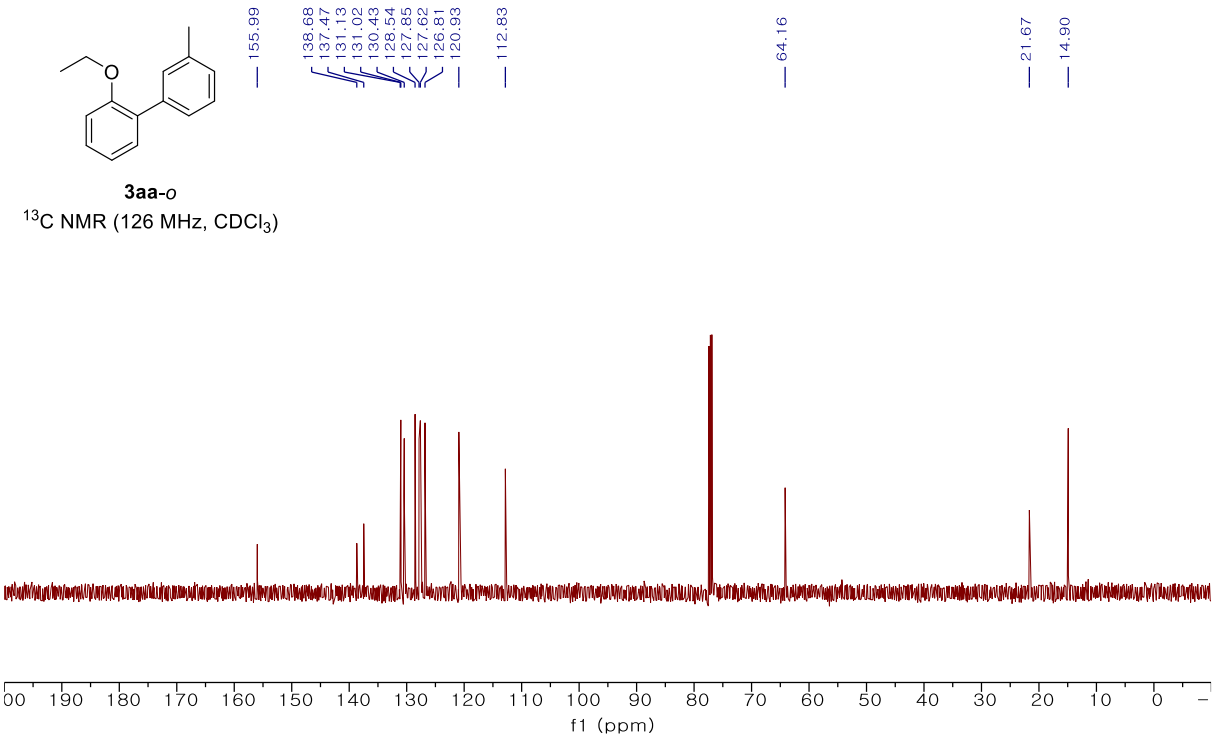

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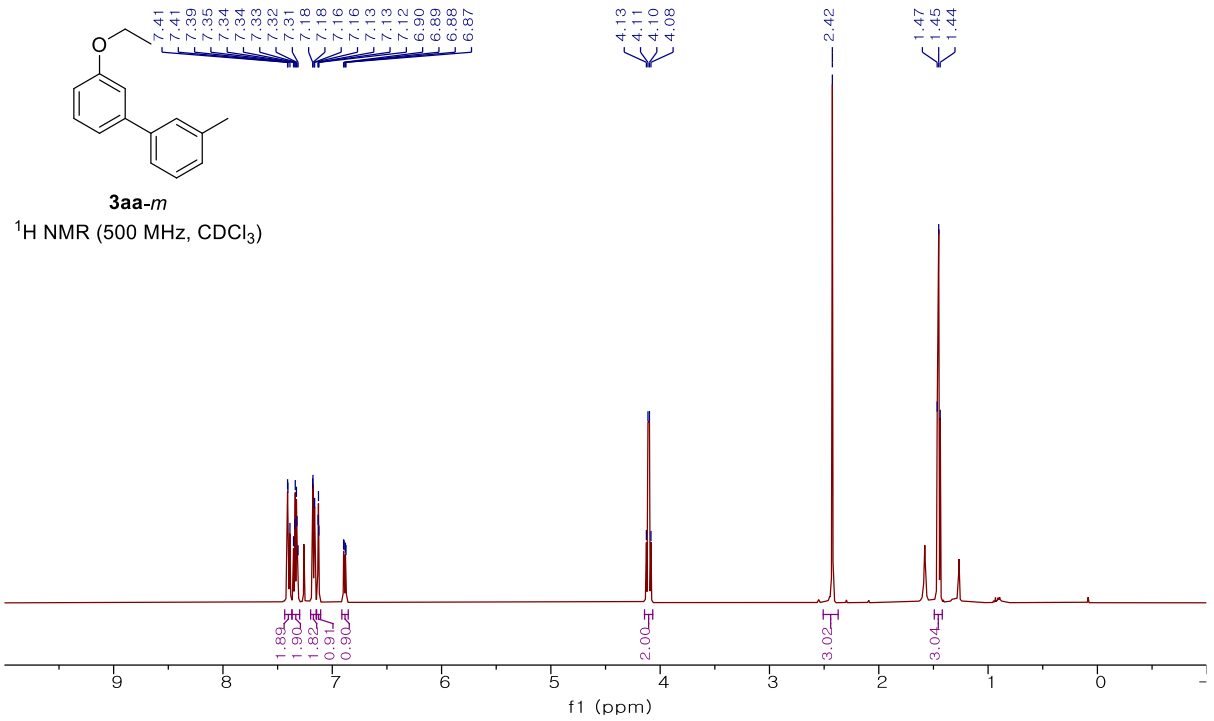

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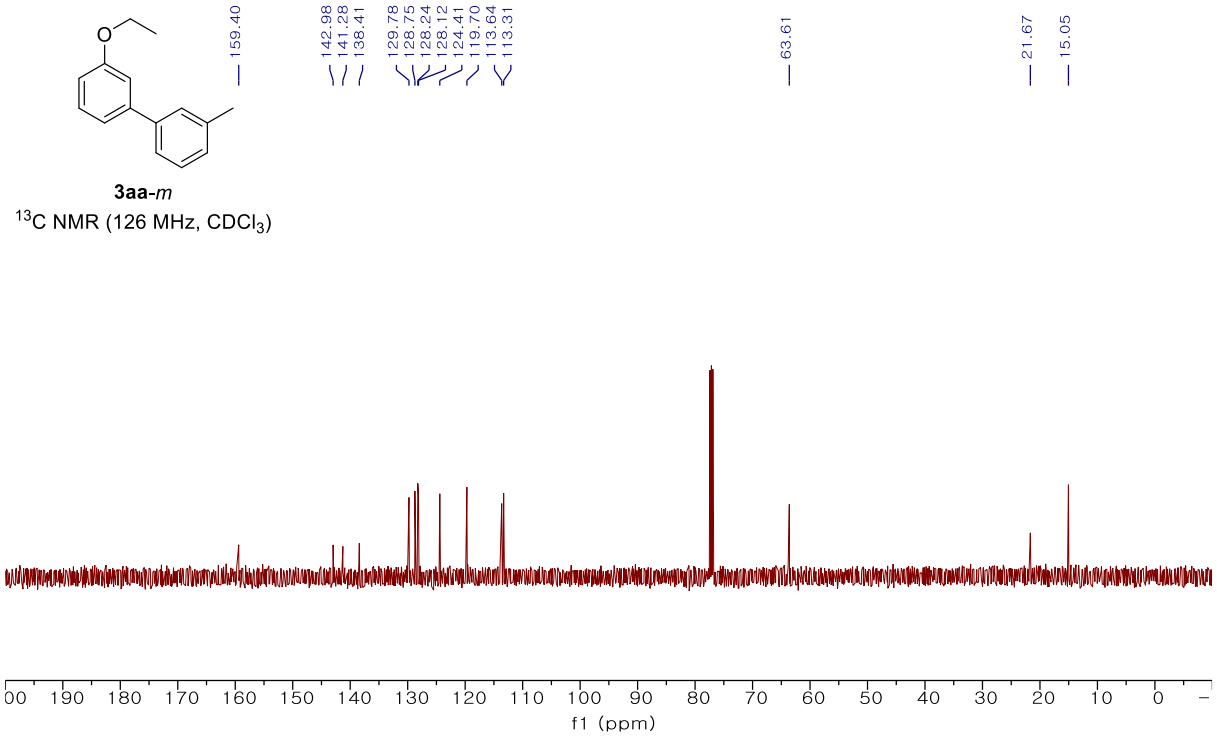

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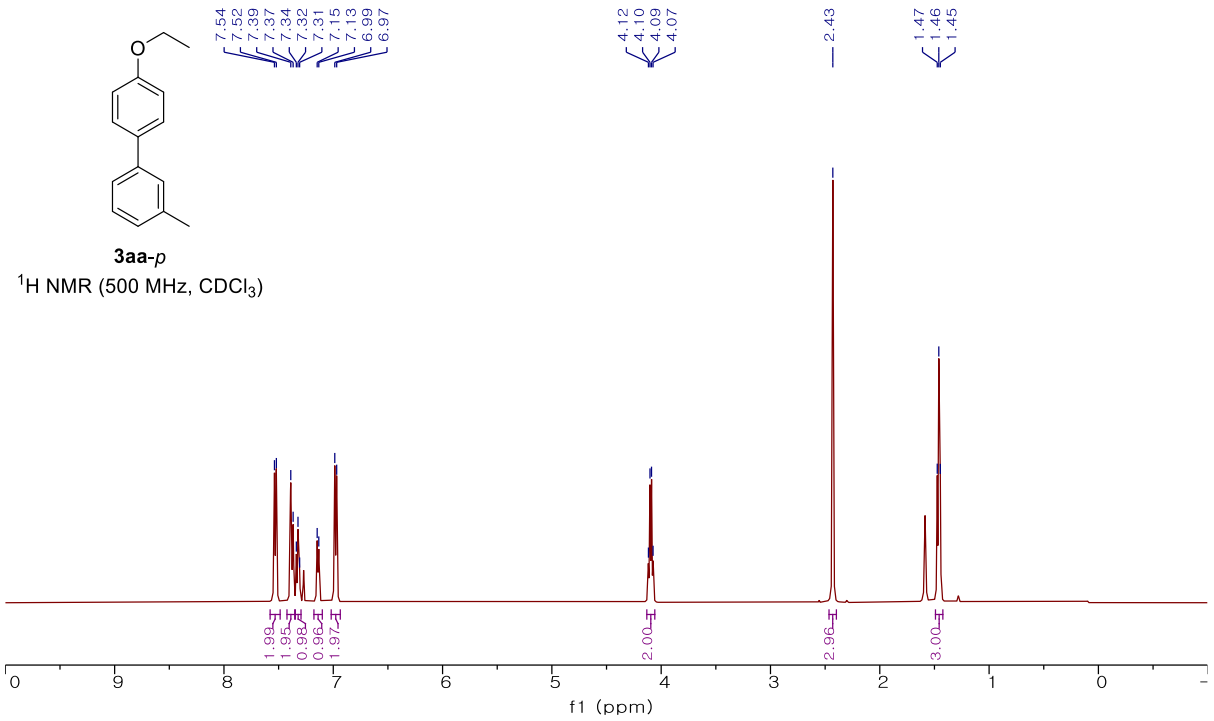

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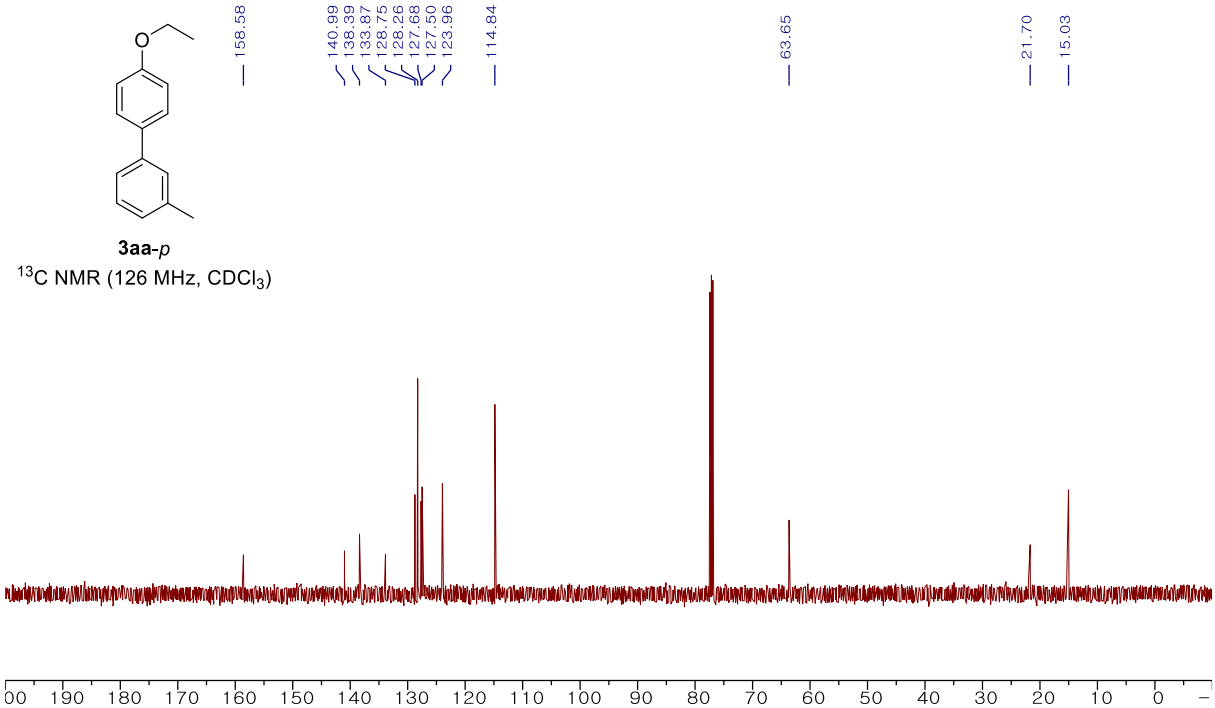

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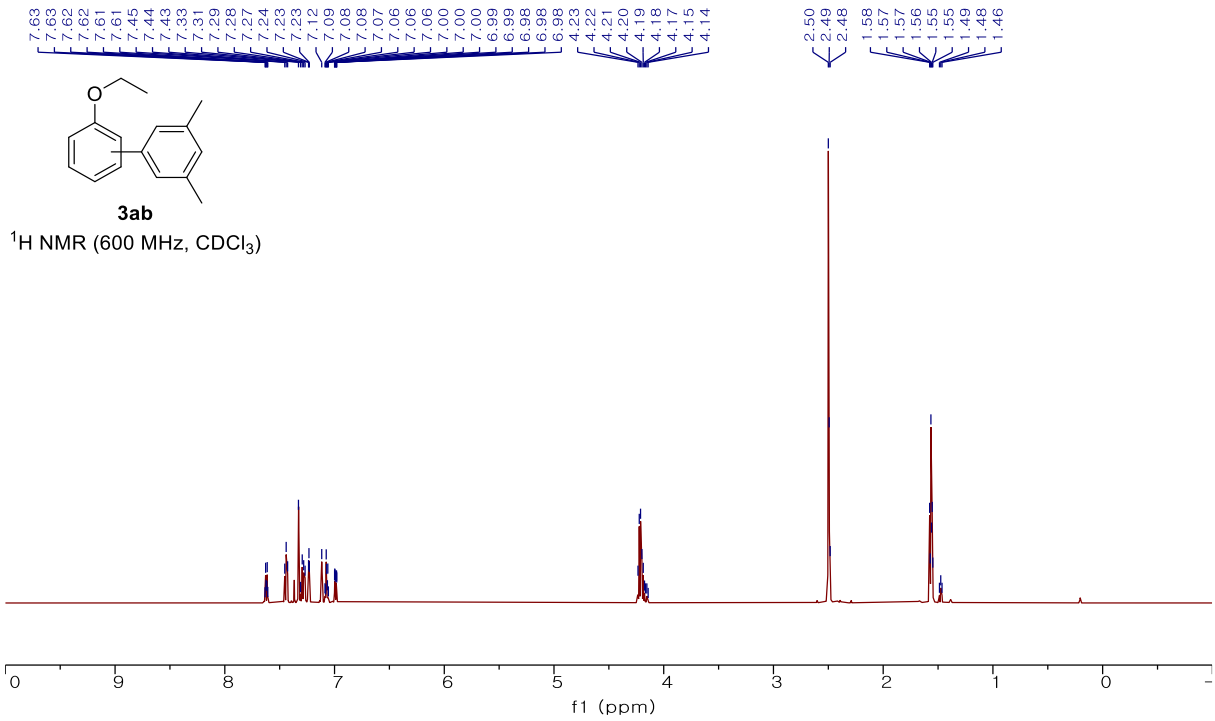

3ab

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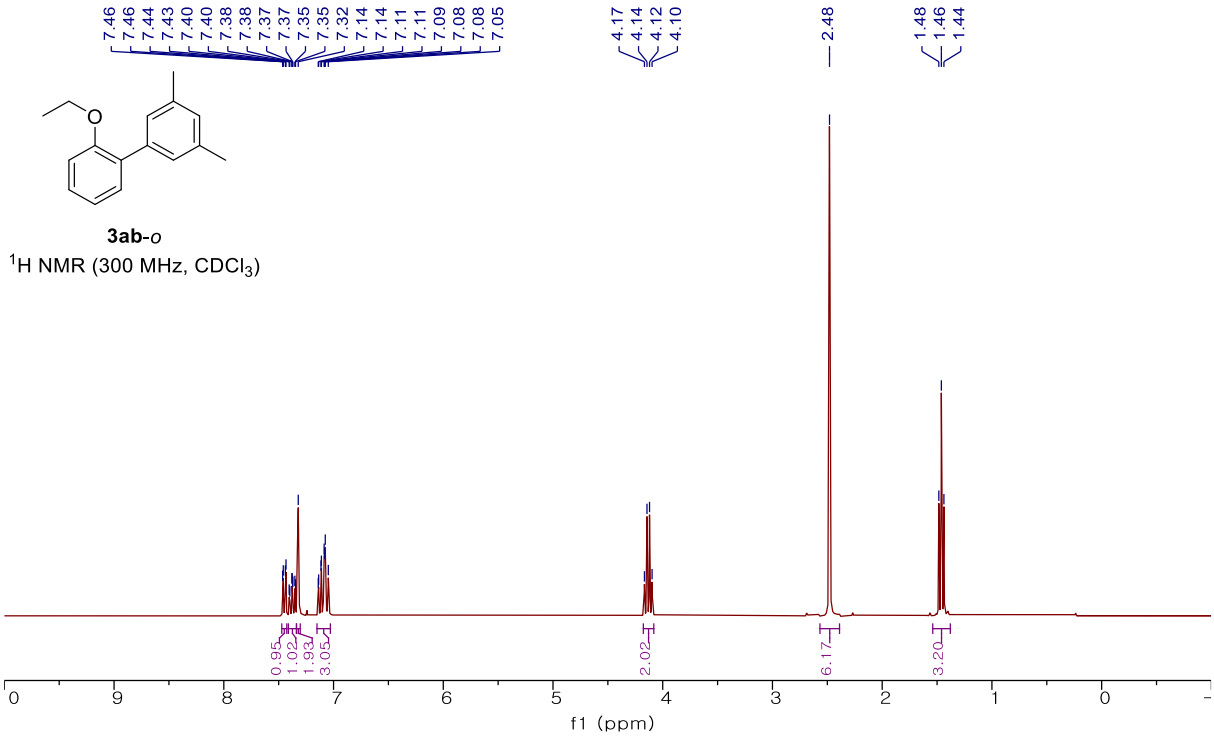

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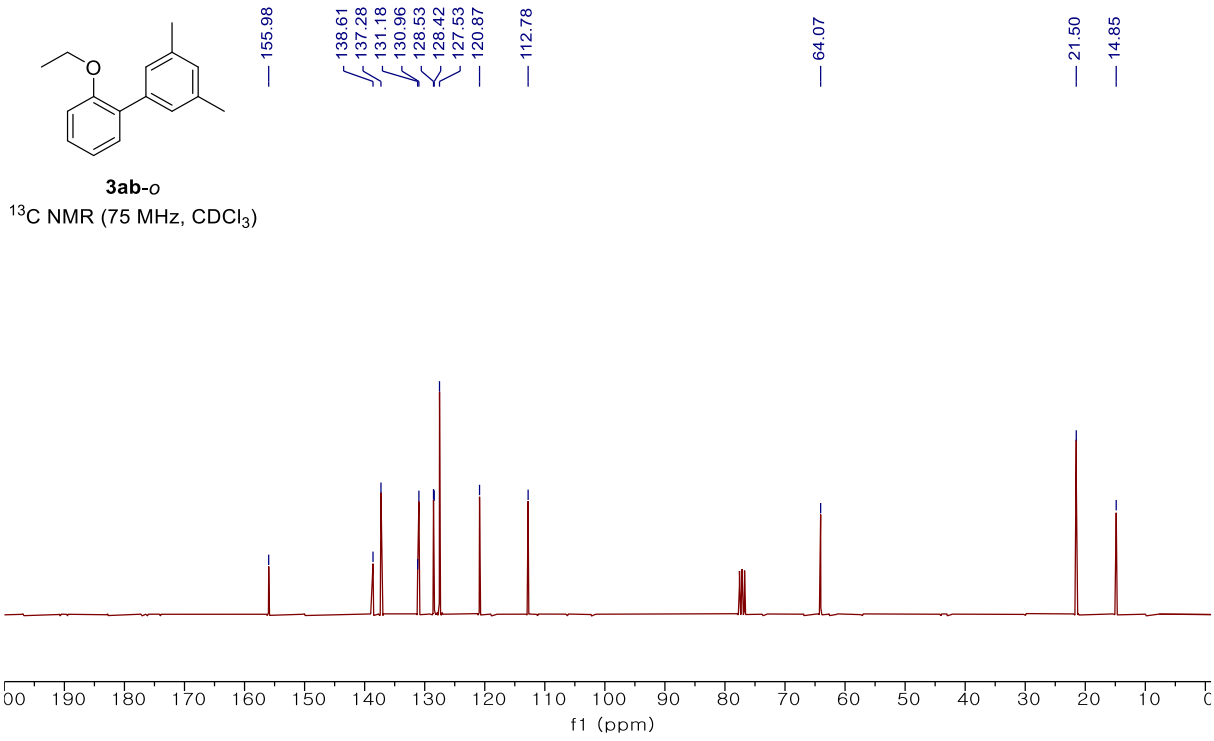

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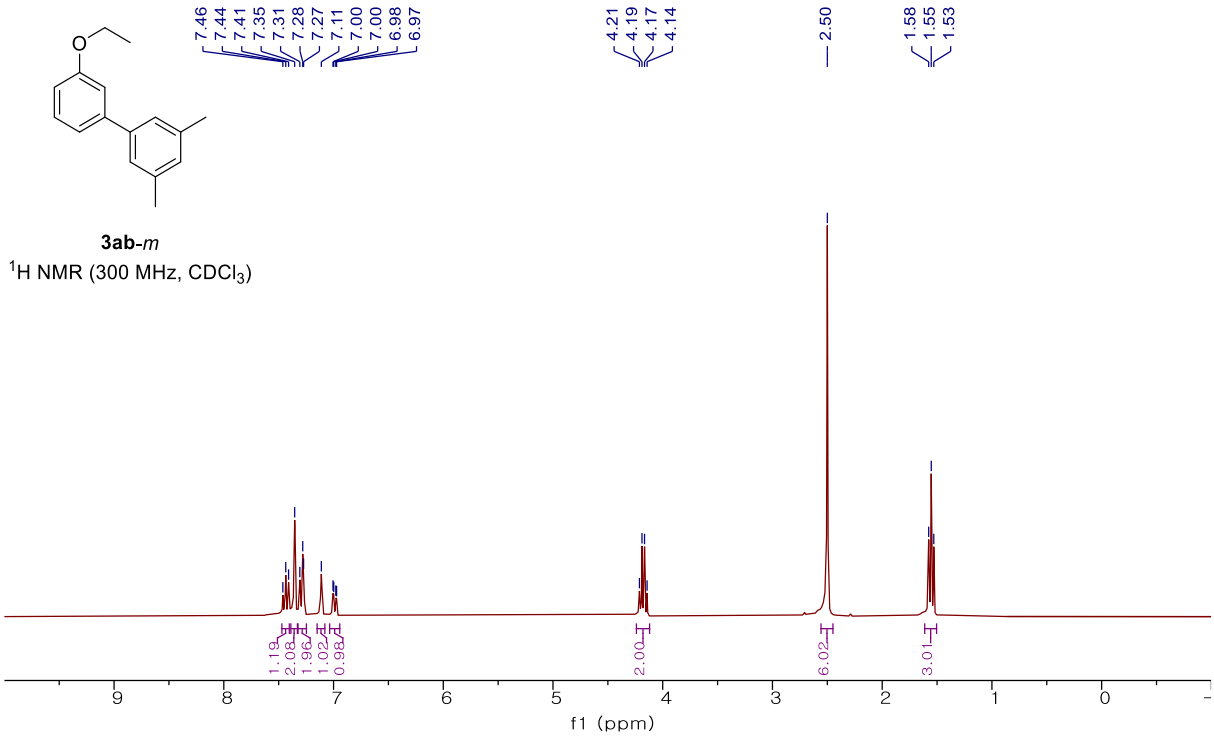

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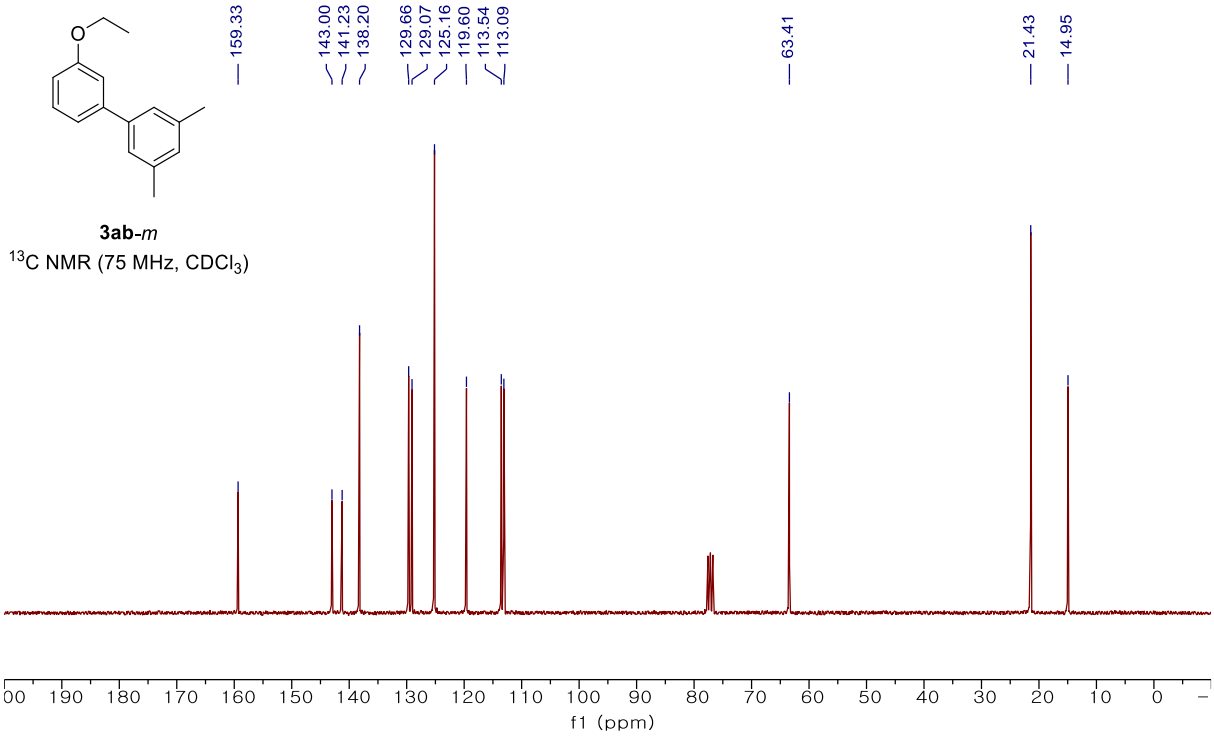

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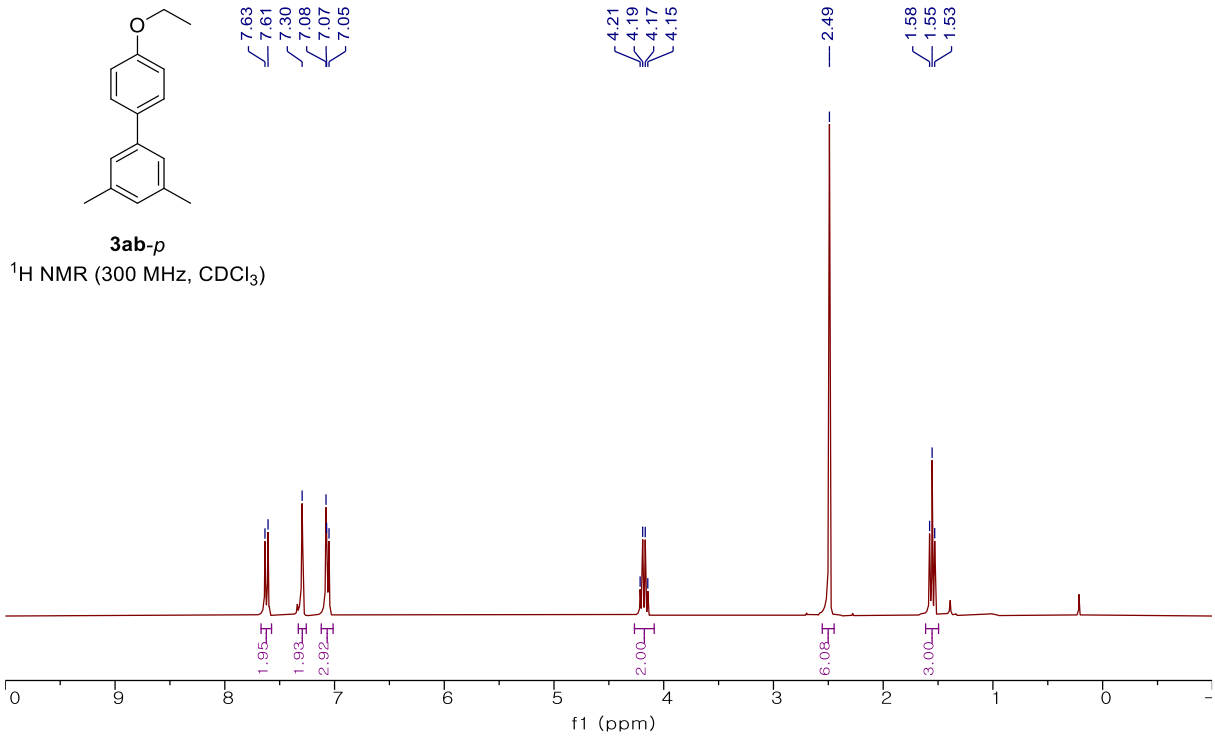

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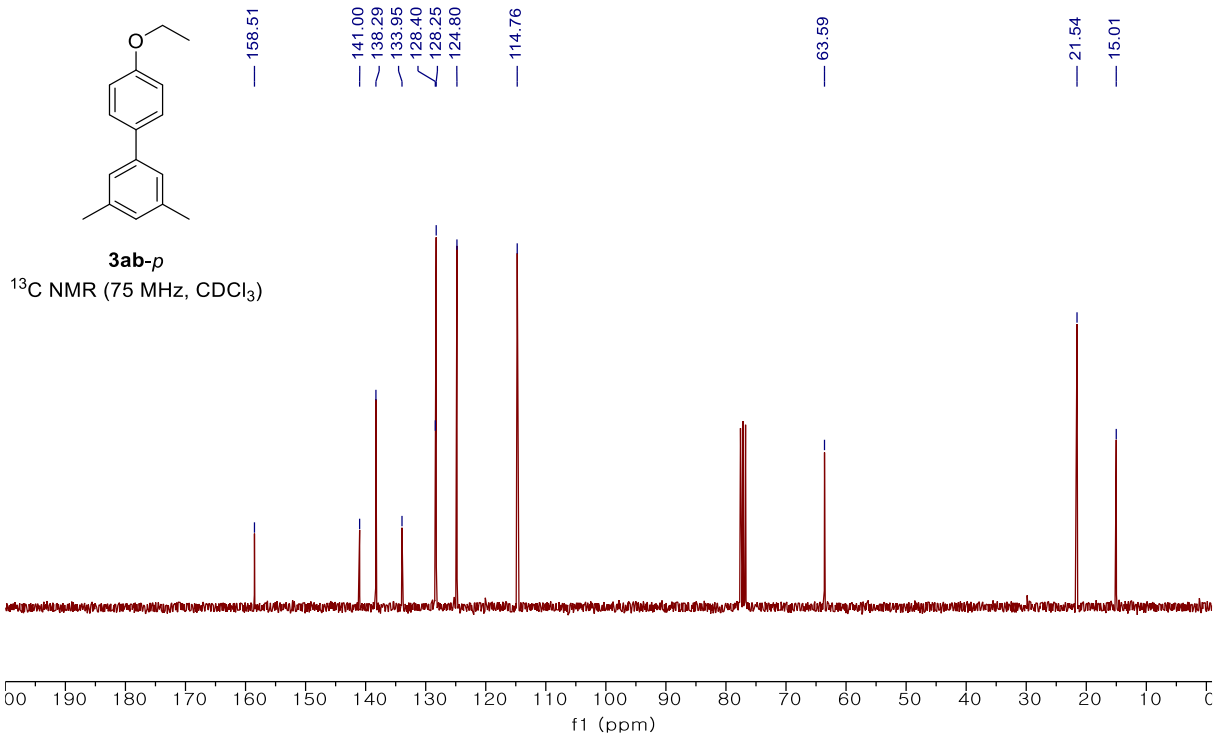

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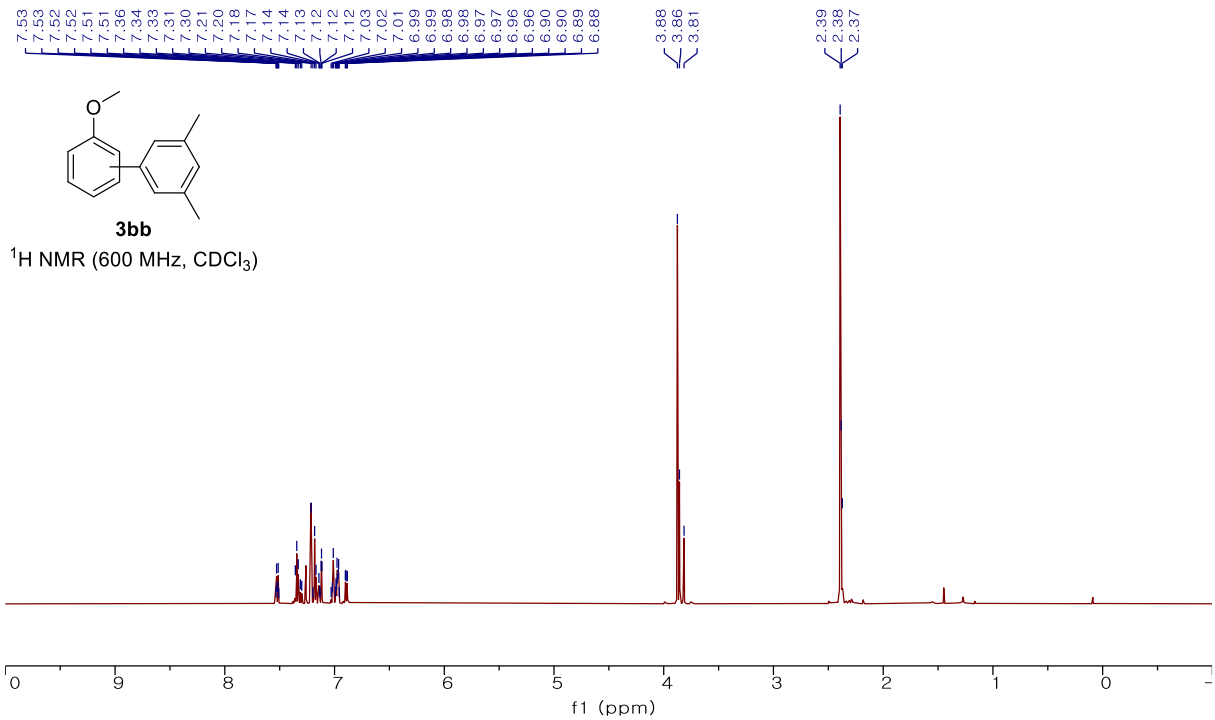
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6.96
6.96
6.90
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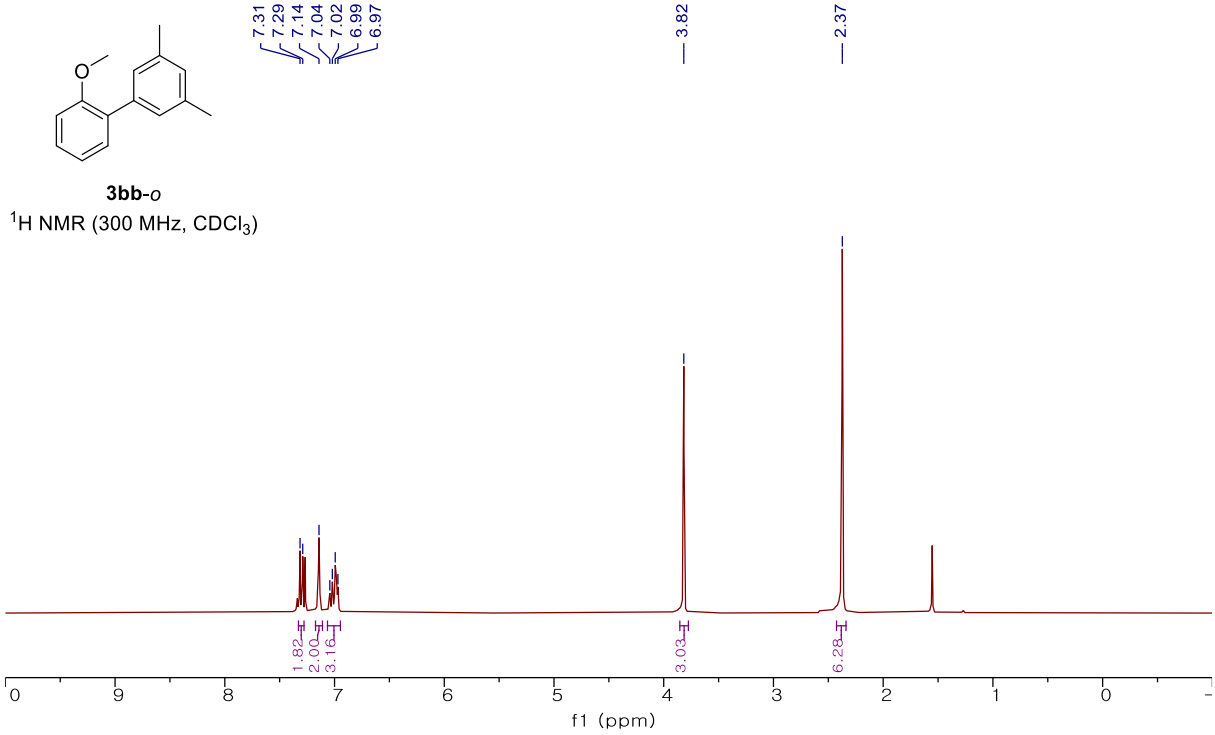
6.89
6.88
3.88
3.86
3.81
2.39
2.38
2.37
O
3bb
1H NMR (600 MHz, CDCl3)
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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7.02
6.99
6.97
3.82
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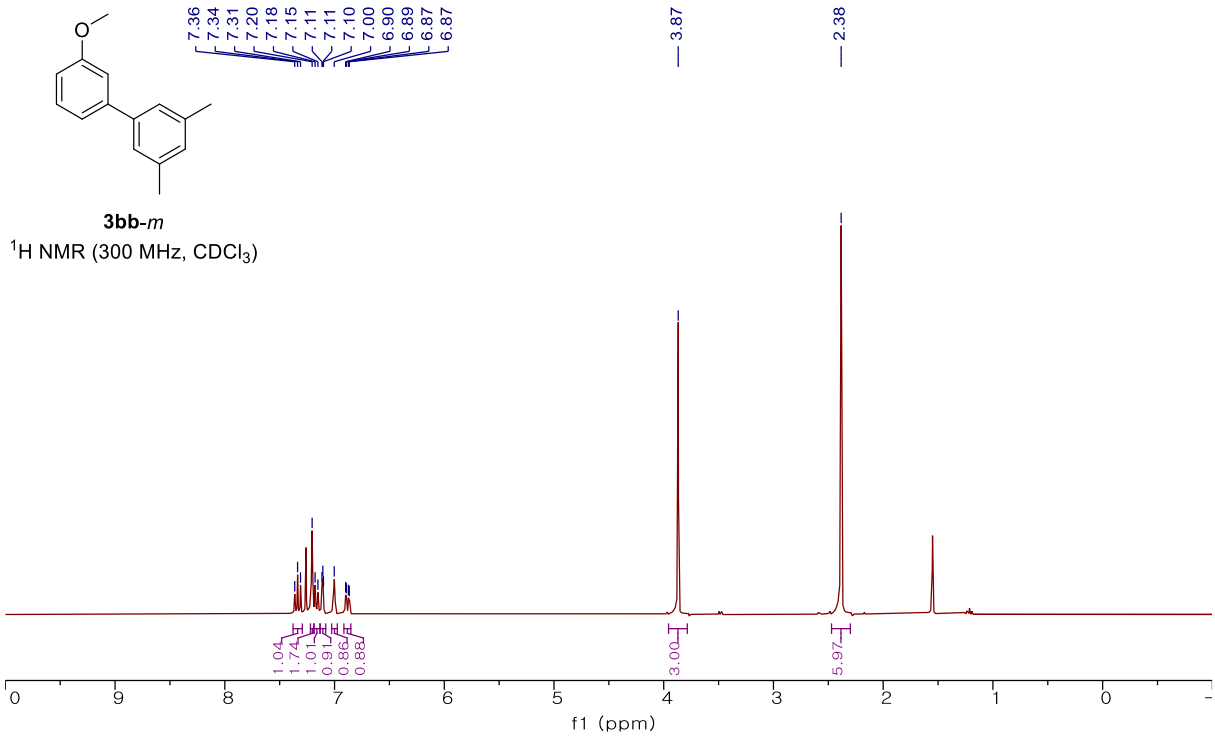
O
3bb-o
1H NMR (300 MHz, CDCl3)
1.82
2.00
3.16
3.03
6.28
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



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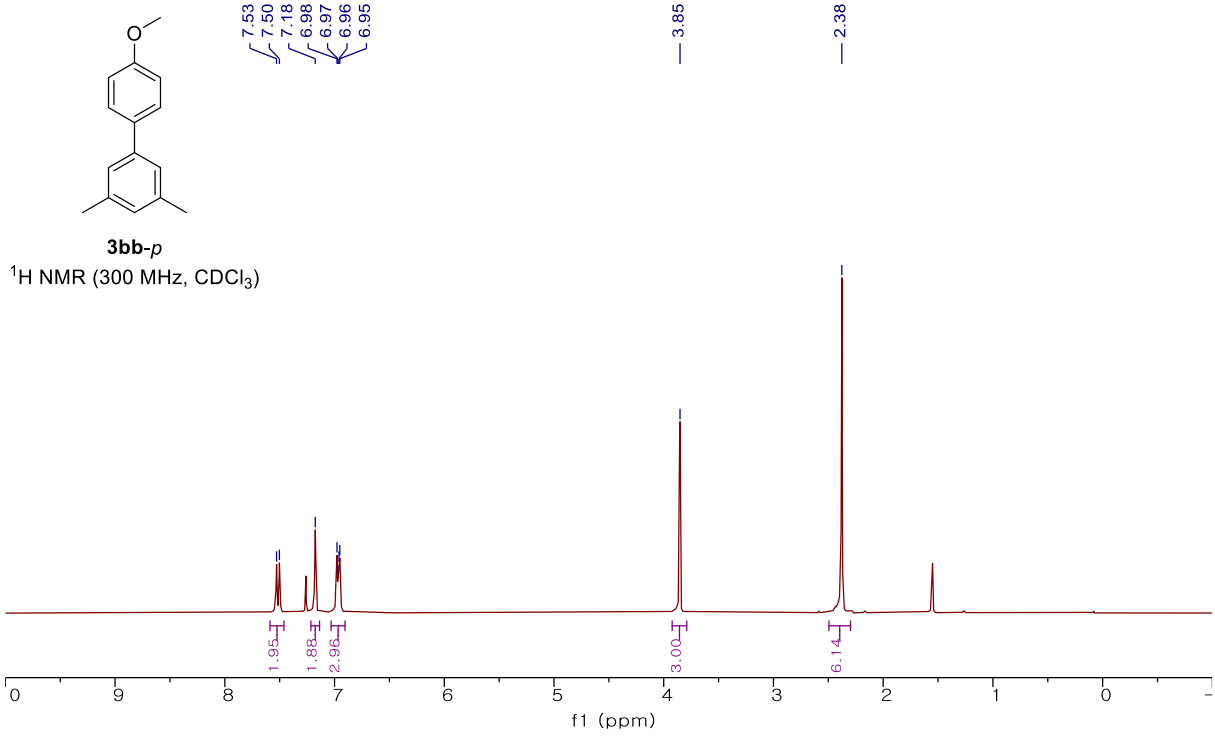

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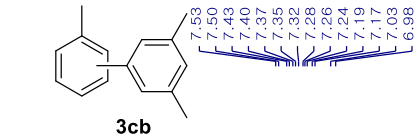

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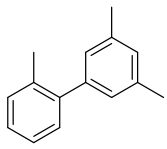

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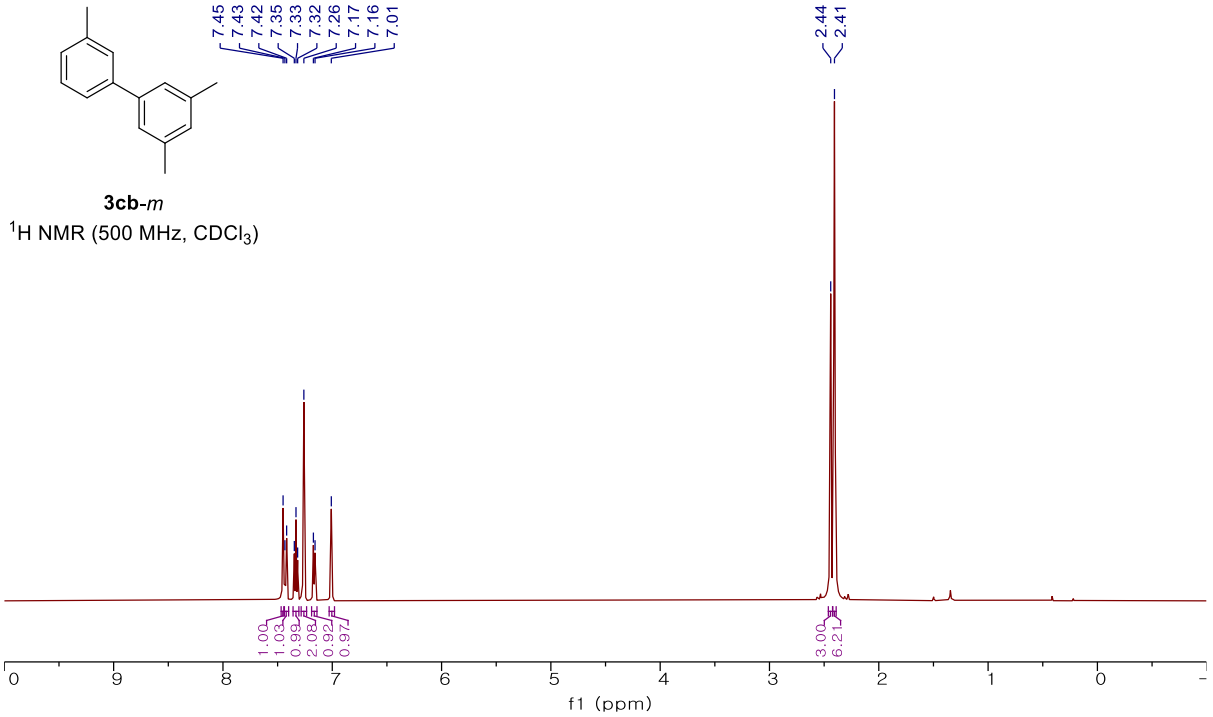

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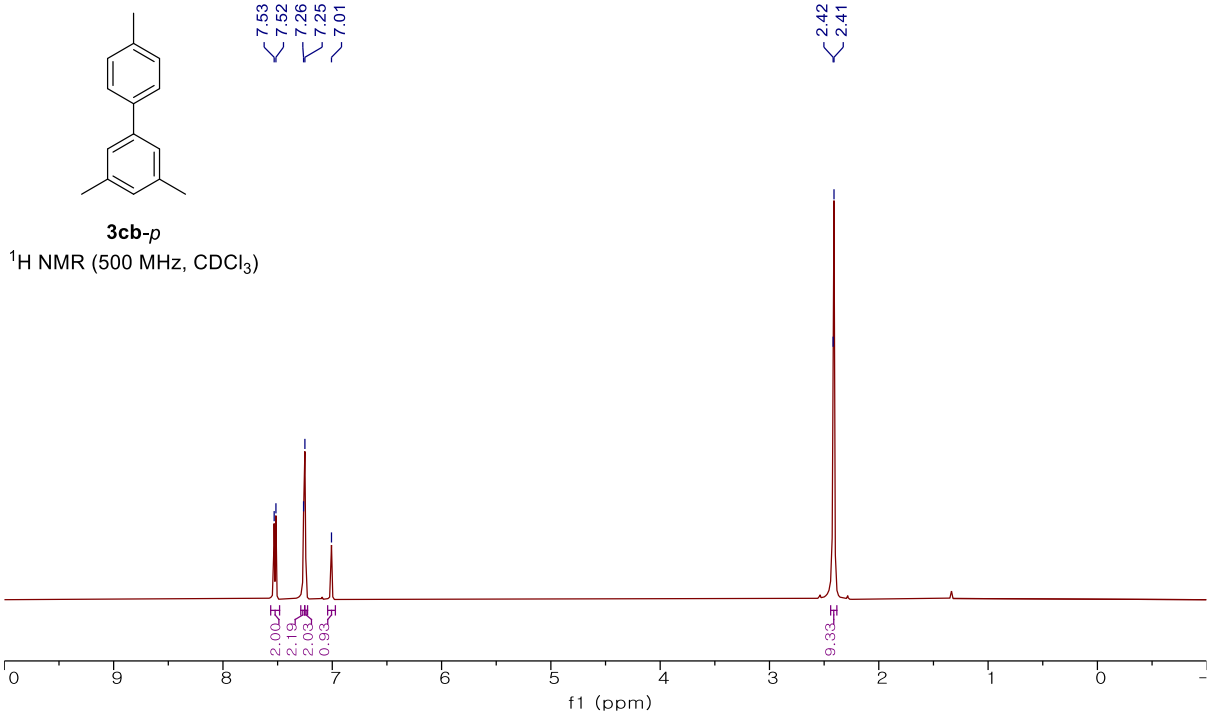

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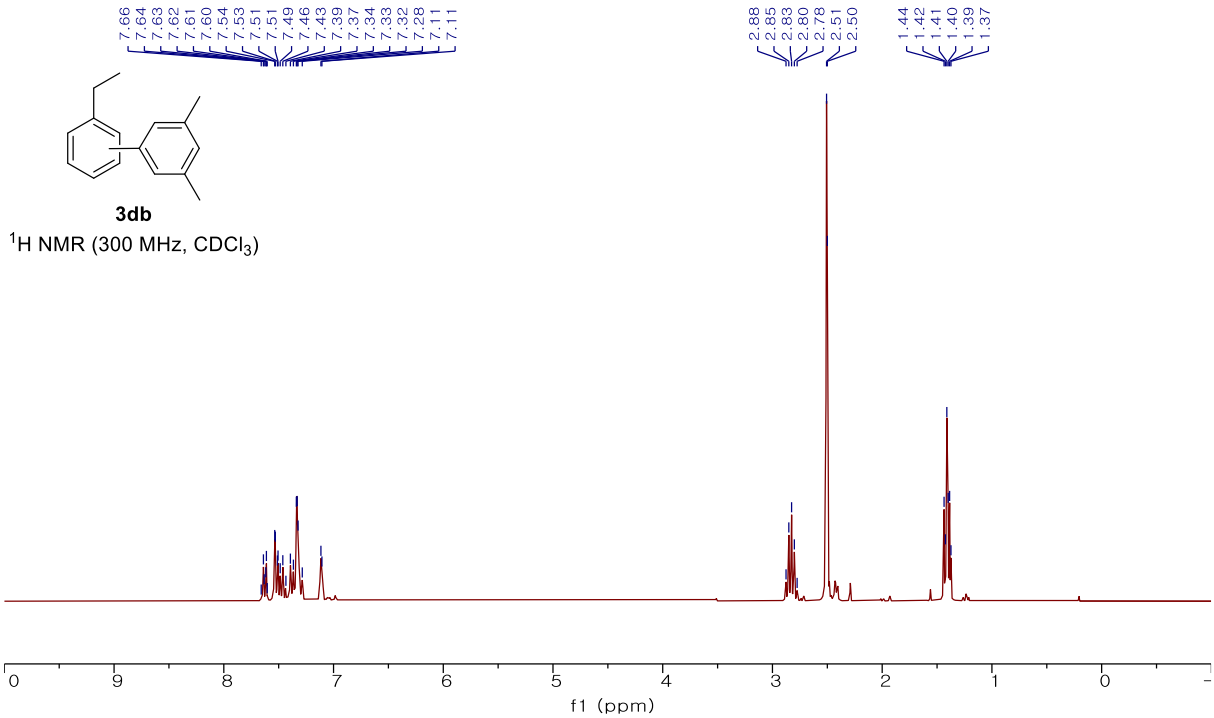

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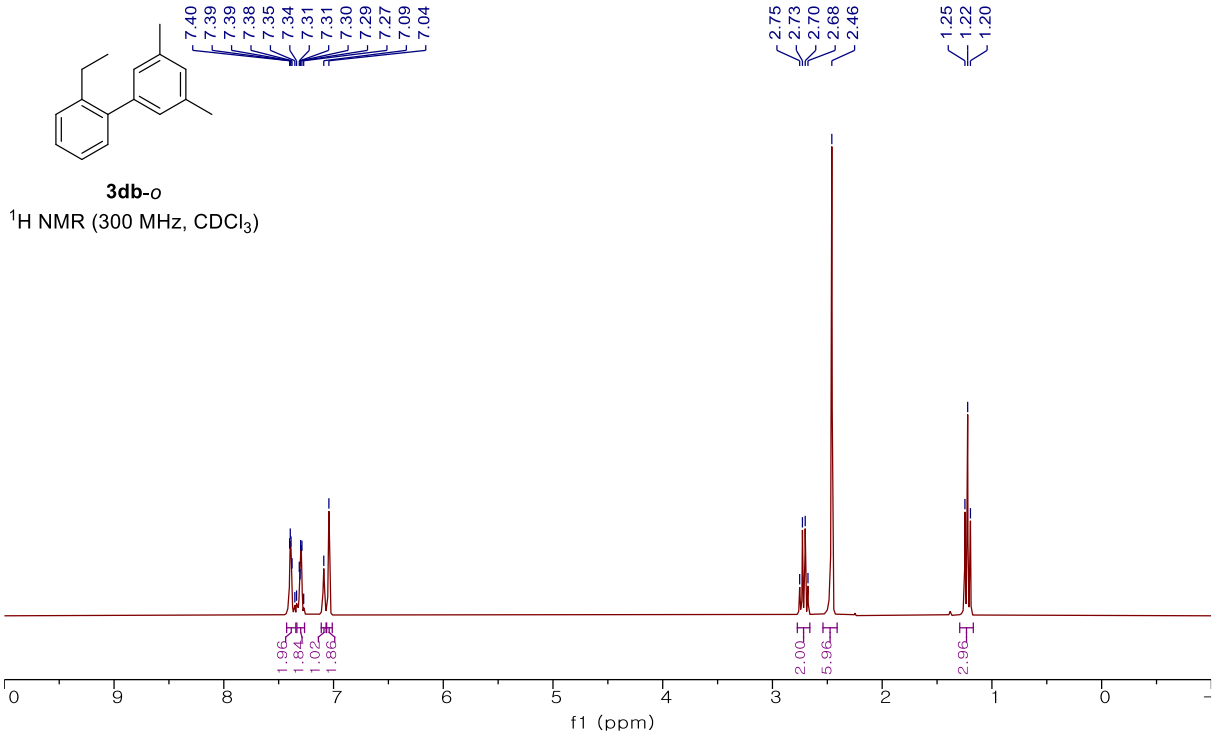

