Supporting Information

Amide-Ligand-Controlled Highly *para*-Selective Arylation of Monosubstituted Simple Arenes with Arylboronic Acids

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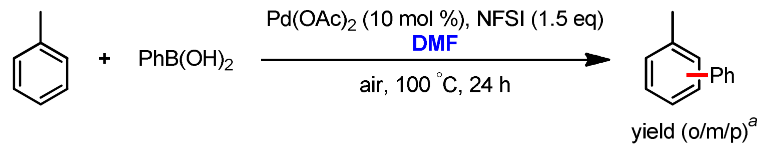
1. General Information

Unless otherwise noted, all solvents were received from commercial sources without further purification. Commercially available reagents were used as received. All reagents were handled under air except for $AgSbF_6$ due to its high hygroscopicity. Non-commercially available compounds were synthesized following reported protocols. Silica gel (particle size 40-63 μm) was used for flash column chromatography. GC-MS spectra were recorded on a Thermo Scientific ISQ Single Quadrupole GC/MS with a flame ionization detector. NMR spectra were recorded on Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR), 376 MHz (^{19}F NMR). Proton and carbon chemical shifts are reported relative to the solvent used as an internal reference. High resolution mass spectra (HRMS) were recorded on an Agilent 6520 Q-TOF LC/MS with Electron Spray Ionization (ESI) resource.

2. Reaction Optimization

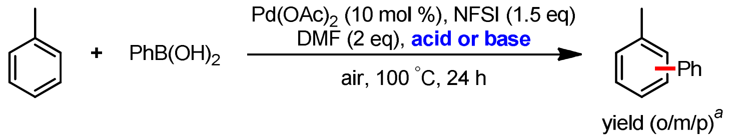
Table S1. DMF Loading Effects



entry	DMF (eq)	yield (o/m/p) [b]
1	0.2 (3 μL)	9% (2.3:1:0)
2	2.0 (30 μL)	13% (0.8:1:6.9)
3	10.0 (154 μL)	8% (0.6:1:8.5)
4	**20.0 (308 μL)**	**7% (0.5:1:9.1)**
5	35.0 (500 μL)	5% (0.2:1:13)
6	140 (2 mL/0.2mL toluene)	4% (0: 0: 1)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $Pd(OAc)_2$ (0.02 mmol), NFSI (0.3 mmol), 100 °C under air for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

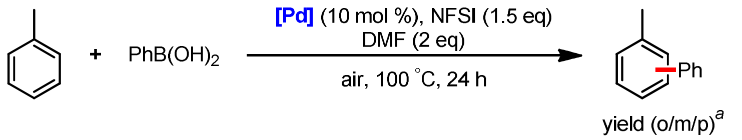
Table S2. Screening of Acids and Bases



entry	acid/base (eq)	yield (o/m/p)[b]
1	K_2CO_3 (0.5)	8% (0:1:15)
2	KOAc (0.5)	7% (0.5:1:21)
3	TFA (10)	9% (1.4:1:0)
4	TFA (5)	12% (1.6:1:0.9)
5	TFA (0.5)	13% (0.8:1:4.0)
6	TFA (10) + KH_2PO_4 (0.5)	5% (1:1:0)
7	HOAc (5)	6% (1:1:16)
8	HOAc (0.5)	10% (1:1:8)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $Pd(OAc)_2$ (0.02 mmol), NFSI (0.3 mmol), DMF (2 eq), 100 °C under air for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

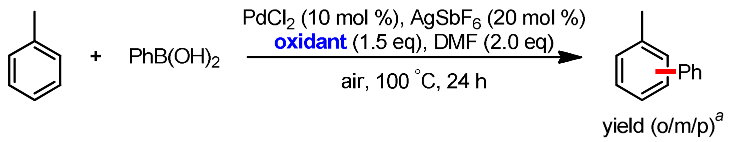
Table S3. Screening of Palladium Catalysts

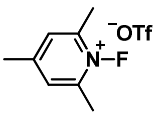


entry	[Pd]	yield (o/m/p)[b]
1	$Pd(OAc)_2$	15% (1:1:7)
2	$Pd(TFA)_2$	14% (1:1:6)
3	$PdCl_2$/AgOTf (1:2)	22% (1:1:10)
4	**$PdCl_2$/$AgSbF_6$ (1:2)**	**41% (0.6:1:16)**
5	$PdCl_2(CH_3CN)_2$	22% (1:2:15)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), [Pd] (0.02 mmol), NFSI (0.3 mmol), DMF (2 eq), 100 °C under air for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

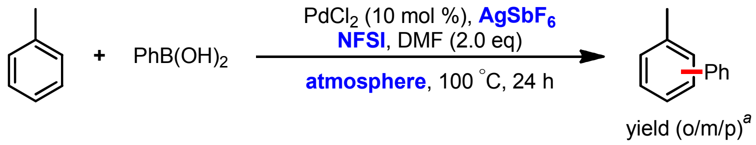
Table S4. Screening of Oxidants



entry	oxidant	yield (o/m/p)[b]
1	**NFSI**	**41% (0.6:1:16)**
2	$PhI(OAc)_2$	0.4% (1:1:1)
3	$Na_2S_2O_8$	0
4	SelectFluor	2% (1:1:15)
5		0

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.04 mmol), DMF (2 eq), 100 °C under air for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

Table S5. Loading Effect of $AgSbF_6$ and NFSI and Atmosphere Effect

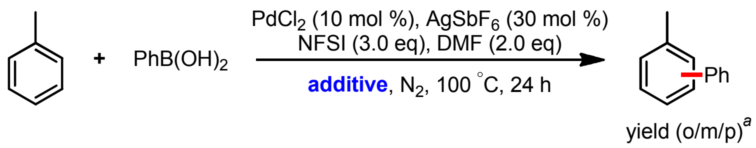


entry	$AgSbF_6$ (mol %)	NFSI (eq)	atmosphere	yield (o/m/p)[b]
1	20	1.5	air	41% (0.6:1:16)
2	30	1.5	air	44% (0.6:1:22)
3	**30**	**3.0**	**air**	**54% (0.6:1:19)**
4	30	3.0	N_2	51% (0.5:1:23)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), DMF (2 eq), 100 °C for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

Note: Due to the high hygroscopicity, $AgSbF_6$ has to be handled under N_2. And thus, the following screening reactions were run under N_2 for convenience because the reaction under either air or N_2 gave almost the same result.

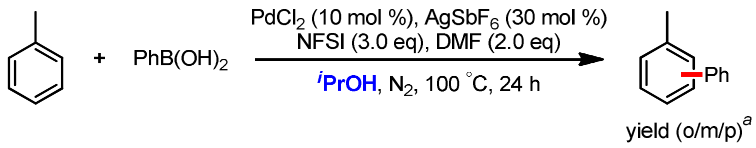
Table S6. Screening of Additives



entry	additive	yield (o/m/p)[b]
1		49% (0.6:1:19)
2	DCM (0.2 mL)	38% (1:1:45)
3	$TBABF_4$ (2 eq)	16% (1:1:23)
4	CH_3CN (0.1 mL)	25% (0.3:1:23)
5	CH_3CN (0.1 mmol)	38% (1:1:80)
6	**^{i}PrOH (0.1 mL)**	**58% (1:1:50)**
7	BQ (0.16 mmol)	3% (0:0:1)
8	BQ (0.04 mmol)	33% (1:1:50)
9	4Å MS (12 mg)	48% (0.5:1:25)
10	$N(^nBu)_3$ (0.04 mmol)	45% (0.5:1:25)
11	NaF (1 mmol)	49% (0.3:1:40)
12	cod (0.08 mmol)	0.7% (0:1:10)
13	cod (0.01 mmol)	47% (0.3:1:40)
14	acetone (0.6 mmol)	43% (0.2:1:30)
15	DMSO (0.02 mmol)	45% (0.3:1:30)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), NFSI (0.6 mmol), DMF (2 eq), 100 °C unde N_2 for 24 h; Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

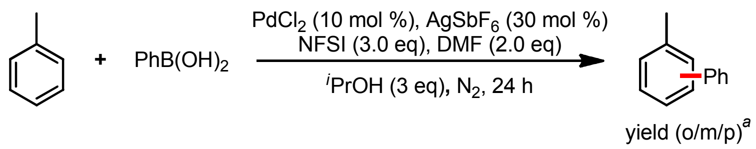
Table S7. Screening of the loading of ^{i}PrOH



entry	^{i}PrOH (eq)	yield (o/m/p) [b]
1	0.5 (8 μL)	36% (0.5:1:24)
2	1.0 (15 μL)	33% (0.5:1:35)
3	**3.0 (46 μL)**	**48% (0:1:50)**
4	6.0 (91 μL)	50% (0:1:35)
5	12.5 (190 μL)	47% (0.3:1:25)
6	25 (380 μL)	24% (1.3:1:20)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $Pd(OAc)_2$ (0.02 mmol), NFSI (0.3 mmol), 100 °C under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

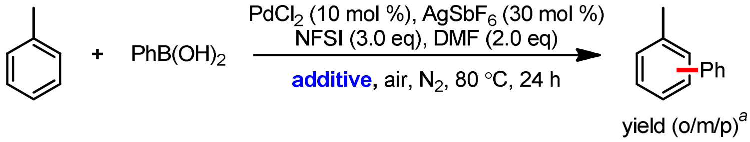
Table S8. Screening of Reaction Temperature



entry	temperature (°C)	yield (o/m/p) [b]
1	50	20% (0:1:80)
2	60	36% (0:1:65)
3	70	57% (0.3:1:53)
4	**80**	**59% (0.1:1:30)**
5	90	55% (0.2:1:40)
6	100	54% (0.2:1:30)
7	110	48% (0.2:1:30)
8	120	51% (0.3:1:30)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), NFSI (0.6 mmol), DMF (2 eq), ^{i}PrOH (3 eq), under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

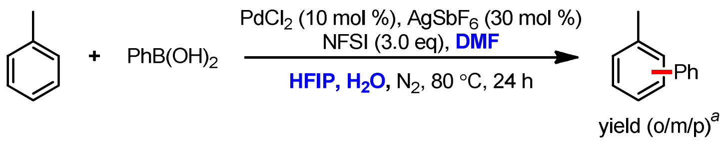
Table S9. Loading Effect of ^{i}PrOH and H_2O



entry	additive	yield (o/m/p)[b]
1	^{i}PrOH (3.0 eq)	59% (0.1:1:26)
2	^{i}PrOH (3.0 eq), H_2O (0.1 mmol, 2 uL)	56% (0.2:1:38)
3	^{i}PrOH (3.0 eq), H_2O (0.2 mmol, 4 uL)	63% (0.2:1:36)
4	^{i}PrOH (3.0 eq), H_2O (0.5 mmol, 9 uL)	58% (0.3:1:37)
5	^{i}PrOH (3.0 eq), H_2O (1.0 mmol, 18 uL)	48% (0.3:1:34)
6	^{i}PrOH (3.0 eq), H_2O (2.0 mmol, 36 uL)	33% (0.3:1:40)
7	**^{i}PrOH/H_2O (v/v = 10:1) (46 uL)**	**63% (0.2:1:30)**
8	^{i}PrOH/H_2O (v/v = 10:1) (100 uL)	57% (0.1:1:30)
9	^{i}PrOH/H_2O (v/v = 10:1) (200 uL)	41% (0.1:1:30)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), NFSI (0.6 mmol), DMF (2 eq), under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

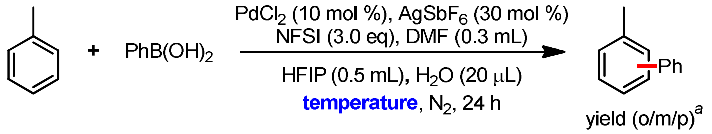
Table S10. HFIP Effect



entry	HFIP, DMF, H_2O	yield (o/m/p)[b]
1	HFIP (0.5 mL), DMF (0.3 mL), ^{i}PrOH/H_2O (10:1,100 uL)	69% (0.3:1:25)
2	HFIP (0.5 mL), DMF (0.3 mL), H_2O (10 uL)	68% (0.3:1:26)
3	**HFIP (0.5 mL), DMF (0.3 mL), H_2O (20 uL)**	**73% (0.3:1:27)**
4	HFIP (0.5 mL), DMF (0.3 mL), H_2O (30 uL)	67% (0.3:1:27)
5	HFIP (0.3 mL), DMF (0.4 mL), H_2O (10 uL)	69% (0.3:1:22)
6	HFIP (0.3 mL), DMF (0.3 mL), H_2O (10 uL)	68% (0.3:1:23)
7	HFIP (0.3 mL), DMF (0.2 mL), H_2O (10 uL)	70% (0.3:1:26)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), NFSI (0.6 mmol), 80 °C under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

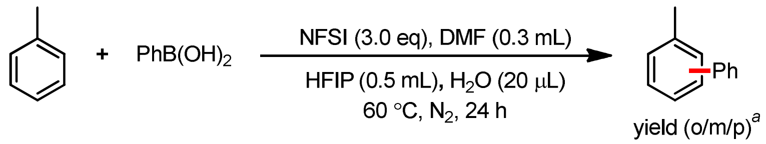
Table S11. Temperature Screening in the Presence of HFIP



entry	temperature (°C)	yield (o/m/p)[b]
1	rt	70% (0.6:1:120)
2	40	80% (0.4:1:89)
3	60	82% (0.6:1:110)
4	80	74% (0.5:1:63)
5	100	75% (0.5:1:45)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), NFSI (0.6 mmol), DMF (0.3 mL), HFIP (0.5 mL), H_2O (20 μL), under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

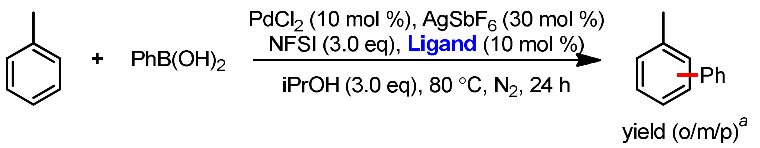
Table S12. Loading Effects of Catalyst and Toluene

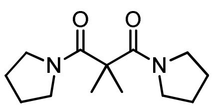


entry	$PdCl_2$ (mol %)/$AgSbF_6$ (mol %)	toluene (mL)	yield (o/m/p)[b]
1	10/30	2.0	82% (0.6:1:110)
2	10/30	1.5	80% (0.4:1:99)
3	10/30	1.0	72% (0.5:1:128)
4	5/15	2.0	78% (0.4:1:91)
5	3/9	2.0	61% (0.3:1:64)

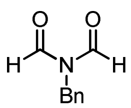
[a] Reaction condition: phenylboronic acid (0.2 mmol), NFSI (0.6 mmol), DMF (0.3 mL), HFIP (0.5 mL), H_2O (20 μL), under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity was determined by GC with dodecane as an internal standard.

Table S13. Screening of Bidentate Amide Ligands

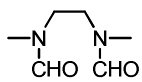




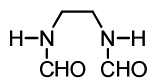
L13, 7% (2.5:1:1.4)



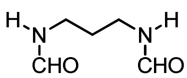
L14, 11% (2.6:1:1.4)



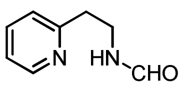
L15, 8% (2.6:1:1.9)



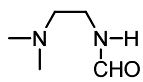
L16, 4% (1.8:1:11)



L17, 7% (2.4:1:3.1)



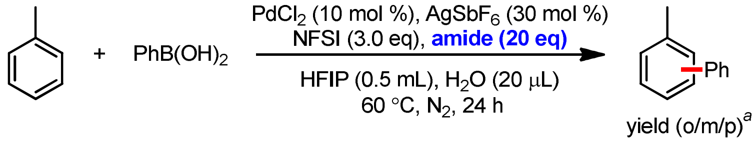
L18, 4% (2.2:1:2.8)

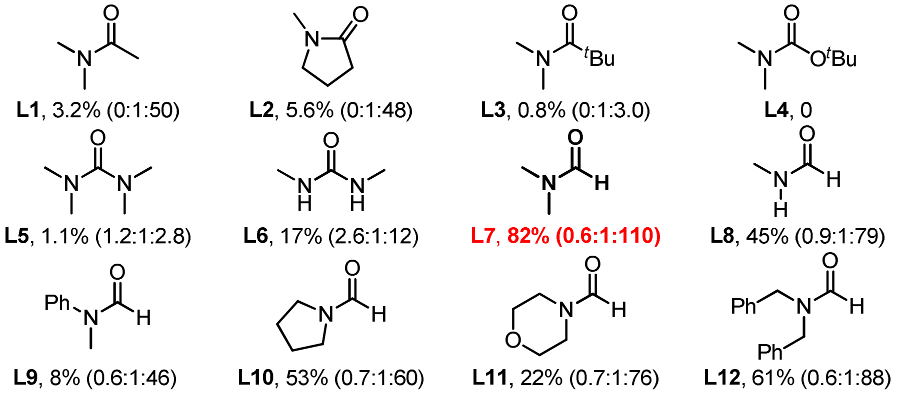


L19, 5% (2.3:1:1.9)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (0.06 mmol), **NFSI** (0.6 mmol), ^{i}PrOH (0.5 mL), 80 °C under N_2 for 24 h; [b] Combined yield and regioselectivity was determined by GC with dodecane as an internal standard.

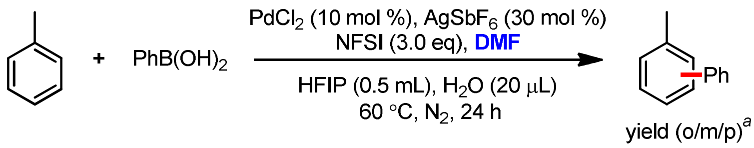
Table S14. Ligand Effects under Optimized Conditions





[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $PdCl_2$ (0.02 mmol), $AgSbF_6$ (30 mol %), amide (20 eq), HFIP (0.5 mL), H_2O (20 μL), N_2, 60 °C for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

Table S15. DMF Loading Effects under Optimized Conditions

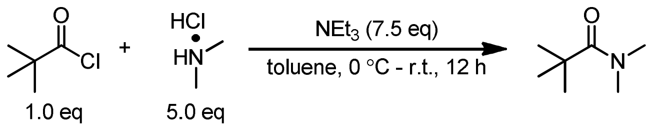


entry	DMF (eq)	yield (o/m/p)[b]
1	0	3% (4.0:1:5)
2	0.5 (8 μL)	7% (0.5:1:23)
3	1.0 (15 μL)	13% (3.3:1:95)
4	2.0 (31 μL)	24% (0.9:1:133)
5	6.5 (100 μL)	43% (1.5:1:296)
6	**20.0 (307 μL)**	**82% (0.6:1:110)**
7	32.5 (500 μL)	74% (0.7:1:117)

[a] Reaction condition: toluene (2.0 mL), phenylboronic acid (0.2 mmol), $Pd(OAc)_2$ (0.02 mmol), $AgSbF_6$ (30 mol %), NFSI (0.3 mmol), HFIP (0.5 mL), H_2O (20 μL), 60 °C under N_2 for 24 h; [b] Combined yield of isomers and regioselectivity were determined by GC with dodecane as an internal standard.

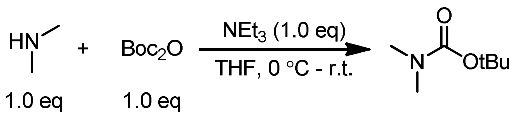
3. Ligand Preparation

2,2,N,N-Tetramethylpropionamide (L3) [1]



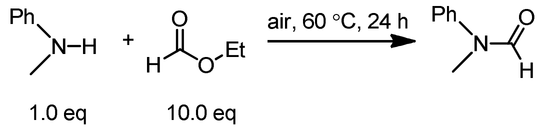
To a stirred solution of N,N-dimethylamine hydrochloride (4.08 g, 50 mmol) in toluene (20 mL) were added NEt_3 (10.4 mL, 75 mmol) at 0 °C. Pivaloyl chloride (1.2 mL, 10 mmol) was subsequently added dropwise and stirred for 1 h. Then the reaction mixture was warmed to room temperature and stirred for another 12 h. The reaction mixture was cooled to 0 °C, quenched by 4 mL of 1 M aqueous HCl and 20 mL of water. The mixture was extracted with ethyl acetate (3×20 mL). The combined organic extracts were washed with saturated aqueous Na_2CO_3 (20 mL) and brine (20 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. Purification by flash column chromatography yielded the amide as a colourless oil (516.5 mg, 40%). **^{1}H NMR** (400 MHz, d_4-MeOH) 3.05 (s, 6H), 1.28 (s, 9H); **^{13}C NMR** (100 MHz, d_4-MeOH) δ 178.3, 39.7, 38.9, 28.4.

***tert*-Butyl-dimethylcarbamate (L4)** [2]



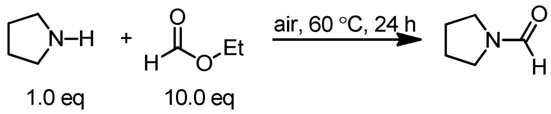
A solution of dimethylamine (33 % in water) (2.73 g, 20 mmol) and NEt_3 (2.8 mL, 20 mmol) in 10 mL of THF was cooled to 0 °C, and di-*tert*-butyl dicarbonate (4.37 mg, 20 mmol) was added portionwise. The mixture was stirred for 10 min, warmed to room temperature and stirred for another 12 h. The mixture was diluted with 15 mL of water and extracted with ethyl acetate (2×20 mL). The organic layers were combined, dried over anhydrous $MgSO_4$, concentrated to give a crude product. Distillation under reduced pressure afforded the desired product as a colorless oil 1.68 g (58%). **^{1}H NMR** (400 MHz, d_4-MeOH) δ 2.88 (s, 6H), 1.48 (s, 9H). **^{13}C NMR** (100 MHz, d_4-MeOH) δ 157.7, 80.8, 36.5, 36.2, 28.7.

N-Methyl-N-phenylformamide (L9) [3]



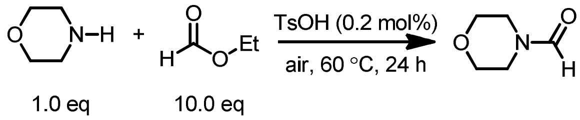
Ethyl formate (4.0 mL, 50.0 mmol) and N-methylaniline (542.8 μL, 5.0 mmol) were combined to form a solution and the mixture was heated at 60 °C for 24 h. After cooled to room temperature, the reaction mixture was evaporated to remove excess ethyl formate and crude products were obtained. Further purification by flash column chromatography afforded the desired product as light yellow oil (601.3 mg, 89%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.35 (t, J = 7.8 Hz, 2H), 7.21 (t, J = 6.8 Hz, 1H), 7.11 (d, J = 7.6 Hz, 2H), 3.25 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.2, 141.9, 129.7, 126.2, 122.2, 32.2.

Pyrrolidine-1-carbaldehyde (L10) [4]



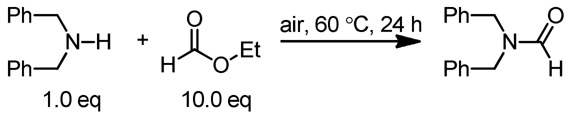
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that pyrrolidine was used. Further purification by distillation afforded pyrrolidine-1-carbaldehyde as colorless oil (302.5 mg, 62%). **^{1}H NMR** (400 MHz, d_4-MeOH) δ 8.23 (s, 1H), 3.59 (t, J = 6.4 Hz, 2H), 3.39 (t, J = 6.6 Hz, 2H), 2.03-1.89 (m, 4H). **^{13}C NMR** (100 MHz, d_4-MeOH) δ 163.0, 47.3, 44.2, 25.8, 25.1.

Morpholine-4-carbaldehyde (L11) [4]



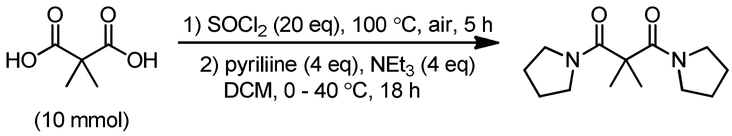
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that morpholine was used and 0.2 mol % TsOH was added. Further purification by distillation afforded morpholine-4-carbaldehyde as colorless oil (322.2 mg, 56%). **^{1}H NMR** (400 MHz, d_4-MeOH) δ 8.08 (s, 1H), 3.71 (t, J = 4.6 Hz, 2H), 3.67 (t, J = 4.8 Hz, 2H), 3.55 (t, J = 4.8 Hz, 2H), 3.49 (t, J = 4.6 Hz, 2H). **^{13}C NMR** (101 MHz, d_4-MeOH) δ 163.1, 68.2, 67.2, 47.0, 41.6.

N,N-Dibenzylformamide (L12) [5]



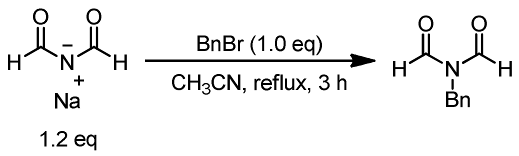
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that dibenzylamine was used. Further purification by flash column chromatography afforded N,N-dibenzylformamide as light yellow solid (968.7 mg, 86%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.42-7.25 (m, 6H), 7.24-7.14 (m, 4H), 4.41 (s, 2H), 4.26 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.0, 136.1, 135.7, 129.1, 128.8, 128.7, 128.3, 127.9, 127.8, 50.3, 44.8.

2,2-Dimethyl-1,3-di(pyrrolidin-1-yl)propane-1,3-dione (L13):



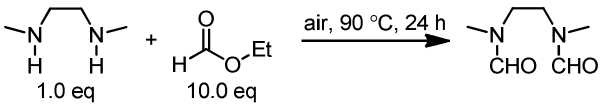
The mixture of dimethylmalonic acid (660.5 mg, 5.0 mmol) in $SOCl_2$ (20 mL) was refluxed for 5 hours. After cooled to room temperature, the solvent was removed under reduced pressure to afford the corresponding crude acid chloride. Then DCM (30 mL) was added and the solution was cooled to 0°C, followed by dropwise addition of NEt_3 (2.8 mL, 20.0 mmol) and pyrrolidine (1.6 mL, 20.0 mmol). The reaction mixture was stirred at room temperature overnight, extracted by DCM. The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated to give a crude product. Purification by flash chromatography afforded the product as light yellow solid (715.0 mg, 60%). m.p. 169-172 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.51 (t, J = 6.8 Hz, 4H), 3.26 (t, J = 6.2 Hz, 4H), 1.94-1.74 (m, 8H), 1.41 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 49.6, 47.3, 46.4, 26.9, 23.6, 23.4. HRMS (ESI) calcd. for $C_{13}H_{22}N_2O_2Na$ ($[M+Na]^+$) 261.1573, Found 261.1576.

N-Benzyl-N-formylformamide (L14) [6]



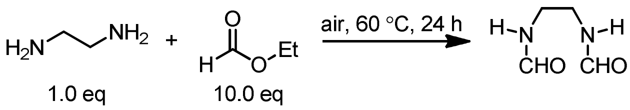
To a solution of sodium diformylamide (1.36 g, 12.0 mmol) in CH_3CN (5 mL) was added benzyl bromide (1.2 mL, 10.0 mmol) under nitrogen. The mixture was refluxed for 3 h. After cooled to room temperature, the reaction mixture was filtered and concentrated. Purification by flash column chromatography afforded N-benzyl-N-formylformamide as white solid (995.4 mg, 61%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (s, 2H), 7.43-7.25 (m, 5H), 4.79 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.0, 135.6, 129.0, 128.8, 128.2, 42.4.

N,N'-(Ethane-1,2-diyl)bis(N-methylformamide) (L15)



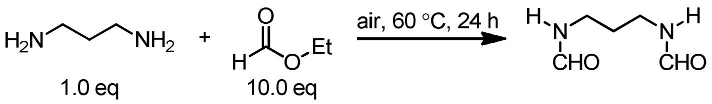
Ethyl formate (4.0 mL, 50.0 mmol) and N,N'-dimethylethane-1,2-diamine (538.1 μL, 5.0 mmol) were combined to form a solution and the mixture was heated at 90 °C for 24 h. After cooled to room temperature, the reaction mixture was washed with 1 mL of 2M HCl and extracted with DCM (3×5 mL). The organic layers were combined and dried over anhydrous Na_2SO_4. Evaporation of the solvent afforded the desired product as light yellow solid (216.3 mg, 30%). m.p. 70-72 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07-7.99 (m, 2H), 3.57-3.40 (m, 4H), 3.01-2.91 (m, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 163.3, 163.0, 162.6, 47.6, 46.5, 42.6, 40.5, 35.5, 34.7, 29.9. HRMS (ESI) calcd. for $C_6H_{13}N_2O_2$ ($[M+H]^+$) 145.0972, Found 145.0977.

N,N'-(Ethane-1,2-diyl)diformamide (L16) [7]



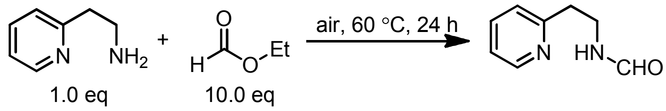
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that ethane-1,2-diamine was used. After removing excess ethyl formate under vacuum, N,N'-(ethane-1,2-diyl)diformamide was obtained as white solid (551.5 mg, 95%). ^{1}**H NMR** (400 MHz, d_6-DMSO) δ 8.18-7.83 (m, 4H), 3.16-3.13 (m, 4H). ^{13}**C NMR** (100 MHz, d_6-DMSO) δ 164.6, 161.4, 36.9.

N,N'-(Propane-1,3-diyl)diformamide (L17)



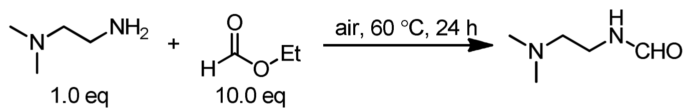
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that propane-1,3-diamine was used. After removing excess ethyl formate under vacuum, N,N'-(propane-1,3-diyl)diformamide was obtained as colorless oil (572.6 mg, 88%). ^{1}**H NMR** (400 MHz, d_6-DMSO) δ 8.02 (br s, 2H), 8.00 (s, 2H), 3.08 (q, J = 6.6 Hz, 4H), 1.54 (p, J = 7.0 Hz, 2H). ^{13}**C NMR** (100 MHz, d_6-DMSO) δδ 161.3, 35.0, 29.2. HRMS (ESI) calcd. for $C_5H_{11}N_2O_2$ ($[M+H]^+$) 131.0815, Found 131.0815.

N-(2-(Pyridin-2-yl)ethyl)formamide (L18)



The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that 2-(pyridin-2-yl)ethanamine was used. Further purification by flash column chromatography afforded N-(2-(pyridin-2-yl)ethyl)formamide as colorless oil (555.6 mg, 74%). ^{1}**H NMR** (400 MHz, d_6-DMSO) δ 8.48 (d, J = 4.0 Hz, 1H), 8.19 (s, 1H), 7.97 (s, 1H), 7.70 (t, J = 7.4 Hz, 1H), 7.25 (d, J = 7.6 Hz, 1H), 7.21 (t, J = 6.0 Hz, 1H), 3.44 (q, J = 6.8 Hz, 2H), 2.87 (t, J = 7.0 Hz, 2H). ^{13}**C NMR** (100 MHz, d_6-DMSO) δ 161.1, 159.0, 148.8, 136.4, 123.2, 121.6, 37.2, 37.0. HRMS (ESI) calcd. for $C_8H_{11}N_2O_1$ ($[M+H]^+$) 151.0866, Found 151.0866.

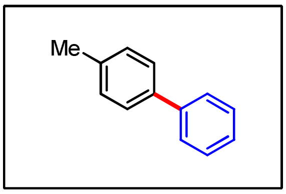
N-(2-(dimethylamino)ethyl)formamide (L19)



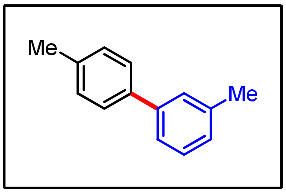
The procedure for the preparation of N-methyl-N-phenylformamide was followed, except that N,N-dimethylethylenediamine was used. Further purification by flash column chromatography afforded N-(2-(dimethylamino)ethyl)formamide as yellow oil (447.2 mg, 77%).**^{1}H NMR** (400 MHz, d_6-DMSO) δ 7.98 (s, 1H), 3.16 (q, J = 6.2 Hz, 2H), 2.27 (t, J = 6.6 Hz, 2H), 2.14 (s, 6H). **^{13}C NMR** (100 MHz, d_6-DMSO) δ160.9, 58.1, 45.2, 35.3. HRMS (ESI) calcd. for $C_5H_{13}N_2O_1$ ($[M+H]^+$) 117.1022, Found 117.1026.

4. Typical Procedure of *para*-Selective Arylation of Simple Arenes

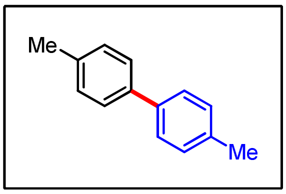
To a 15 mL sealed tube were added $PdCl_2$ (3.5 mg, 0.02 mmol, 10 mol %), $AgSbF_6$ (20.6 mg, 0.06 mmol, 30 mol %), NFSI (189.2 mg, 0.6 mmol, 3.0 eq), arylboronic acid (0.2 mmol, 1.0 eq), and arene (2.0 mL) under N_2 atmosphere, then HFIP (0.5 mL), DMF (0.3 mL), and H_2O (20 μL) were subsequently added. The tube was sealed with a Teflon cap and the mixture was stirred at 60 °C for 24 h. After cooled to room temperature, the crude product was diluted with EtOAc, and detected by GC with dodecane (10.0 μL, 0.044 mmol) as an internal standard to obtain regioisomer ratios. The minor isomers were determined by contrasting with GC spectra of corresponding compounds obtained by Suzuki-Miyaura cross-coupling reactions. Then the mixture was filtered through a short pad of Celite, and the filtrate was concentrated under vacuum. The resulting residue was purified by column chromatography to give an isolated combined yield of all regioisomers. The pure major *para*-isomer for characterization was obtained by further purification on a silica gel column with a gradient eluent (hexane to hexane/dichloromethane).



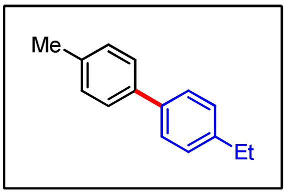
3a: 4-methylbiphenyl.[8] White solid (78% yield). m.p. 44-45 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (d, J = 7.2 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.30 (t, J = 6.8 Hz, 1H), 7.22 (d, J = 7.6 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.3, 138.5, 137.1, 129.6, 128.8, 127.1, 21.2.



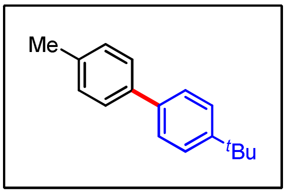
3b: 3,4'-dimethylbiphenyl.[9] Colorless oil (82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.0 Hz, 2H), 7.30-7.26 (m, 2H), 7.21 (t, J = 7.6 Hz, 1H), 7.13 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 7.2 Hz, 1H), 2.31 (s, 3H), 2.28 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.3, 138.6, 138.4, 137.0, 129.5, 128.7, 127.9, 127.8, 127.1, 124.2, 21.7, 21.2.



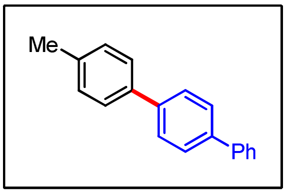
3c: 4,4'-dimethylbiphenyl.[10] White solid (62% yield). m.p. 123-124 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.0 Hz, 4H), 7.23 (d, J = 8.0 Hz, 4H), 2.38 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.4, 136.8, 129.6, 126.9, 21.2.



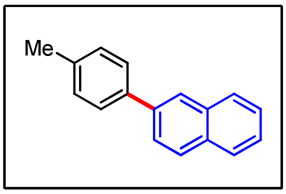
3d: 4-methyl-4'-ethyl-biphenyl.[11] White solid (76% yield). m.p. 56-58 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51-7.47 (m, 4H), 7.27-7.22 (m, 4H), 2.69 (q, J = 7.6 Hz, 2H), 2.39 (s, 3H), 1.27 (t, J = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.2, 138.7, 138.4, 136.8, 129.6, 128.4, 127.0, 126.9, 28.6, 21.2, 15.8.



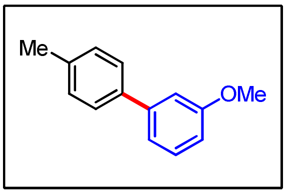
3e: 4-methyl-4'-tertiary butyl-biphenyl.[12] White solid (77% yield). m.p. 74-77 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45-7.36 (m, 6H), 7.15 (d, J = 6.0 Hz, 2H), 2.30 (s, 3H), 1.28 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.1, 138.4, 138.3, 136.8, 129.6, 127.0, 126.7, 125.8, 34.6, 31.5, 21.2.



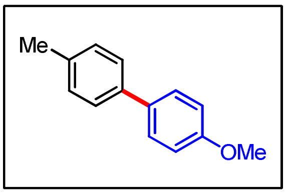
3f: 4-(4-methylphenyl)biphenyl.[13] White solid (84% yield). m.p. 198-200 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (s, 4H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.9, 140.2, 140.0, 137.9, 137.3, 129.7, 128.9, 127.6, 127.4, 127.2, 127.0, 21.3.



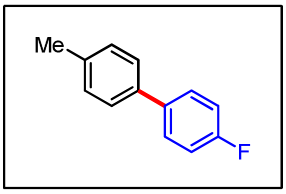
3g: 2-p-tolylnaphthalene.[11] White solid (64% yield). m.p. 91-92 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.94-7.84 (m, 3H), 7.75 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.54-7.46 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.6, 138.4, 137.3, 133.8, 132.6, 129.7, 128.5, 128.3, 127.8, 127.43, 126.4, 125.9, 125.7, 125.6, 21.1.



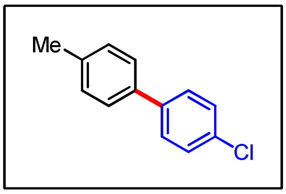
3h: 3-methoxyl-4'-methyl-biphenyl.[14] White solid (57% yield). m.p. 72-74 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.10 (s, 1H), 6.86 (dd, *J* = 8.4, 2.8 Hz, 1H), 3.82 (s, 3H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.0, 142.8, 138.3, 137.3, 129.8, 129.5, 127.1, 119.6, 112.8, 112.4, 55.2, 21.2.



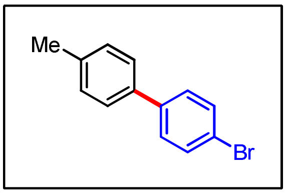
3i: 4-methyl-4'-methoxyl-biphenyl.[11] White solid (41% yield). m.p. 103-105 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H), 2.38 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.0, 138.1, 136.5, 133.9, 129.7, 128.0, 126.6, 114.1, 55.2, 21.2.



3j: 4-fluoro-4'-methyl-biphenyl.[15] White solid (68% yield). m.p. 73-75 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56-7.49 (m, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 7.6 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.4 (d, *J* = 244 Hz), 137.5, 137.4 (d, *J* = 3 Hz), 137.2, 129.7, 128.6 (d, *J* = 8 Hz), 127.0, 115.6 (d, *J* = 21 Hz), 21.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.3.

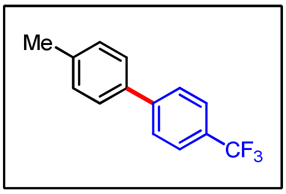


3k: 4-chloro-4'-methyl-biphenyl.[10] White solid (78% yield). m.p. 116-118 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 2H), 2.38 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 139.7, 137.6, 137.2, 133.2, 129.7, 129.0, 128.3, 126.9, 21.2.

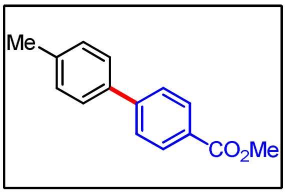


3l: 4-methyl-4'-bromo-biphenyl.[12] White solid (73% yield). m.p. 128-129 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.46-7.40 (m, 4H), 7.24 (d, *J* =

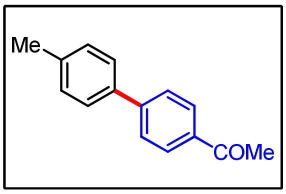
8.0 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.2, 137.6, 137.2, 131.9, 129.8, 128.6, 126.9, 121.3, 21.2.



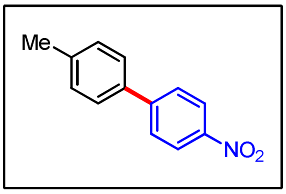
3m: 4-methyl-4'-trifluomethyl-biphenyl.[16] White solid (61% yield). m.p. 123-125 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.66 (s, 4H), 7.49 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.8, 138.3, 136.9, 129.9, 129.2 (q, J = 32.6 Hz), 127.3, 127.2, 125.8 (q, J = 4.0 Hz), 123.2, 21.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.3.



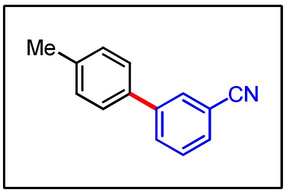
3n: 4-methoxycarbonyl-4'-methyl-biphenyl.[16] White solid (80% yield). m.p. 111-113 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 (d, J = 8.8 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 3.93 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.2, 145.7, 138.1, 137.2, 130.2, 129.8, 128.7, 127.2, 126.9, 52.1, 21.3.



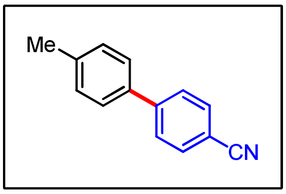
3o: 4-acetyl-4'-methyl-biphenyl.[16] White solid (59% yield). m.p. 112-113 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 2.63 (s, 3H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.0, 145.9, 138.3, 137.0, 135.7, 129.8, 129.0, 127.2, 127.1, 26.9, 21.3.



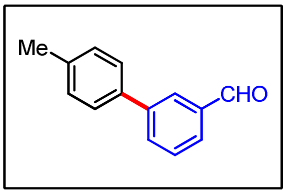
3p: 4-methyl-4'-nitro-biphenyl.[17] White solid (77% yield). m.p. 139-140 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 2H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 147.7, 146.9, 139.2, 135.9, 130.0, 127.6, 127.3, 124.2, 21.0.



3q: 3-cyano-4'-methyl-biphenyl.[18] White solid (71% yield). m.p. 72-75 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.5, 138.5, 136.1, 131.4, 130.6, 130.5, 130.0, 129.7, 127.0, 119.1, 113.0, 21.3.

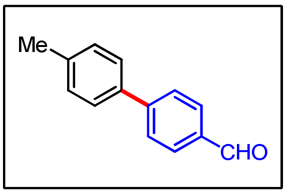


3r: 4-cyano-4'-methyl-biphenyl.[11] White solid (56% yield). m.p. 109-110 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76-7.68 (m, 4H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.7, 138.8, 136.4, 132.7, 130.0, 127.6, 127.2, 119.1, 110.6, 21.0.

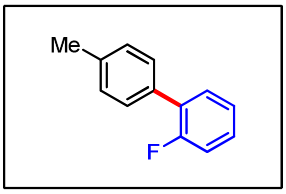


3s: 3-formyl-4'-methyl-biphenyl.[19] White solid (82% yield). m.p. 125-127 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.08 (s, 1H), 7.85-7.82 (m, 2H), 7.58 (t, *J* =

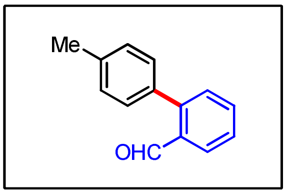
7.6 Hz, 1H), 7.52 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.6, 142.2, 138.0, 137.0, 136.9, 133.0, 129.8, 129.6, 128.5, 128.1, 127.1, 21.3.



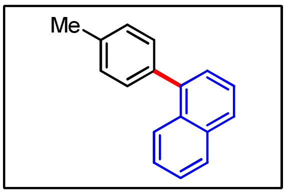
3t: 4-formyl-4’-methyl-biphenyl.[18] White solid (57% yield). m.p. 108-110 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 2H), 2.41 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.1, 147.3, 138.7, 136.9, 135.1, 130.4, 129.9, 127.5, 127.3, 21.3.



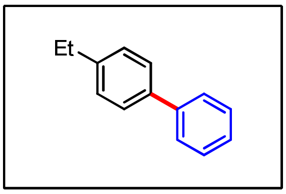
3v: 2-fluoro-4'-methylbiphenyl.[20] Colorless oil (74% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40-7.24 (m, 3H), 7.23-7.01 (m, 5H), 2.31 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.9 (d, J = 248.5 Hz), 137.6, 133.0, 130.8 (d, J = 3.03 Hz), 129.3, 129.0 (d, J = 3.0 Hz), 128.8, 128.7, 124.4 (d, J = 3.0 Hz), 116.2 (d, J = 22.2 Hz), 21.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -118.1.



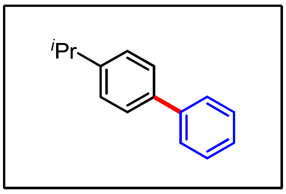
3w: 2-formyl-4’-methyl-biphenyl.[21] Light yellow oil (64% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.02 (d, J = 7.6 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.50-7.43 (m, 2H), 7.28 (s, 4H), 2.43 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.5, 146.2, 138.2, 134.9, 133.9, 133.7, 130.9, 130.2, 129.3, 128.5, 127.7, 21.3.



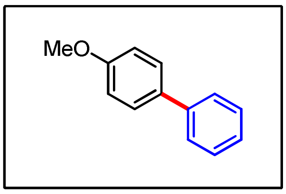
3x: 1-p-tolylnaphthalene.[11] Colorless oil (43% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96-7.81 (m, 3H), 7.54-7.36 (m, 6H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.4, 137.9, 137.0, 133.9, 131.8, 130.1, 129.1, 128.4, 127.6, 127.0, 126.2, 126.1, 125.8, 125.5, 21.3.



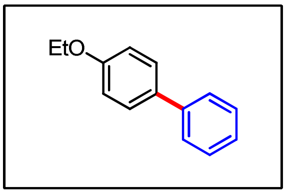
4a: 4-ethyl-biphenyl.[22] Colorless oil (79% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.35-7.27 (m, 3H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 141.3, 138.7, 128.8, 128.4, 127.2, 127.1, 127.1, 28.7, 15.8.



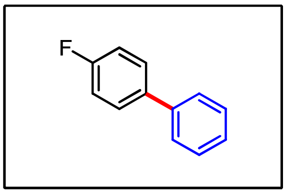
4b: 4-isopropyl-biphenyl.[23] Colorless oil (61% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.2 Hz, 2H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.34-7.27 (m, 3H), 3.01-2.89 (m, 1H), 1.29 (d, *J* = 6.8 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.1, 141.3, 138.9, 128.8, 127.2, 127.1, 127.0, 126.9, 33.9, 24.2.



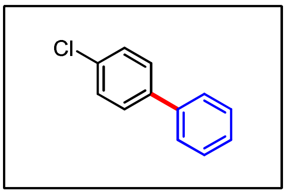
4c: 4-methoxy-biphenyl.[24] White solid (87% yield). m.p. 83-84 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57-7.49 (m, 4H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 6.97 (d, J = 8.4 Hz, 2H), 3.83 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 159.3, 140.9, 133.9, 128.9, 128.3, 126.9, 126.8, 114.3, 55.5.



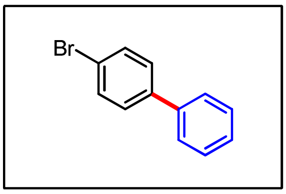
4d: 4-ethoxy-biphenyl.[25] White solid (52% yield). m.p. 74-75 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59-7.53 (m, 4H), 7.44 (t, J = 7.4 Hz, 2H), 7.32 (t, J = 7.4 Hz, 1H), 6.99 (d, J = 8.0 Hz, 2H), 4.09 (q, J = 6.9 Hz, 2H), 1.46 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.6, 141.0, 133.7, 128.8, 128.3, 126.8, 126.7, 114.9, 63.6, 15.0.



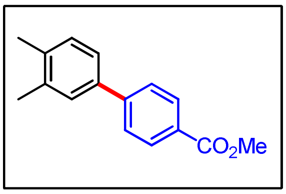
4e: 4-fluoro-biphenyl.[26] White solid (79% yield). m.p. 72-73 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63-7.55 (m, 4H), 7.47-7.43 (m, 2H), 7.36 (t, J = 7.0 Hz, 1H), 7.16-7.12 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.6 (d, J = 244.6 Hz), 140.4, 137.5 (d, J = 2.9 Hz), 129.0, 128.8 (d, J = 8.0 Hz), 127.4, 127.2, 115.7 (d, J = 21.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -115.8.



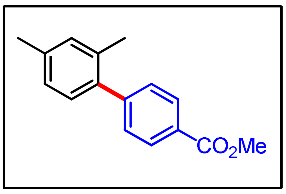
4f: 4-chloro-biphenyl.[10] White solid (38% yield). m.p. 73-76 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56-7.51 (m, 4H), 7.46-7.34 (m, 5H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.1, 139.8, 133.5, 129.0, 129.0, 128.5, 127.7, 127.1.



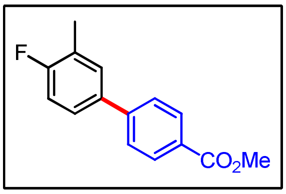
4g: 4-bromo-biphenyl.[27] White solid (36% yield). m.p. 87-89 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59-7.53 (m, 4H), 7.48-7.42 (m, 4H), 7.36 (t, *J* = 7.4 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.3, 140.2, 132.0, 129.0, 128.9, 127.8, 127.1, 121.7.



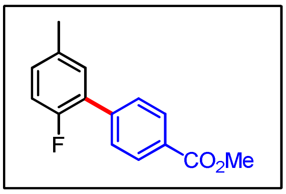
4h: methyl 3',4'-dimethyl-[1,1'-biphenyl]-4-carboxylate. White solid (80% yield). m.p. 97-100 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.40 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 3.93 (s, 3H), 2.33 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 145.8, 137.7, 137.3, 136.9, 130.3, 130.2, 128.6, 126.9, 124.7, 52.2, 20.1, 19.6. HRMS (ESI) calcd. for $C_{16}H_{17}O_2$ ($[M+H]^+$) 241.1229, Found 241.1229.



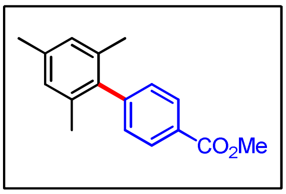
4i: methyl 2',4'-dimethyl-[1,1'-biphenyl]-4-carboxylate. White solid (72% yield). m.p. 62-64 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.15-7.06 (m, 3H), 3.95 (s, 3H), 2.38 (s, 3H), 2.25 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.2, 146.9, 138.1, 137.7, 135.1, 131.4, 129.6, 129.5, 129.5, 128.5, 126.8, 52.3, 21.2, 20.5. HRMS (ESI) calcd. for $C_{16}H_{17}O_2$ ($[M+H]^+$) 241.1229, Found 241.1221.



4j: methyl 4'-fluoro-3'-methyl-[1,1'-biphenyl]-4-carboxylate. White solid (67% yield). m.p. 92-94 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.46-7.36 (m, 2H), 7.08 (t, *J* = 8.8 Hz, 1H), 3.94 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.1, 161.6 (d, *J* = 245.0 Hz), 144.9, 135.9 (d, *J* = 3.6 Hz), 130.5 (d, *J* = 5.3 Hz), 130.2, 128.9, 127.0, 126.3 (d, *J* = 8.1 Hz), 125.5 (d, *J* = 17.5 Hz), 115.6 (d, *J* = 22.5 Hz), 52.26, 14.84. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -118.4. HRMS (ESI) calcd. for $C_{15}H_{14}FO_2$ ($[M+H]^+$) 245.0972, Found 245.0970.



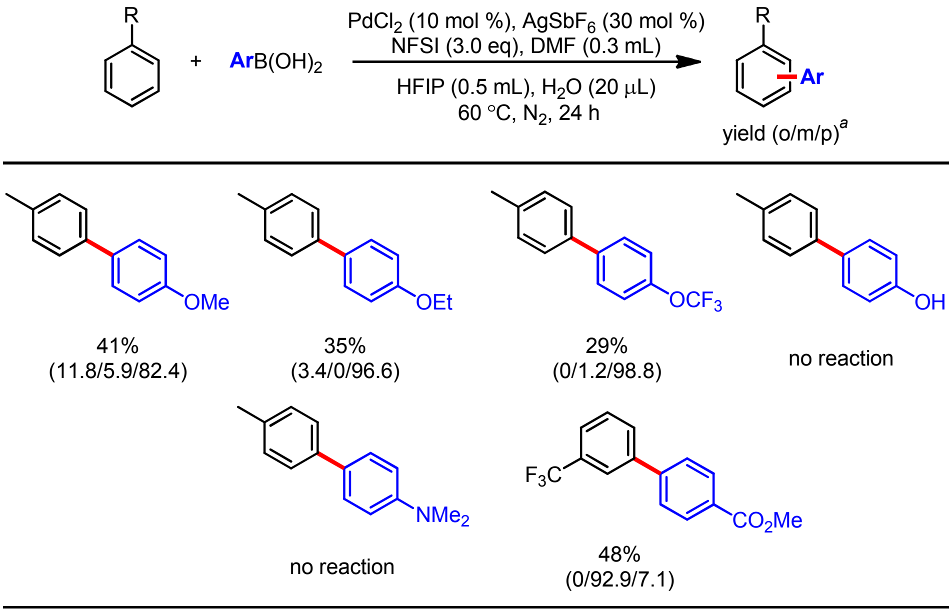
4k: methyl 2'-fluoro-5'-methyl-[1,1'-biphenyl]-4-carboxylate. White solid (65% yield). m.p. 59-62 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 6.2 Hz, 1H), 7.05 (t, *J* = 9.4 Hz, 1H), 3.94 (s, 3H), 2.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.1, 158.0 (d, *J* = 244.5 Hz), 140.7, 134.0 (d, *J* = 3.7 Hz), 131.1 (d, *J* = 2.9 Hz), 130.3 (d, *J* = 8.0 Hz), 129.8, 129.2, 129.1 (d, *J* = 3.1 Hz), 127.6 (d, *J* = 13.2 Hz), 116.1 (d, *J* = 22.5 Hz), 52.3, 20.8. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -122.9. HRMS (ESI) calcd. for $C_{15}H_{14}FO_2$ ($[M+H]^+$) 245.0972, Found 245.0972.



4l: methyl 2',4',6'-trimethyl-[1,1'-biphenyl]-4-carboxylate.[28] White solid (56% yield). m.p. 117-119 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.95 (s, 2H), 3.94 (s, 3H), 2.33 (s, 3H), 1.98 (s, 6H). **^{13}C NMR** (100

MHz, $CDCl_3$) δ 167.3, 146.4, 138.1, 137.2, 135.6, 130.0, 129.6, 128.6, 128.3, 52.3, 21.12, 20.8.