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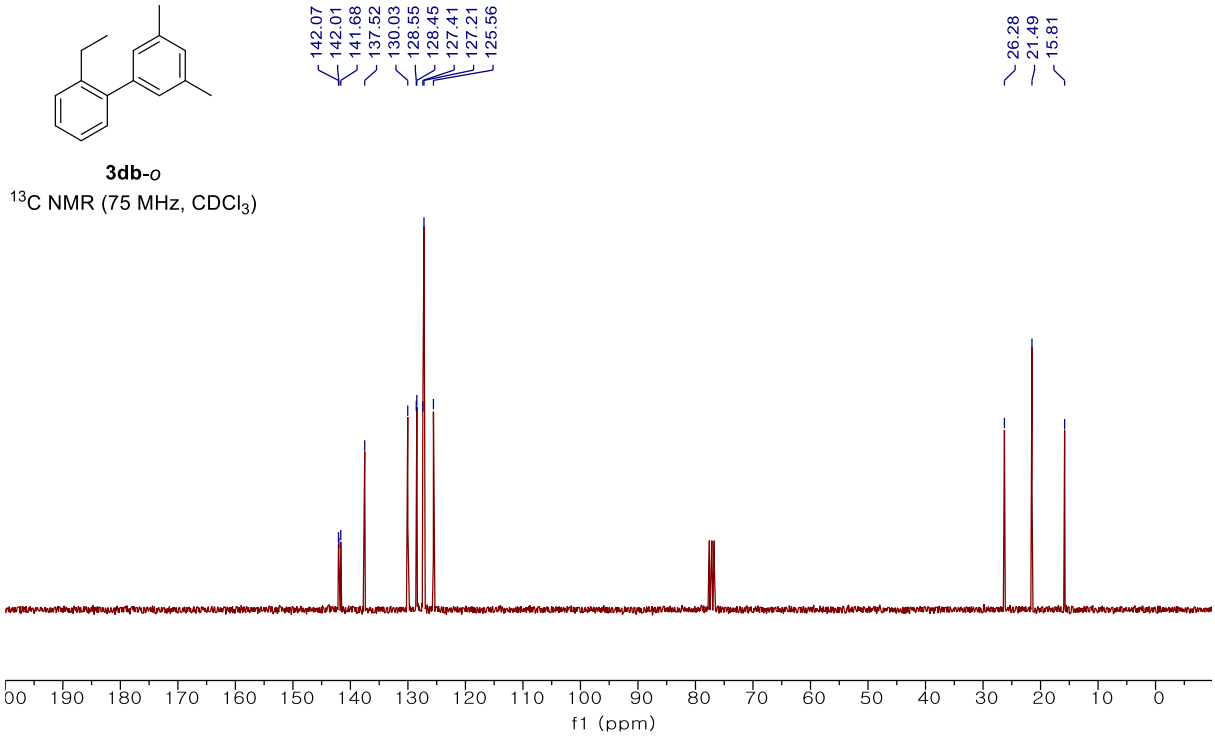

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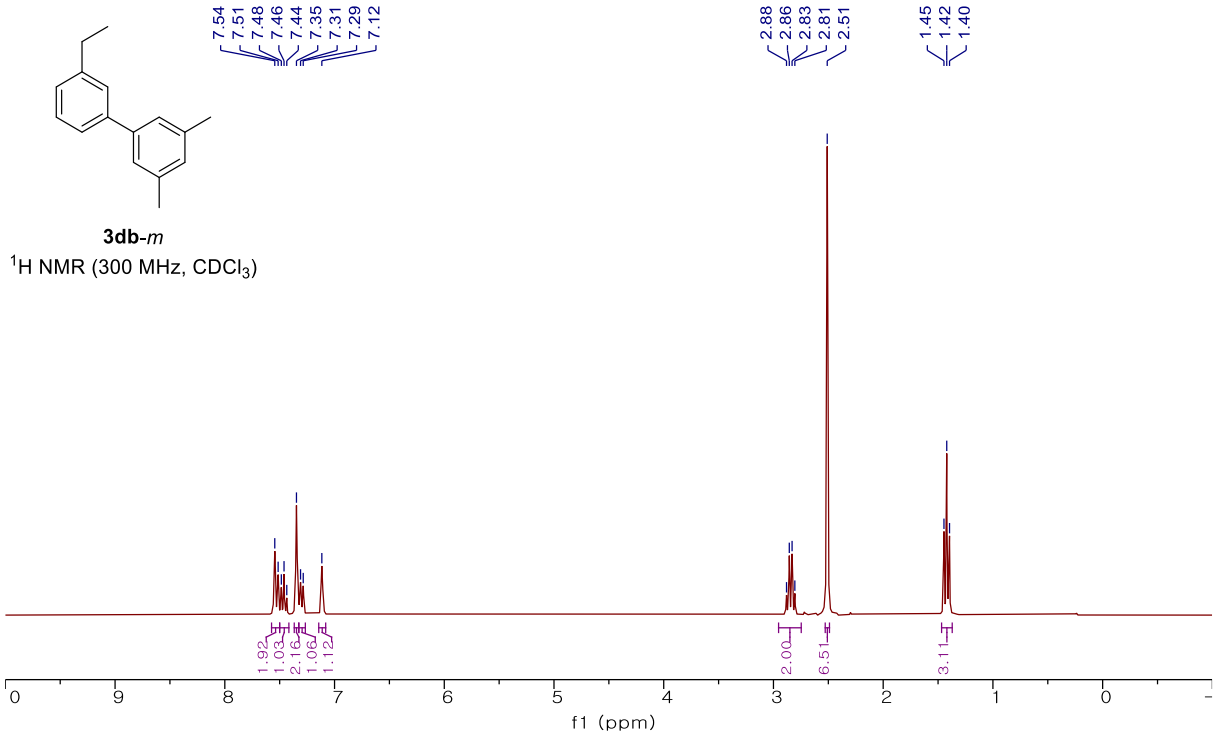

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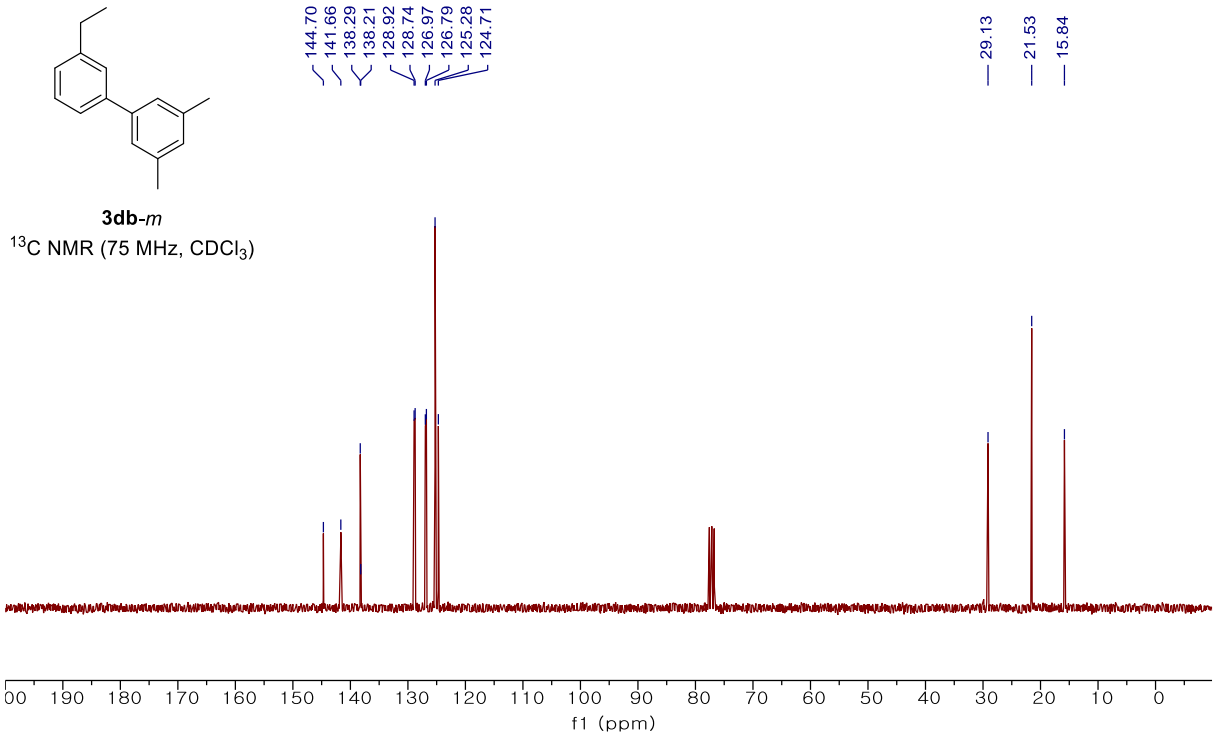

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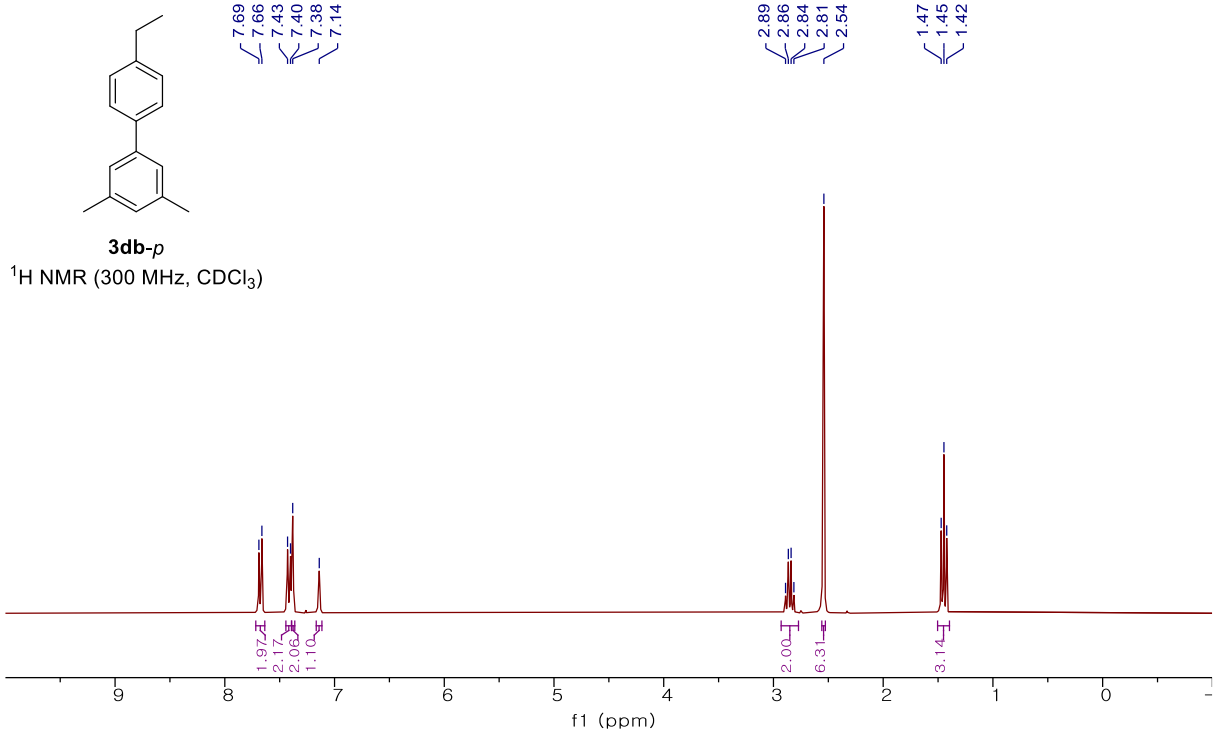

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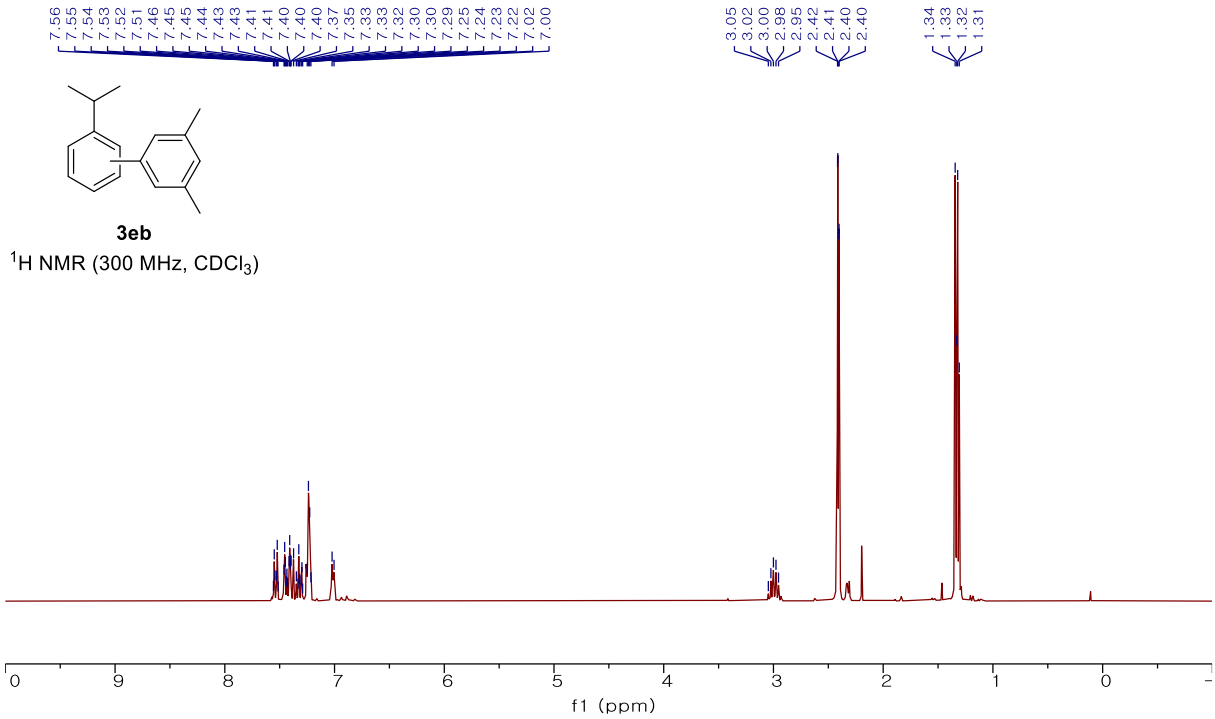

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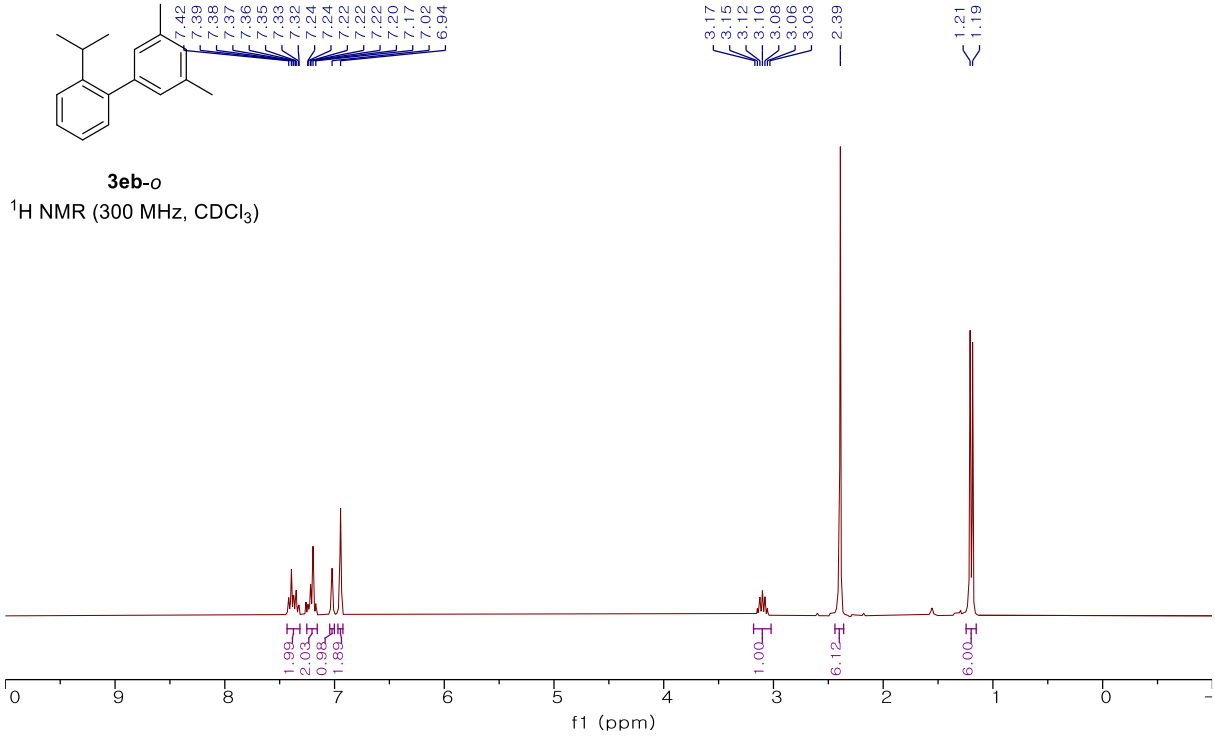

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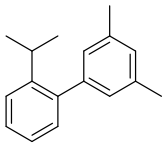
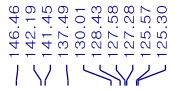
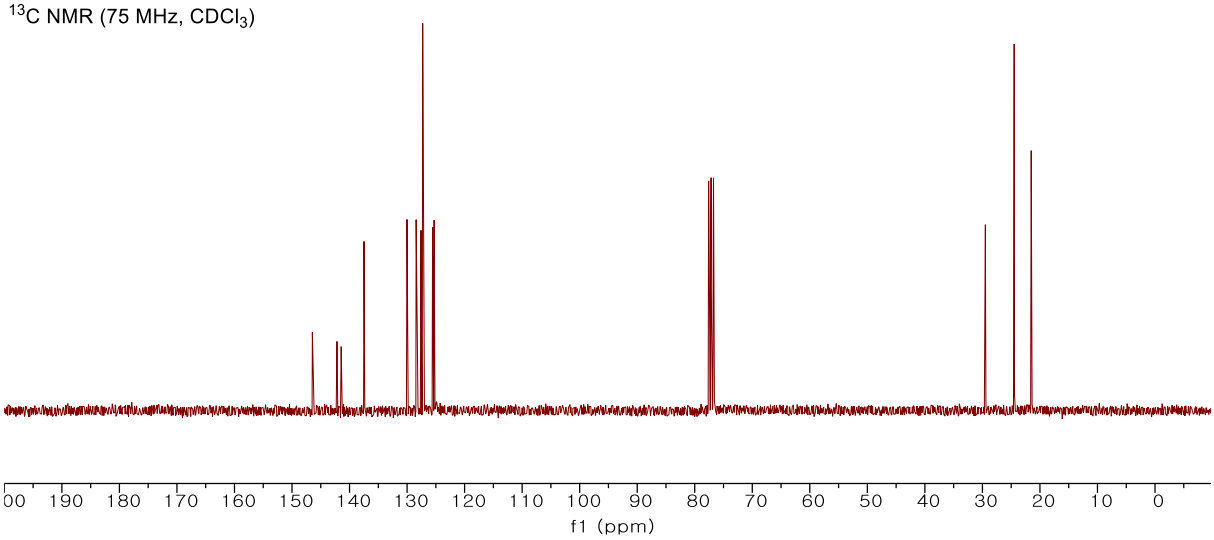
^{1}H NMR (300 MHz, $CDCl_3$)

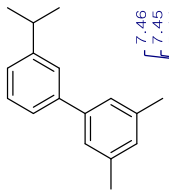


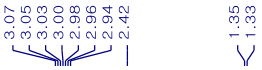


3eb-*o*

^{13}C NMR (75 MHz, $CDCl_3$)

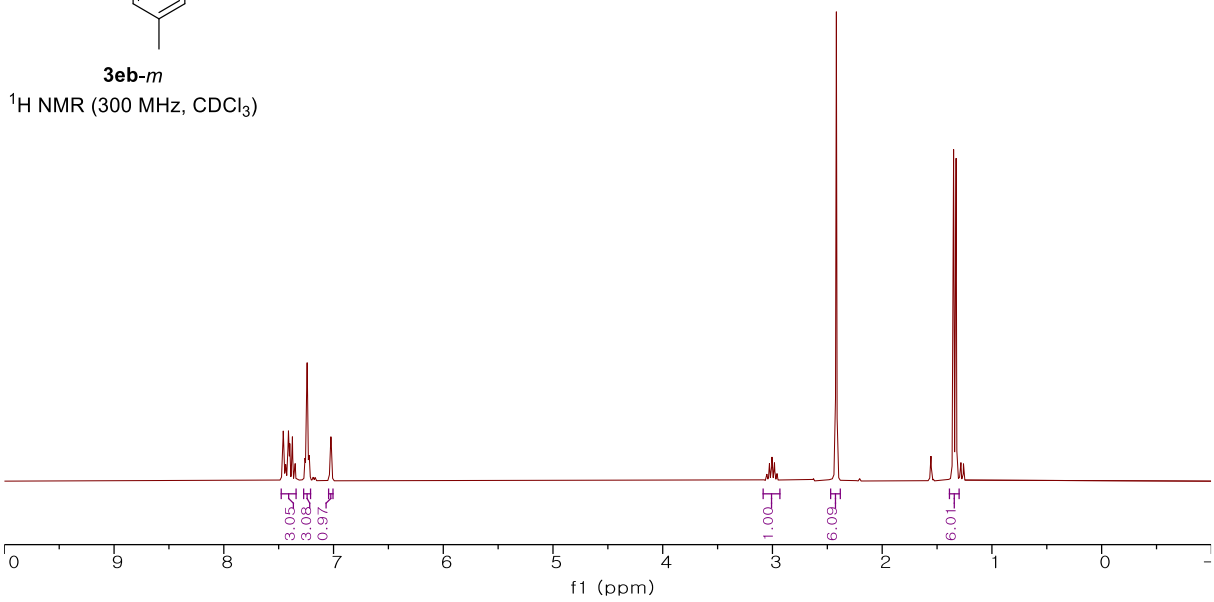


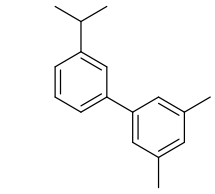




3eb-*m*

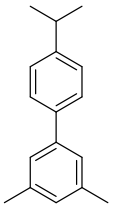
^{1}H NMR (300 MHz, $CDCl_3$)





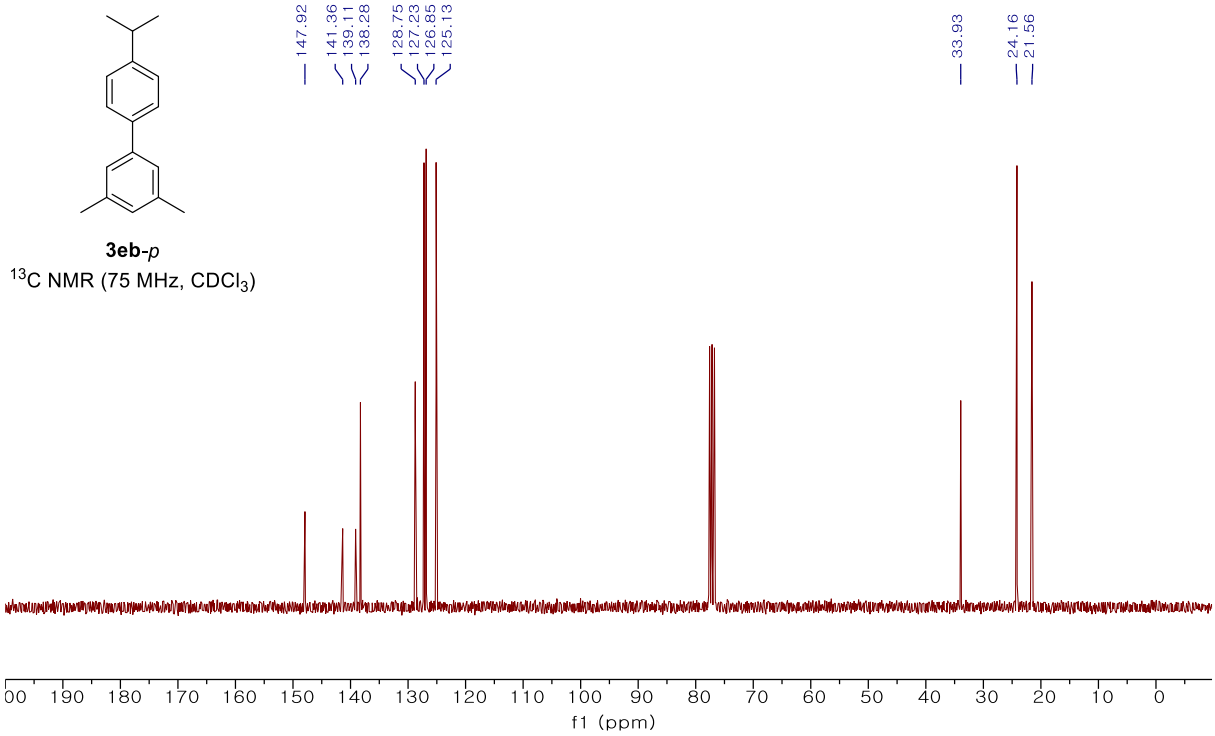
3eb-*m*

^{13}C NMR (75 MHz, $CDCl_3$)



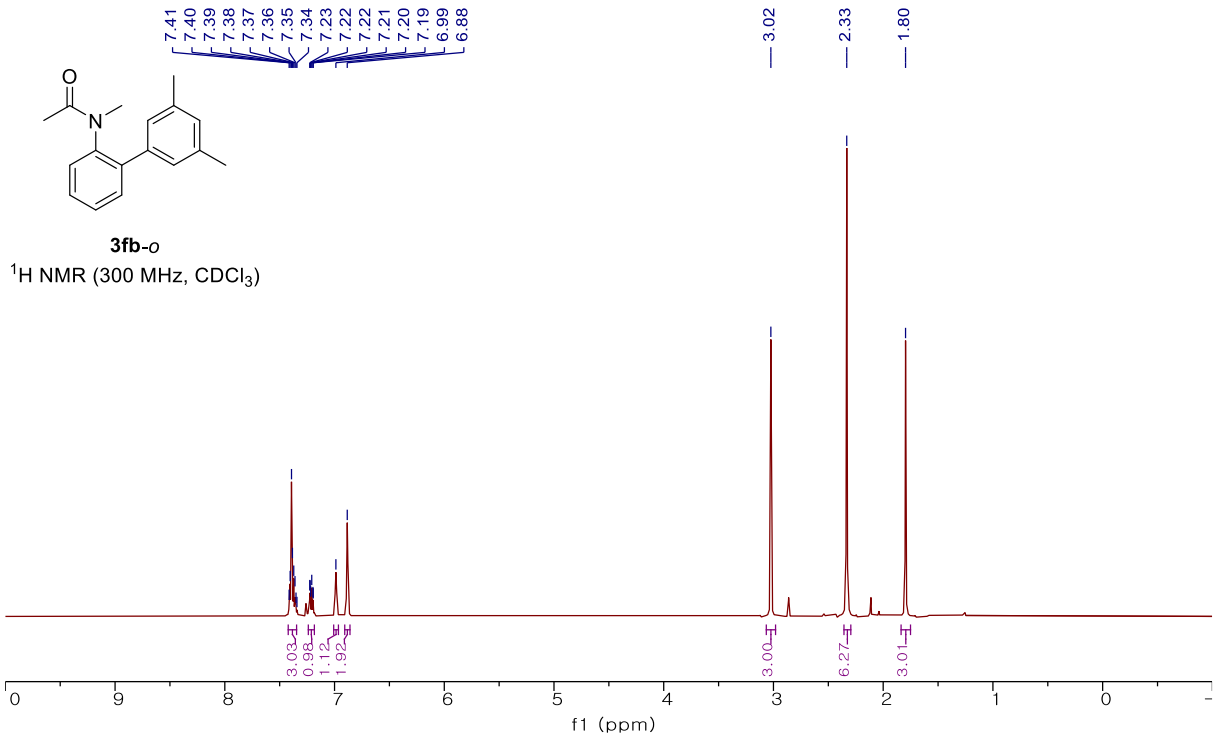
3eb-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



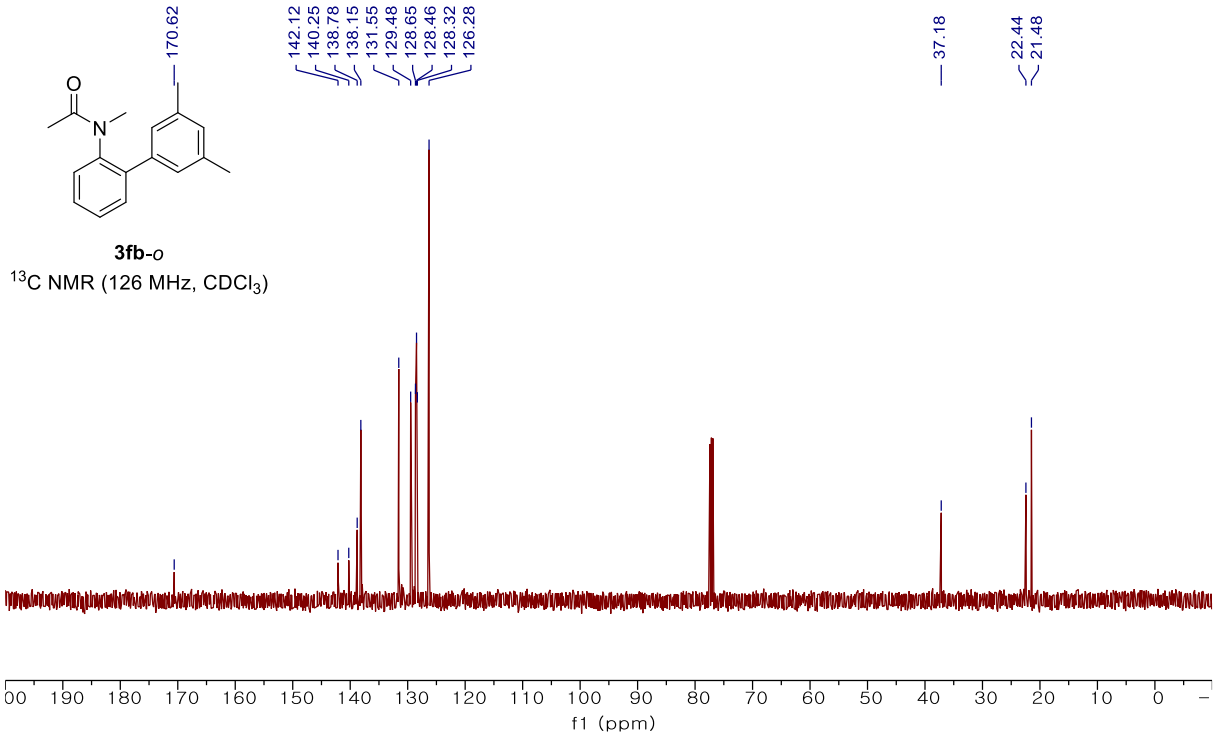
3eb-*p*

^{13}C NMR (75 MHz, $CDCl_3$)



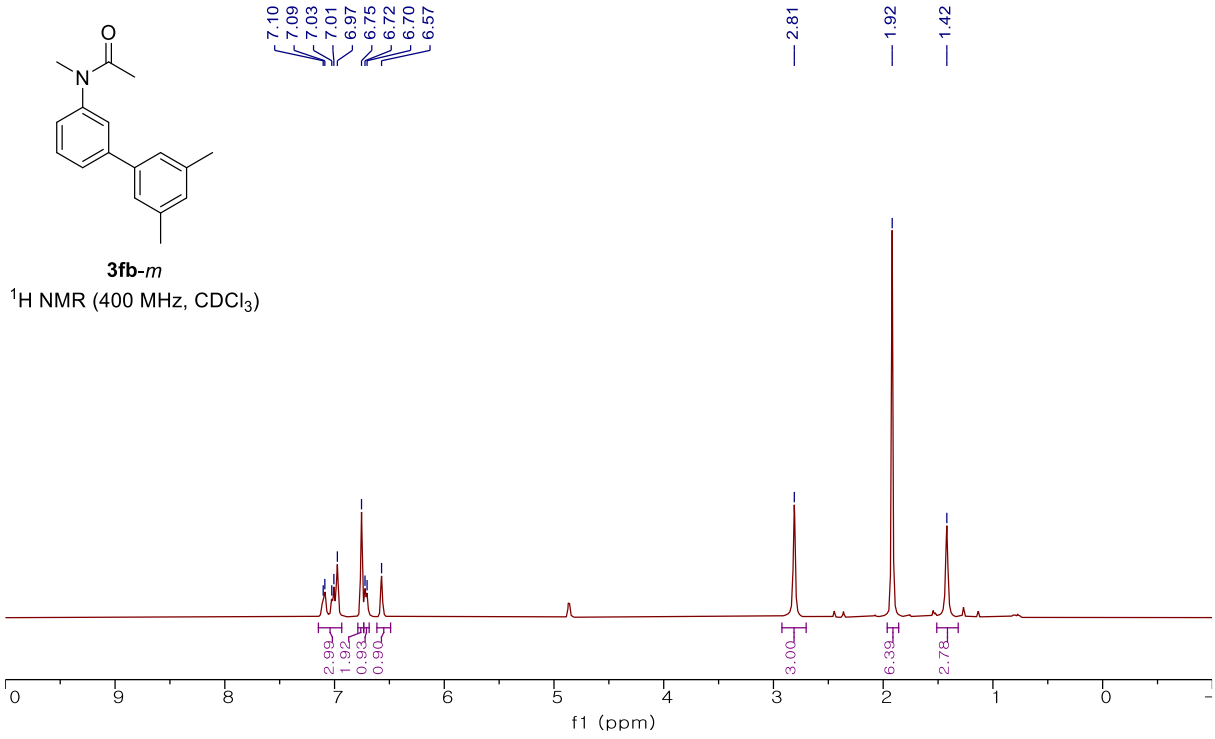
3fb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



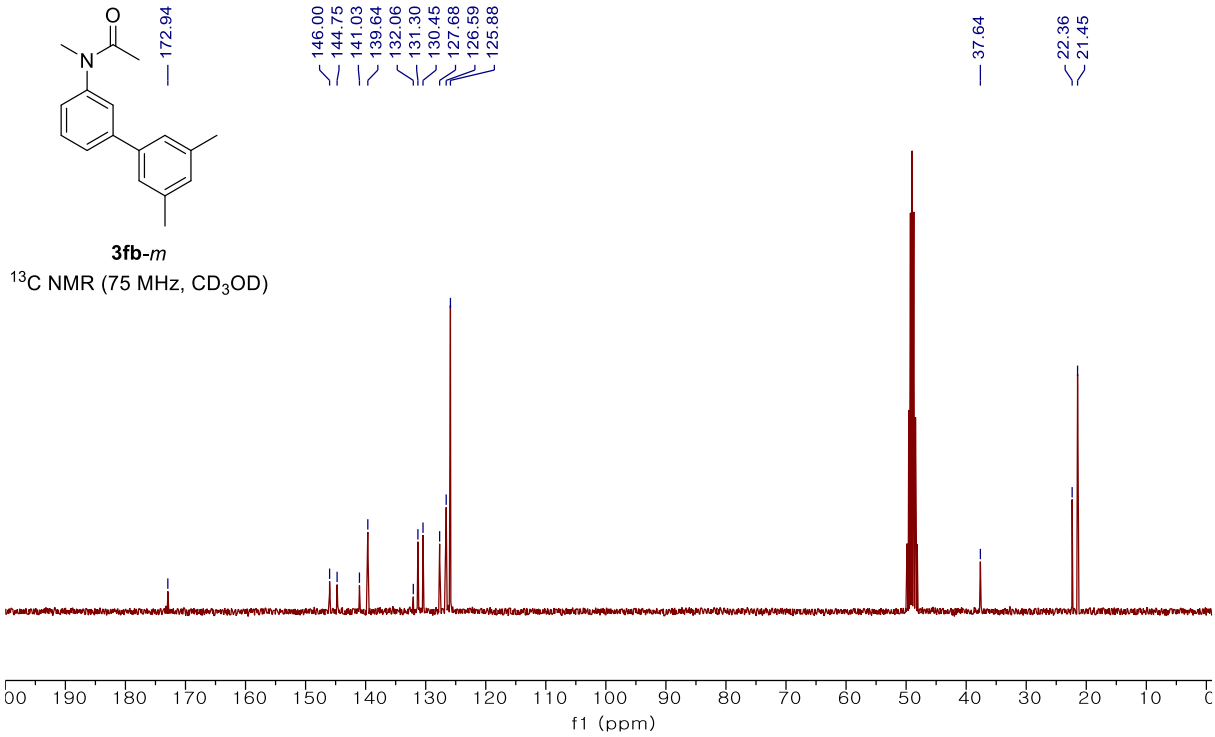
3fb-*o*

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



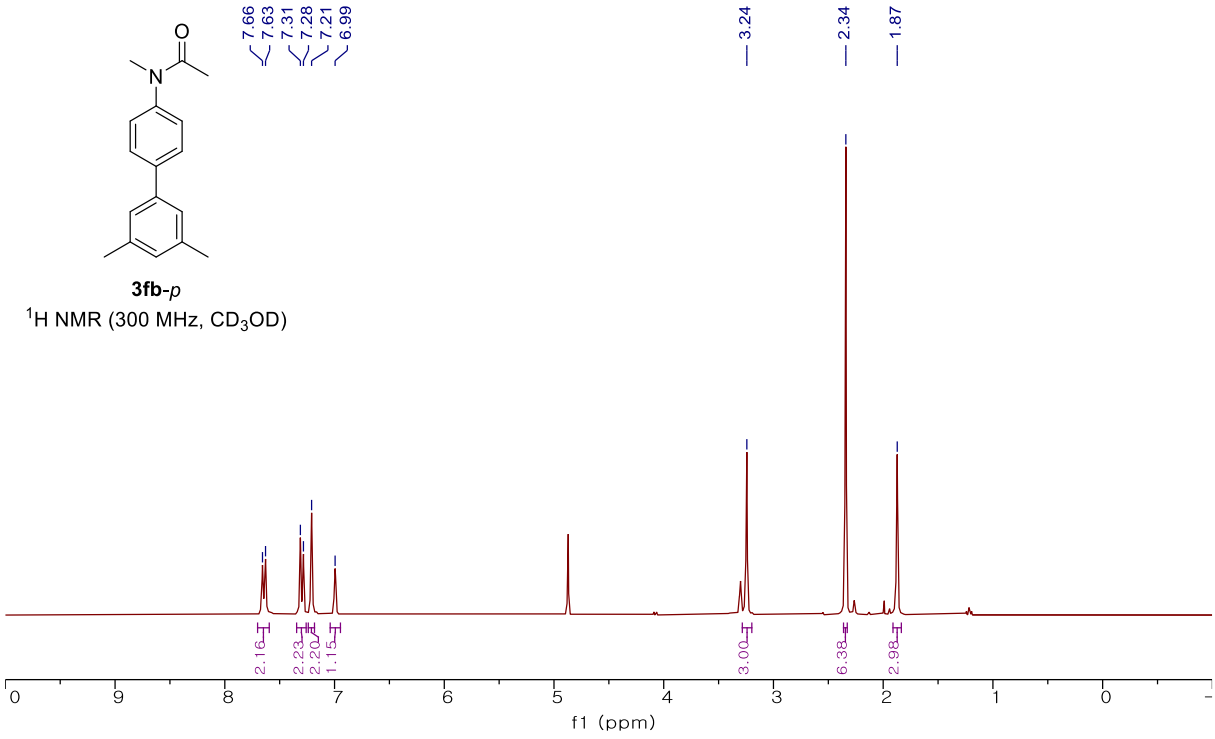
3fb-*m*

^{1}H NMR (400 MHz, $CDCl_3$)



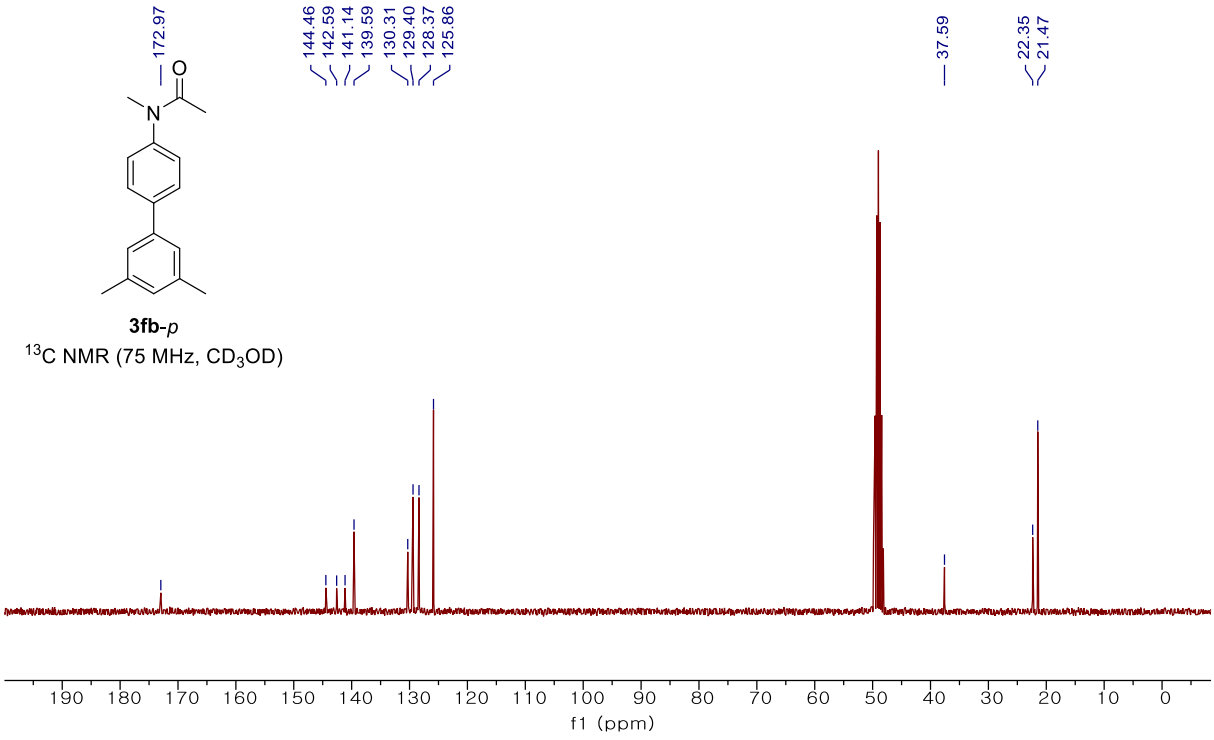
3fb-*m*

^{13}C NMR (75 MHz, CD_3OD)



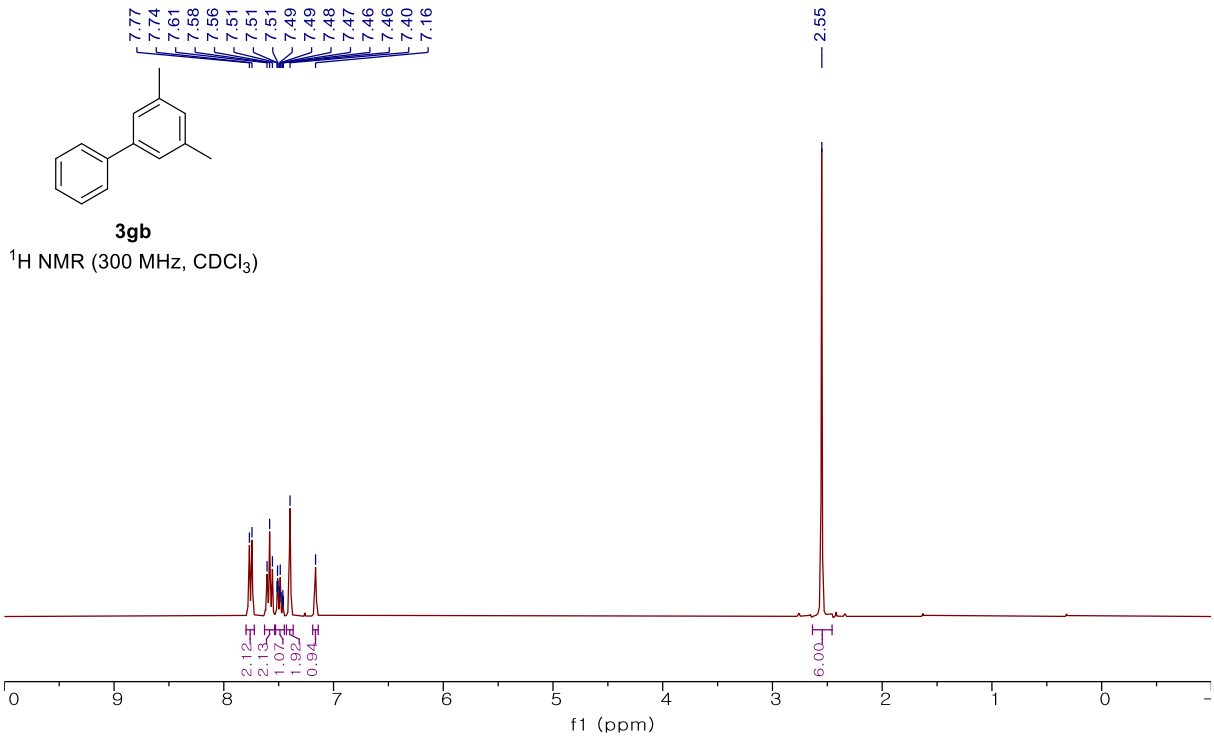
3fb-*p*

^{1}H NMR (300 MHz, CD_3OD)



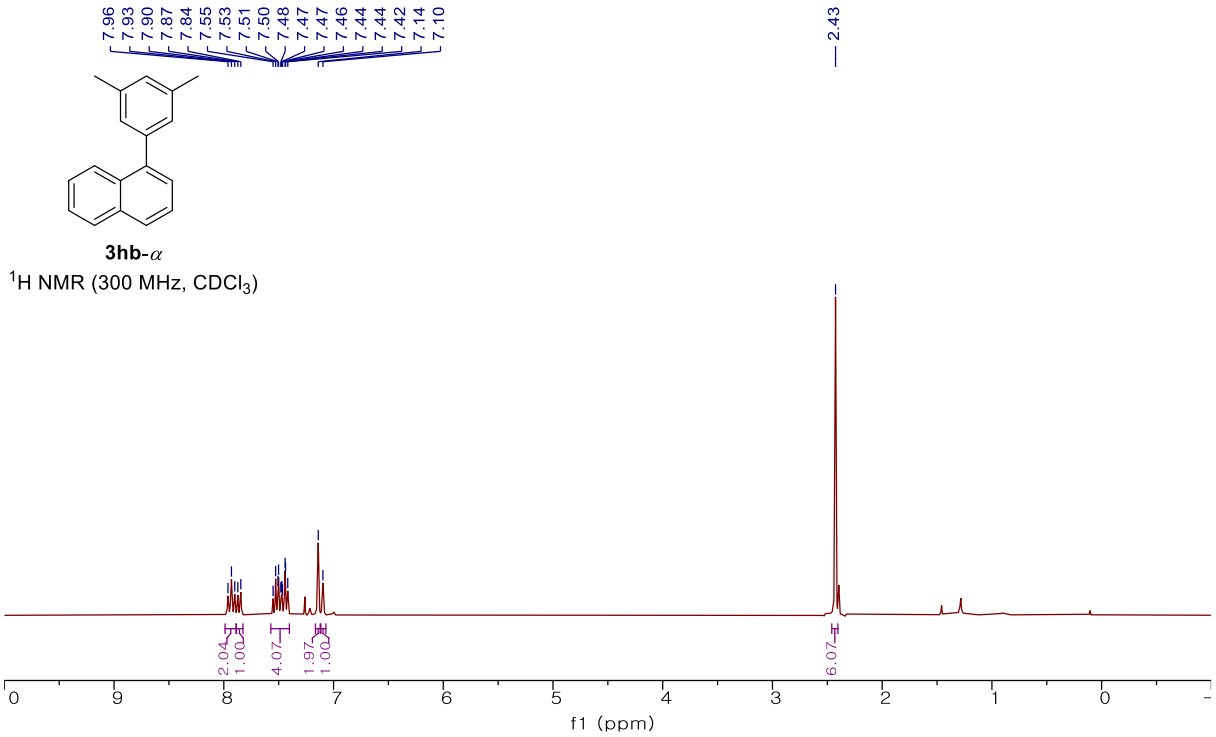
3fb-*p*

^{13}C NMR (75 MHz, CD_3OD)



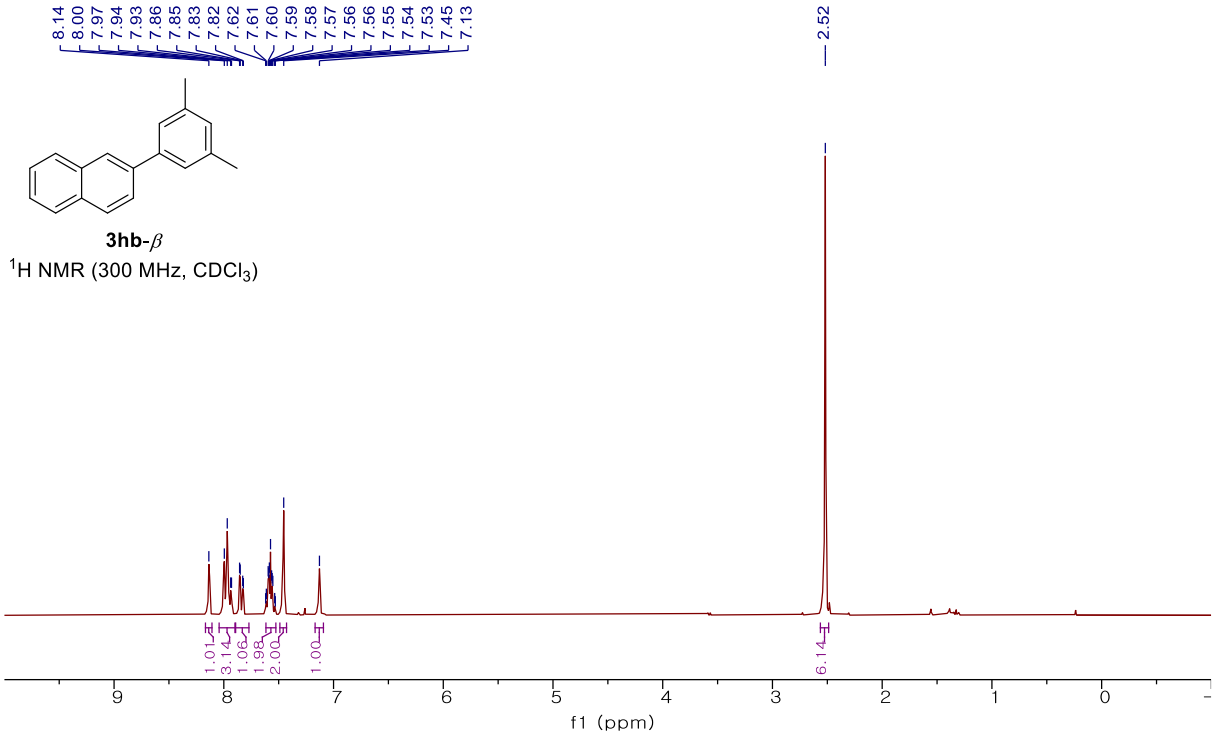
3gb

^{1}H NMR (300 MHz, $CDCl_3$)



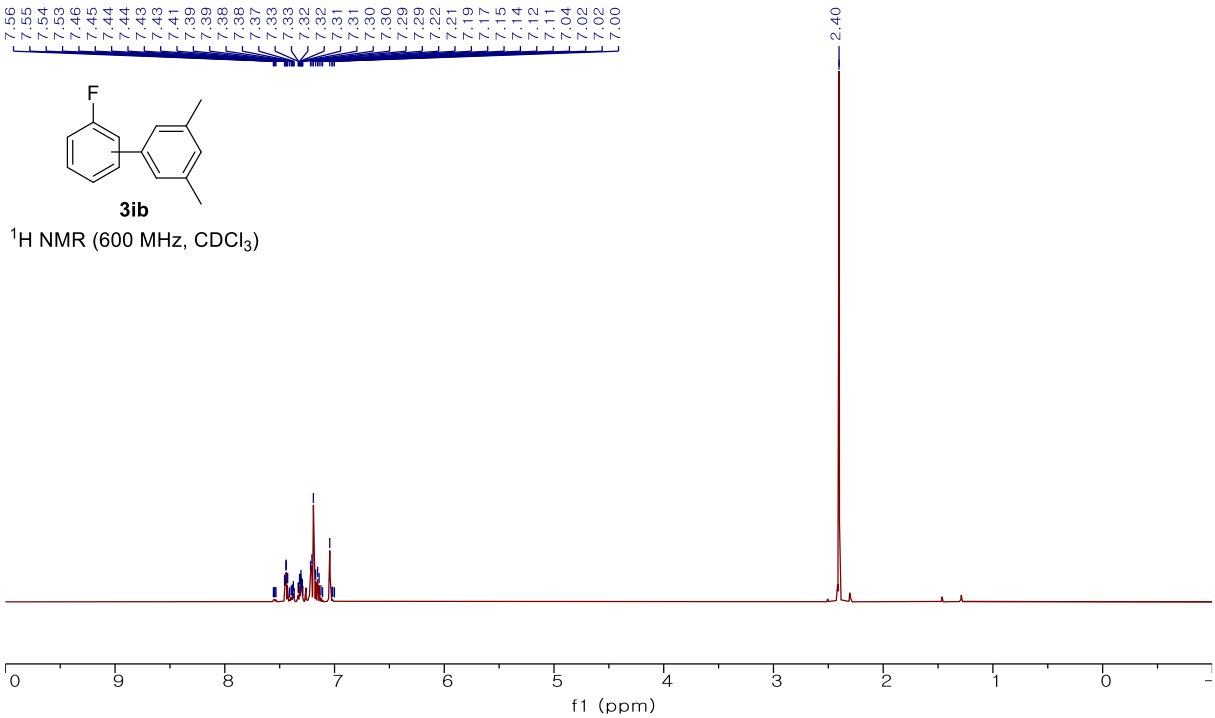
3hb-α

^{1}H NMR (300 MHz, $CDCl_3$)



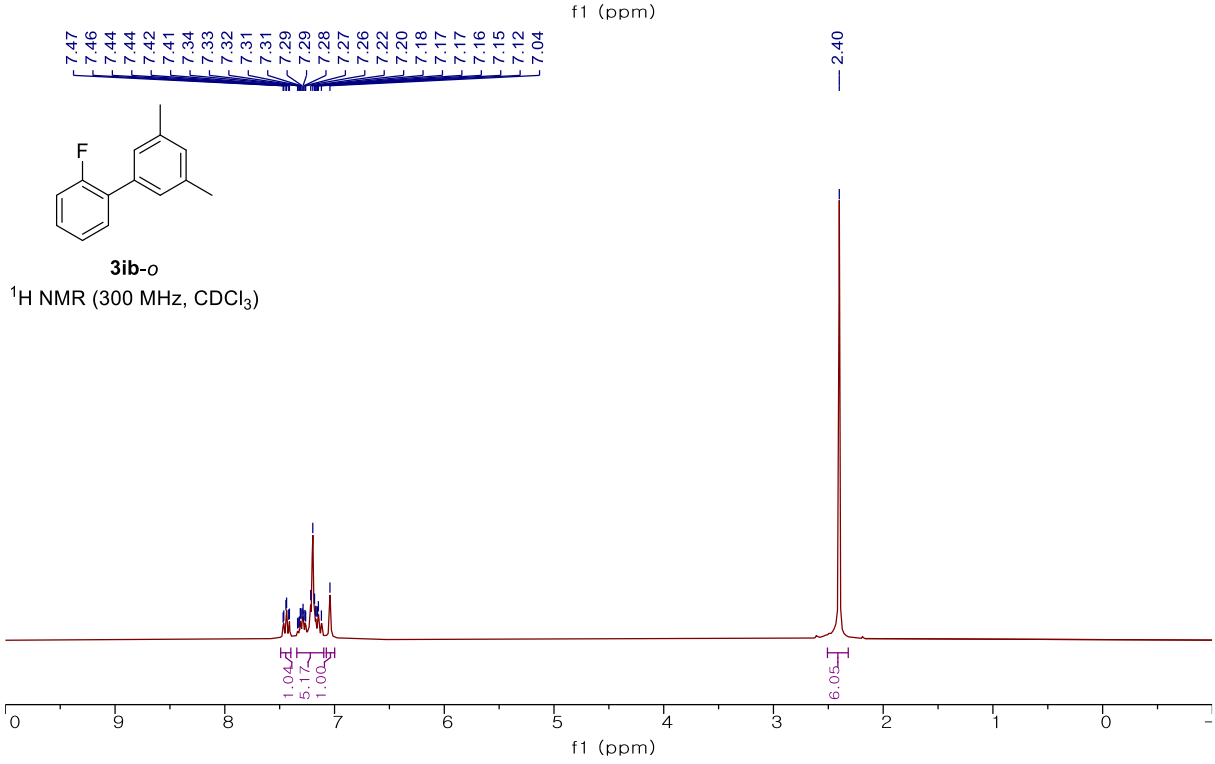
3hb-β

^{1}H NMR (300 MHz, $CDCl_3$)