Table S16. Electronic effect of substituted group on arene and arylboronic acid



5. Mechanistic Study

5.1 KIE determined by competition reaction

To a 15 mL sealed tube were added $PdCl_2$ (3.5 mg, 0.02 mmol, 10 mol%), $AgSbF_6$ (20.6 mg, 0.06 mmol, 30 mol%), NFSI (189.2 mg, 0.6 mmol, 3.0 eq), and phenylboronic acid (0.2 mmol, 1.0 eq) under N_2 atmosphere. Then toluene (1.0 mL), toluene-d_8 (1.0 mL), HFIP (0.5 mL), DMF (0.3 mL), and H_2O (20 μL) were subsequently added. The tube was sealed with a Teflon cap and the mixture was stirred at 60 °C for 24 h. After cooled to room temperature, the reaction mixture was concentrated under vacuum and biaryl products were obtained by preparative thin-layer chromatography.

The KIE was determined by [1]H NMR analysis as shown in **Figure S1**.

3a/(*d*7-**3a**) = {2.28-[(1.97+2.41)/4]}/ [(1.97+2.41)/4] = 1.1/1

Scheme S1. KIE determined by competition reaction

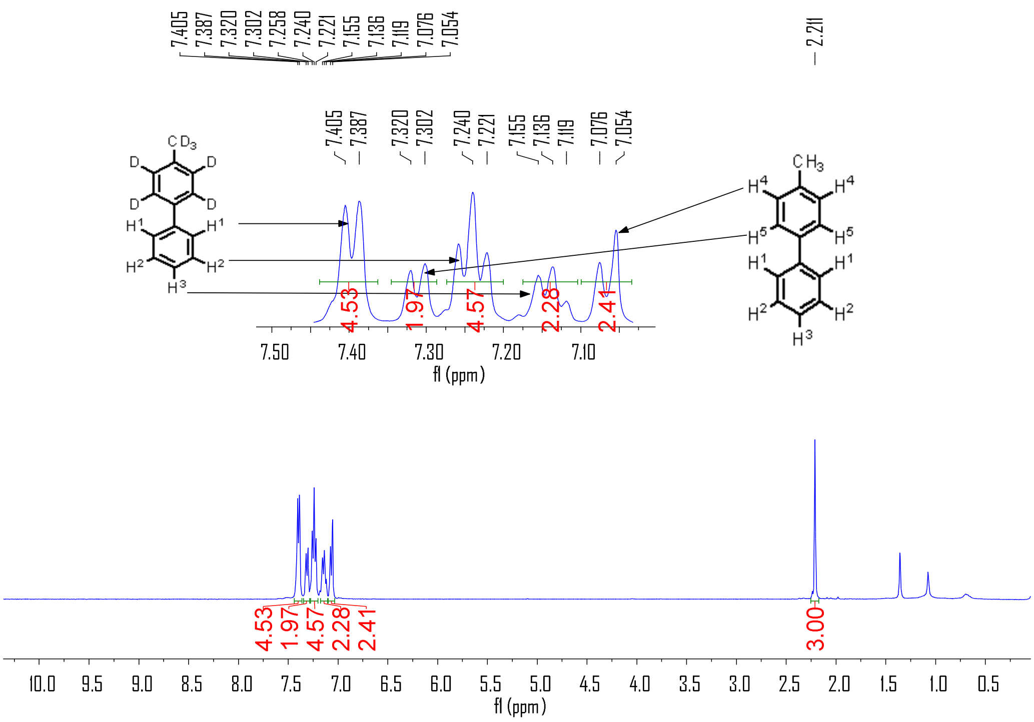
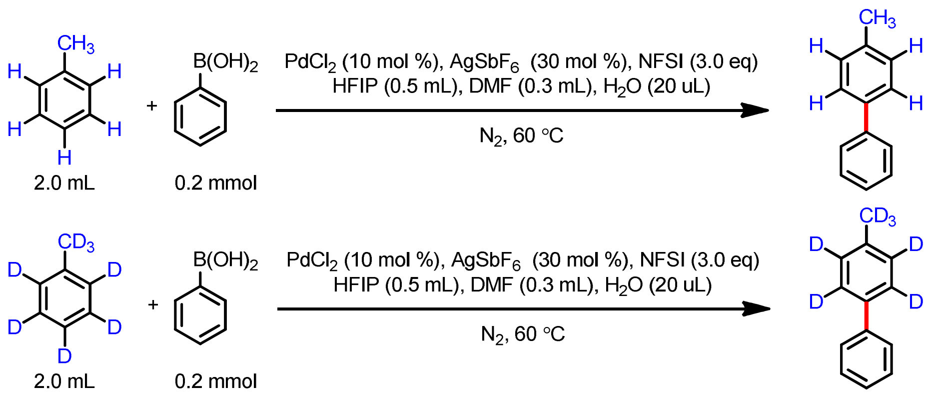


Figure S1. ^{1}H NMR spectrum of the mixture of 3a and *d*$_7$-3a

5.2 KIE determined by initial rate measurements of two parallel reactions

Side-by-side reactions were set-up following general procedure for the arylation of simple arenes with toluene (2.0 mL) and d$_8$-toluene (2.0 mL). Aliquots were taken at 5 minute intervals for the first half an hour. Product yield was determined by GC/MS using n-dodecane as an internal standard. Data points represent the average of two runs.



The KIE was determined by initial rates of these two pallaral reactions as shown in **Figure S2**.

KIE = k_H / k_D = 0.2706/ 0.2560 = 1.05

Scheme S2. KIE determined by initial rate measurements of parallel reactions

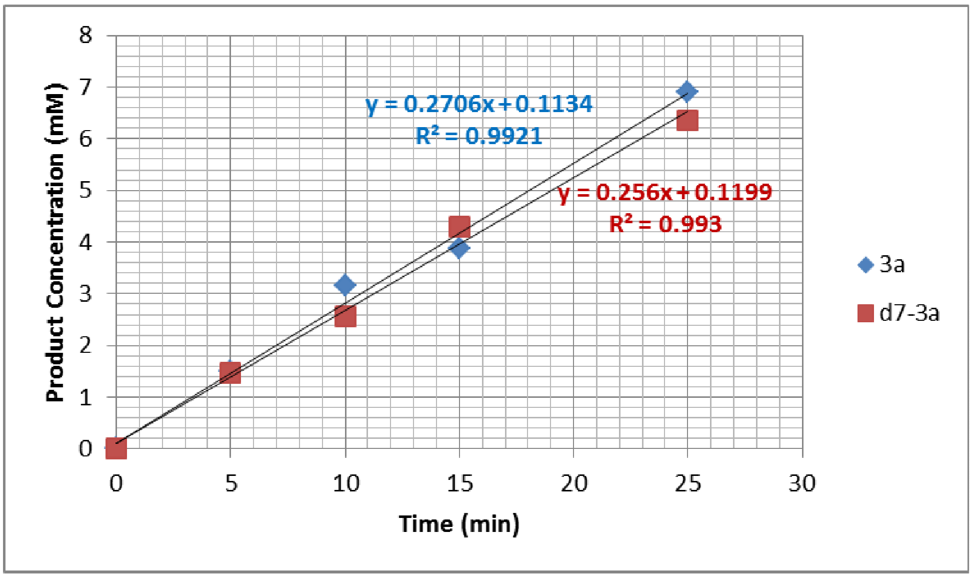
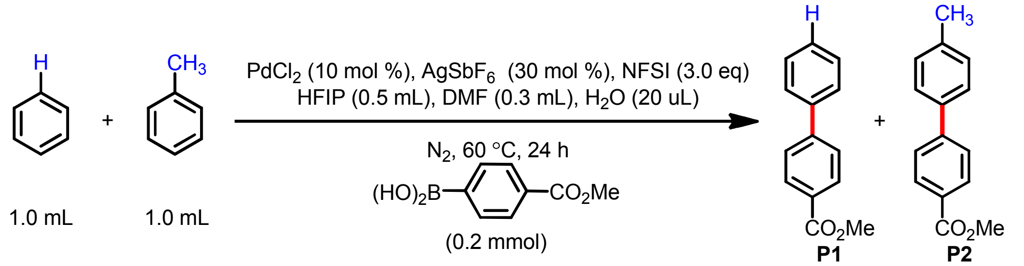


Figure S2. Initial reaction rate measurement for arylations of toluene (blue) and *d_8*-toluene (red). Data points represent the average of two runs.

5.3 Competition reactions between benzene and *para*-substituted arenes

To a 15 mL sealed tube were added $PdCl_2$ (3.5 mg, 0.02 mmol, 10 mol%), $AgSbF_6$ (20.6 mg, 0.06 mmol, 30 mol%), NFSI (189.2 mg, 0.6 mmol, 3.0 eq), and 4-(methoxycarbonyl)phenylboronic acid (0.2 mmol, 1.0 eq) under N_2 atmosphere. Then benzene (1.0 mL) and the other arene (1.0 mL) [toluene, fluorobenzene or anisole], HFIP (0.5 mL), DMF (0.3 mL), and H_2O (20 μL) were subsequently added. The tube was sealed with a Teflon cap and the mixture was stirred at 60 °C for 24 h. After cooled to room temperature, the reaction mixture was filtered and concentrated under vacuum and the cross coupling products were obtained by preparative thin-layer chromatography. The ratios of products were determined by ^{1}H NMR analysis.



The ratio of products was determined by ^{1}H NMR analysis as shown in **Figure S3**.

P1/P2 = (6.2-3.0)/3.0 = 1.07

Scheme S3. Competition reaction between benzene and toluene (1:1)

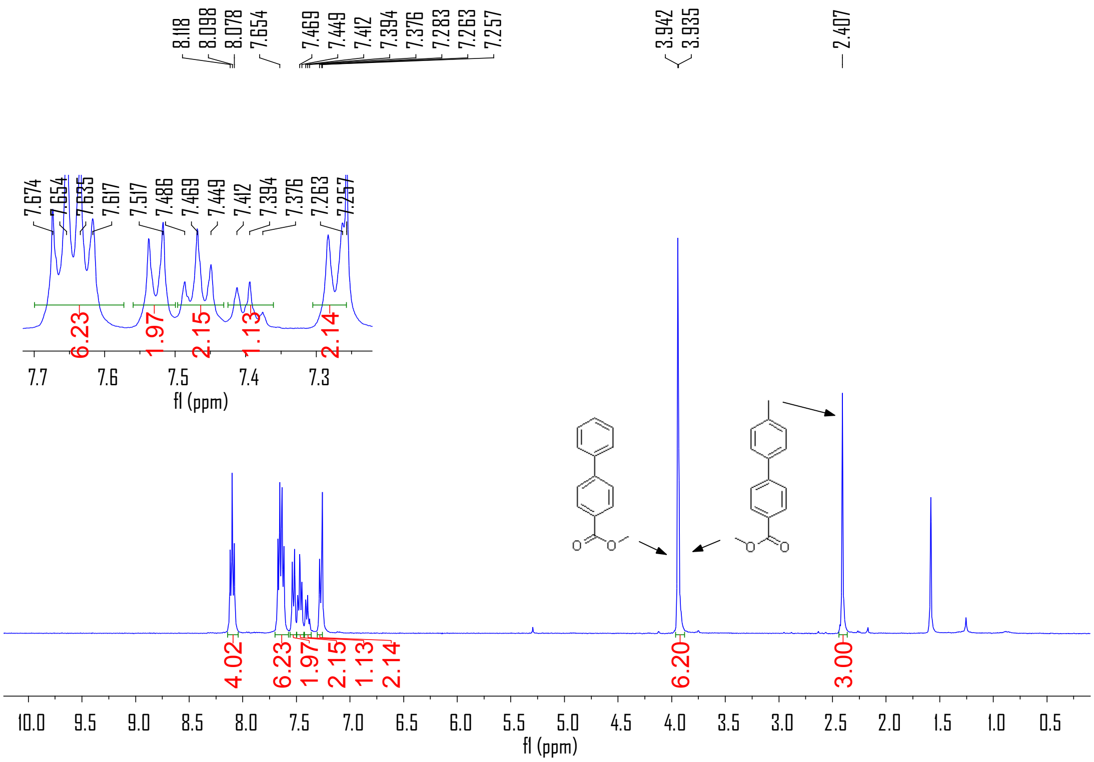
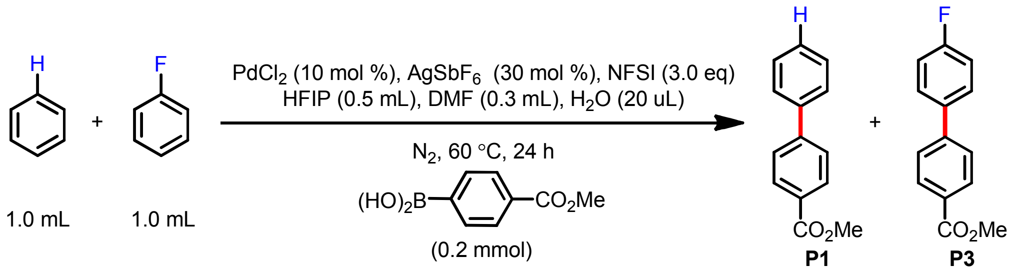


Figure S3. ^{1}H NMR spectrum of the mixture of products



The ratio of products was determined by 1H NMR analysis as shown in **Figure S4**.

P1/P3 = 3.0 / (4.7-3.0) = 1.76

Scheme S4. Competition reaction between benzene and fluorobenzene (1:1)

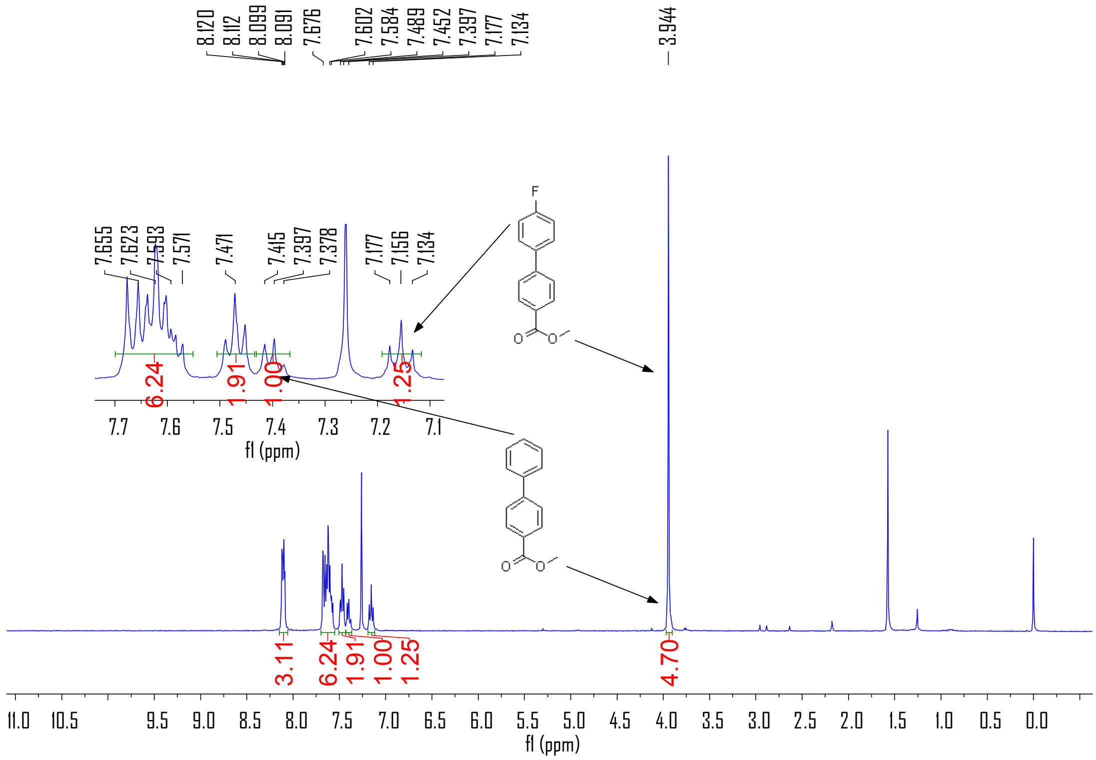
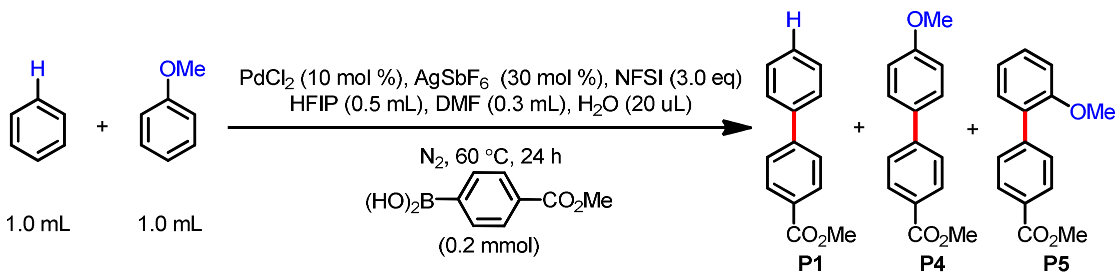


Figure S4. ^{1}H NMR spectrum of the mixture of products



The ratio of products was determined by 1H NMR analysis as shown in **Figure S5**.

P1(**P4+P5**) = (6.05-3.0) / 3.0 = 1.01

Scheme S5. Competition reaction between benzene and anisole (1:1)

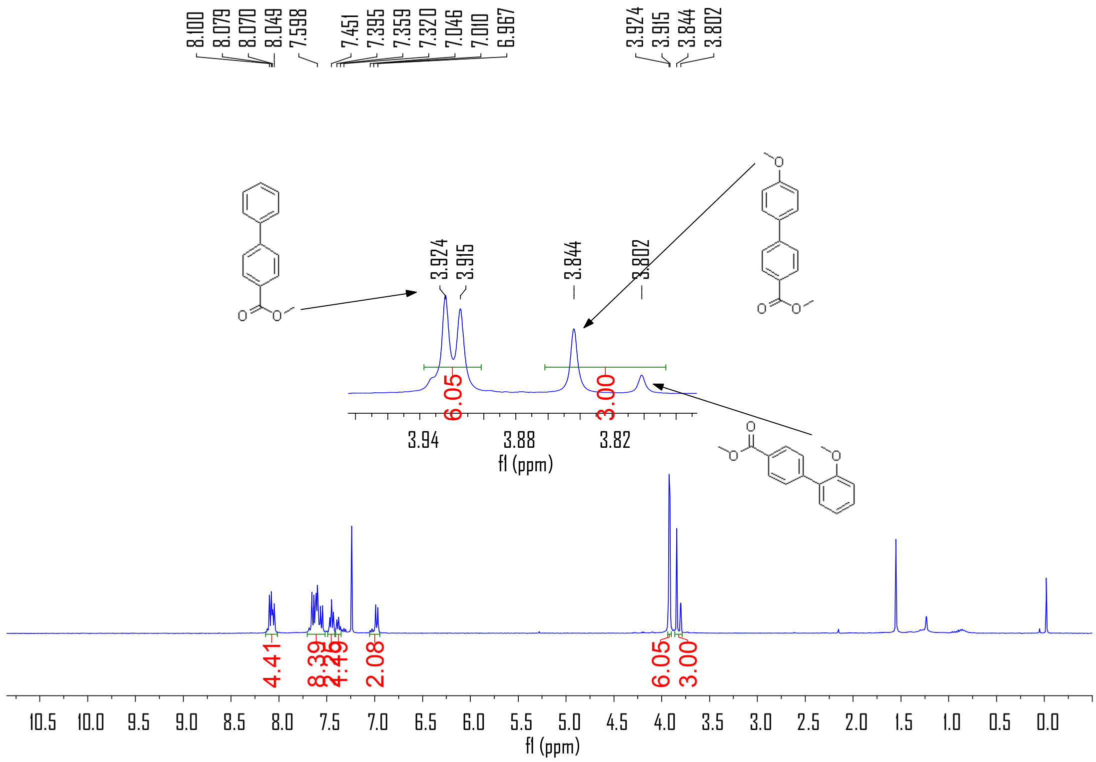


Figure S5. ^{1}H NMR spectrum of the mixture of products

References:

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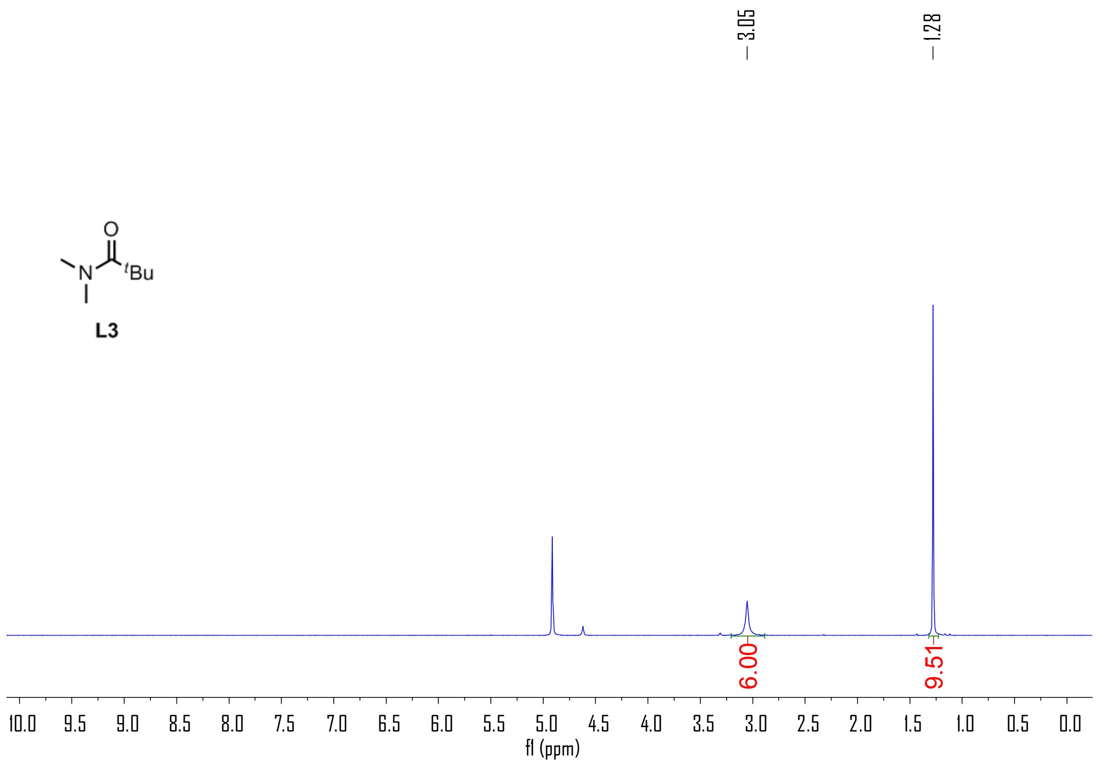
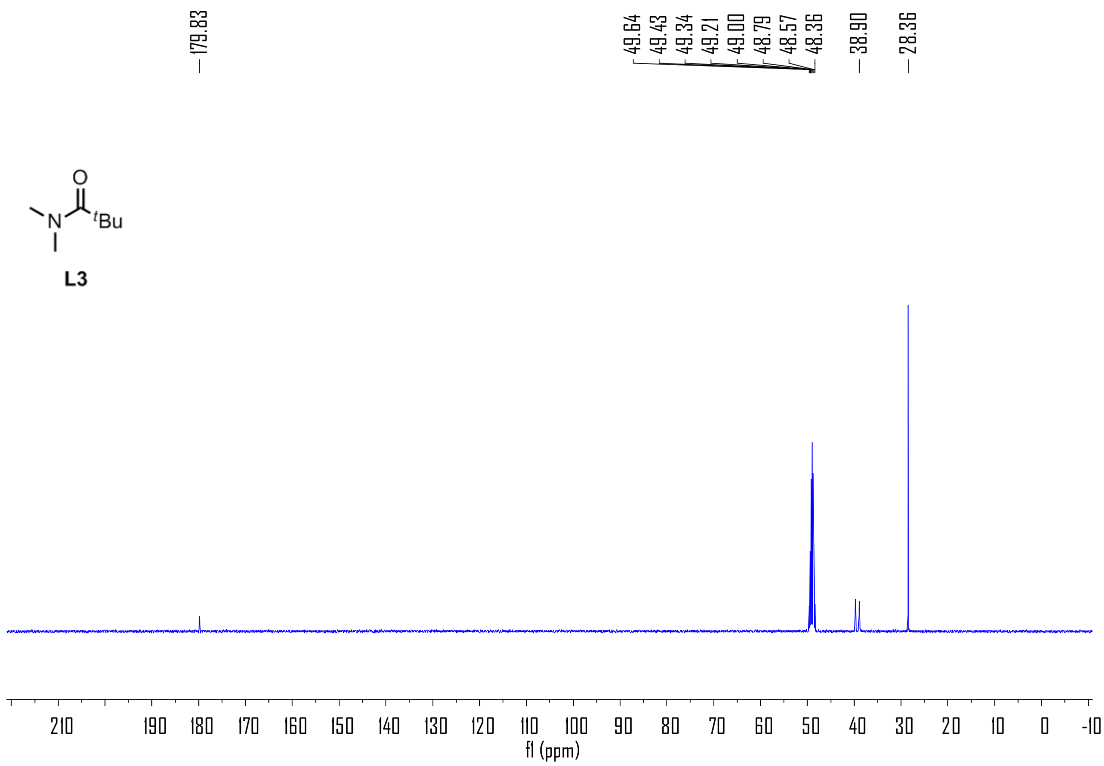
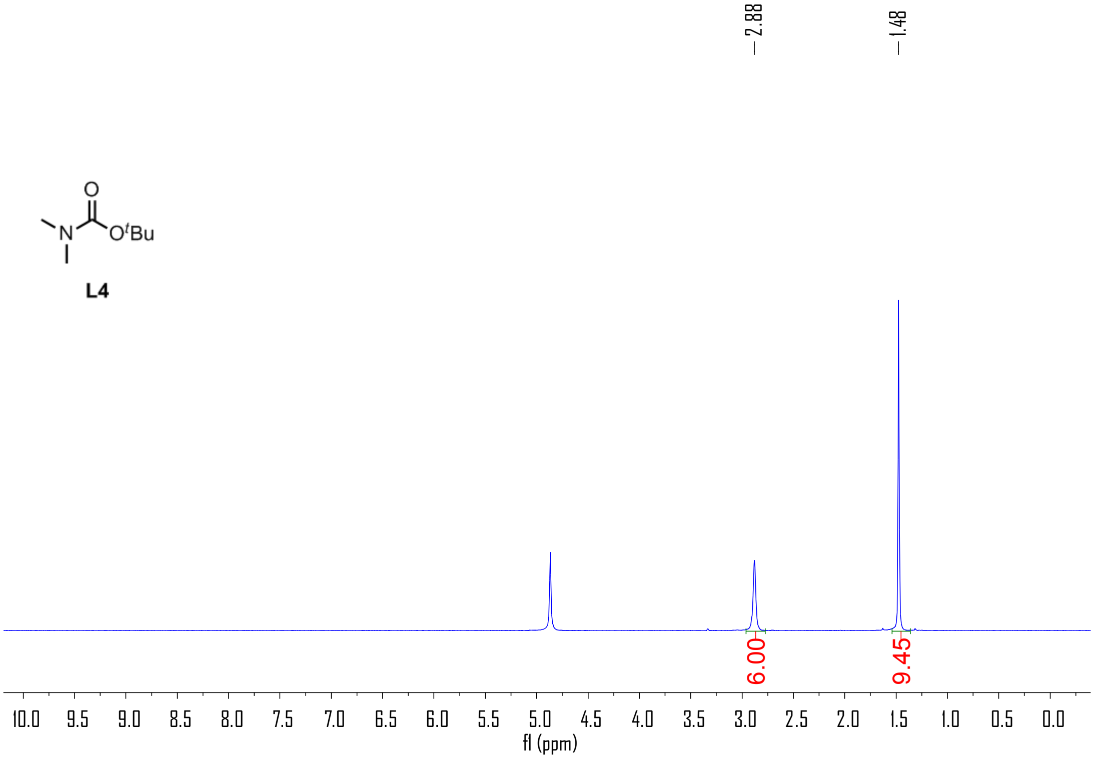
6. NMR Spectra







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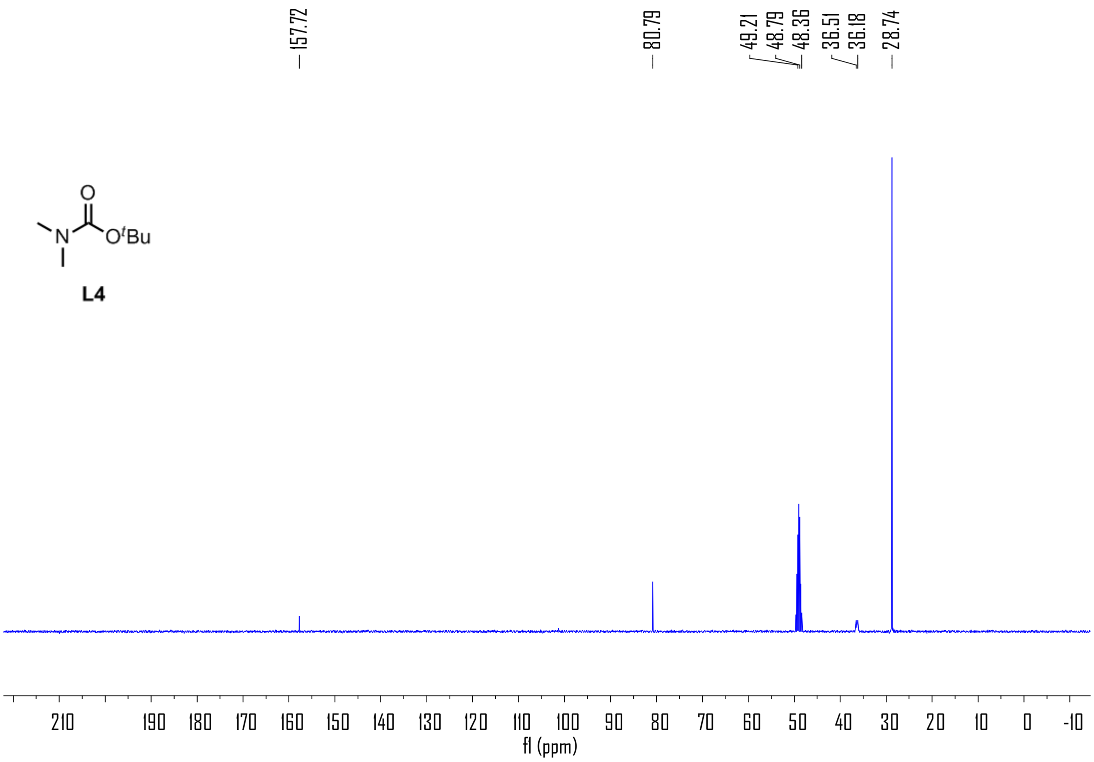
O^tBu
2.88
1.48
6.00
9.45
fl (ppm)



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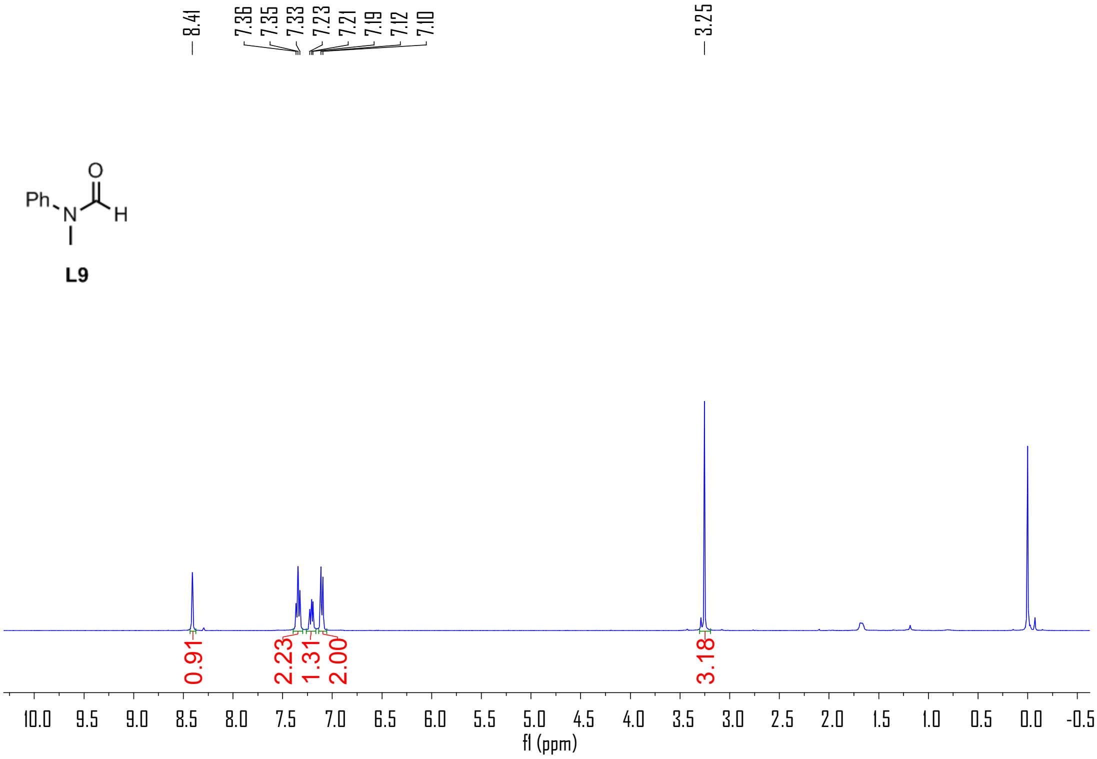
157.72
80.79
49.21
48.79
48.36
36.51
36.18
28.74
fl (ppm)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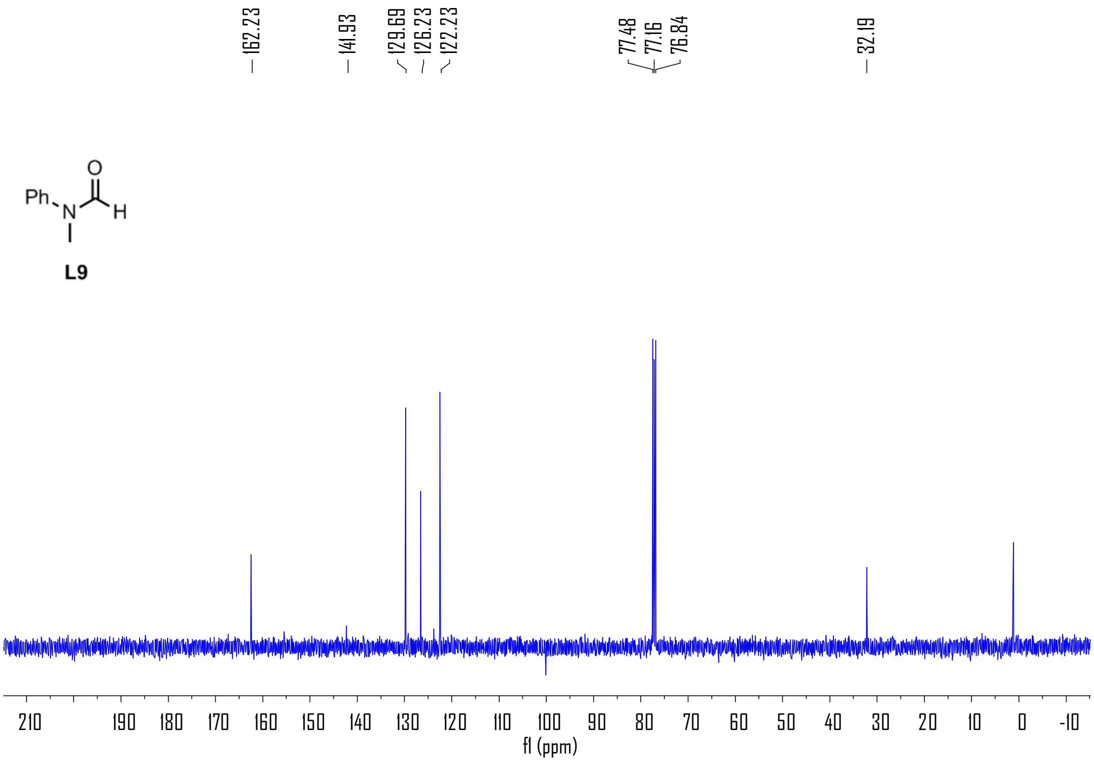
7.36
7.35
7.33
7.23
7.21
7.19
7.12
7.10
3.25
Ph
N
O
H
L9
0.91
2.23
1.31
2.00
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.23
141.93
129.69
126.23
122.23
77.48
77.16
76.84
32.19
Ph
N
O
H
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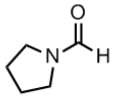
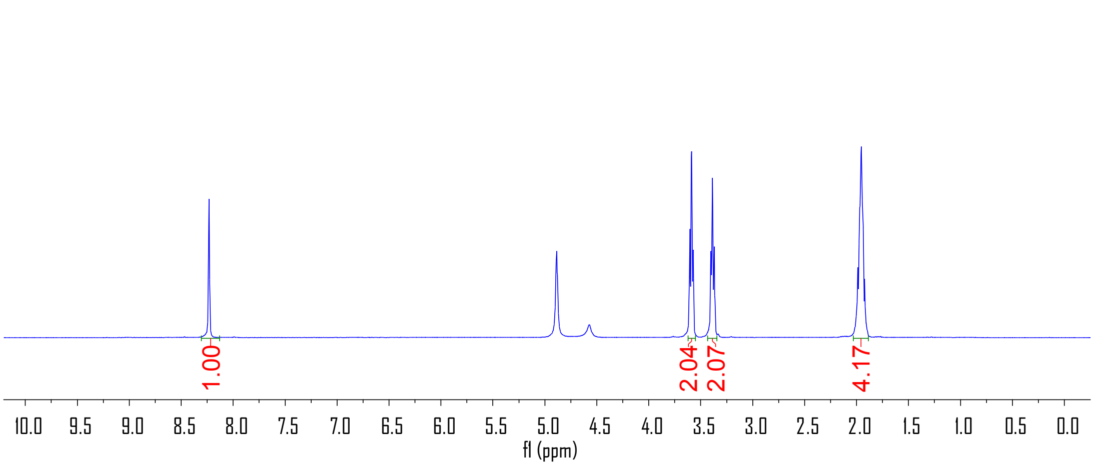
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



L10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3.40
3.39
3.37
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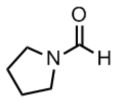
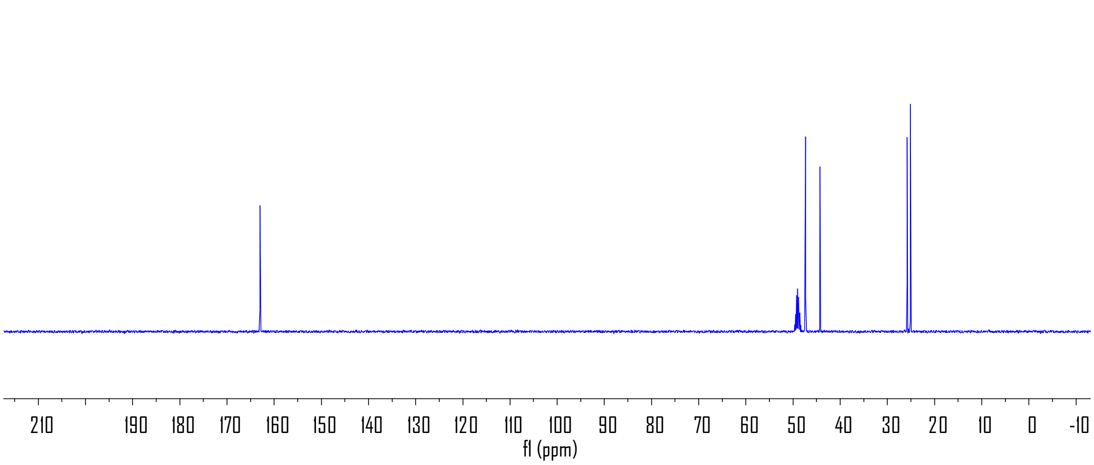
1.99
1.97
1.95
1.94
1.92
1.91
1.00
2.04
2.07
4.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



L10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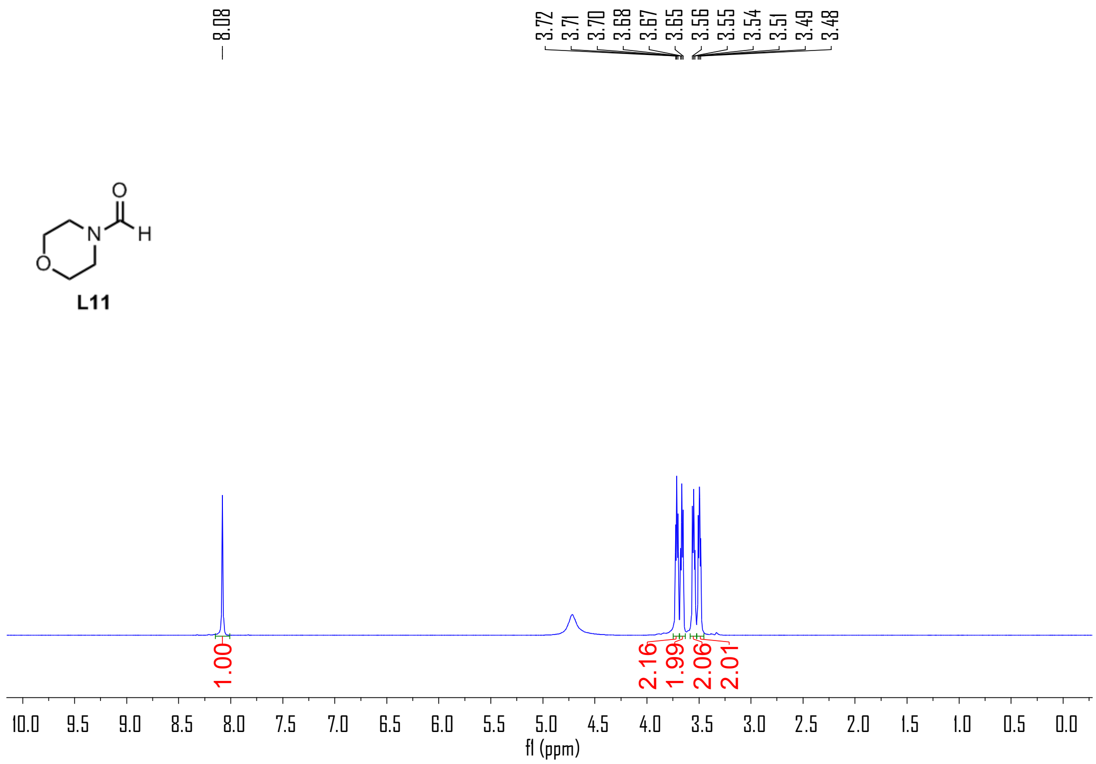
49.64
49.43
49.21
49.00
48.79
48.58
48.36
47.35
44.24
25.79
25.10
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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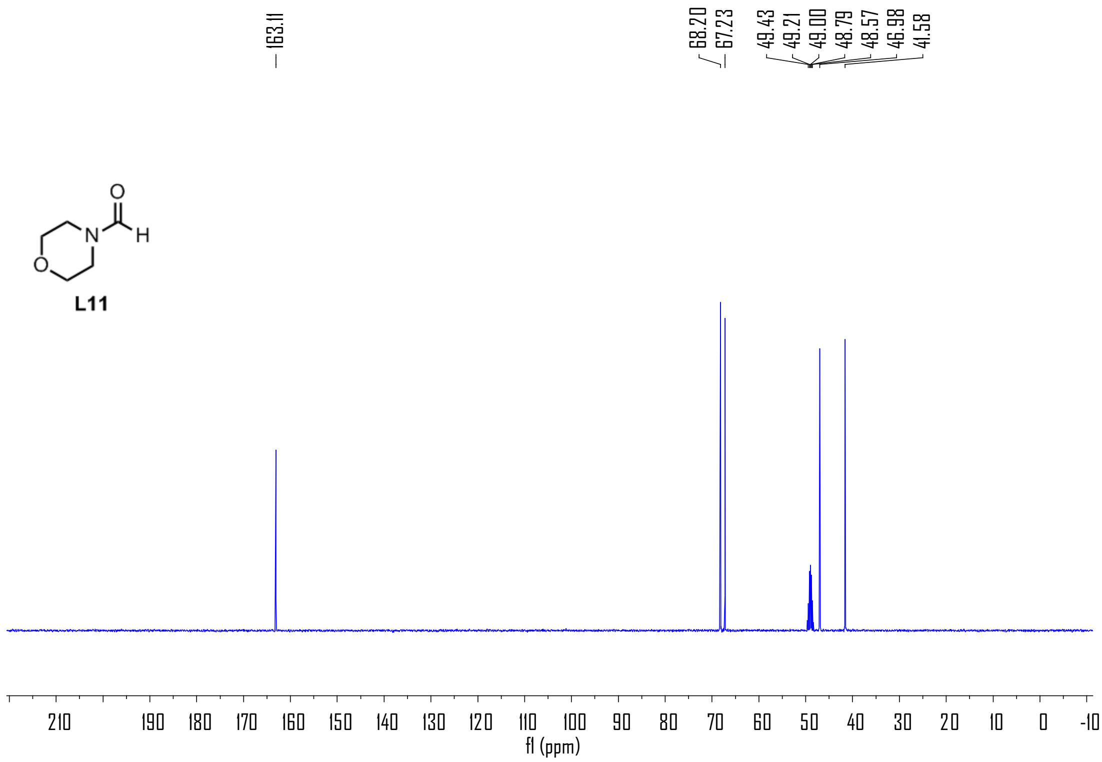
3.72
3.71
3.70
3.68
3.67
3.65
3.56
3.55
3.54
3.51
3.49
3.48
L11
1.00
2.16
1.99
2.06
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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67.23
49.43
49.21
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48.57
46.98
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L11
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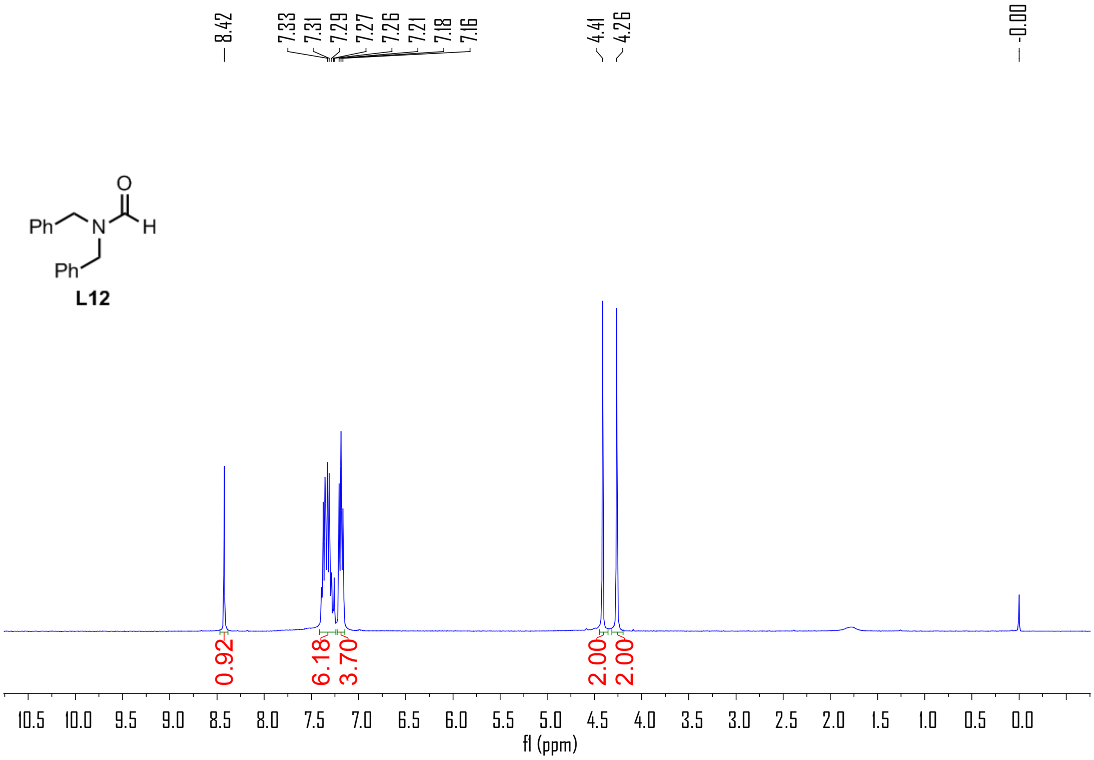
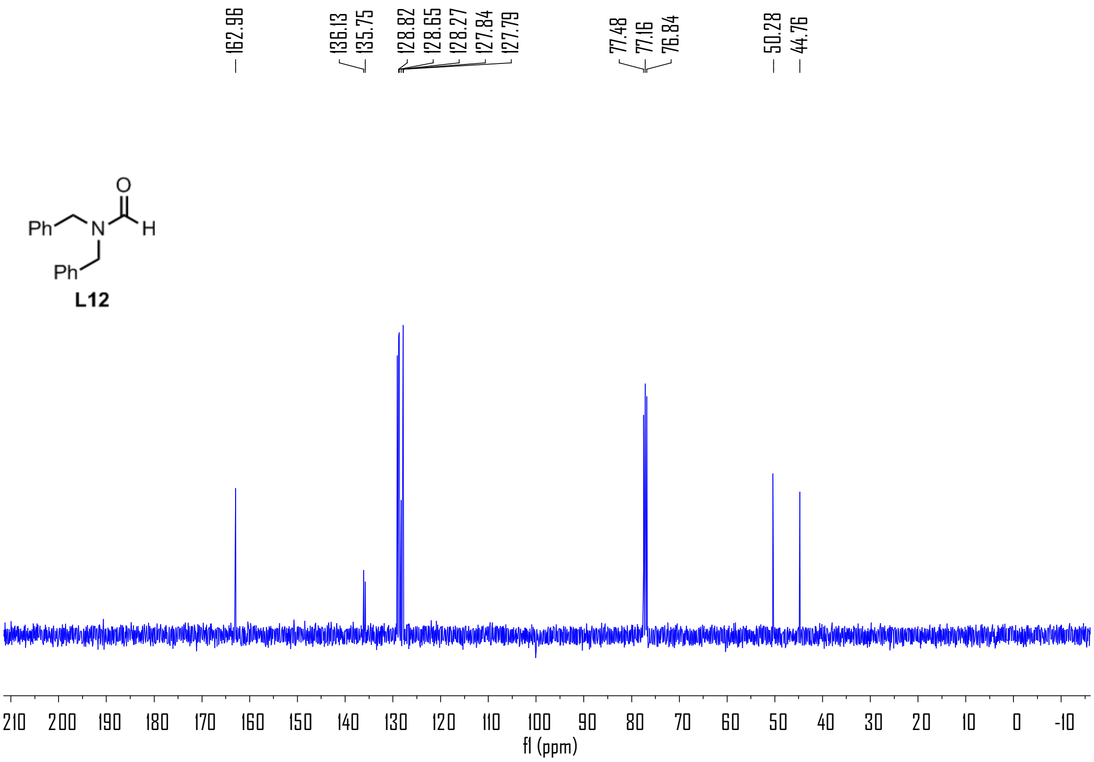
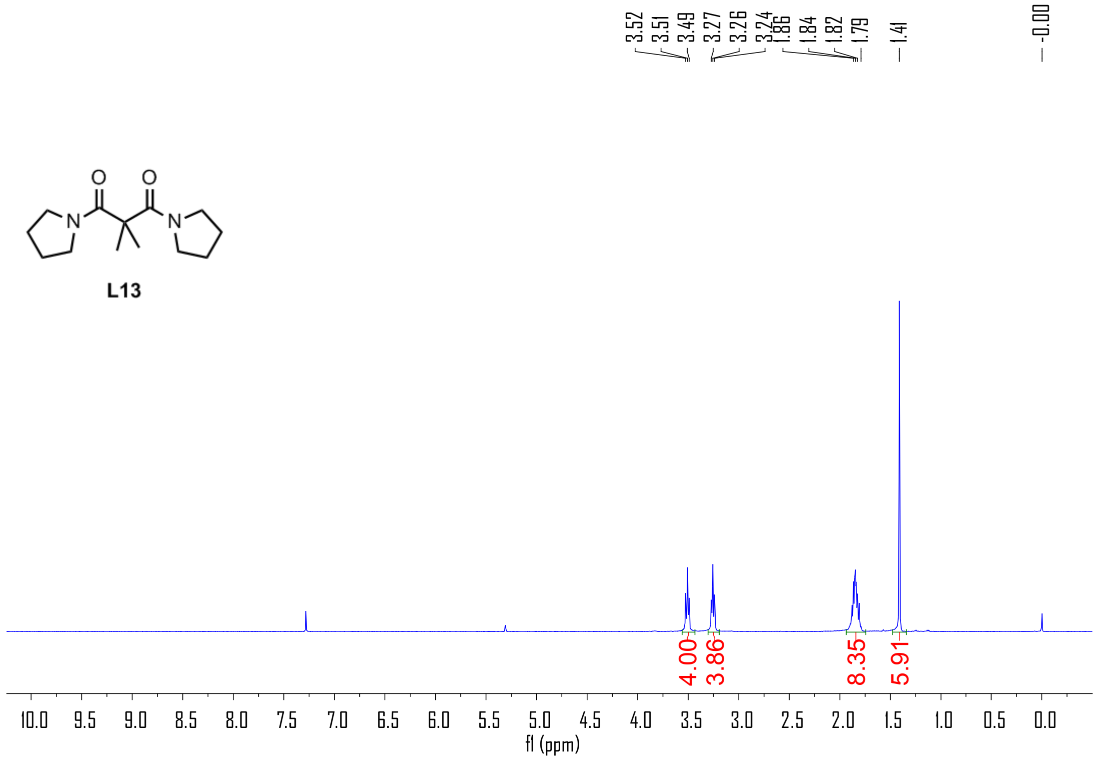
f1 (ppm)