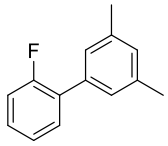
3ib

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



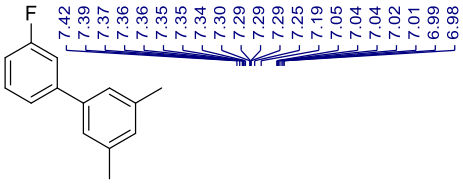
3ib-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



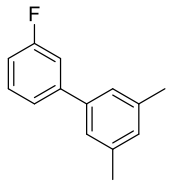
3ib-*o*

^{19}F NMR (376 MHz, $CDCl_3$)



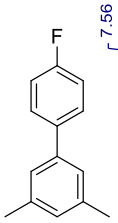
3ib-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



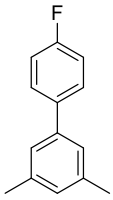
3ib-*m*

^{19}F NMR (376 MHz, $CDCl_3$)



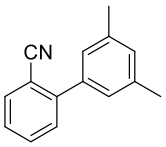
3ib-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



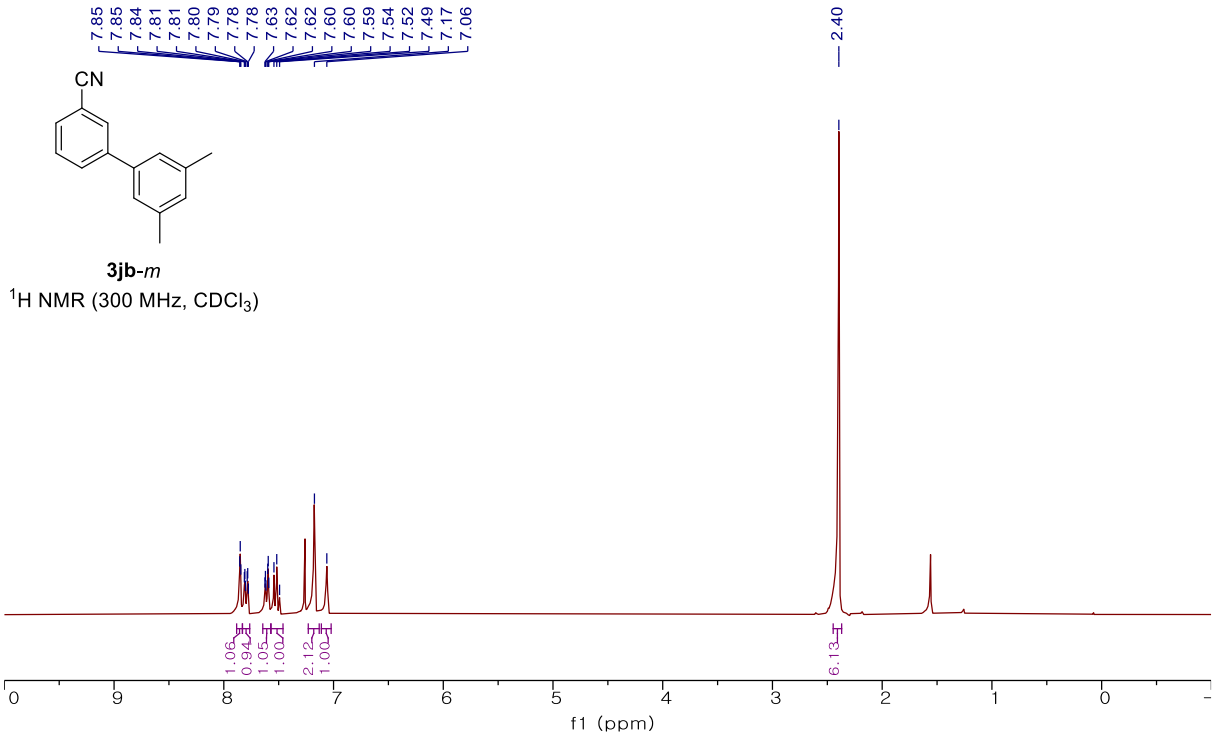
3ib-*p*

^{19}F NMR (376 MHz, $CDCl_3$)



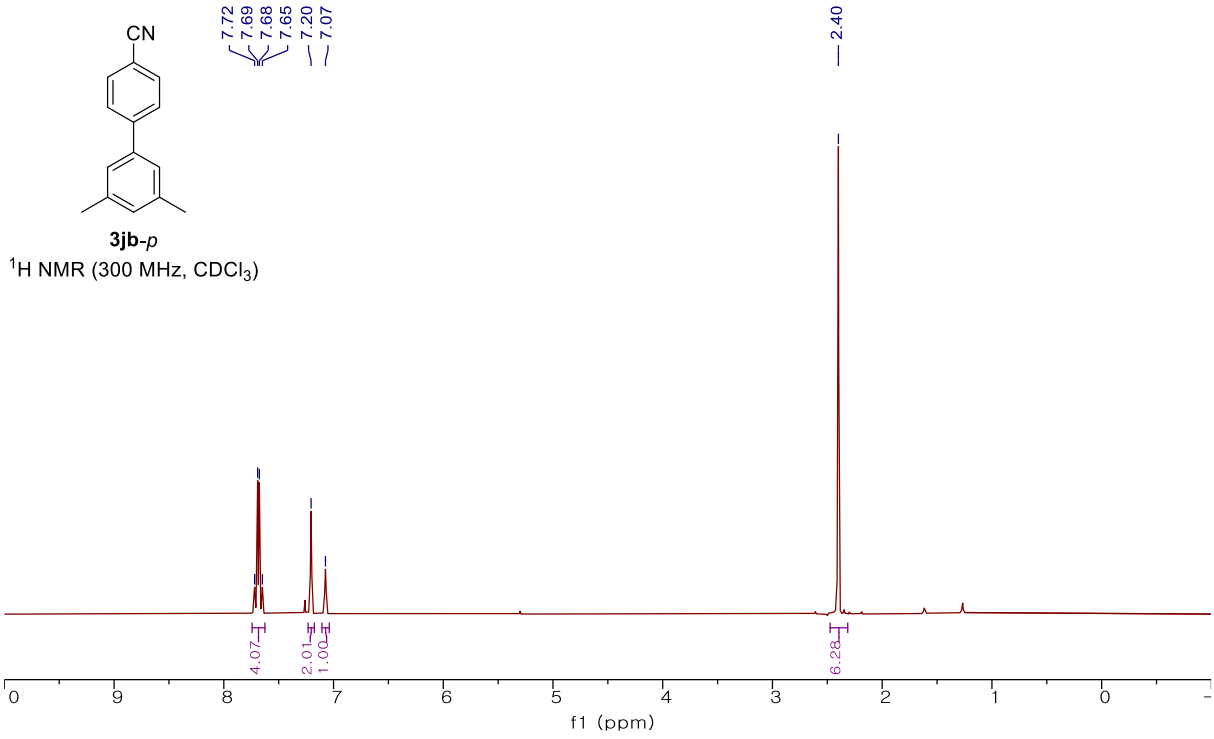
3jb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



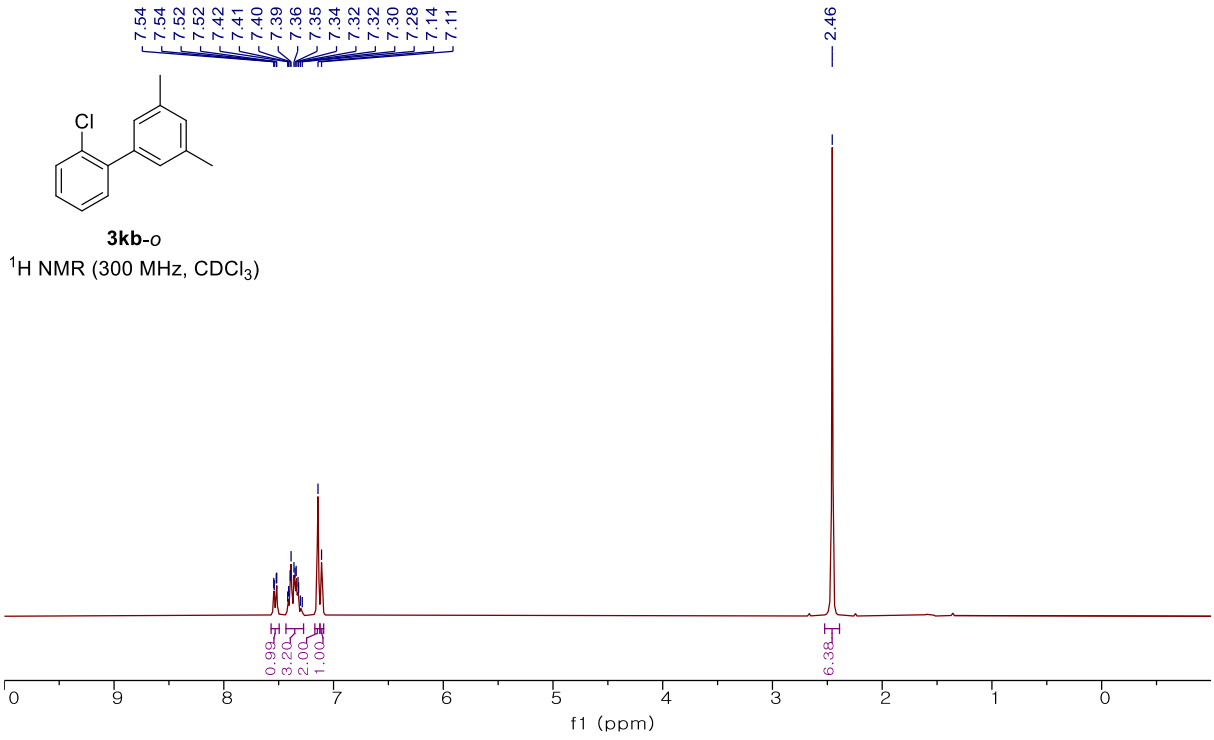
3jb-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



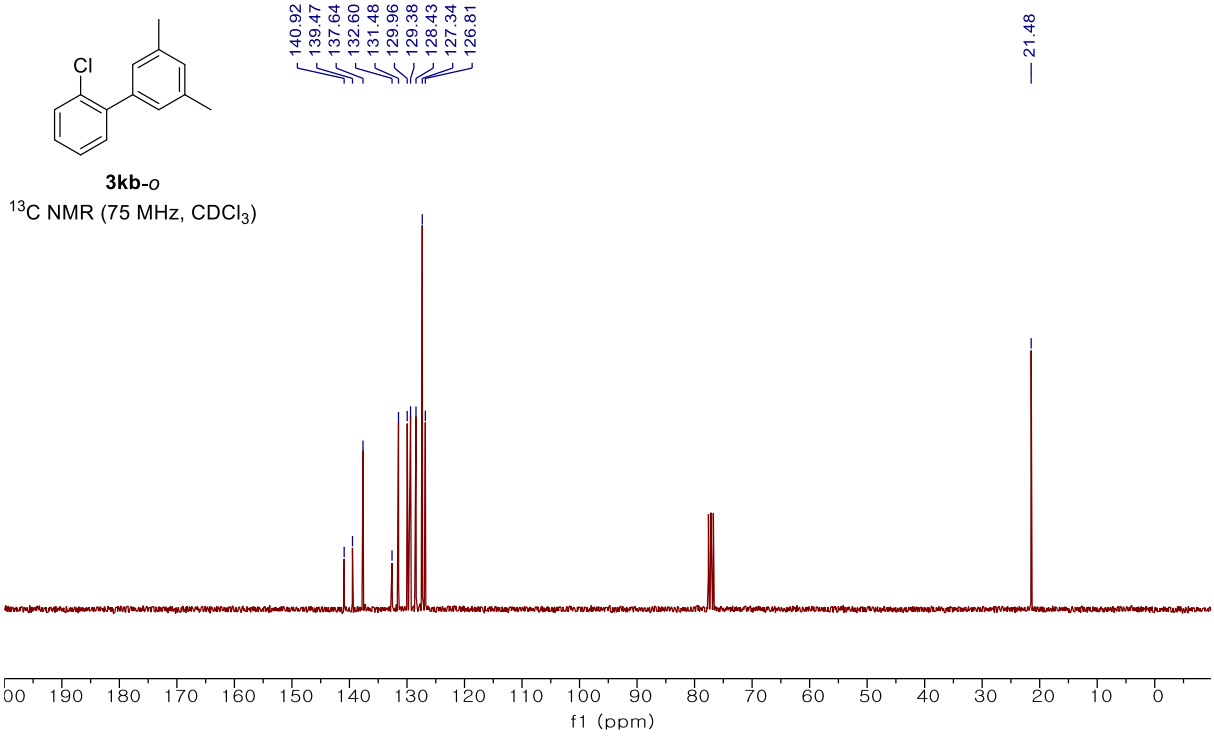
3jb-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



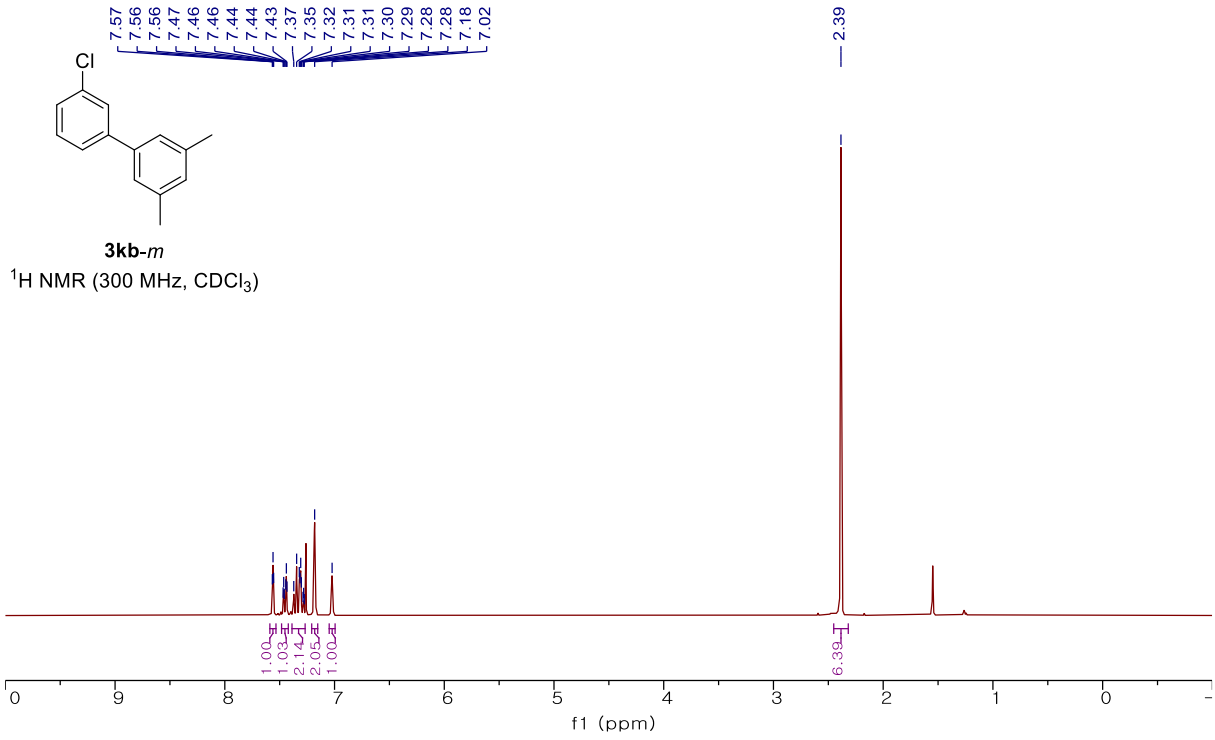
3kb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



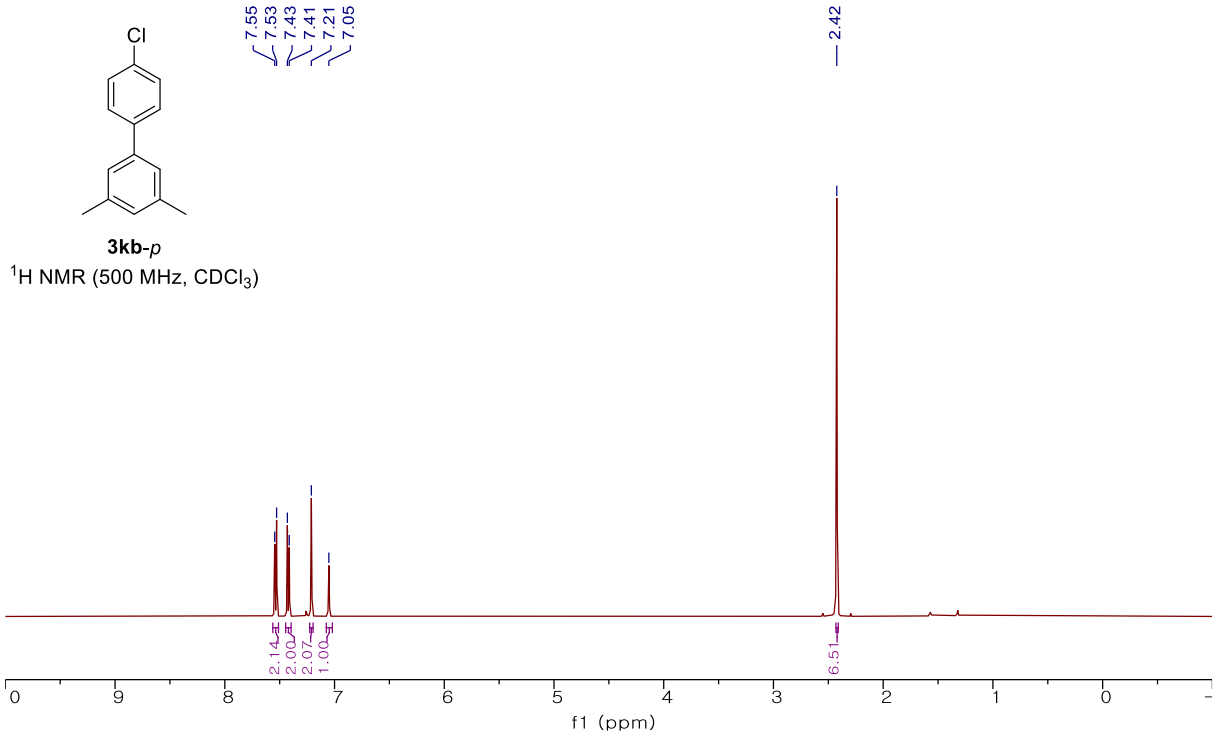
3kb-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



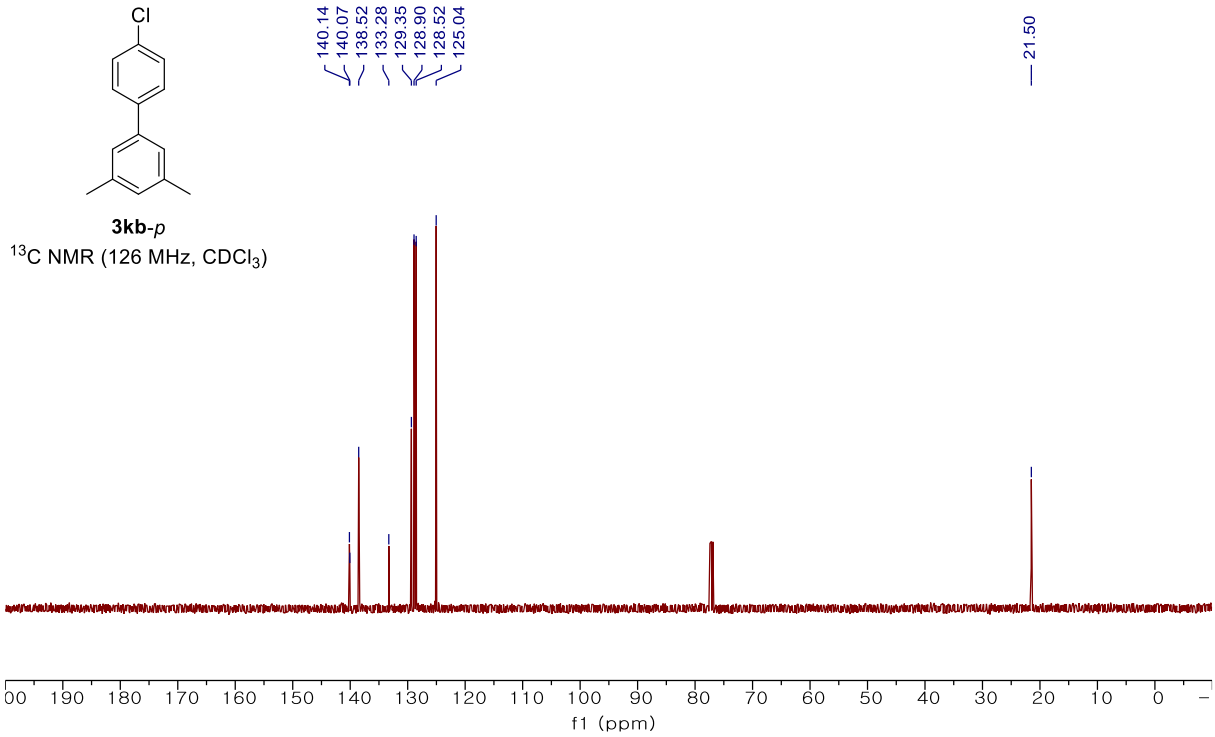
3kb-*m*

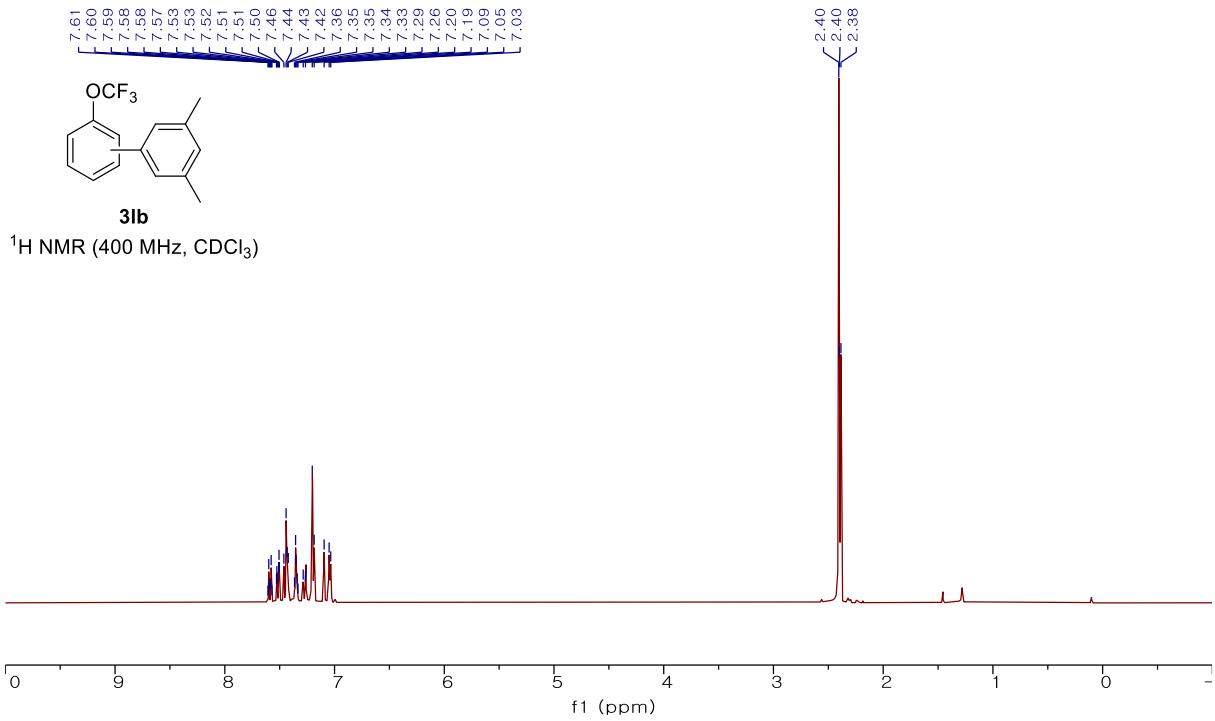
^{1}H NMR (300 MHz, $CDCl_3$)

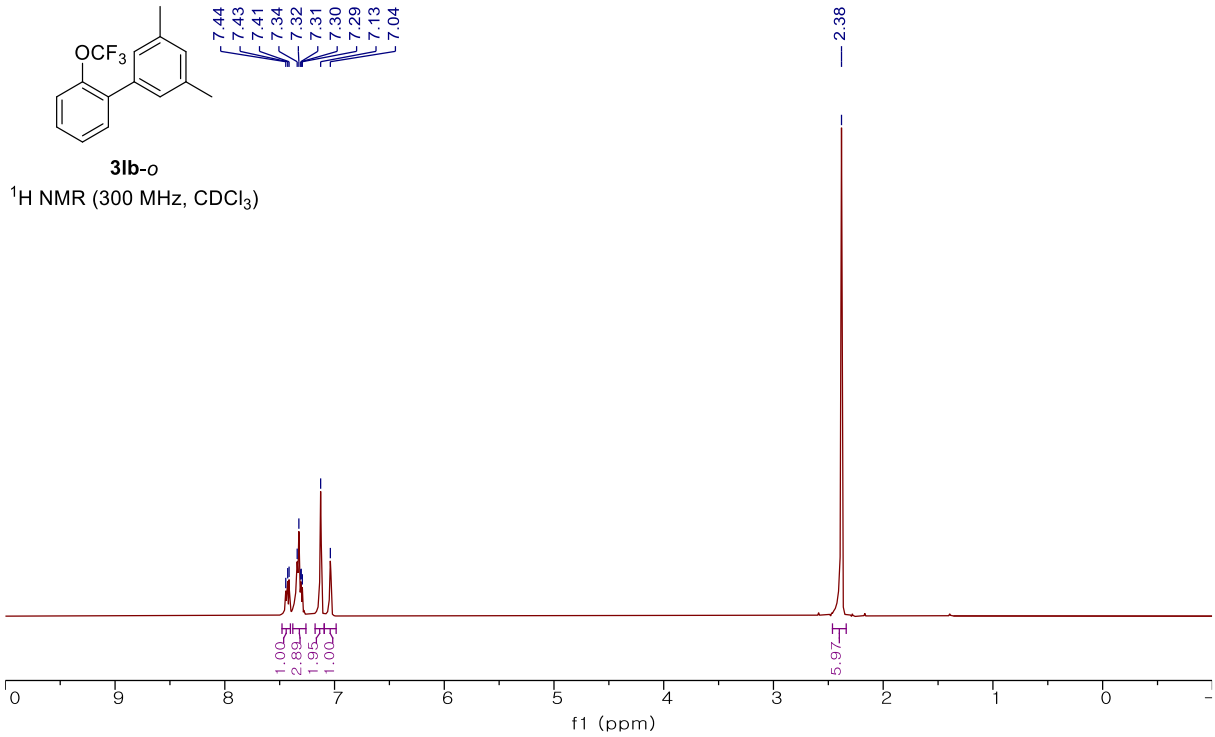


3kb-*p*

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

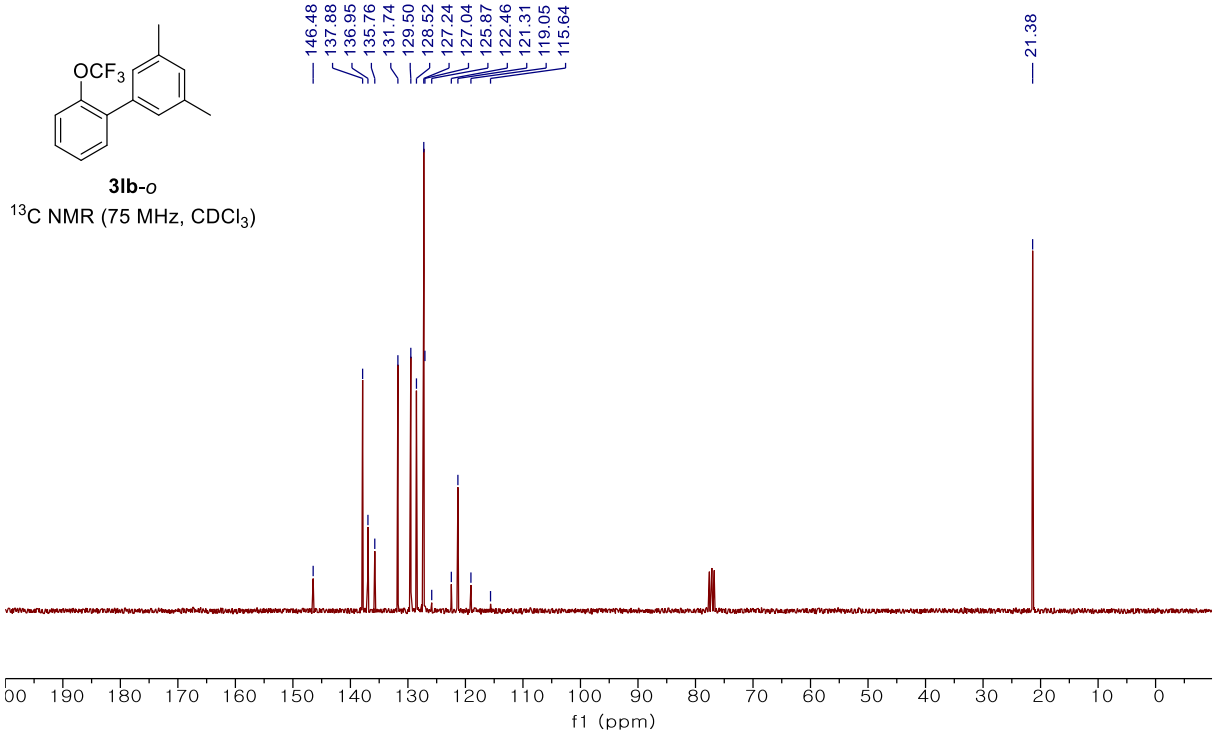

Cl
140.14
140.07
138.52
133.28
129.35
128.90
128.52
125.04
21.50
3kb-p
13C NMR (126 MHz, CDCl3)
f1 (ppm)


7.61
7.60
7.59
7.58
7.58
7.57
7.53
7.53
7.52
7.51
7.51
7.50
7.46
7.44
7.43
7.42
7.36
7.35
7.35
7.34
7.33
7.29
7.26
7.20
7.19
7.09
7.05
7.03
2.40
2.40
2.38
OCF3
3lb
1H NMR (400 MHz, CDCl3)
f1 (ppm)



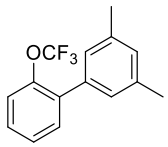
3lb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



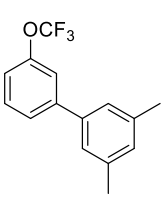
3lb-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



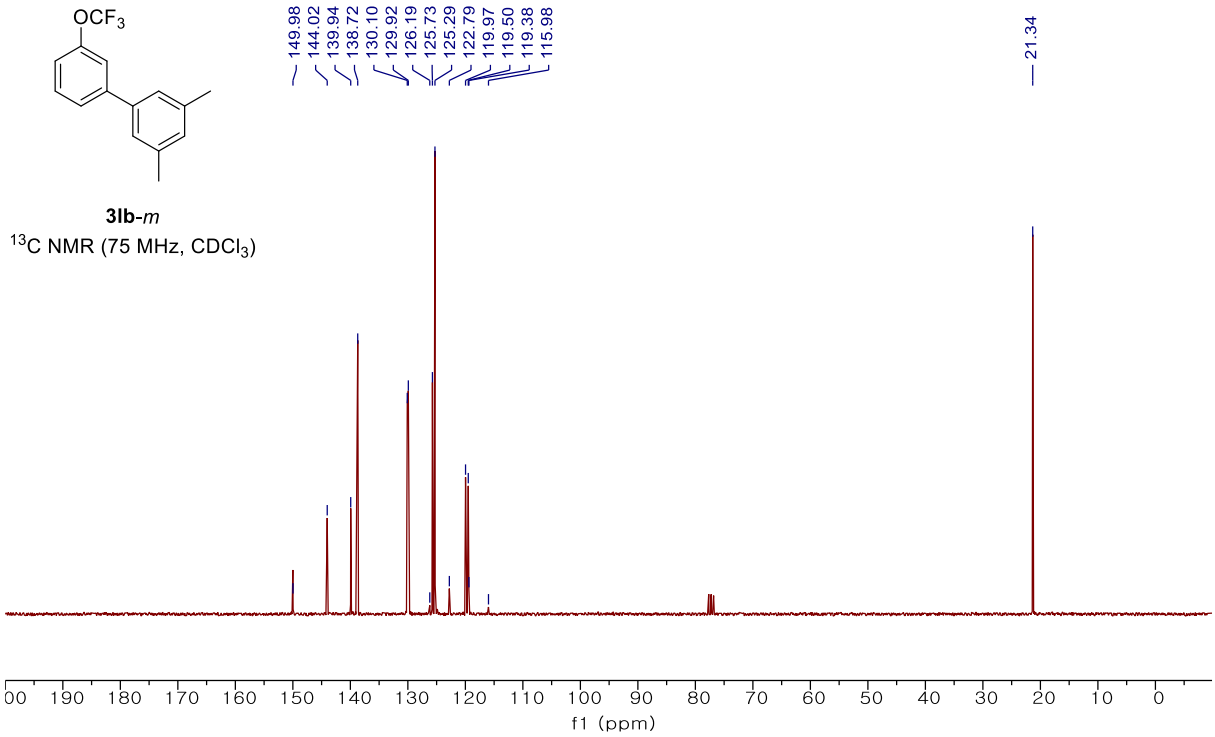
3lb-*o*

^{19}F NMR (376 MHz, $CDCl_3$)



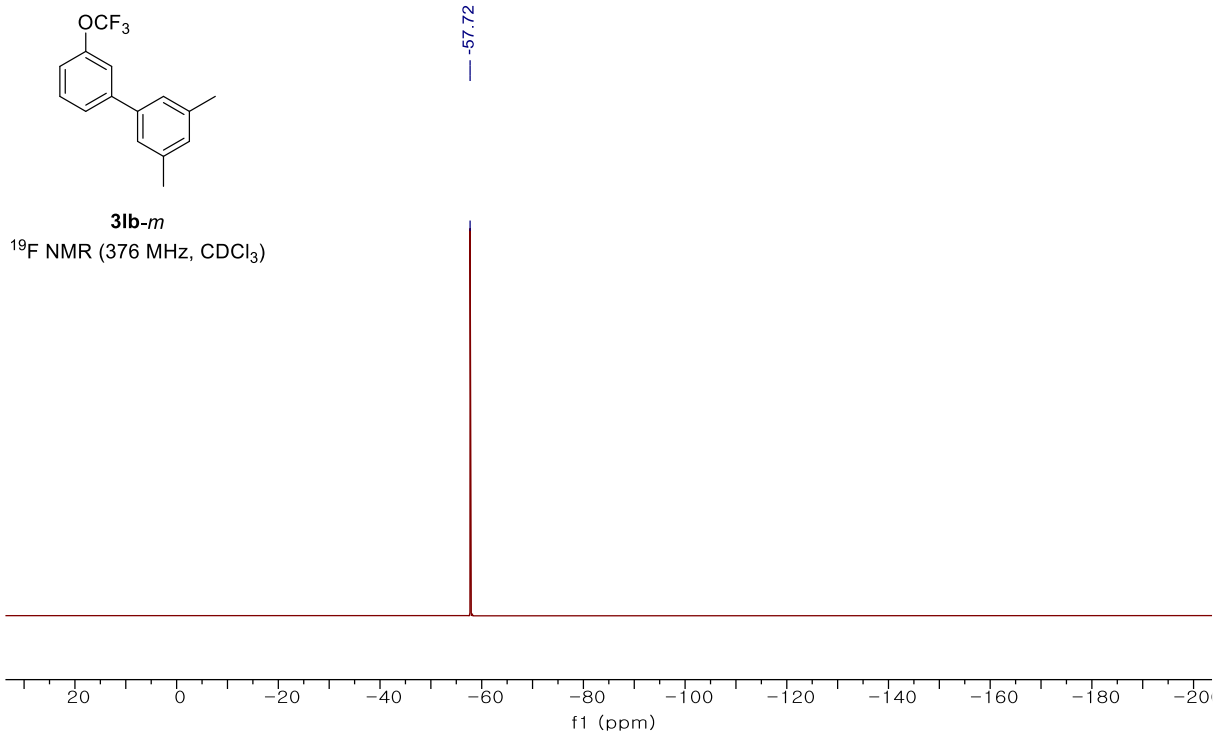
3lb-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



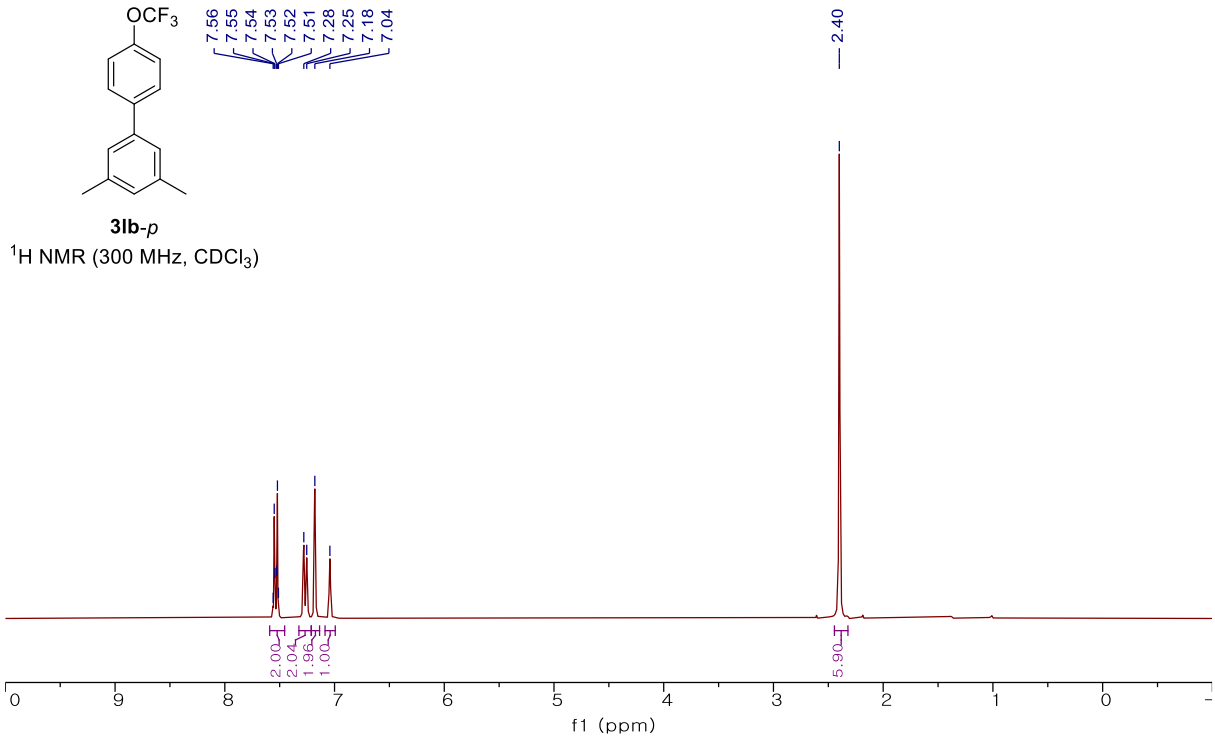
3lb-*m*

^{13}C NMR (75 MHz, $CDCl_3$)



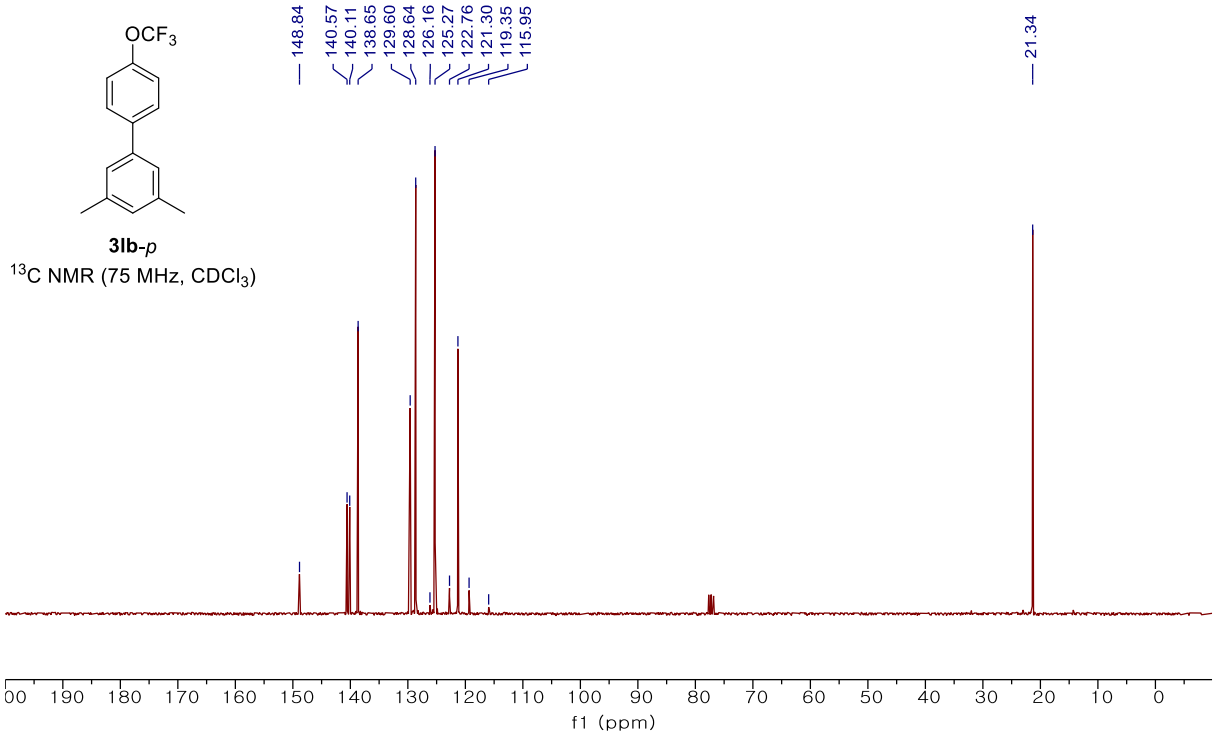
3lb-*m*

^{19}F NMR (376 MHz, $CDCl_3$)



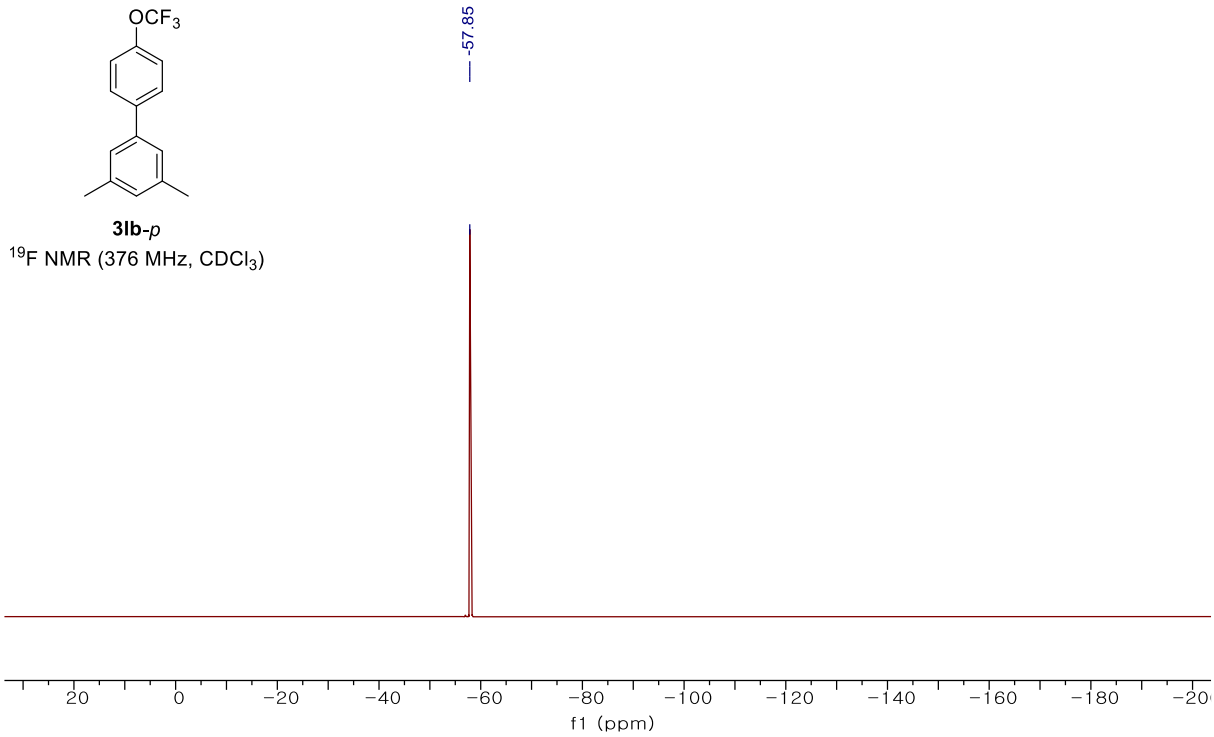
3lb-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



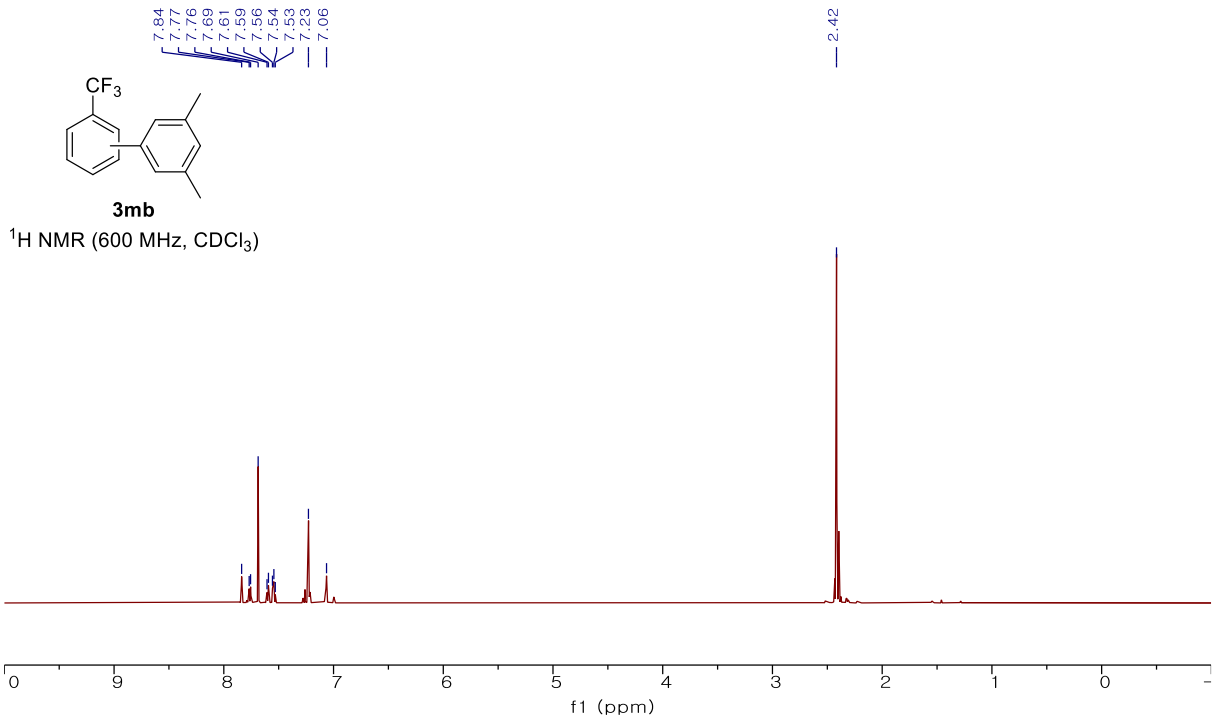
3lb-*p*

^{13}C NMR (75 MHz, $CDCl_3$)



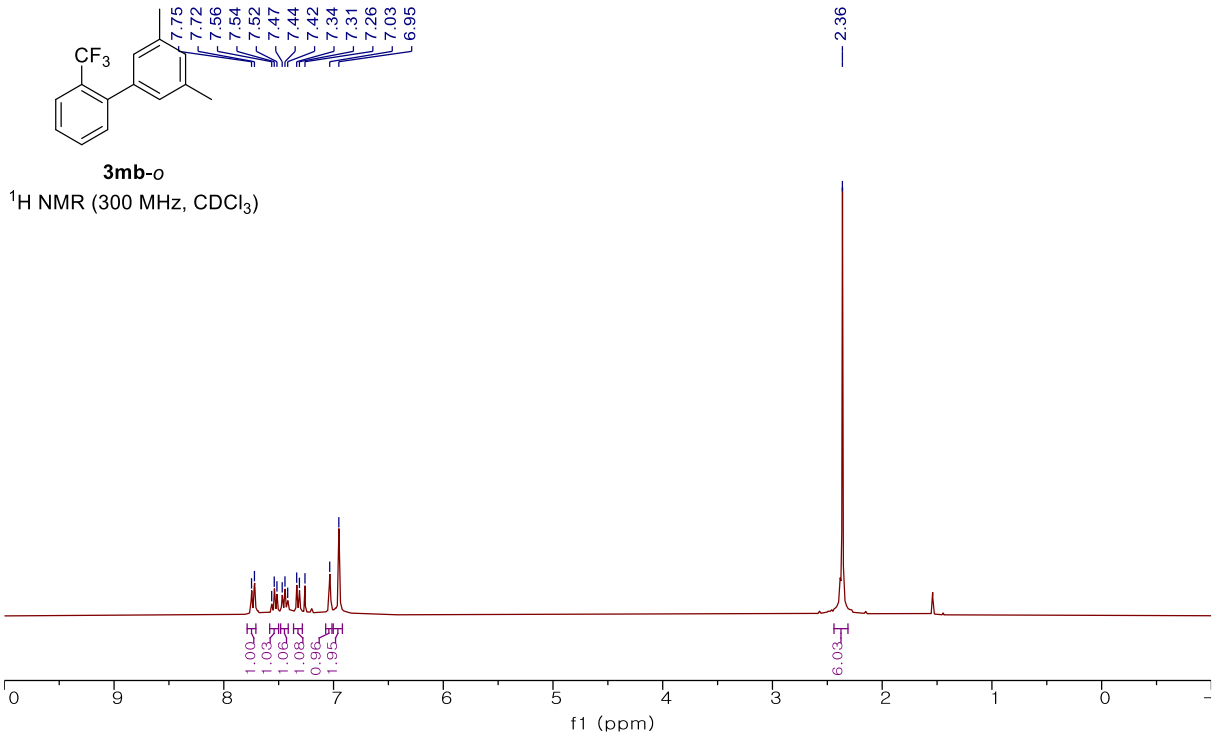
3lb-*p*

^{19}F NMR (376 MHz, $CDCl_3$)



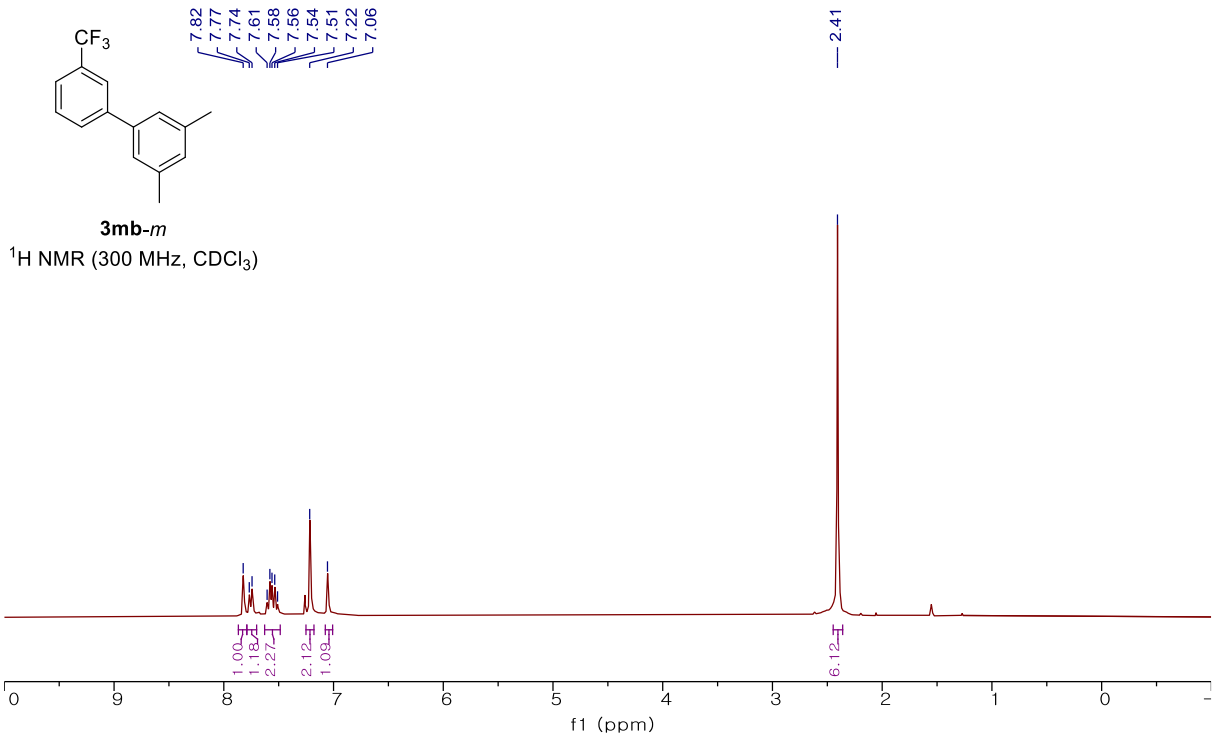
3mb

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



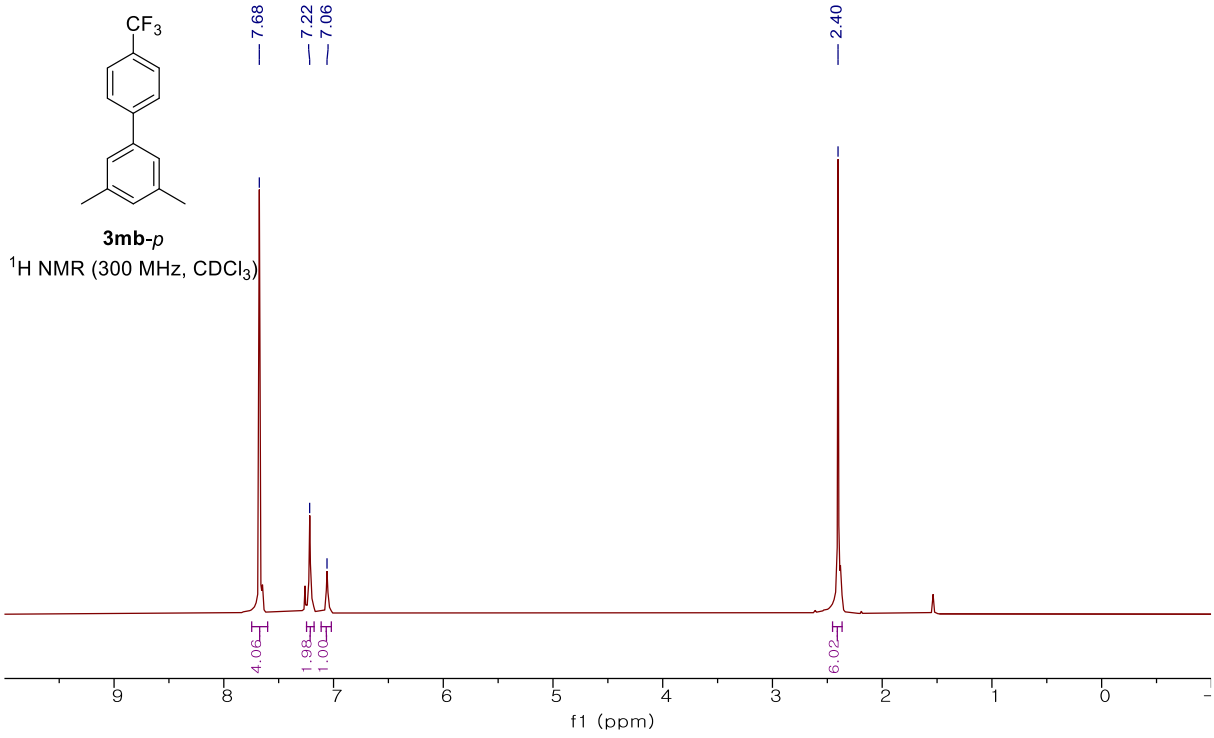
3mb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