L12


L12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3.49
3.27
3.26
3.24
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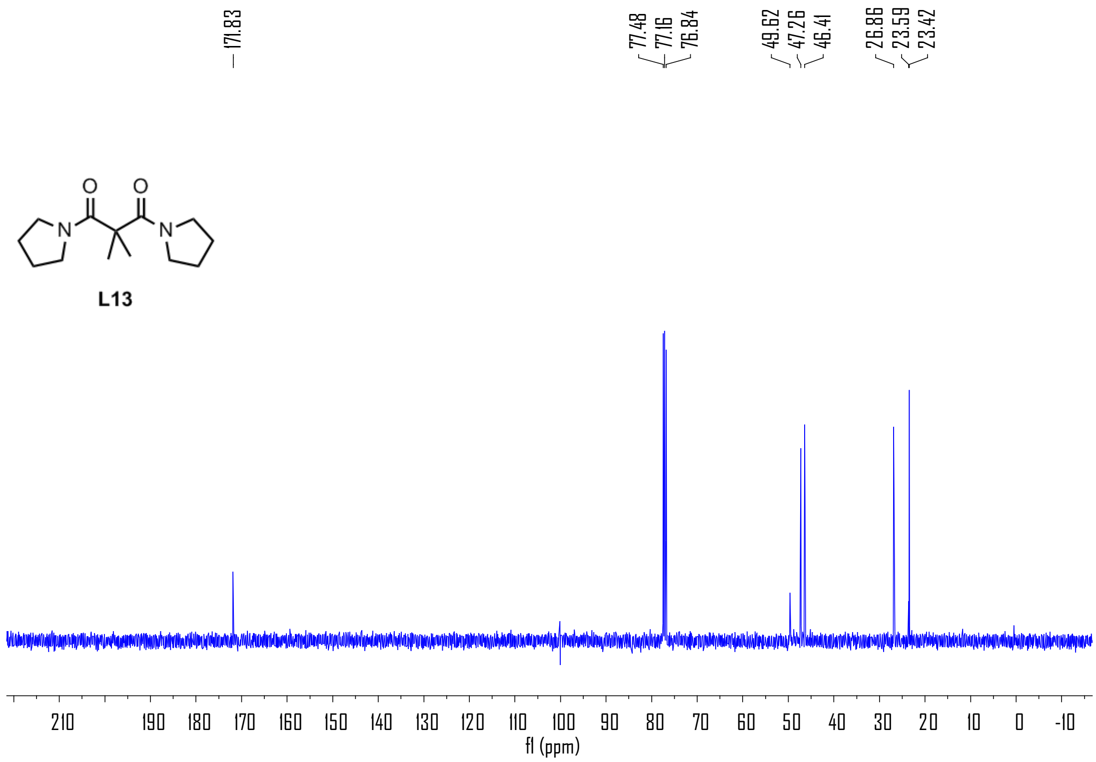
1.84
1.82
1.79
1.41
-0.00
O
O
N
N
L13
4.00
3.86
8.35
5.91
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)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49.62
47.26
46.41
26.86
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O
O
N
N
L13
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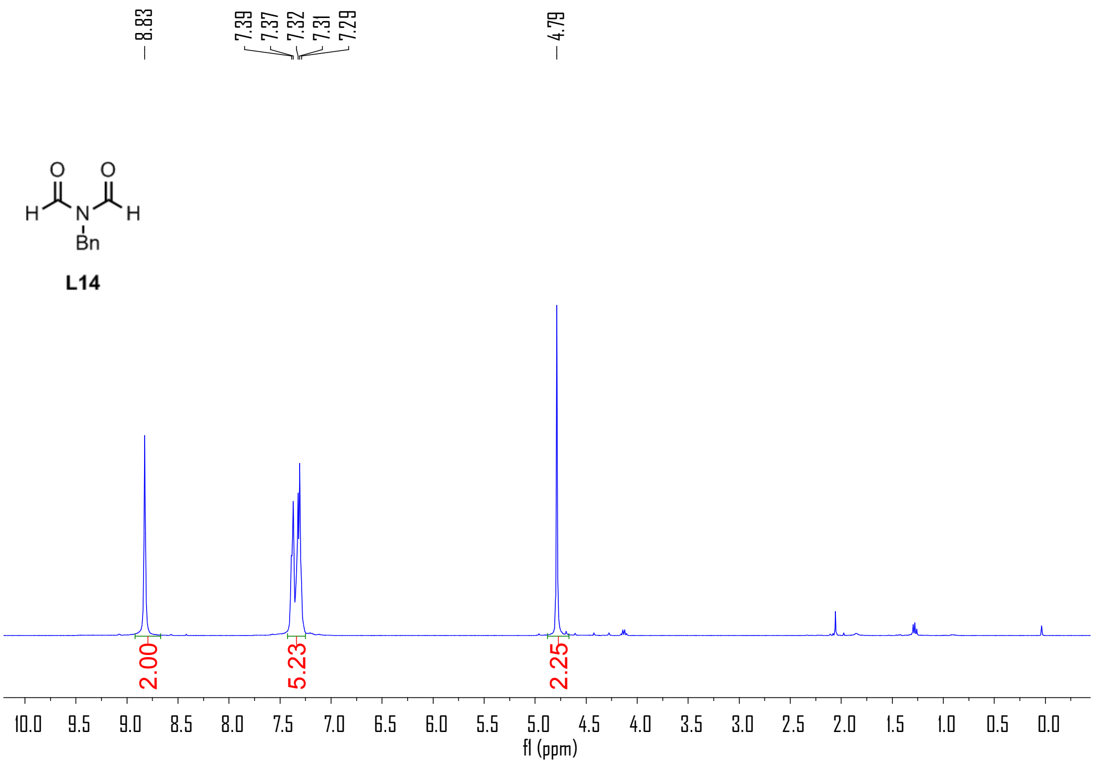
fl (ppm)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O
O
H
N
H
Bn
L14
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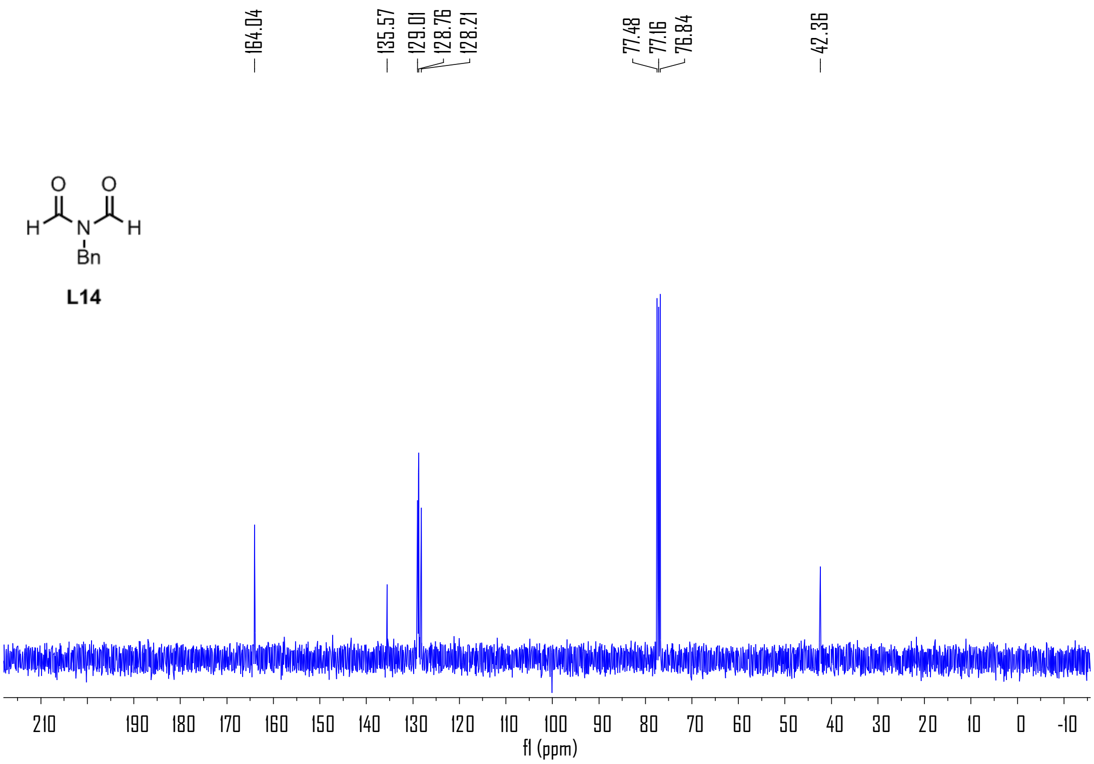
5.23
2.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.84
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H
N
H
Bn
L14
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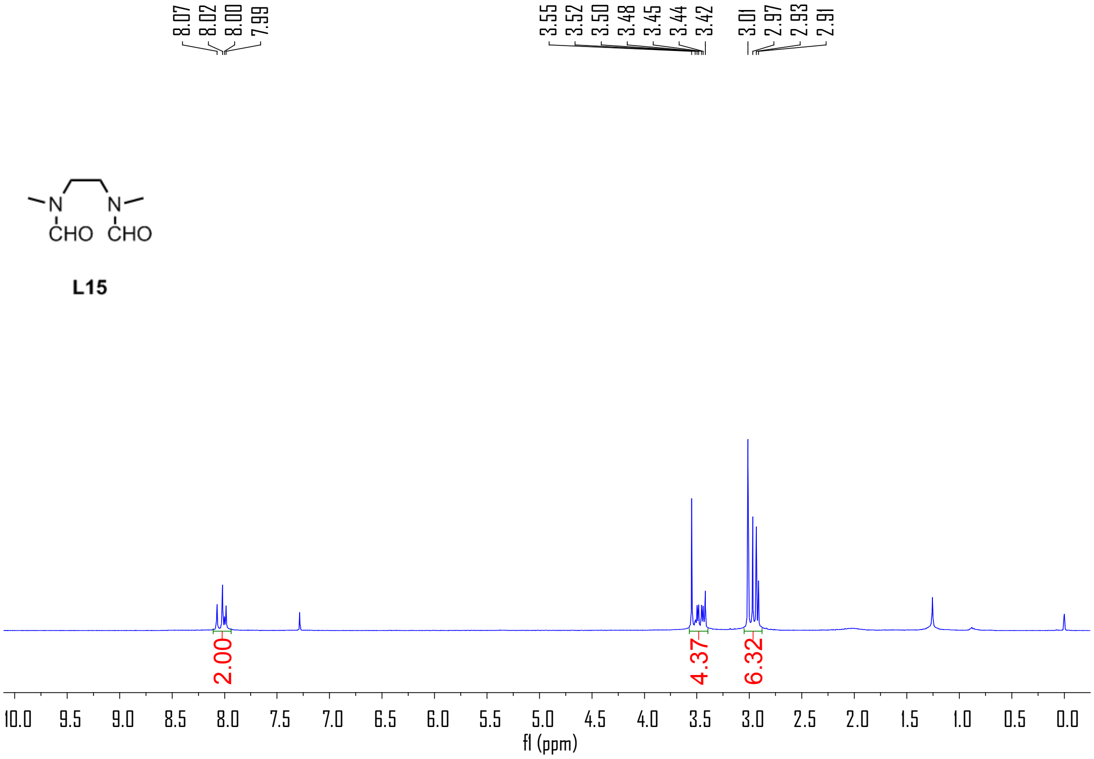
f1 (ppm)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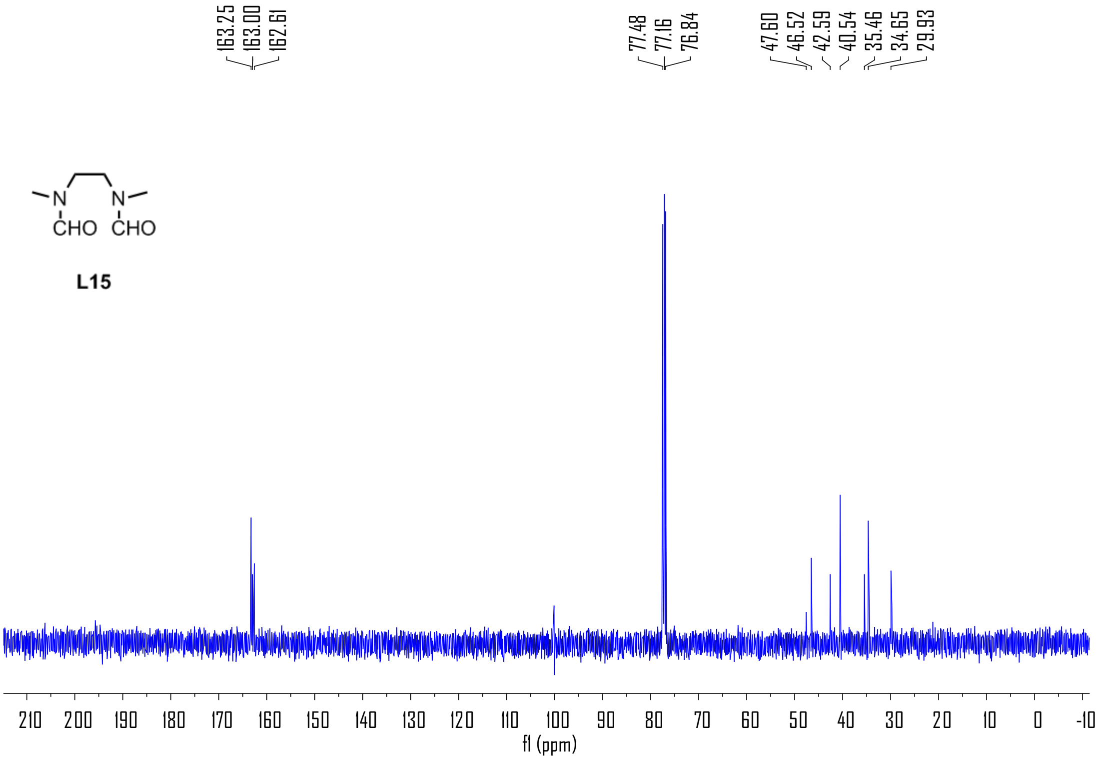
3.52
3.50
3.48
3.45
3.44
3.42
3.01
2.97
2.93
2.91
CHO CHO
2.00
4.37
6.32
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)

L15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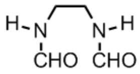
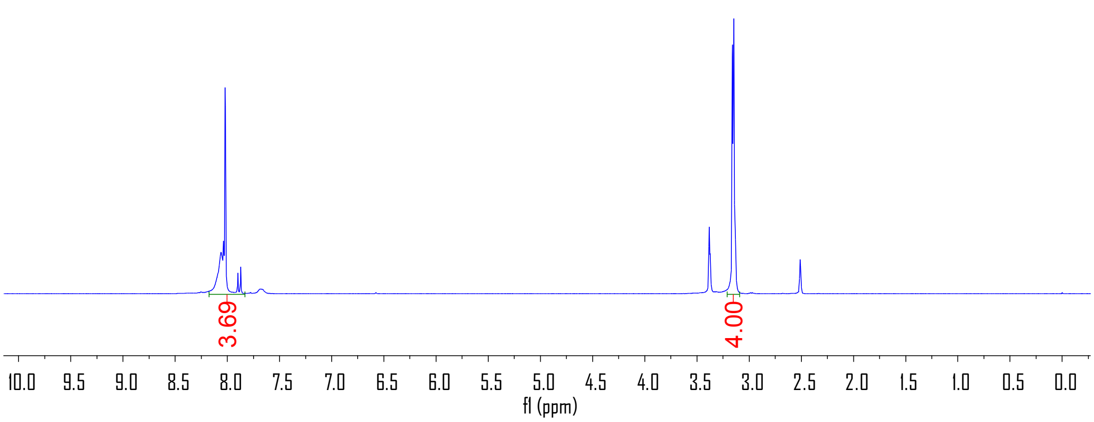
fl (ppm)

L15



L16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3.15
3.13
3.69
4.00
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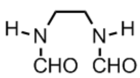
f1 (ppm)



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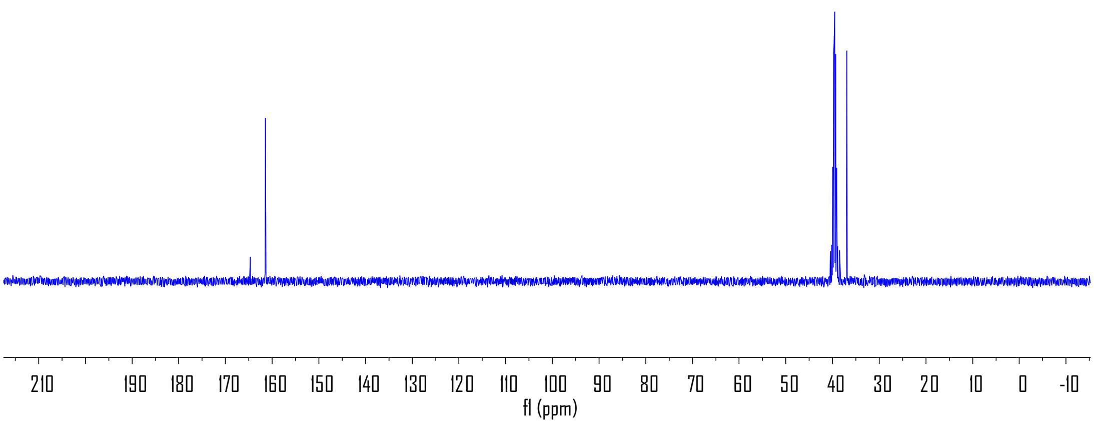
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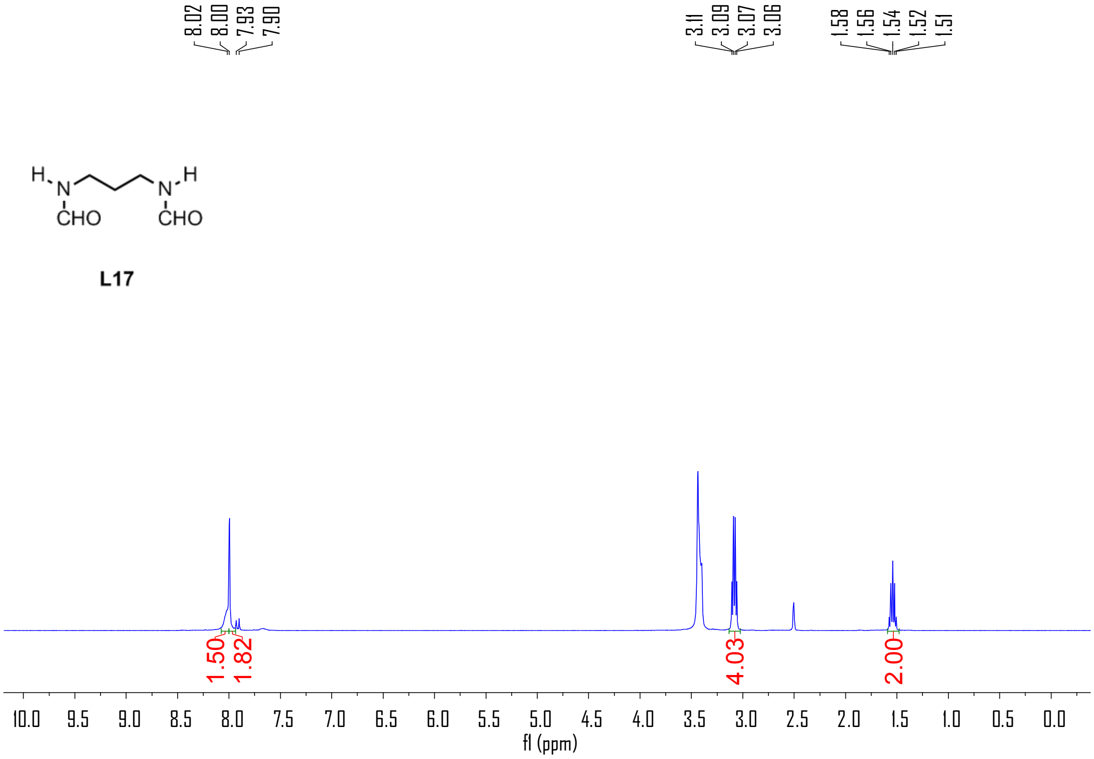
f1 (ppm)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3.07
3.06
1.58
1.56
1.54
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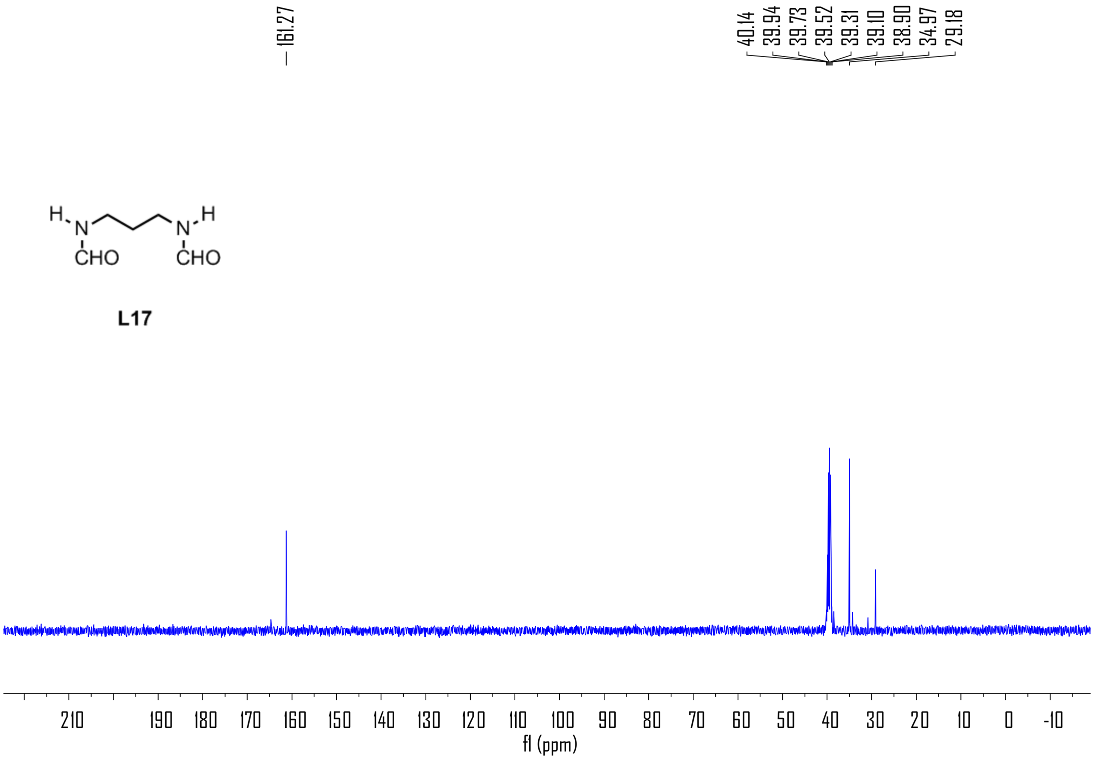
1.51
H
N
N
H
CHO
CHO
1.50
1.82
4.03
2.00
fl (ppm)

L17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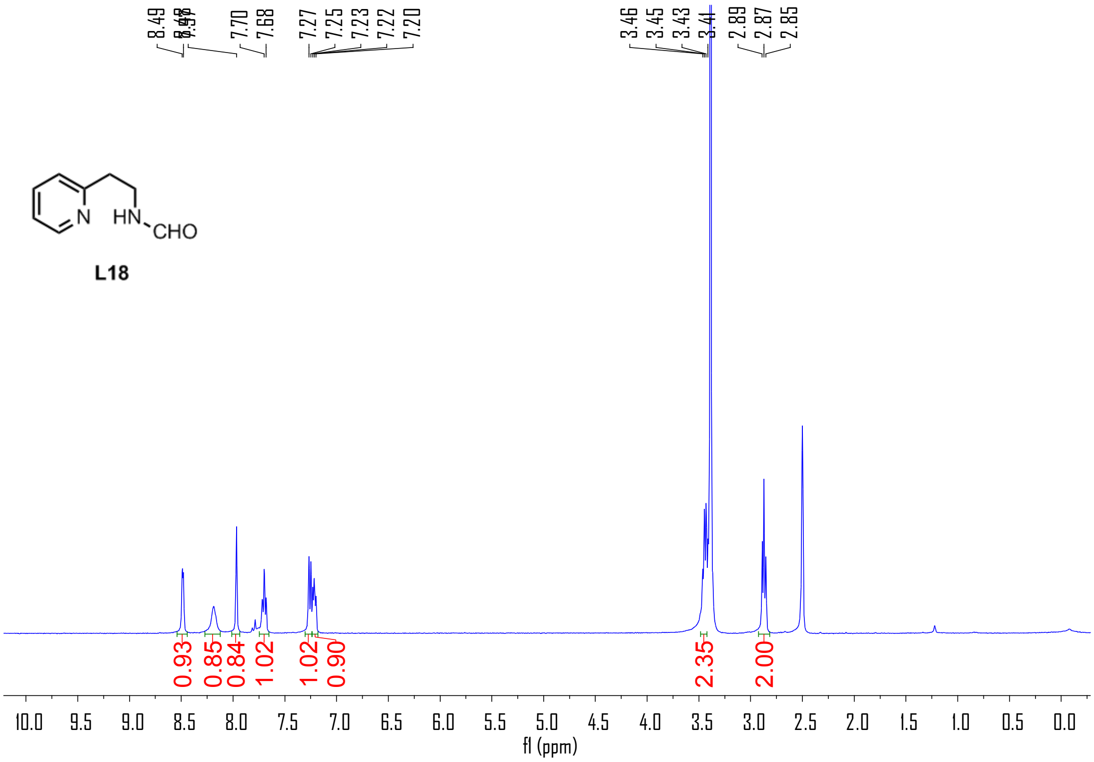
CHO
CHO
fl (ppm)

L17



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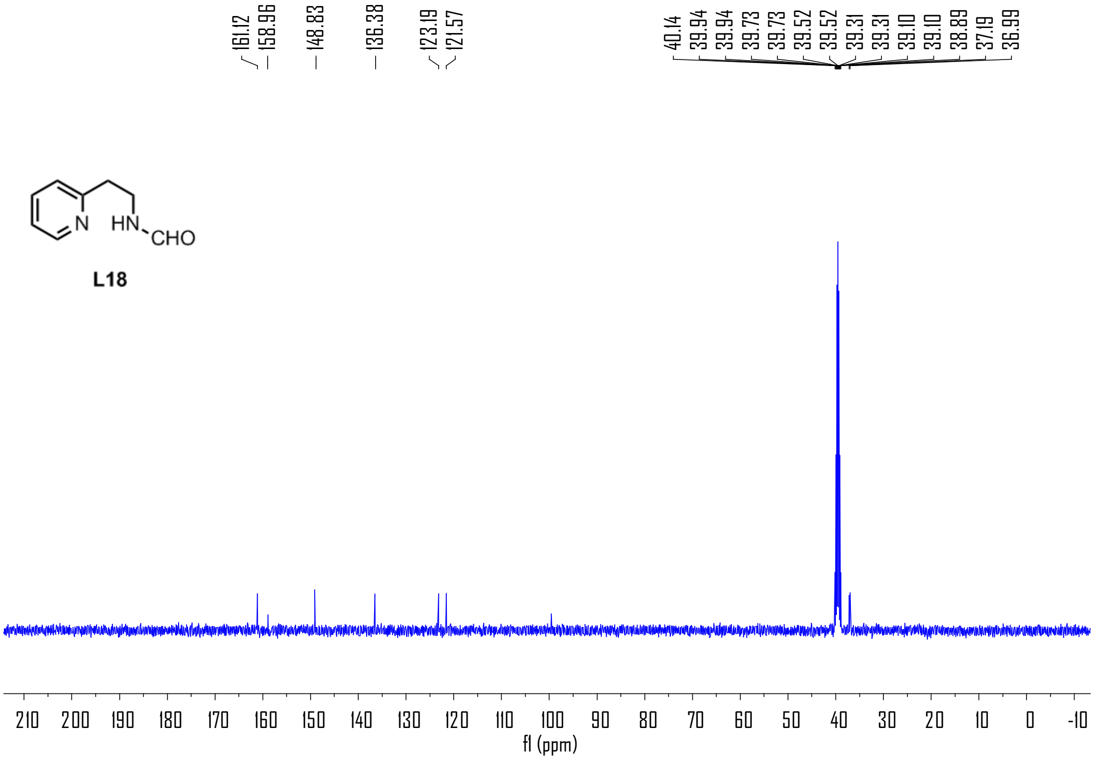
7.27
7.25
7.23
7.22
7.20
3.46
3.45
3.43
3.41
2.89
2.87
2.85
0.93
0.85
0.84
1.02
1.02
0.90
2.35
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

L18



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39.52
39.31
39.31
39.10
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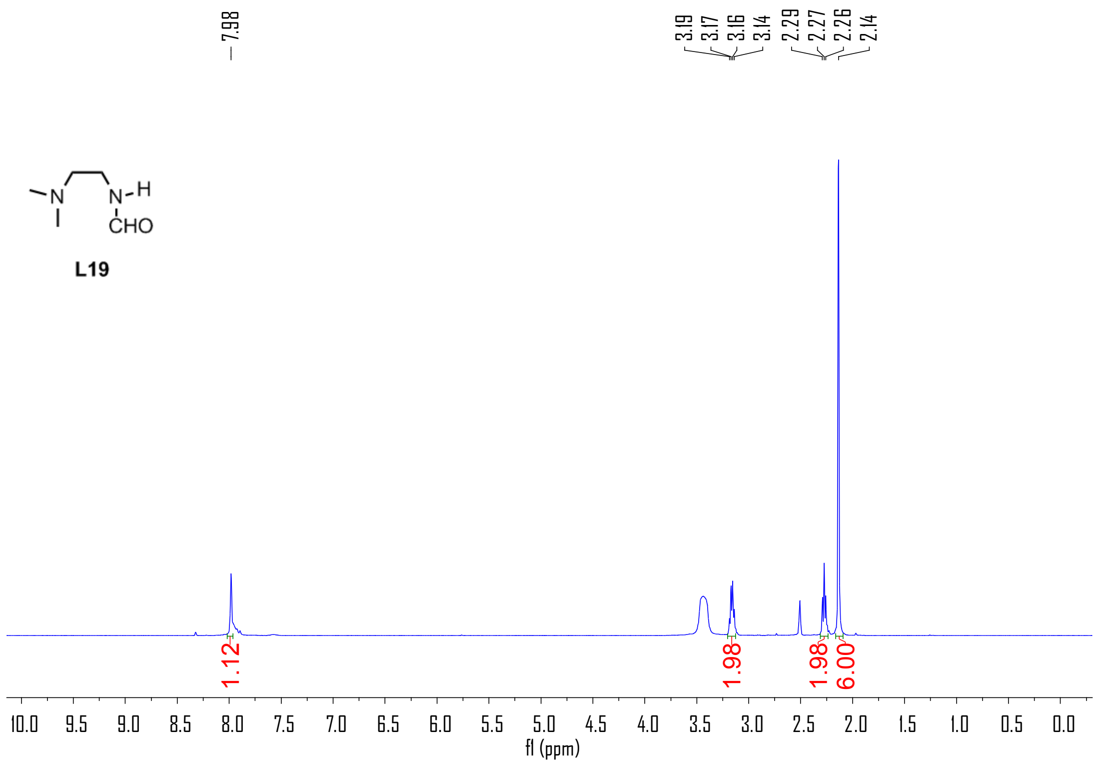
37.19
36.99
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

L18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3.14
2.29
2.27
2.26
2.14
N-H
CHO
L19
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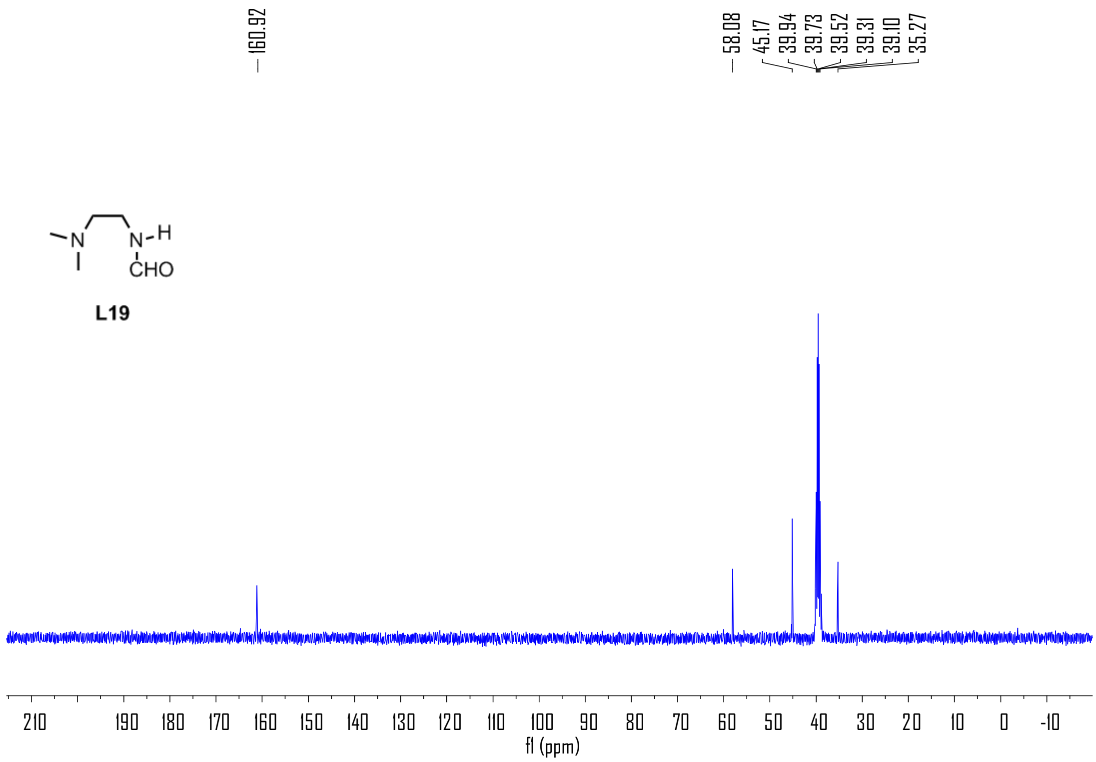
1.98
1.98
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)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N-H
CHO
L19
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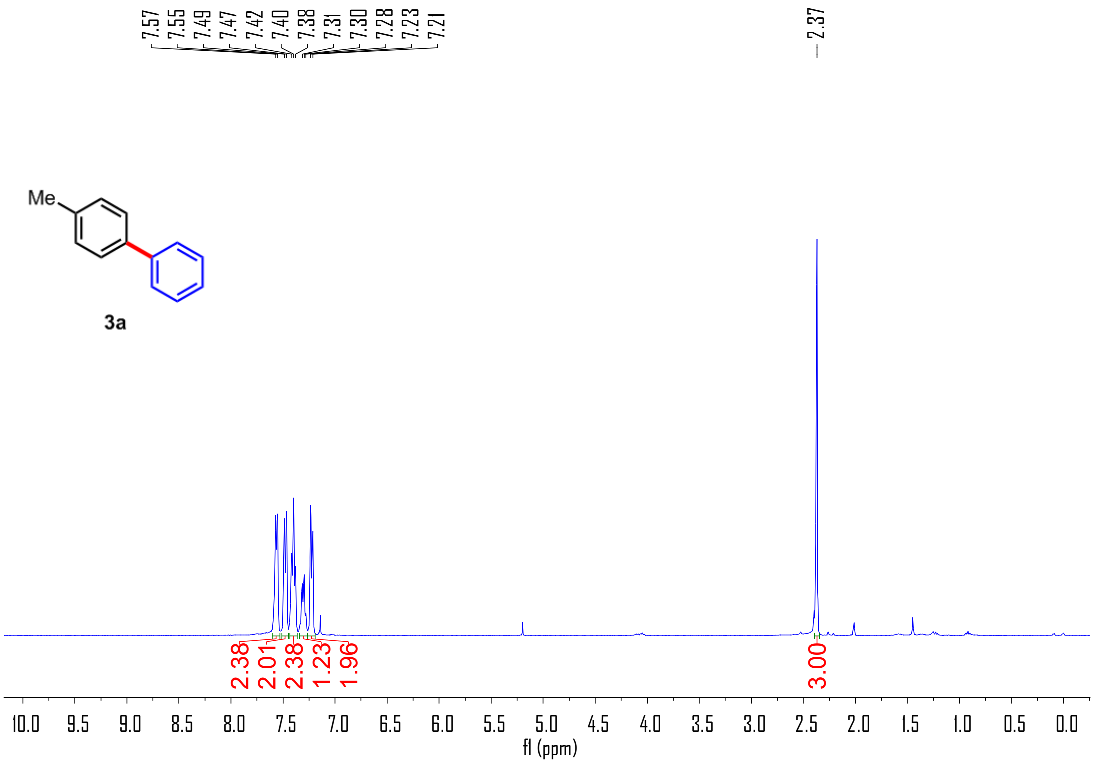
fl (ppm)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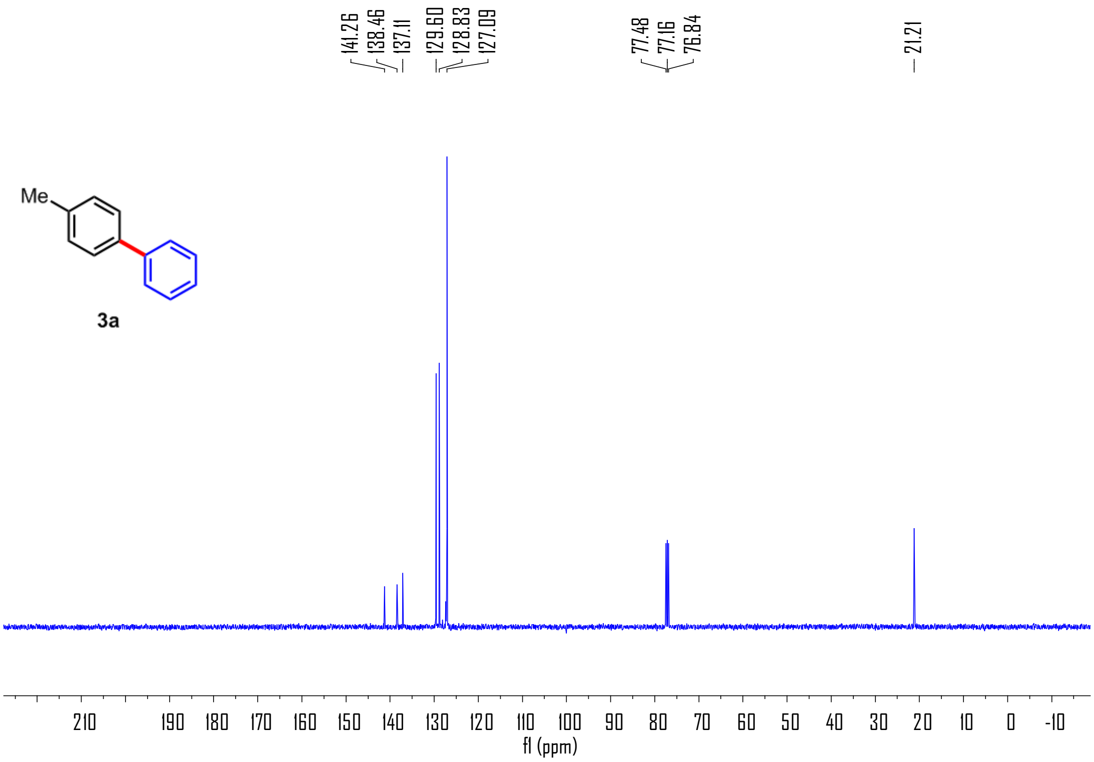
7.23
7.21
2.37
Me
3a
2.38
2.01
2.38
1.23
1.96
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.84
21.21
Me
3a
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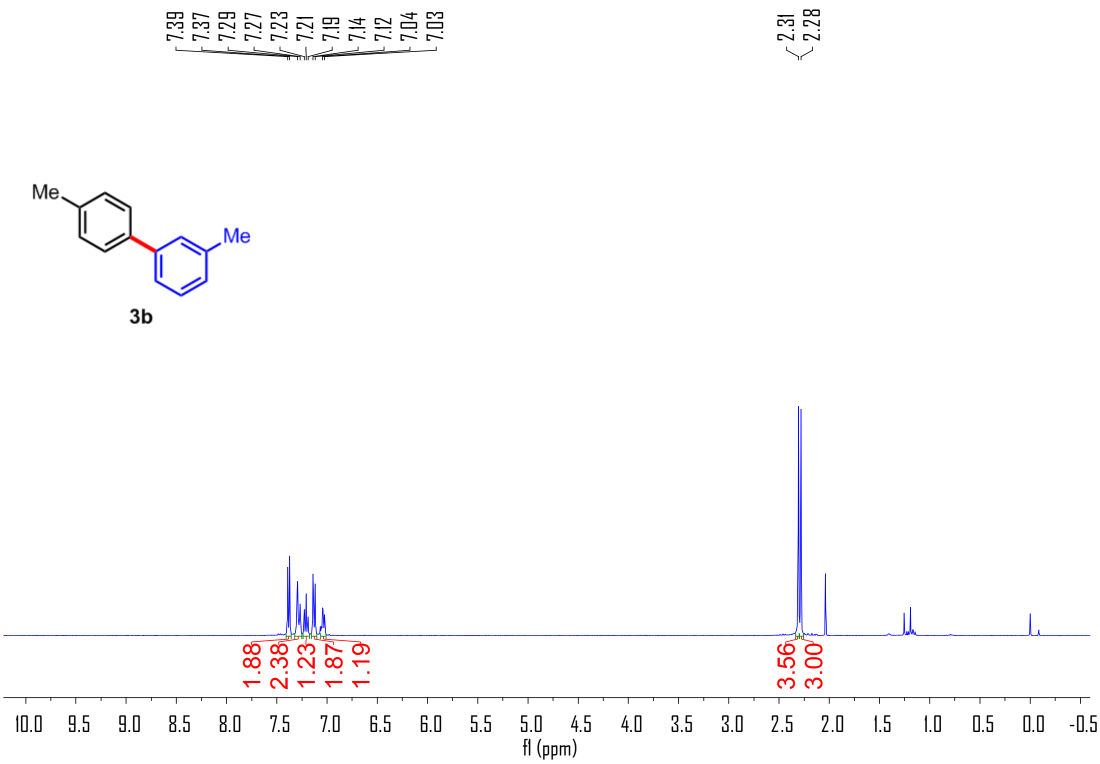
f1 (ppm)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7.03
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Me
3b
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1.87
1.19
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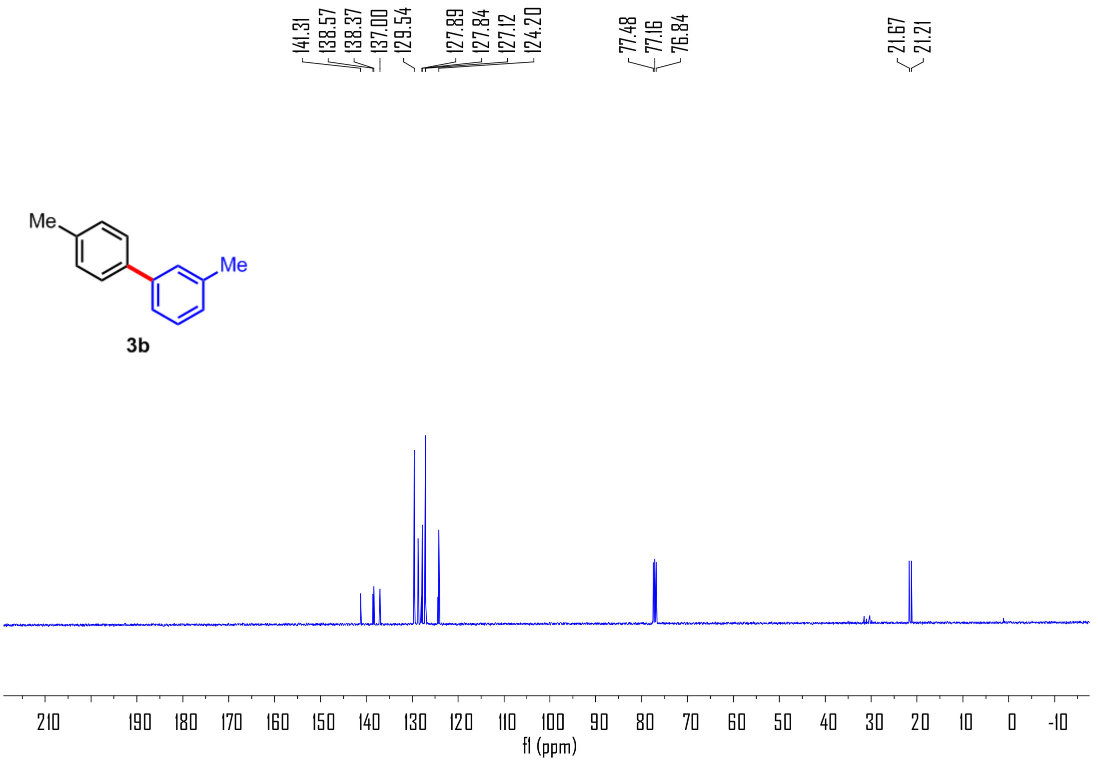
3.00
fl (ppm)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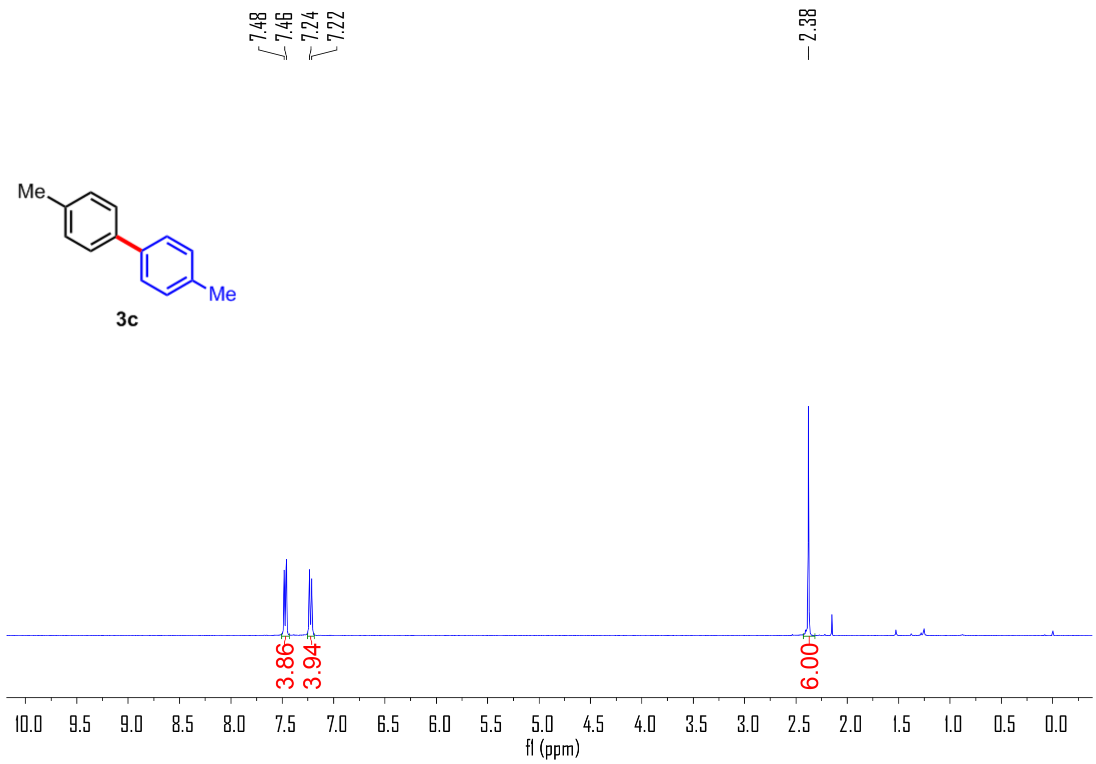
21.21
Me
Me
3b
fl (ppm)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3.86
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6.00
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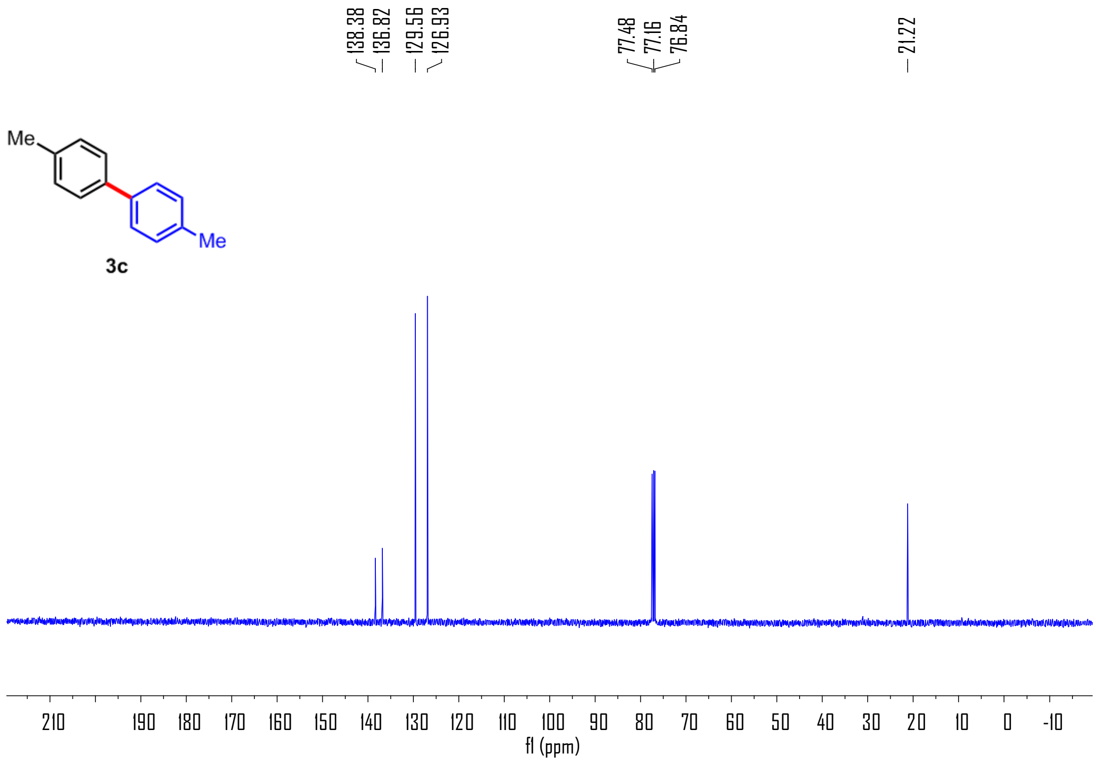
fl (ppm)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Me
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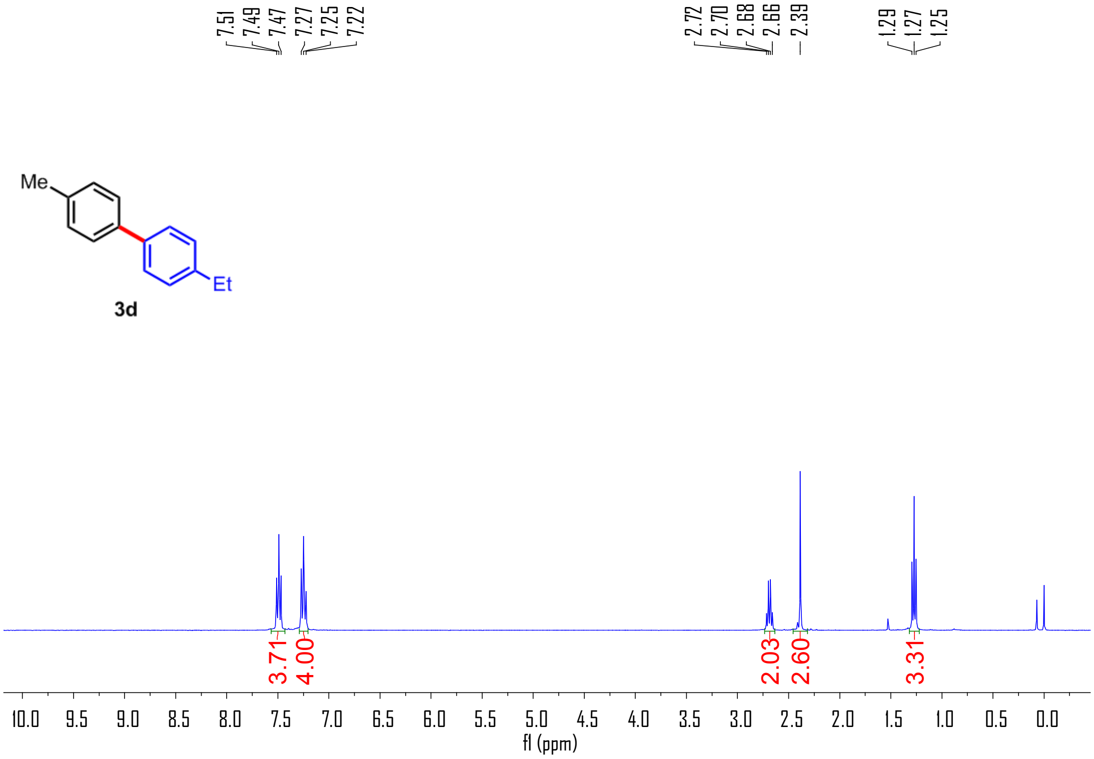
fl (ppm)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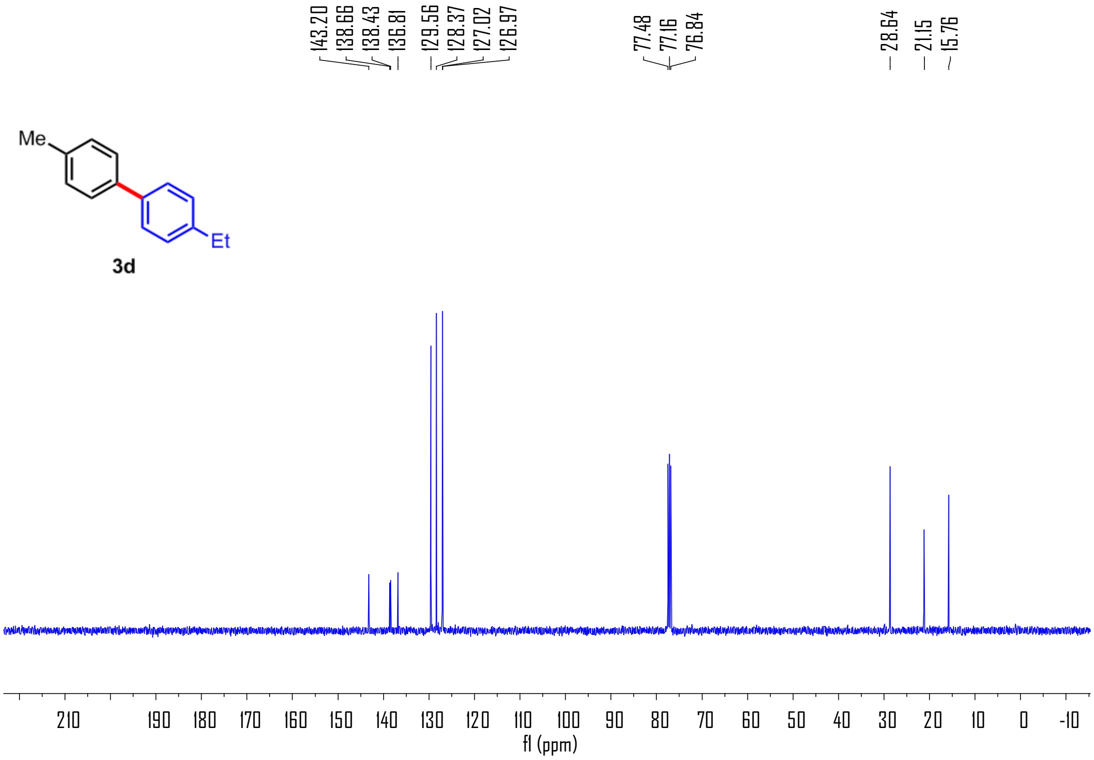
fl (ppm)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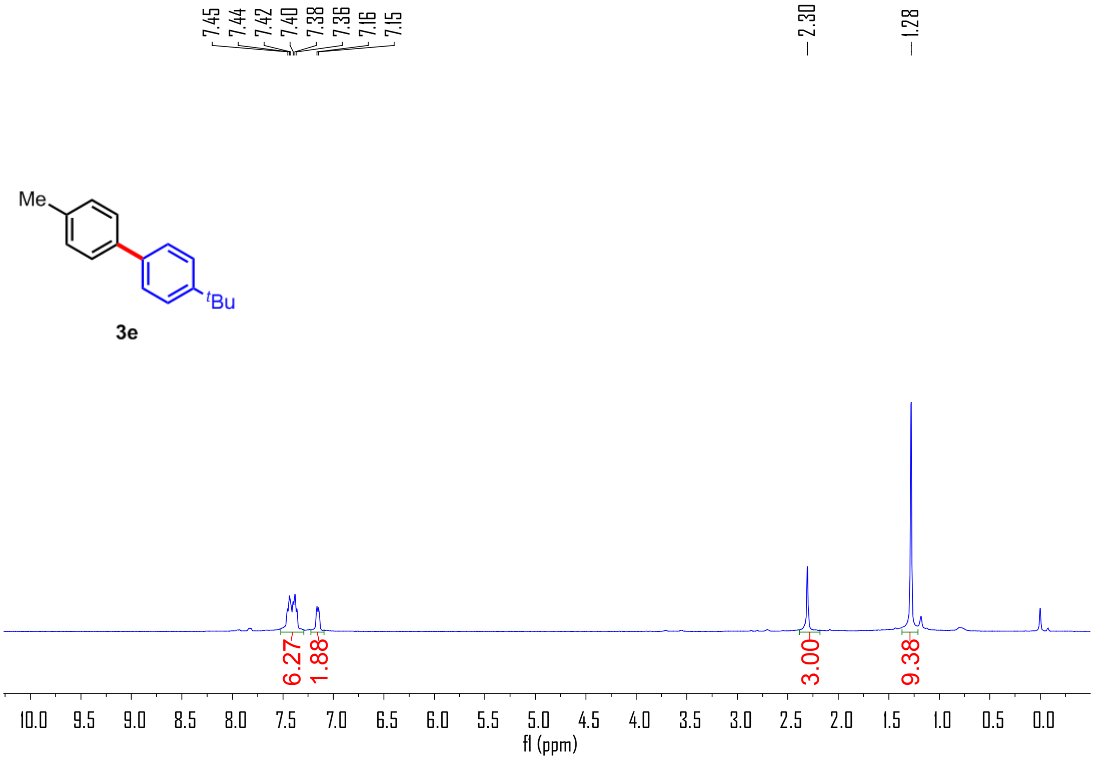
Et
3d
fl (ppm)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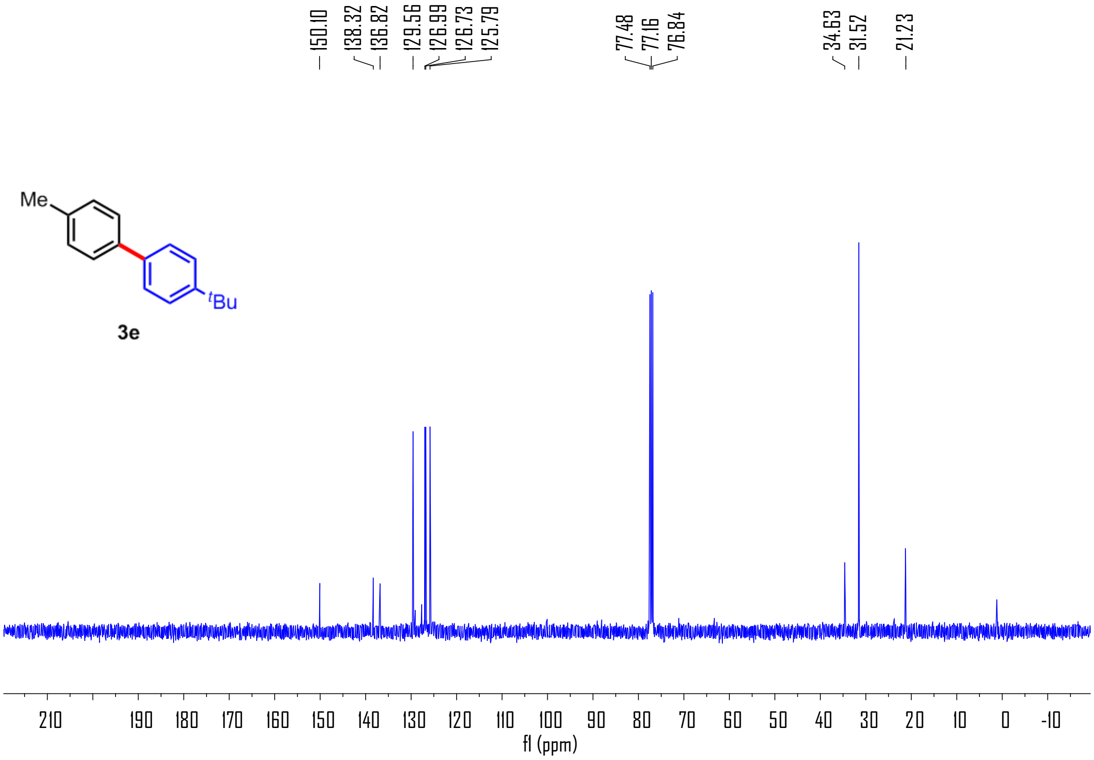
Me
tBu
3e
6.27
1.88
3.00
9.38
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)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125.79
77.48
77.16
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21.23
Me
tBu
3e
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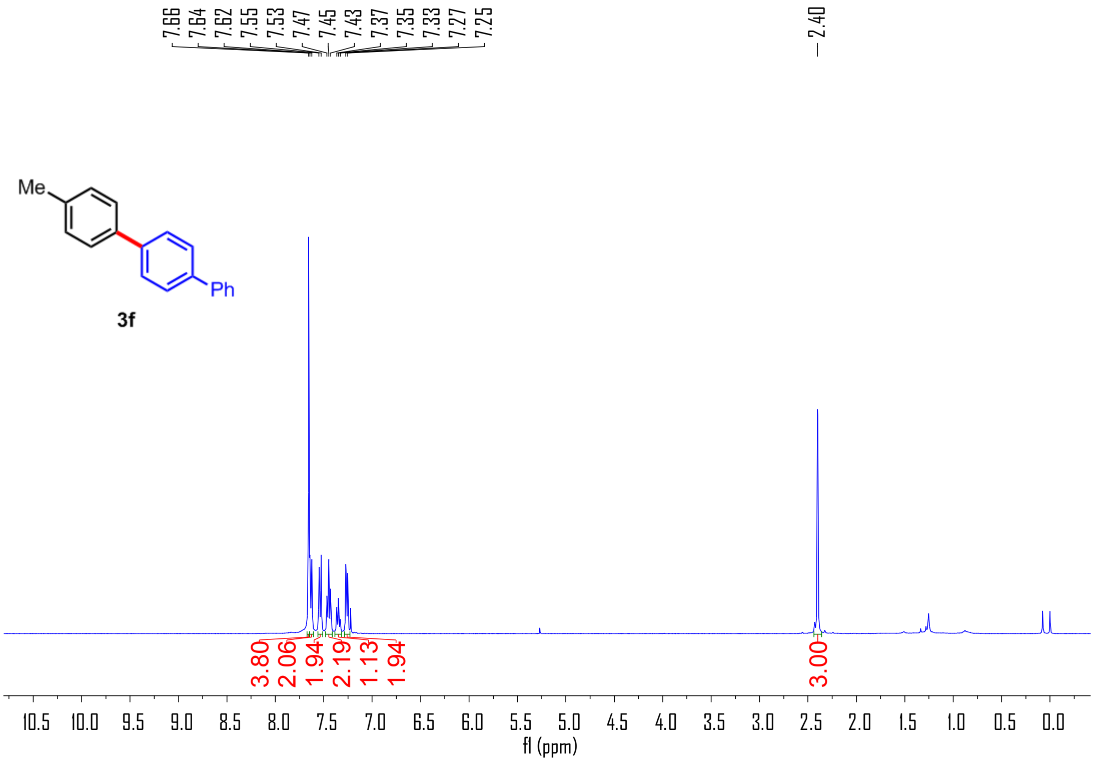
fl (ppm)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7.43
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7.35
7.33
7.27
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Ph
3f
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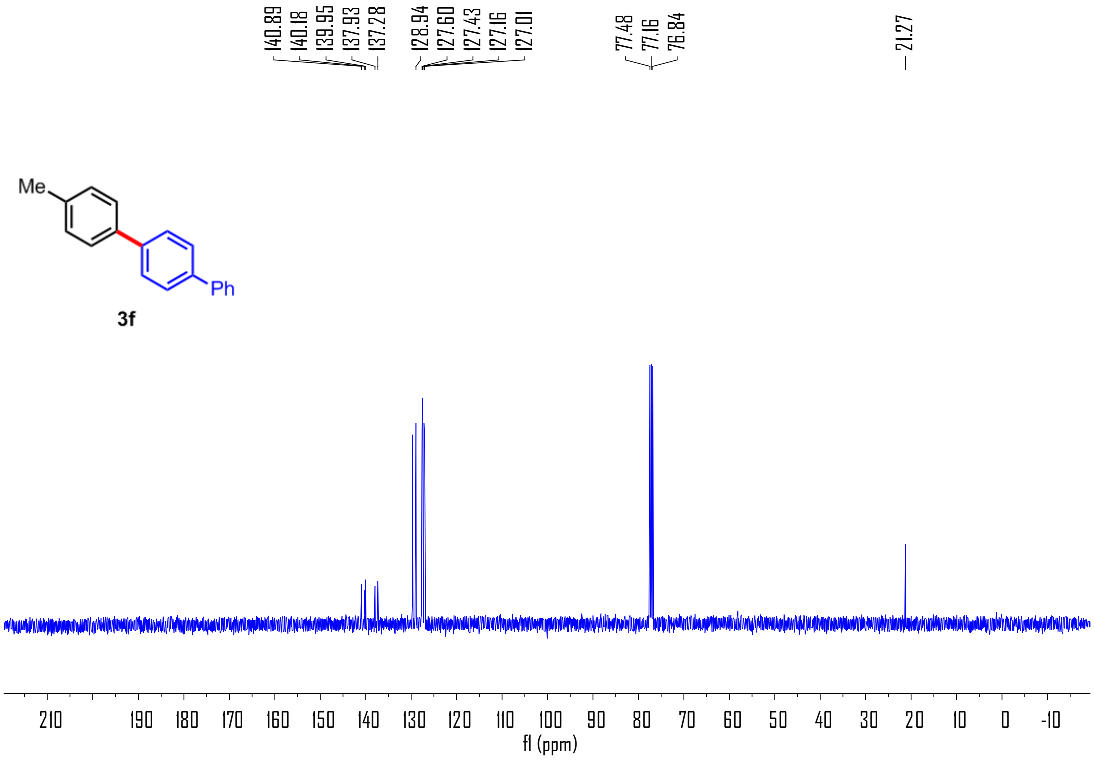
2.06
1.94
2.19
1.13
1.94
3.00
fl (ppm)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139.95
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137.28
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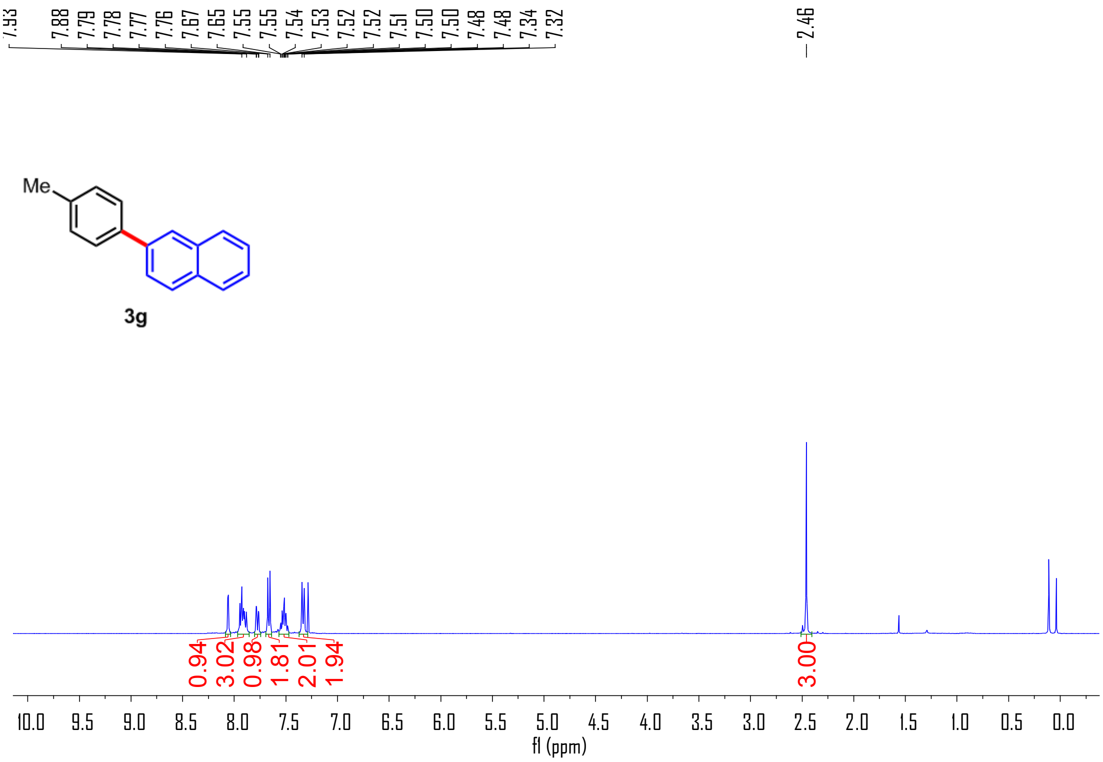
Ph
3f
fl (ppm)



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7.79
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7.77
7.76
7.67
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7.55
7.54
7.53
7.52
7.52
7.51
7.50
7.50
7.48
7.48
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3.02
0.98
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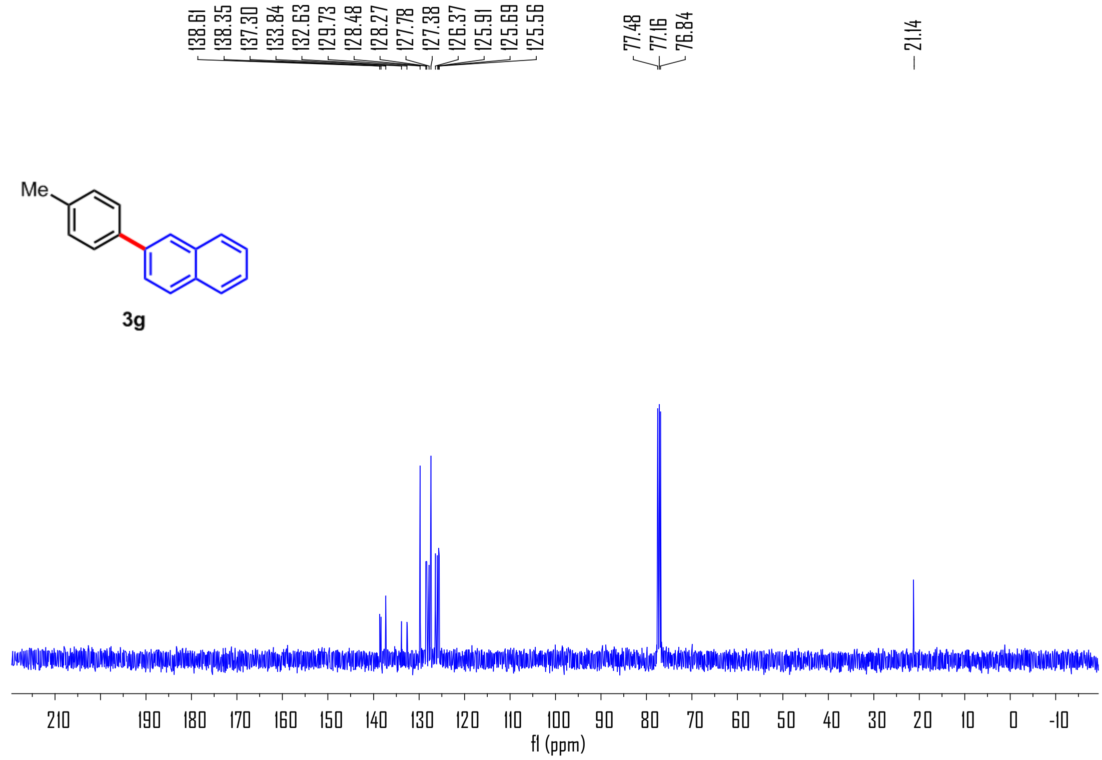
2.01
1.94
3.00
fl (ppm)



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132.63
129.73
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128.27
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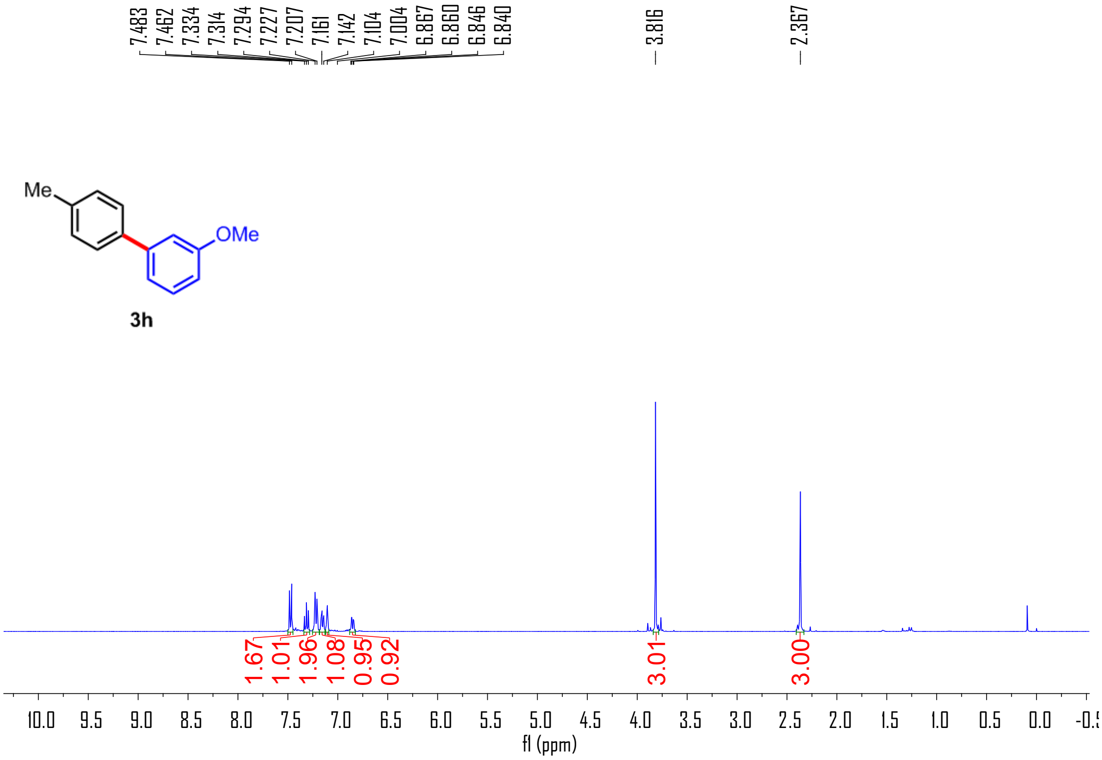
125.69
125.56
77.48
77.16
76.84
21.14
Me
3g
fl (ppm)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6.860
6.846
6.840
3.816
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Me
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3h
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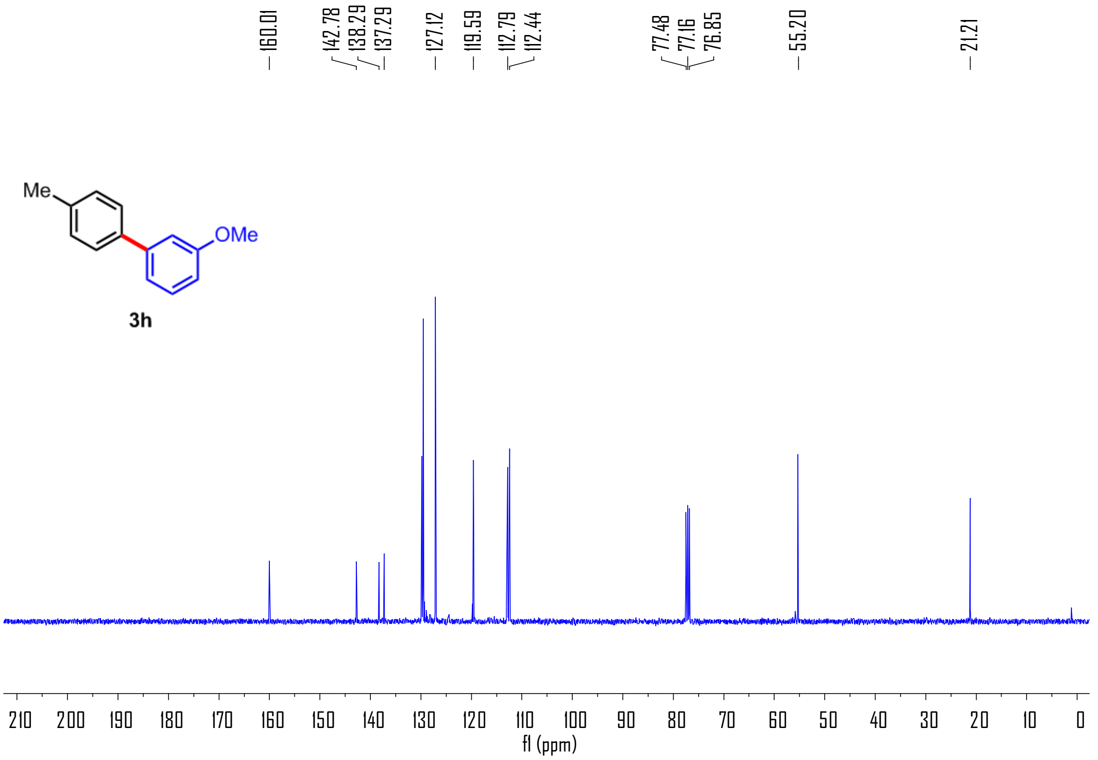
0.95
0.92
3.01
3.00
fl (ppm)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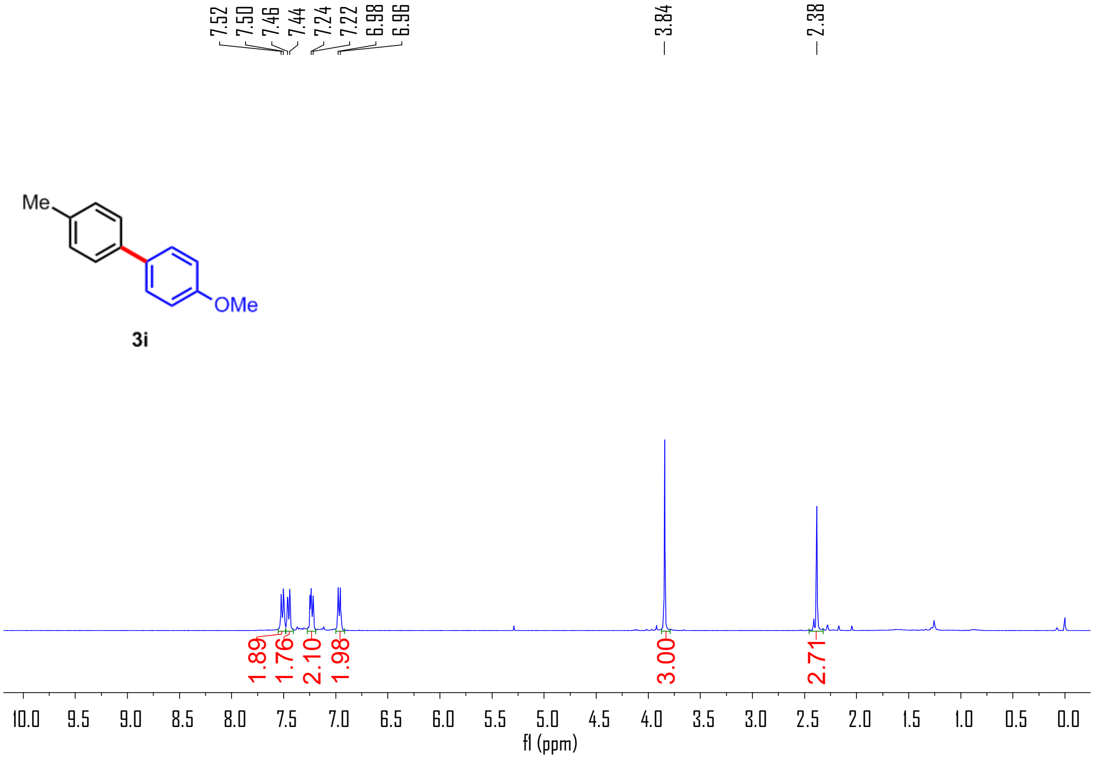
OMe
3h
fl (ppm)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2.38
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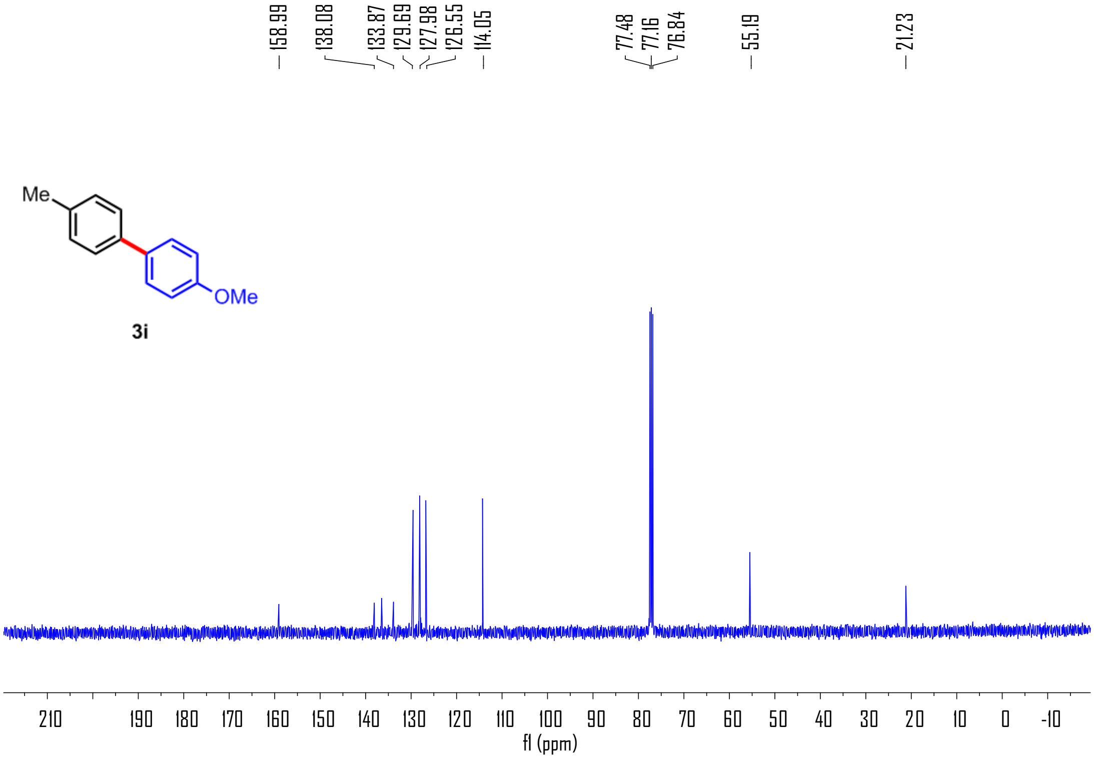
OMe
3i
1.89
1.76
2.10
1.98
3.00
2.71
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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21.23
Me
OMe
3i
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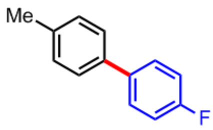
f1 (ppm)



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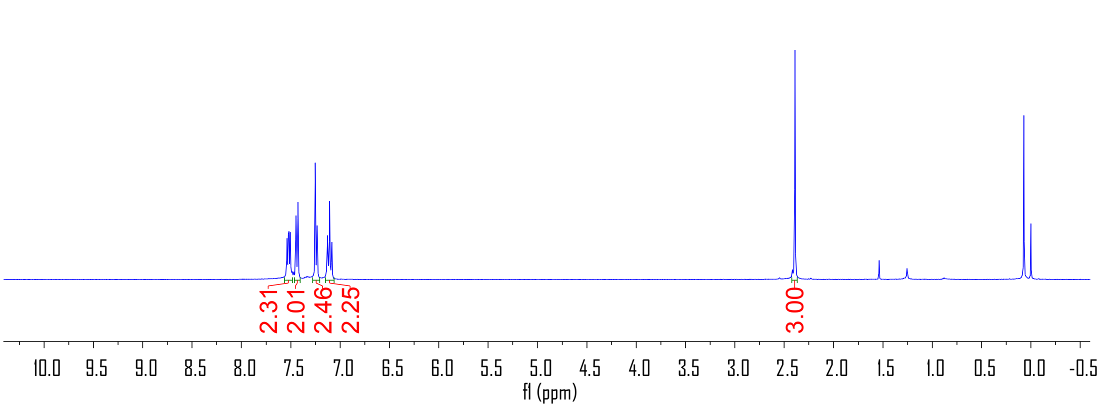

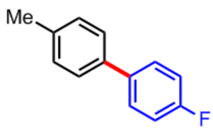

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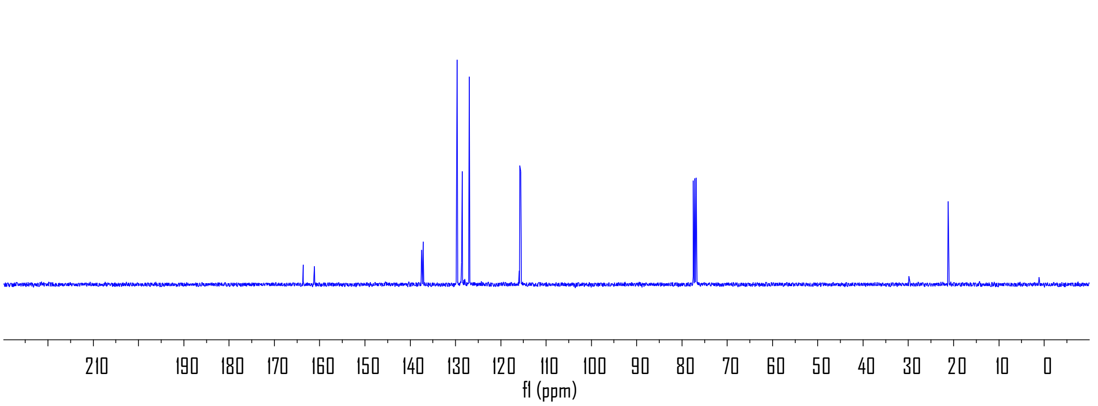

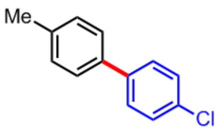

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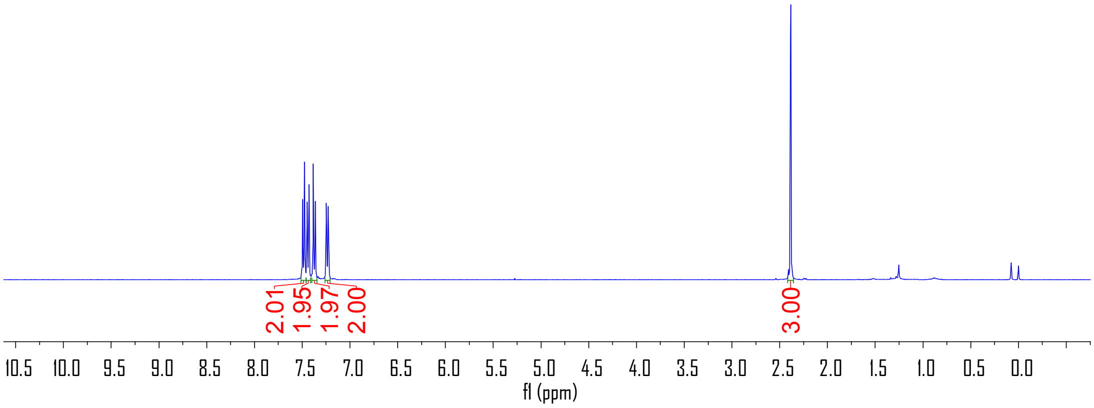

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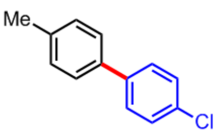
1.97
2.00
3.00
fl (ppm)



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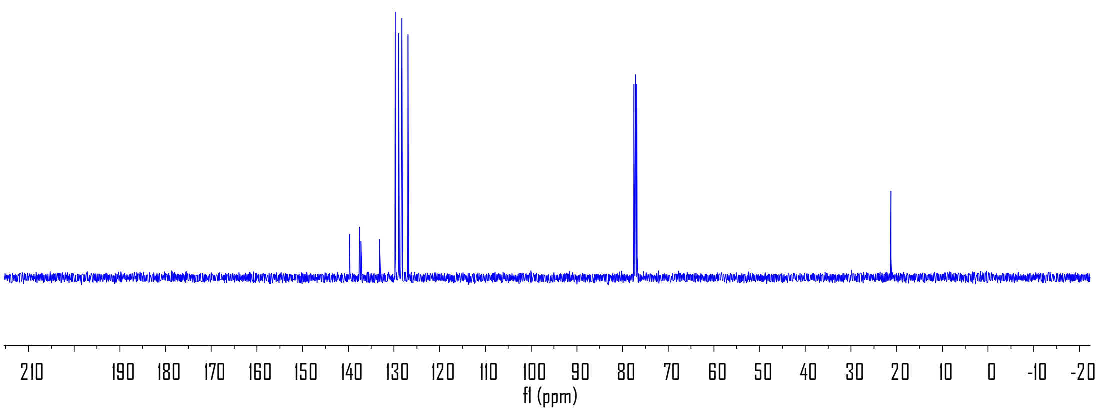