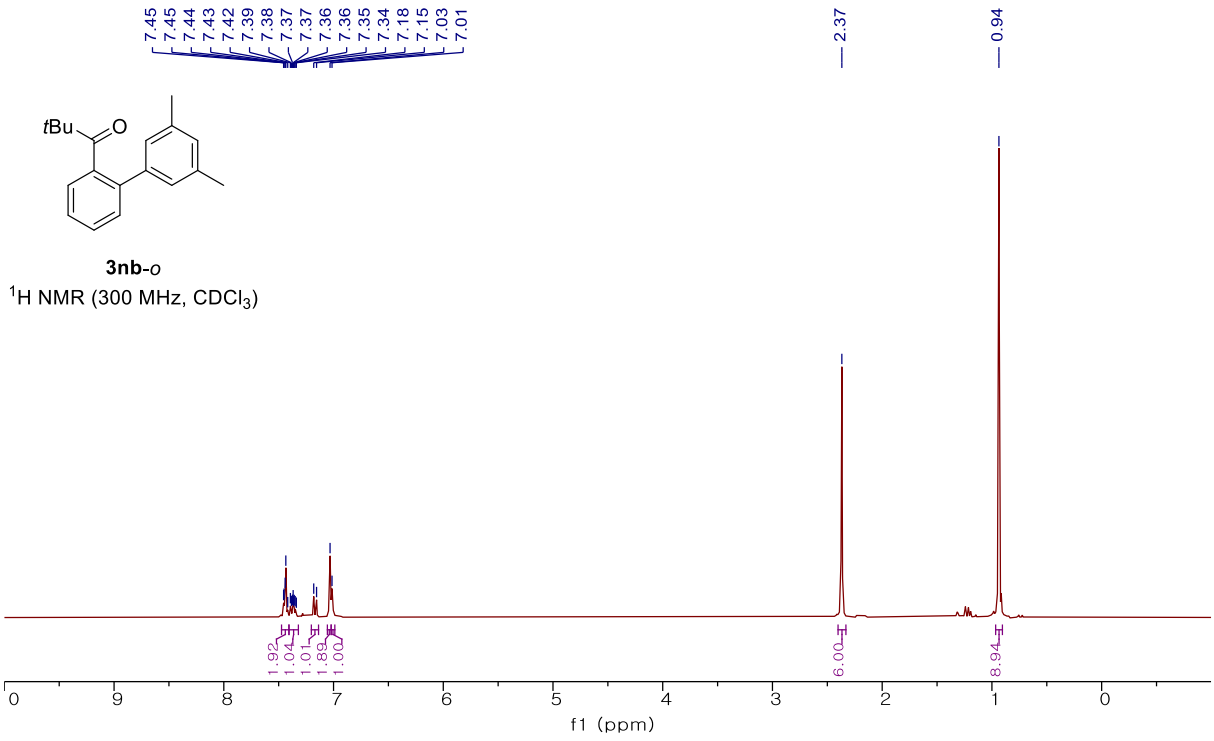
3mb-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



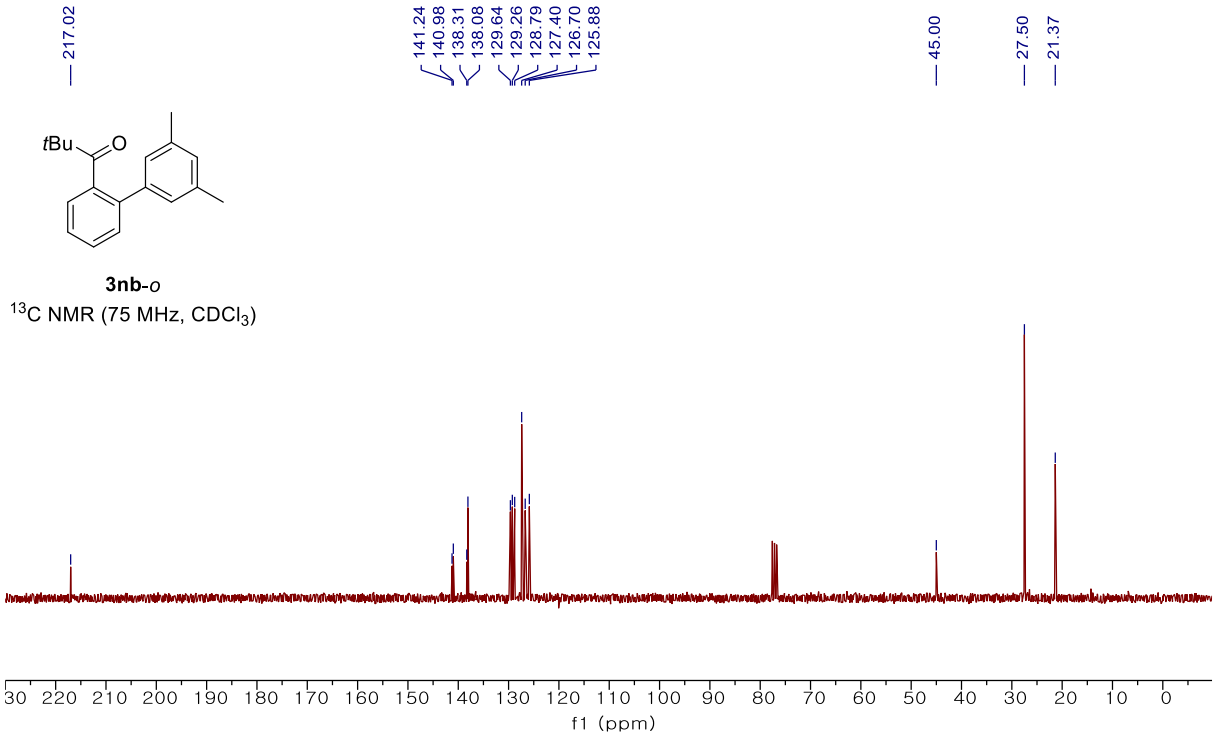
3mb-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



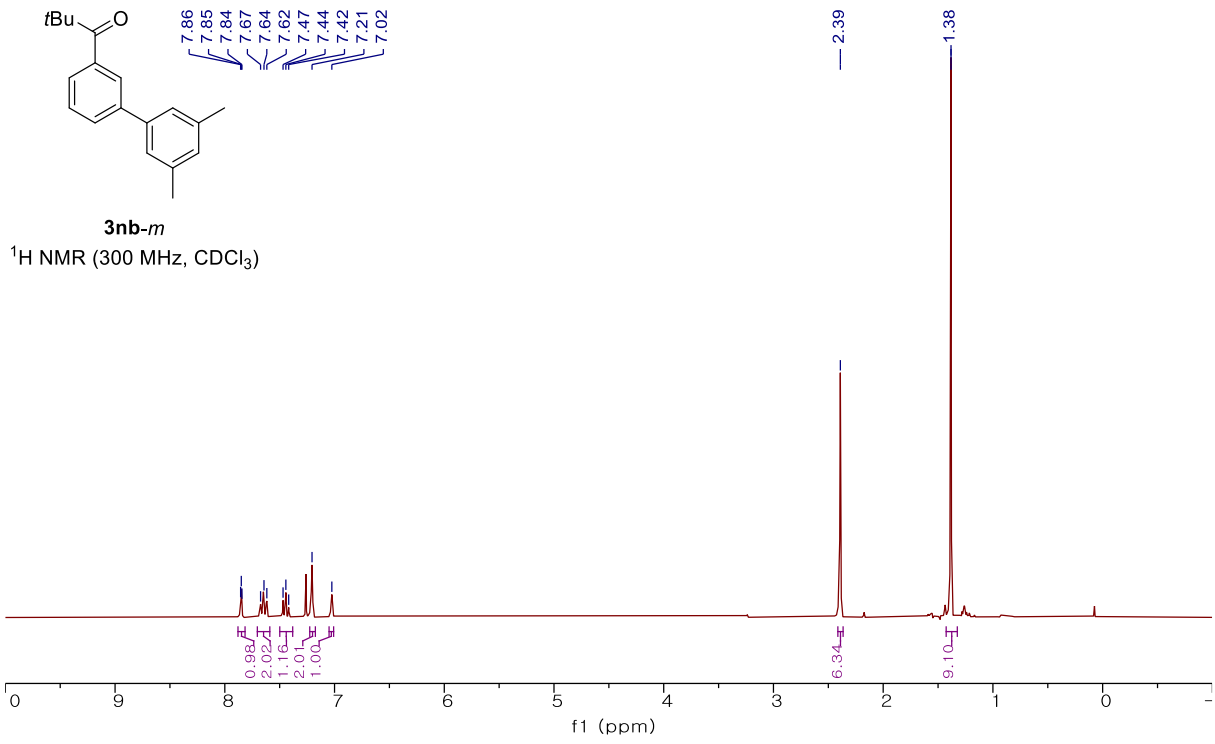
3nb-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



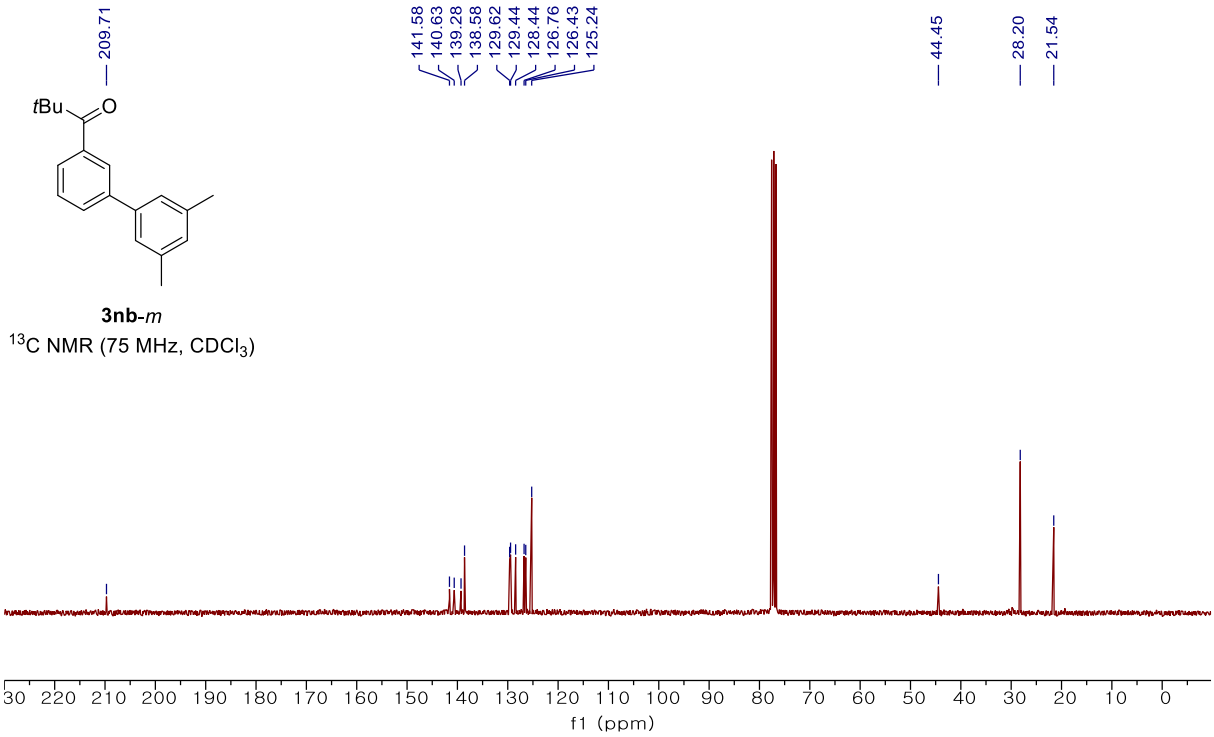
3nb-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



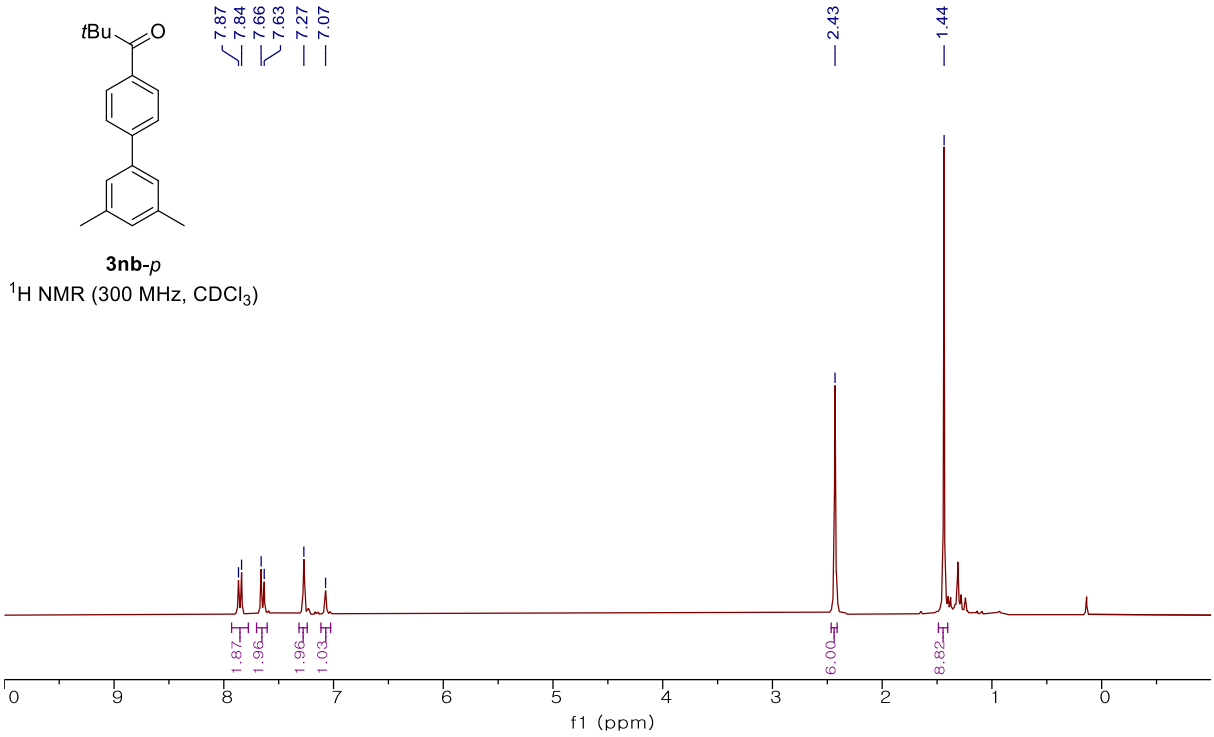
3nb-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



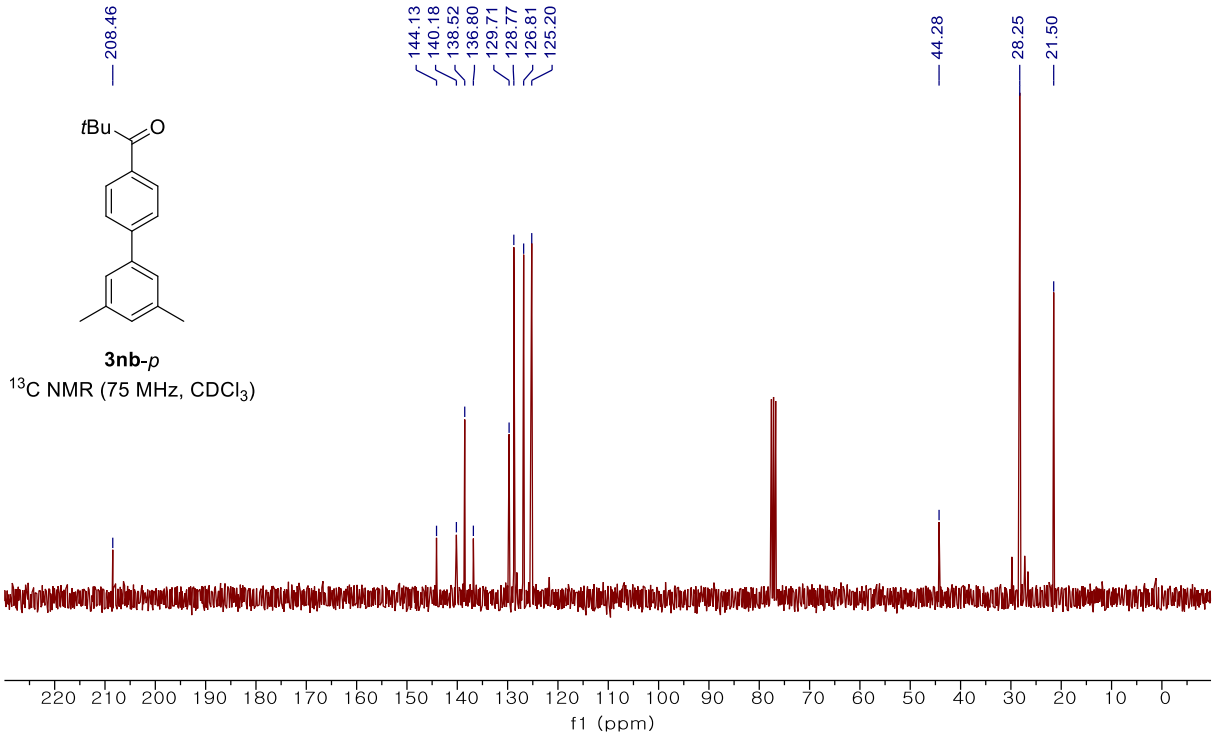
3nb-*m*

^{13}C NMR (75 MHz, $CDCl_3$)



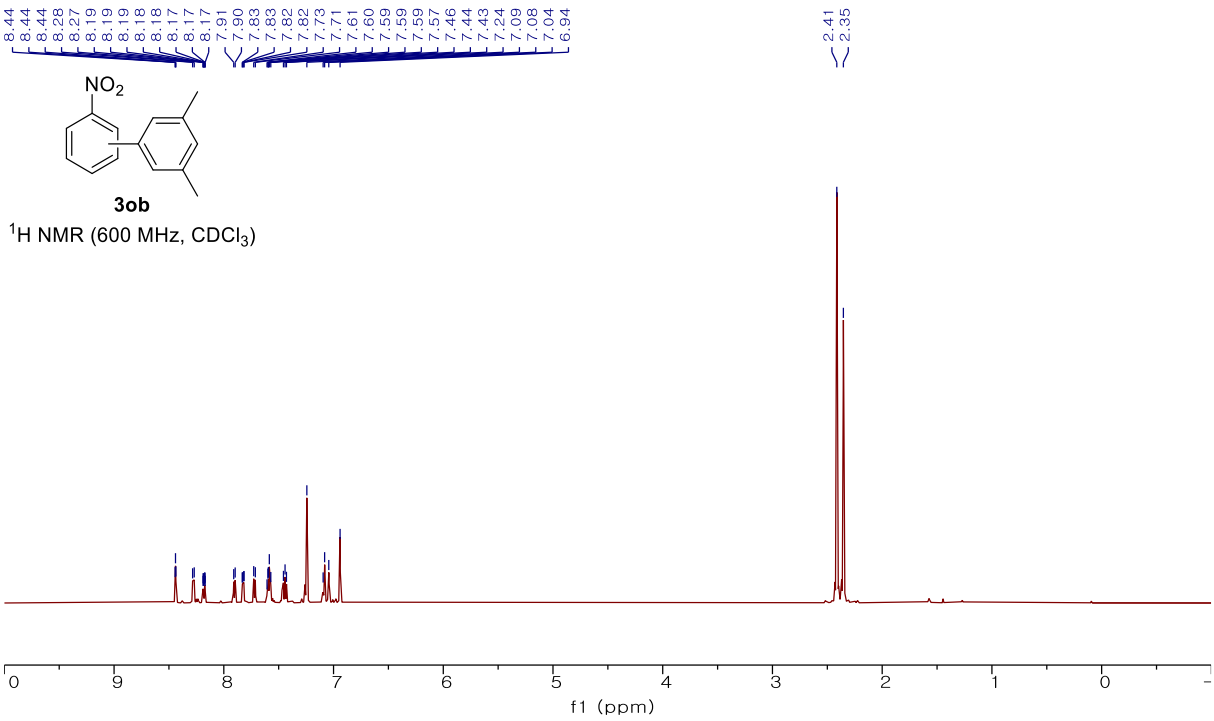
3nb-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



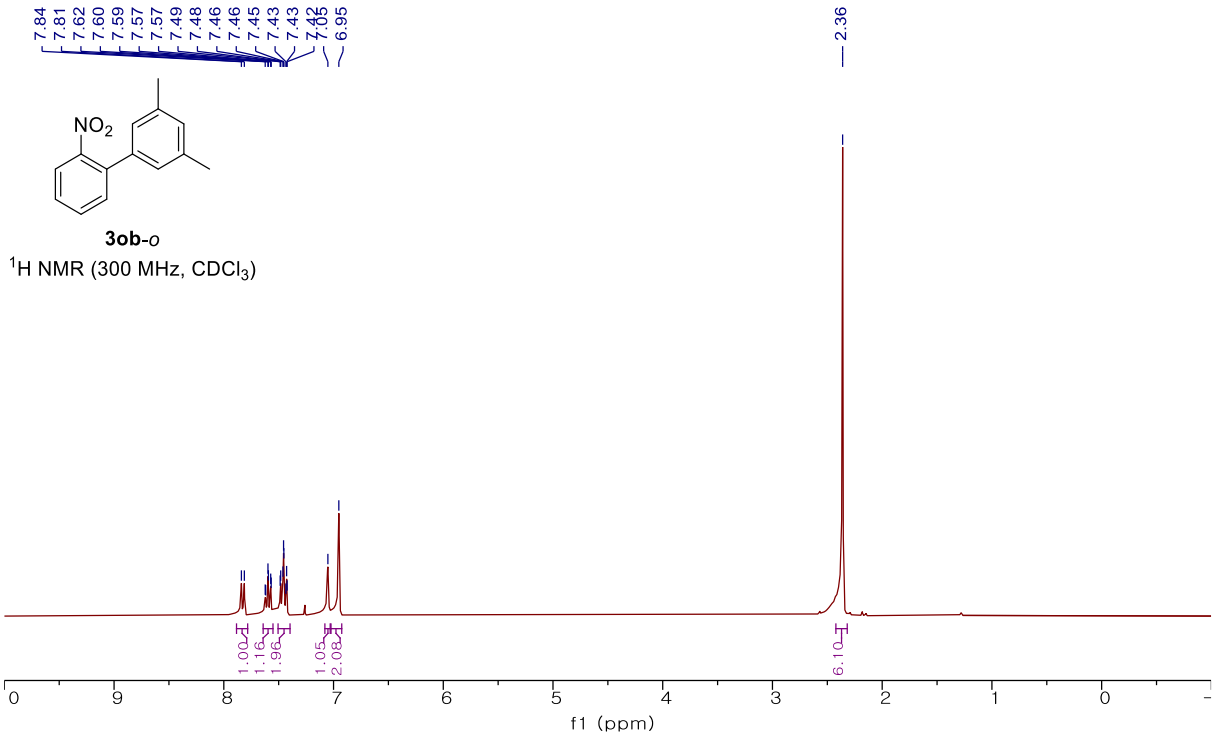
3nb-*p*

^{13}C NMR (75 MHz, $CDCl_3$)



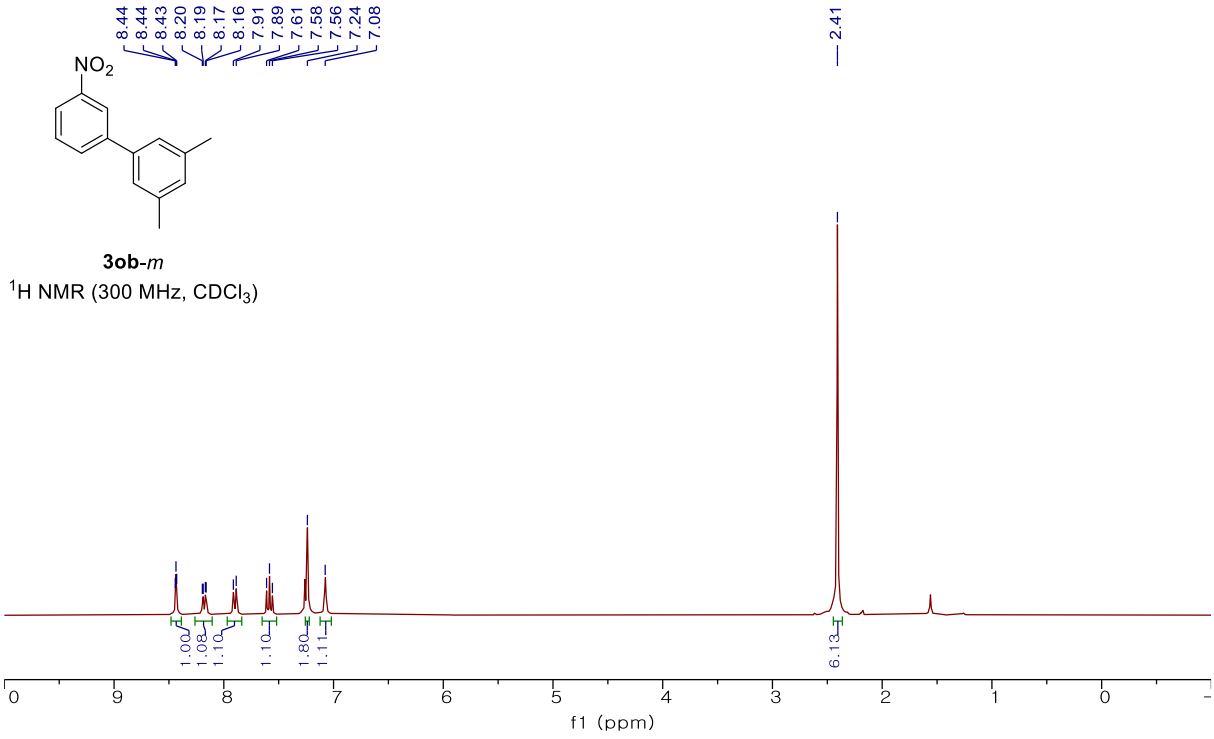
3ob

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



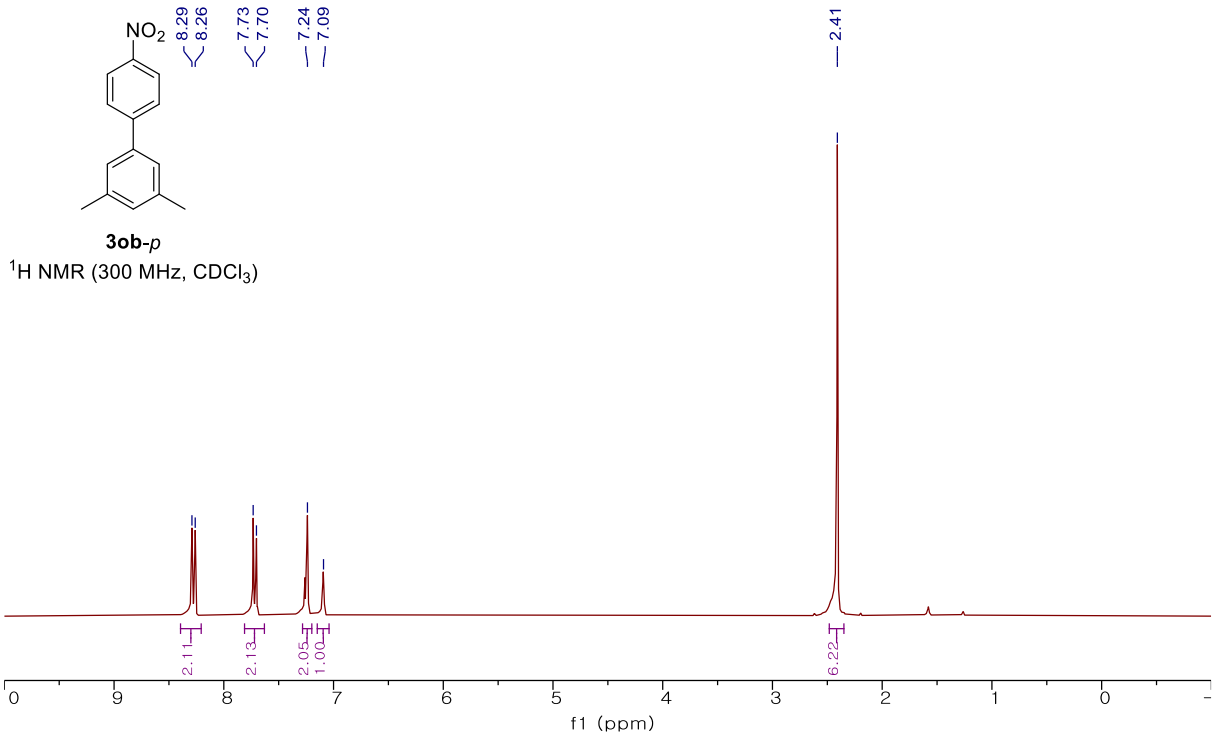
3ob-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



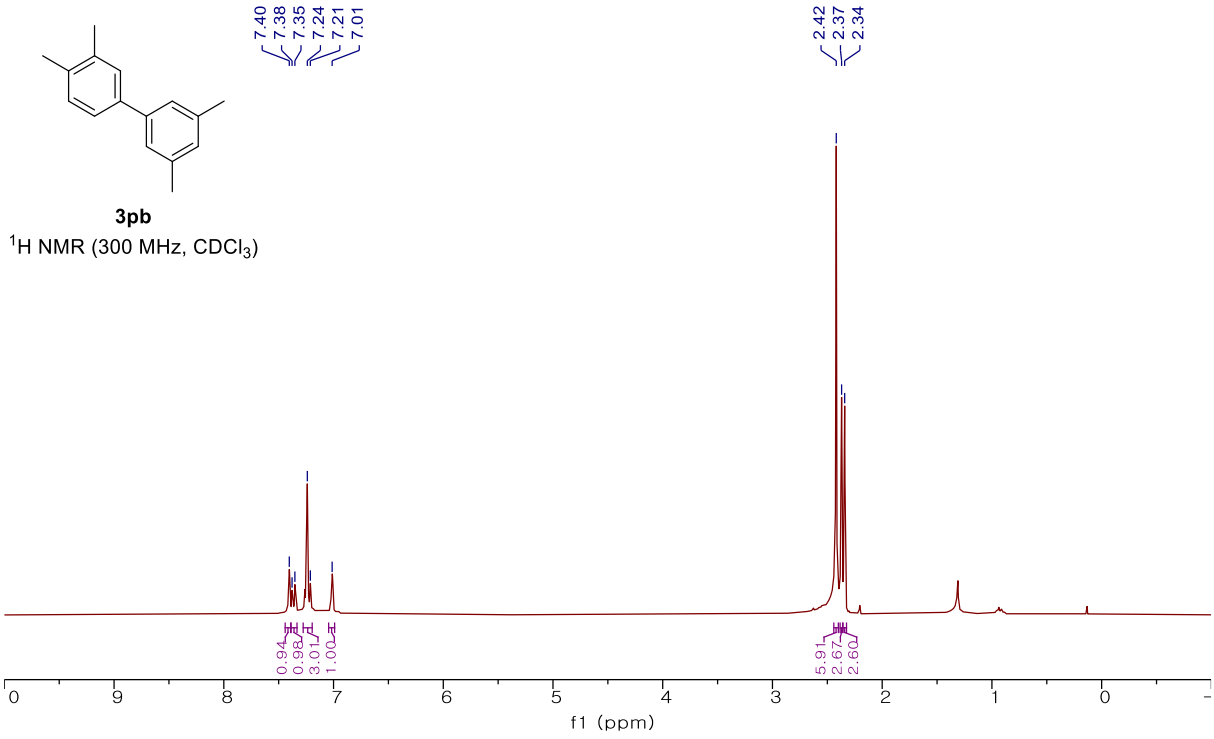
3ob-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



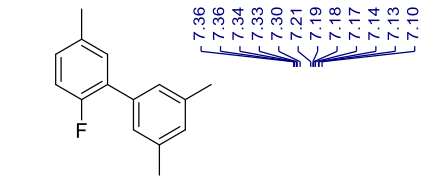
3ob-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



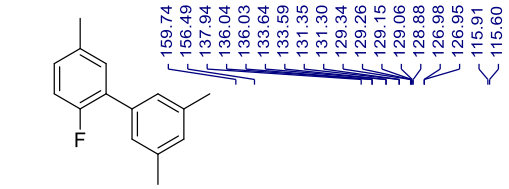
3pb

^{1}H NMR (300 MHz, $CDCl_3$)



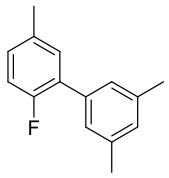
3qb

^{1}H NMR (300 MHz, $CDCl_3$)



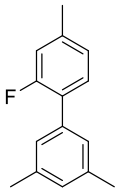
3qb

^{13}C NMR (75 MHz, $CDCl_3$)



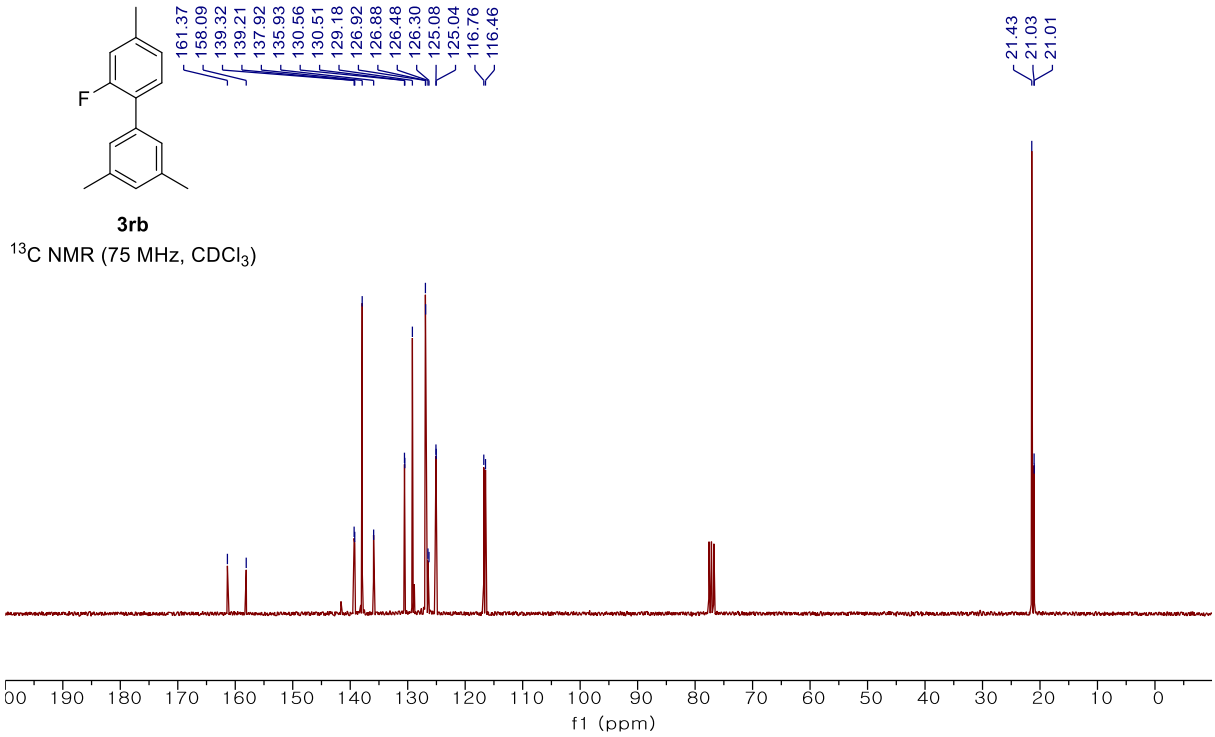
3qb

^{19}F NMR (376 MHz, $CDCl_3$)



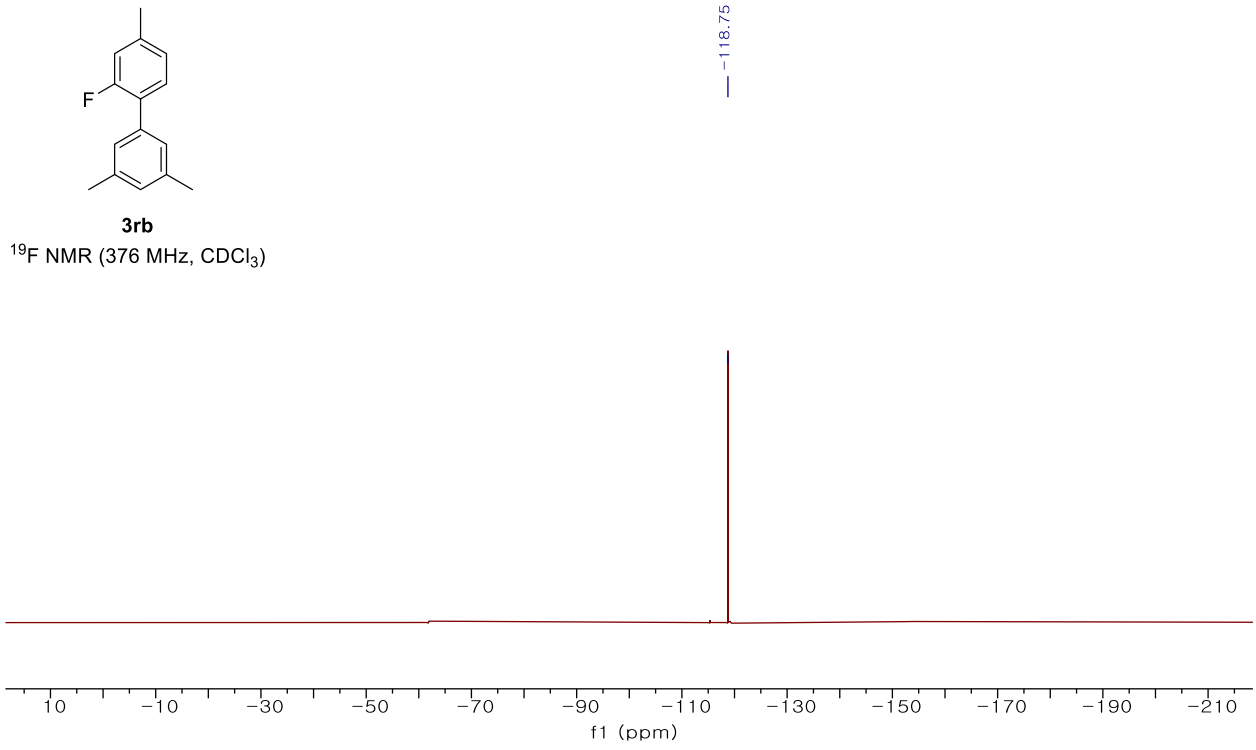
3rb

^{1}H NMR (300 MHz, $CDCl_3$)



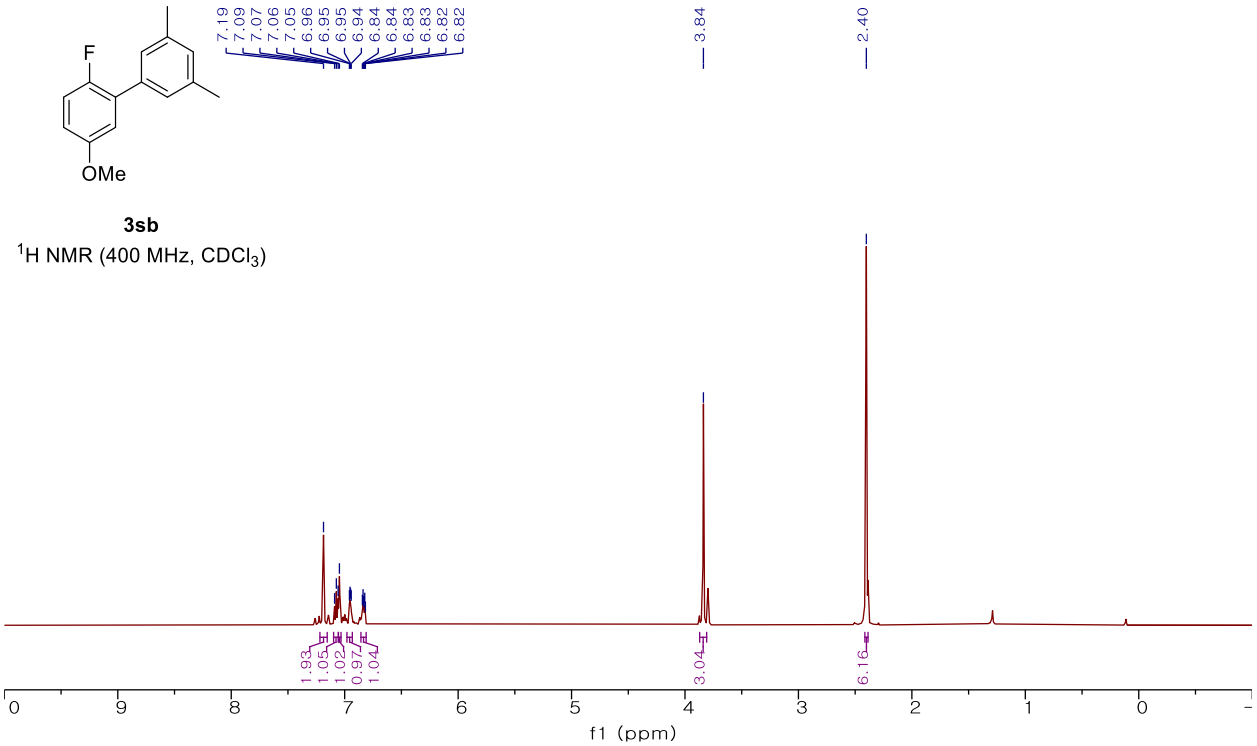
3rb

^{13}C NMR (75 MHz, $CDCl_3$)



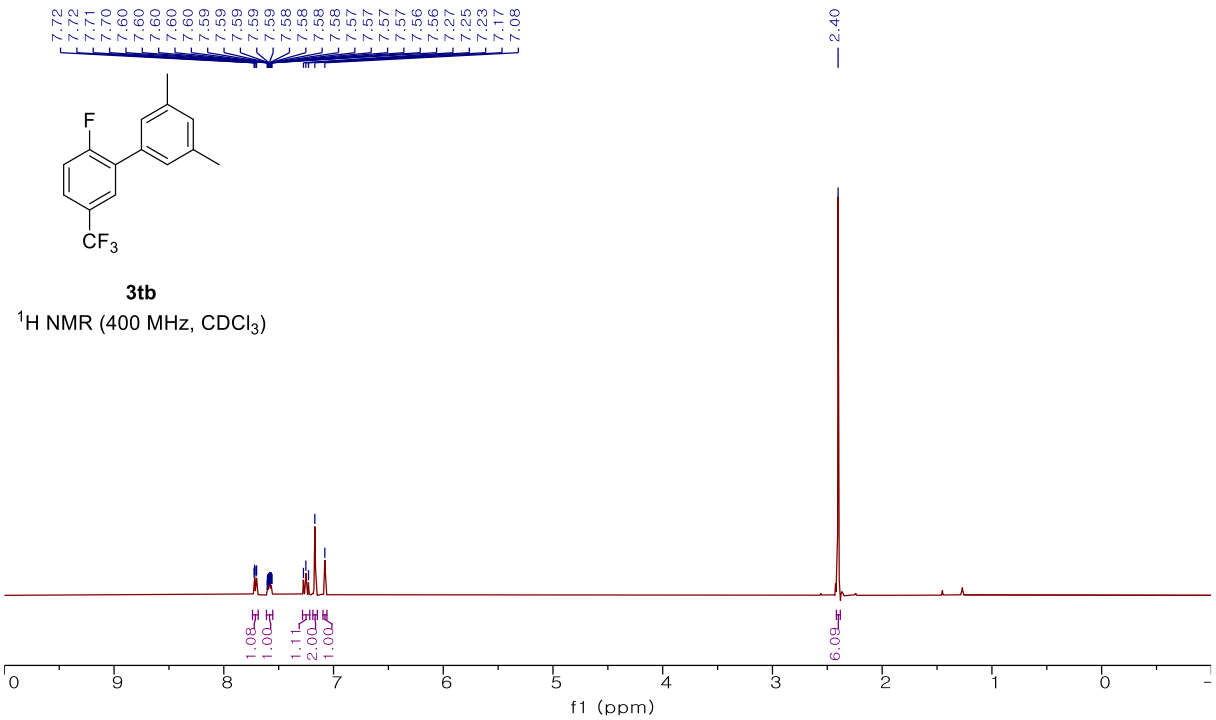
3rb

^{19}F NMR (376 MHz, $CDCl_3$)



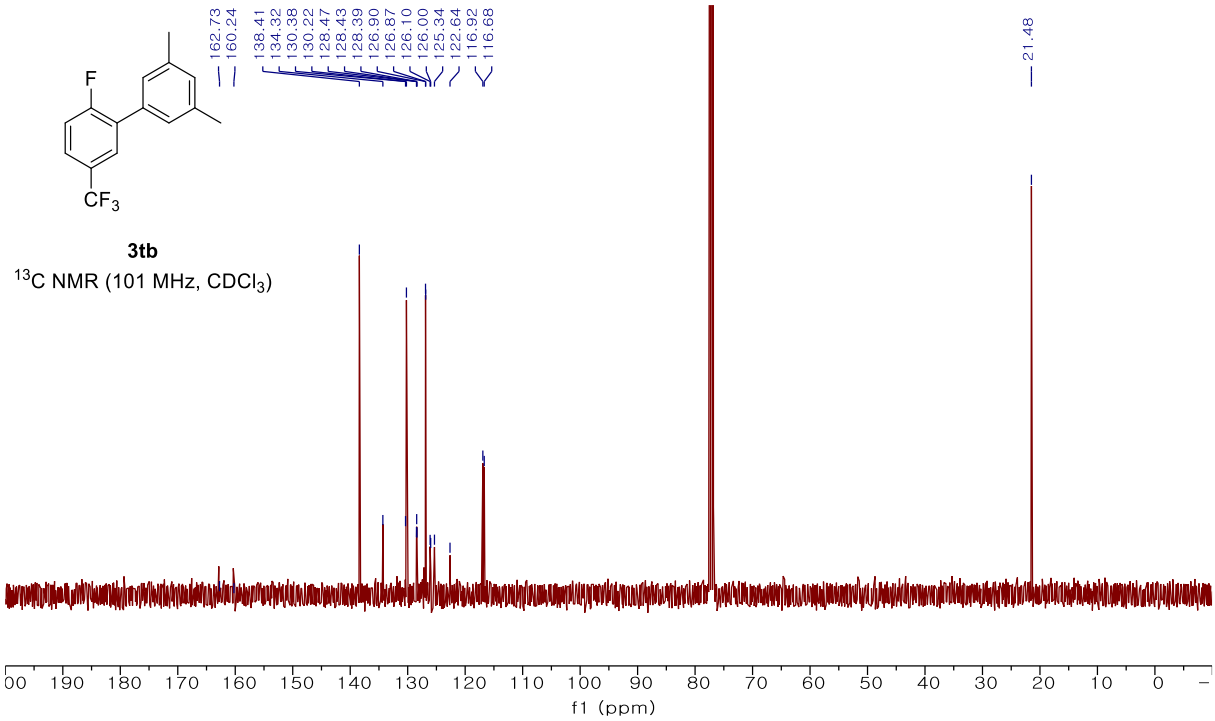
3sb

^{1}H NMR (400 MHz, $CDCl_3$)



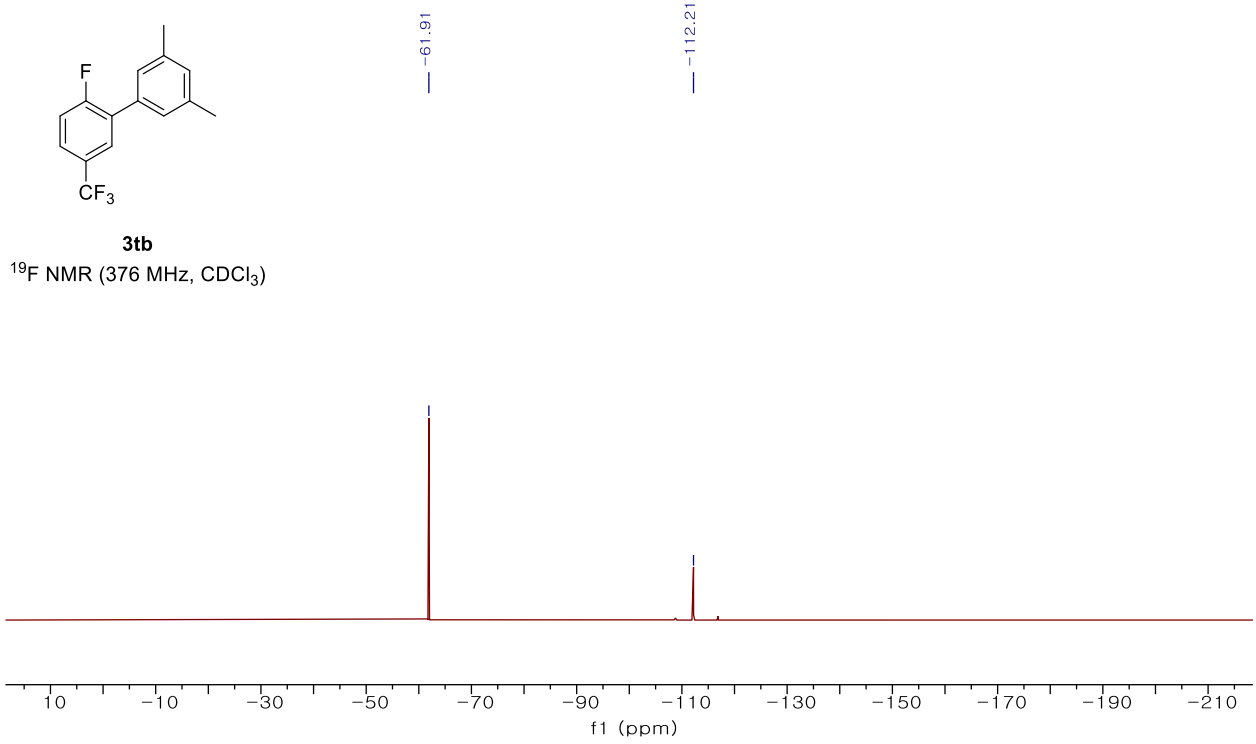
3tb

^{1}H NMR (400 MHz, $CDCl_3$)



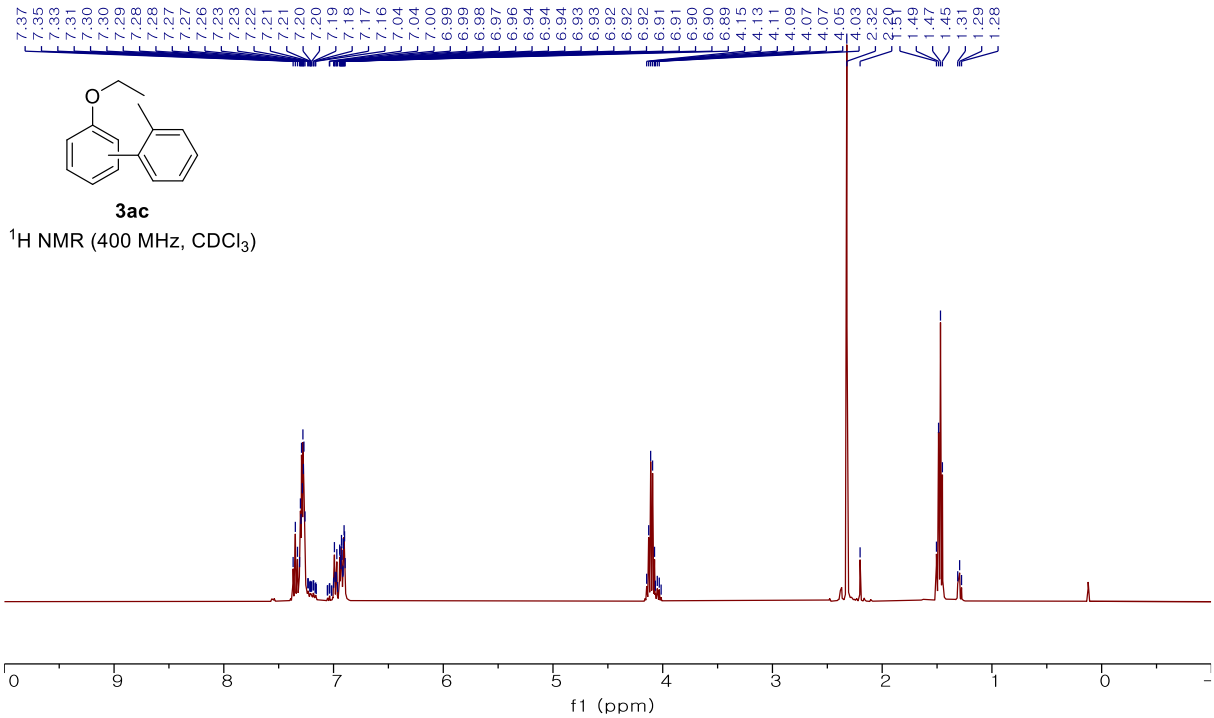
3tb

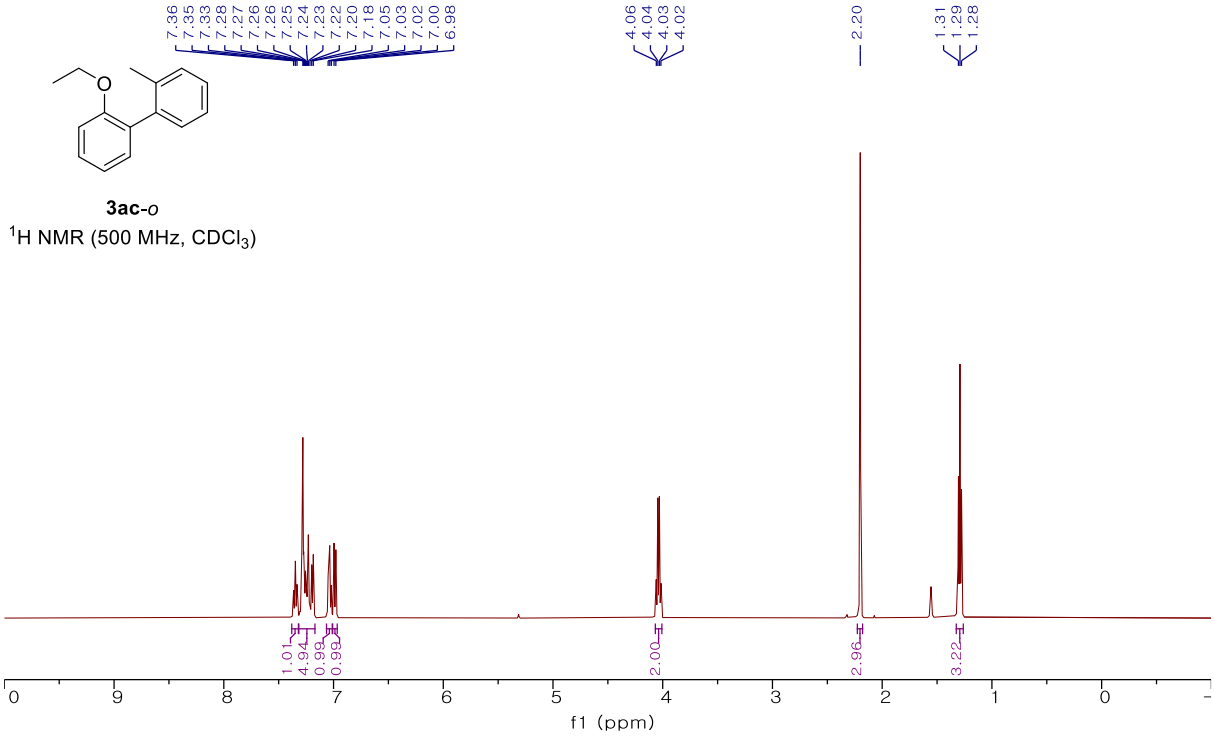
^{13}C NMR (101 MHz, $CDCl_3$)

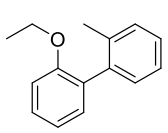


3tb

^{19}F NMR (376 MHz, $CDCl_3$)

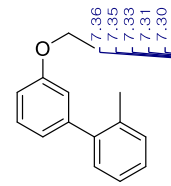

7.37 7.35 7.33 7.31 7.30 7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.23 7.23 7.22 7.21 7.21 7.20 7.20 7.19 7.18 7.17 7.16 7.04 7.04 7.00 6.99 6.99 6.98 6.97 6.96 6.94 6.94 6.94 6.93 6.93 6.92 6.92 6.92 6.91 6.91 6.90 6.90 6.89 4.15 4.13 4.11 4.09 4.07 4.07 4.05 4.03 2.32 2.20 1.51 1.49 1.47 1.45 1.31 1.29 1.28
O
3ac
1H NMR (400 MHz, CDCl3)
0 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


7.36 7.35 7.33 7.28 7.27 7.26 7.26 7.25 7.24 7.23 7.22 7.20 7.18 7.05 7.03 7.02 7.00 6.98
4.06 4.04 4.03 4.02
2.20
1.31 1.29 1.28
O
3ac-o
1H NMR (500 MHz, CDCl3)
1.01 4.94 0.99 0.99 2.00 2.96 3.22
0 9 8 7 6 5 4 3 2 1 0
f1 (ppm)