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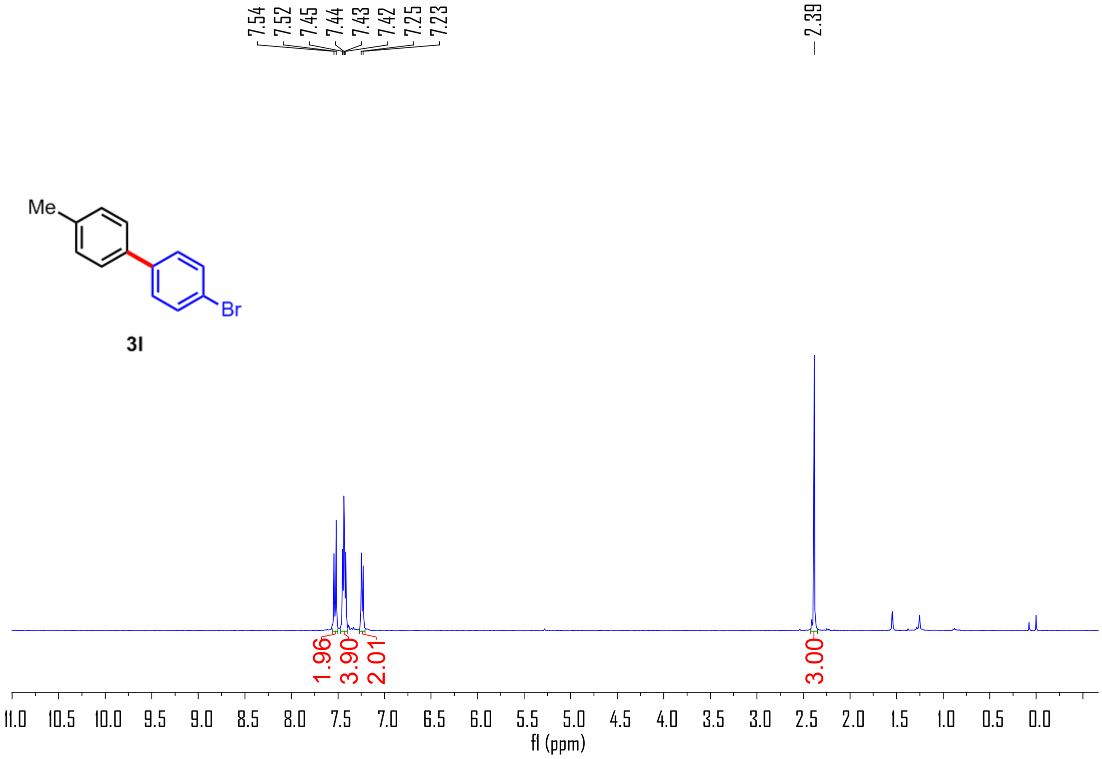
fl (ppm)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Me
Br
3l
1.96
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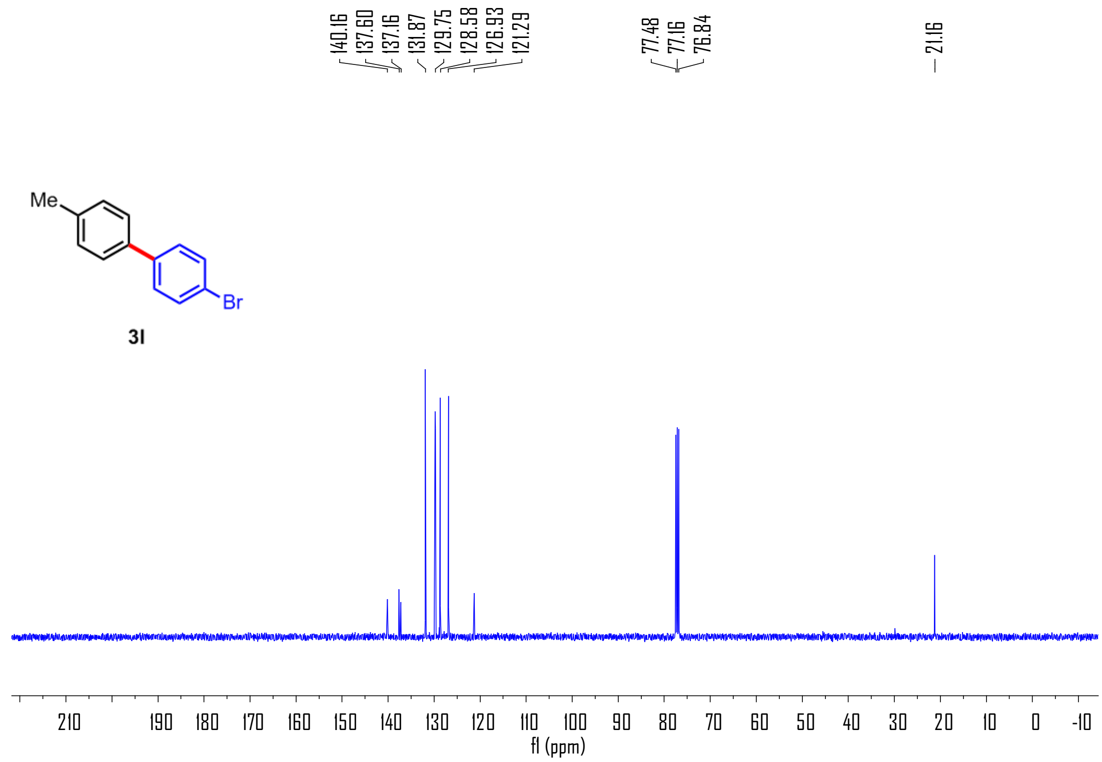
2.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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21.16
Me
Br
3l
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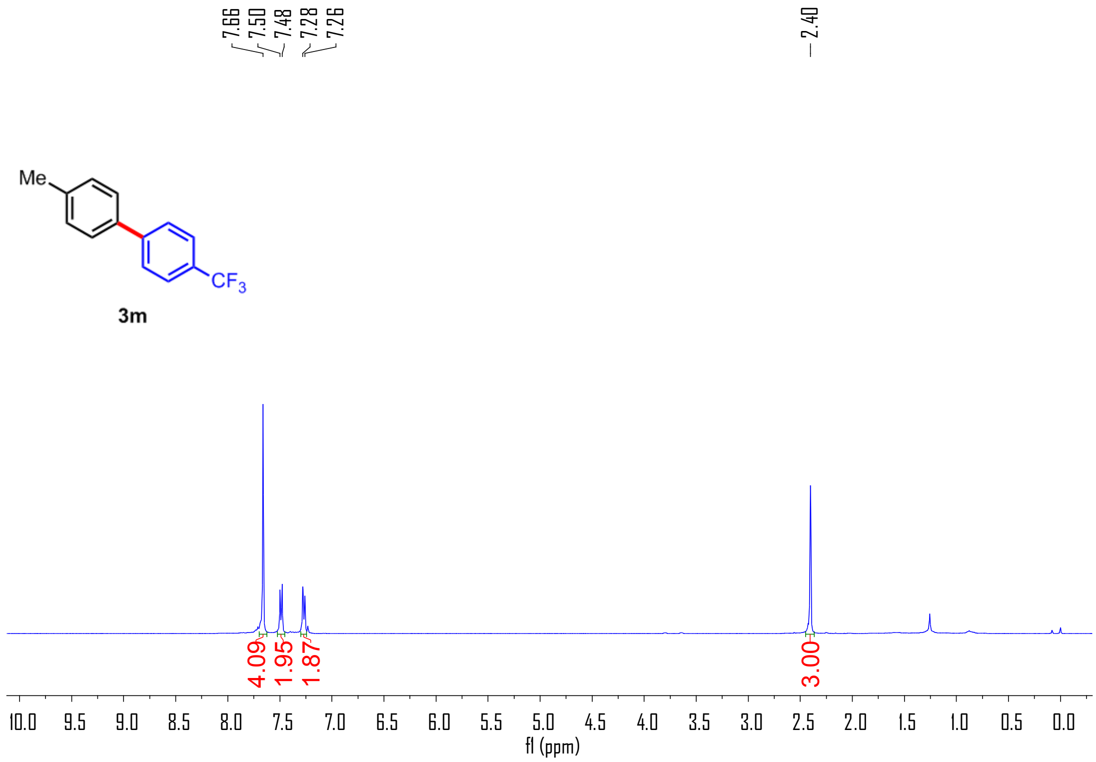
f1 (ppm)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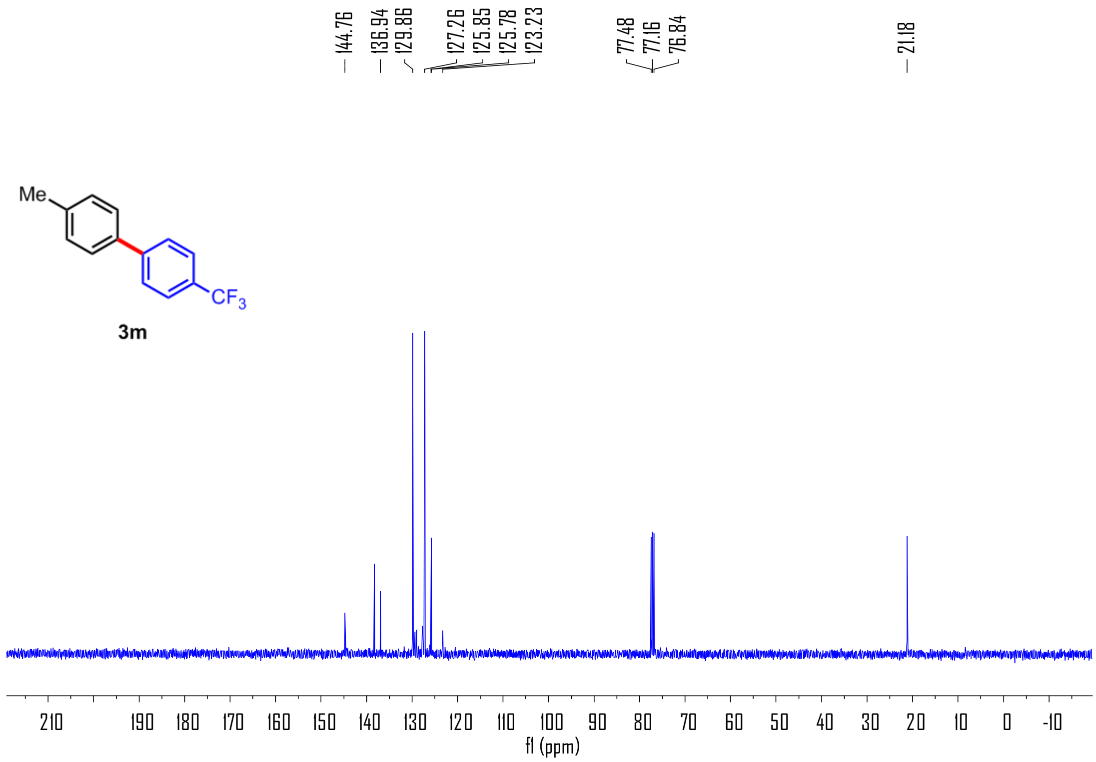
CF3
3m
4.09
1.95
1.87
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.85
125.78
123.23
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77.16
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21.18
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CF3
3m
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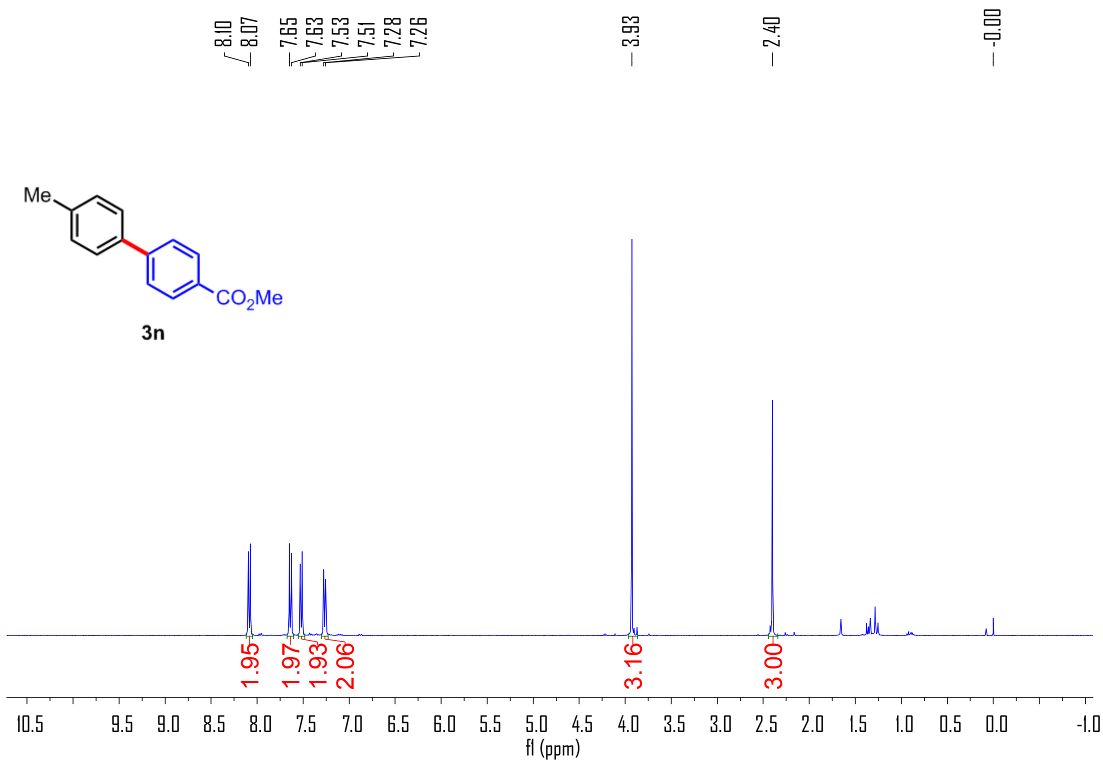
f1 (ppm)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7.28
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CO2Me
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1.97
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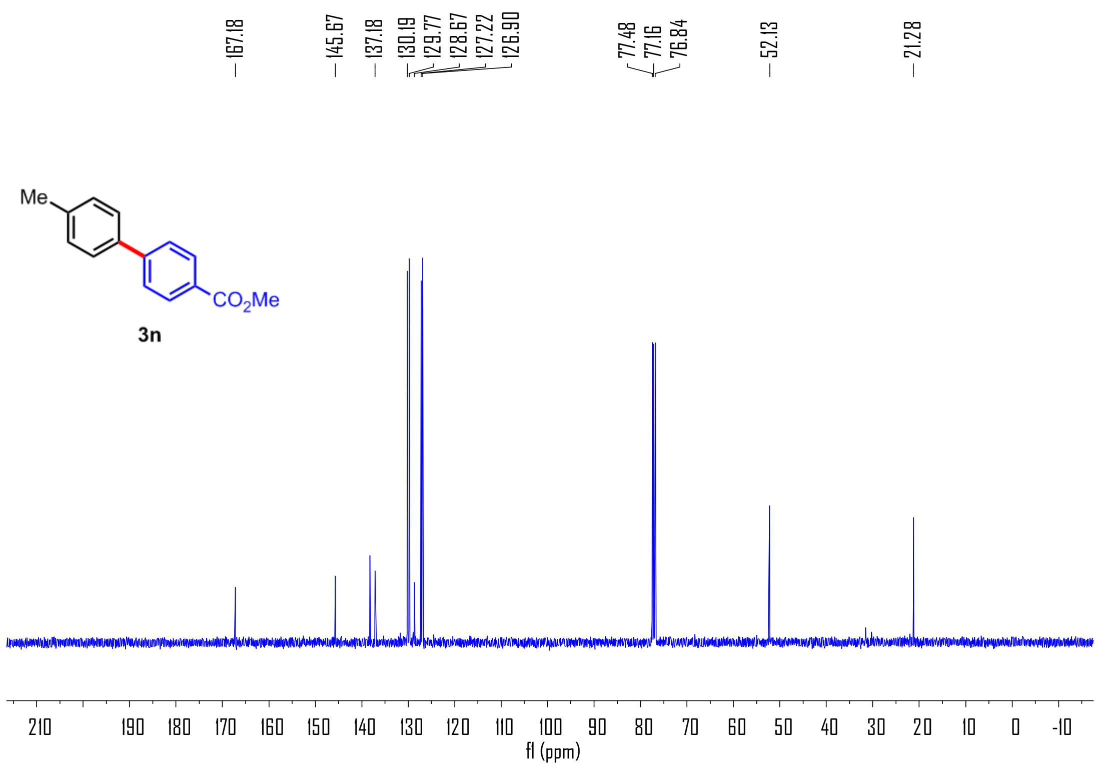
3.00
fl (ppm)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76.84
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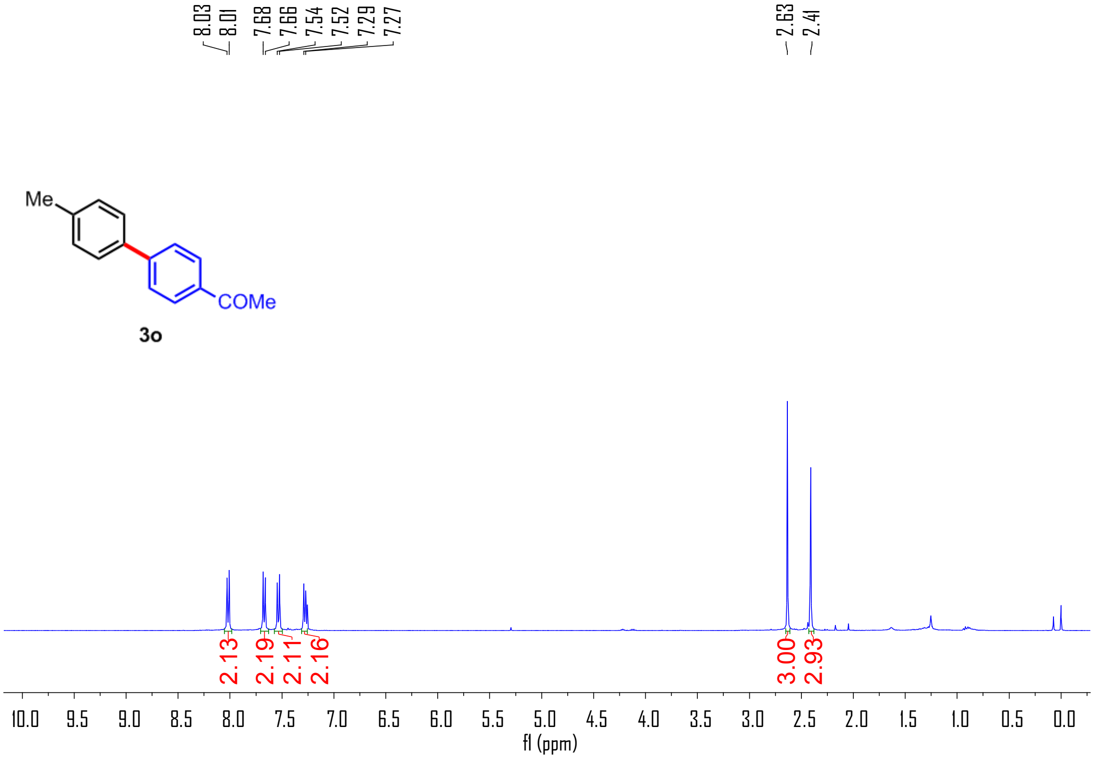
CO2Me
3n
fl (ppm)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7.29
7.27
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2.41
Me
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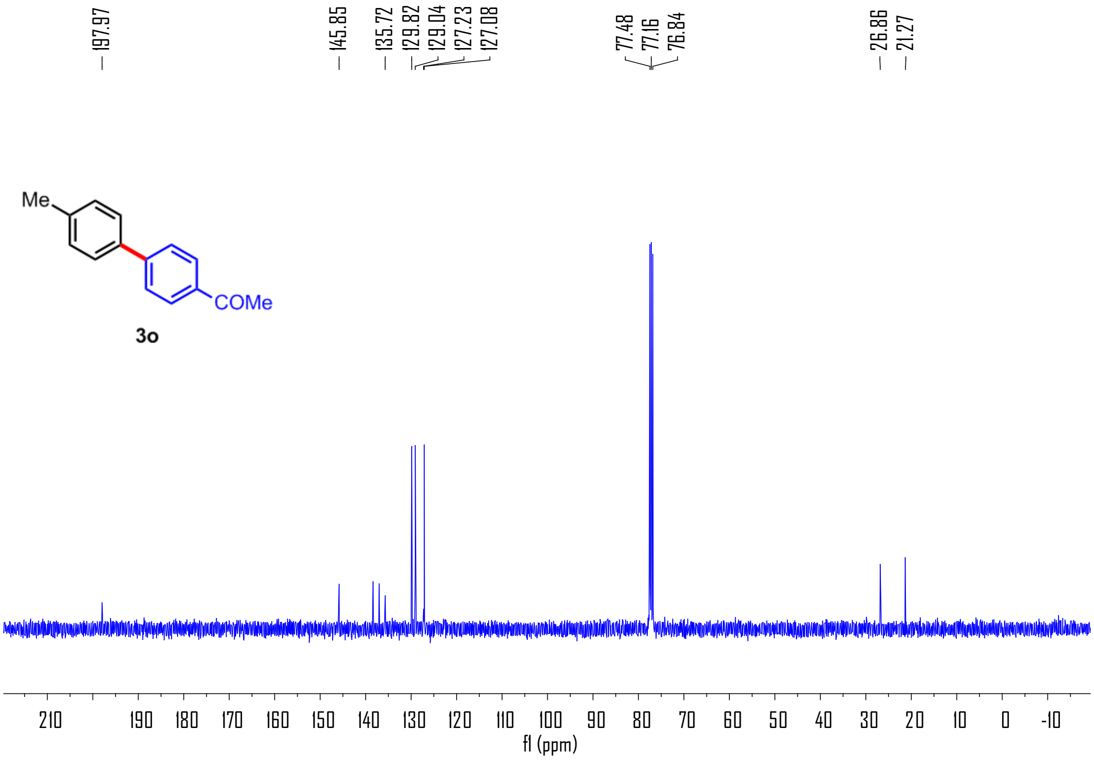
3o
2.13
2.19
2.11
2.16
3.00
2.93
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.08
77.48
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21.27
Me
COMe
3o
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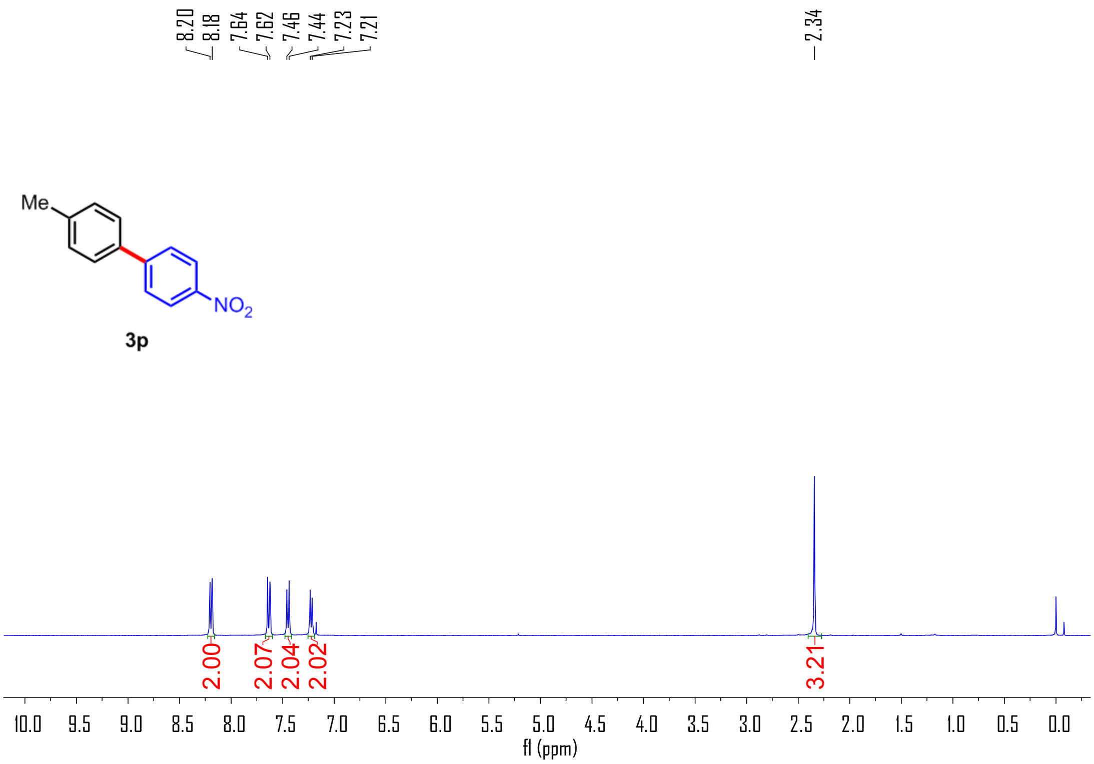
f1 (ppm)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7.23
7.21
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Me
NO2
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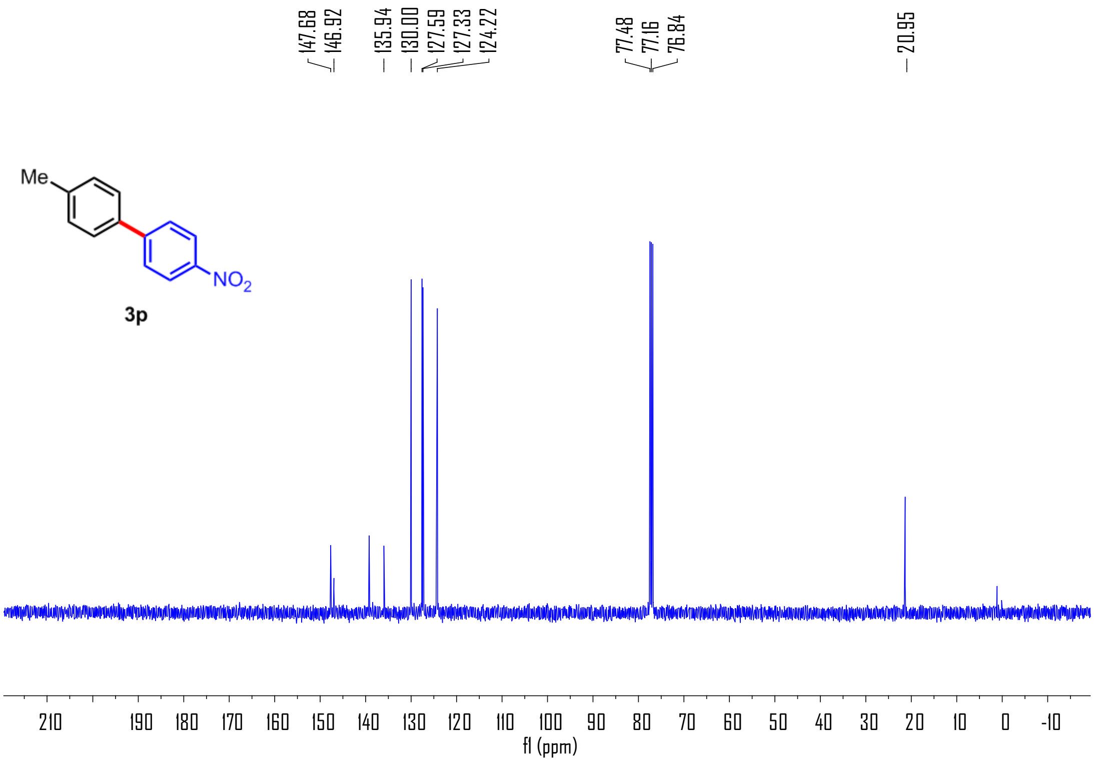
2.04
2.02
3.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)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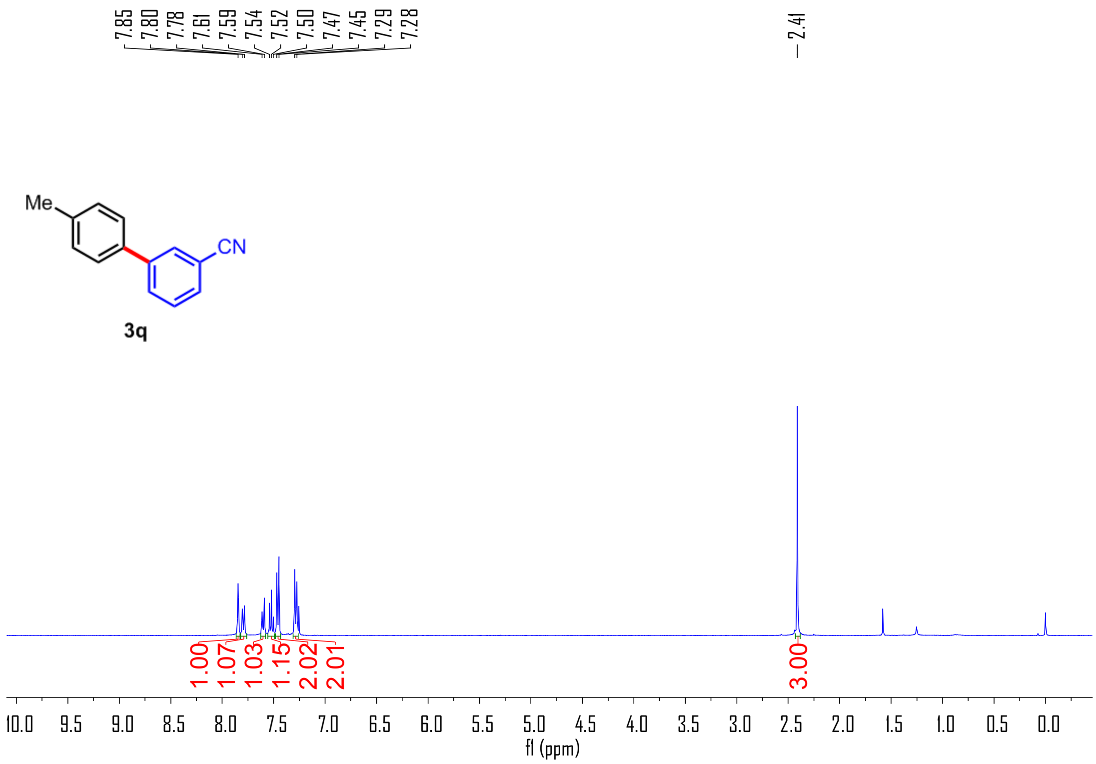
fl (ppm)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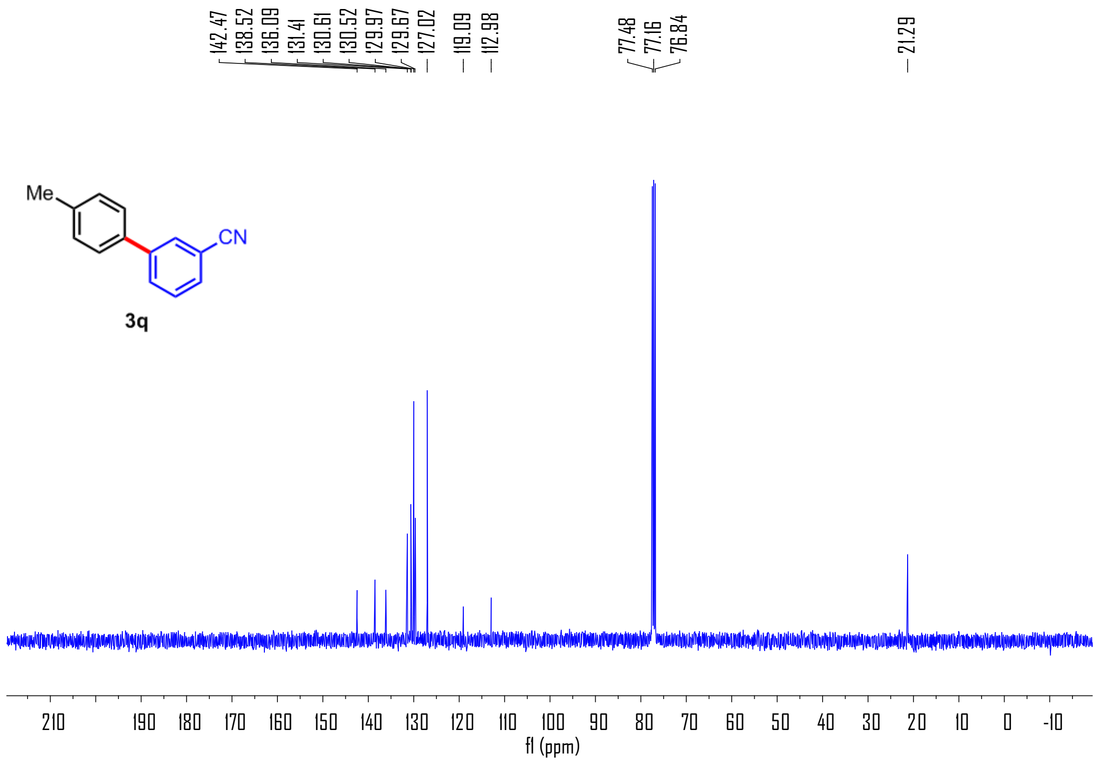
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CN
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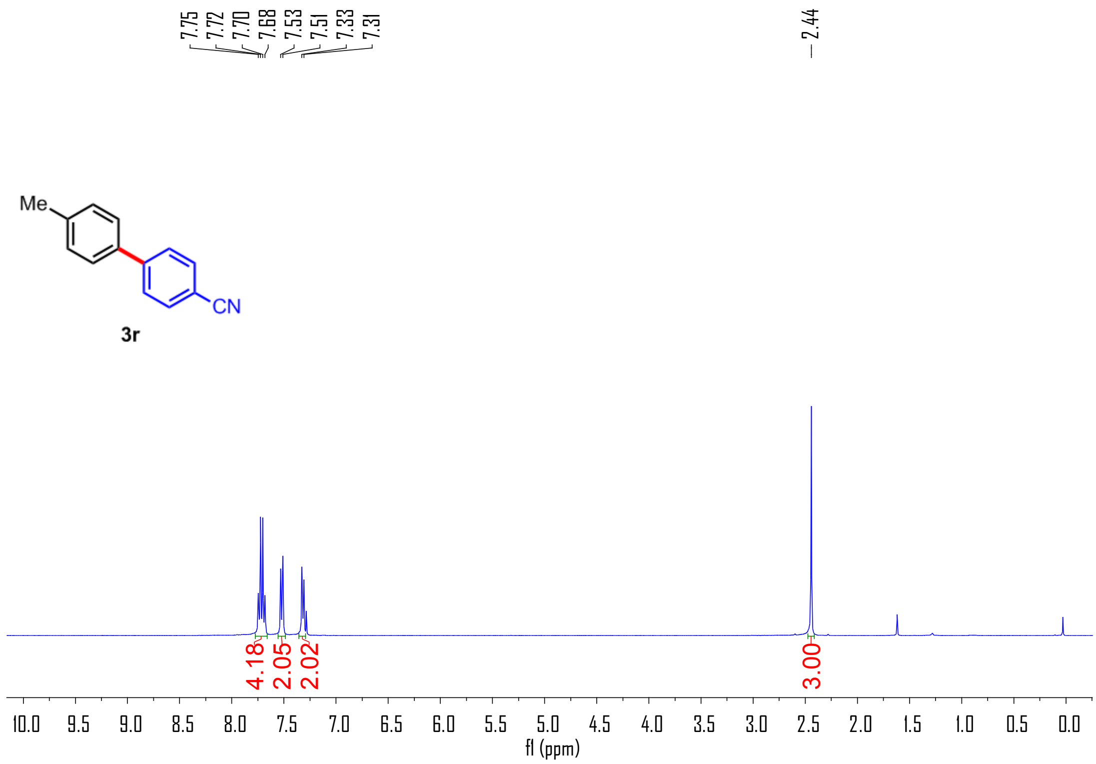
fl (ppm)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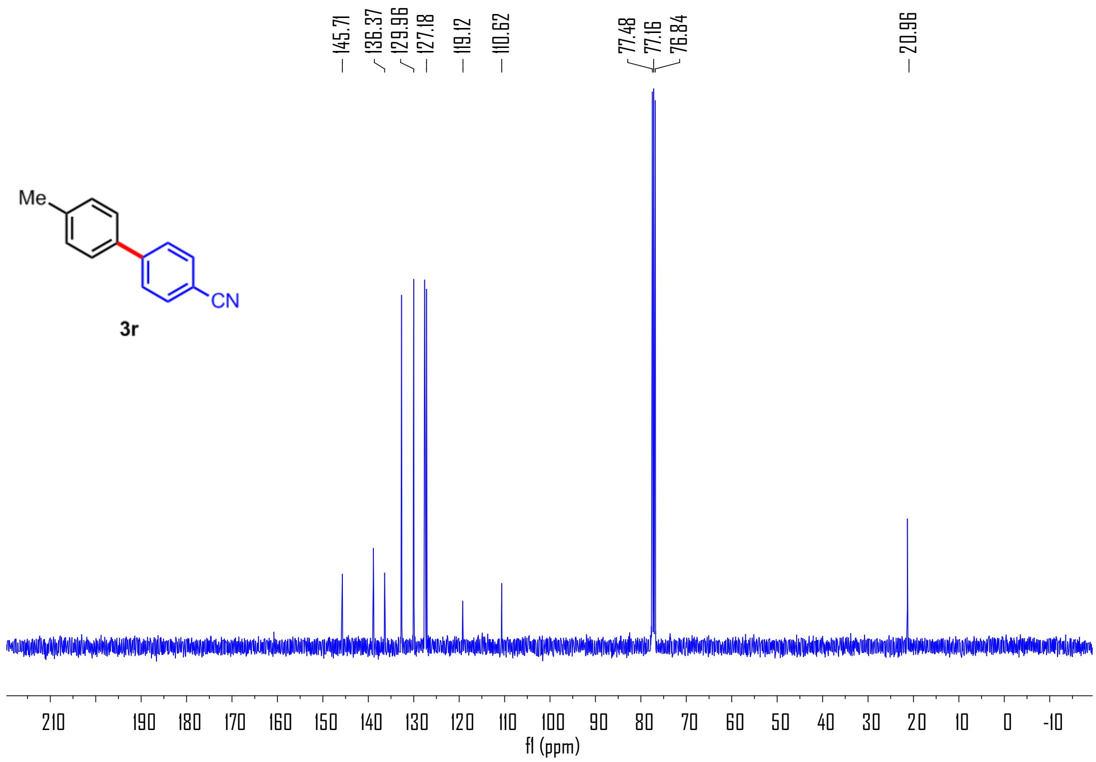
fl (ppm)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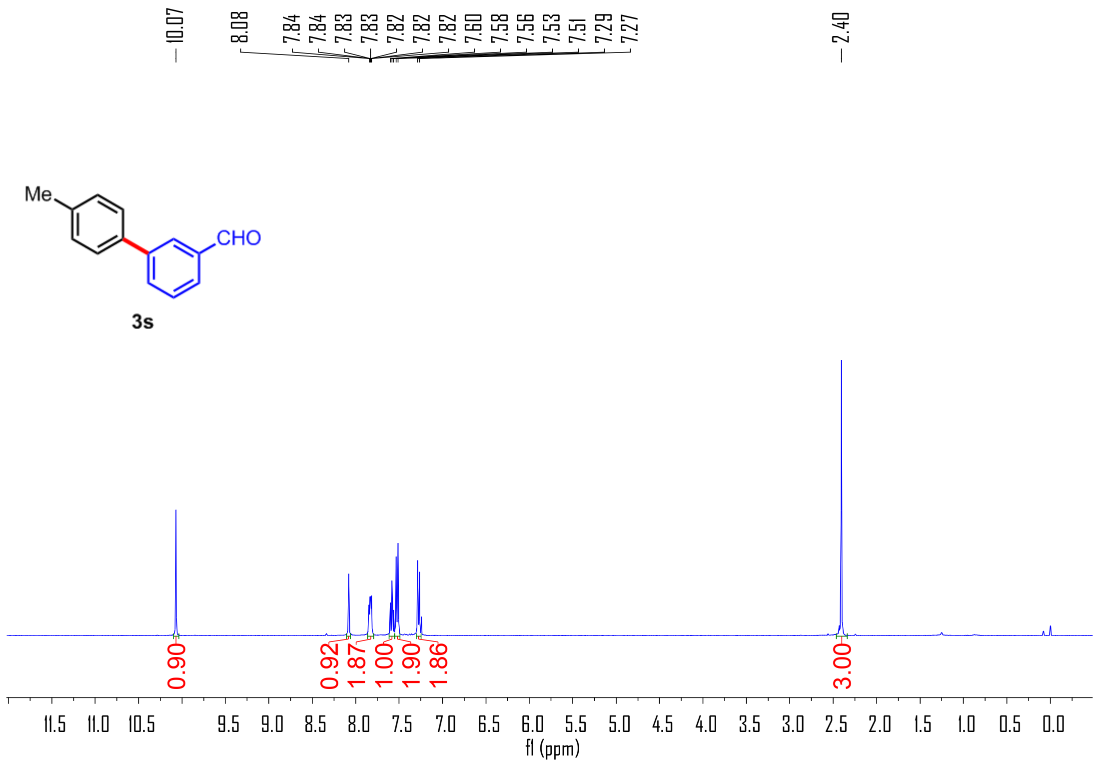
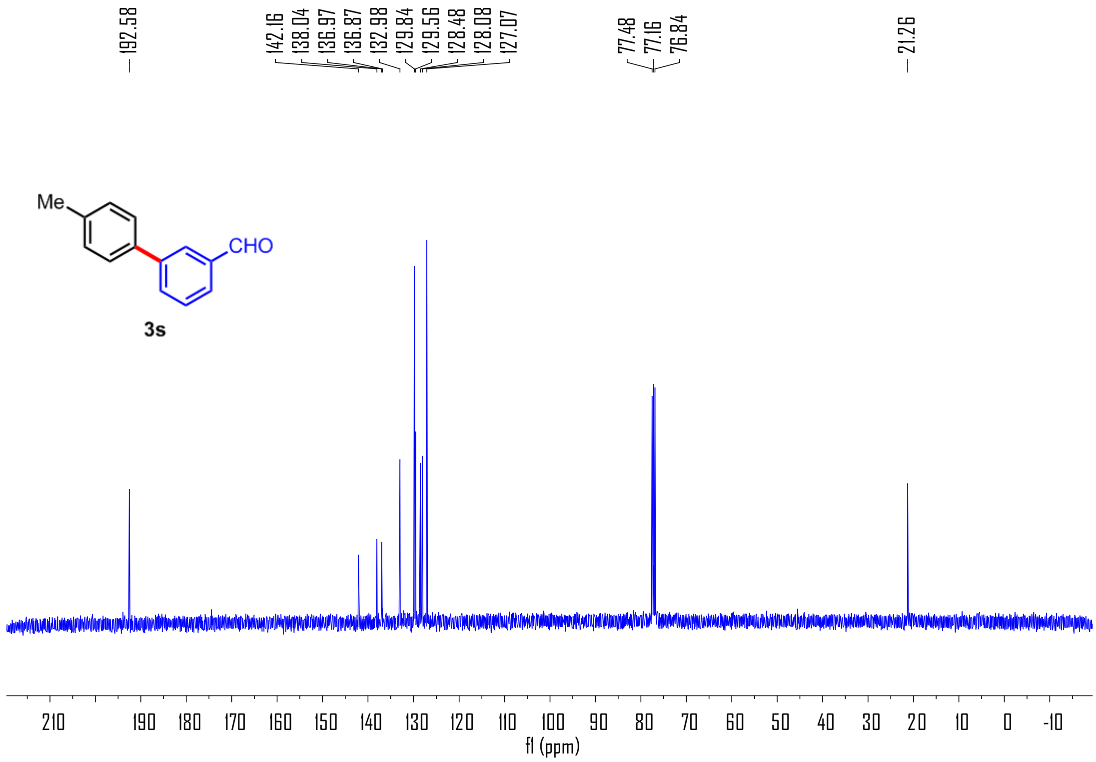
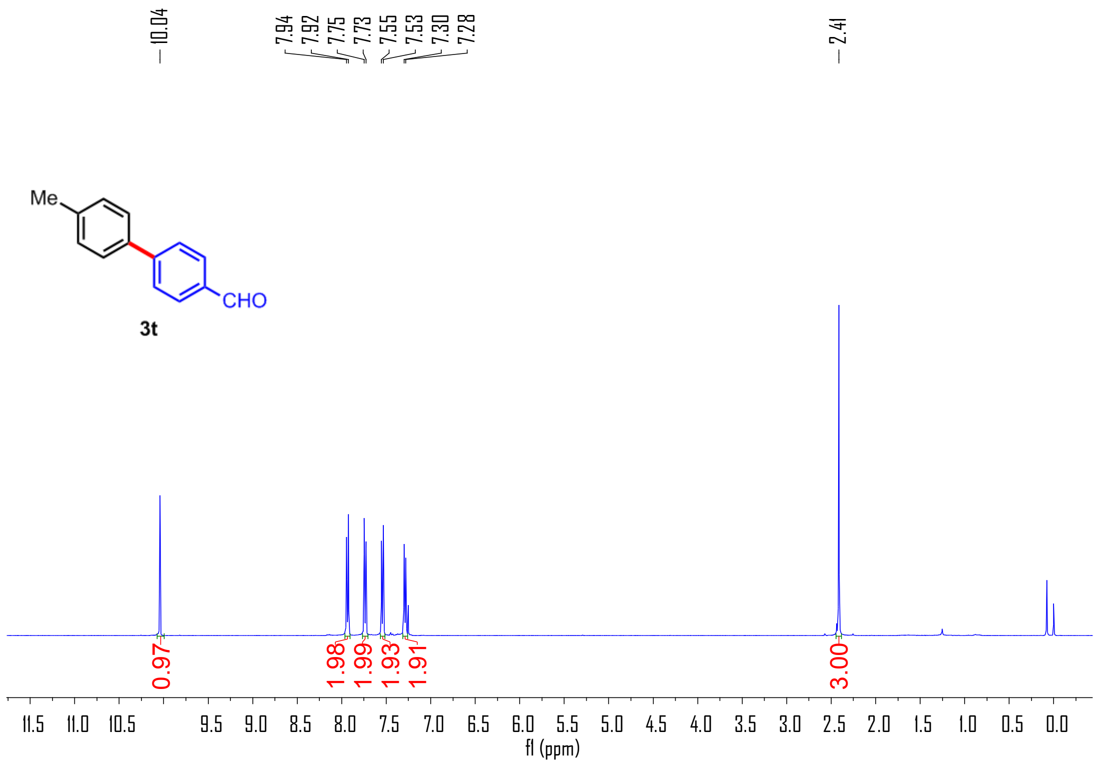
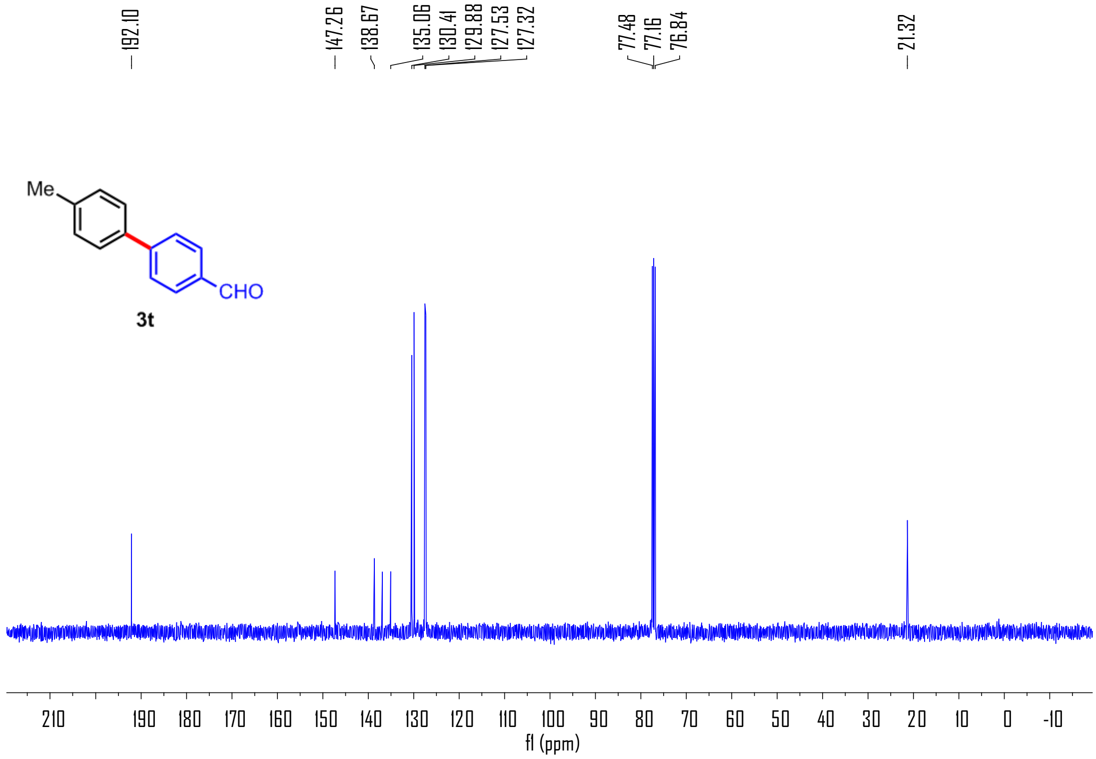
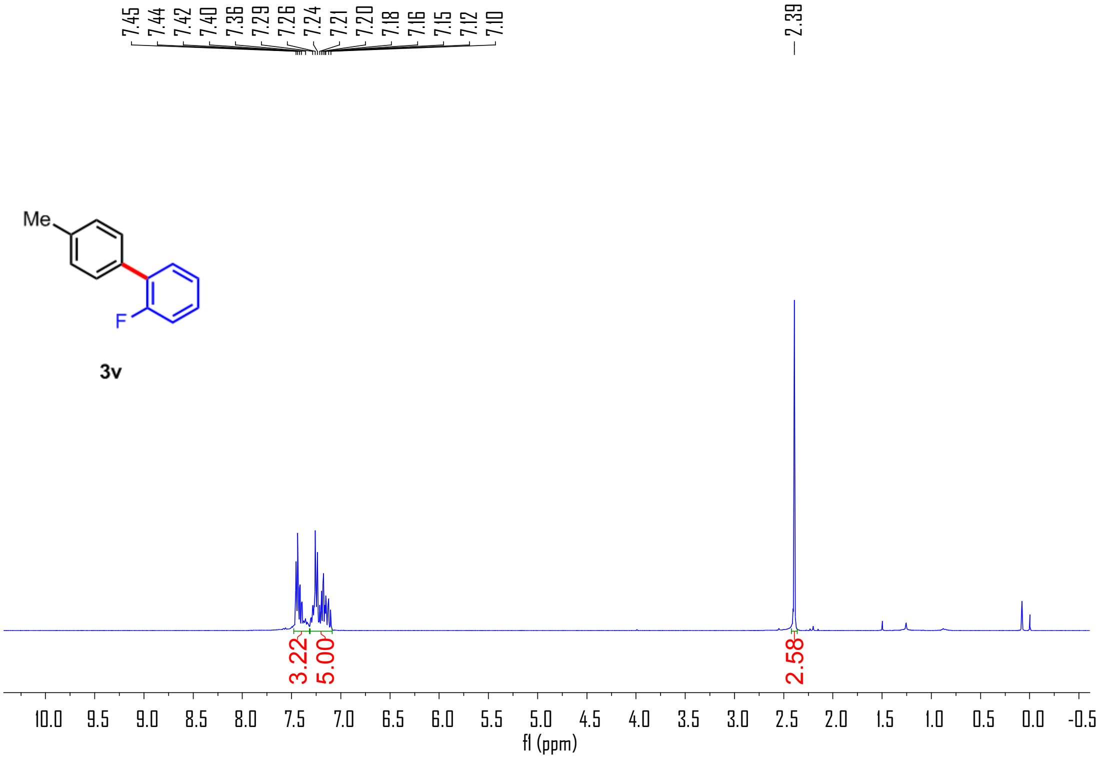
76.84
20.96
Me
CN
3r
fl (ppm)

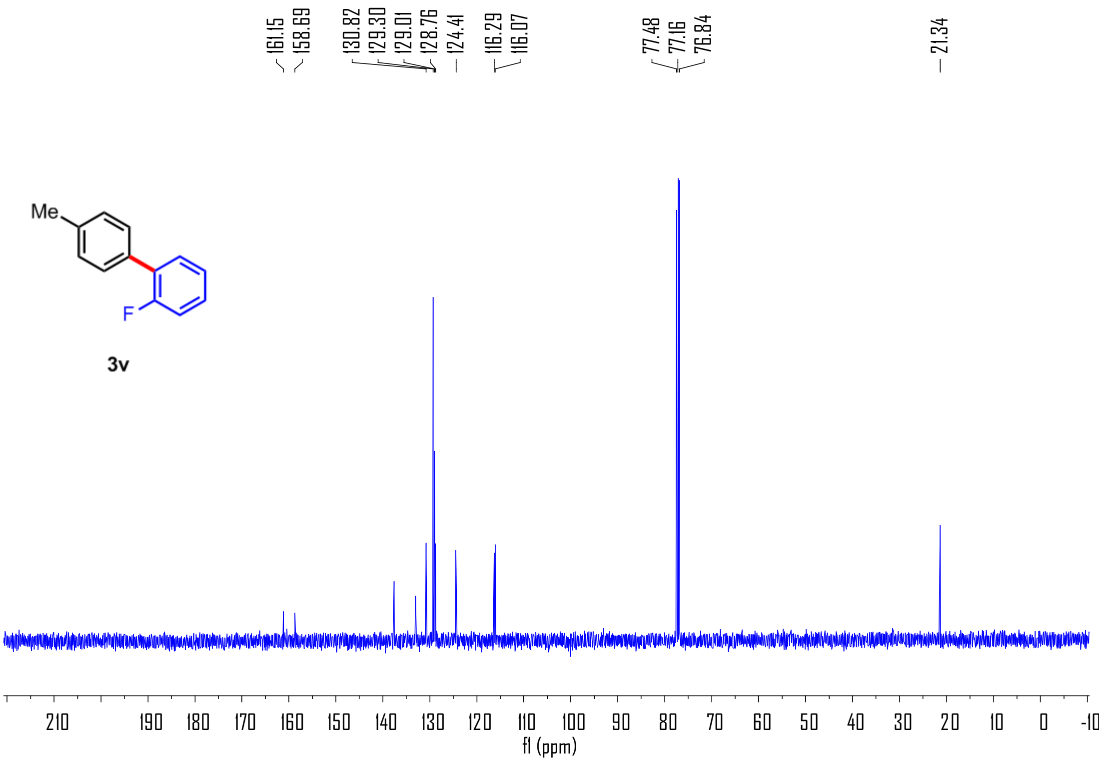

10.07
8.08
7.84
7.84
7.83
7.83
7.82
7.82
7.82
7.60
7.58
7.56
7.53
7.51
7.29
7.27
2.40
Me
CHO
3s
0.90
0.92
1.87
1.00
1.90
1.86
3.00
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)

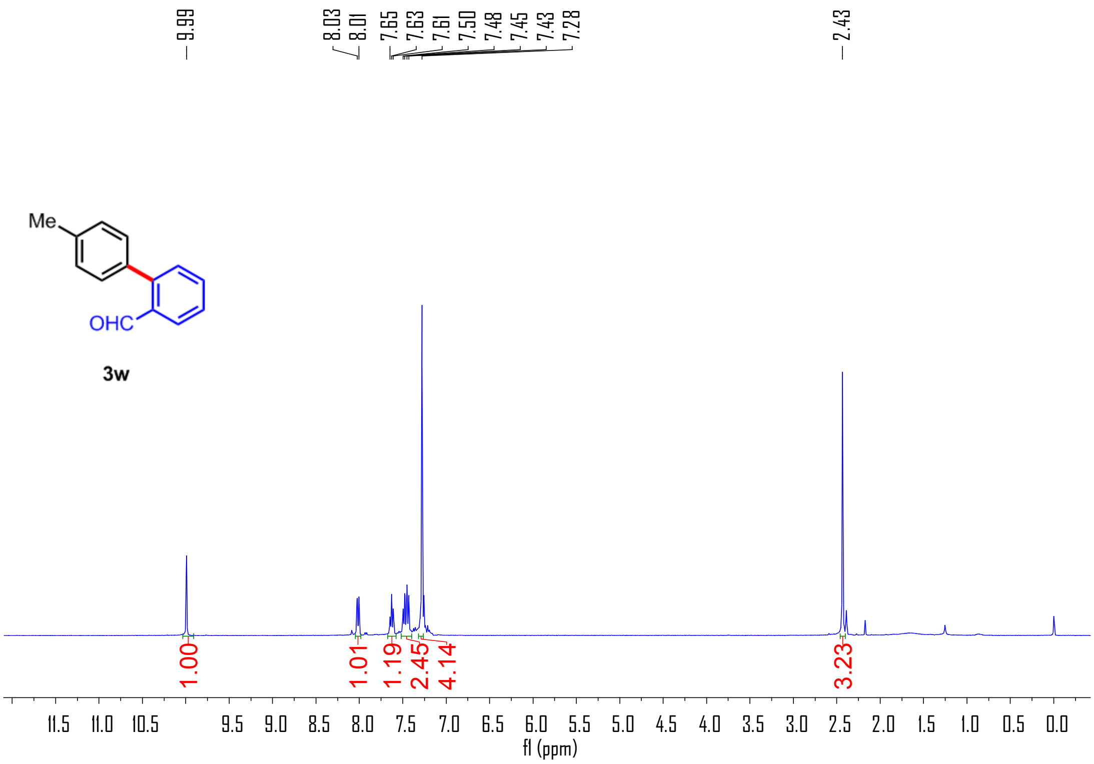

192.58
142.16
138.04
136.97
136.87
132.98
129.84
129.56
128.48
128.08
127.07
77.48
77.16
76.84
21.26
Me
CHO
3s
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
fl (ppm)

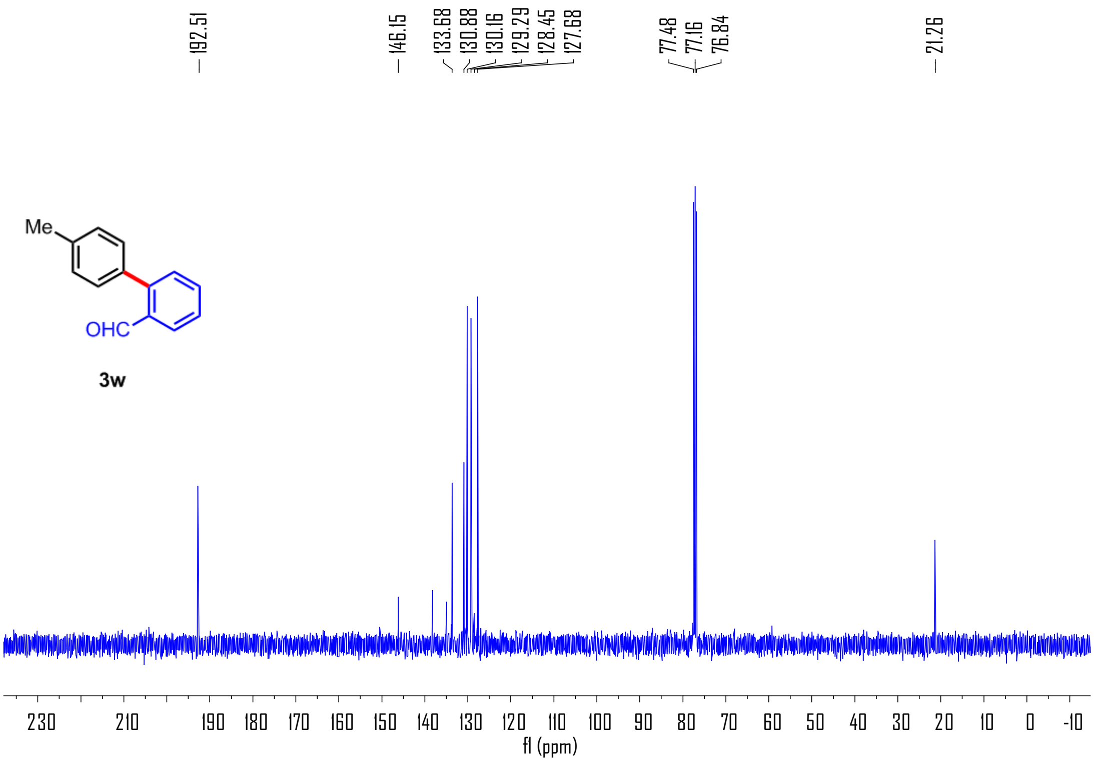

10.04
7.94
7.92
7.75
7.73
7.55
7.53
7.30
7.28
2.41
Me
CHO
3t
0.97
1.98
1.99
1.93
1.91
3.00
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

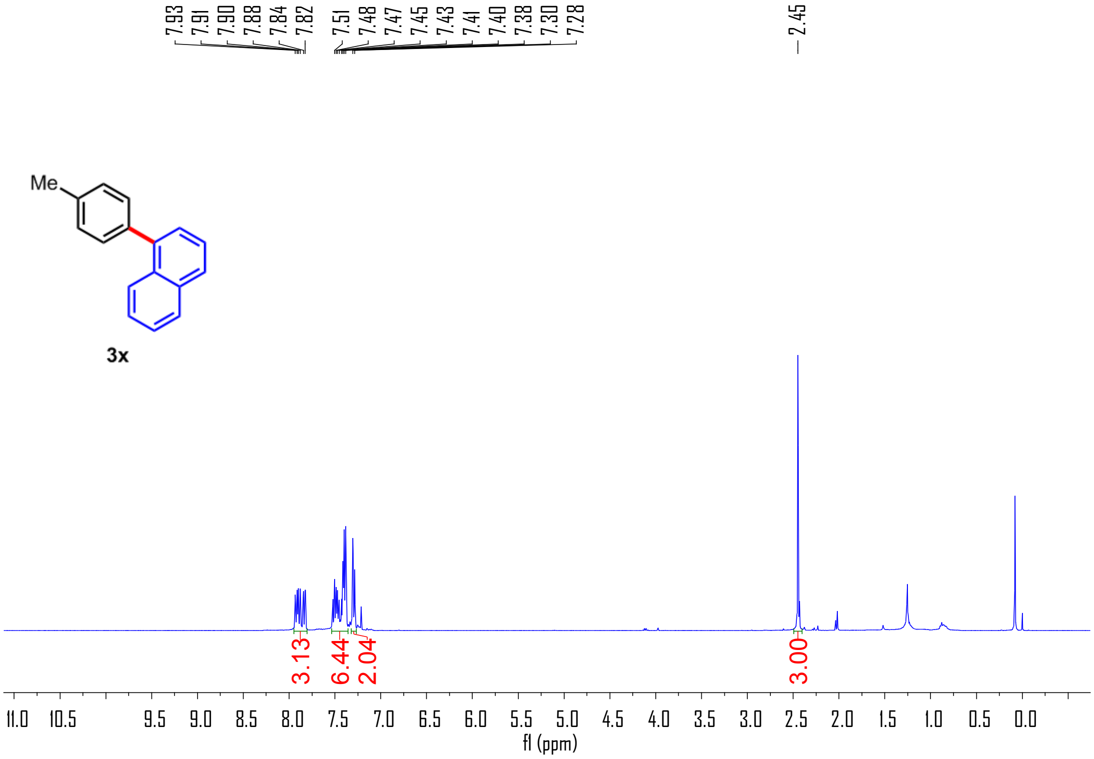

192.10
147.26
138.67
135.06
130.41
129.88
127.53
127.32
77.48
77.16
76.84
21.32
Me
CHO
3t
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.45
7.44
7.42
7.40
7.36
7.29
7.26
7.24
7.21
7.20
7.18
7.16
7.15
7.12
7.10
2.39
Me
F
3v
3.22
5.00
2.58
fl (ppm)

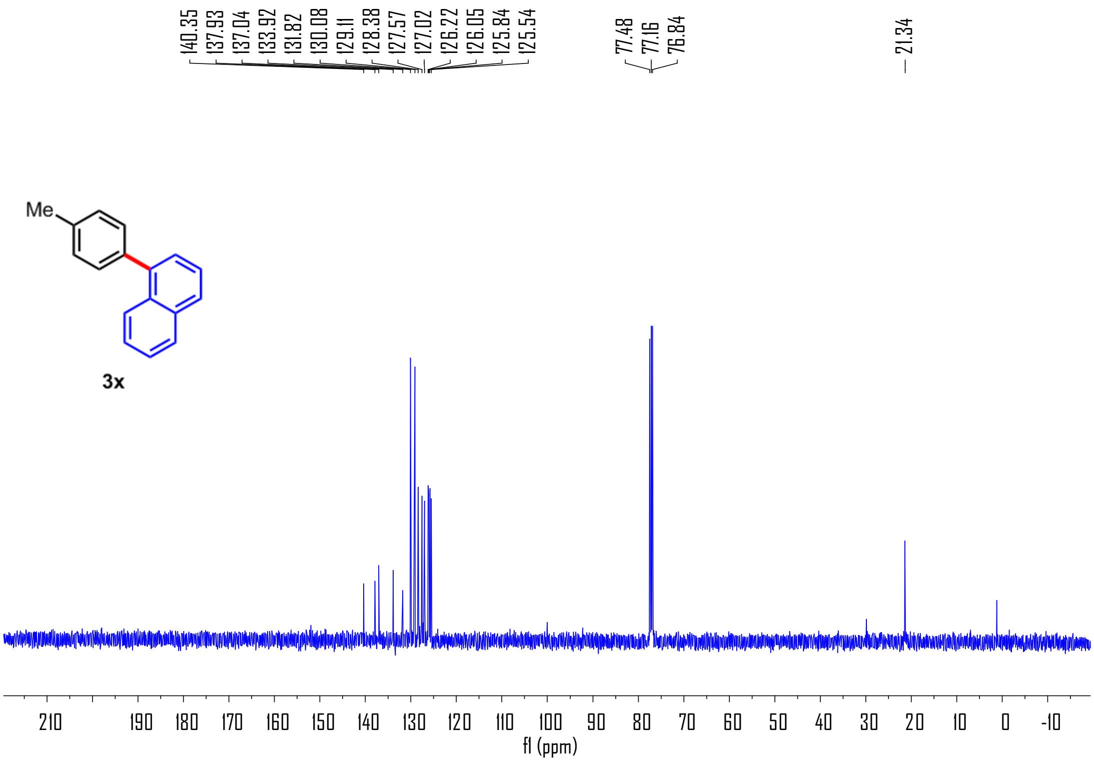

161.15
158.69
130.82
129.30
129.01
128.76
124.41
116.29
116.07
77.48
77.16
76.84
21.34
Me
F
3v
fl (ppm)


9.99
8.03
8.01
7.65
7.63
7.61
7.50
7.48
7.45
7.43
7.28
2.43
Me
OHC
3w
1.00
1.01
1.19
2.45
4.14
3.23
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

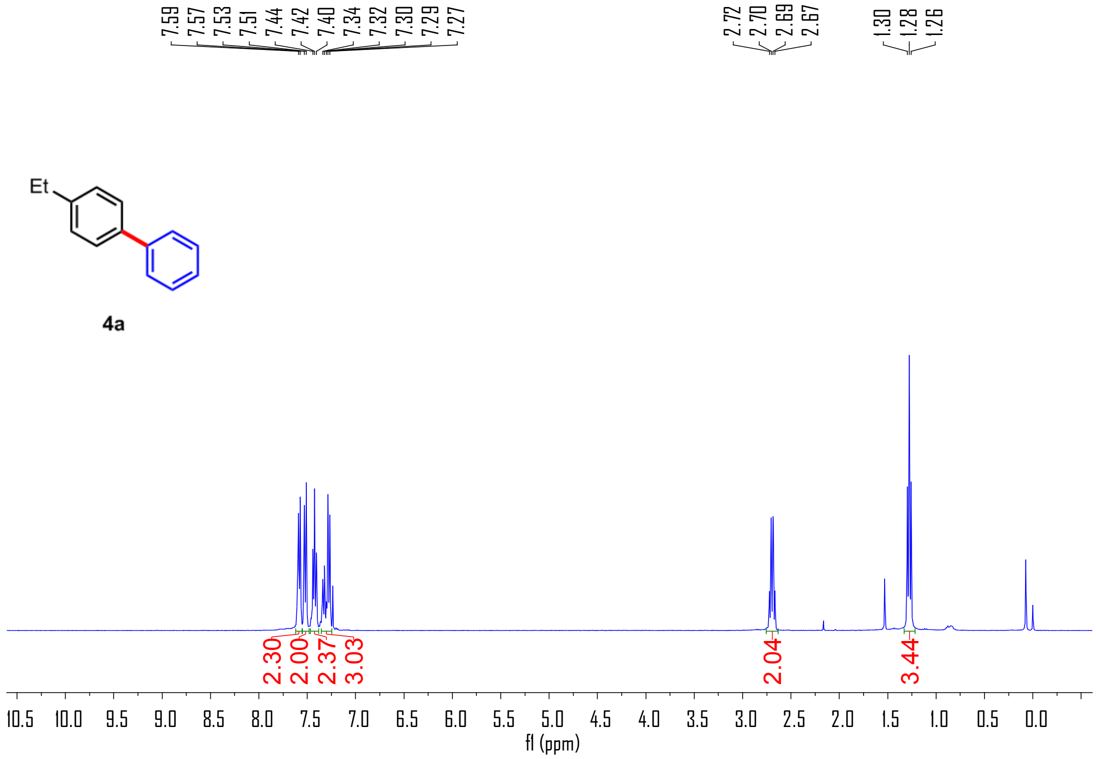

192.51
146.15
133.68
130.88
130.16
129.29
128.45
127.68
77.48
77.16
76.84
21.26
Me
OHC
3w
230 210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

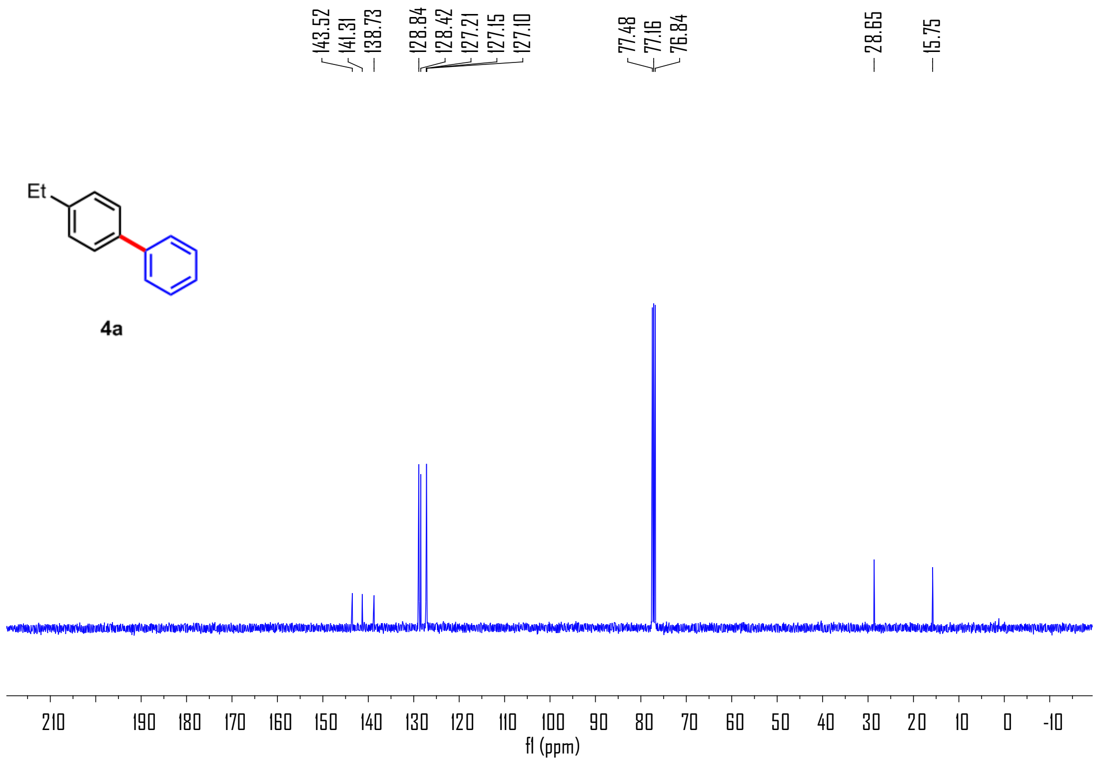


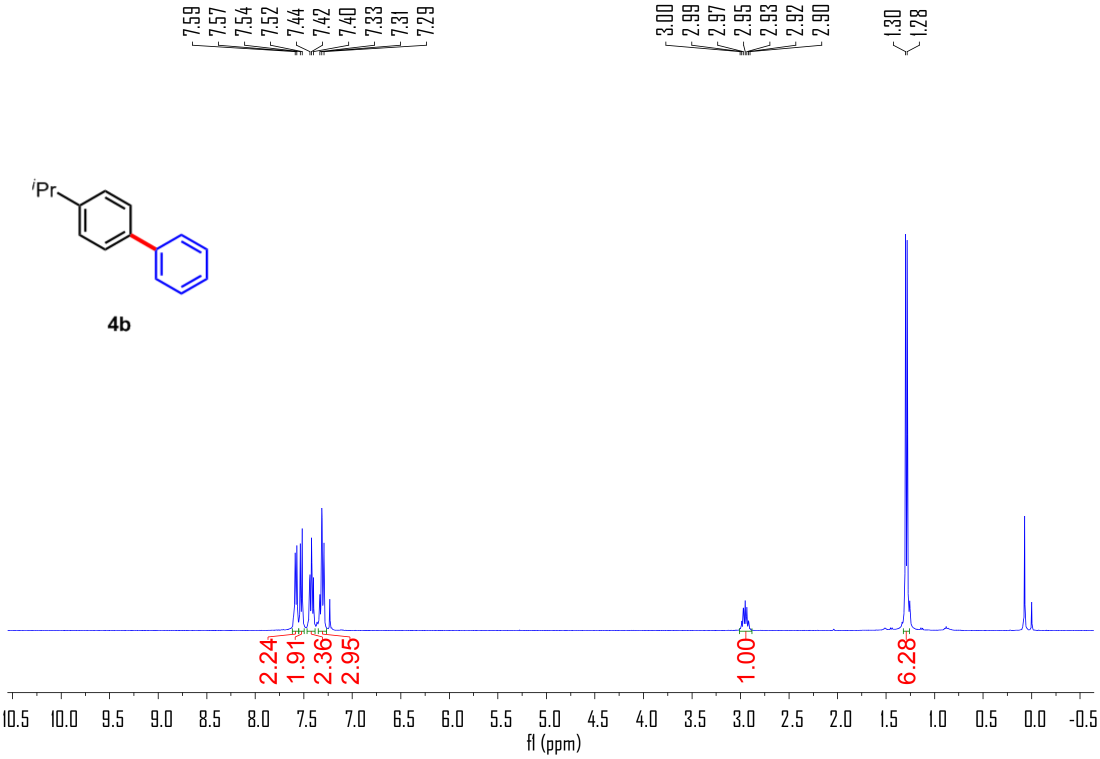
7.93
7.91
7.90
7.88
7.84
7.82
7.51
7.48
7.47
7.45
7.43
7.41
7.40
7.38
7.30
7.28
2.45
Me
3.13
6.44
2.04
3.00
fl (ppm)

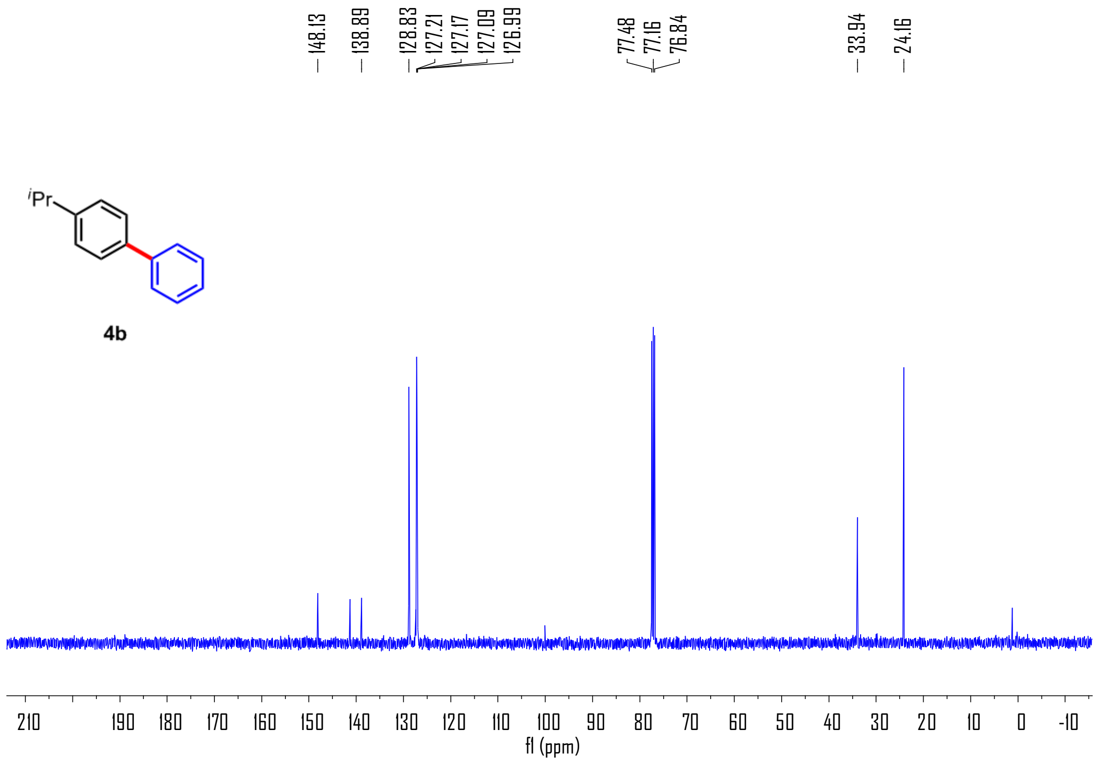


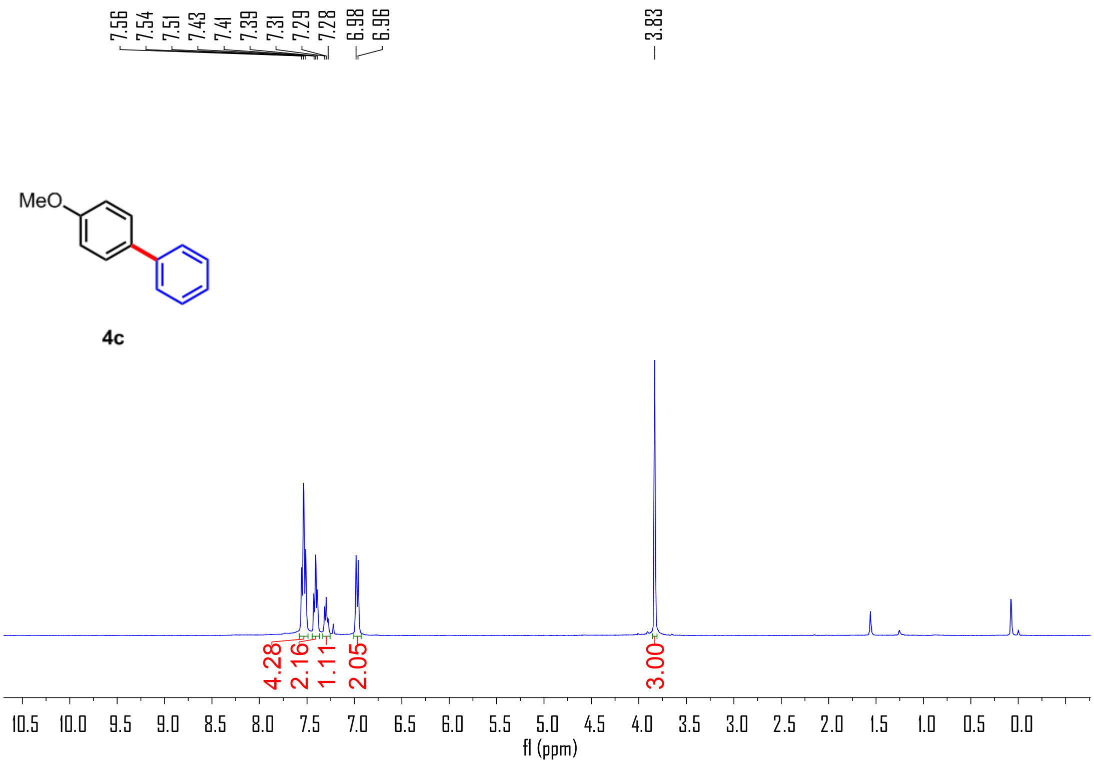
140.35
137.93
137.04
133.92
131.82
130.08
129.11
128.38
127.57
127.02
126.22
126.05
125.84
125.54
77.48
77.16
76.84
21.34
Me
fl (ppm)

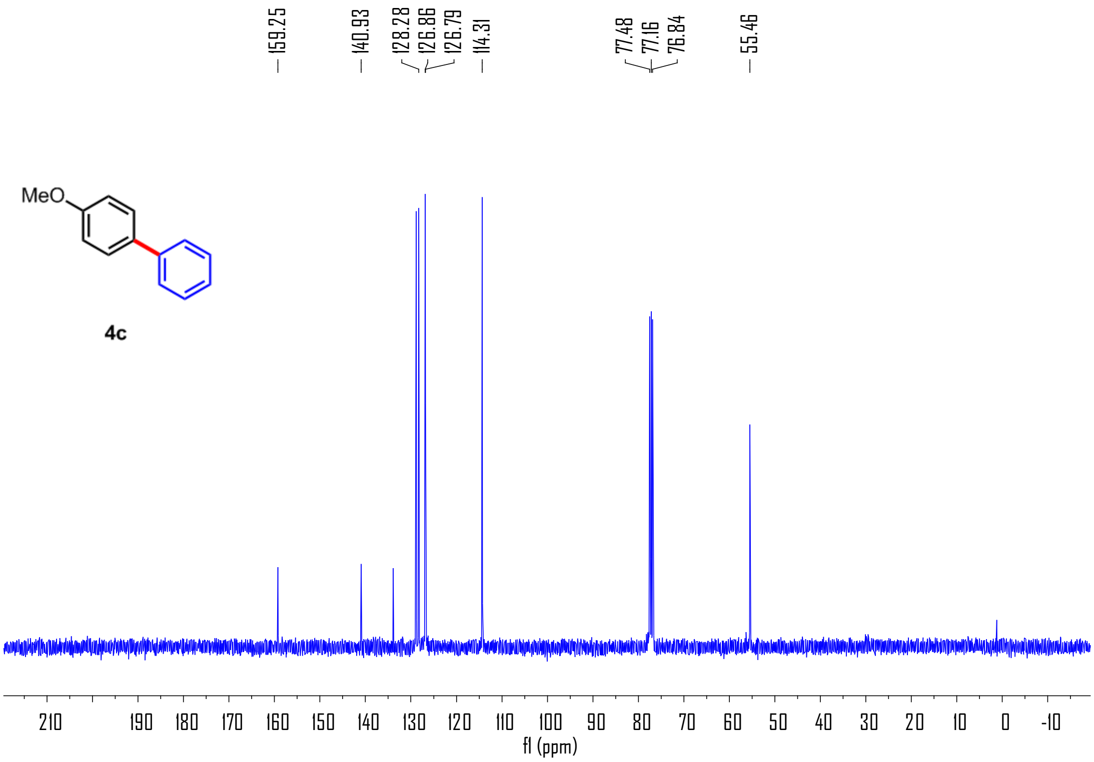

7.59
7.57
7.53
7.51
7.44
7.42
7.40
7.34
7.32
7.30
7.29
7.27
2.72
2.70
2.69
2.67
1.30
1.28
1.26
Et
4a
2.30
2.00
2.37
3.03
2.04
3.44
fl (ppm)

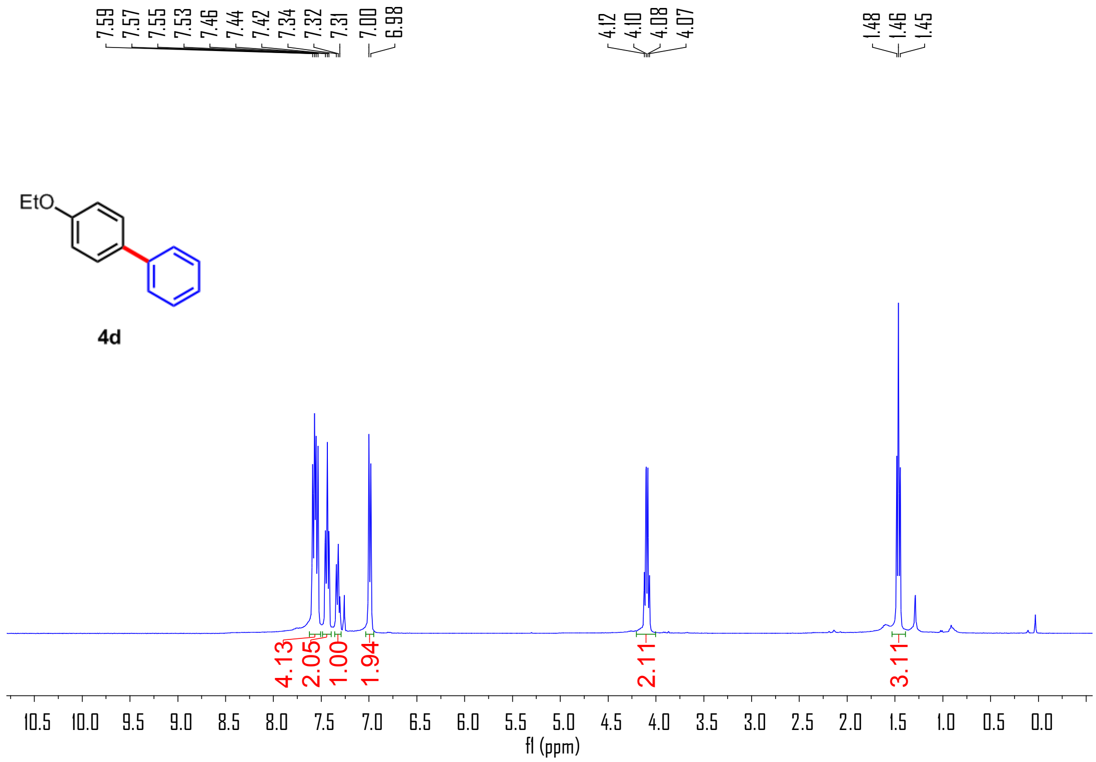

143.52
141.31
138.73
128.84
128.42
127.21
127.15
127.10
77.48
77.16
76.84
28.65
15.75
Et
4a
fl (ppm)

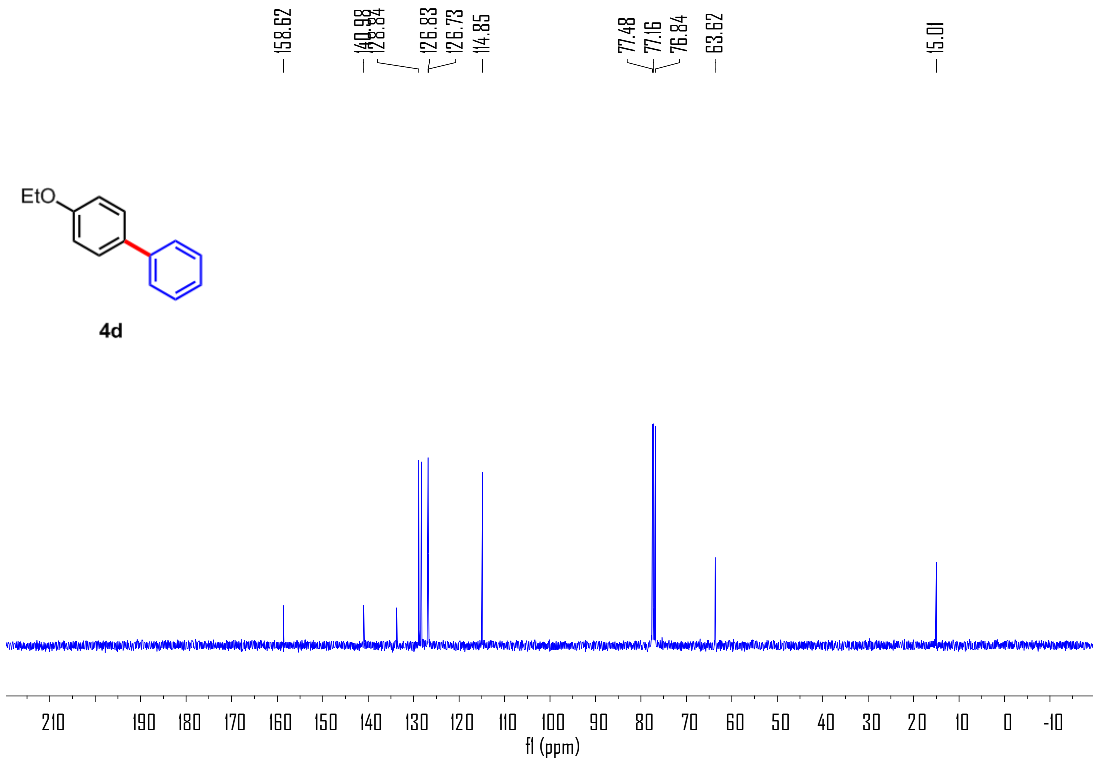

7.59
7.57
7.54
7.52
7.44
7.42
7.40
7.33
7.31
7.29
3.00
2.99
2.97
2.95
2.93
2.92
2.90
1.30
1.28
iPr
4b
2.24
1.91
2.36
2.95
1.00
6.28
fl (ppm)

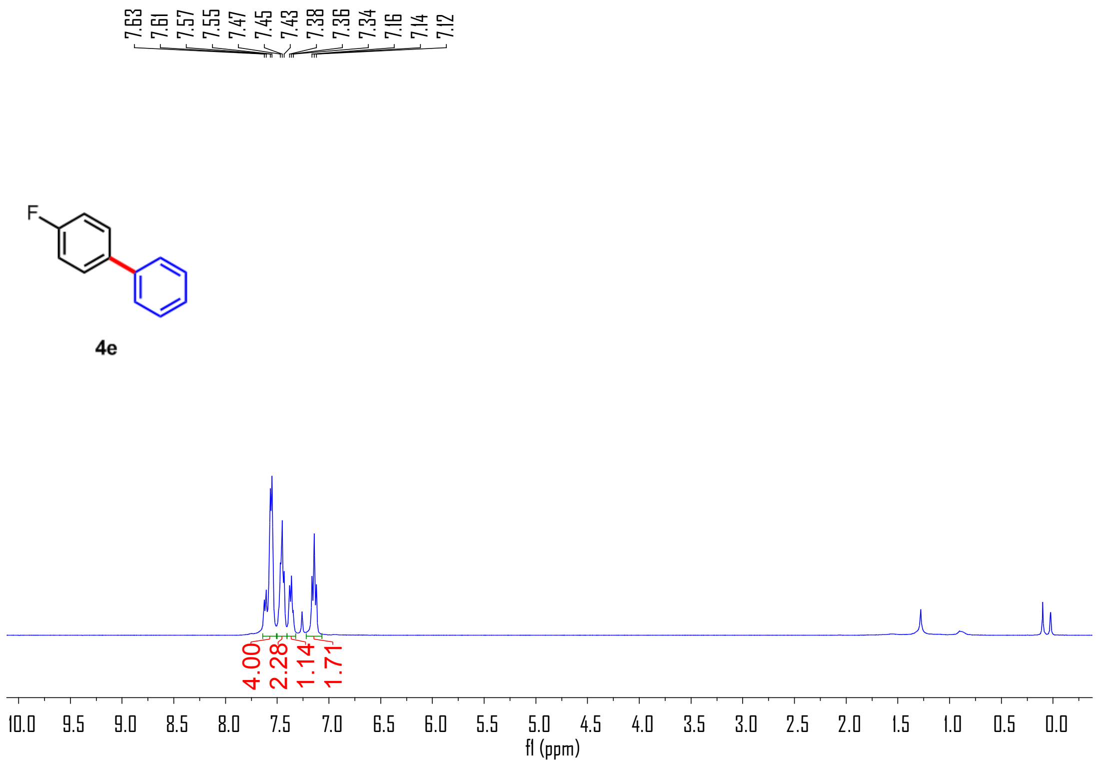

148.13
138.89
128.83
127.21
127.17
127.09
126.99
77.48
77.16
76.84
33.94
24.16
iPr
4b
fl (ppm)

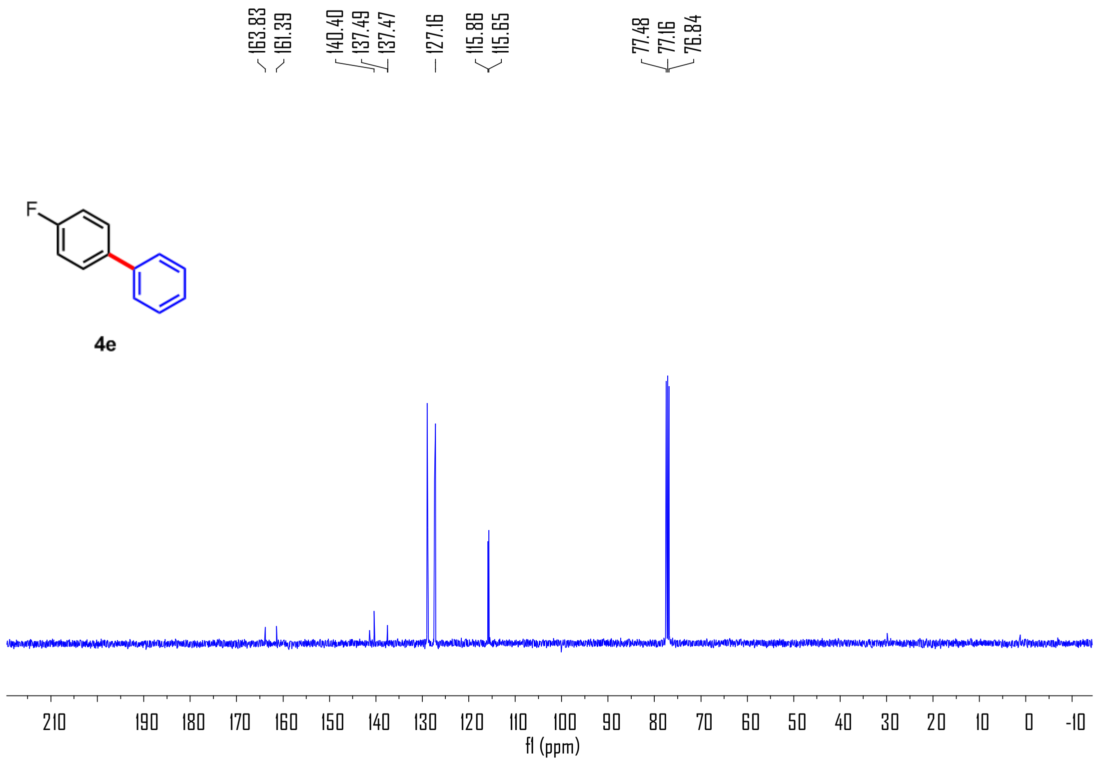

7.56
7.54
7.51
7.43
7.41
7.39
7.31
7.29
7.28
6.98
6.96
3.83
MeO
4c
4.28
2.16
1.11
2.05
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

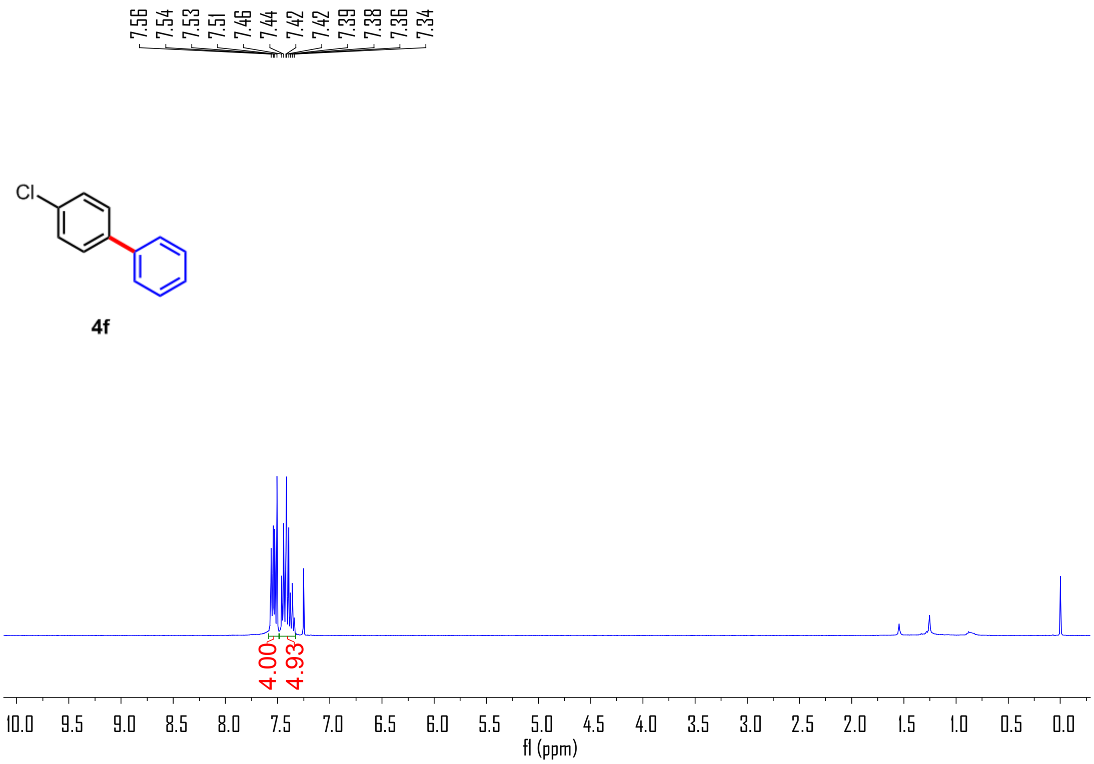

159.25
140.93
128.28
126.86
126.79
114.31
77.48
77.16
76.84
55.46
MeO
4c
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

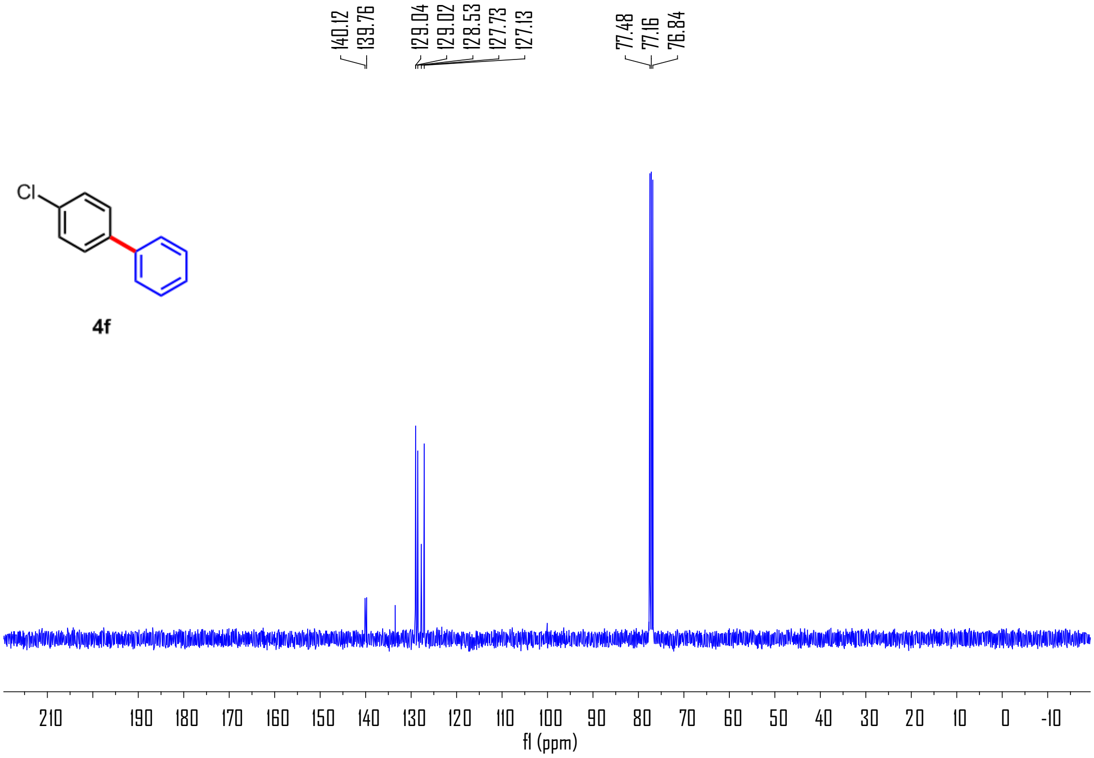

7.59
7.57
7.55
7.53
7.46
7.44
7.42
7.34
7.32
7.31
7.00
6.98
4.12
4.10
4.08
4.07
1.48
1.46
1.45
EtO
4d
4.13
2.05
1.00
1.94
2.11
3.11
f1 (ppm)

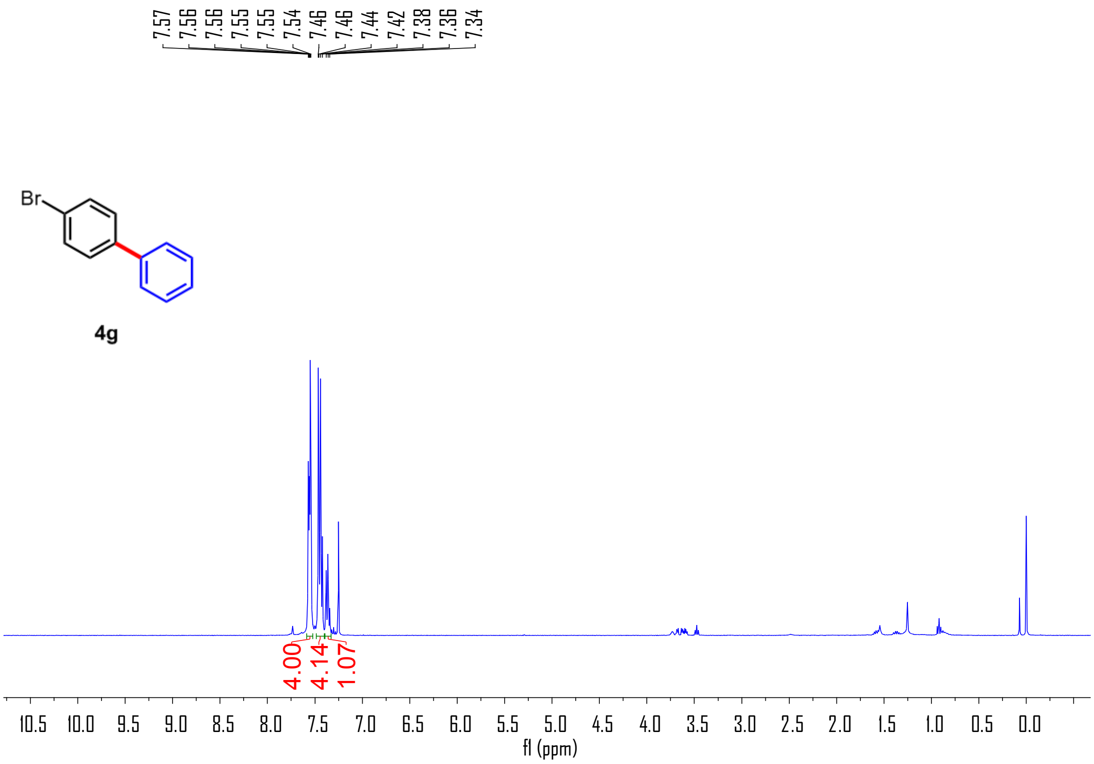

158.62
140.98
128.84
126.83
126.73
114.85
77.48
77.16
76.84
63.62
15.01
EtO
4d
f1 (ppm)

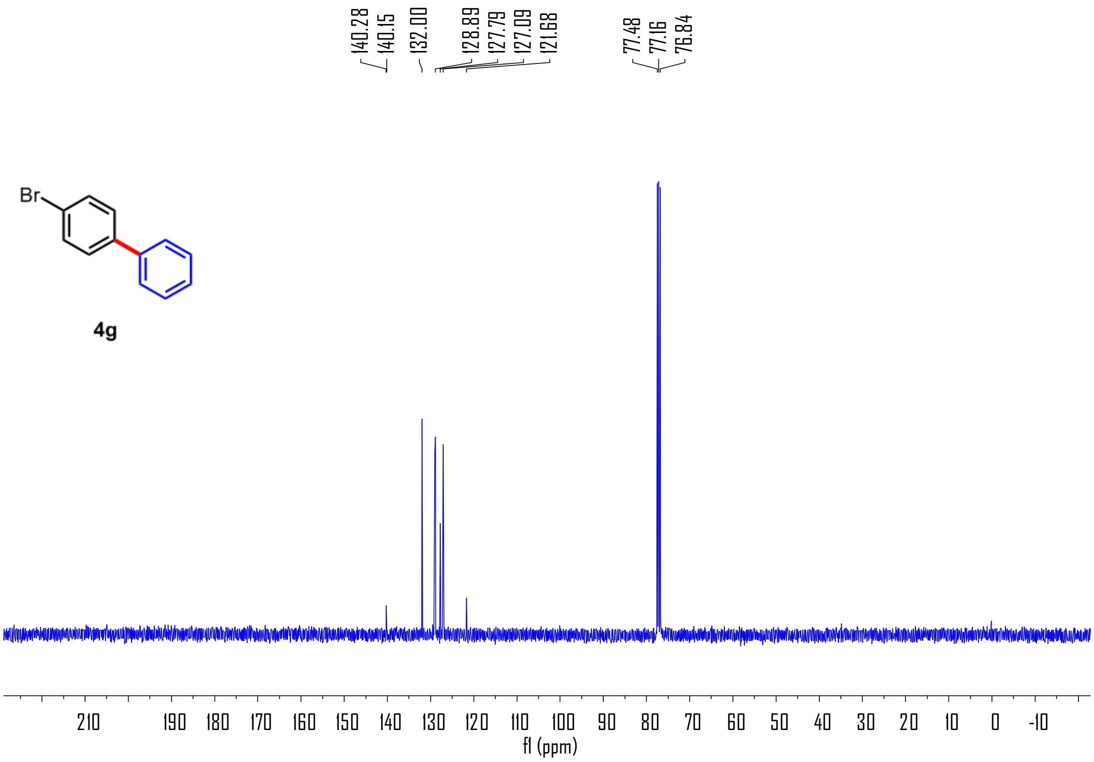

7.63
7.61
7.57
7.55
7.47
7.45
7.43
7.38
7.36
7.34
7.16
7.14
7.12
F
4e
4.00
2.28
1.14
1.71
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
fl (ppm)

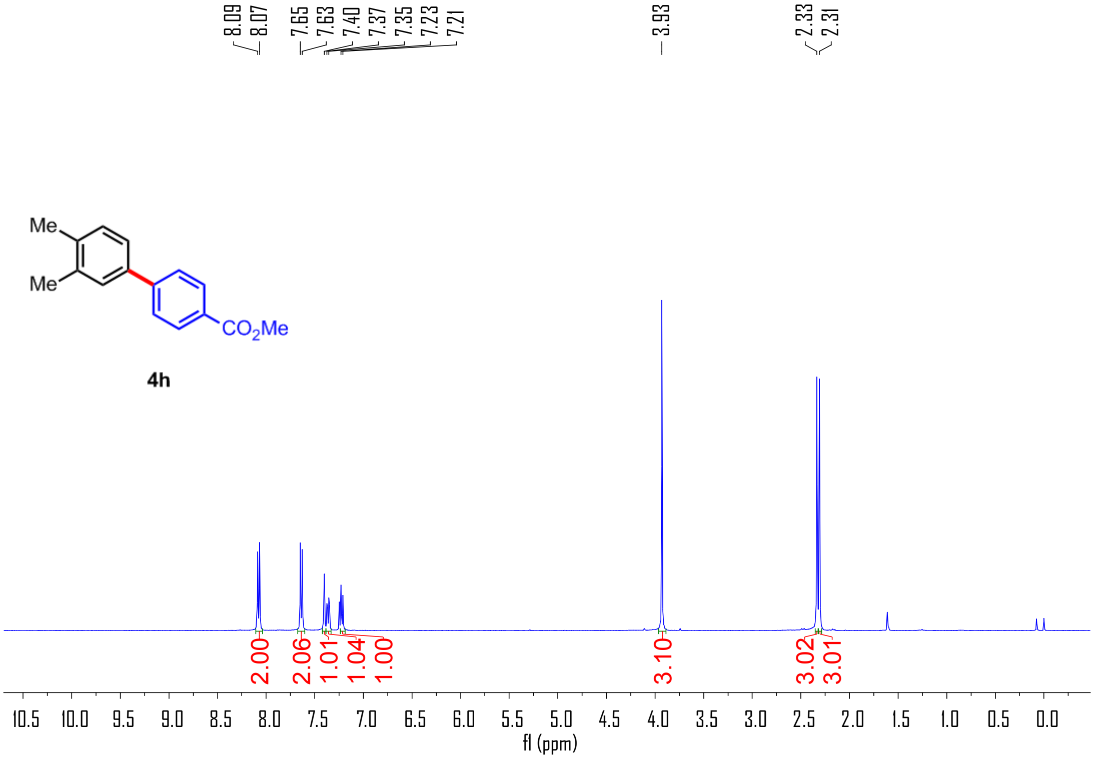

163.83
161.39
140.40
137.49
137.47
127.16
115.86
115.65
77.48
77.16
76.84
F
4e
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
fl (ppm)

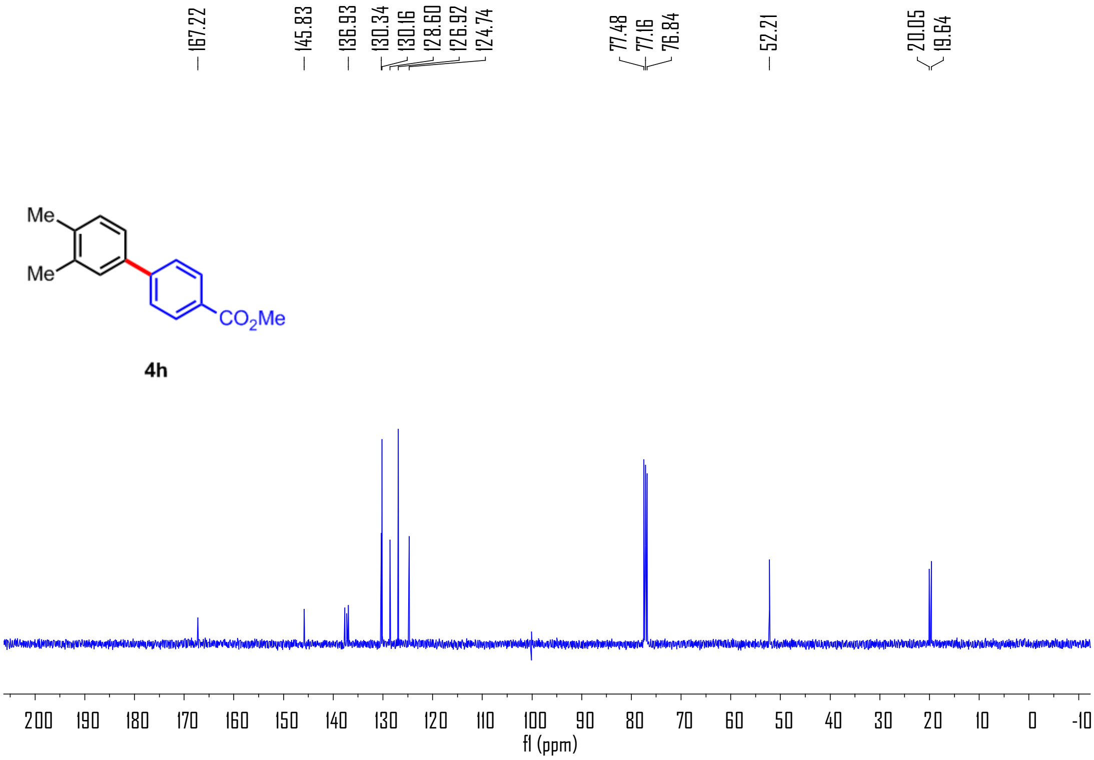

7.56
7.54
7.53
7.51
7.46
7.44
7.42
7.42
7.39
7.38
7.36
7.34
Cl
4f
4.00
4.93
fl (ppm)

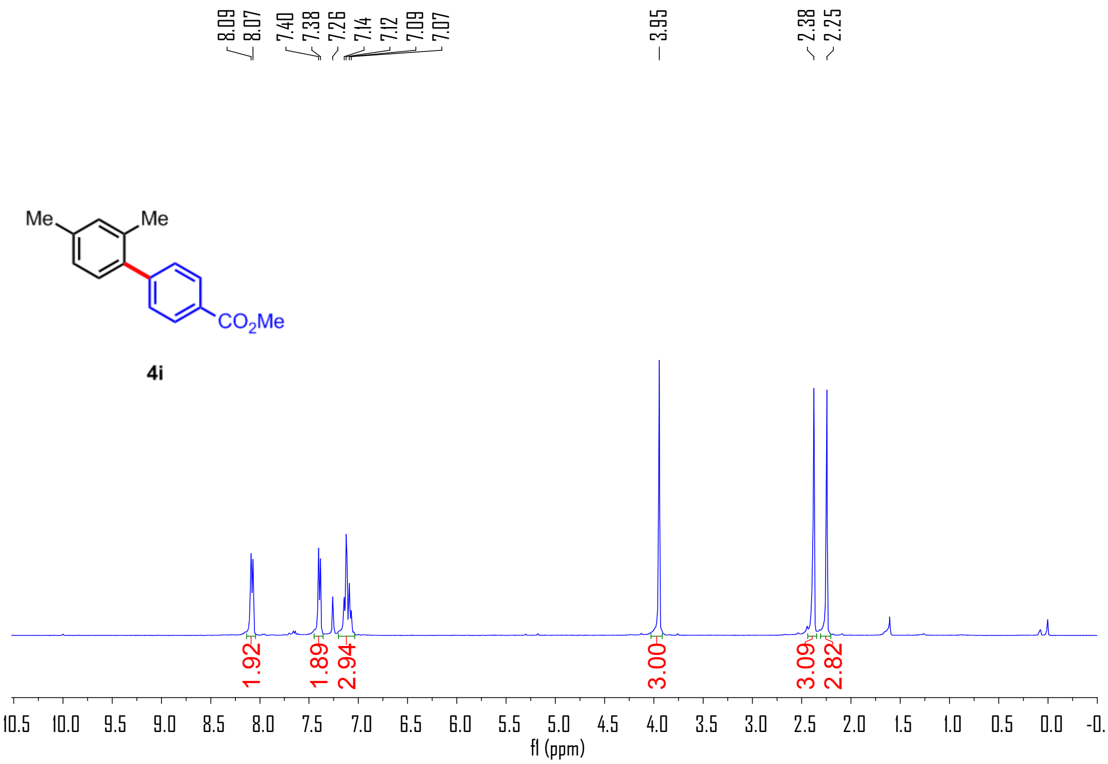

140.12
139.76
129.04
129.02
128.53
127.73
127.13
77.48
77.16
76.84
Cl
4f
fl (ppm)

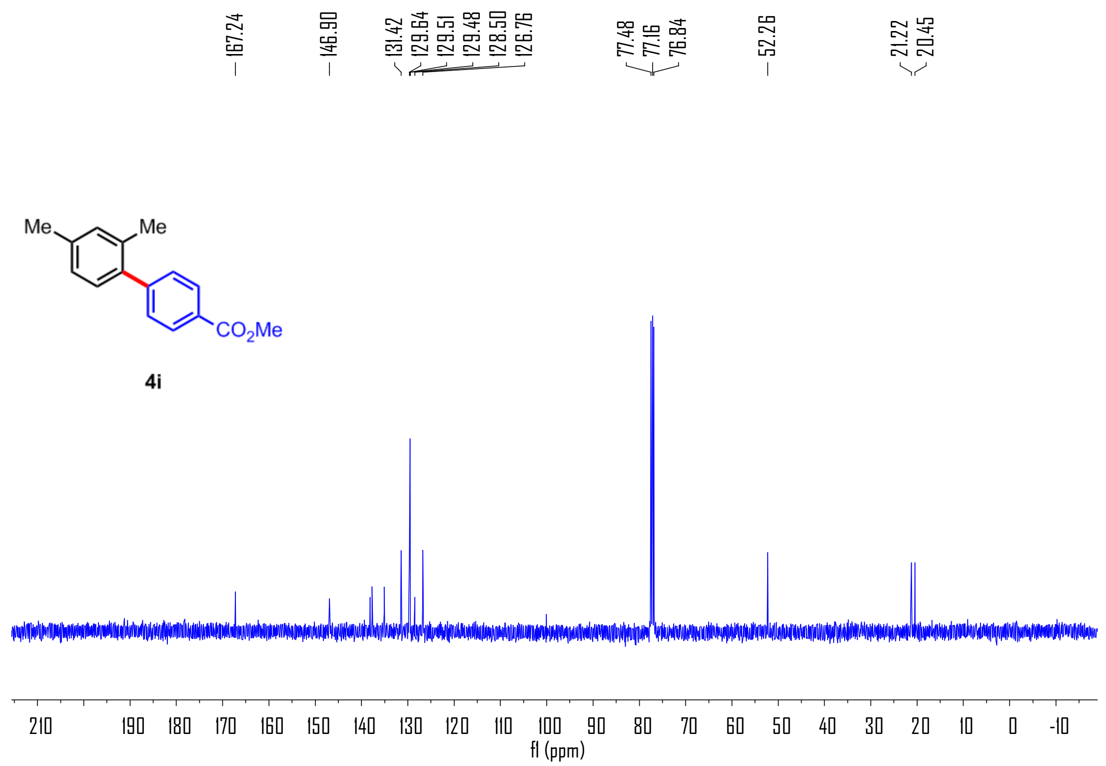

7.57 7.56 7.56 7.55 7.55 7.54 7.46 7.46 7.44 7.42 7.38 7.36 7.34
Br
4g
4.00
4.14
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

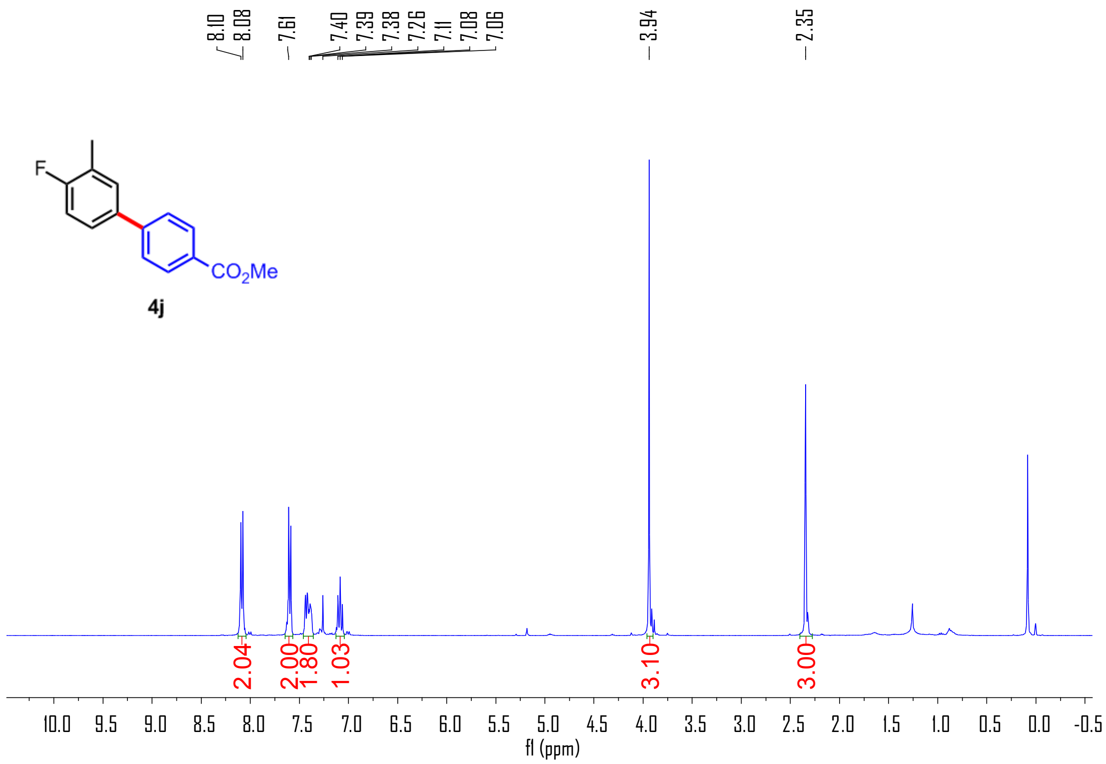

140.28 140.15 132.00 128.89 127.79 127.09 121.68 77.48 77.16 76.84
Br
4g
210 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

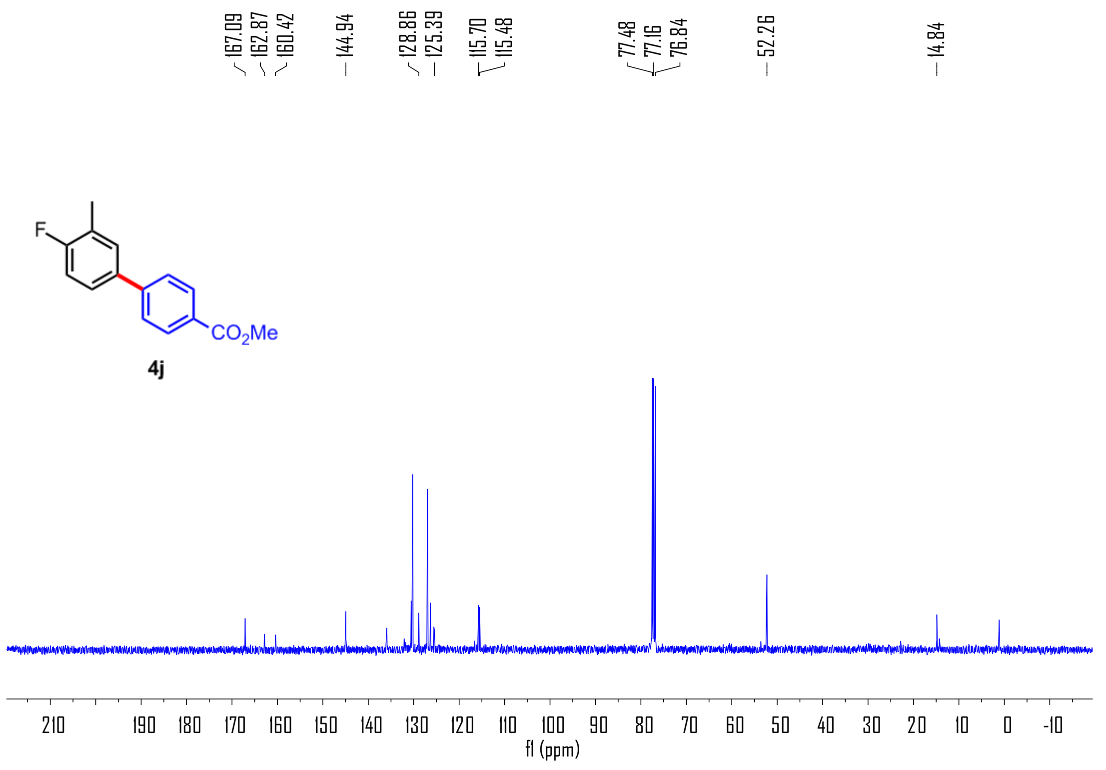

8.09
8.07
7.65
7.63
7.40
7.37
7.35
7.23
7.21
3.93
2.33
2.31
Me
Me
CO2Me
4h
2.00
2.06
1.01
1.04
1.00
3.10
3.02
3.01
fl (ppm)

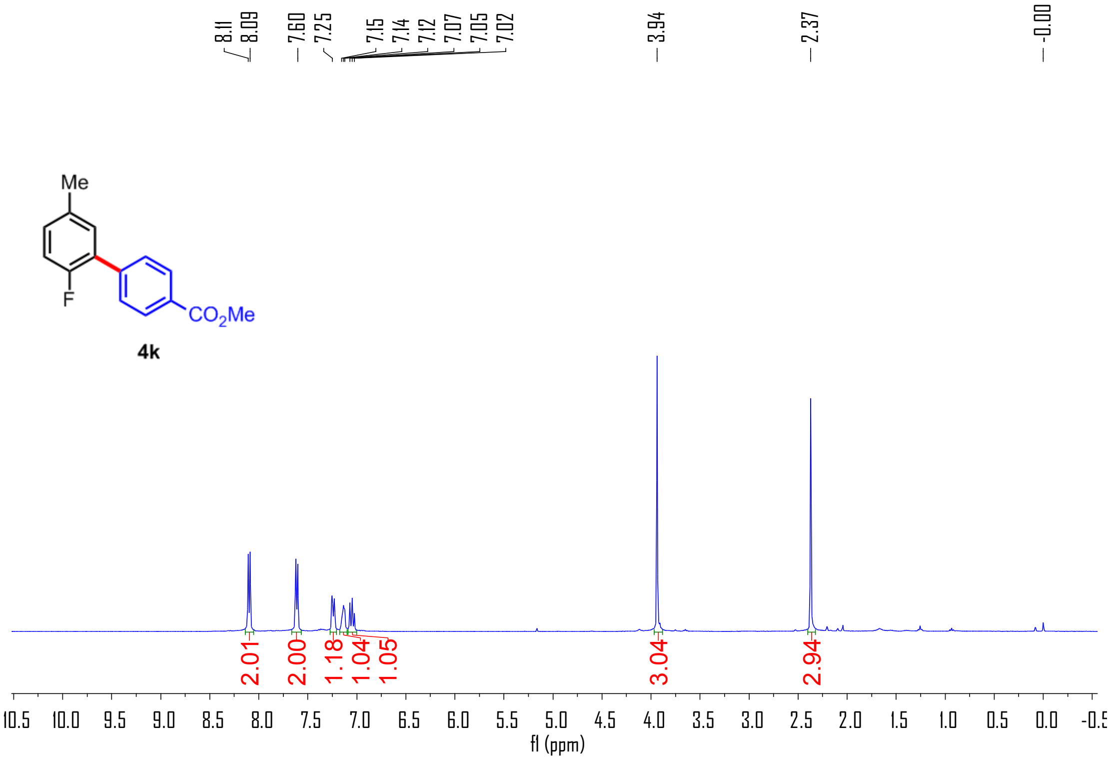

167.22
145.83
136.93
130.34
130.16
128.60
126.92
124.74
77.48
77.16
76.84
52.21
20.05
19.64
Me
Me
CO2Me
4h
fl (ppm)