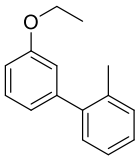
3ac-*o*

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



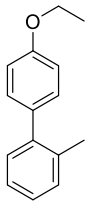
3ac-*m*

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



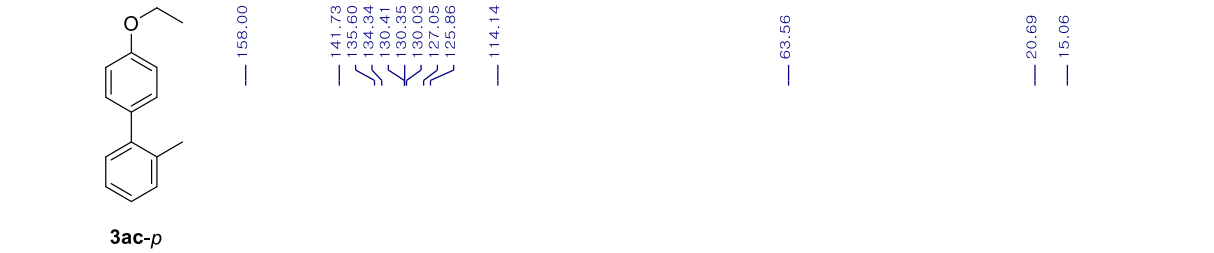
3ac-*m*

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



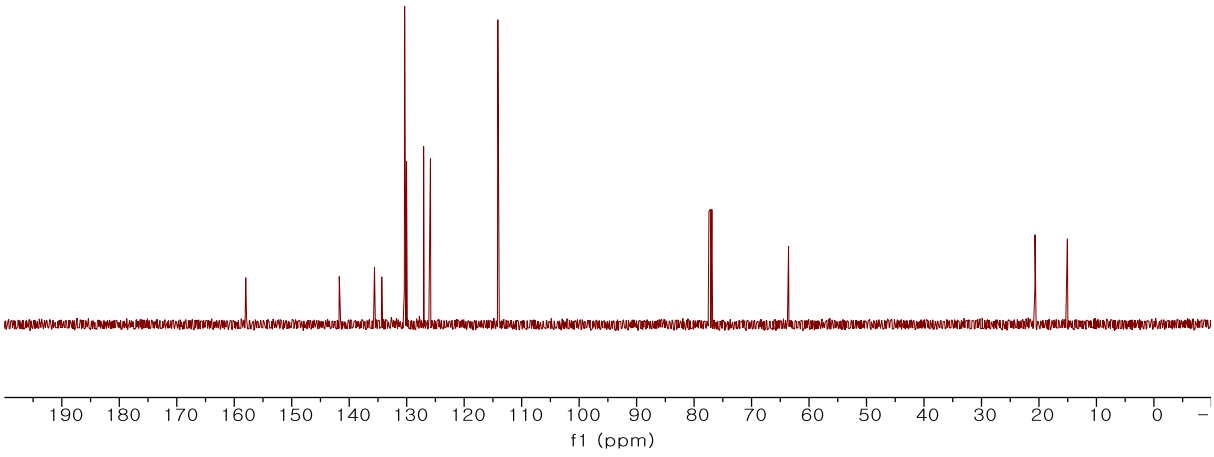
3ac-*p*

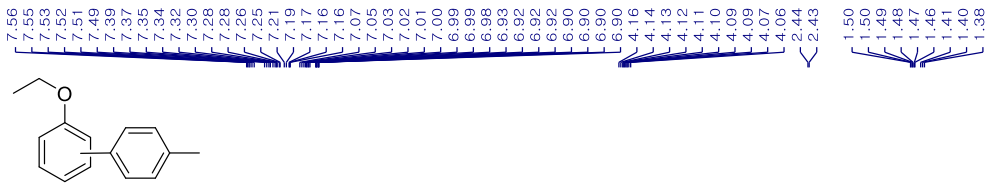
^{1}H NMR (500 MHz, $CDCl_3$)



3ac-*p*

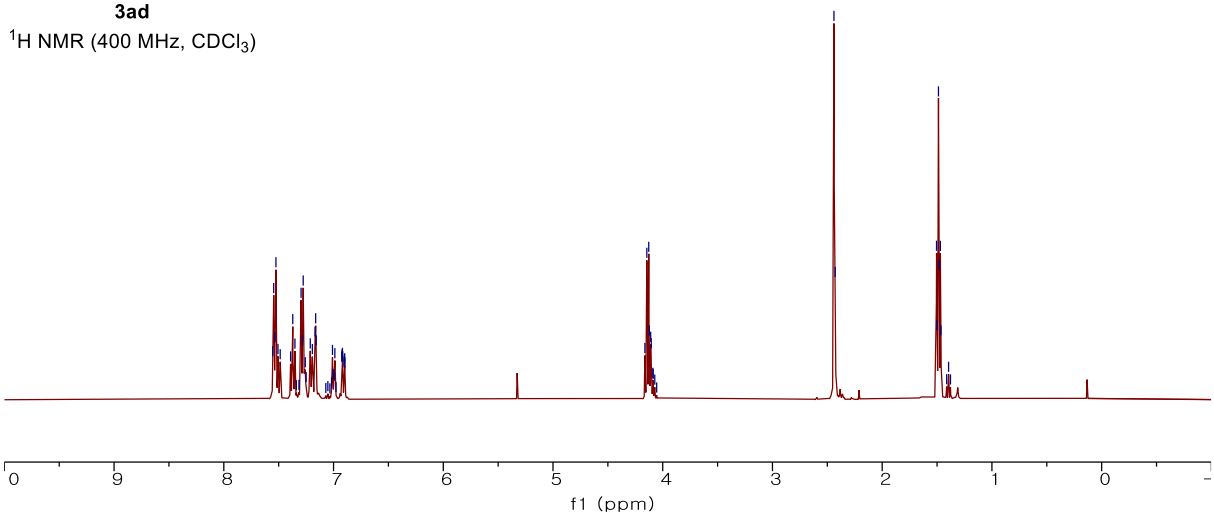
^{13}C NMR (126 MHz, $CDCl_3$)

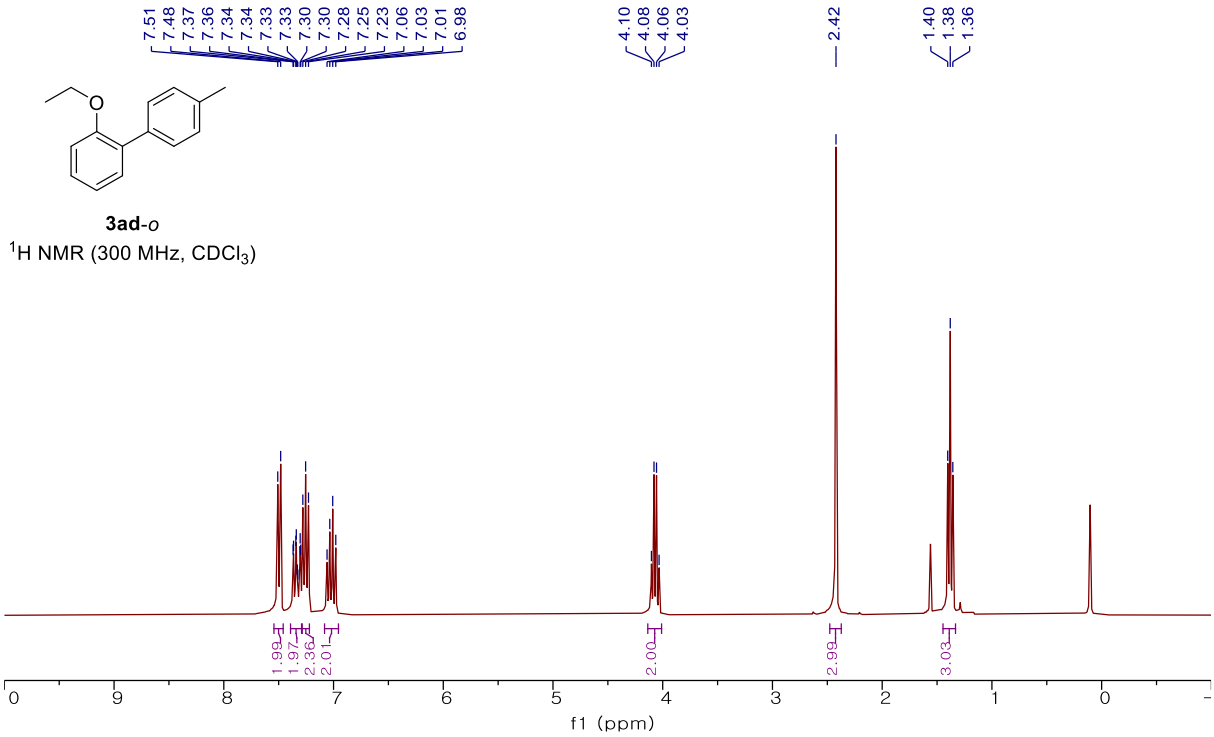




3ad

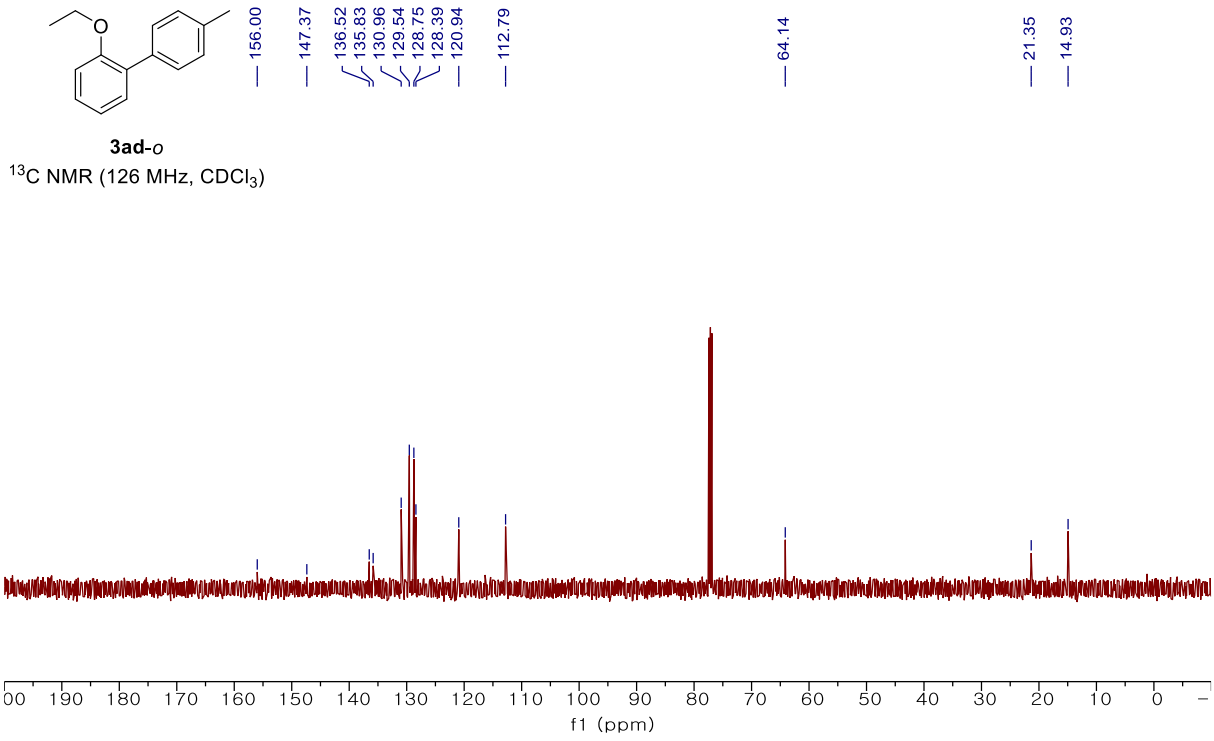
^{1}H NMR (400 MHz, $CDCl_3$)





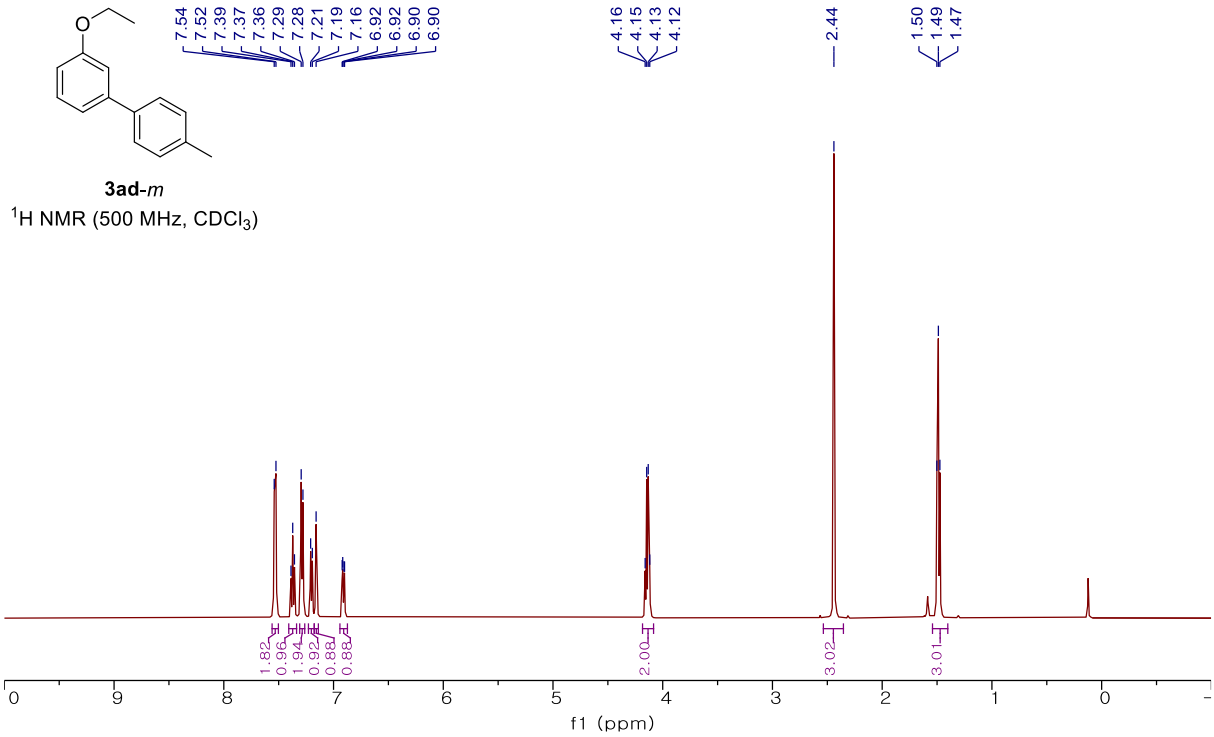
3ad-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



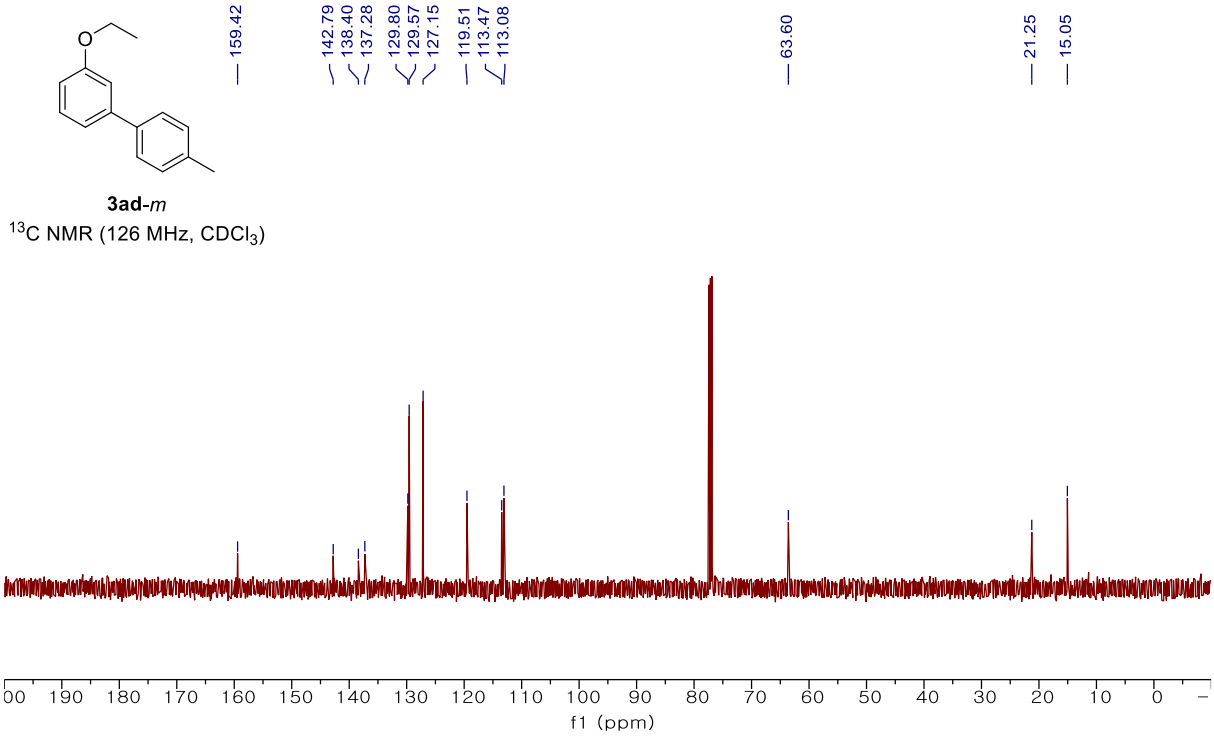
3ad-*o*

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



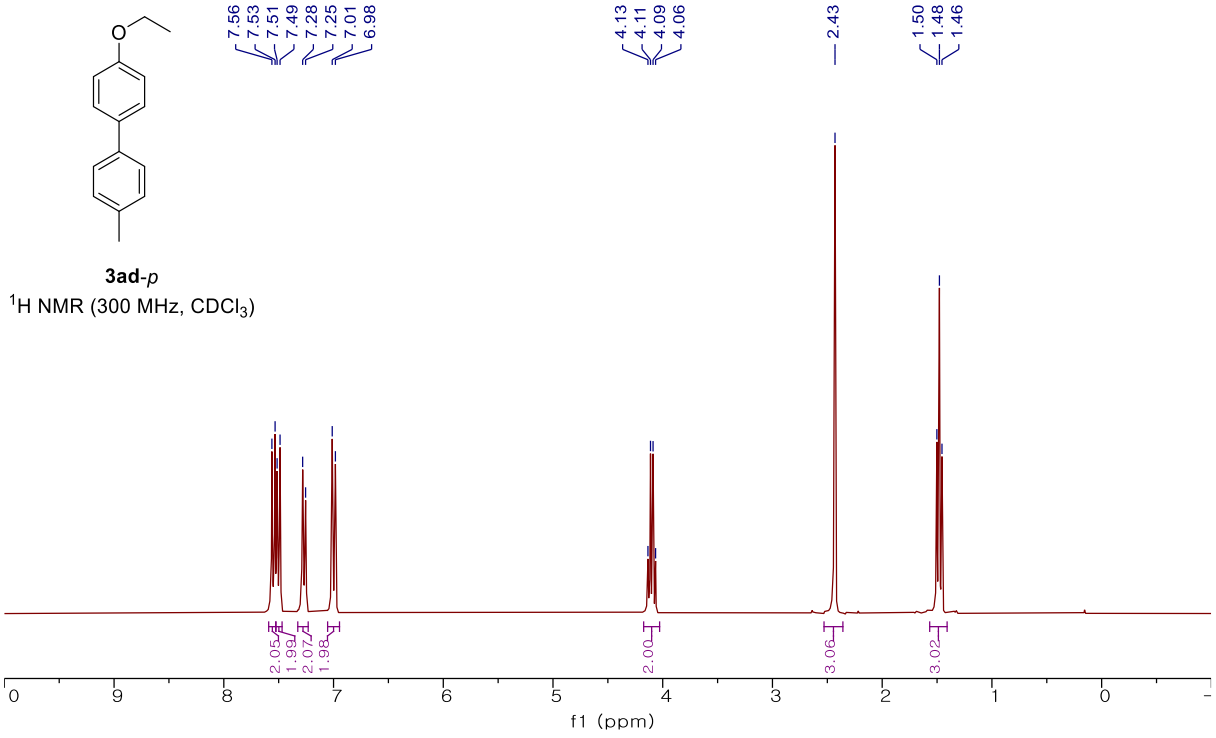
3ad-*m*

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



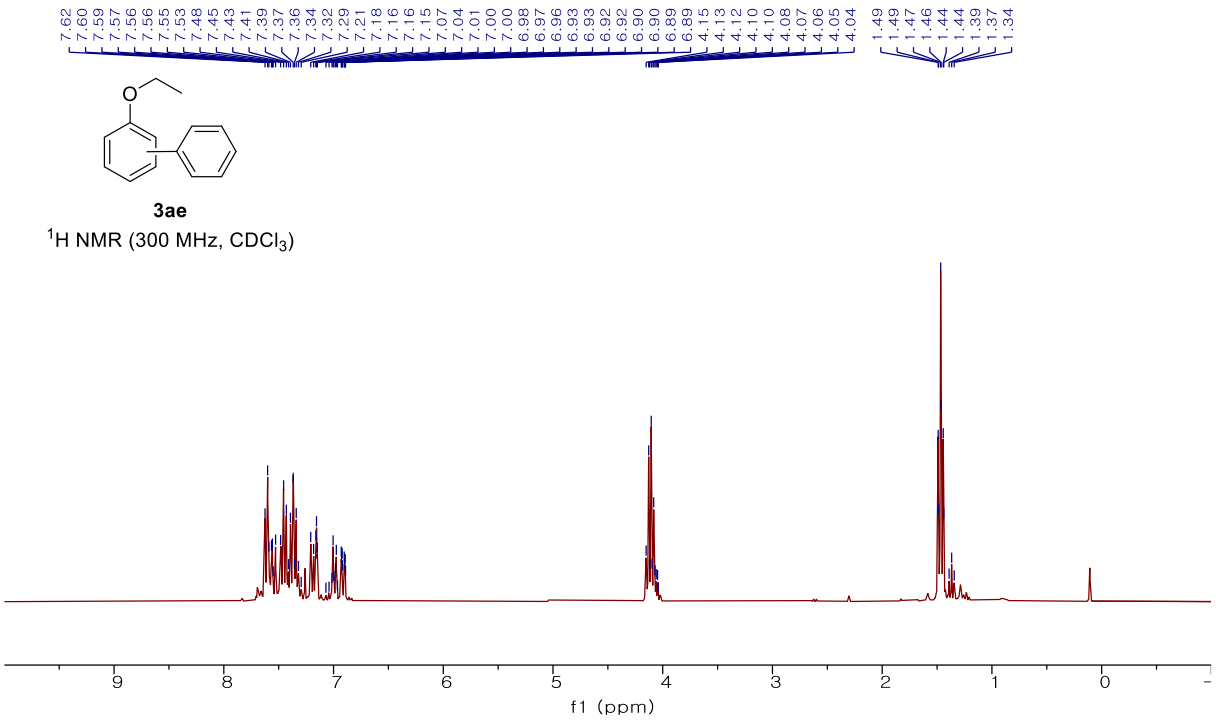
3ad-*m*

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



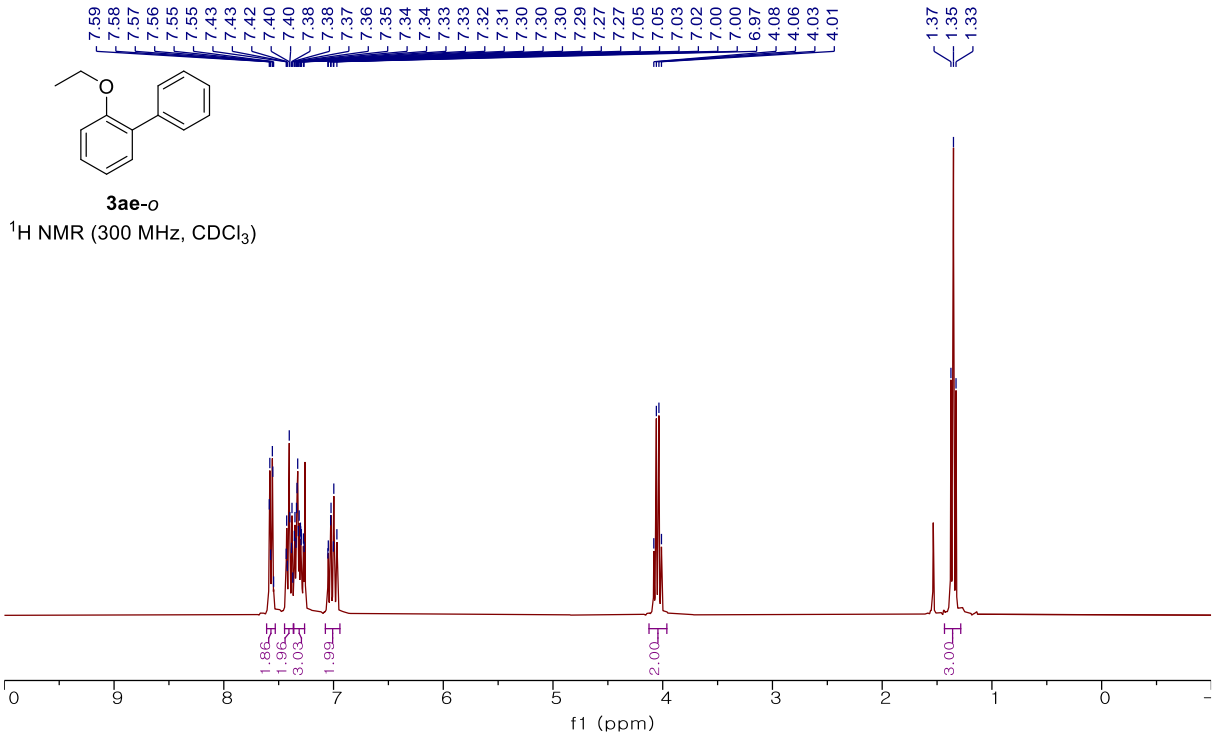
3ad-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



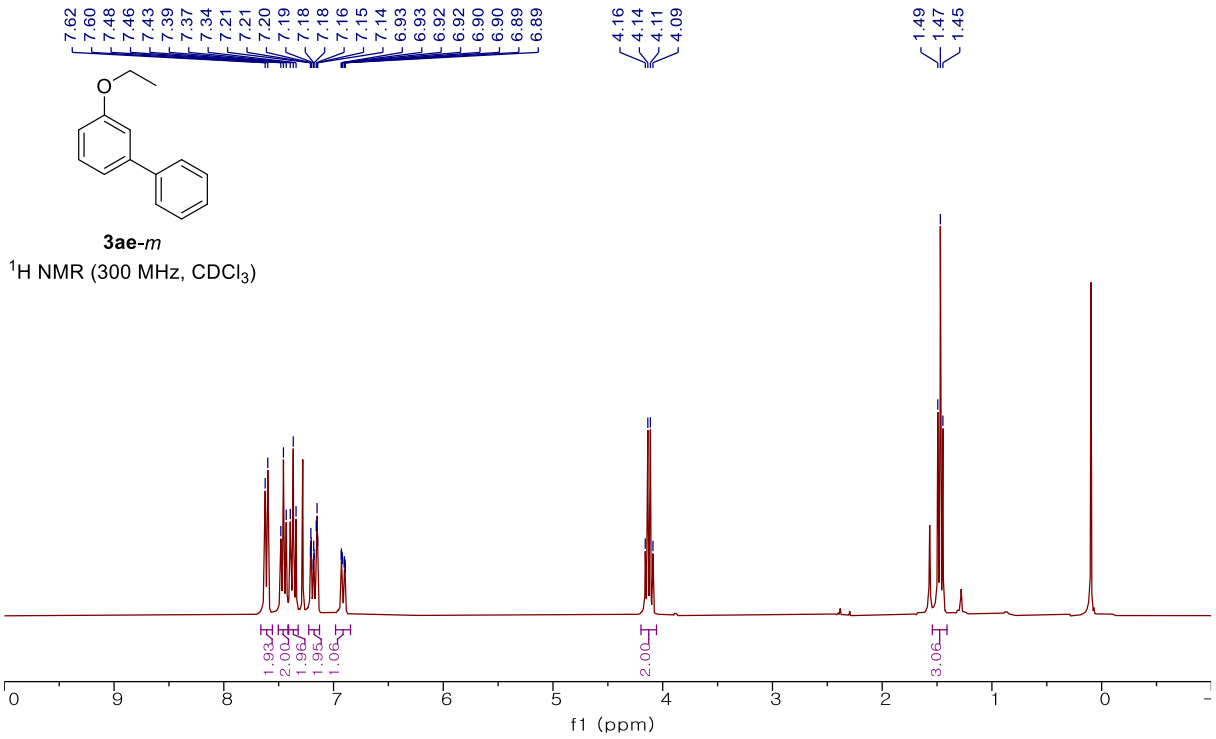
3ae

^{1}H NMR (300 MHz, $CDCl_3$)



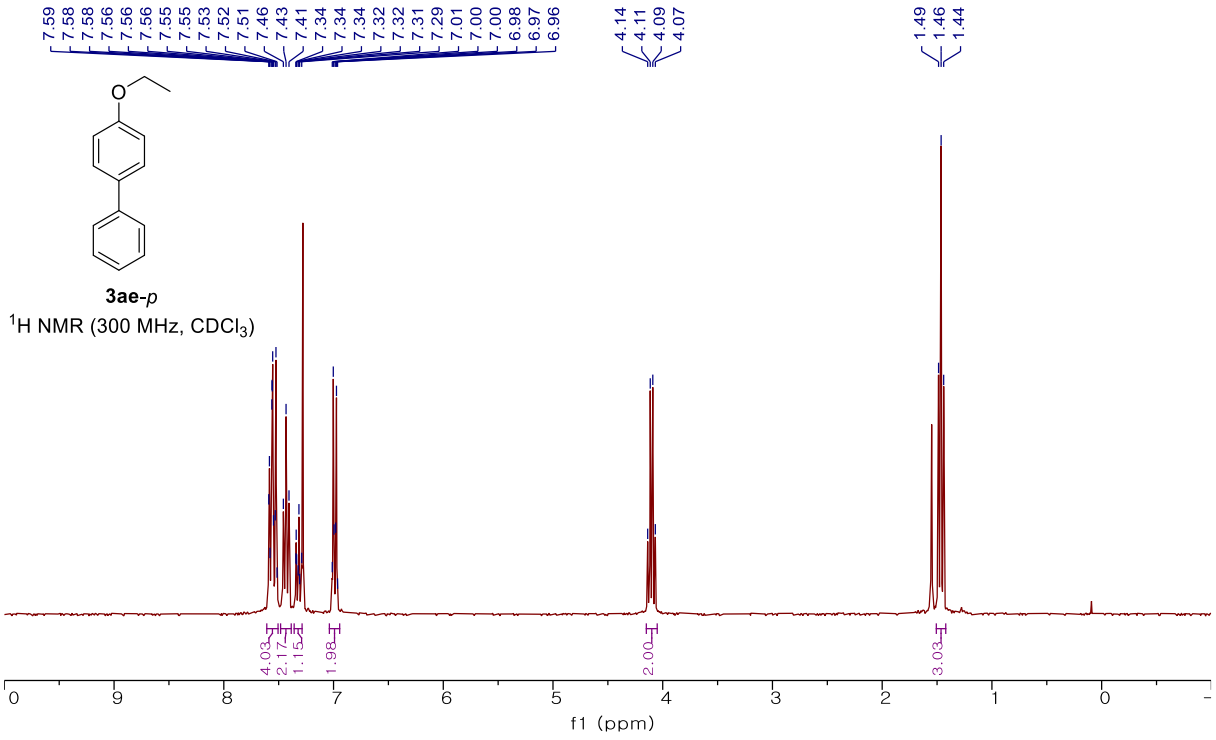
3ae-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



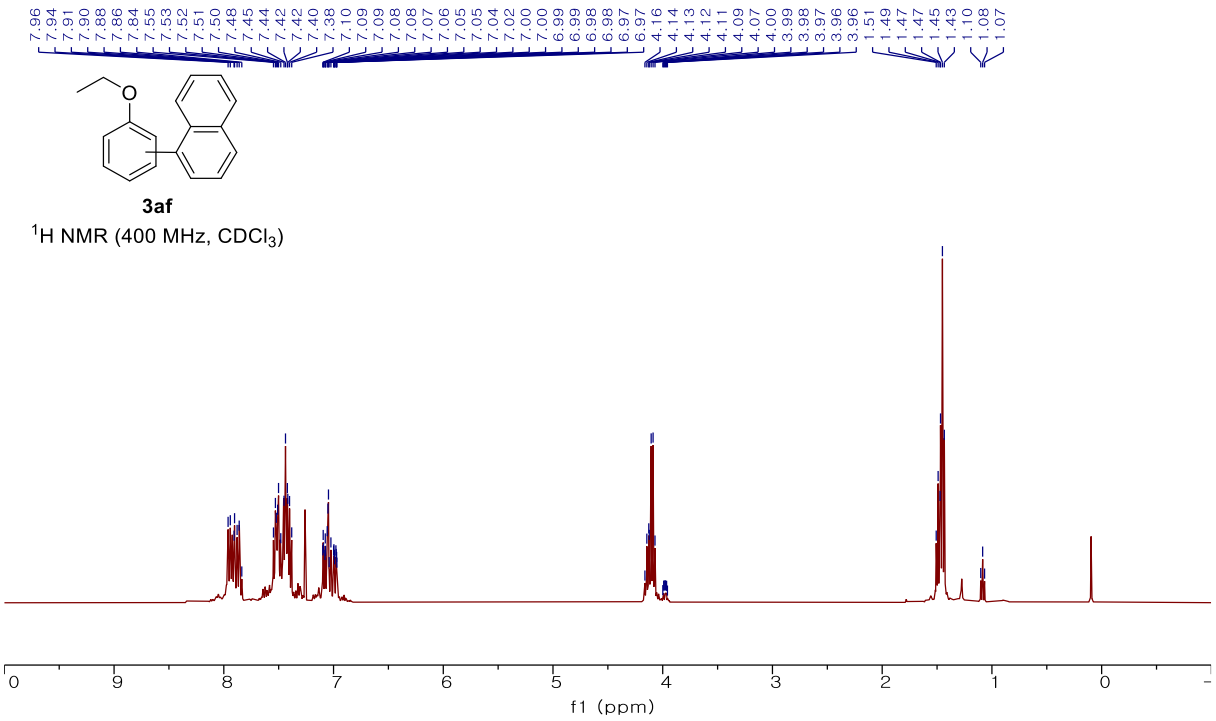
3ae-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



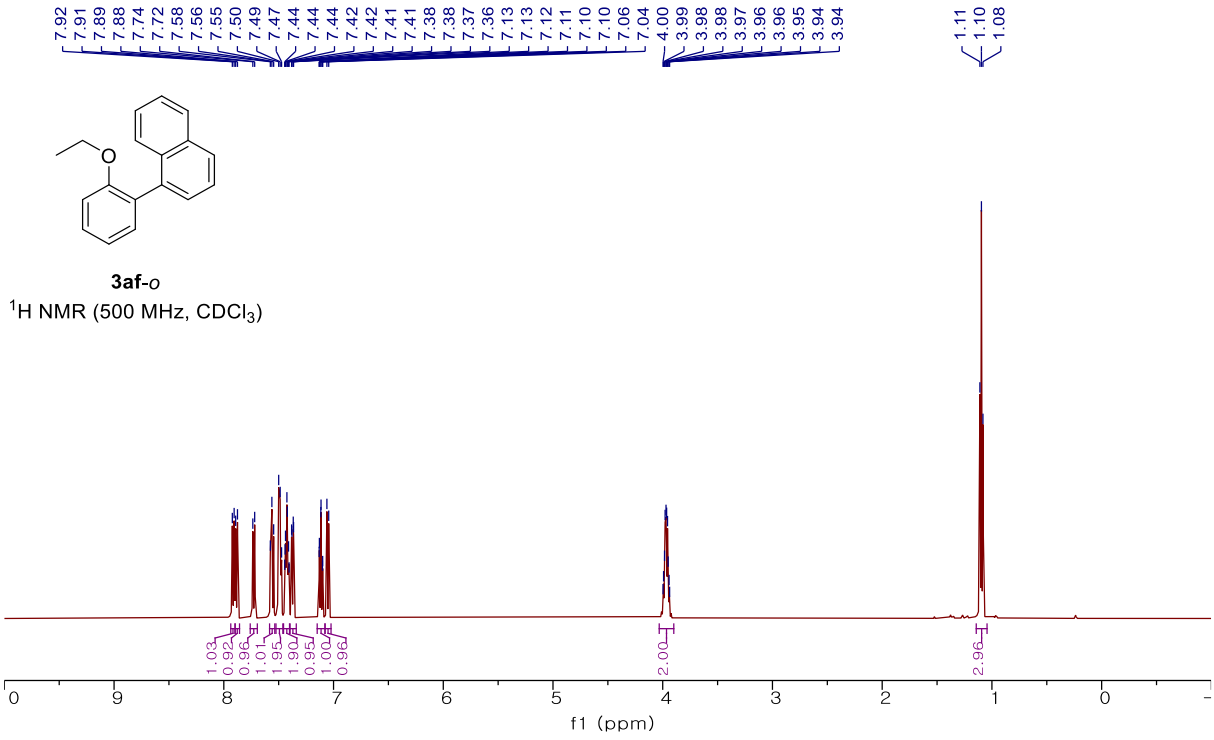
3ae-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



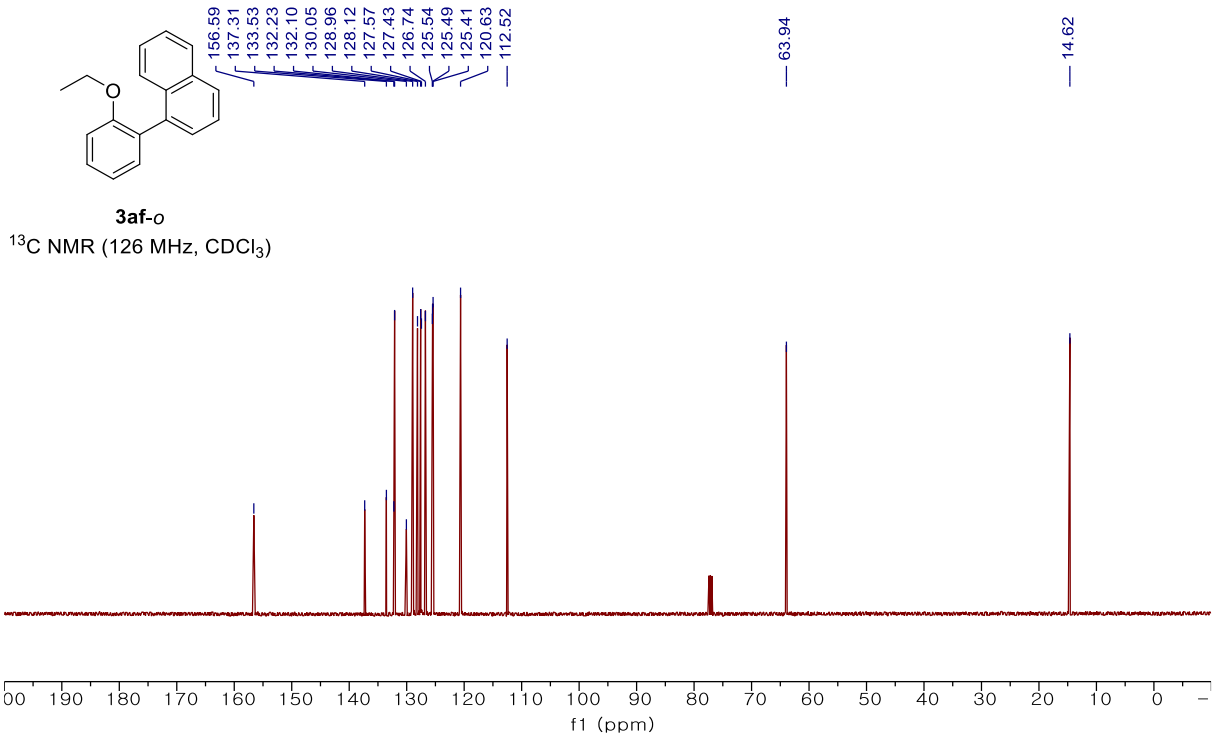
3af

^{1}H NMR (400 MHz, $CDCl_3$)



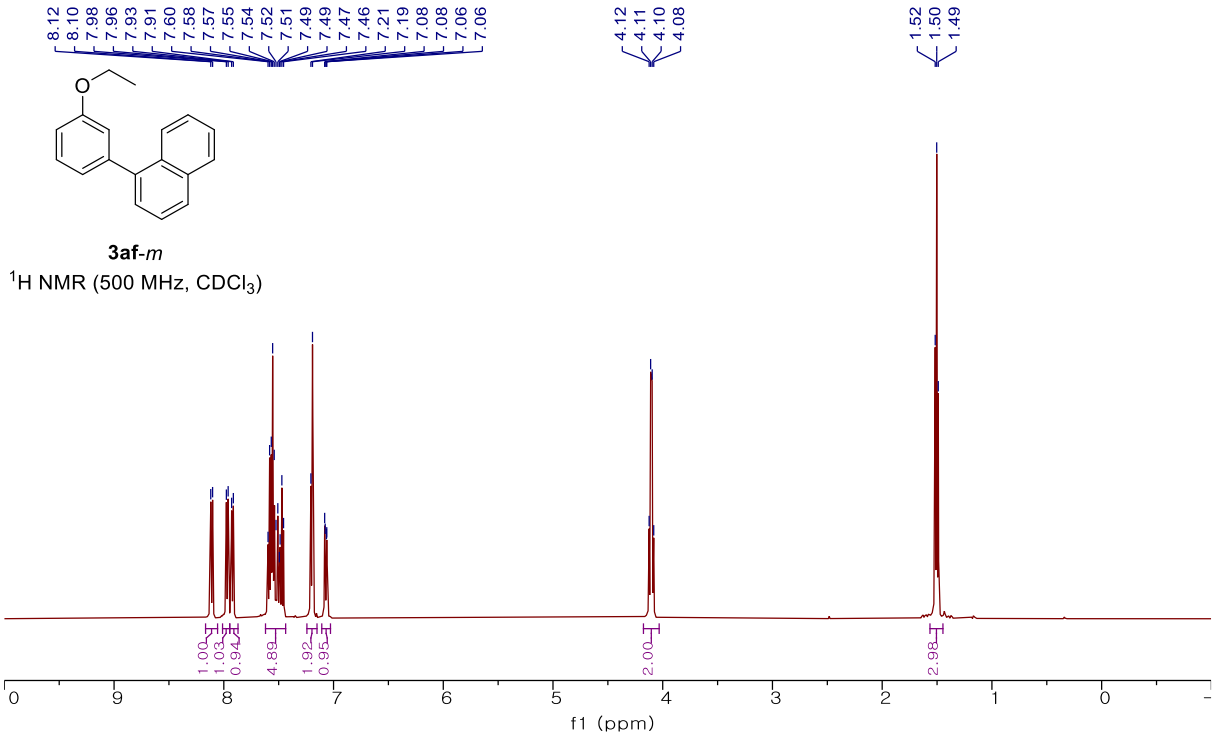
3af-*o*

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



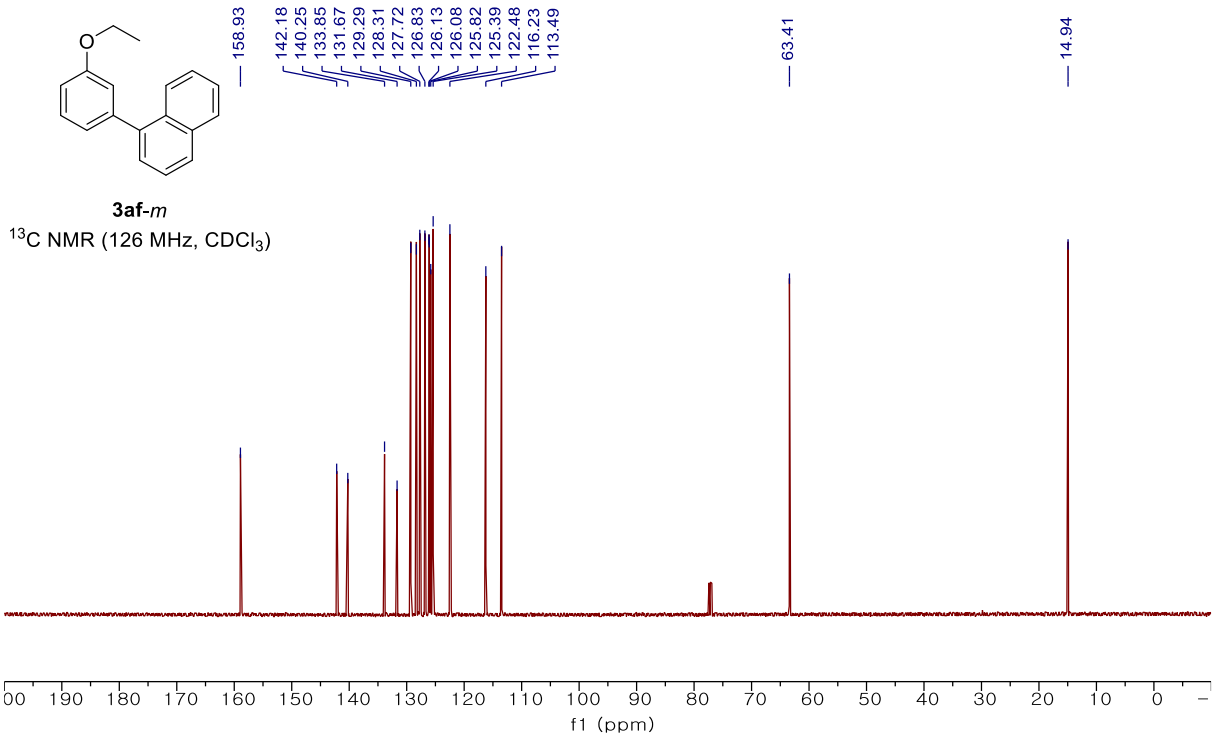
3af-*o*

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



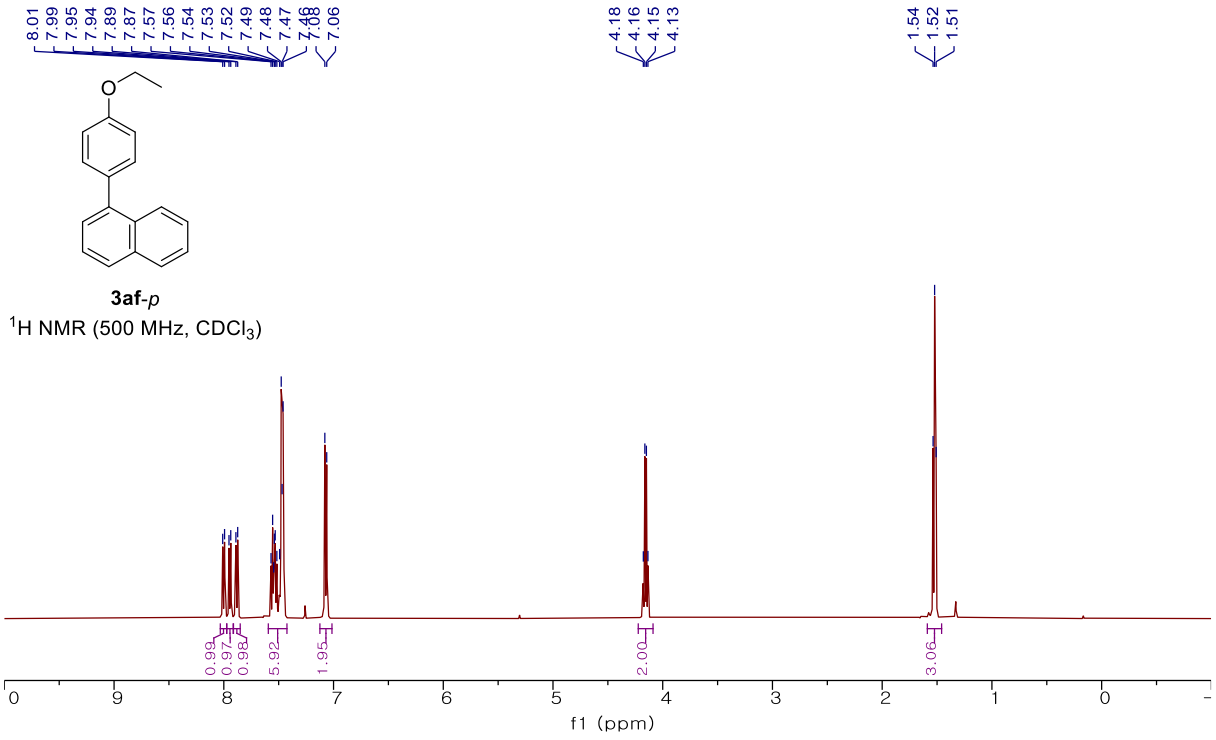
3af-*m*

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



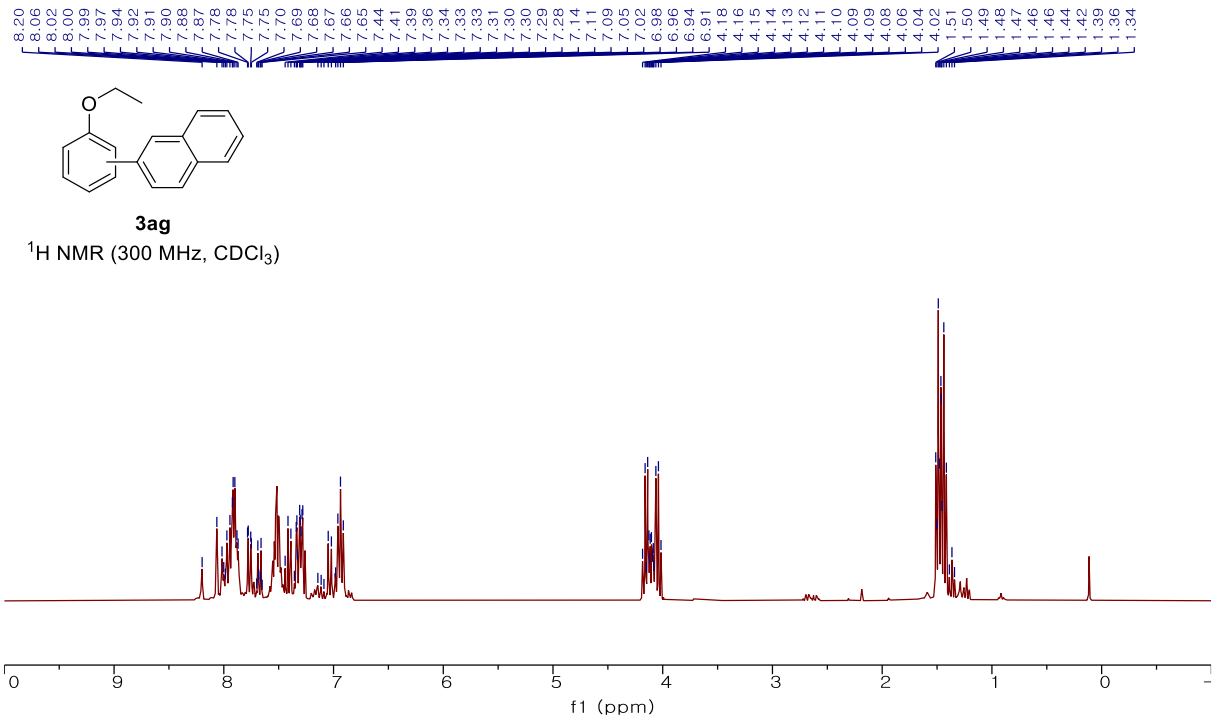
3af-*m*

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



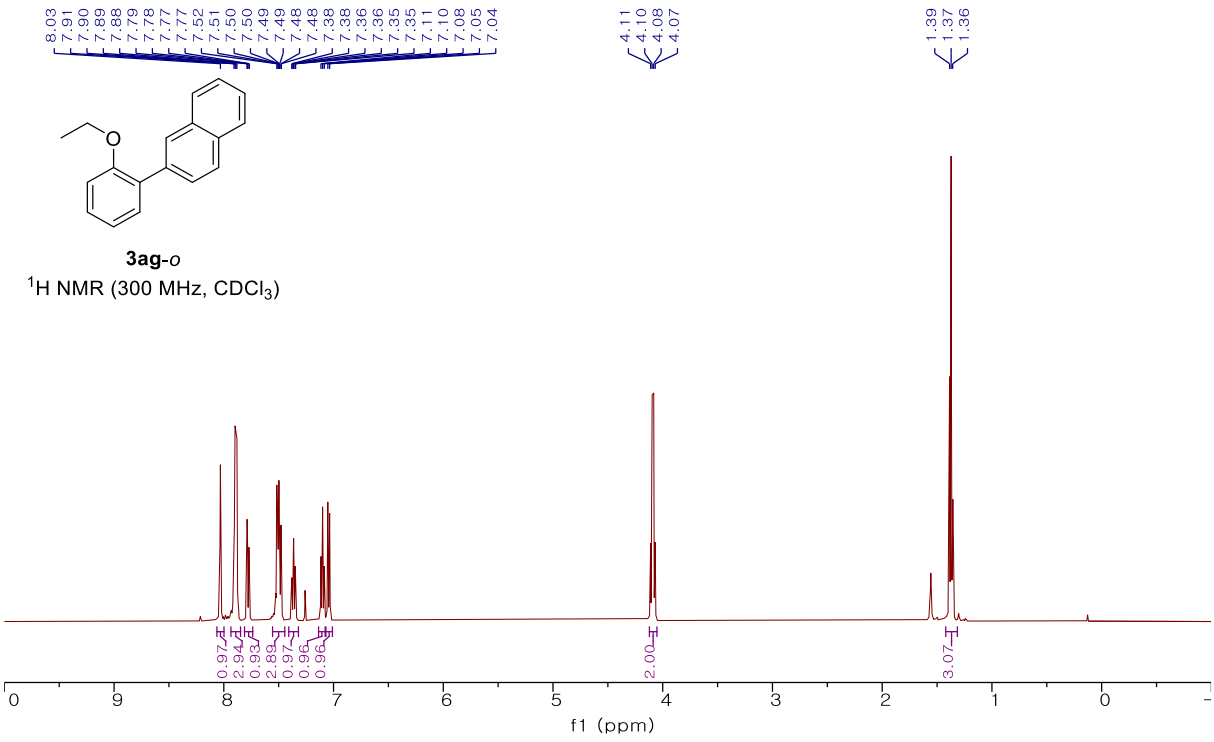
3af-*p*

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



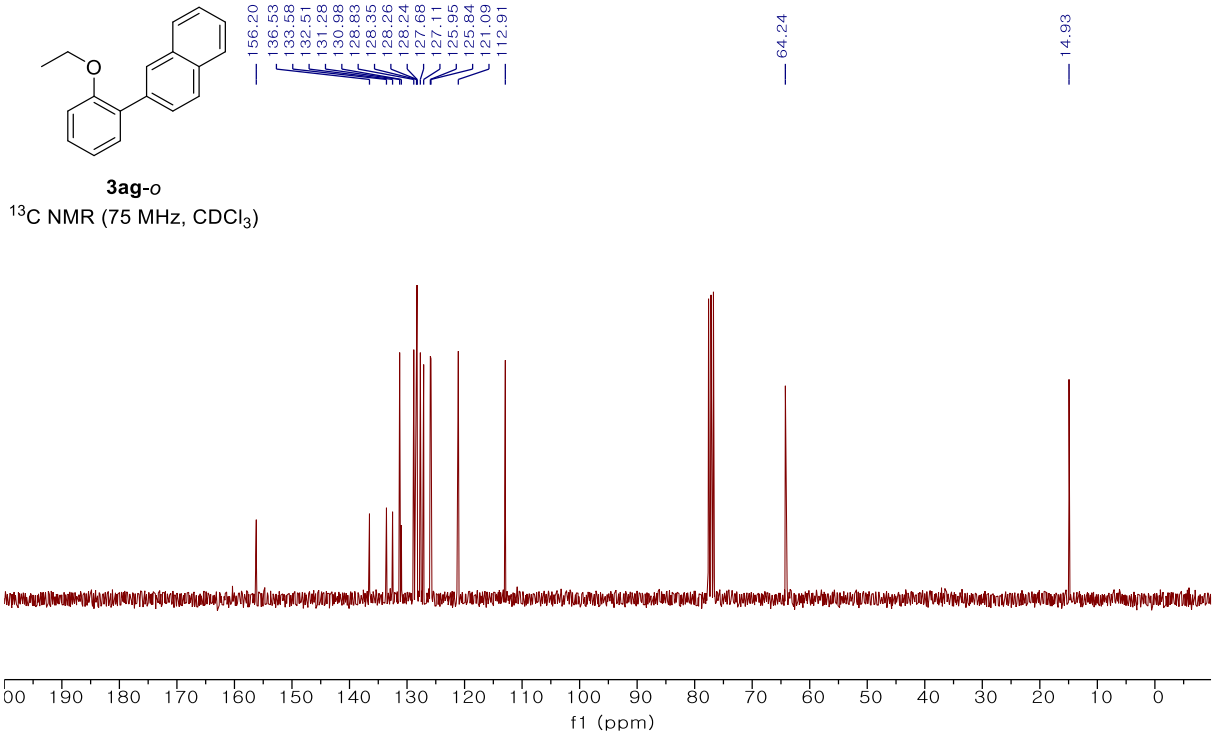
3ag

^{1}H NMR (300 MHz, $CDCl_3$)