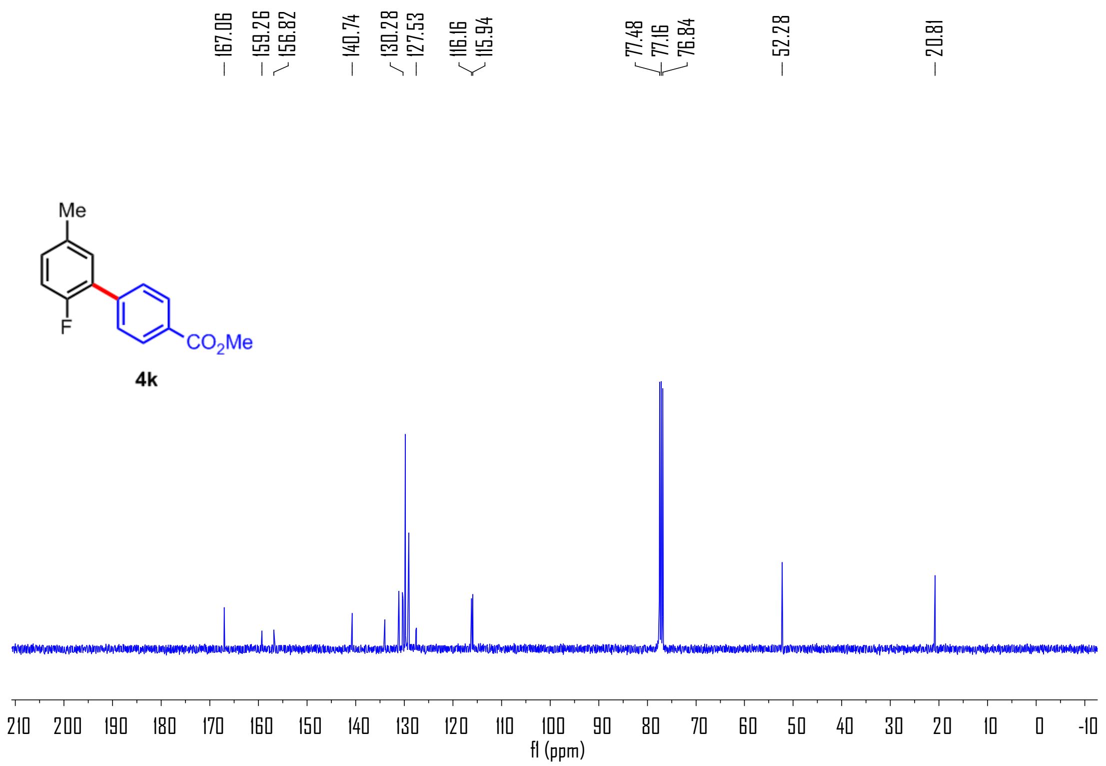


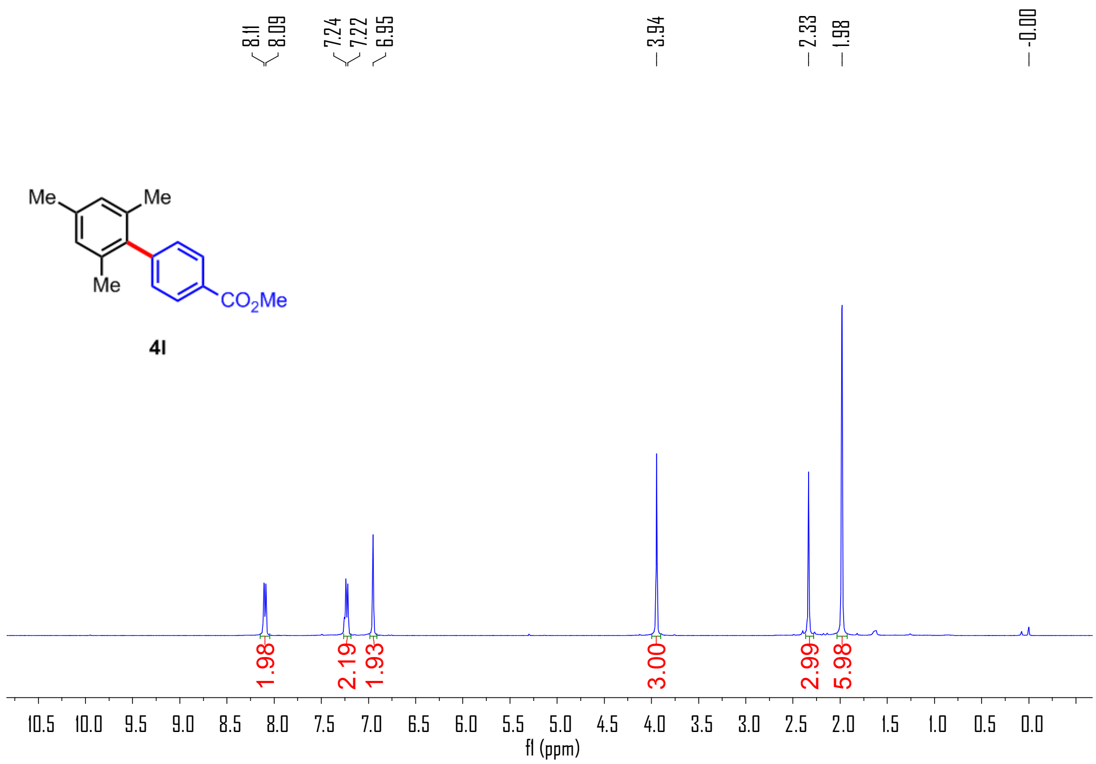


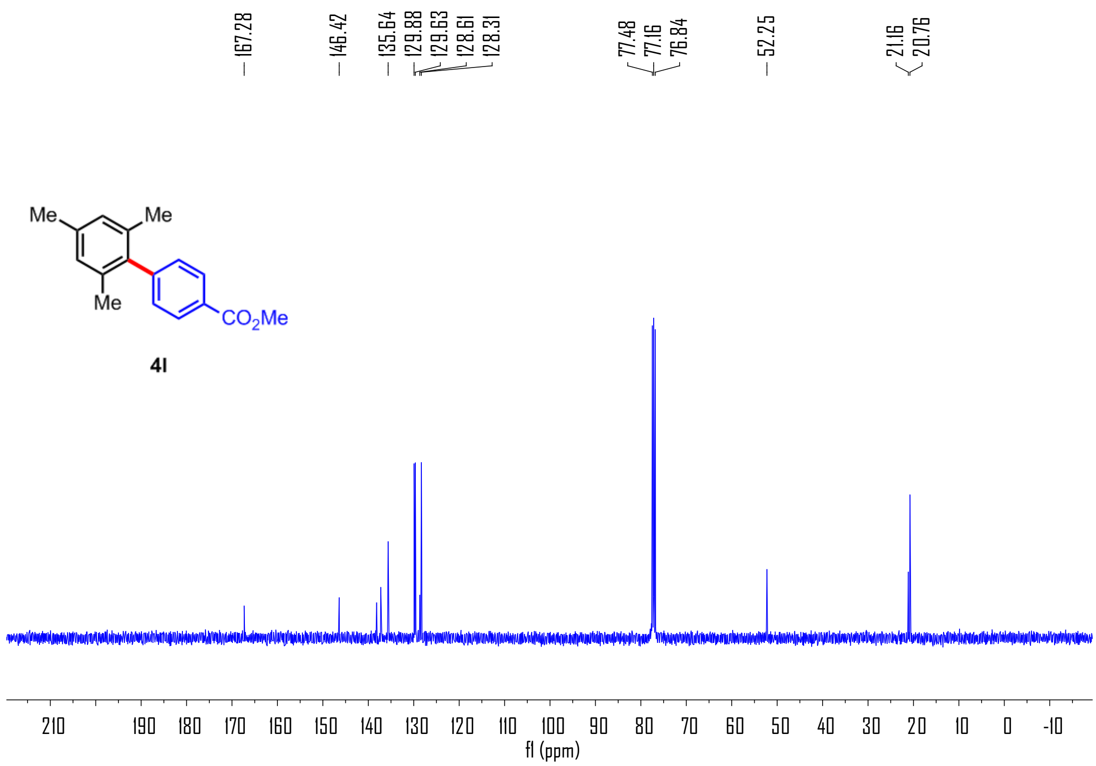

8.10
8.08
7.61
7.40
7.39
7.38
7.26
7.11
7.08
7.06
3.94
2.35
F
CO2Me
4j
2.04
2.00
1.80
1.03
3.10
3.00
fl (ppm)


167.09
162.87
160.42
144.94
128.86
125.39
115.70
115.48
77.48
77.16
76.84
52.26
14.84
F
CO2Me
4j
fl (ppm)

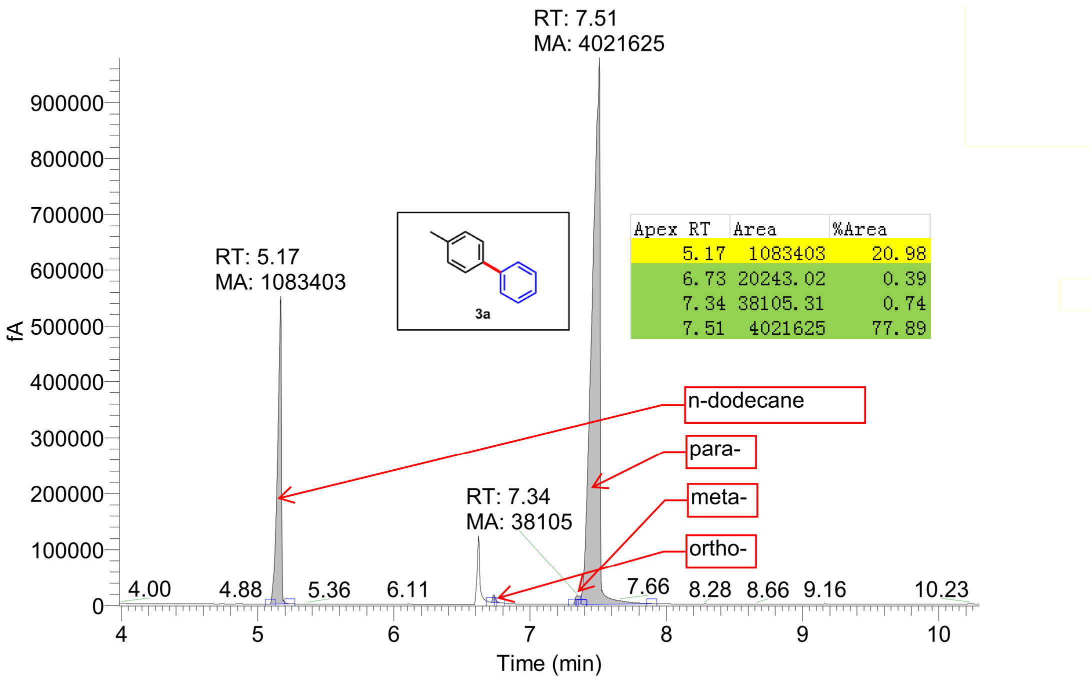

8.11
8.09
7.60
7.25
7.15
7.14
7.12
7.07
7.05
7.02
3.94
2.37
-0.00
Me
F
CO2Me
4k
2.01
2.00
1.18
1.04
1.05
3.04
2.94
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

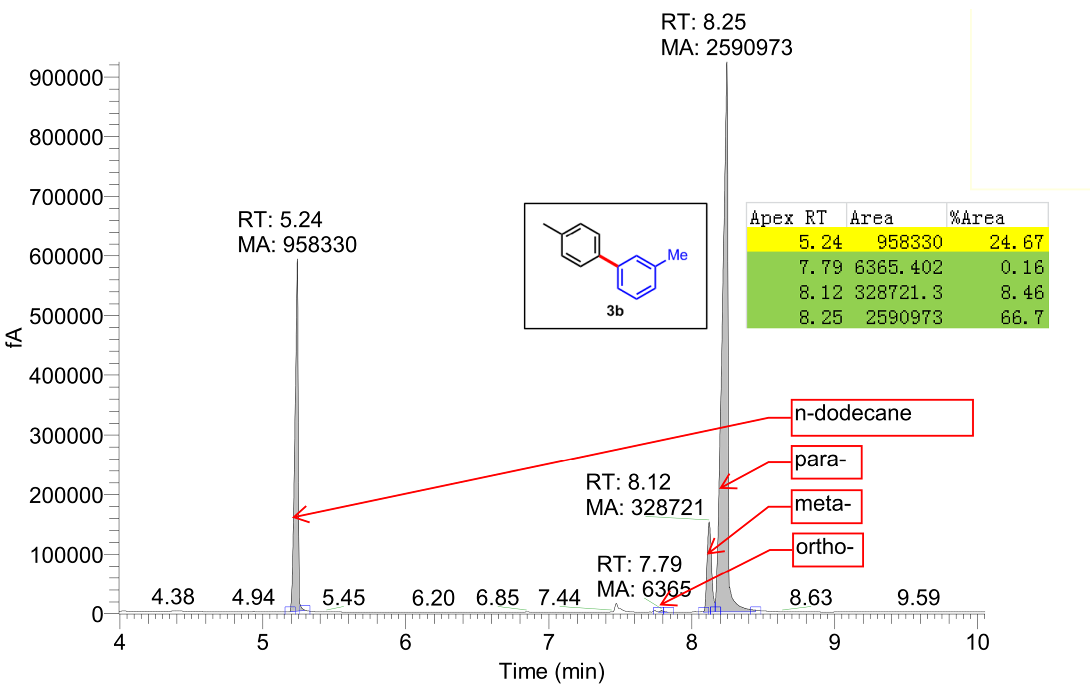

167.06
159.26
156.82
140.74
130.28
127.53
116.16
115.94
77.48
77.16
76.84
52.28
20.81
Me
F
CO2Me
4k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

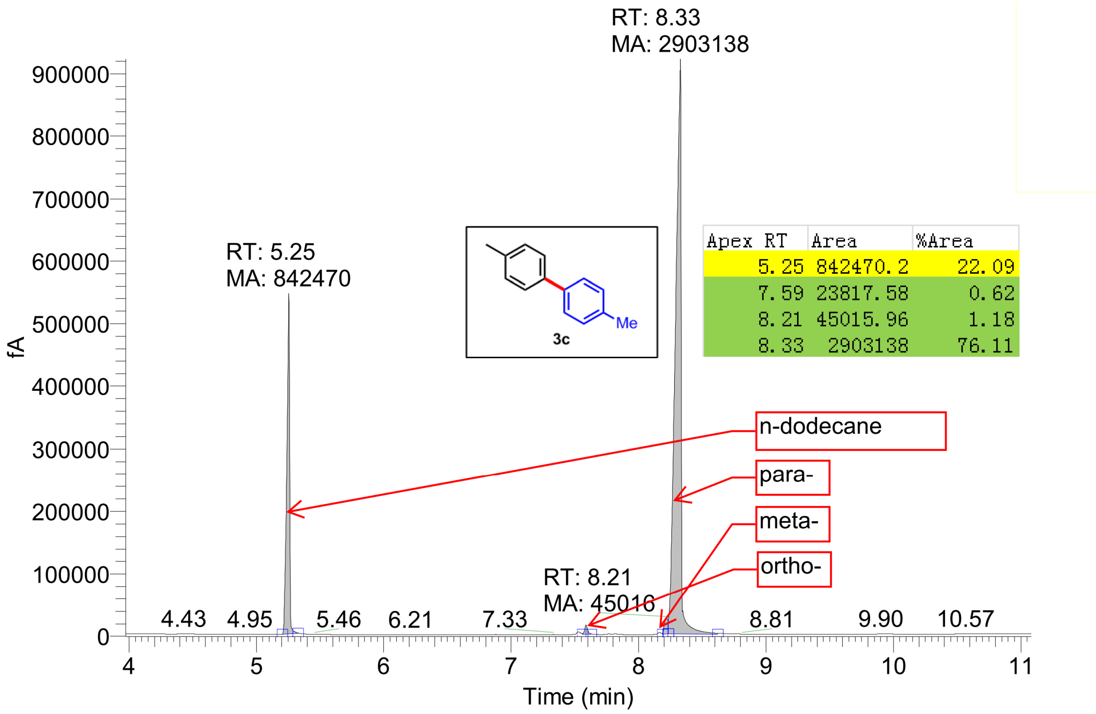

8.11
8.09
7.24
7.22
6.95
3.94
2.33
1.98
-0.00
Me
Me
Me
CO2Me
4l
1.98
2.19
1.93
3.00
2.99
5.98
fl (ppm)

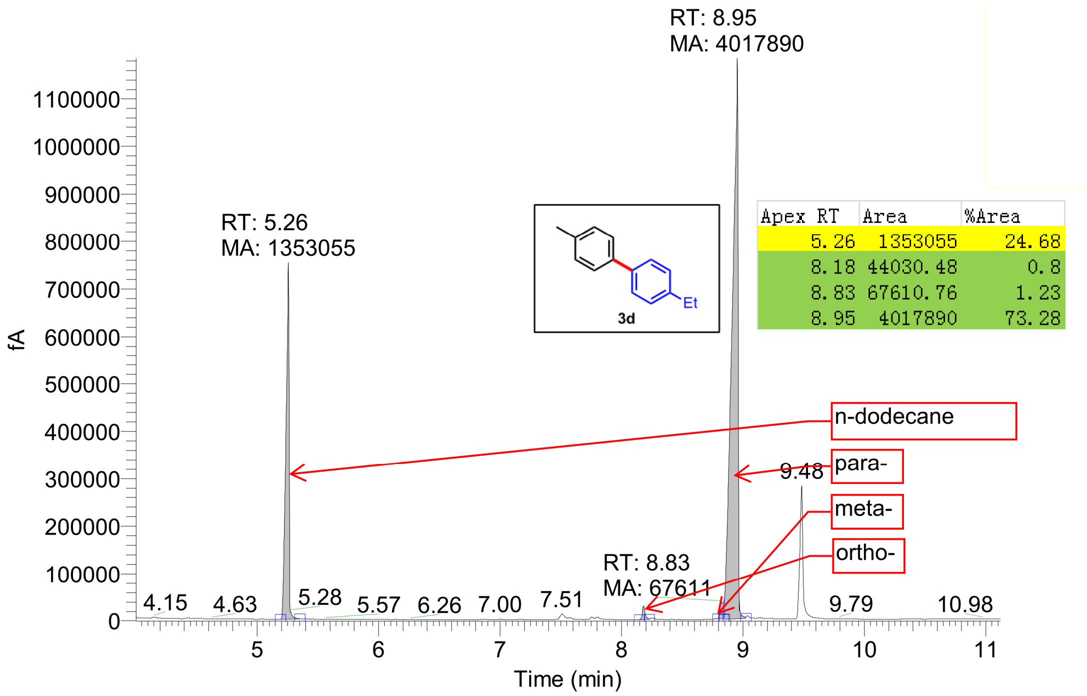

167.28
146.42
135.64
129.88
129.63
128.61
128.31
77.48
77.16
76.84
52.25
21.16
20.76
Me
Me
Me
CO2Me
4l
fl (ppm)

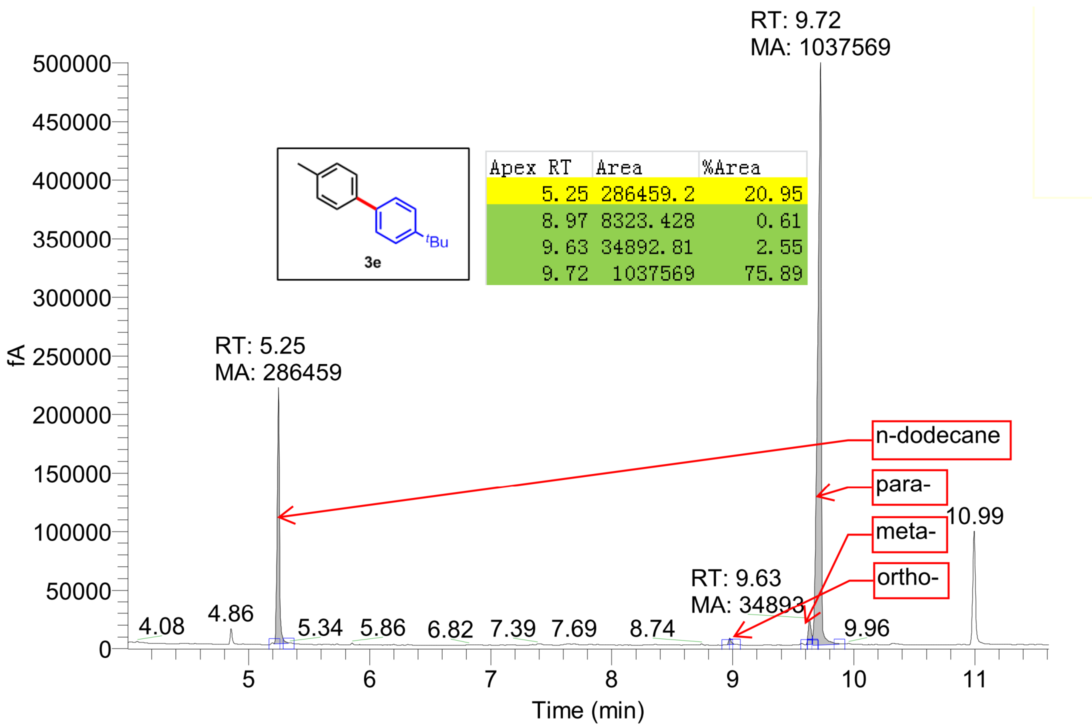
7. GC Charts of Crude Products



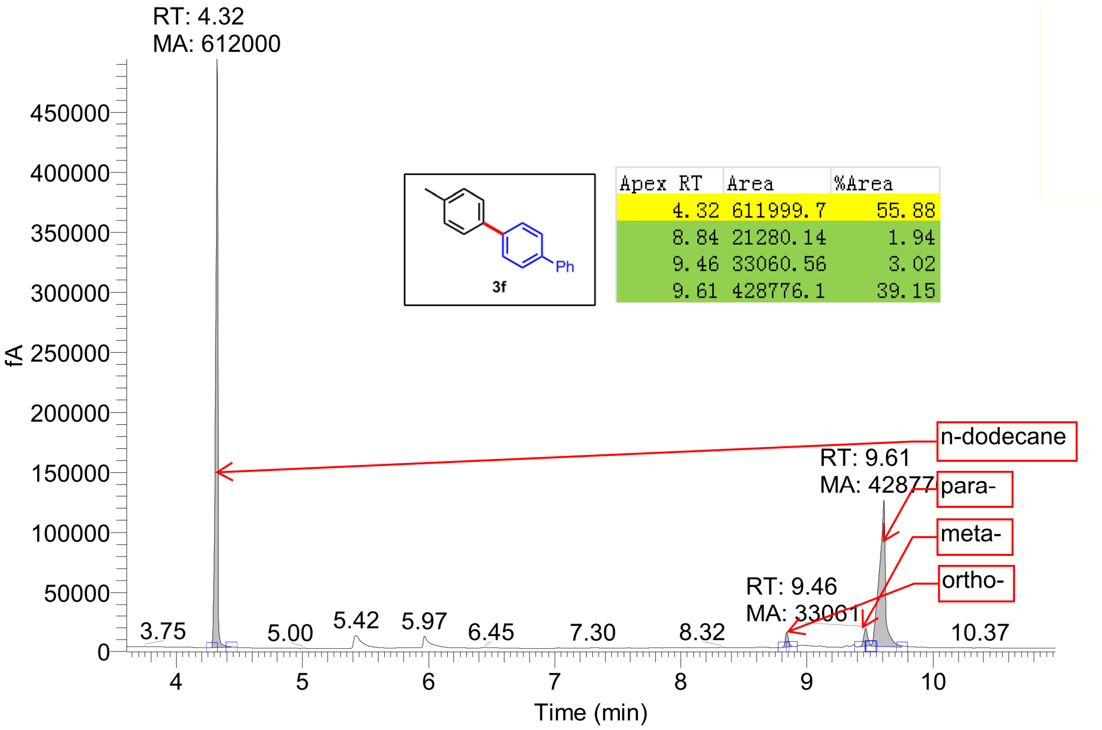



RT: 8.33
MA: 2903138
RT: 5.25
MA: 842470
RT: 8.21
MA: 45016
3c
Me
Apex RT | Area | %Area
5.25 | 842470.2 | 22.09
7.59 | 23817.58 | 0.62
8.21 | 45015.96 | 1.18
8.33 | 2903138 | 76.11
n-dodecane
para-
meta-
ortho-
fA
Time (min)

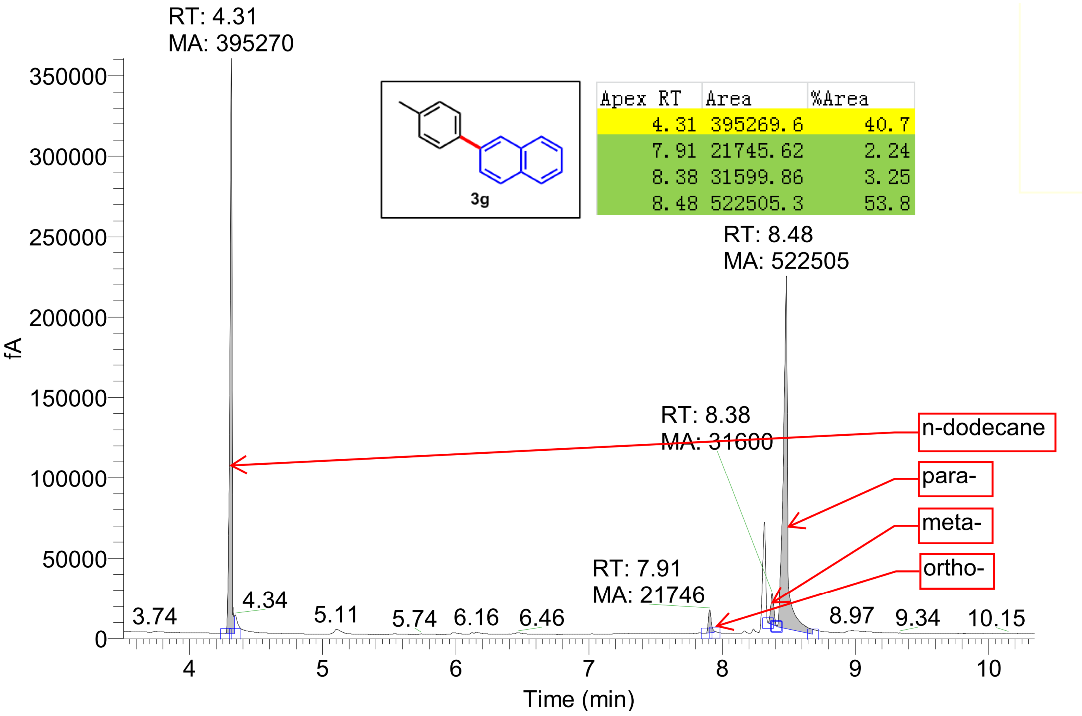

RT: 8.95
MA: 4017890
RT: 5.26
MA: 1353055
RT: 8.83
MA: 67611
3d
Et
Apex RT | Area | %Area
5.26 | 1353055 | 24.68
8.18 | 44030.48 | 0.8
8.83 | 67610.76 | 1.23
8.95 | 4017890 | 73.28
n-dodecane
para-
meta-
ortho-
9.48
fA
Time (min)



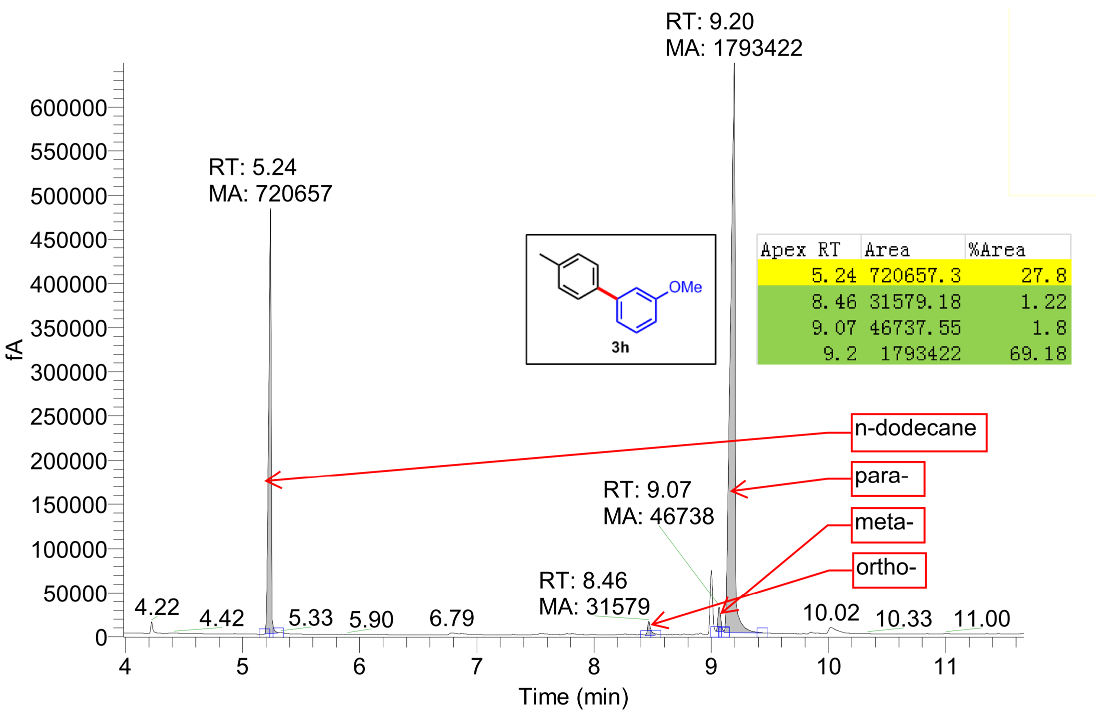
Apex RT	Area	%Area
5.25	286459.2	20.95
8.97	8323.428	0.61
9.63	34892.81	2.55
9.72	1037569	75.89



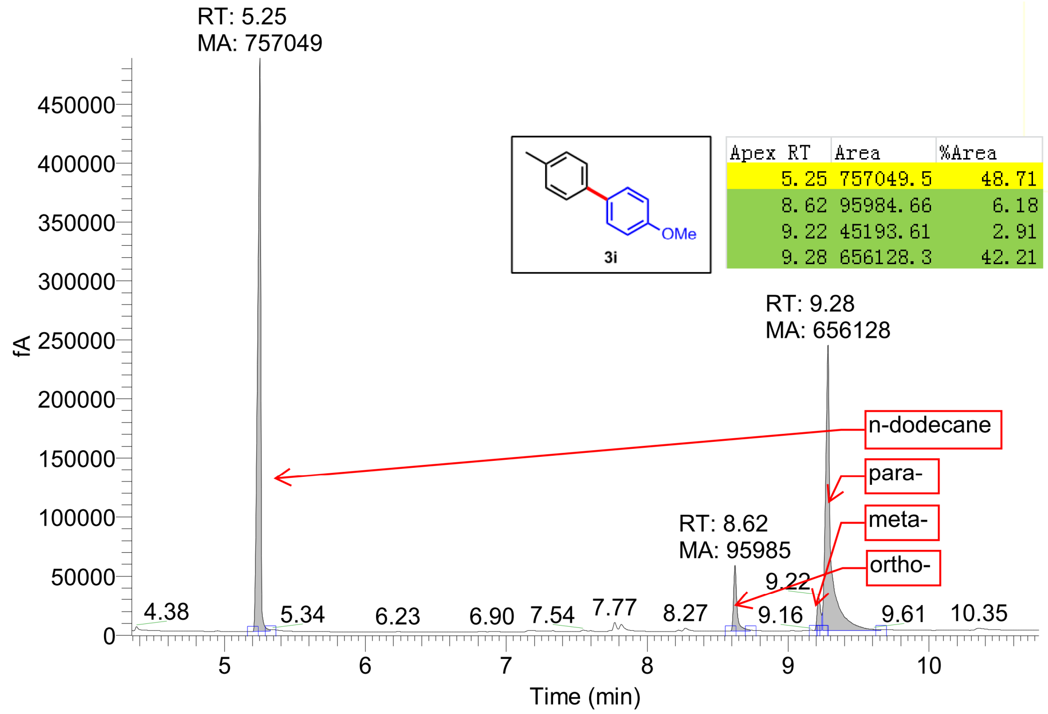
Apex RT	Area	%Area
4.32	611999.7	55.88
8.84	21280.14	1.94
9.46	33060.56	3.02
9.61	428776.1	39.15



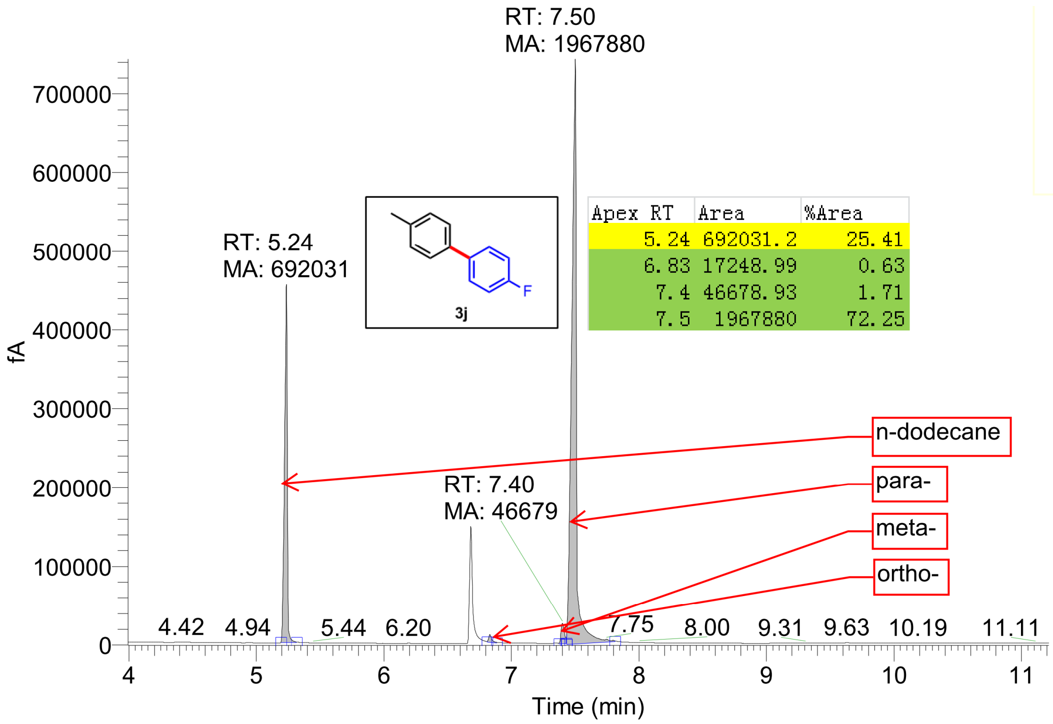
Apex RT	Area	%Area
4.31	395269.6	40.7
7.91	21745.62	2.24
8.38	31599.86	3.25
8.48	522505.3	53.8



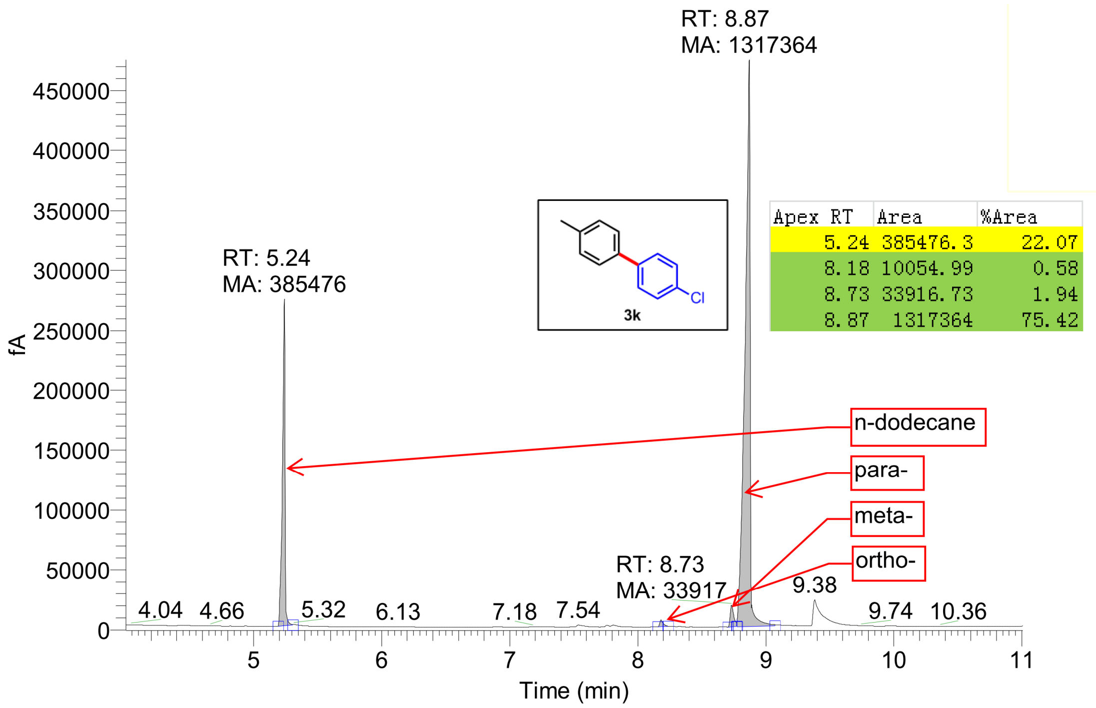
Apex RT	Area	%Area
5.24	720657.3	27.8
8.46	31579.18	1.22
9.07	46737.55	1.8
9.2	1793422	69.18



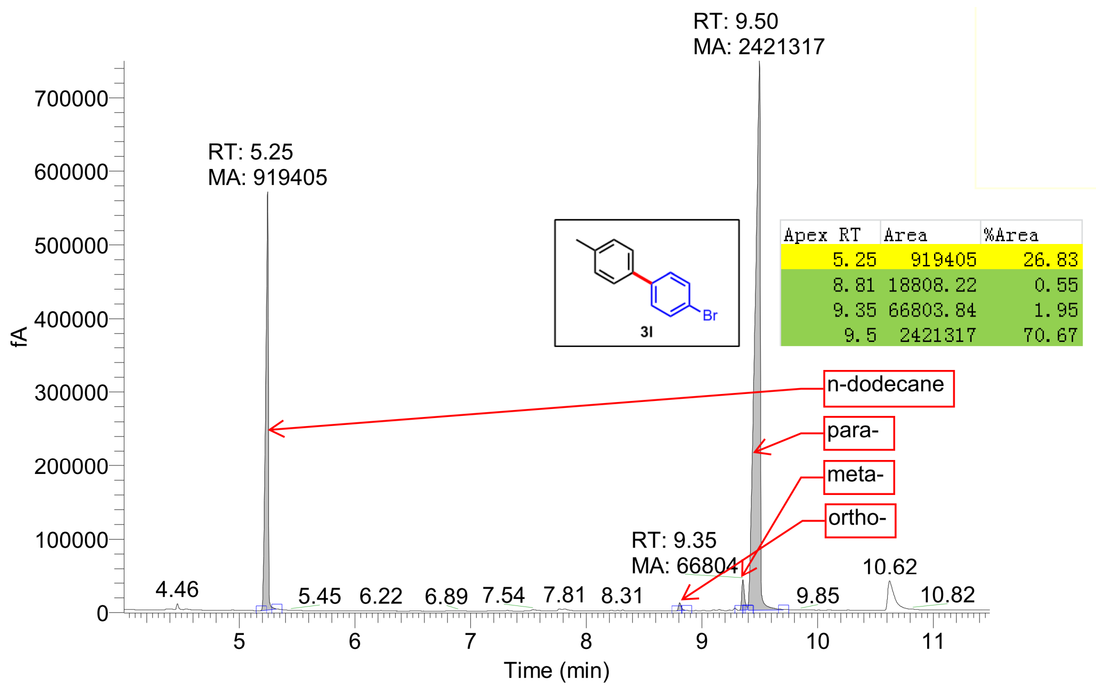
Apex RT	Area	%Area
5.25	757049.5	48.71
8.62	95984.66	6.18
9.22	45193.61	2.91
9.28	656128.3	42.21



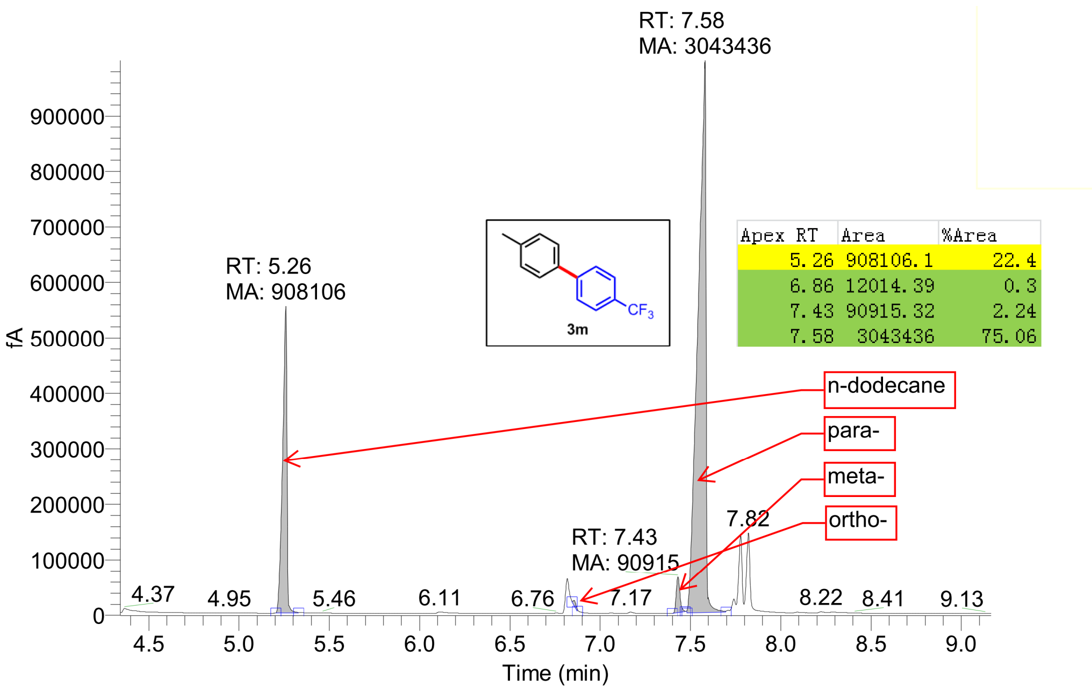
Apex RT	Area	%Area
5.24	692031.2	25.41
6.83	17248.99	0.63
7.4	46678.93	1.71
7.5	1967880	72.25

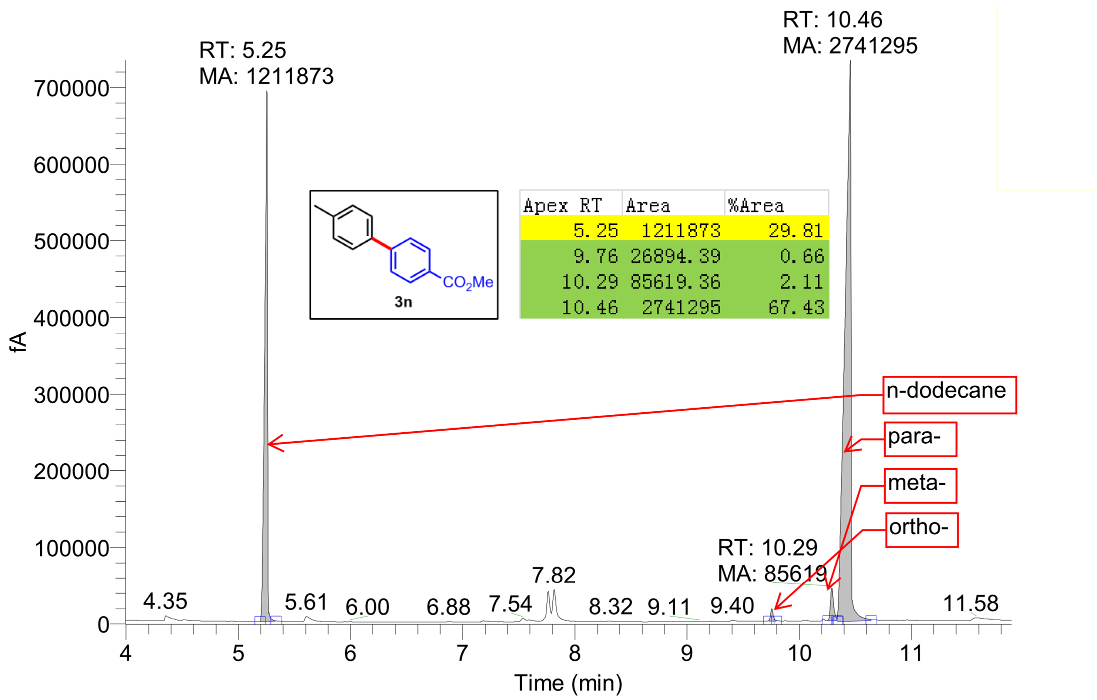


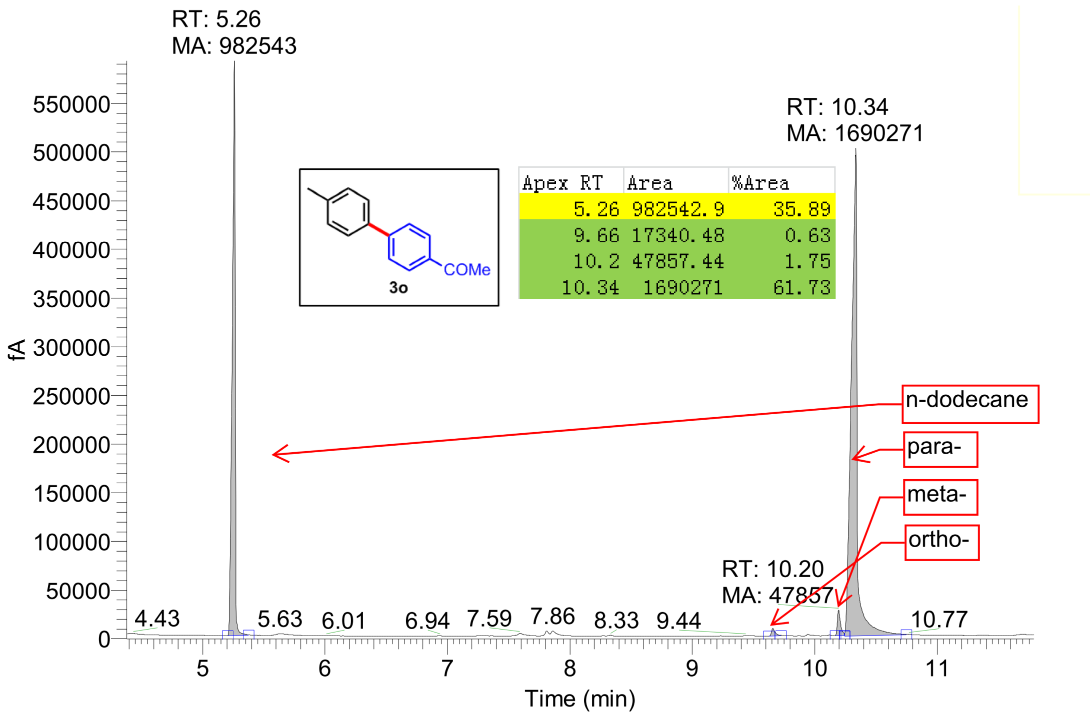
Apex RT	Area	%Area
5.24	385476.3	22.07
8.18	10054.99	0.58
8.73	33916.73	1.94
8.87	1317364	75.42

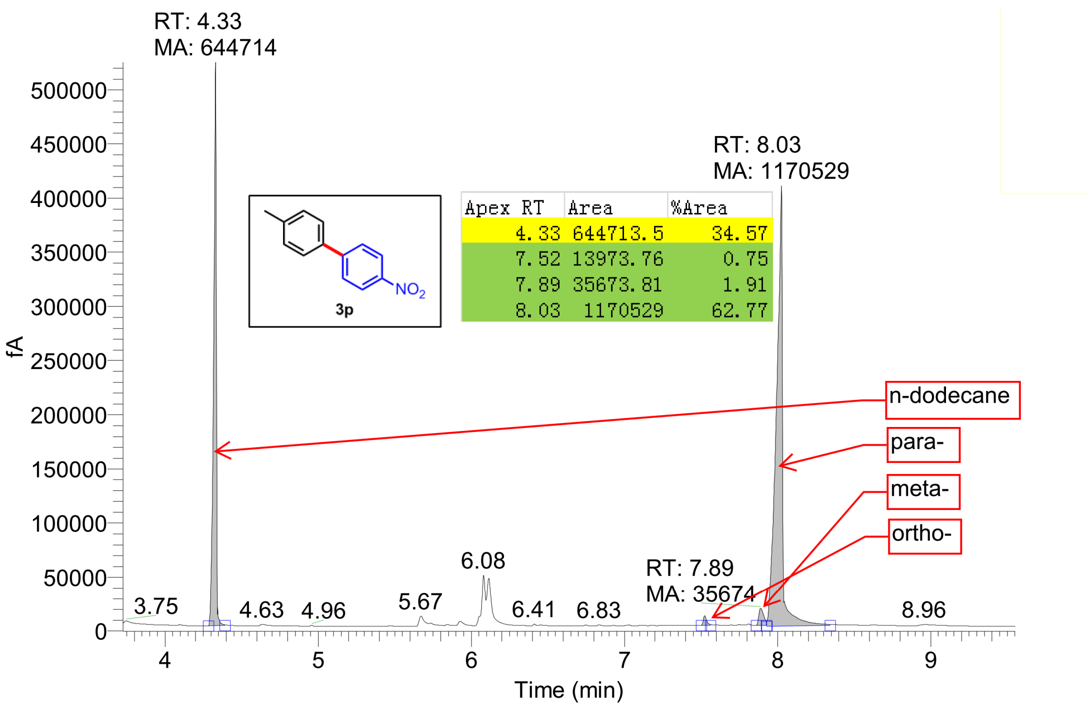


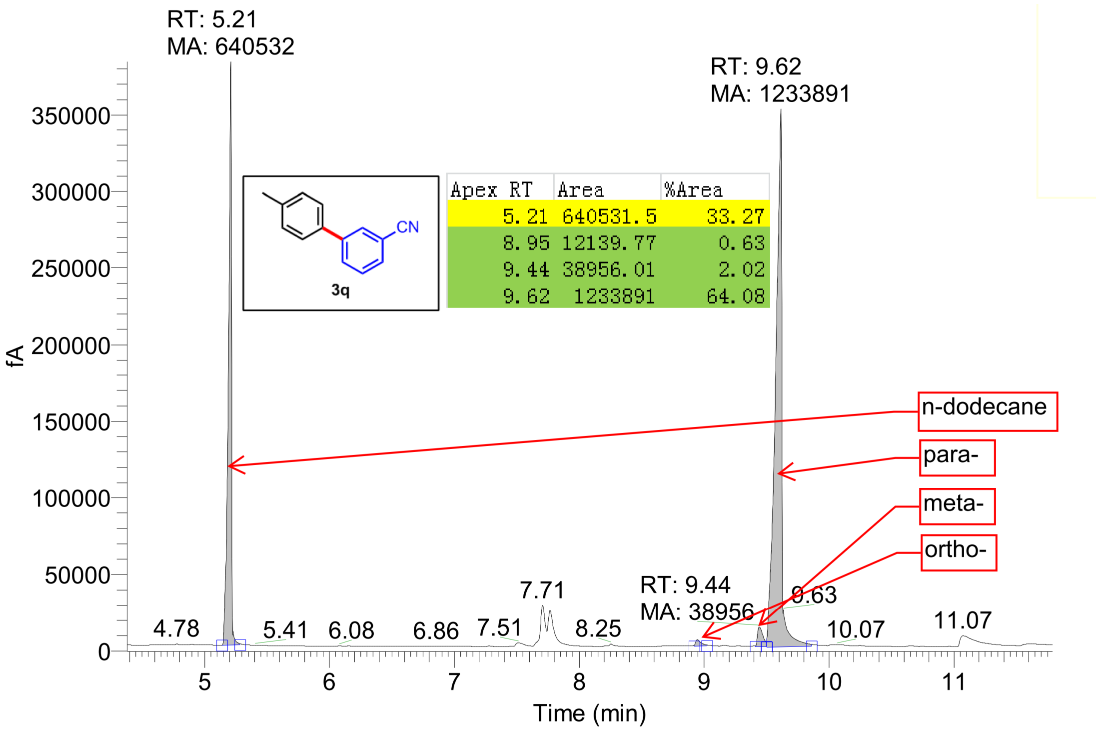
Apex RT	Area	%Area
5.25	919405	26.83
8.81	18808.22	0.55
9.35	66803.84	1.95
9.5	2421317	70.67


RT: 7.58
MA: 3043436
RT: 5.26
MA: 908106
RT: 7.43
MA: 90915
3m
Apex RT Area %Area
5.26 908106.1 22.4
6.86 12014.39 0.3
7.43 90915.32 2.24
7.58 3043436 75.06
n-dodecane
para-
meta-
ortho-
fA
Time (min)

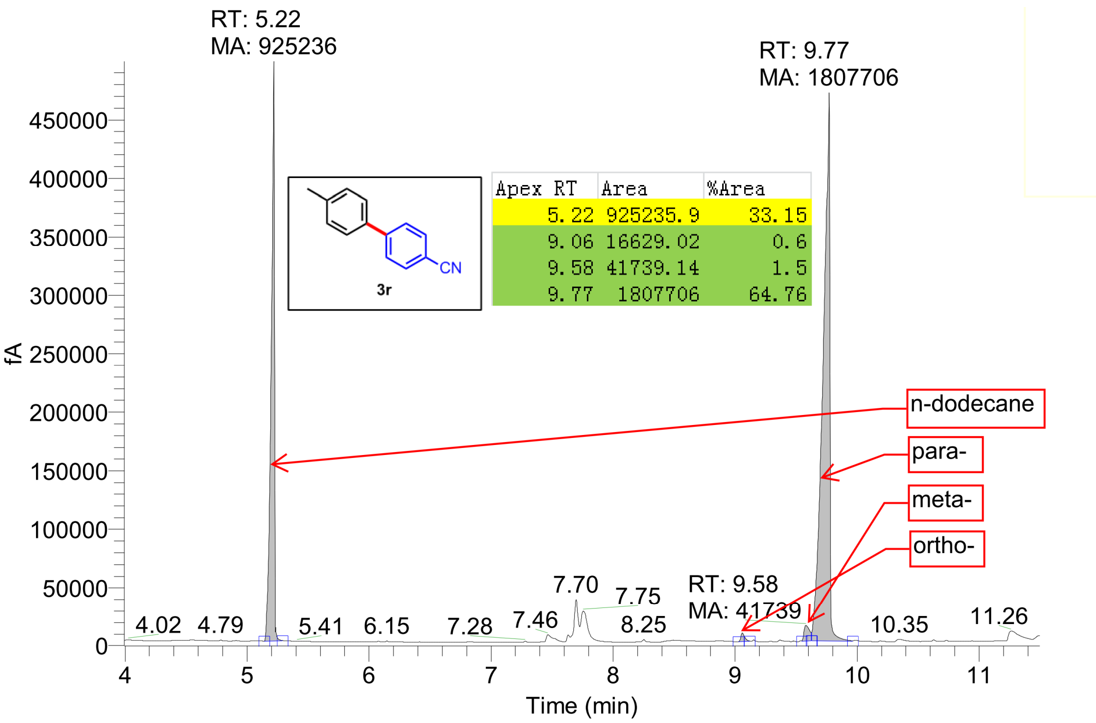

RT: 5.25
MA: 1211873
RT: 10.46
MA: 2741295
RT: 10.29
MA: 85619
3n
Apex RT Area %Area
5.25 1211873 29.81
9.76 26894.39 0.66
10.29 85619.36 2.11
10.46 2741295 67.43
n-dodecane
para-
meta-
ortho-
fA
Time (min)