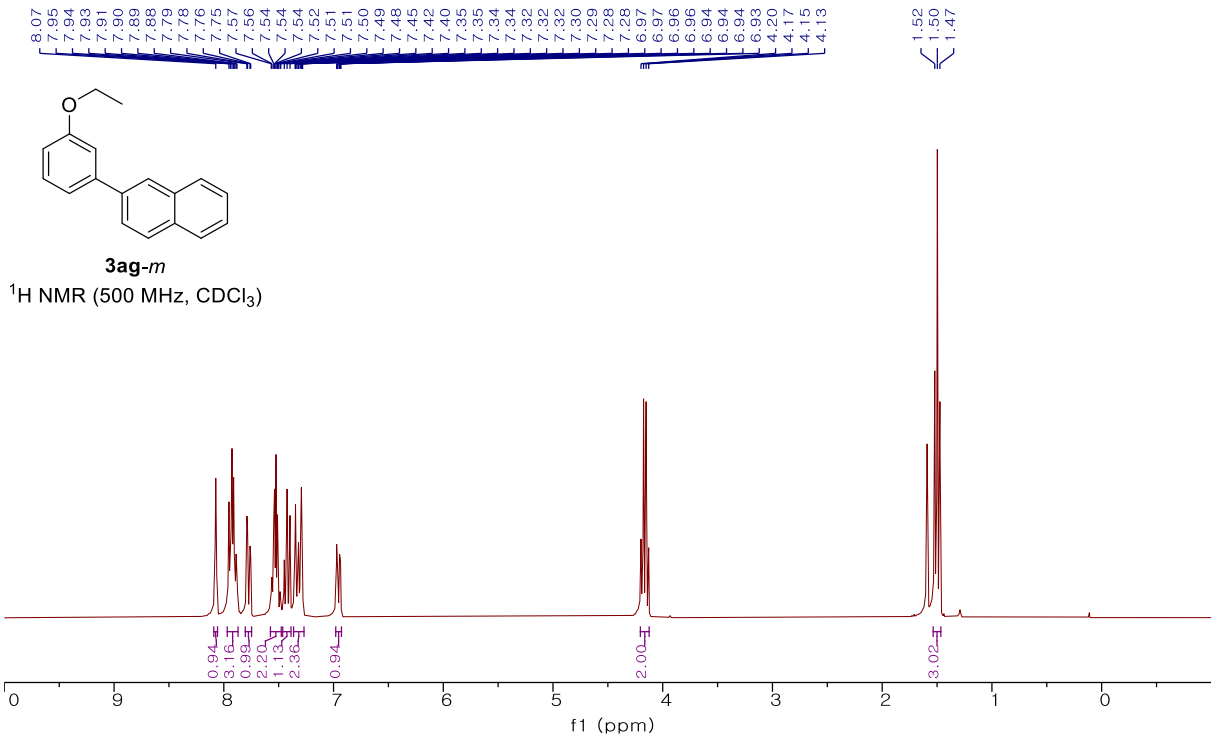
3ag-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



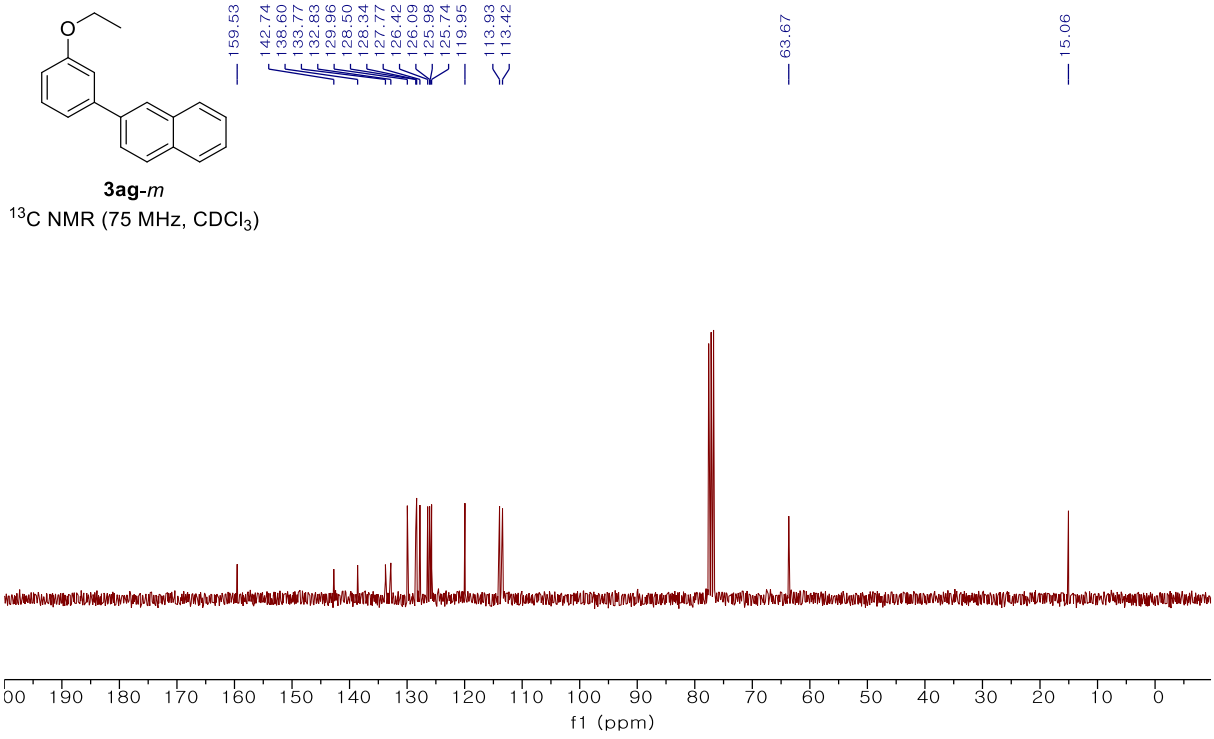
3ag-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



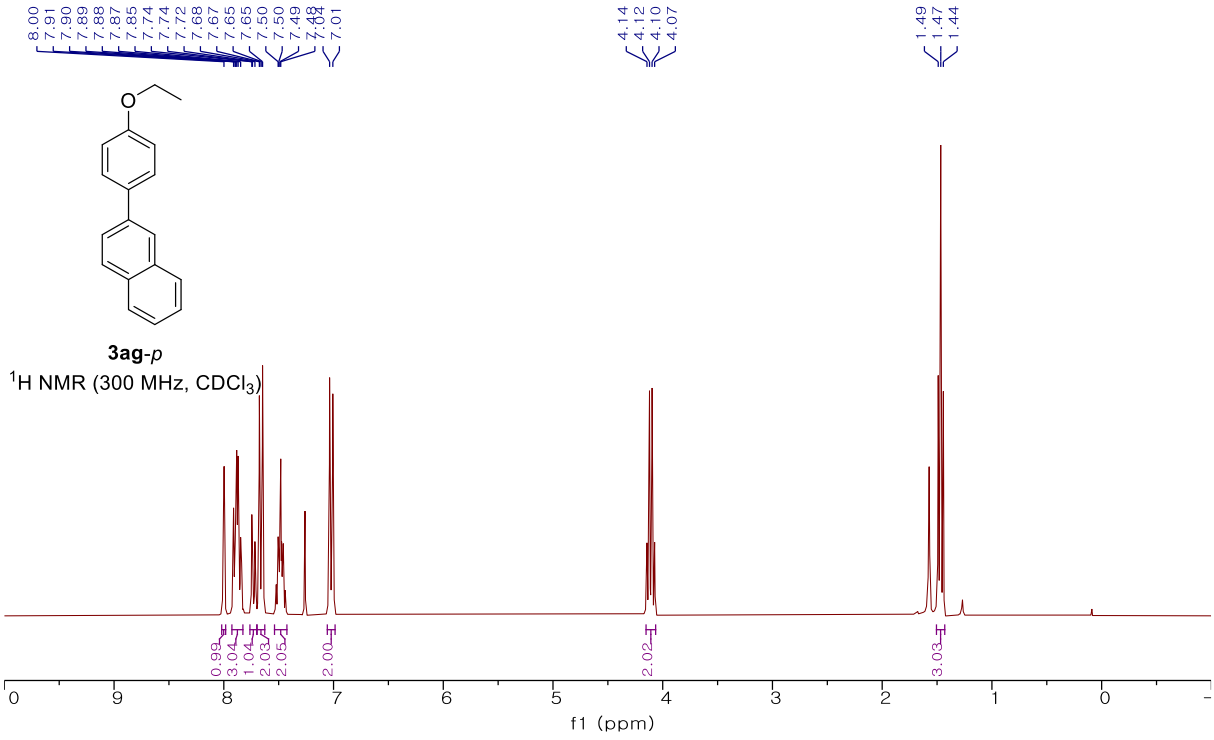
3ag-*m*

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



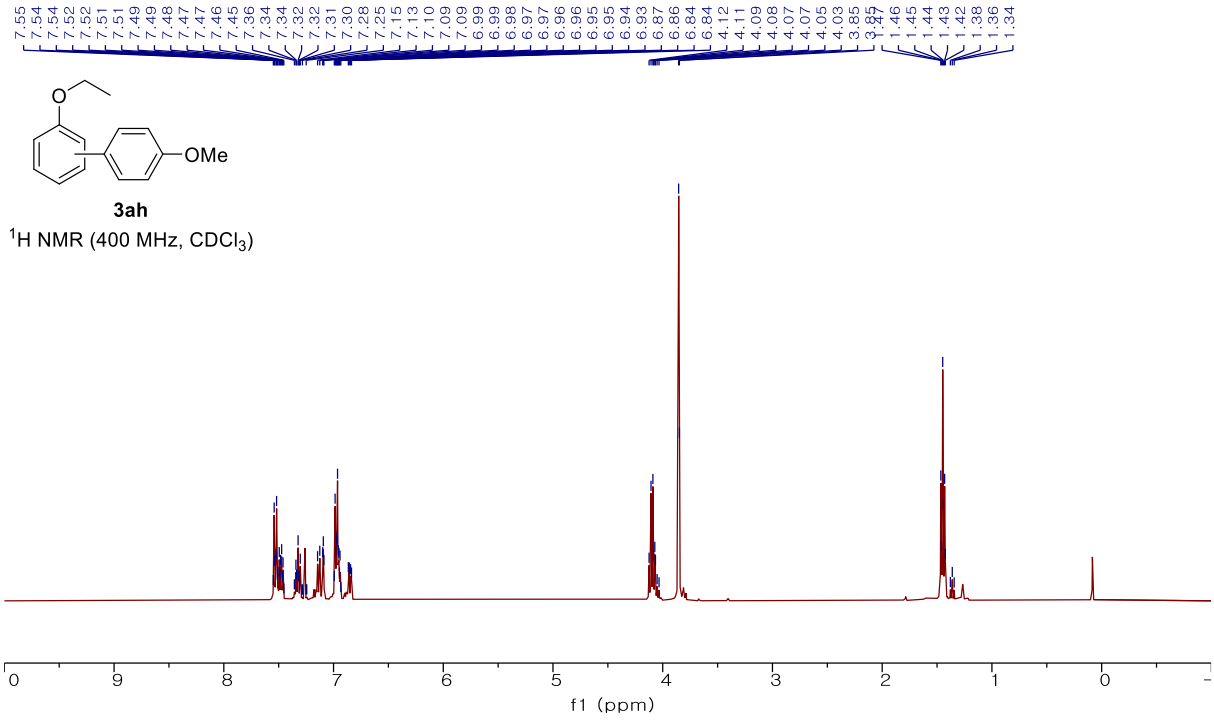
3ag-*m*

^{13}C NMR (75 MHz, $CDCl_3$)



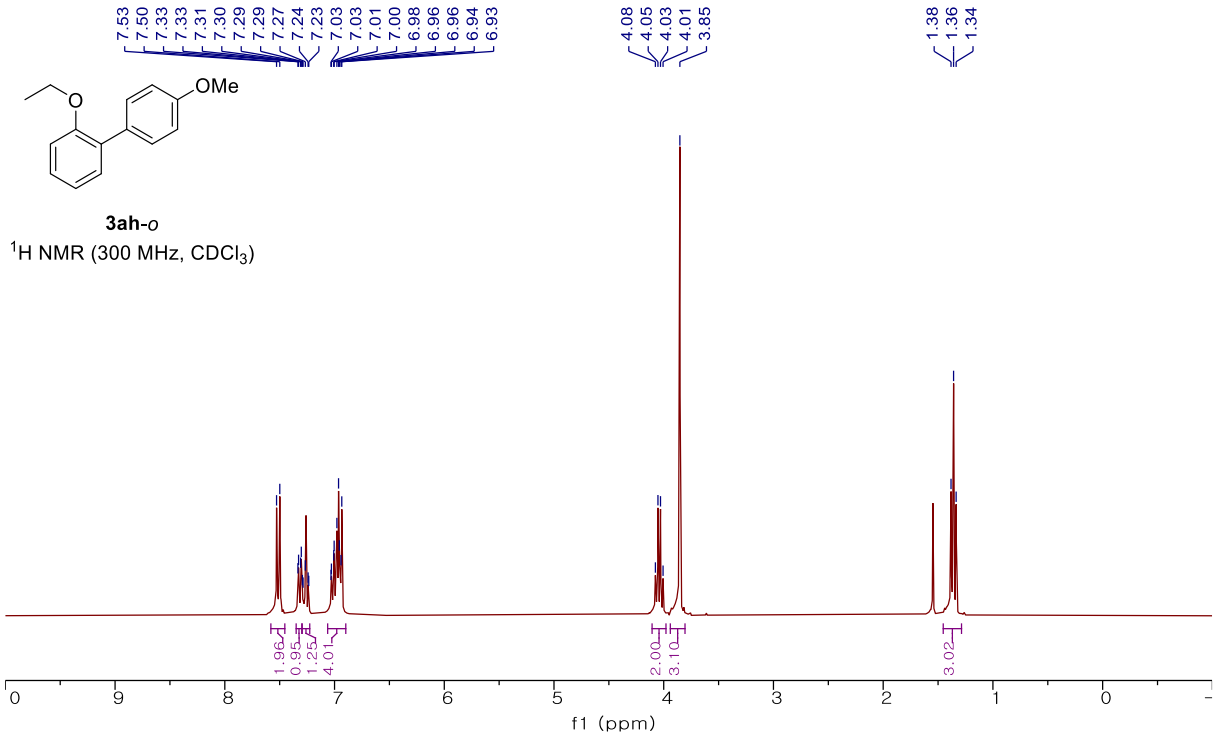
3ag-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



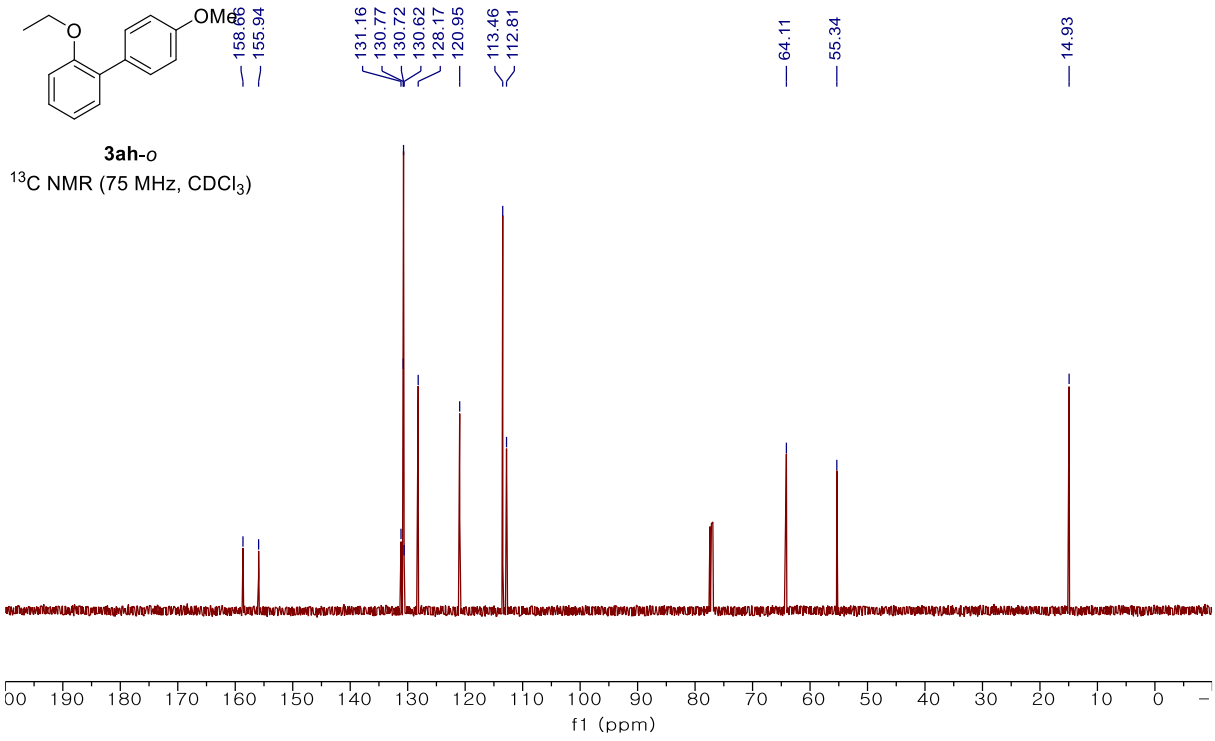
3ah

^{1}H NMR (400 MHz, $CDCl_3$)



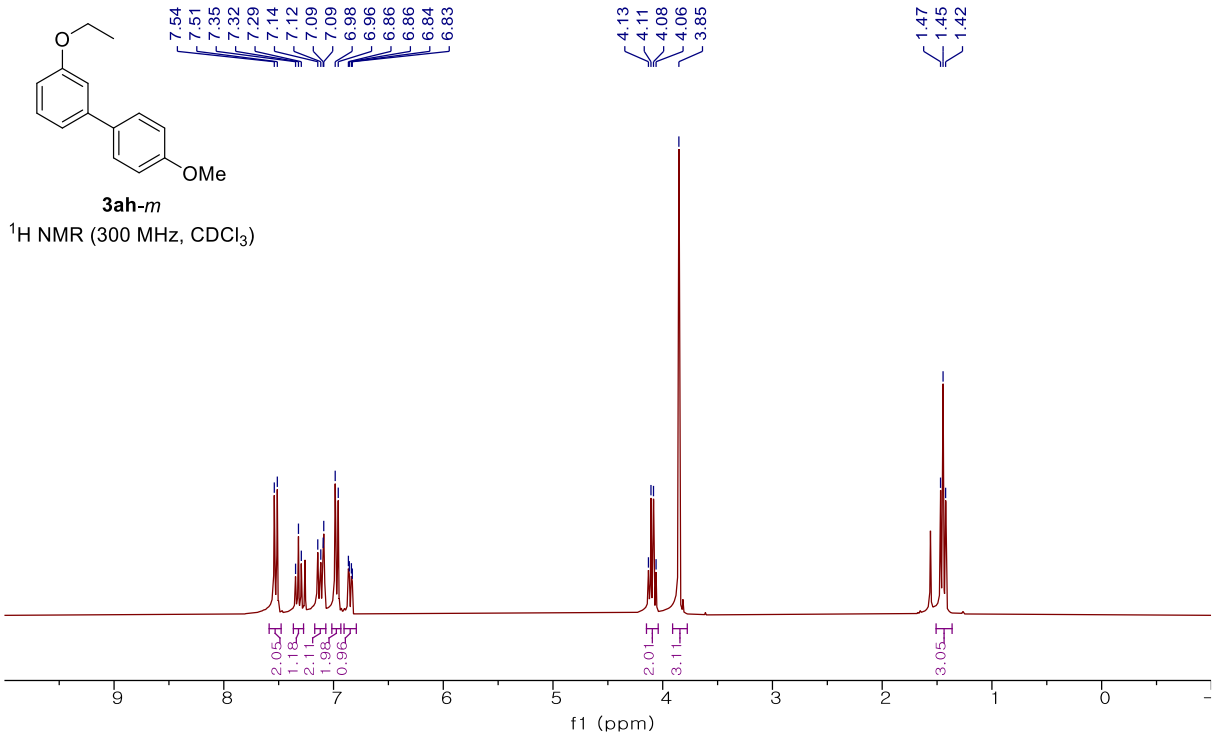
3ah-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



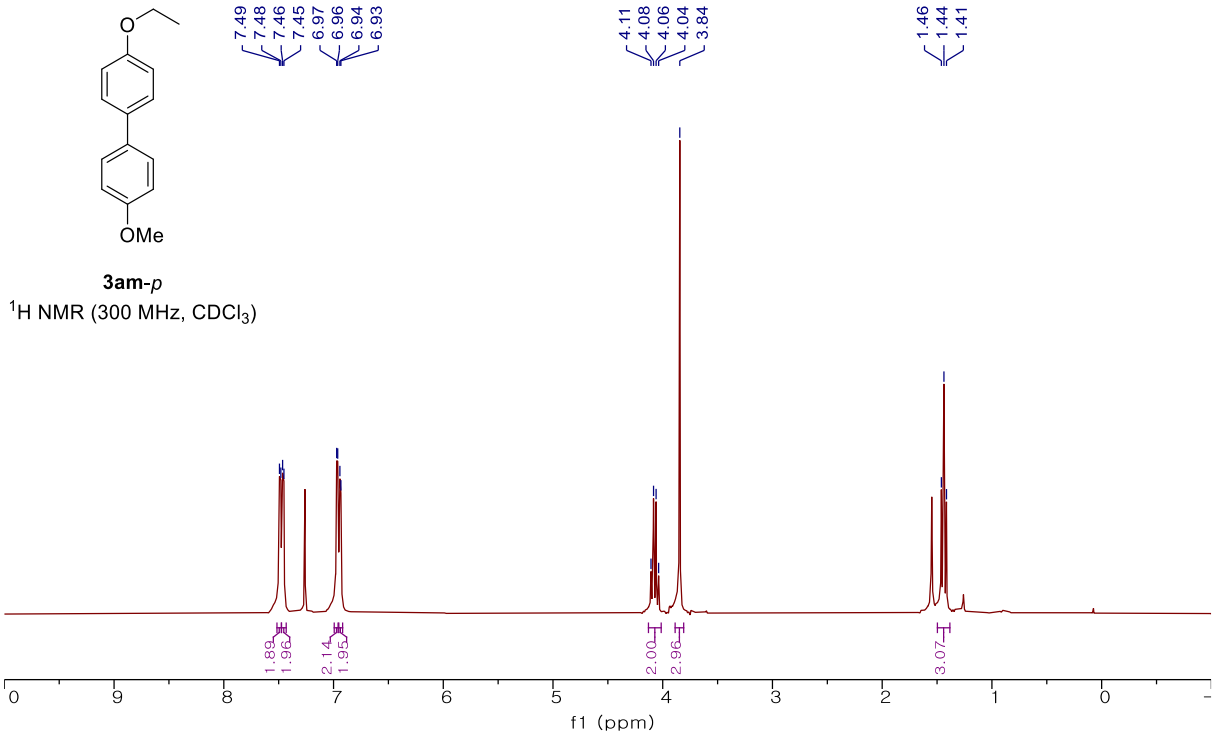
3ah-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



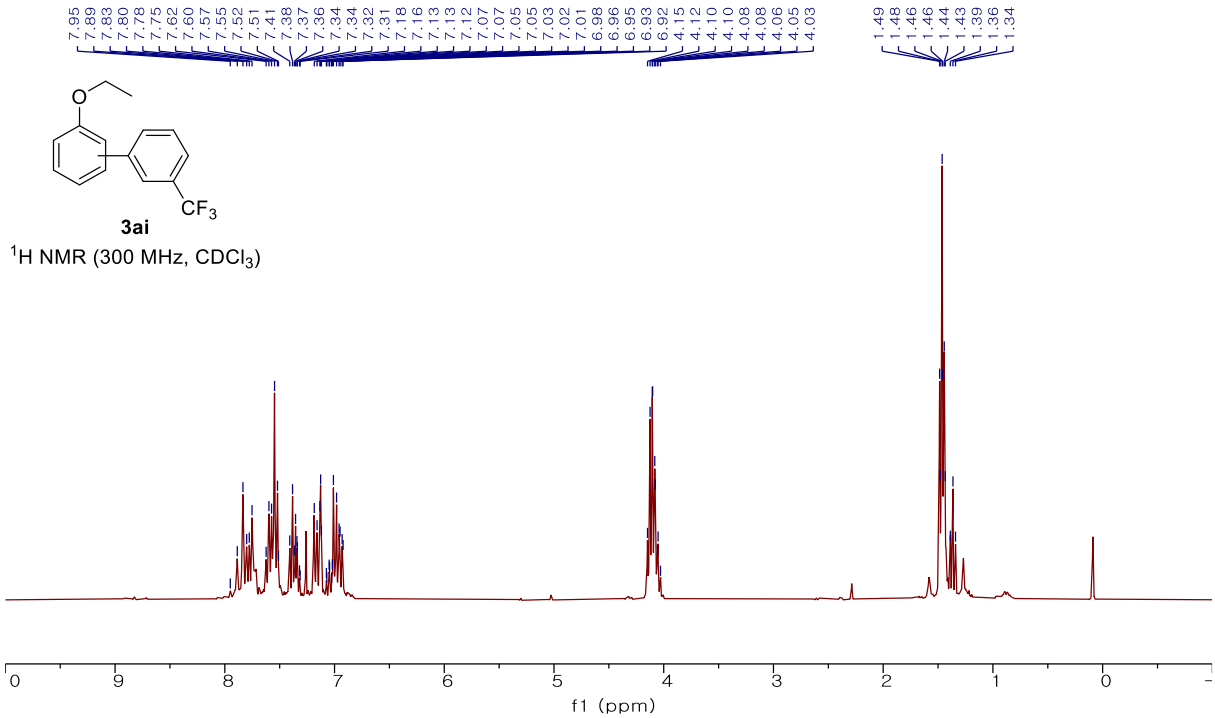
3ah-*m*

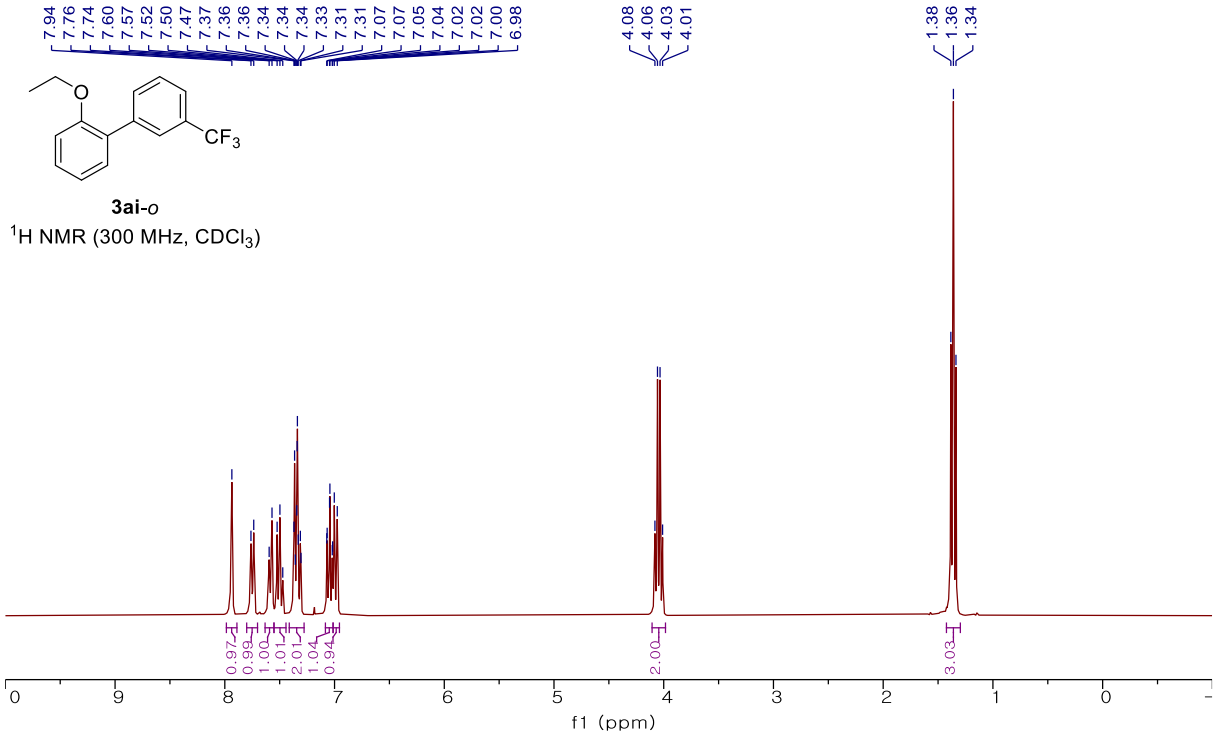
^{1}H NMR (300 MHz, $CDCl_3$)

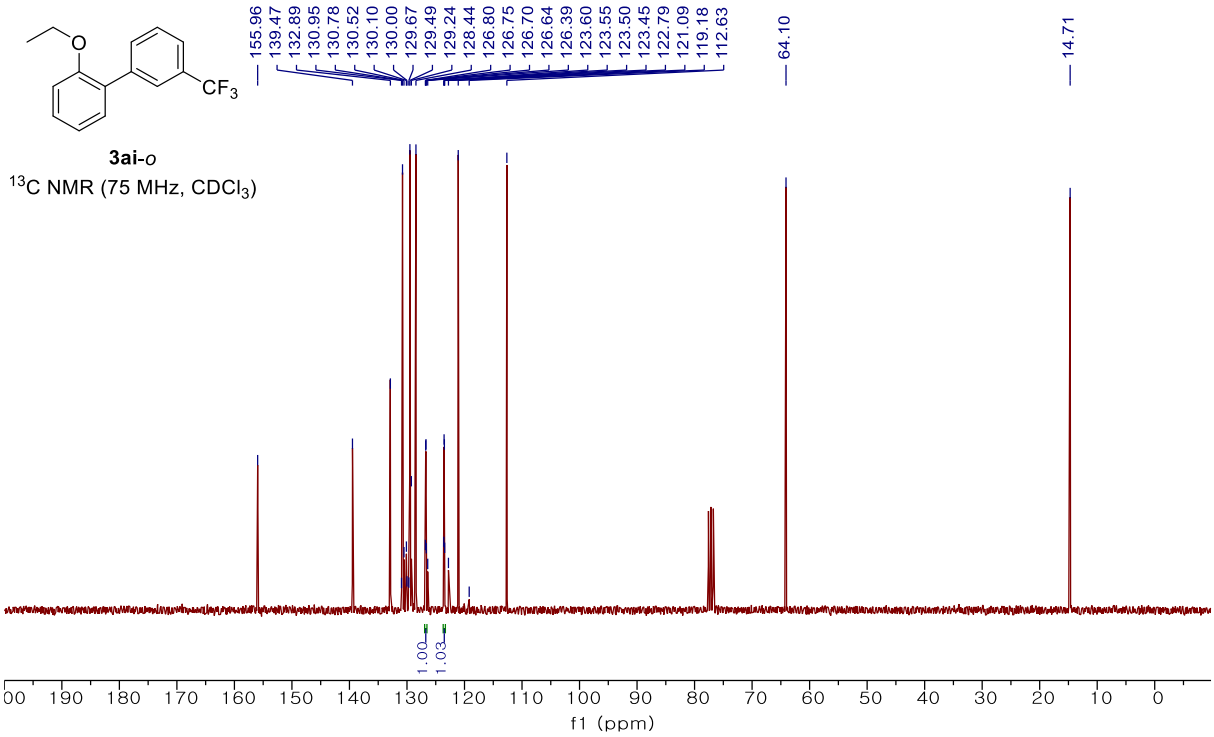


3am-*p*

^{1}H NMR (300 MHz, $CDCl_3$)

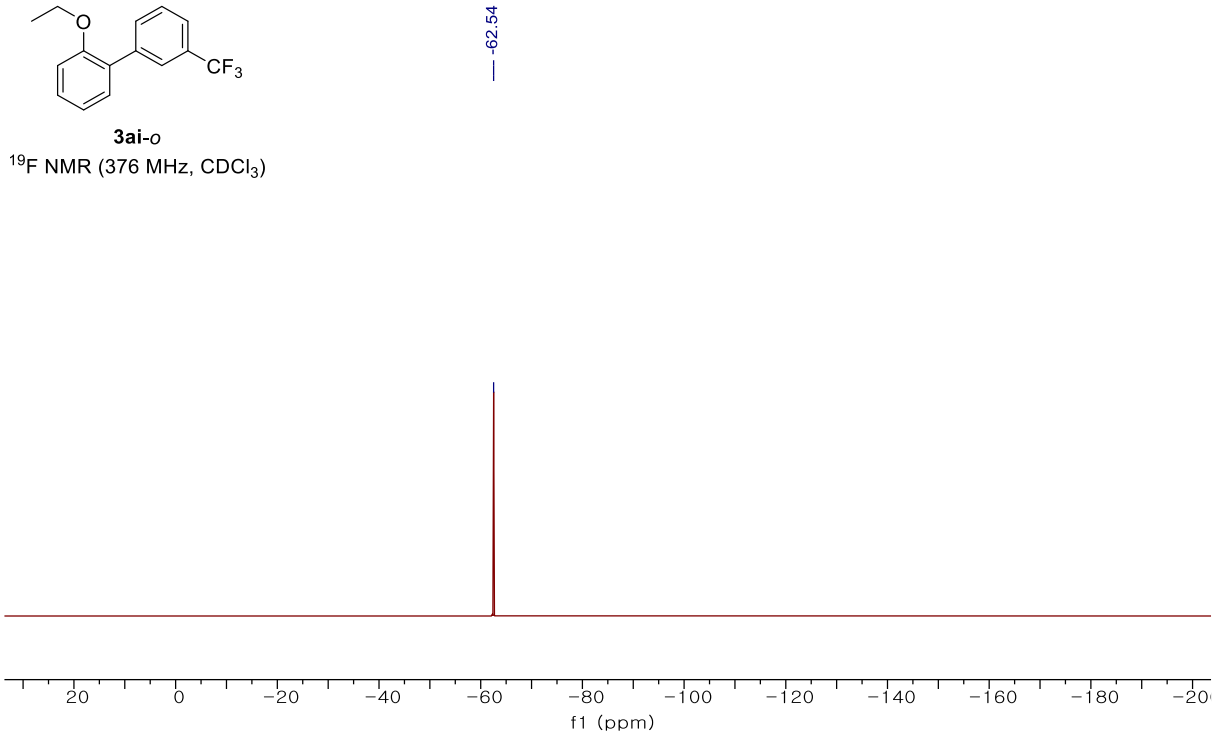

7.95
7.89
7.83
7.80
7.78
7.75
7.62
7.60
7.57
7.55
7.52
7.51
7.41
7.38
7.37
7.36
7.34
7.34
7.32
7.31
7.18
7.16
7.13
7.13
7.12
7.07
7.07
7.05
7.05
7.03
7.02
7.01
6.98
6.96
6.95
6.93
6.92
4.15
4.12
4.10
4.10
4.08
4.08
4.06
4.05
4.03
1.49
1.48
1.46
1.46
1.44
1.43
1.39
1.36
1.34
O
CF3
3ai
1H NMR (300 MHz, CDCl3)
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


7.94
7.76
7.74
7.60
7.57
7.52
7.50
7.47
7.37
7.36
7.36
7.34
7.34
7.34
7.33
7.31
7.31
7.07
7.07
7.05
7.04
7.02
7.02
7.00
6.98
4.08
4.06
4.03
4.01
1.38
1.36
1.34
O
CF3
3ai-o
1H NMR (300 MHz, CDCl3)
0.97
0.99
1.00
1.01
2.01
1.04
0.94
2.00
3.03
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



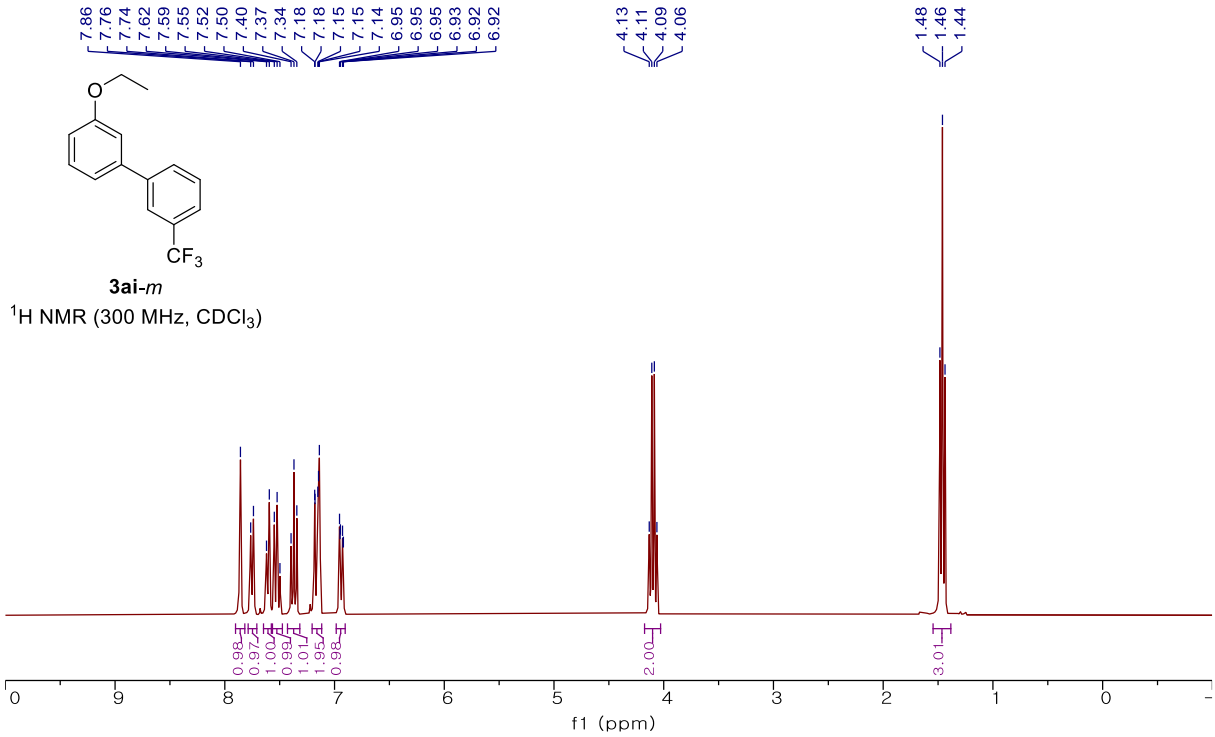
3ai-*o*

^{13}C NMR (75 MHz, $CDCl_3$)



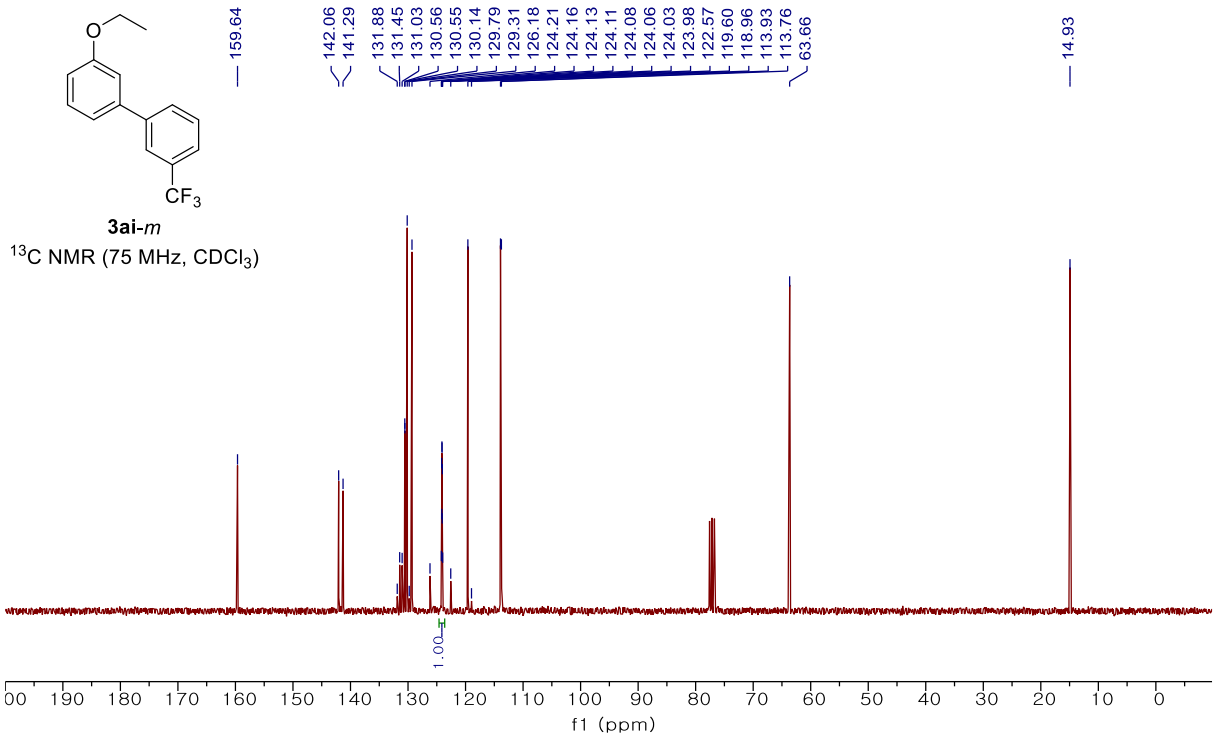
3ai-*o*

^{19}F NMR (376 MHz, $CDCl_3$)



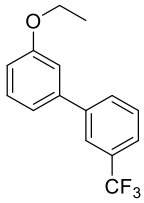
3ai-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



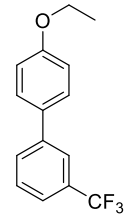
3ai-*m*

^{13}C NMR (75 MHz, $CDCl_3$)



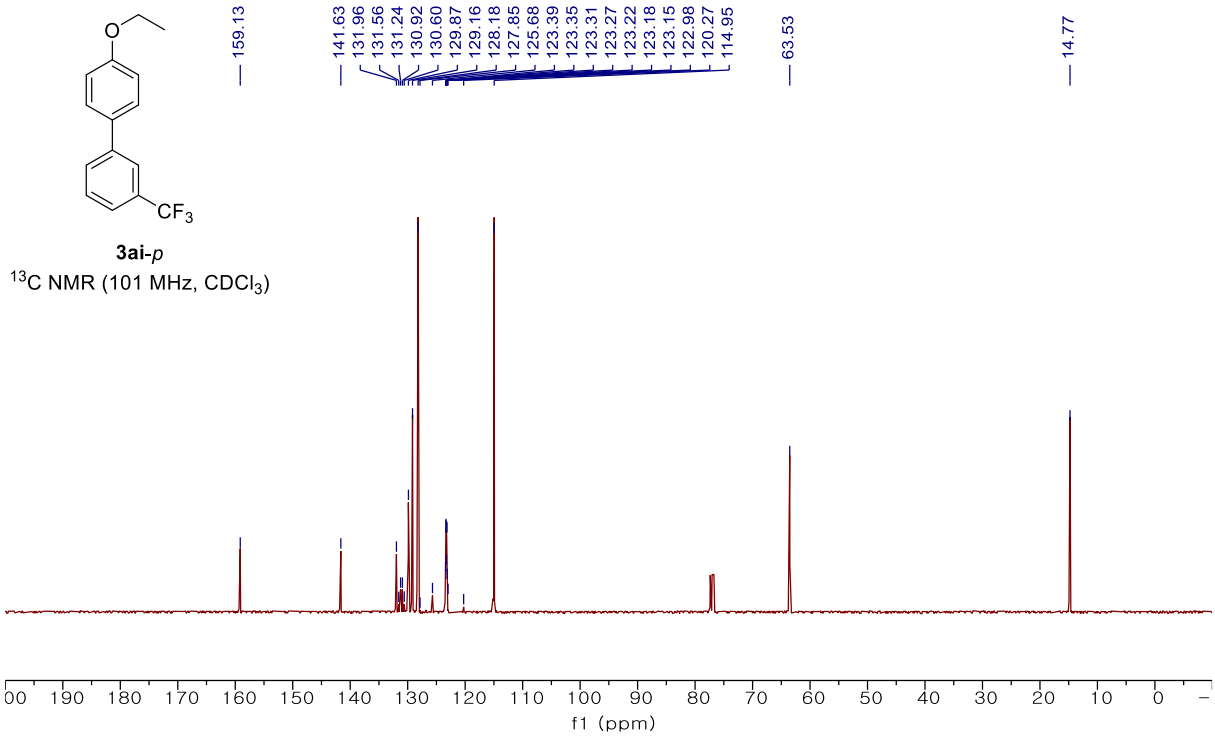
3ai-*m*

^{19}F NMR (376 MHz, $CDCl_3$)



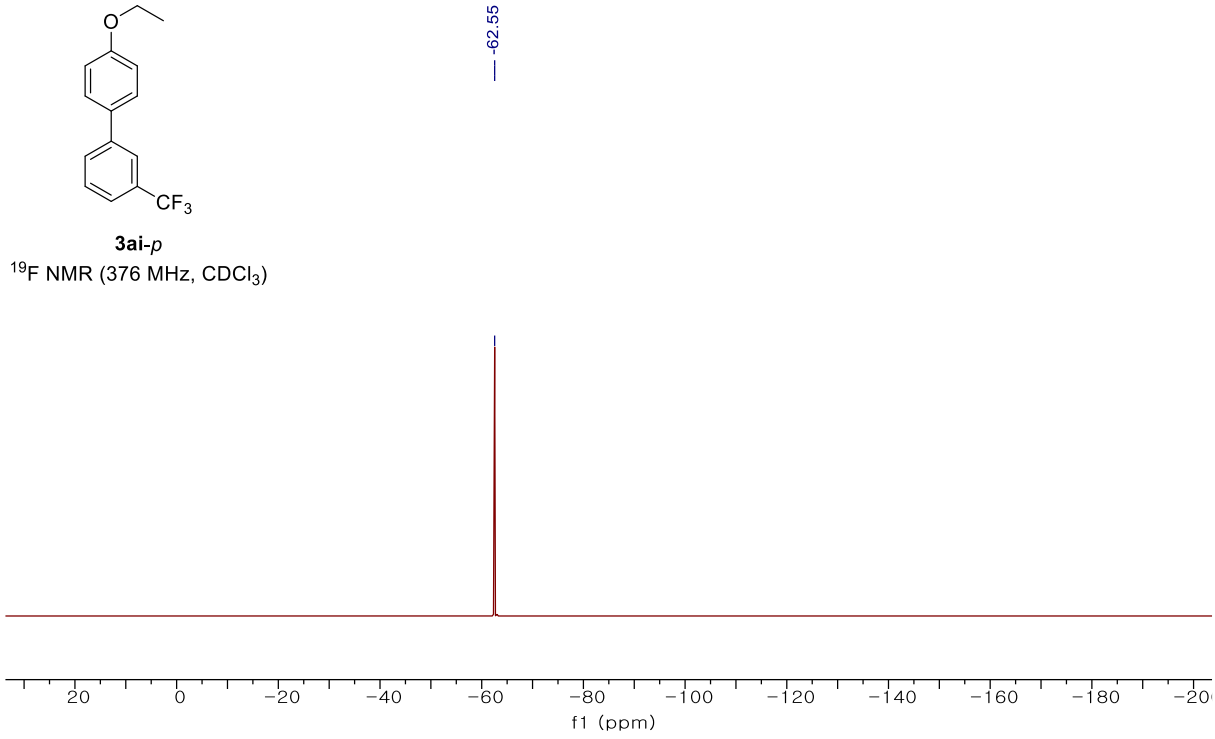
3ai-*p*

^{1}H NMR (300 MHz, $CDCl_3$)



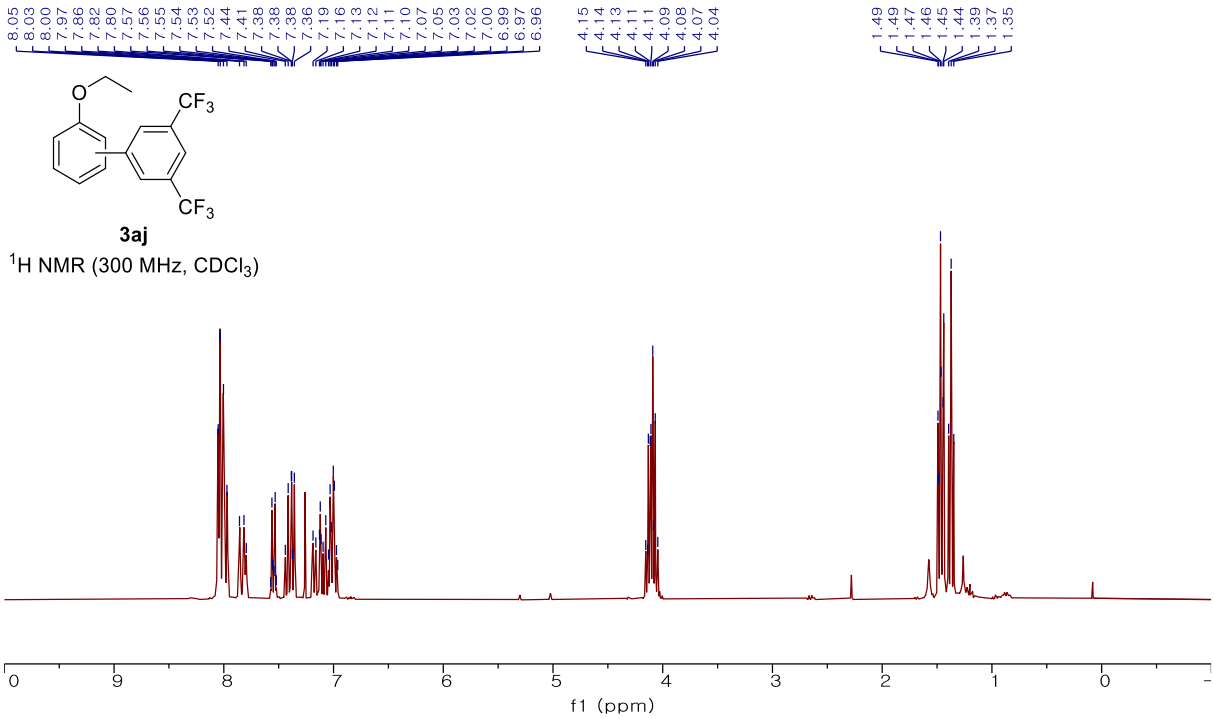
3ai-*p*

^{13}C NMR (101 MHz, $CDCl_3$)



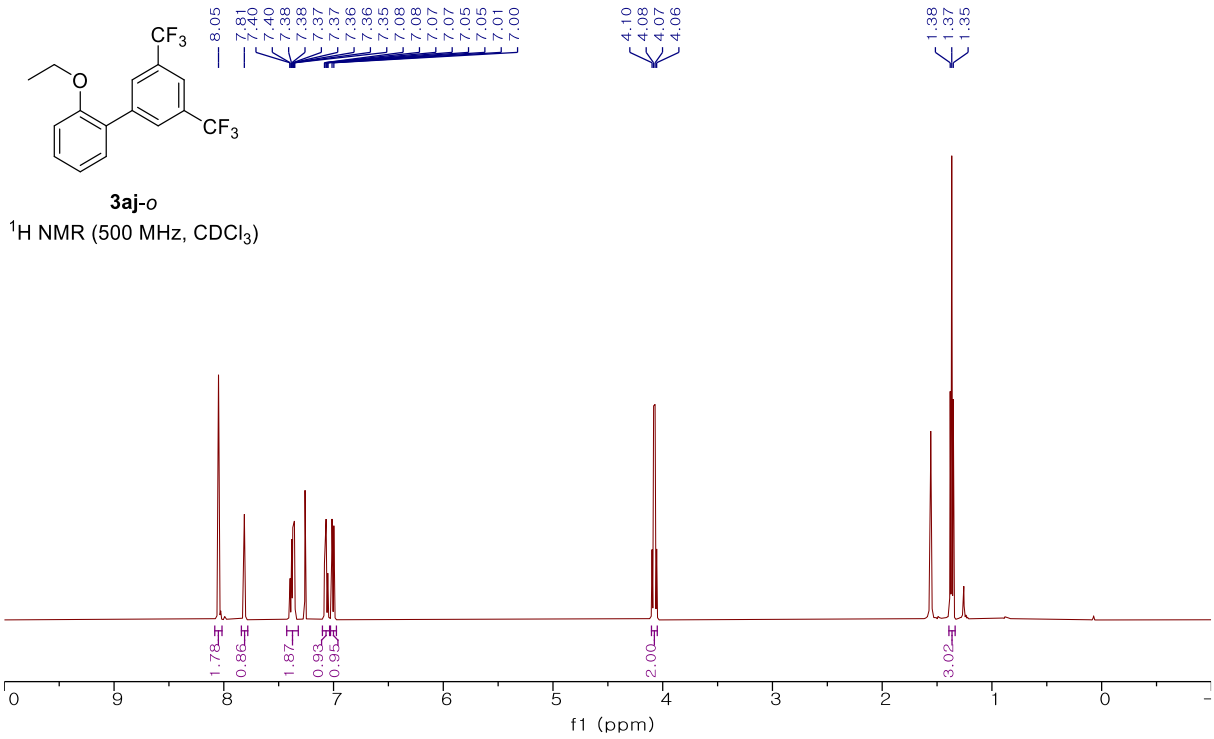
3ai-*p*

^{19}F NMR (376 MHz, $CDCl_3$)



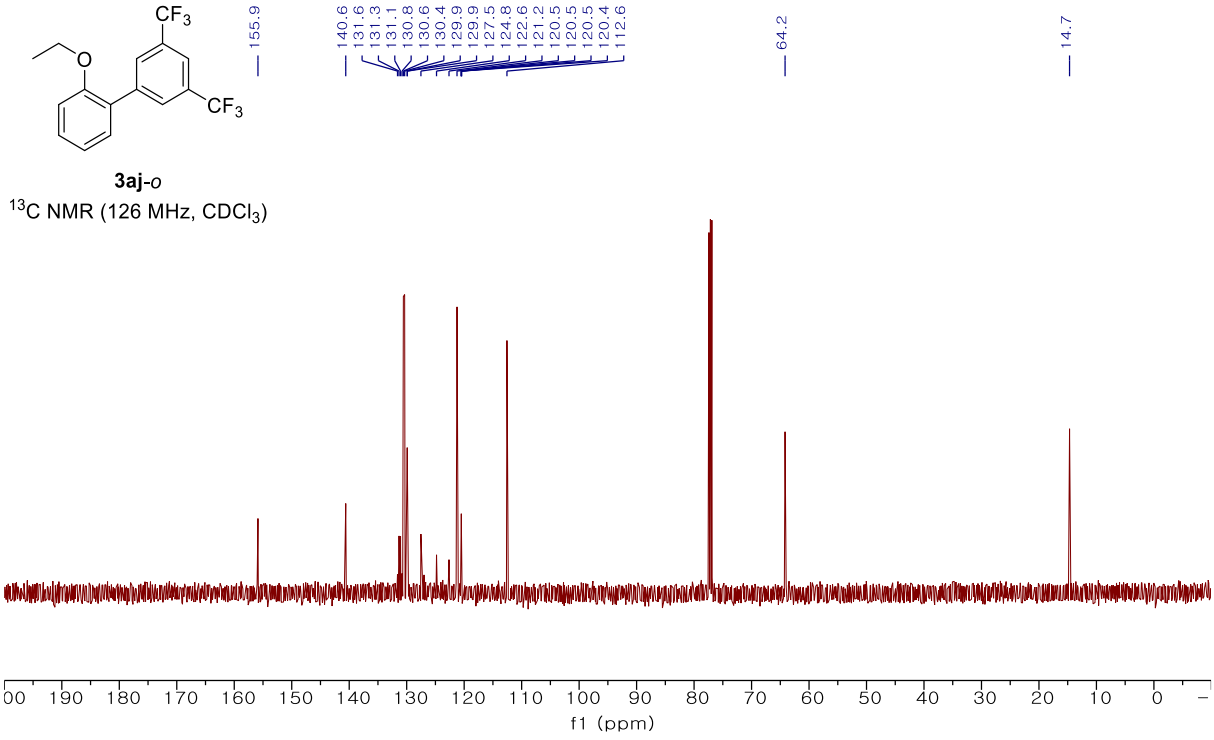
3aj

^{1}H NMR (300 MHz, $CDCl_3$)



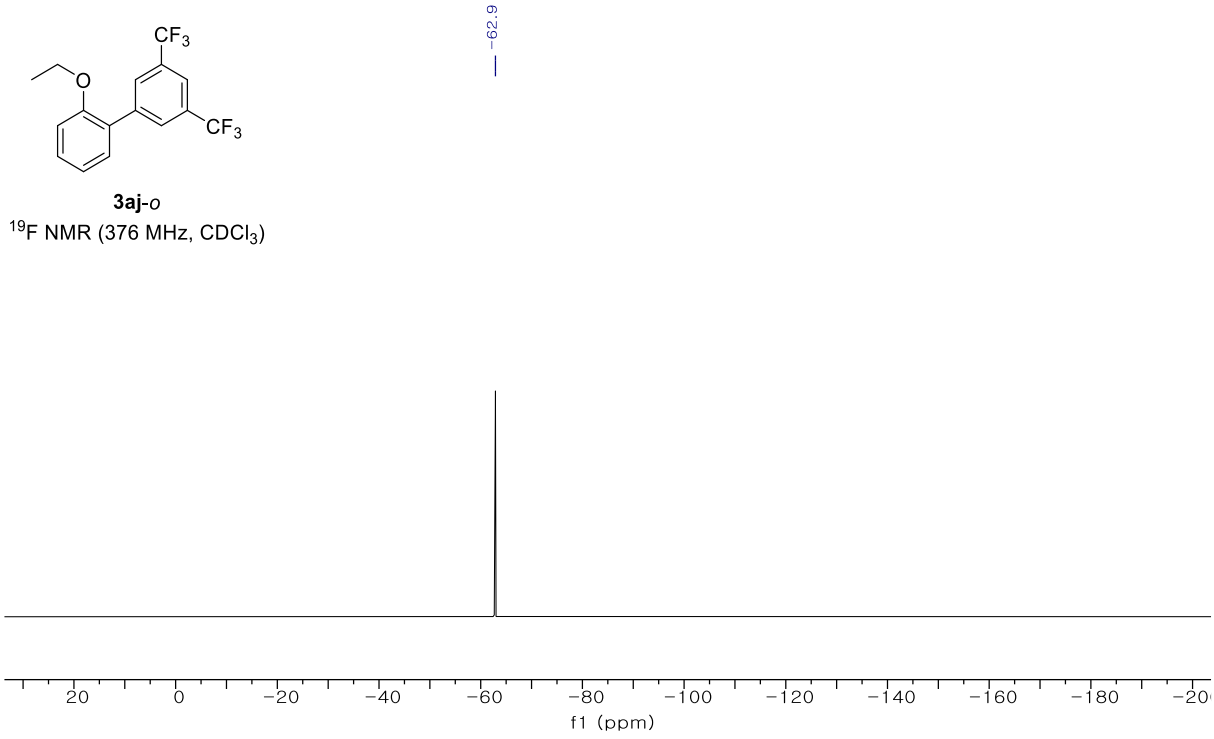
3aj-*o*

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



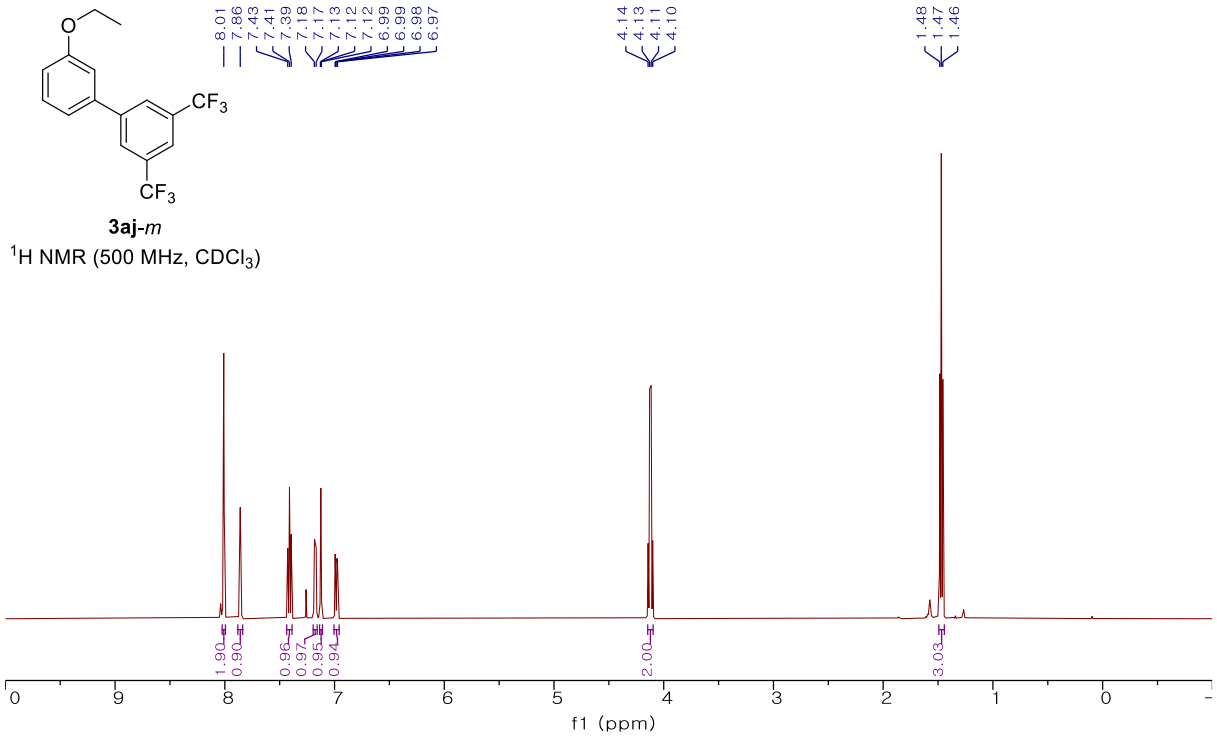
3aj-*o*

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



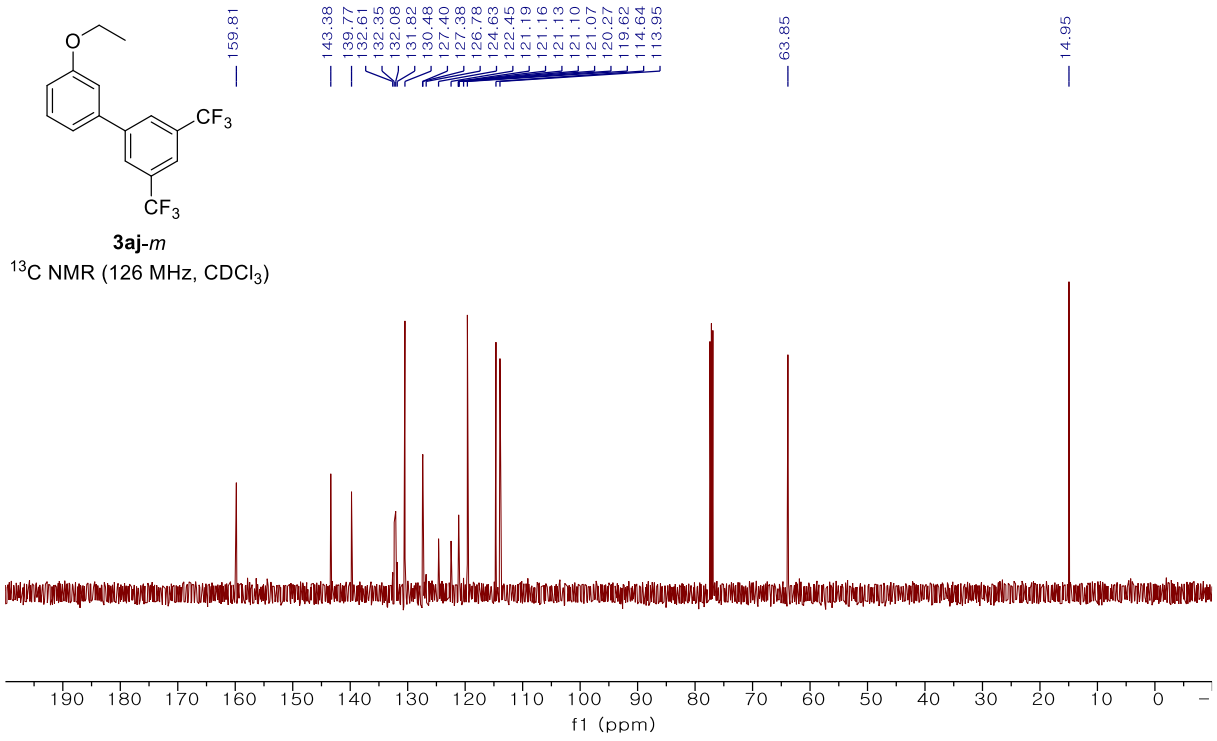
3aj-*o*

^{19}F NMR (376 MHz, $CDCl_3$)



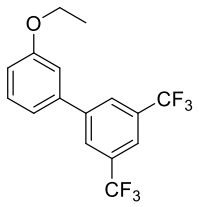
3aj-*m*

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



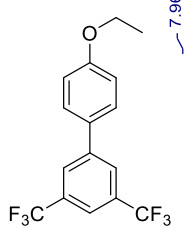
3aj-*m*

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



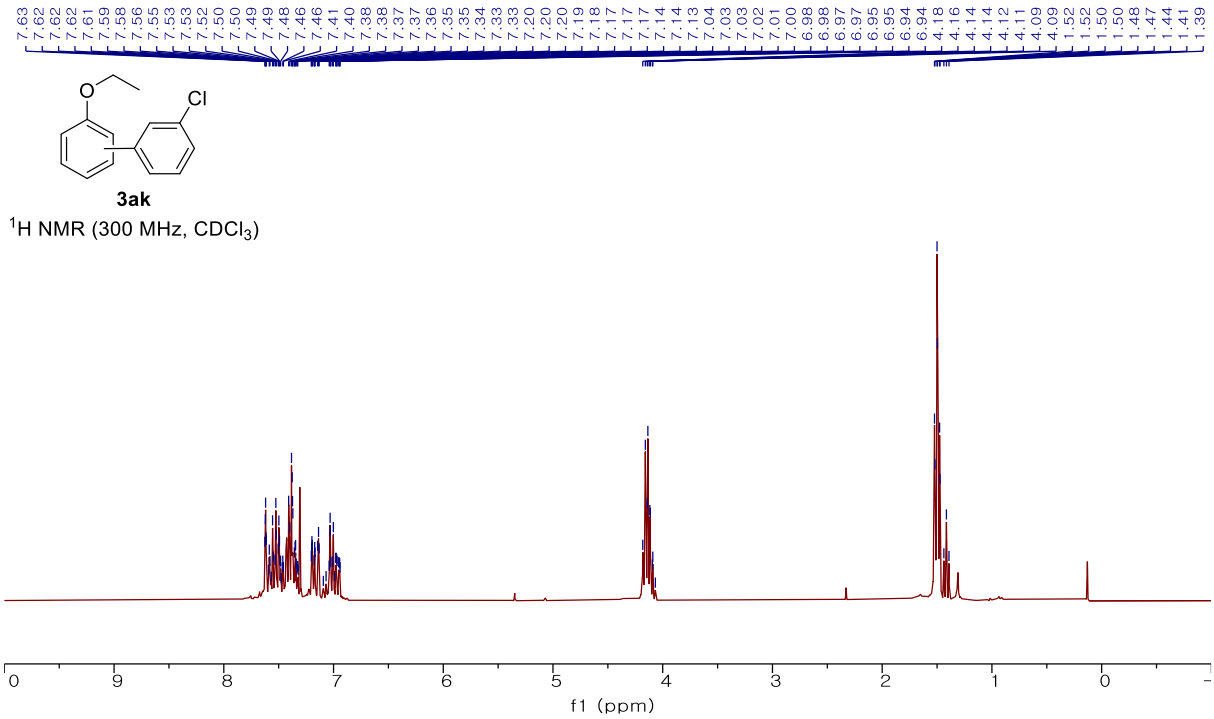
3aj-*m*

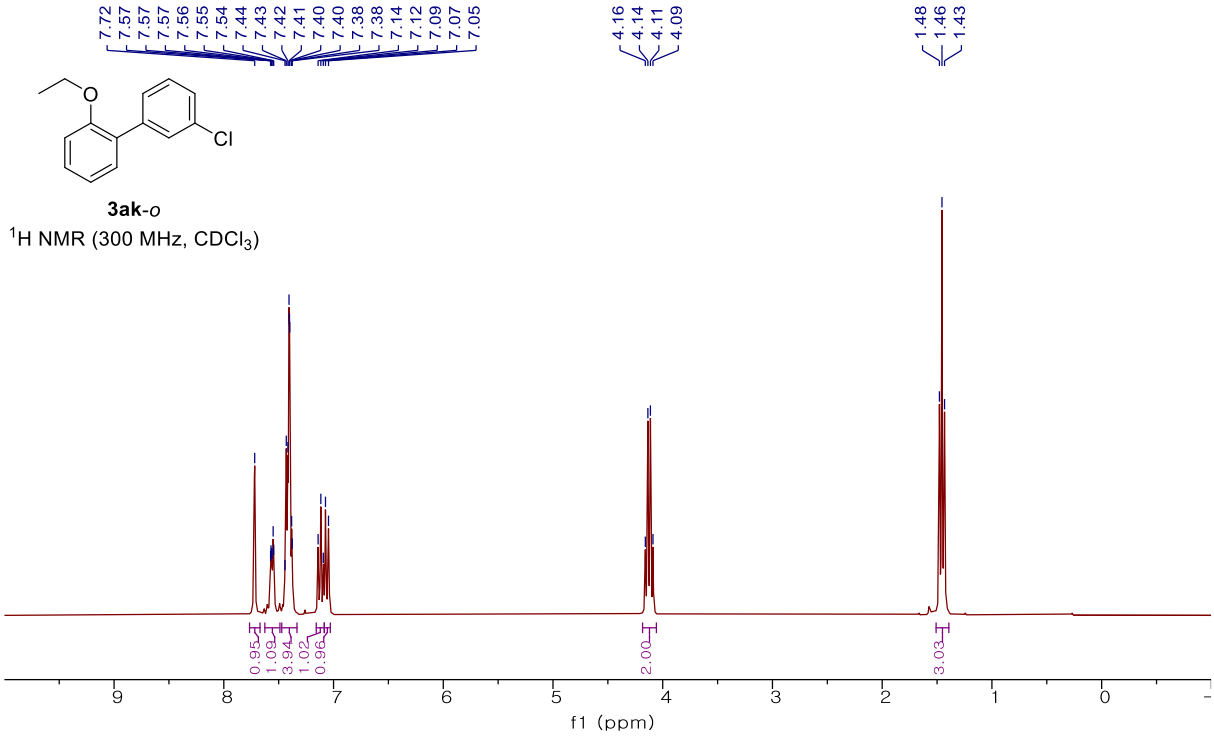
^{19}F NMR (376 MHz, $CDCl_3$)

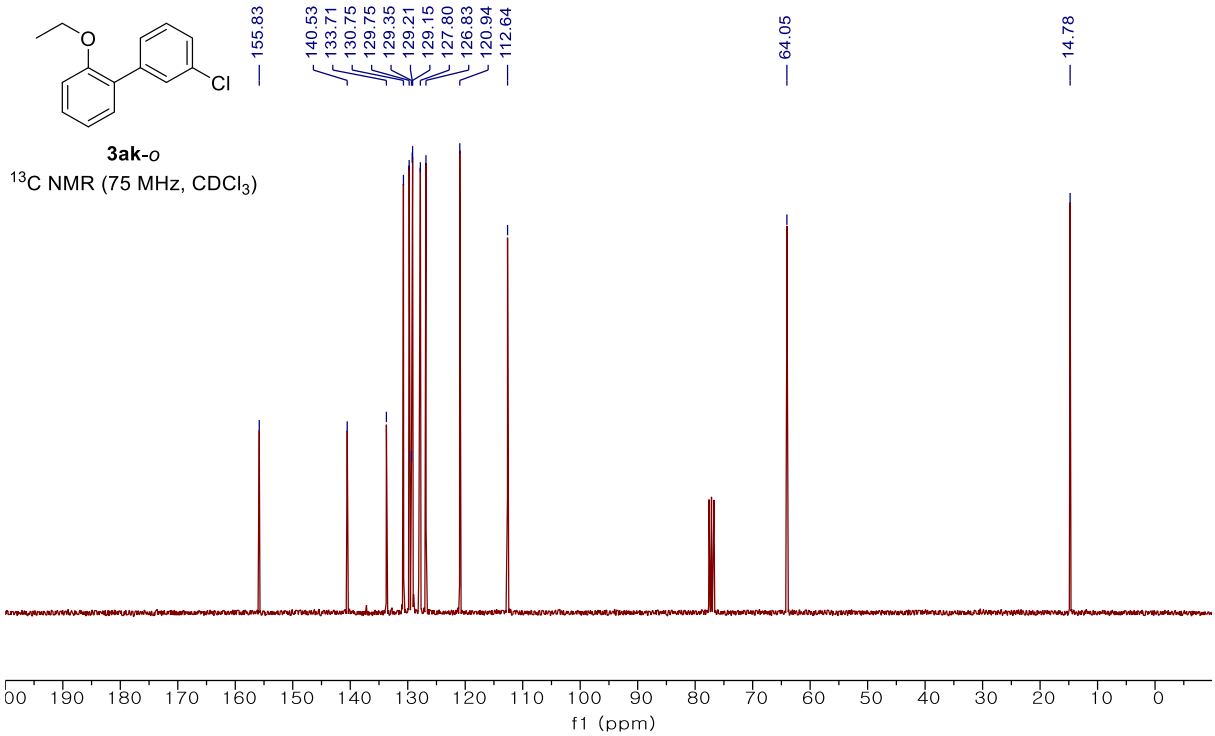


3aj-*p*

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

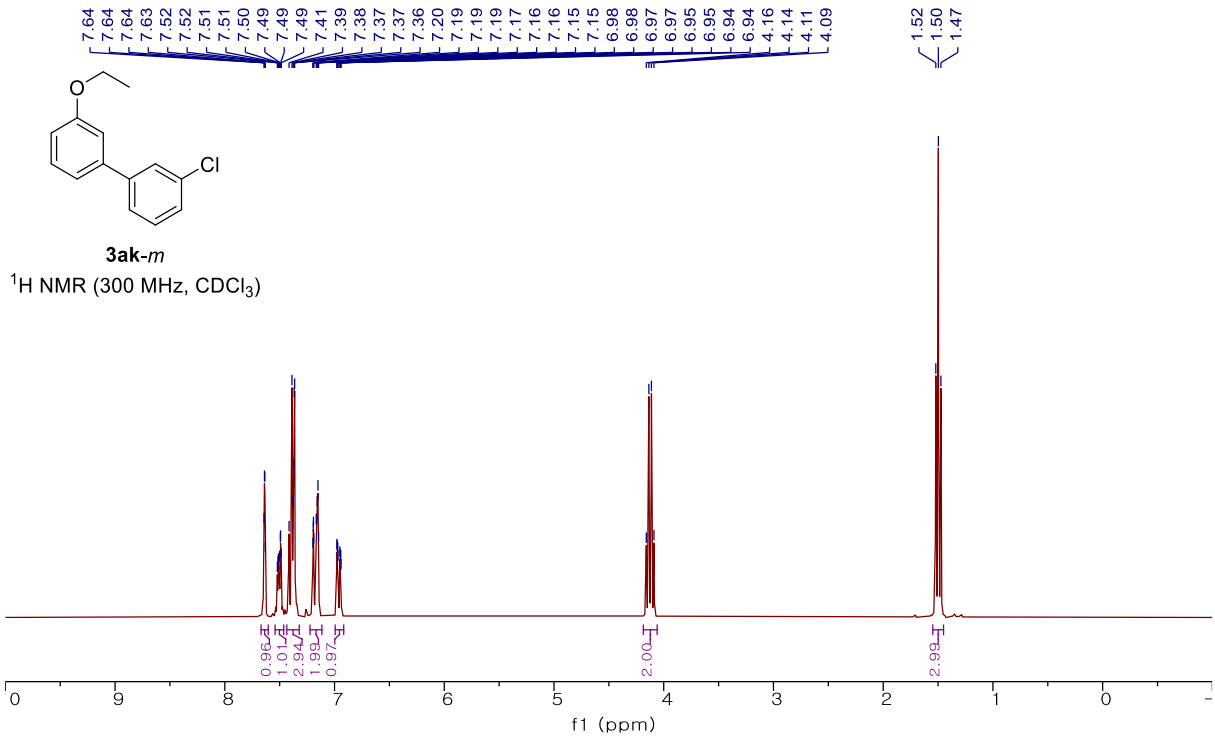

7.63 7.62 7.62 7.62 7.61 7.59 7.58 7.56 7.55 7.53 7.53 7.52 7.50 7.50 7.49 7.49 7.48 7.46 7.46 7.41 7.40 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.20 7.20 7.19 7.18 7.17 7.17 7.17 7.14 7.14 7.13 7.04 7.03 7.03 7.02 7.01 7.00 6.98 6.98 6.97 6.97 6.95 6.95 6.94 6.94 4.18 4.16 4.14 4.14 4.12 4.11 4.09 4.09 1.52 1.52 1.50 1.50 1.48 1.47 1.44 1.41 1.39
O
Cl
3ak
1H NMR (300 MHz, CDCl3)
0 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


7.72 7.57 7.57 7.57 7.56 7.55 7.54 7.44 7.43 7.42 7.41 7.40 7.40 7.38 7.38 7.14 7.12 7.09 7.07 7.05
4.16 4.14 4.11 4.09
1.48 1.46 1.43
O
Cl
3ak-o
1H NMR (300 MHz, CDCl3)
0.95 1.09 3.94 1.02 0.96 2.00 3.03
9 8 7 6 5 4 3 2 1 0
f1 (ppm)



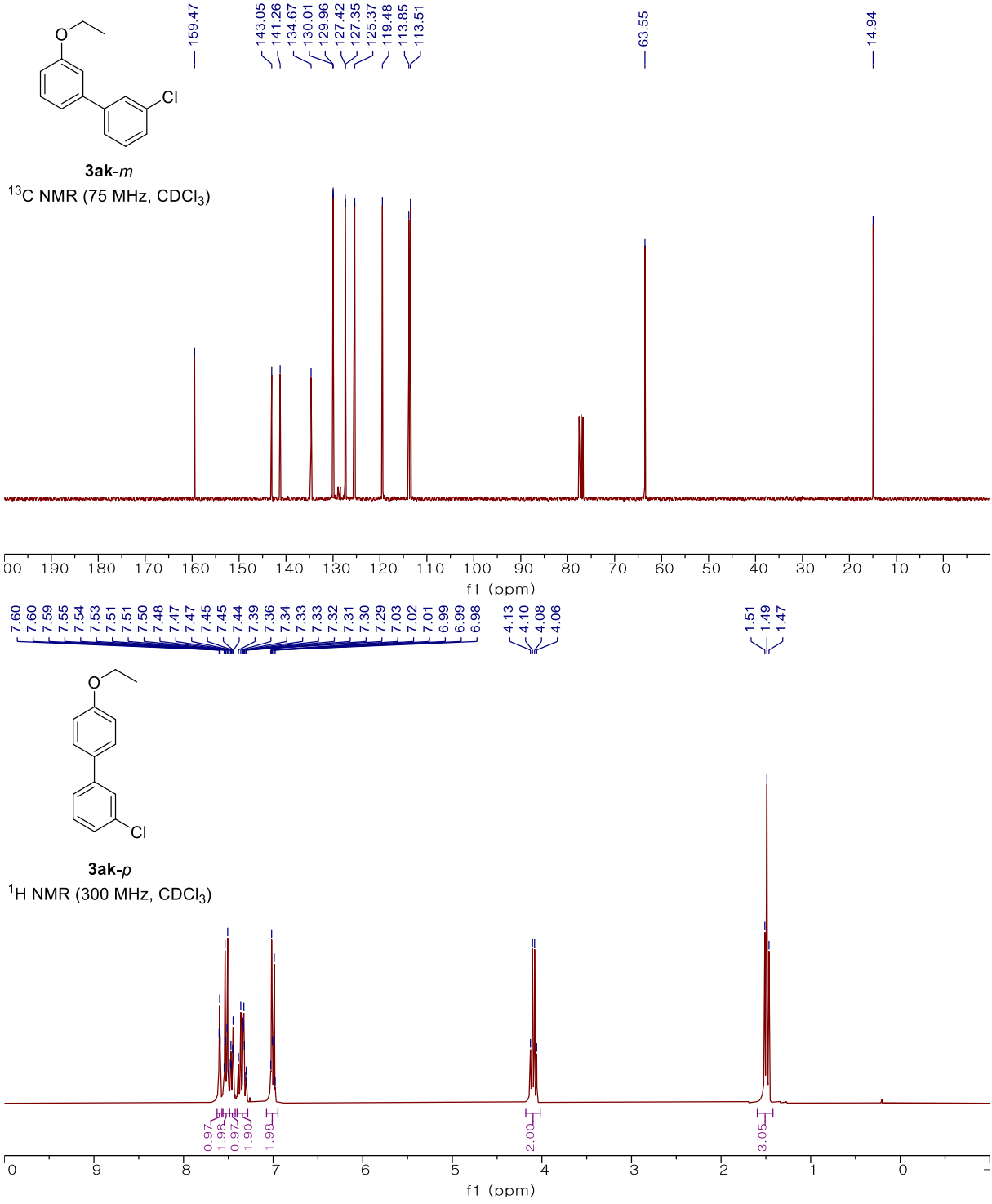
3ak-*o*

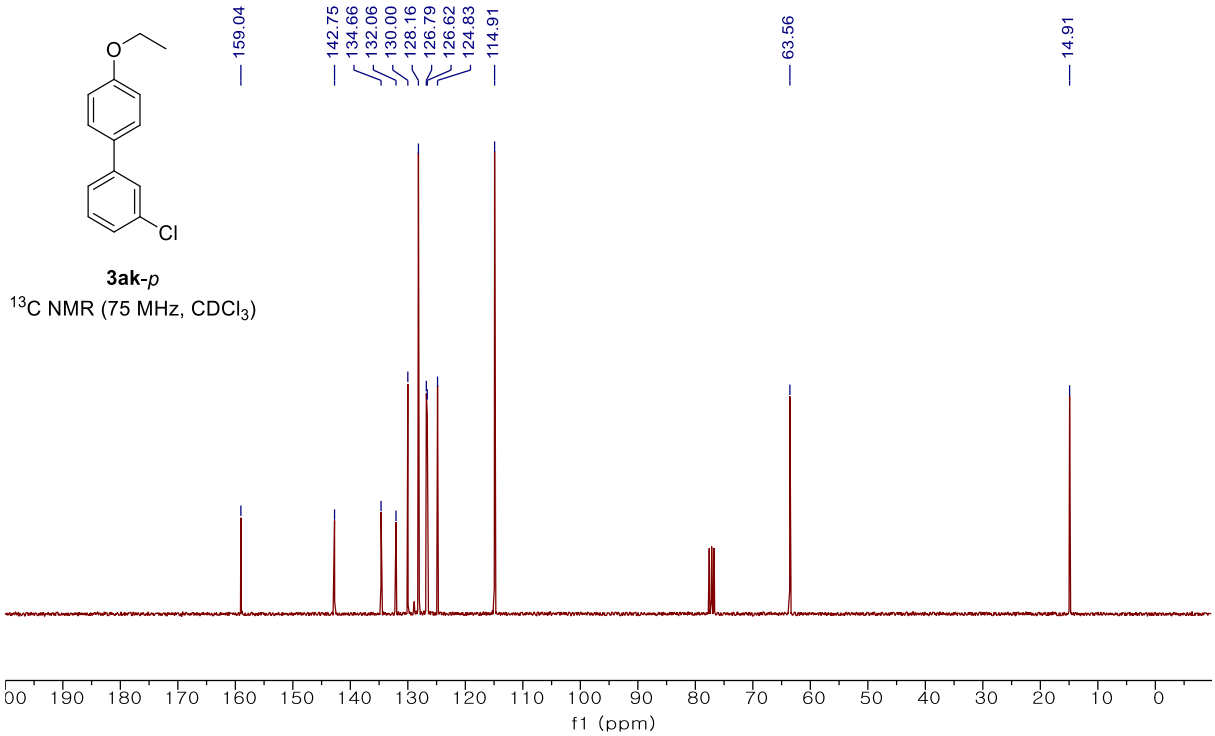
^{13}C NMR (75 MHz, $CDCl_3$)



3ak-*m*

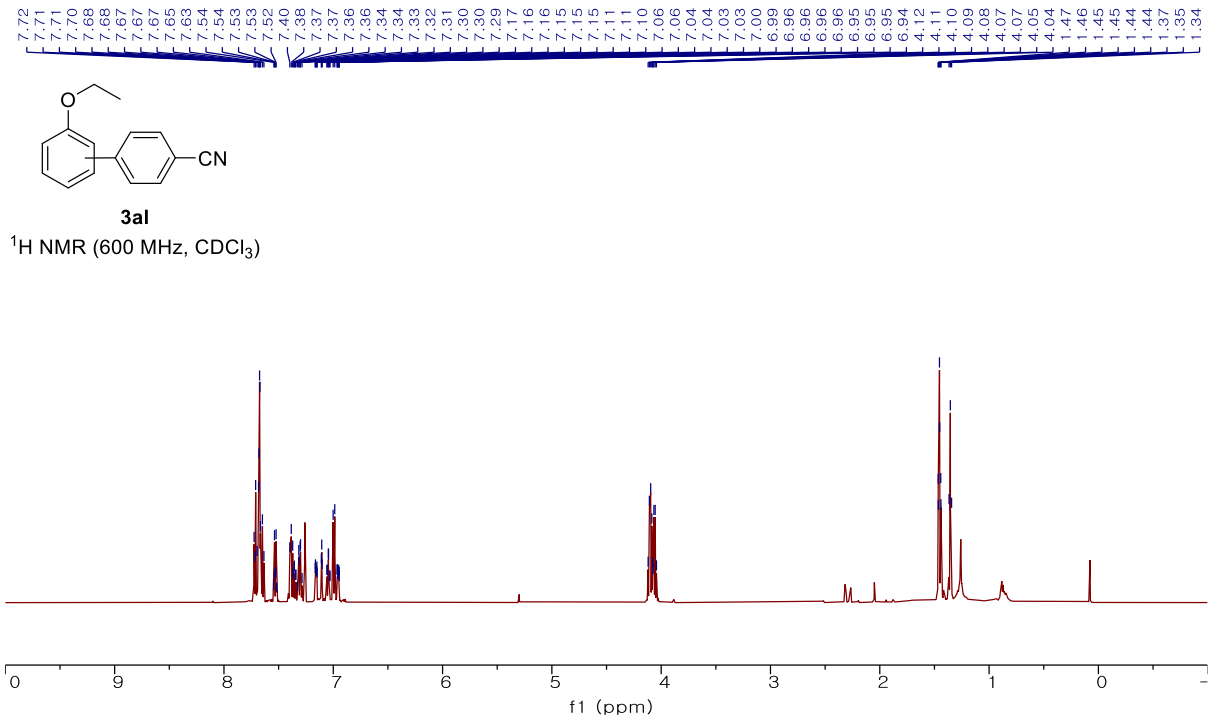
^{1}H NMR (300 MHz, $CDCl_3$)


159.47
143.05
141.26
134.67
130.01
129.96
127.42
127.35
125.37
119.48
113.85
113.51
63.55
14.94
O
Cl
3ak-m
13C NMR (75 MHz, CDCl3)
f1 (ppm)
7.60
7.60
7.59
7.55
7.54
7.53
7.51
7.51
7.50
7.48
7.47
7.47
7.45
7.45
7.44
7.39
7.36
7.34
7.33
7.33
7.32
7.31
7.30
7.29
7.03
7.02
7.01
6.99
6.99
6.98
4.13
4.10
4.08
4.06
1.51
1.49
1.47
O
Cl
3ak-p
1H NMR (300 MHz, CDCl3)
0.97
1.98
0.97
1.90
1.98
2.00
3.05
f1 (ppm)



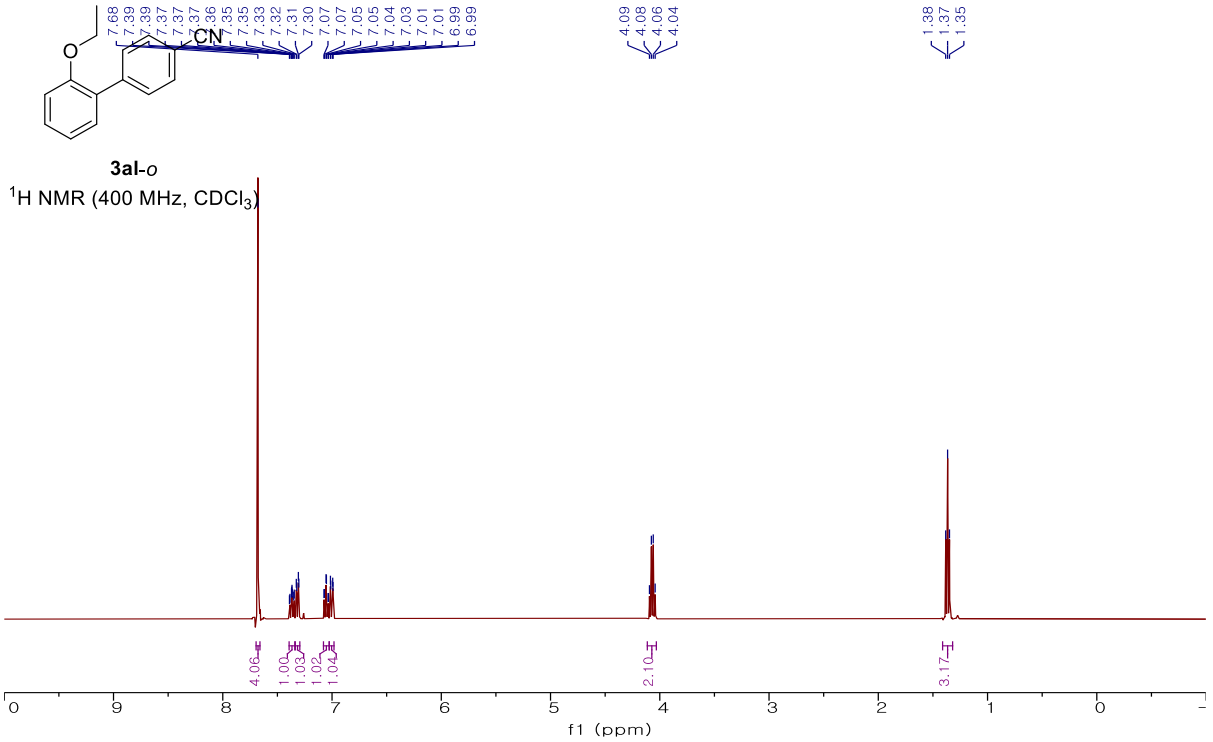
3ak-*p*

^{13}C NMR (75 MHz, $CDCl_3$)



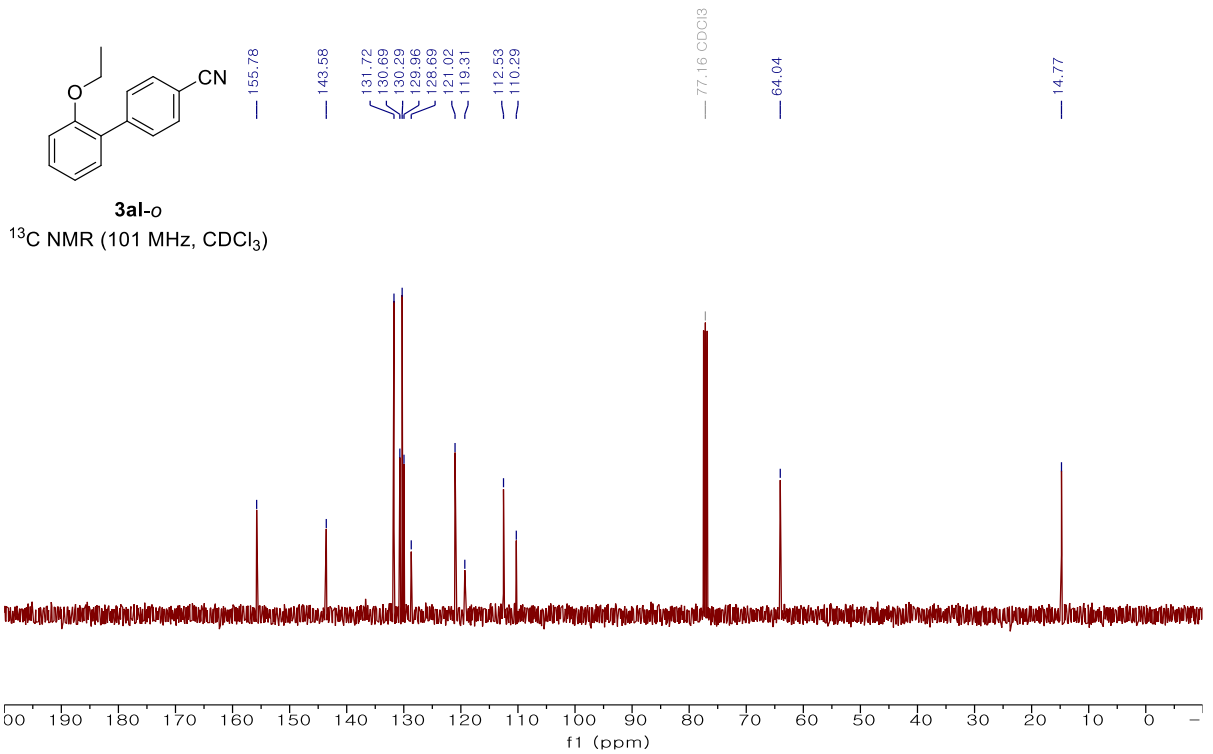
3al

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



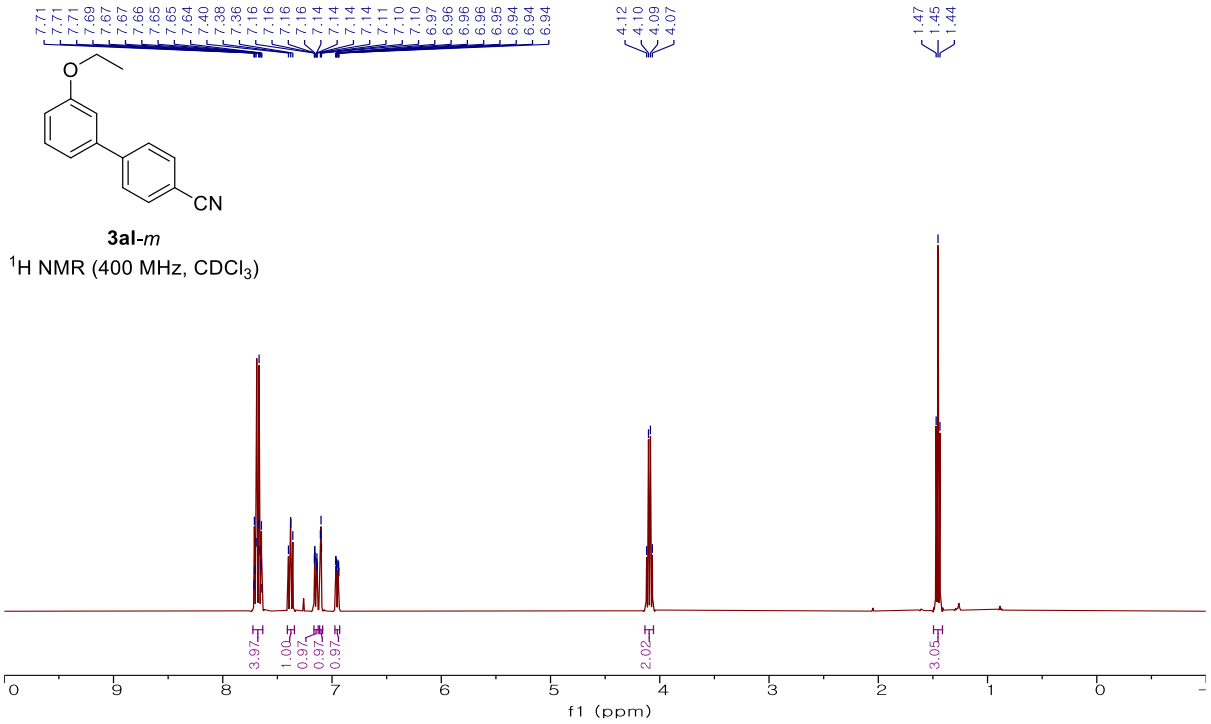
3al-*o*

^{1}H NMR (400 MHz, $CDCl_3$)



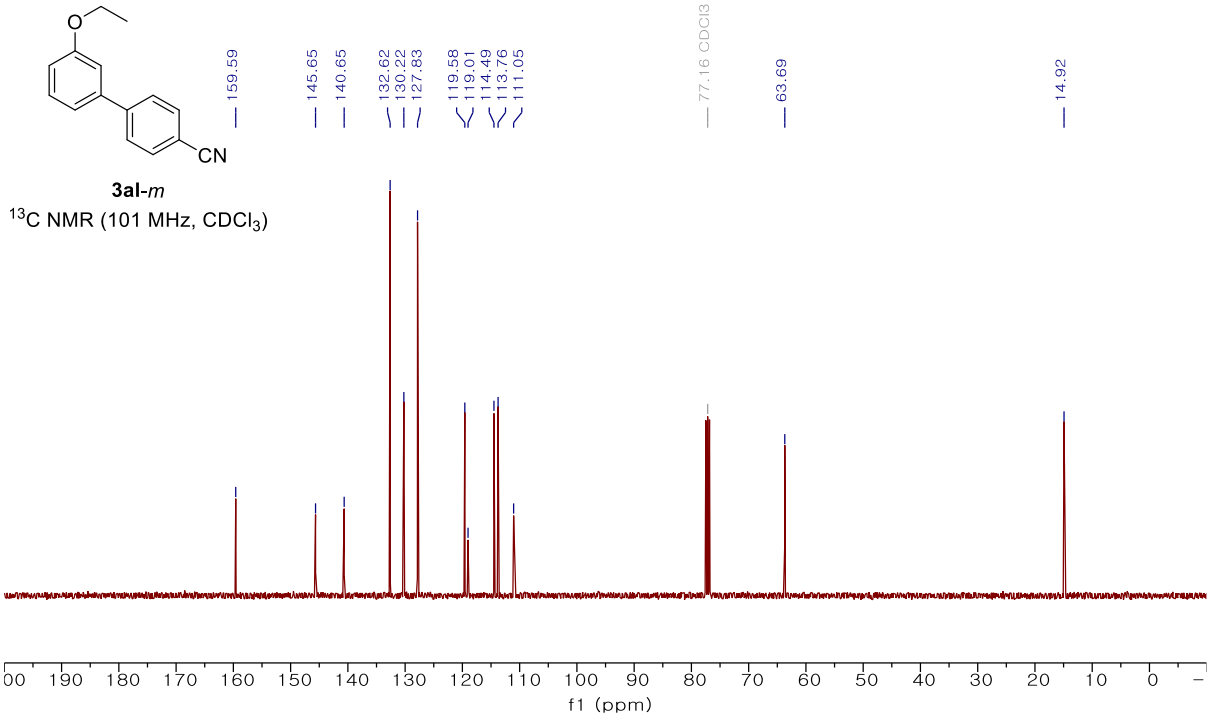
3al-*o*

^{13}C NMR (101 MHz, $CDCl_3$)



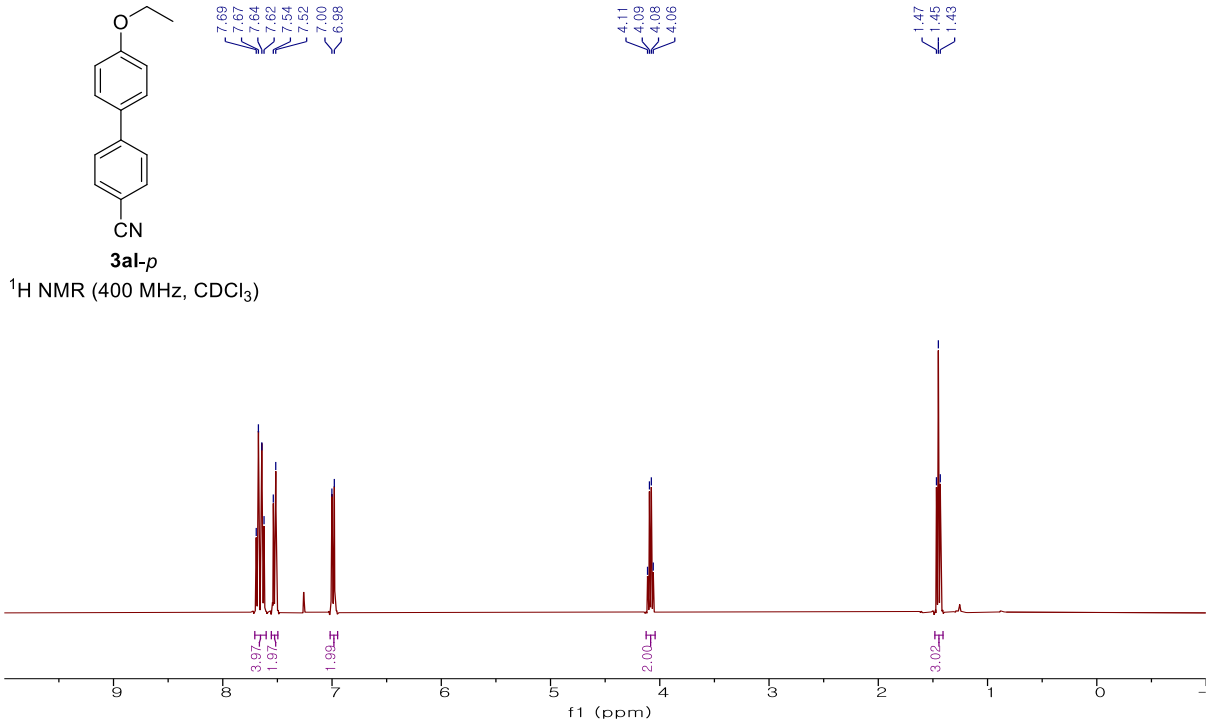
3al-*m*

^{1}H NMR (400 MHz, $CDCl_3$)



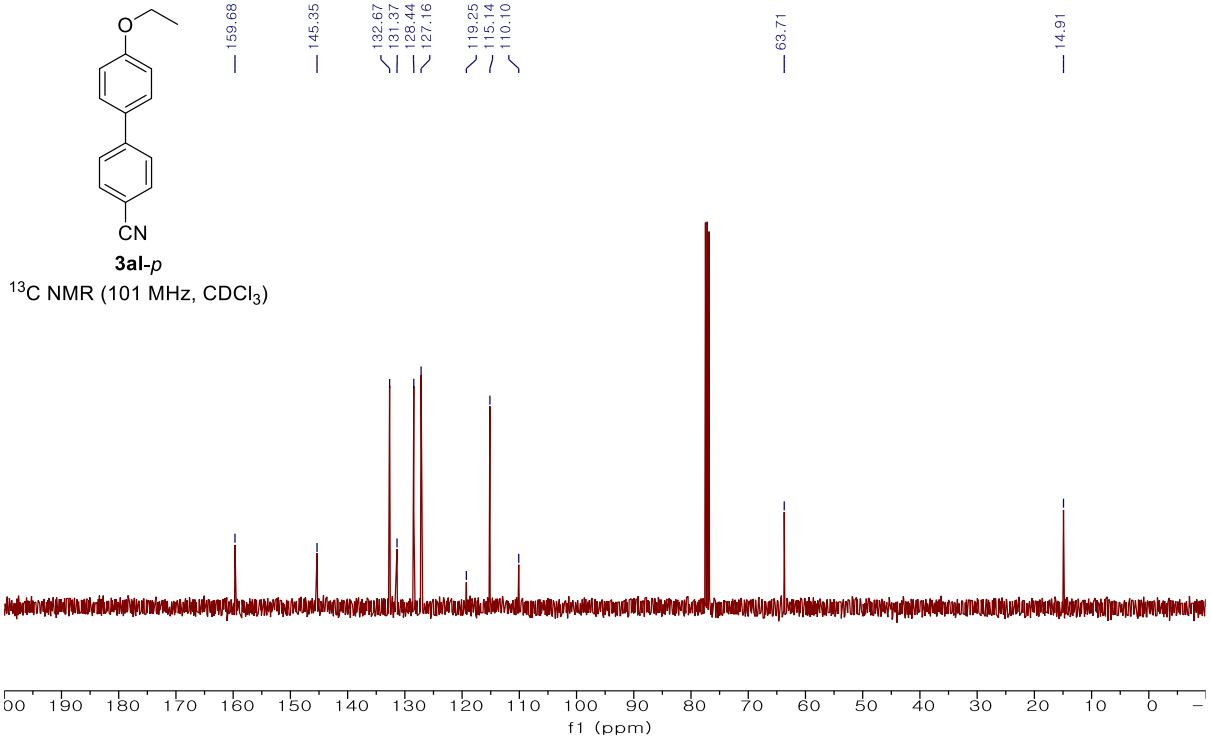
3al-*m*

^{13}C NMR (101 MHz, $CDCl_3$)



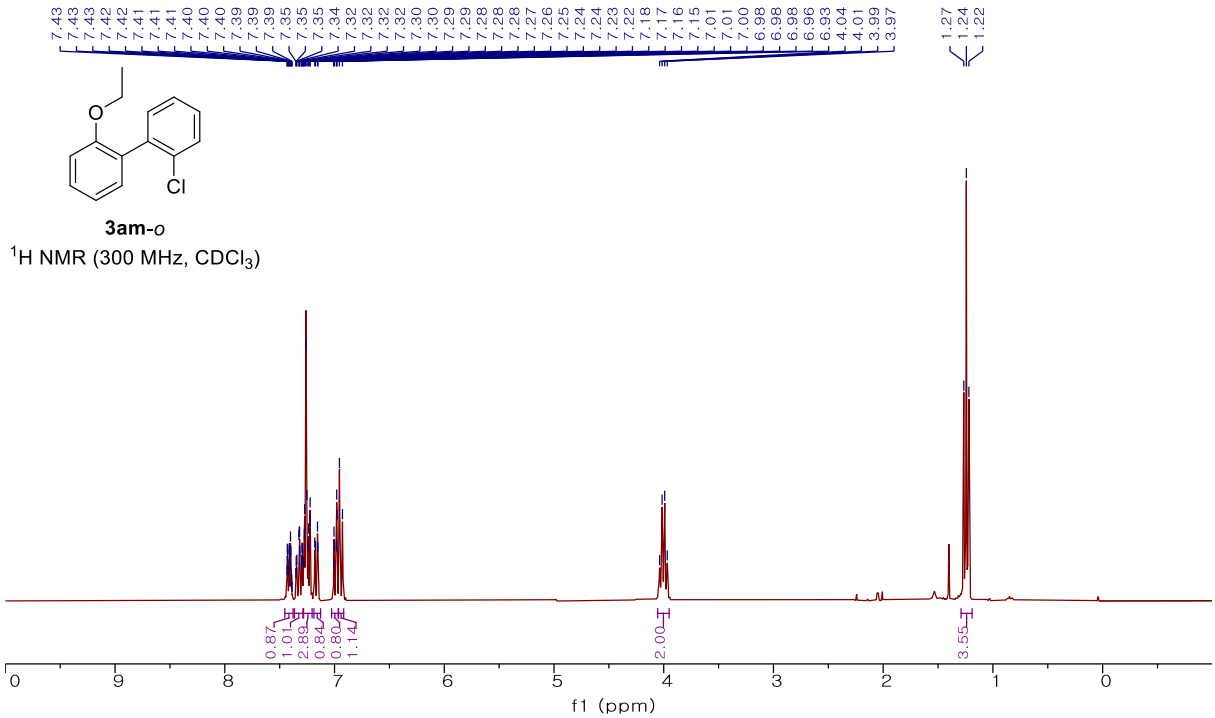
3al-*p*

^{1}H NMR (400 MHz, $CDCl_3$)



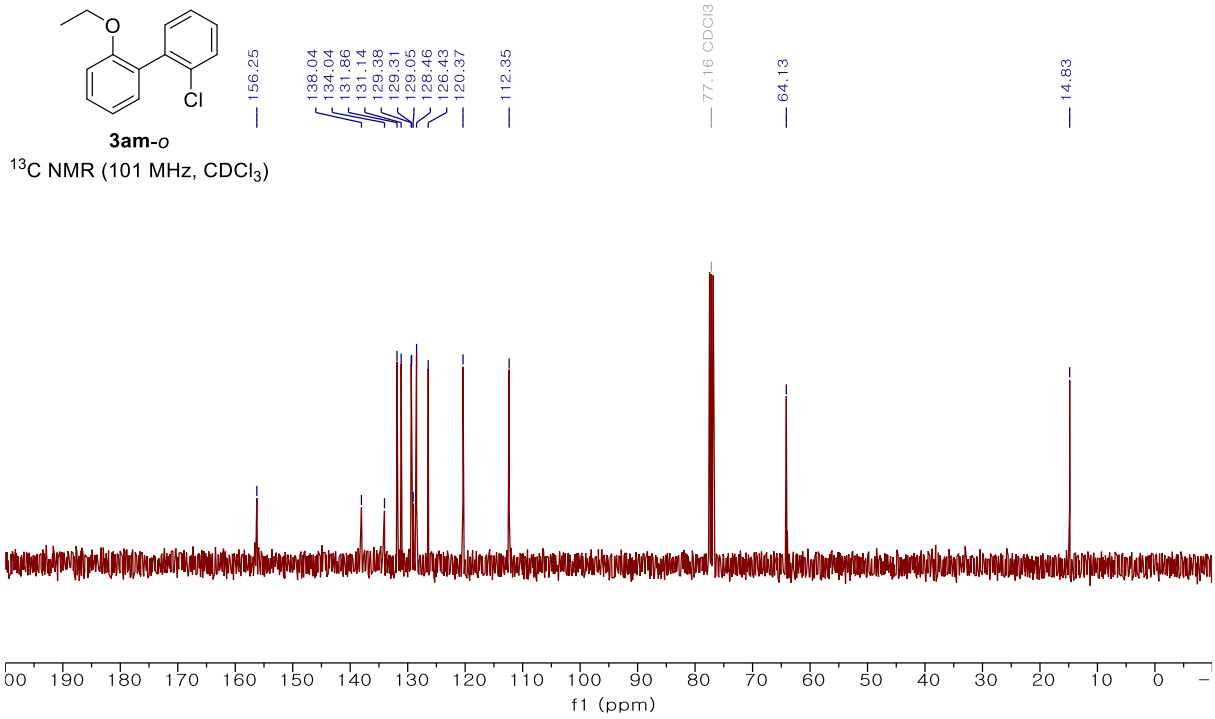
3al-*p*

^{13}C NMR (101 MHz, $CDCl_3$)



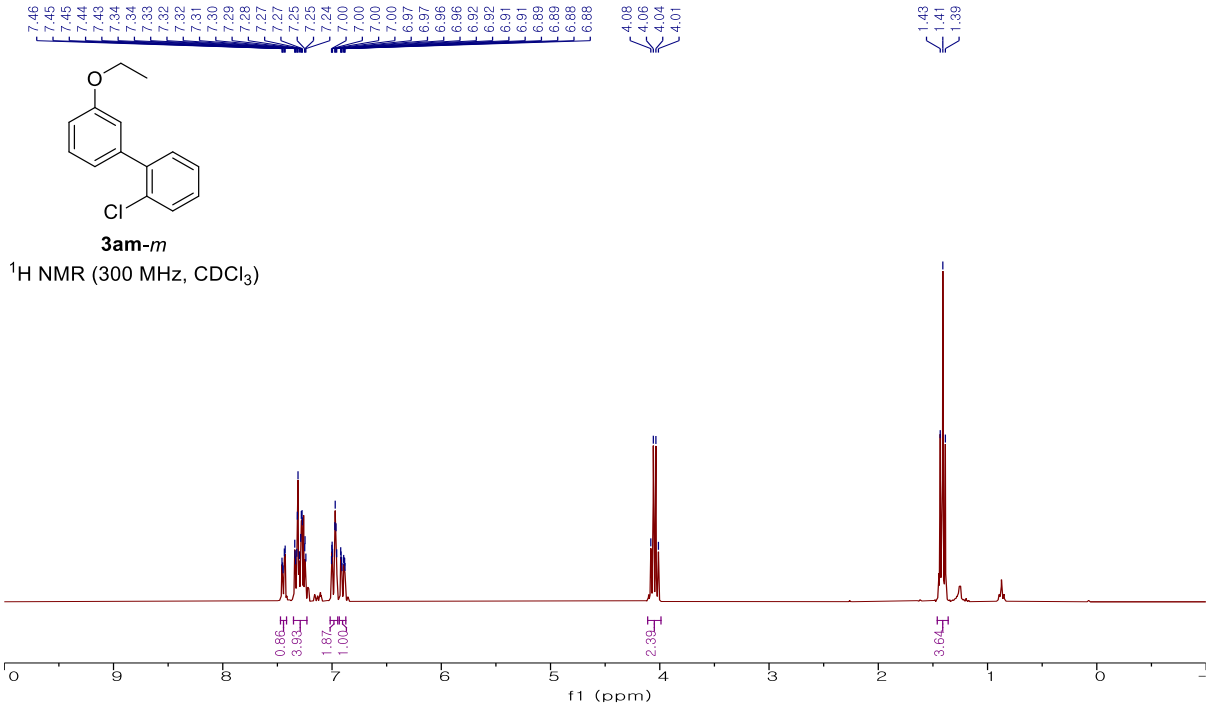
3am-*o*

^{1}H NMR (300 MHz, $CDCl_3$)