RT: 5.26
MA: 982543
RT: 10.34
MA: 1690271
3o
COMe
Apex RT | Area | %Area
5.26 | 982542.9 | 35.89
9.66 | 17340.48 | 0.63
10.2 | 47857.44 | 1.75
10.34 | 1690271 | 61.73
n-dodecane
para-
meta-
ortho-
RT: 10.20
MA: 47857
fA
Time (min)

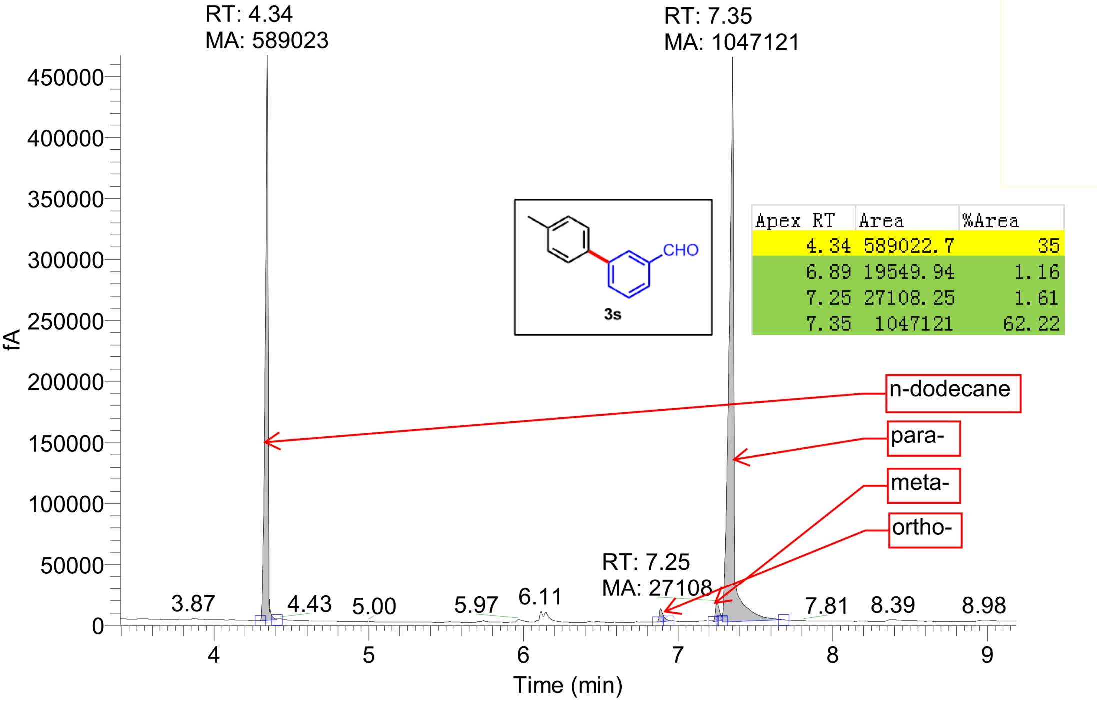

RT: 4.33
MA: 644714
RT: 8.03
MA: 1170529
3p
NO2
Apex RT | Area | %Area
4.33 | 644713.5 | 34.57
7.52 | 13973.76 | 0.75
7.89 | 35673.81 | 1.91
8.03 | 1170529 | 62.77
n-dodecane
para-
meta-
ortho-
RT: 7.89
MA: 35674
fA
Time (min)



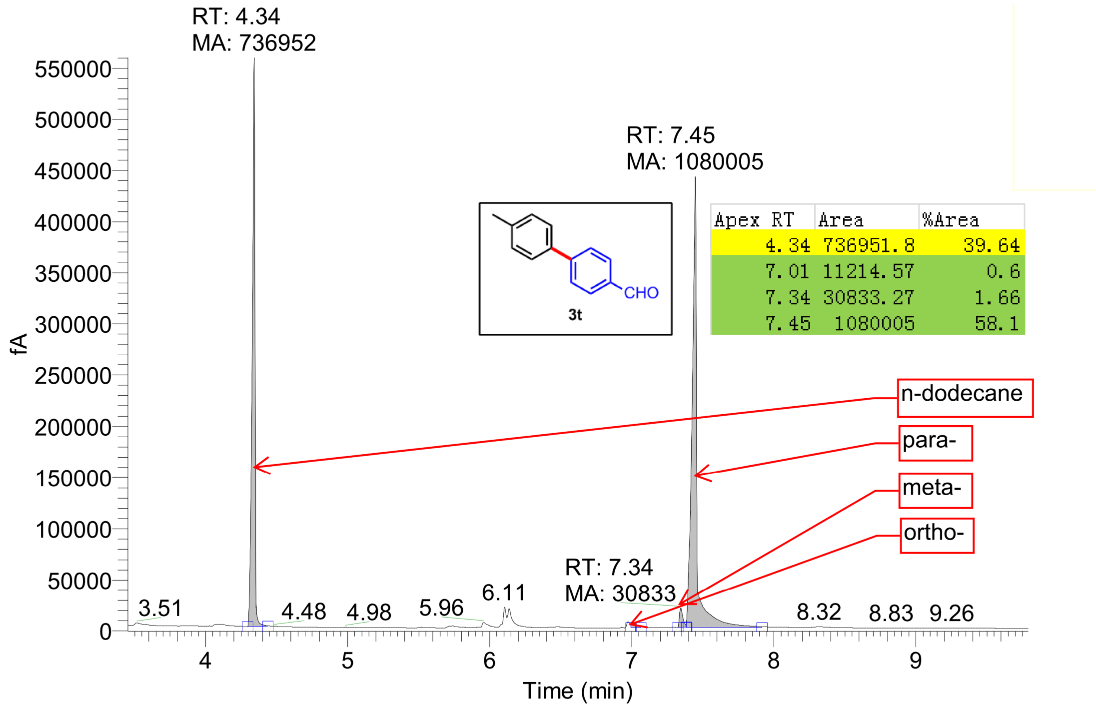
Apex RT	Area	%Area
5.21	640531.5	33.27
8.95	12139.77	0.63
9.44	38956.01	2.02
9.62	1233891	64.08



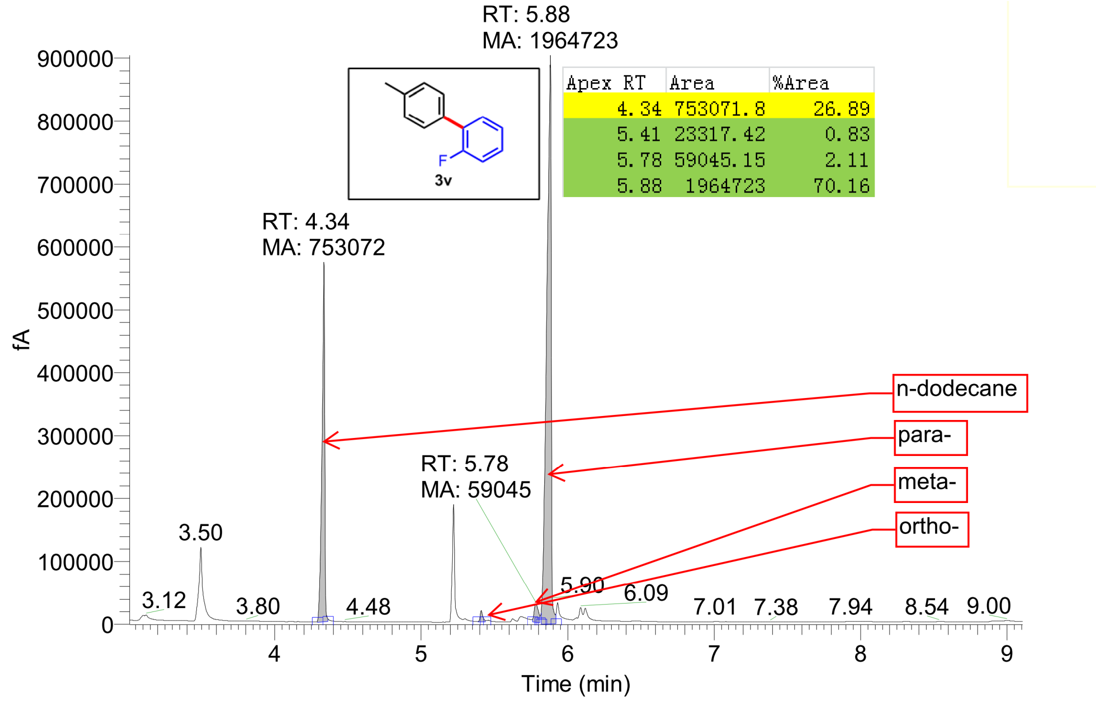
Apex RT	Area	%Area
5.22	925235.9	33.15
9.06	16629.02	0.6
9.58	41739.14	1.5
9.77	1807706	64.76



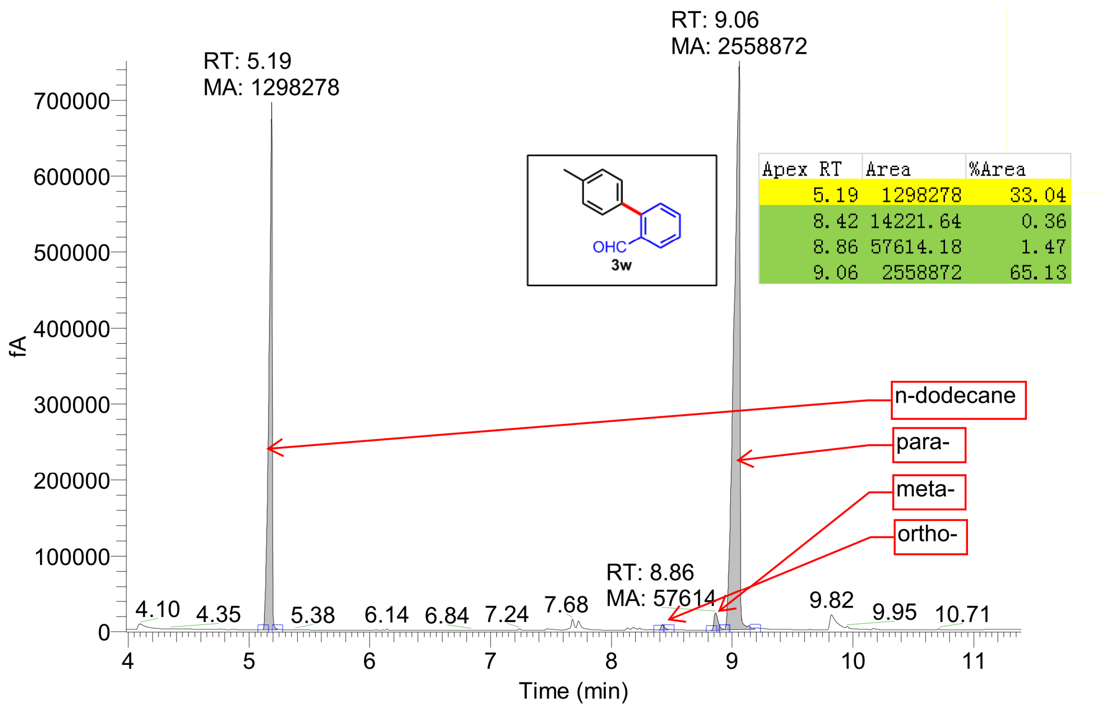
Apex RT	Area	%Area
4.34	589022.7	35
6.89	19549.94	1.16
7.25	27108.25	1.61
7.35	1047121	62.22



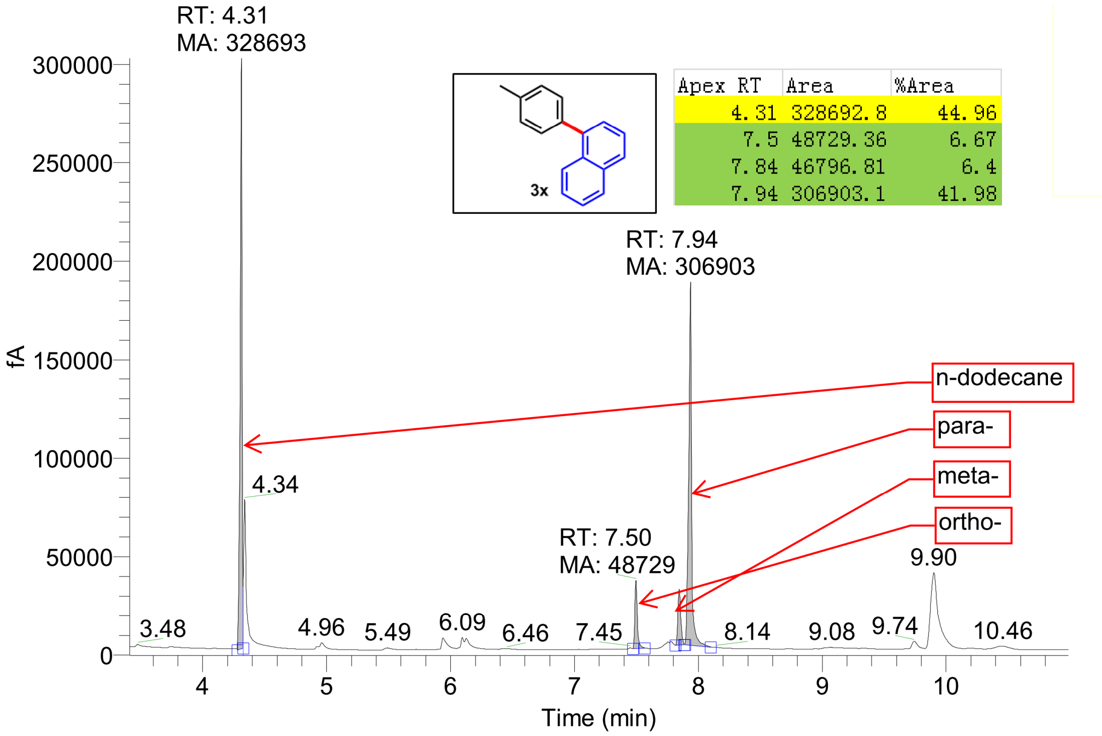
Apex RT	Area	%Area
4.34	736951.8	39.64
7.01	11214.57	0.6
7.34	30833.27	1.66
7.45	1080005	58.1

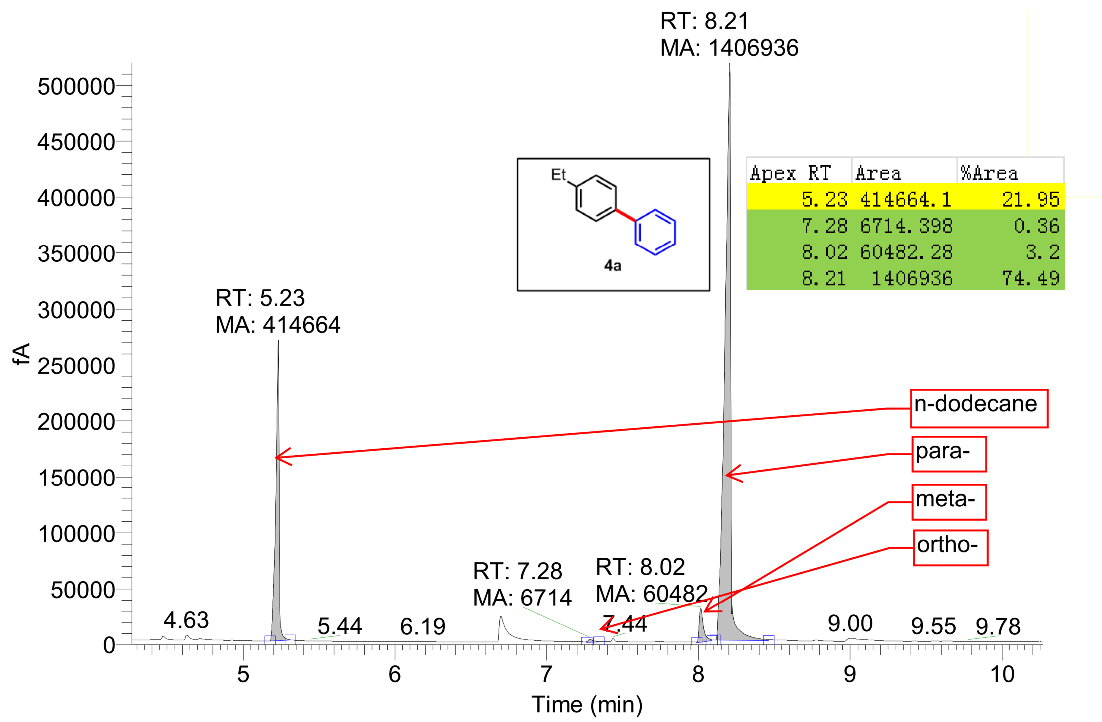


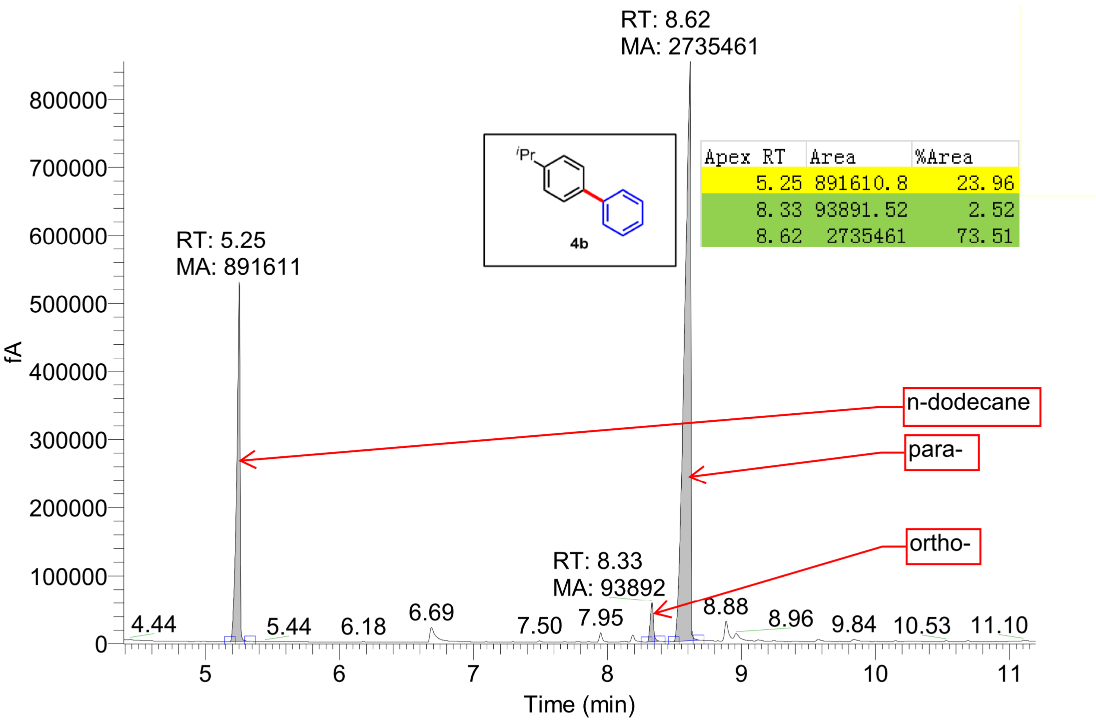
Apex RT	Area	%Area
4.34	753071.8	26.89
5.41	23317.42	0.83
5.78	59045.15	2.11
5.88	1964723	70.16

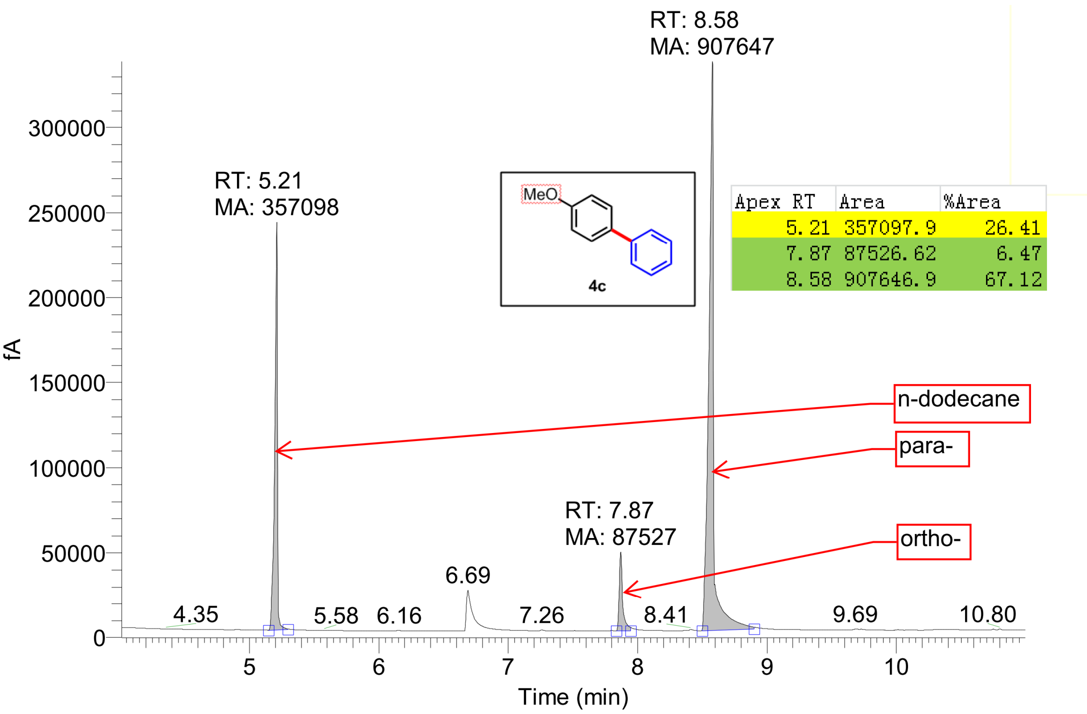


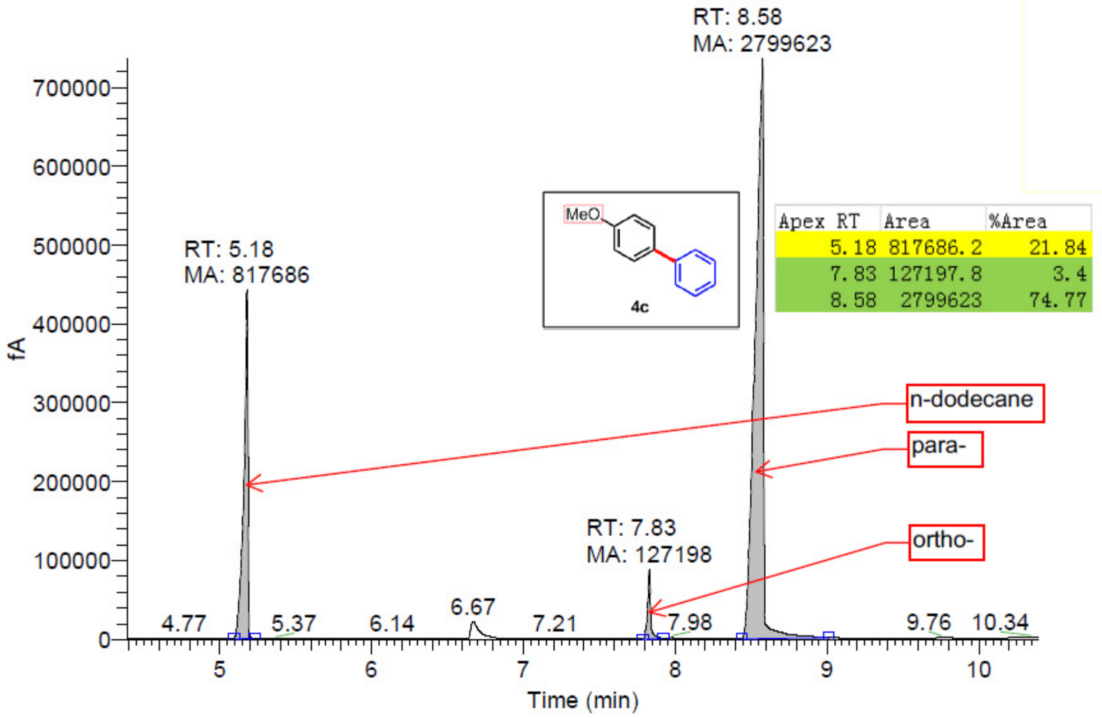
Apex RT	Area	%Area
5.19	1298278	33.04
8.42	14221.64	0.36
8.86	57614.18	1.47
9.06	2558872	65.13

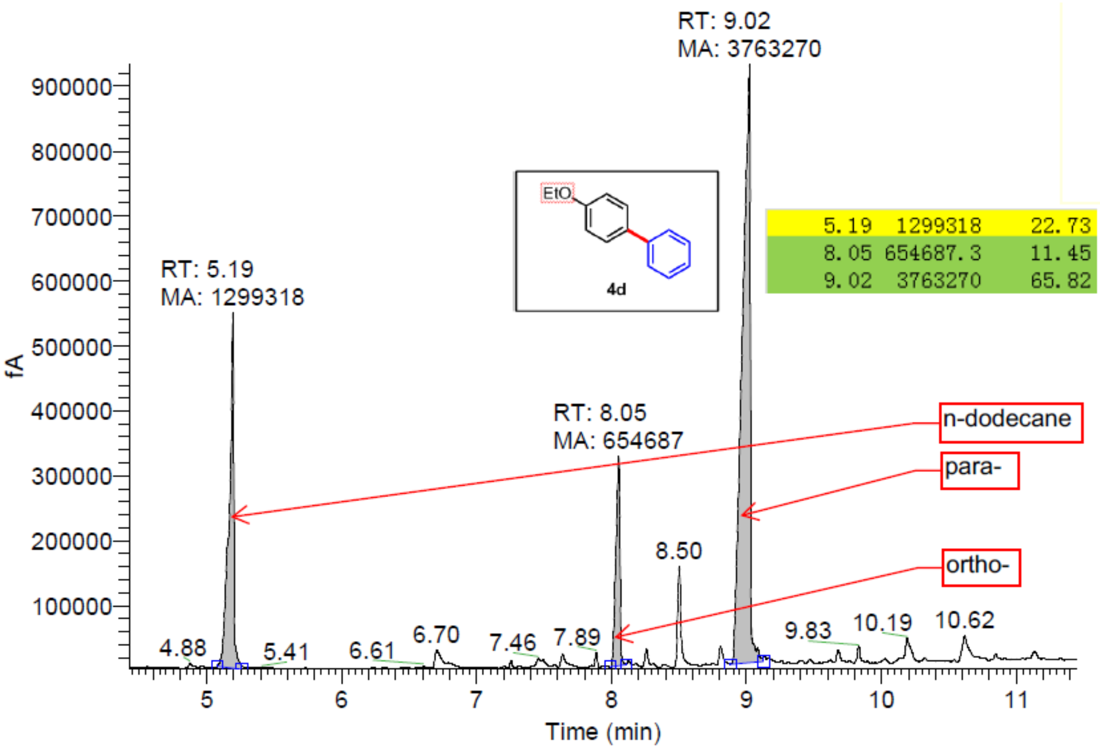

RT: 4.31
MA: 328693
RT: 7.94
MA: 306903
RT: 7.50
MA: 48729
3x
Apex RT | Area | %Area
4.31 | 328692.8 | 44.96
7.5 | 48729.36 | 6.67
7.84 | 46796.81 | 6.4
7.94 | 306903.1 | 41.98
n-dodecane
para-
meta-
ortho-
4.34
3.48
4.96
5.49
6.09
6.46
7.45
8.14
9.08
9.74
9.90
10.46
fA
Time (min)

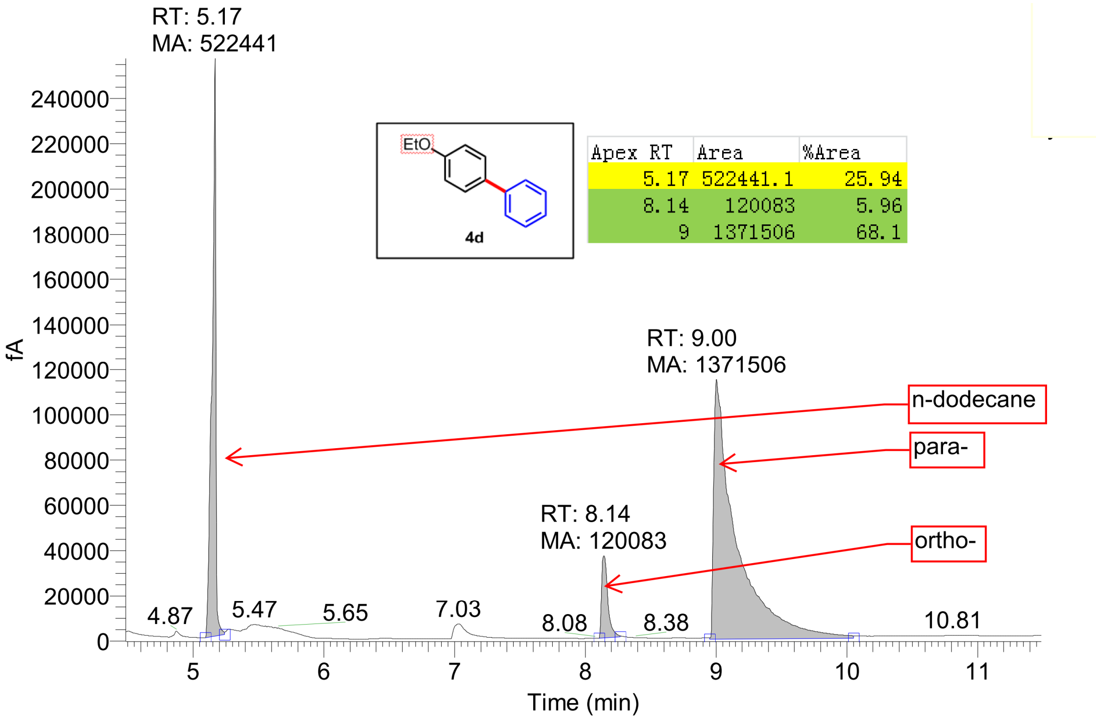

RT: 8.21
MA: 1406936
RT: 5.23
MA: 414664
RT: 7.28
MA: 6714
RT: 8.02
MA: 60482
Et
4a
Apex RT | Area | %Area
5.23 | 414664.1 | 21.95
7.28 | 6714.398 | 0.36
8.02 | 60482.28 | 3.2
8.21 | 1406936 | 74.49
n-dodecane
para-
meta-
ortho-
4.63
5.44
6.19
7.44
9.00
9.55
9.78
fA
Time (min)


RT: 8.62
MA: 2735461
RT: 5.25
MA: 891611
RT: 8.33
MA: 93892
4b
Apex RT Area %Area
5.25 891610.8 23.96
8.33 93891.52 2.52
8.62 2735461 73.51
n-dodecane
para-
ortho-
fA
Time (min)

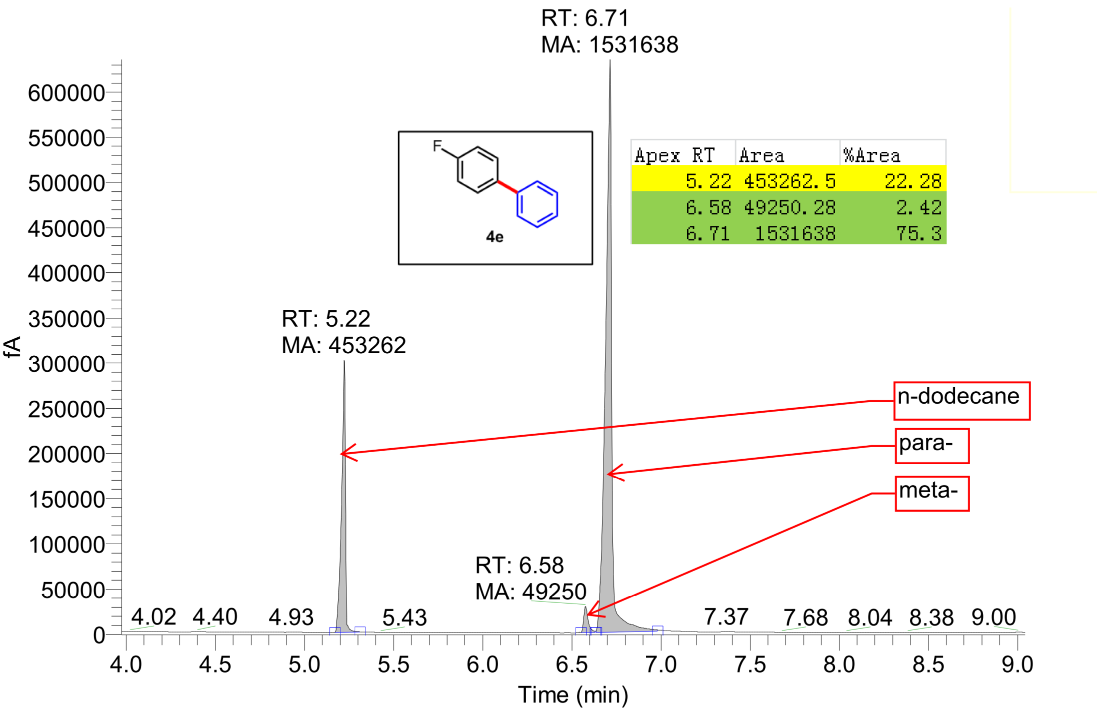

RT: 8.58
MA: 907647
RT: 5.21
MA: 357098
RT: 7.87
MA: 87527
MeO
4c
Apex RT Area %Area
5.21 357097.9 26.41
7.87 87526.62 6.47
8.58 907646.9 67.12
n-dodecane
para-
ortho-
fA
Time (min)


RT: 8.58
MA: 2799623
RT: 5.18
MA: 817686
RT: 7.83
MA: 127198
MeO
4c
Apex RT Area %Area
5.18 817686.2 21.84
7.83 127197.8 3.4
8.58 2799623 74.77
n-dodecane
para-
ortho-
4.77
5.37
6.14
6.67
7.21
7.98
9.76
10.34
fA
Time (min)

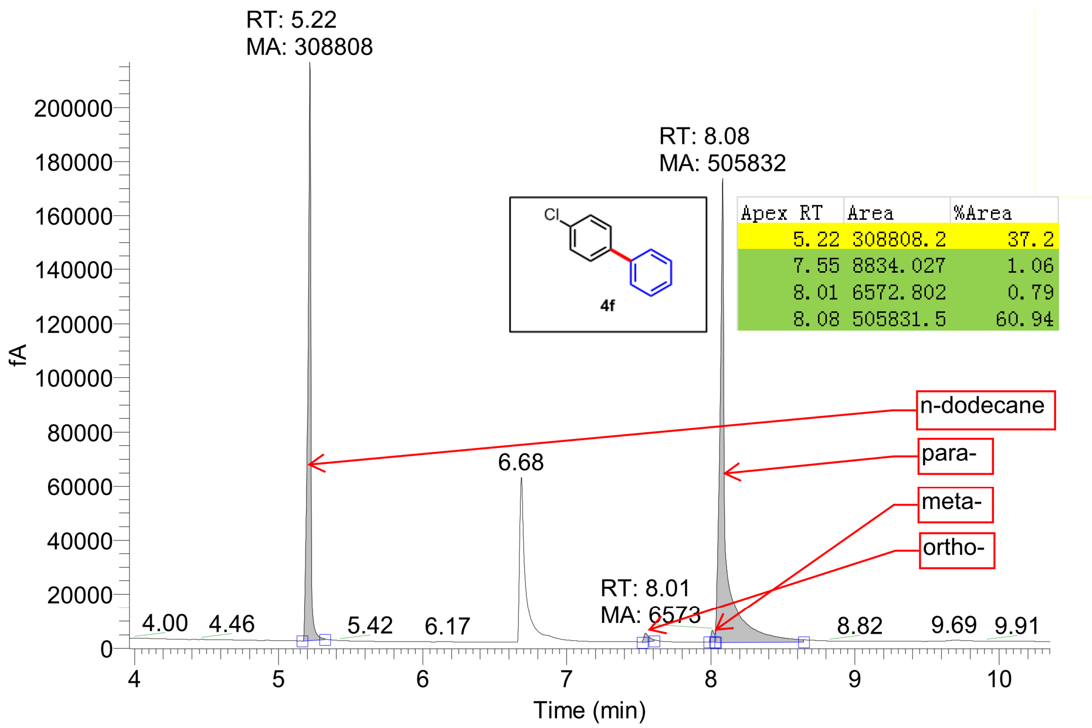

RT: 9.02
MA: 3763270
RT: 5.19
MA: 1299318
RT: 8.05
MA: 654687
EtO
4d
5.19 1299318 22.73
8.05 654687.3 11.45
9.02 3763270 65.82
n-dodecane
para-
ortho-
8.50
4.88
5.41
6.61
6.70
7.46
7.89
9.83
10.19
10.62
fA
Time (min)



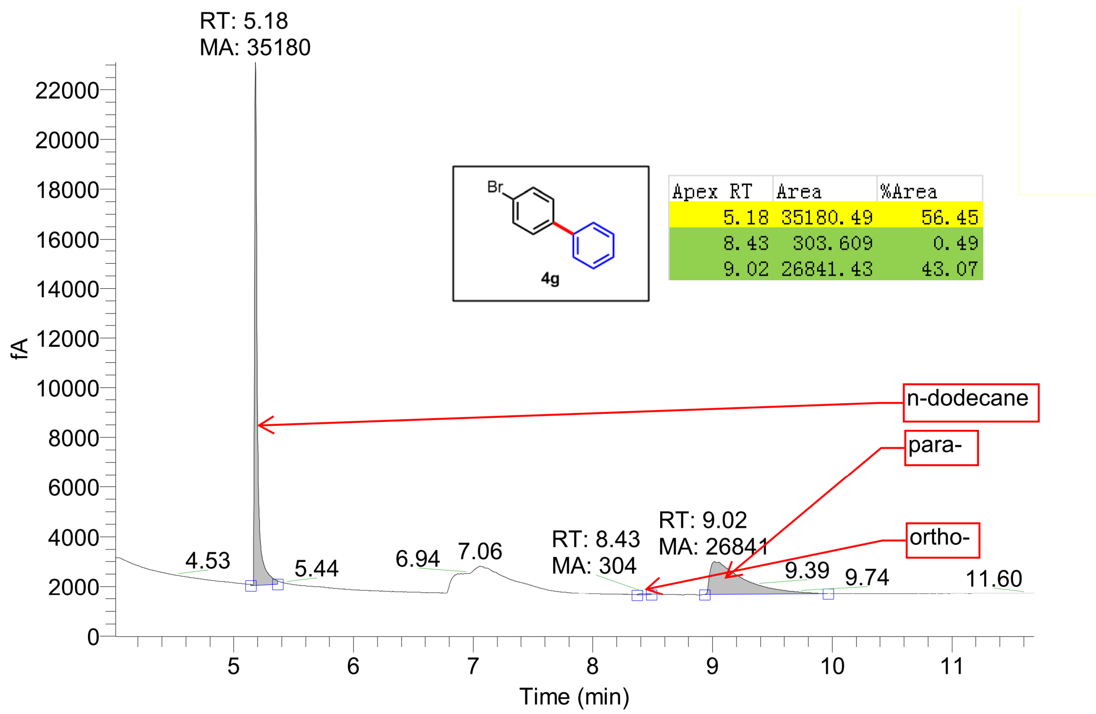
Apex RT	Area	%Area
5.17	522441.1	25.94
8.14	120083	5.96
9	1371506	68.1



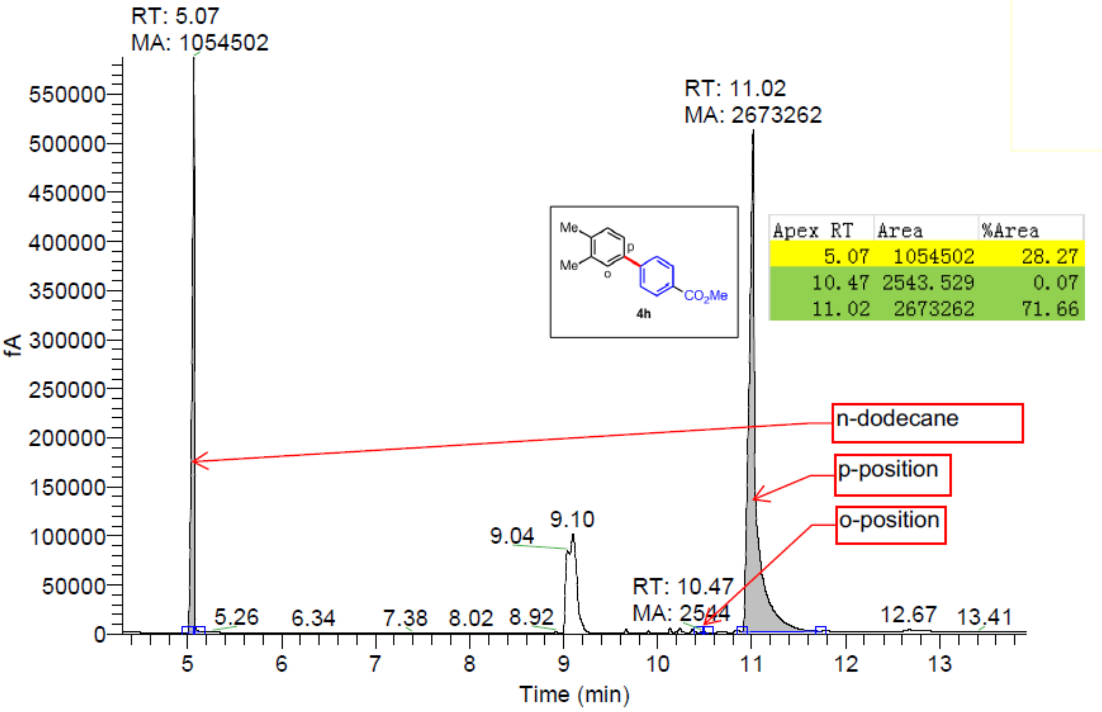
Apex RT	Area	%Area
5.22	453262.5	22.28
6.58	49250.28	2.42
6.71	1531638	75.3



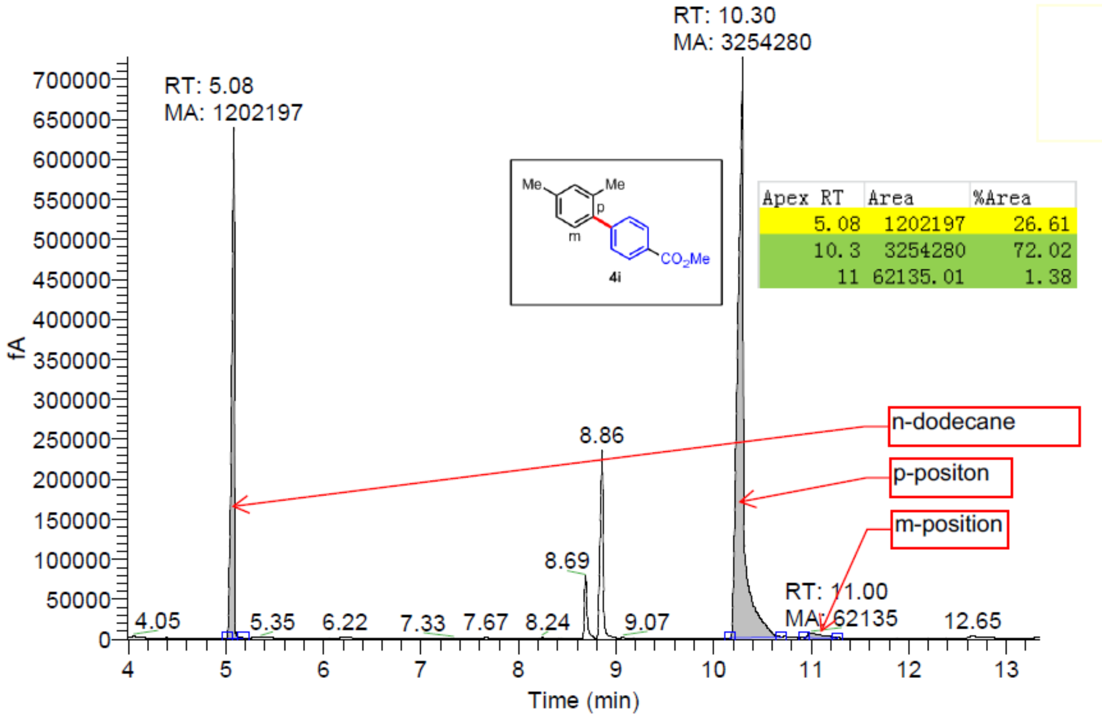
Apex RT	Area	%Area
5.22	308808.2	37.2
7.55	8834.027	1.06
8.01	6572.802	0.79
8.08	505831.5	60.94



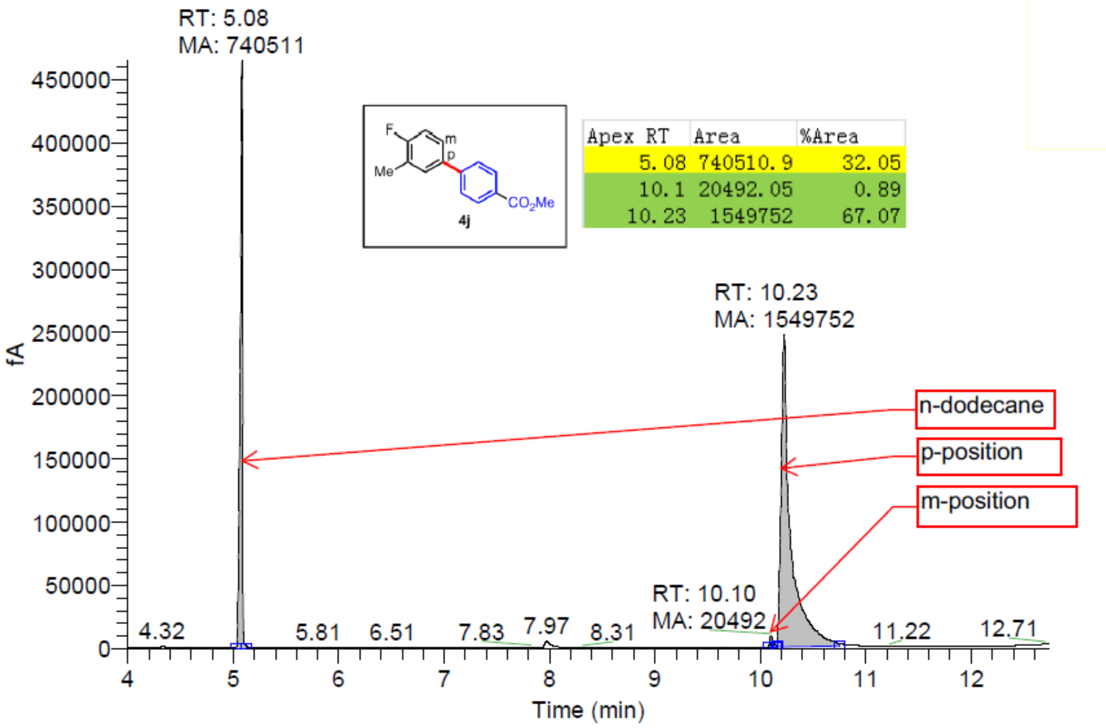
Apex RT	Area	%Area
5.18	35180.49	56.45
8.43	303.609	0.49
9.02	26841.43	43.07

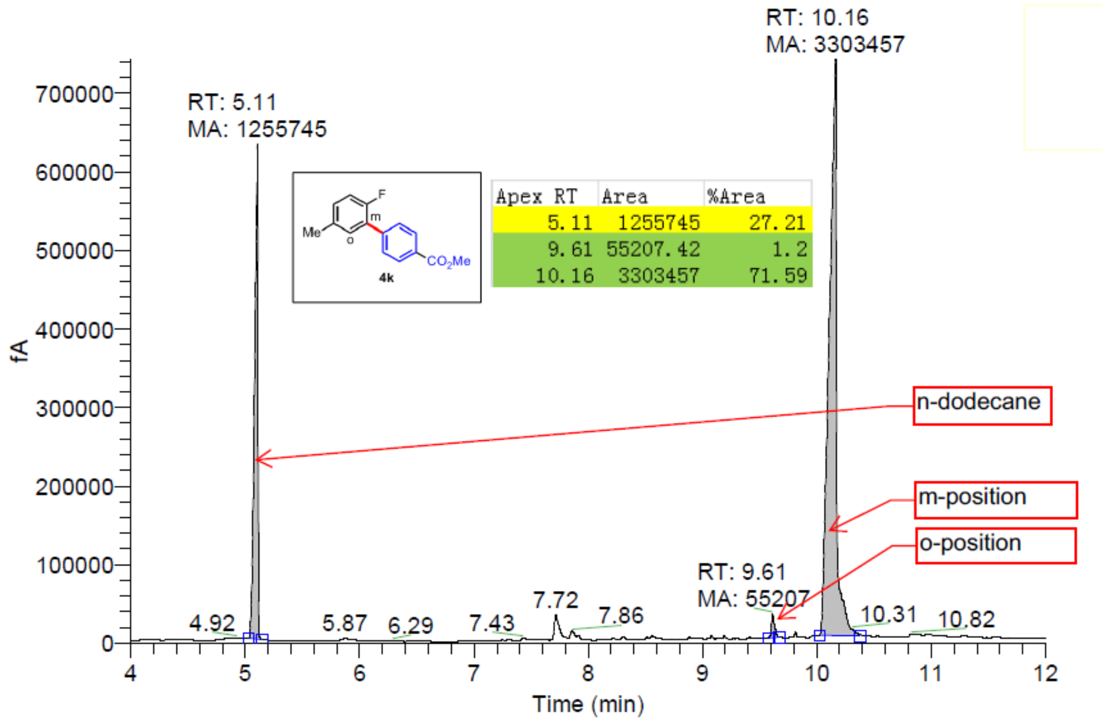


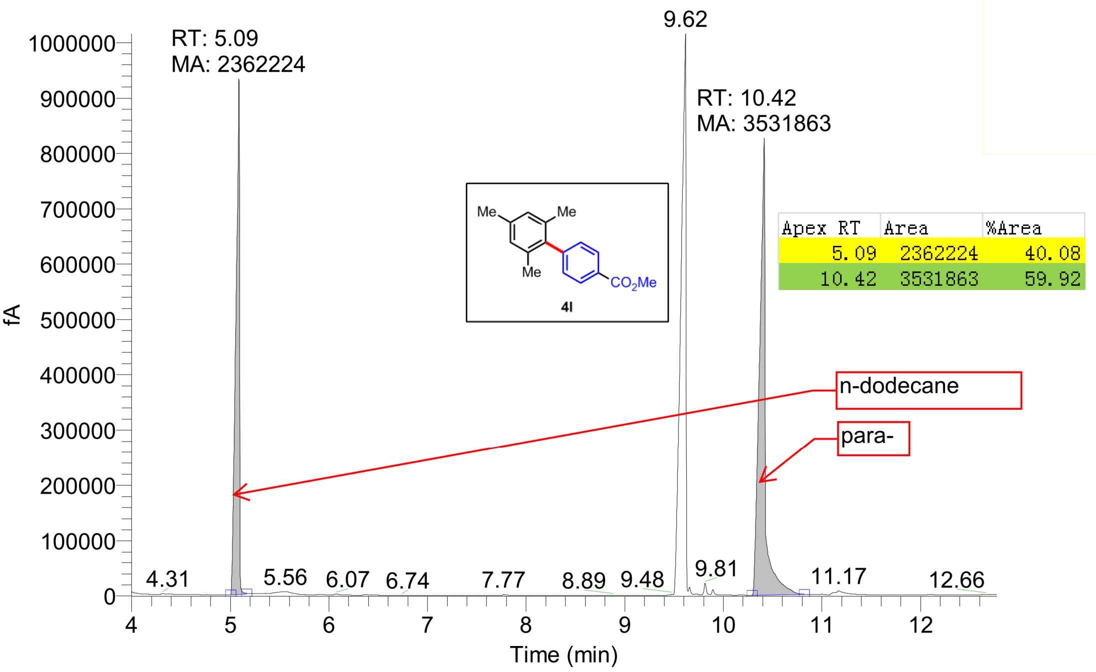
Apex RT	Area	%Area
5.07	1054502	28.27
10.47	2543.529	0.07
11.02	2673262	71.66



Apex RT	Area	%Area
5.08	1202197	26.61
10.3	3254280	72.02
11	62135.01	1.38


RT: 5.08
MA: 740511
4j
Apex RT | Area | %Area
5.08 | 740510.9 | 32.05
10.1 | 20492.05 | 0.89
10.23 | 1549752 | 67.07
RT: 10.23
MA: 1549752
n-dodecane
p-position
m-position
RT: 10.10
MA: 20492
fA
Time (min)


RT: 10.16
MA: 3303457
RT: 5.11
MA: 1255745
4k
Apex RT | Area | %Area
5.11 | 1255745 | 27.21
9.61 | 55207.42 | 1.2
10.16 | 3303457 | 71.59
n-dodecane
m-position
o-position
RT: 9.61
MA: 55207
fA
Time (min)



RT: 5.09
MA: 2362224
9.62
RT: 10.42
MA: 3531863
Me
Me
Me
CO2Me
4l
Apex RT | Area | %Area
5.09 | 2362224 | 40.08
10.42 | 3531863 | 59.92
n-dodecane
para-
fA
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.31
5.56
6.07
6.74
7.77
8.89
9.48
9.81
11.17
12.66
4
5
6
7
8
9
10
11
12
Time (min)