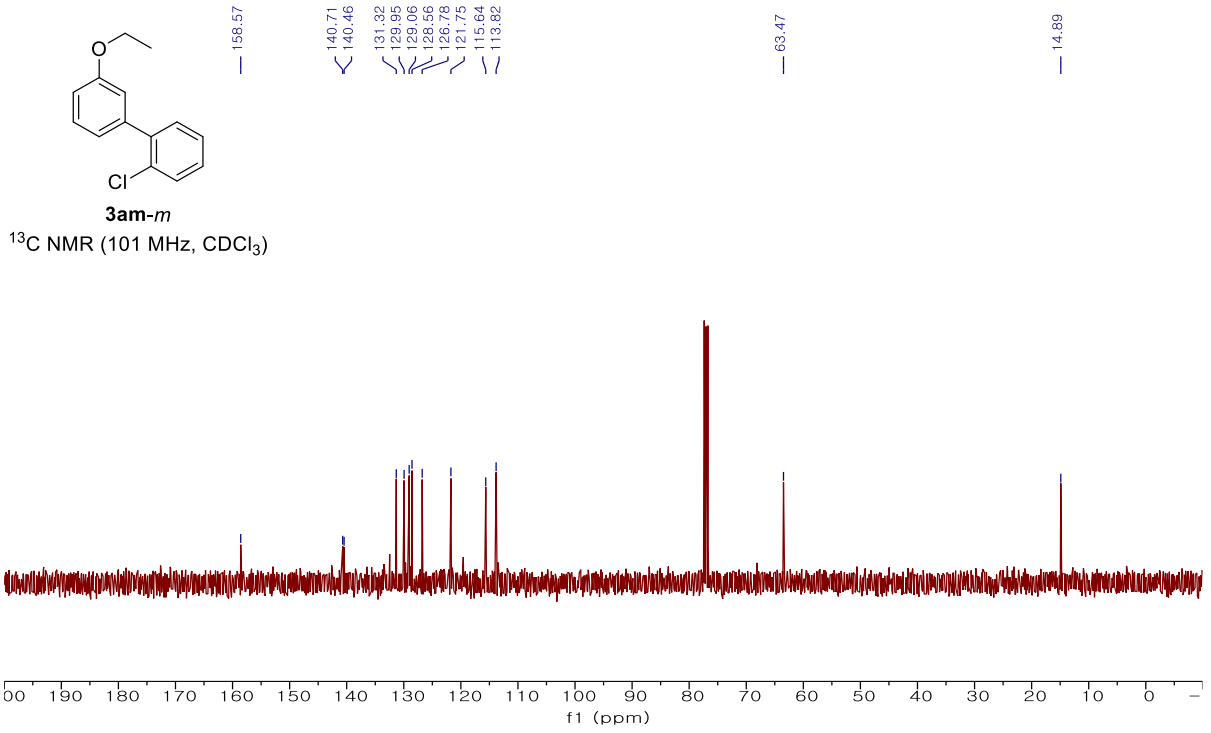
3am-*o*

^{13}C NMR (101 MHz, $CDCl_3$)



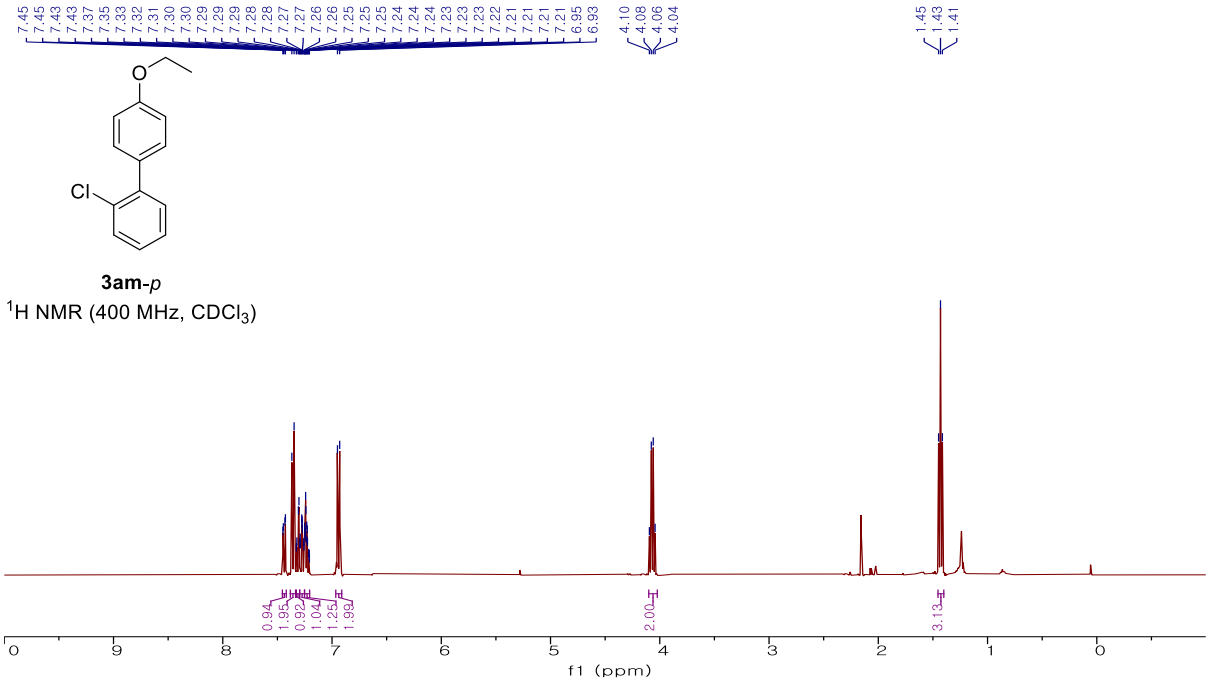
3am-*m*

^{1}H NMR (300 MHz, $CDCl_3$)



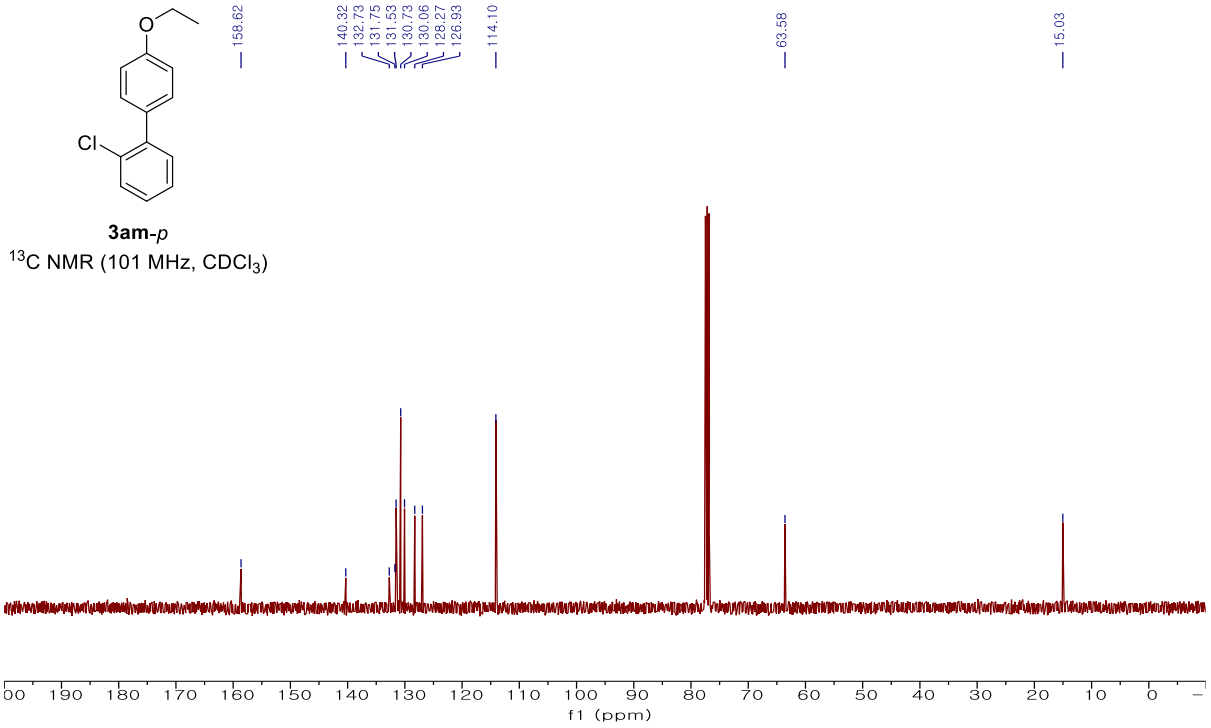
3am-*m*

^{13}C NMR (101 MHz, $CDCl_3$)



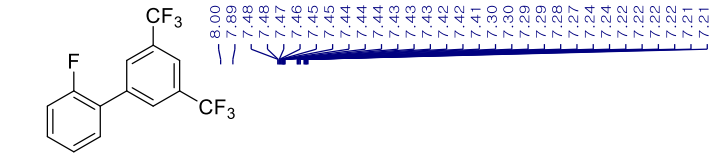
3am-*p*

^{1}H NMR (400 MHz, $CDCl_3$)



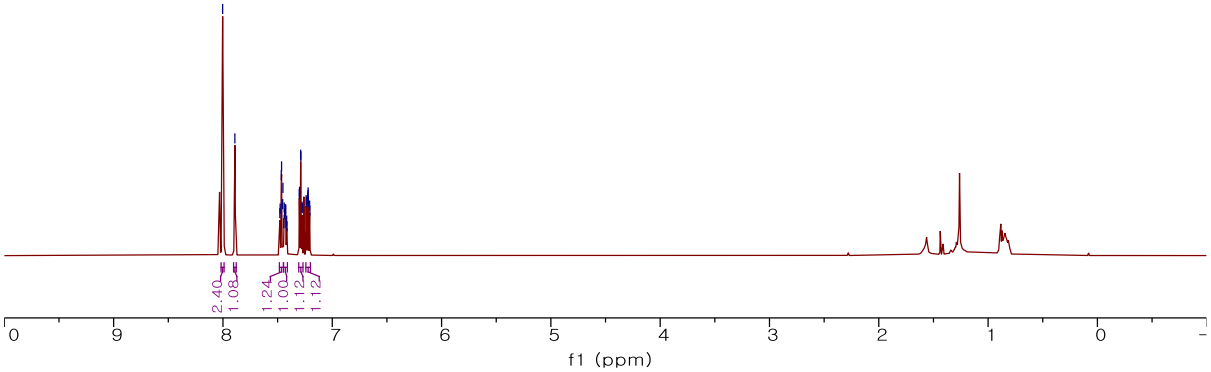
3am-*p*

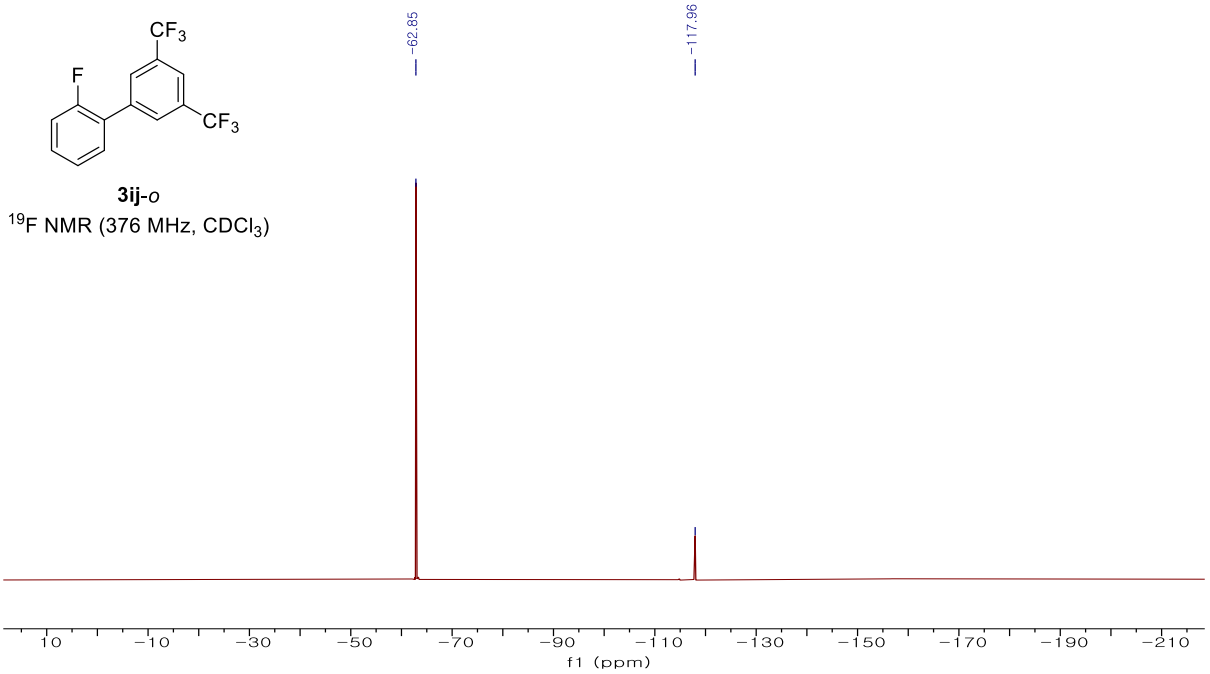
^{13}C NMR (101 MHz, $CDCl_3$)



3ij-*o*

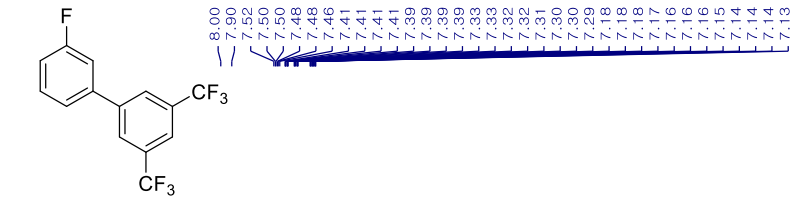
^{1}H NMR (600 MHz, $CDCl_3$)





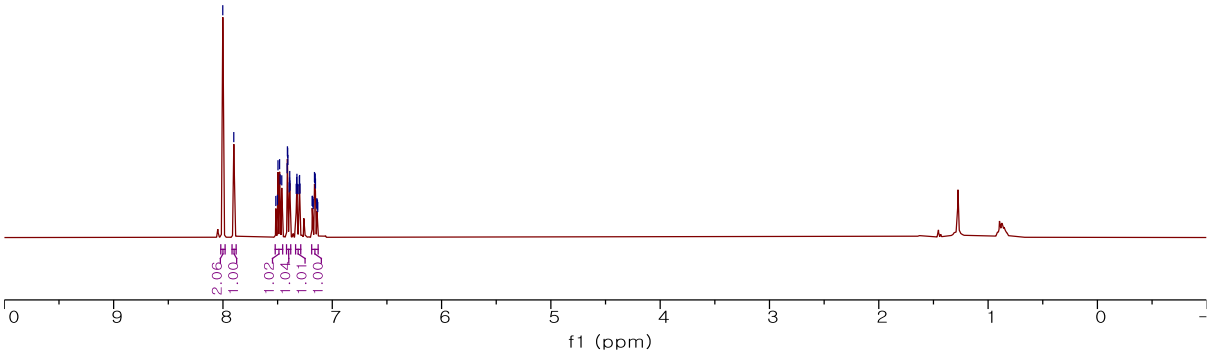
3ij-*o*

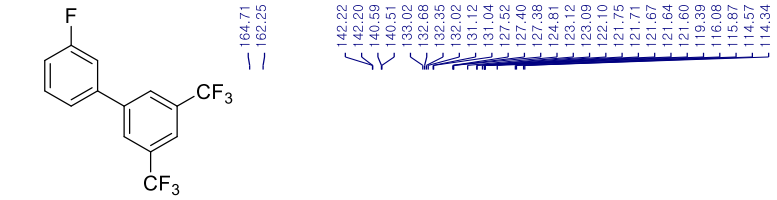
^{19}F NMR (376 MHz, $CDCl_3$)



3ij-*m*

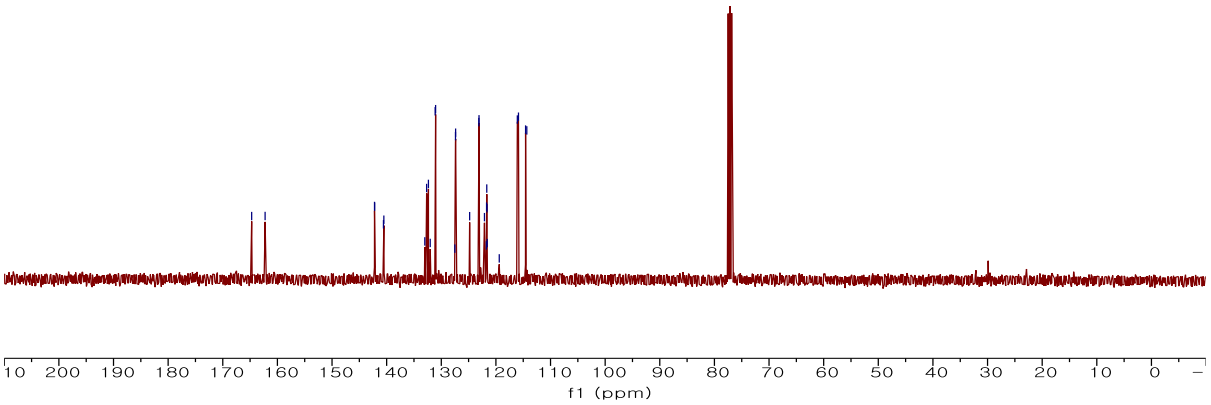
^{1}H NMR (400 MHz, $CDCl_3$)

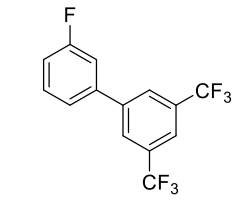




3ij-*m*

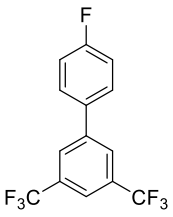
^{13}C NMR (101 MHz, $CDCl_3$)





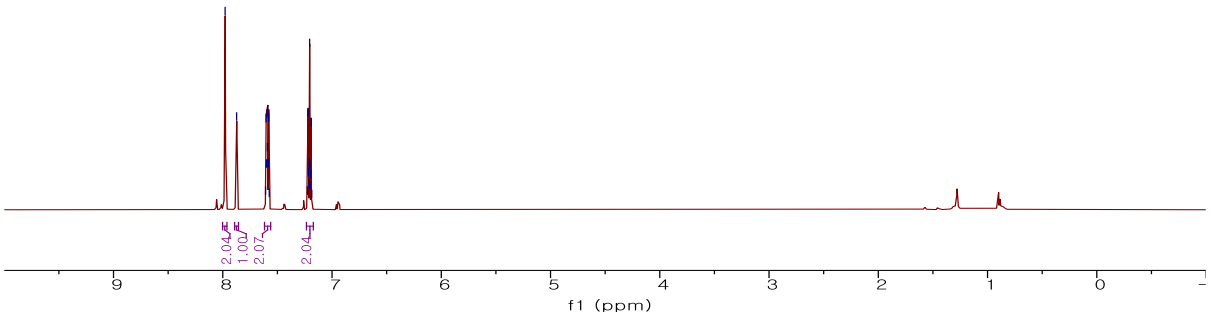
3ij-*m*

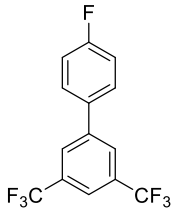
^{19}F NMR (376 MHz, $CDCl_3$)



3ij-*p*

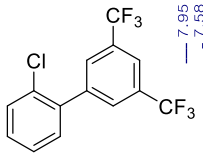
^{1}H NMR (600 MHz, $CDCl_3$)





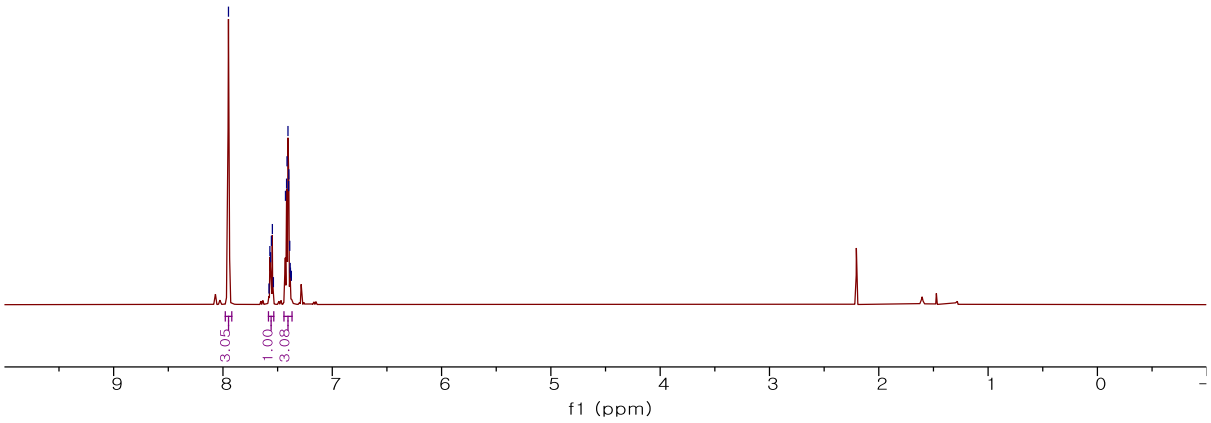
3ij-*p*

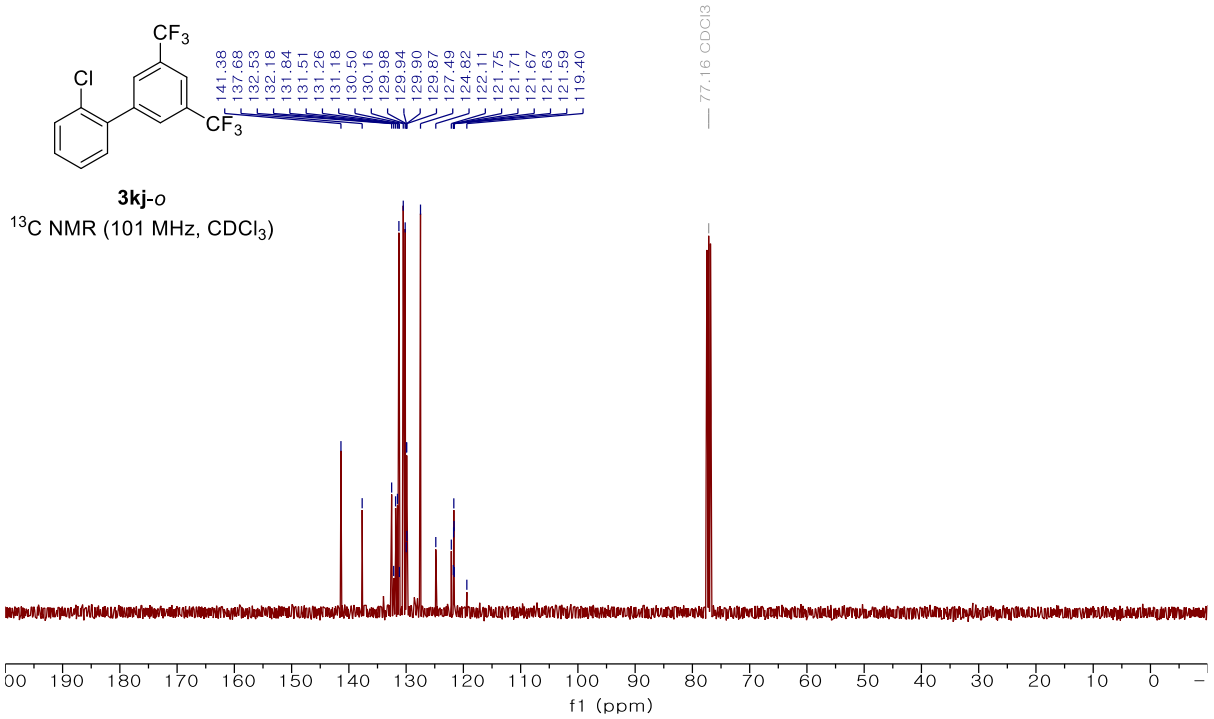
^{19}F NMR (376 MHz, $CDCl_3$)



3kj-*o*

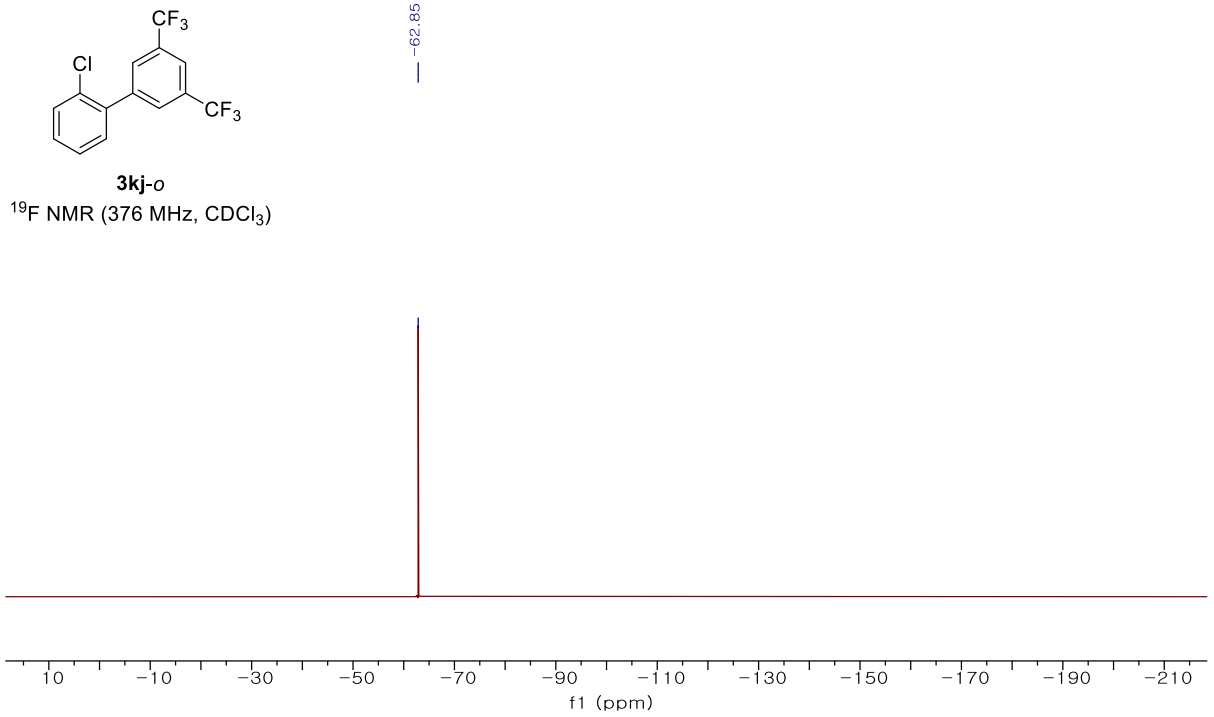
^{1}H NMR (400 MHz, $CDCl_3$)





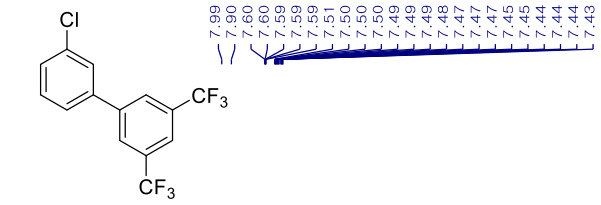
3kj-*o*

^{13}C NMR (101 MHz, $CDCl_3$)



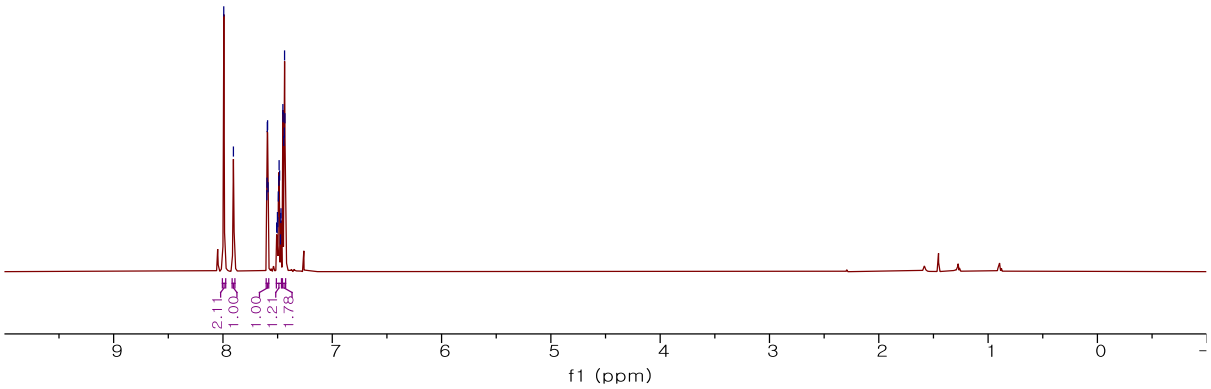
3kj-*o*

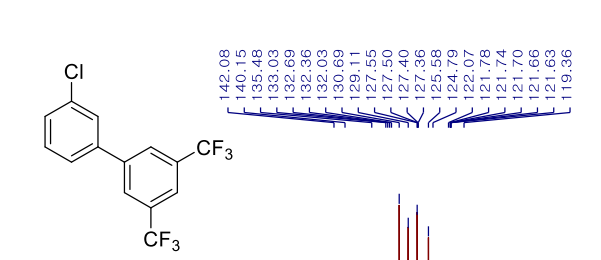
^{19}F NMR (376 MHz, $CDCl_3$)



3kj-*m*

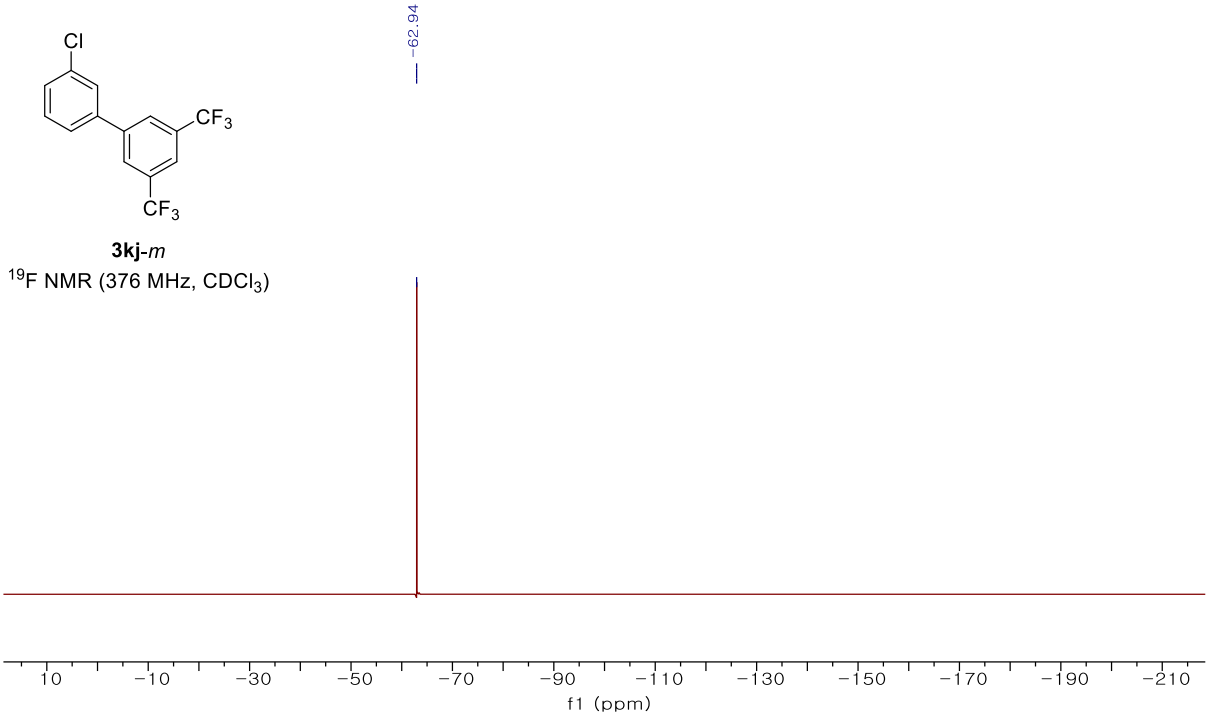
^{1}H NMR (400 MHz, $CDCl_3$)





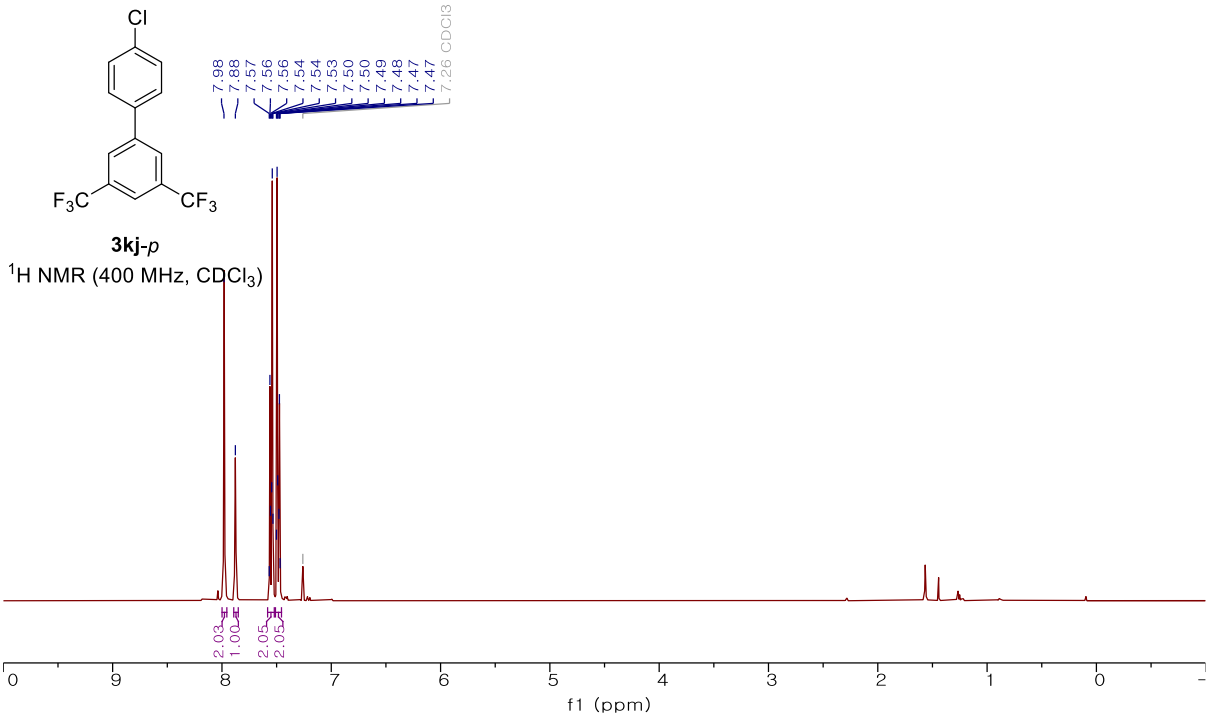
3kj-*m*

^{13}C NMR (101 MHz, $CDCl_3$)



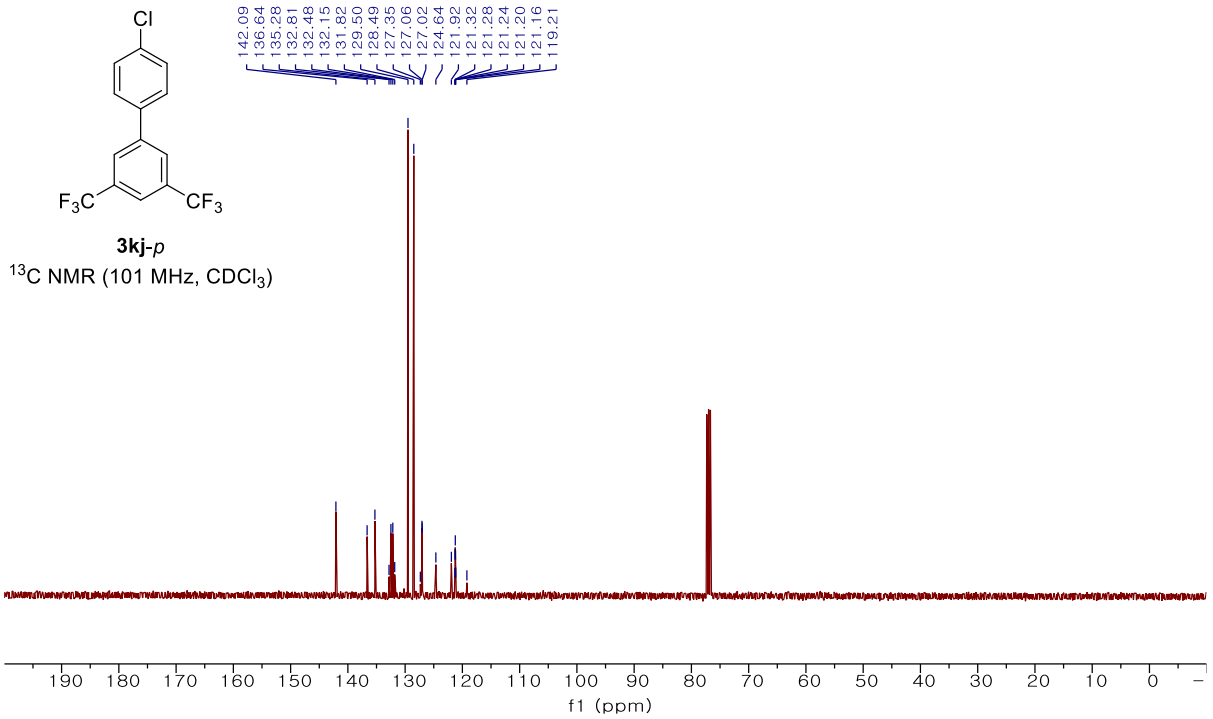
3kj-*m*

^{19}F NMR (376 MHz, $CDCl_3$)



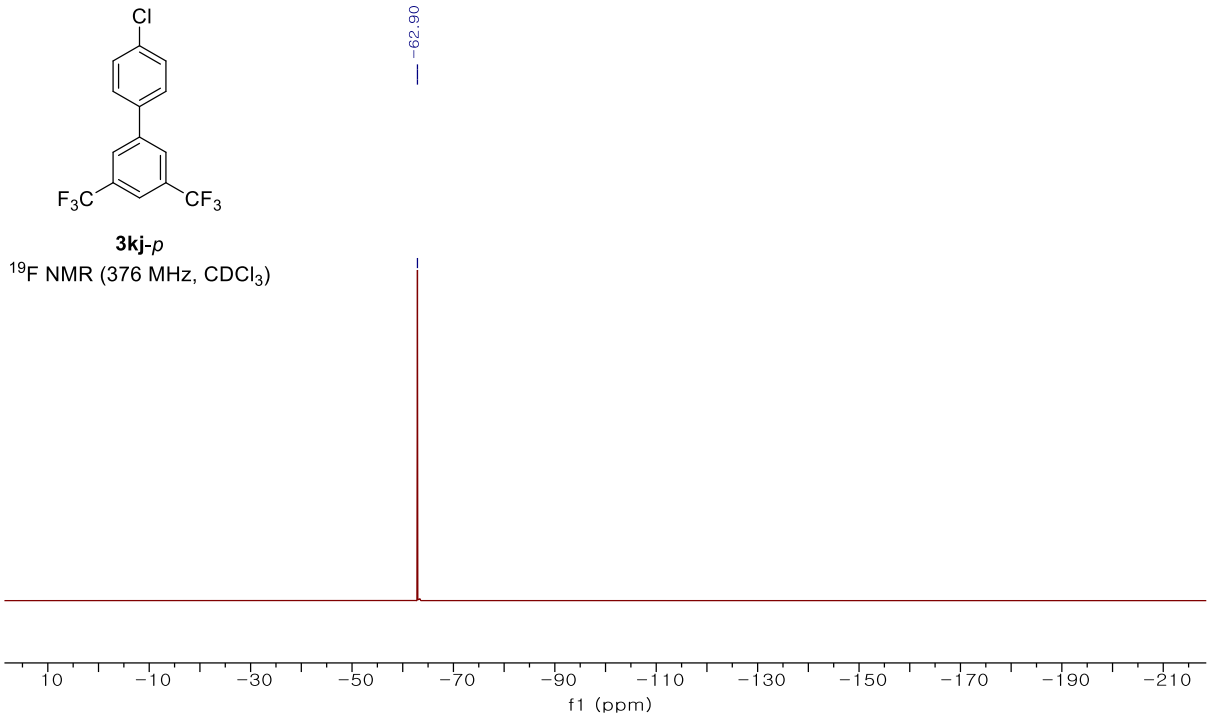
3kj-*p*

^{1}H NMR (400 MHz, $CDCl_3$)



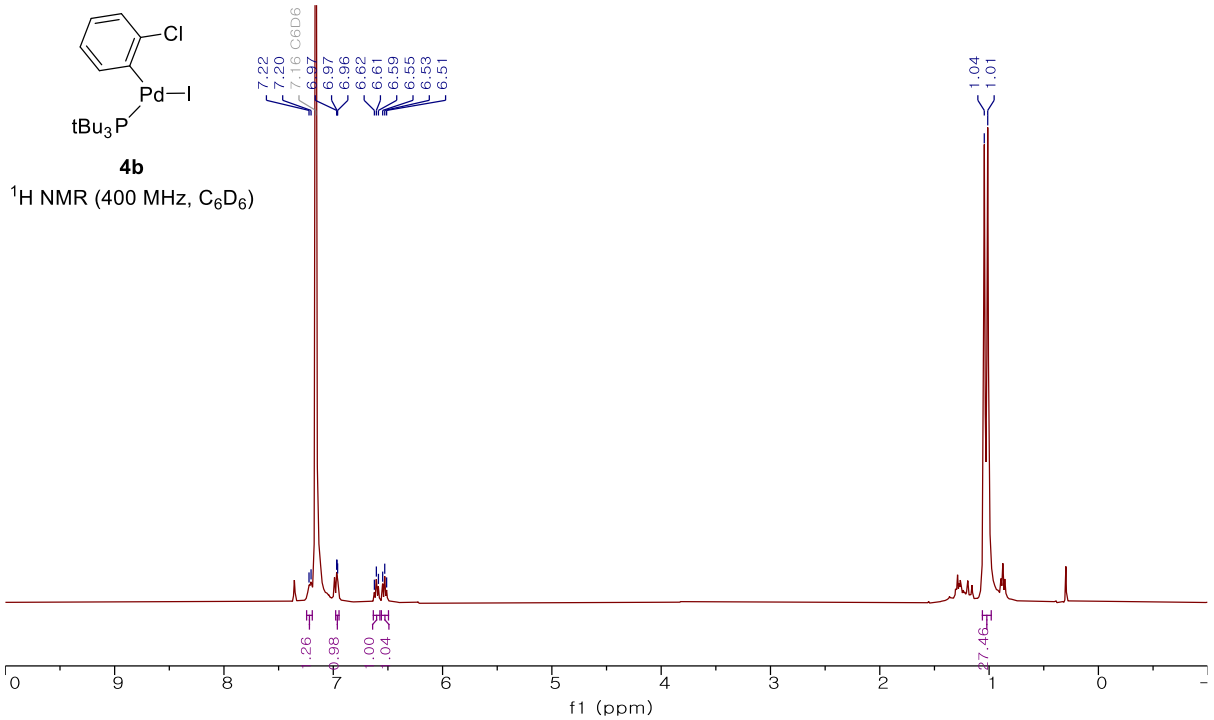
3kj-*p*

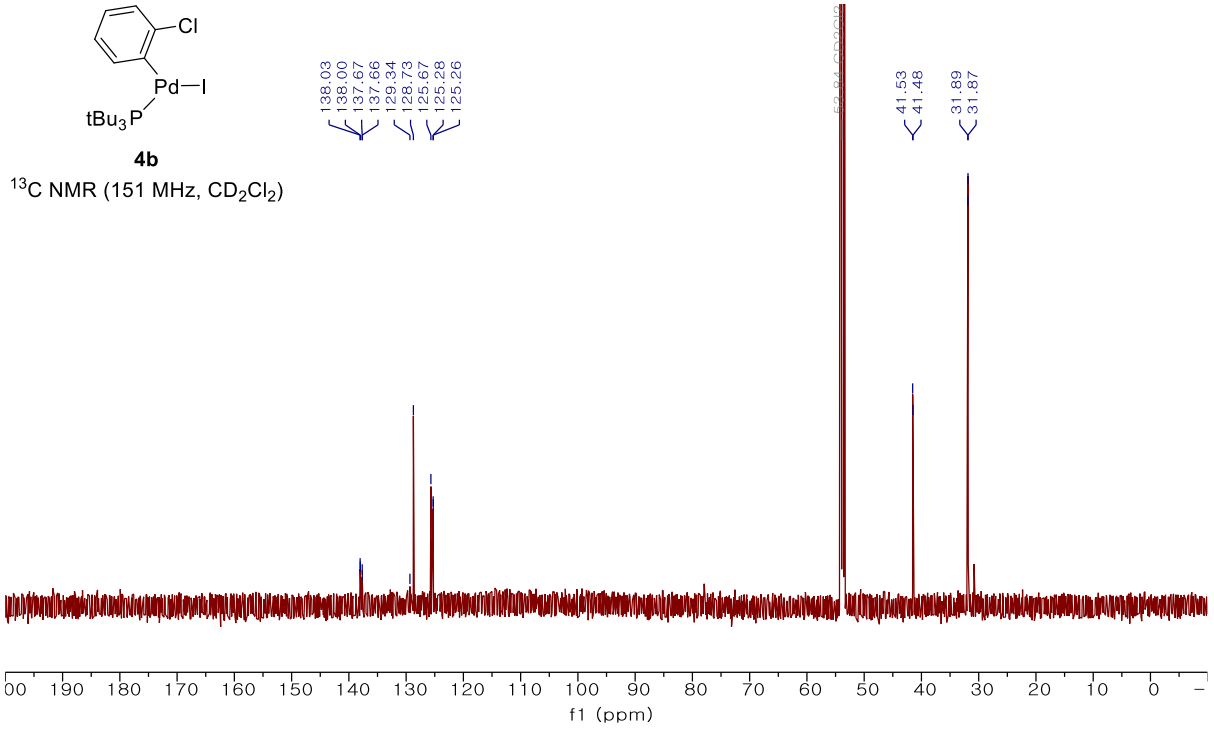
^{13}C NMR (101 MHz, $CDCl_3$)

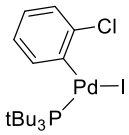


3kj-*p*

^{19}F NMR (376 MHz, $CDCl_3$)

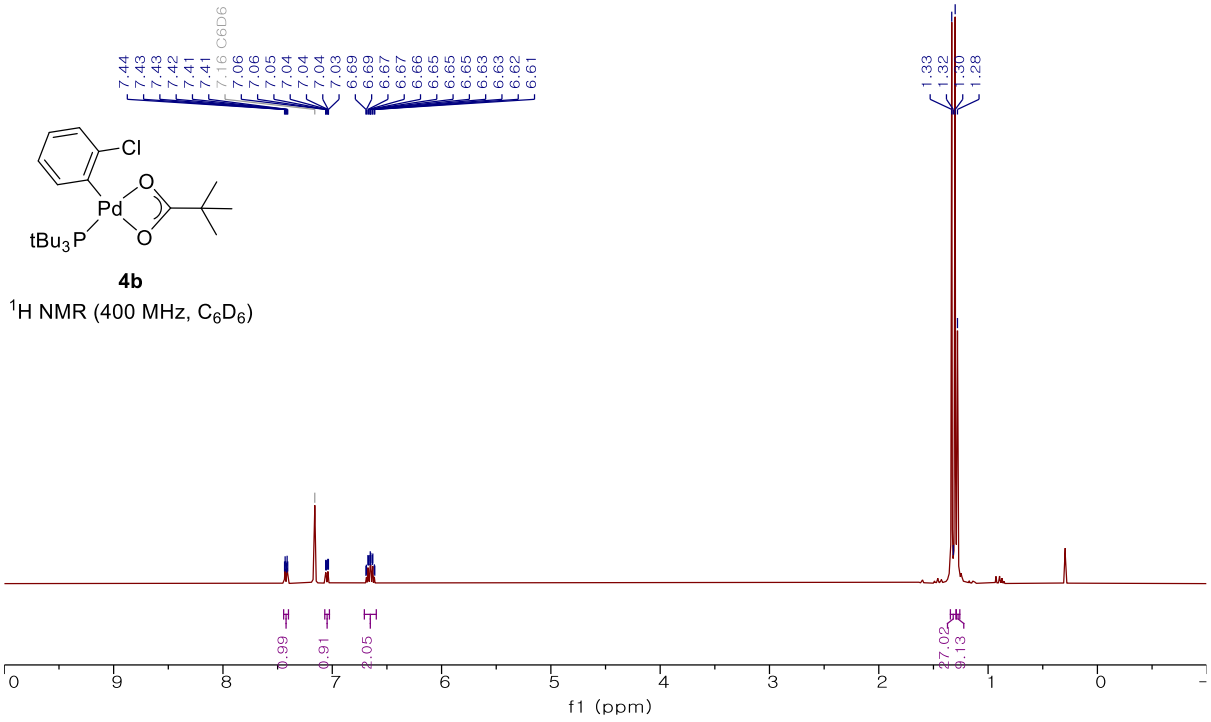

Cl
Pd—I
tBu3P
4b
1H NMR (400 MHz, C6D6)
7.22
7.20
7.16 C6D6
6.97
6.97
6.96
6.62
6.61
6.59
6.55
6.53
6.51
1.04
1.01
1.26
0.98
1.00
1.04
27.46
f1 (ppm)


Cl
Pd—I
tBu3P
4b
13C NMR (151 MHz, CD2Cl2)
138.03
138.00
137.67
137.66
129.34
128.73
125.67
125.28
125.26
53.84 CD2Cl2
41.53
41.48
31.89
31.87
f1 (ppm)



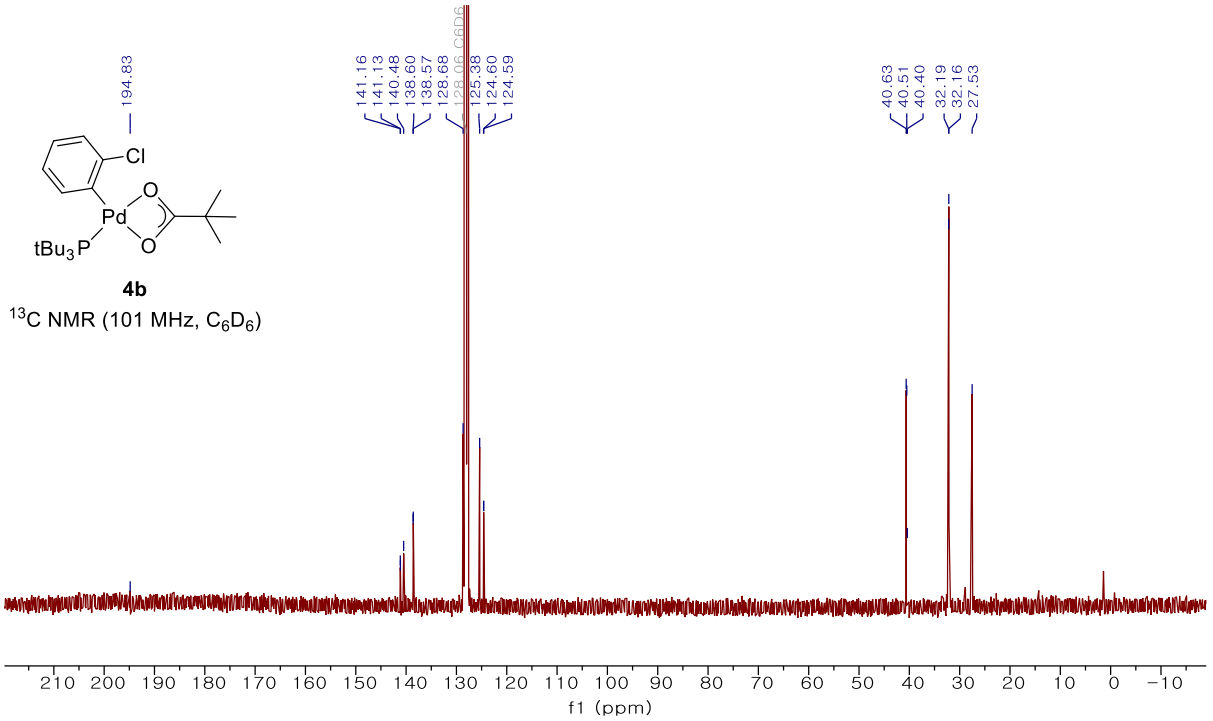
4b

^{31}P NMR (162 MHz, C_6D_6)



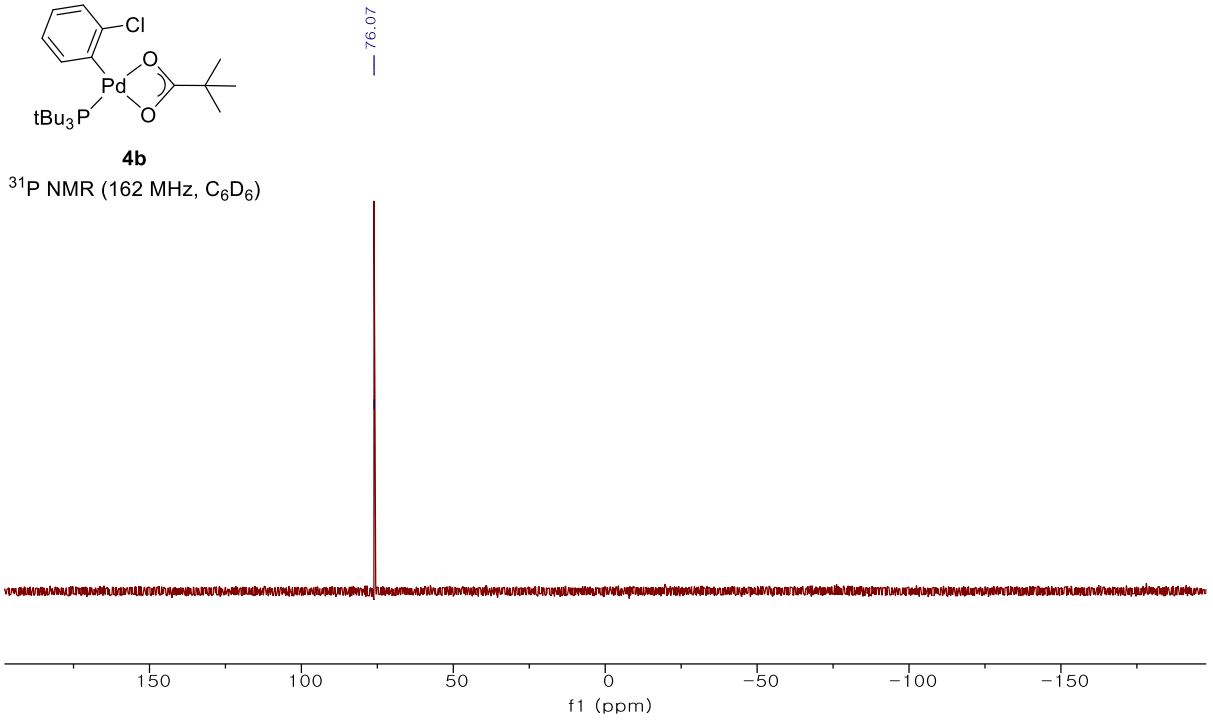
4b

^{1}H NMR (400 MHz, C_6D_6)



4b

^{13}C NMR (101 MHz, C_6D_6)



4b

^{31}P NMR (162 MHz, C_6D_6)

12. X-ray Crystallographic Data

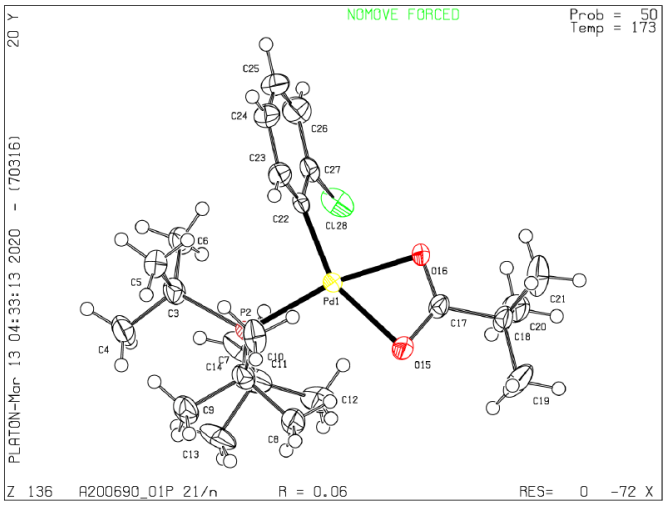


Table S20. Crystal Data and Structure Refinement for **4b**

Identification code	**4b** (CCDC 2000400)	
Empirical formula	$C_{23}H_{40}O_2PClPd$	
Formula weight	521.37	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.7932(5) Å	α = 90°
	b = 13.0955(6) Å	β = 93.9044(18)°
	c = 19.8473(10) Å	γ = 90°
Volume	2539.4(2) Å ^{3}	
Z	4	
Density (calculated)	1.364 Mg/m^3	
Absorption coefficient	0.914 mm^{-1}	
F(000)	1088	
Crystal size	0.157 x 0.112 x 0.087 mm^3	
Theta range for data collection	2.601 to 24.299°.	
Index ranges	–11<=h<=11, –15<=k<=15, –22<=l<=22	
Reflections collected	49846	
Independent reflections	4109 [R(int) = 0.0589]	
Completeness to theta = 24.299°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7455 and 0.6665	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4109 / 0 / 265	
Goodness-of-fit on F^2	1.225	
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.1539	
R indices (all data)	R1 = 0.0629, wR2 = 0.1551	
Largest diff. peak and hole	0.913 and –2.224 e·Å $^{-3}$	