

Supporting Information

Rapid Room-Temperature, Chemoselective C_{sp²}–C_{sp²} Coupling of Poly(pseudo)halogenated Arenes Enabled by Palladium(I) Catalysis in Air

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1. General Information

^1H , ^{13}C and ^{19}F NMR spectra were recorded either on Varian V-NMRS 600, Varian V-NMRS 400 or Varian Mercury 300 spectrometer. ^1H and ^{13}C spectra are referenced to residual solvent signals; CDCl_3 7.26 ppm for ^1H and 77.0 ppm for ^{13}C and benzene- d_6 7.16 ppm for ^1H . Chemical shifts (δ) of ^{19}F NMR spectra are reported in ppm relative to trifluorotoluene (-62.78 ppm). Chemical shifts (δ) of ^{31}P NMR spectra are given in ppm relative to trimethyl phosphate (2.36 ppm). Coupling constants (J) are reported in Hz and coupling patterns are described as br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High resolution mass spectra (HRMS) were recorded on Thermo Scientific LTQ Orbitrap XL (ESI) or Finnigan MAT 95 (EI) spectrometer in positive ion mode. Melting points were measured with a Büchi Melting Point B-540 apparatus. Flash column chromatography was performed with Merck silica gel 60 (35–70 mesh). Thin layer chromatography (TLC) analyses were performed with aluminum sheets silica gel 60 F254 from Merck with detection by UV light.

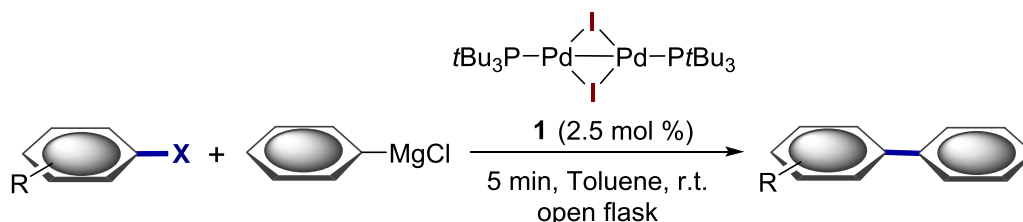
In-situ FTIR reaction analysis was performed using a Mettler-Toledo ReactIRTM 15 instrument fitted with a DST Series AgX Fiber Conduit probe.

Toluene, THF, hexane and DCM were dried by solvent purification system (Innovative Technology PS-MD-5). Unless stated otherwise, other anhydrous solvents as well as all starting materials, ligands and Pd-complexes were commercially available and used as received. Solvents used for column chromatography (pentane, hexane, ethyl acetate and DCM) were received in technical grade and distilled prior to use. $\text{Pd}^{(I)}$ -dimer^[1] and $\text{Pd}(\text{P}t\text{Bu}_3)_2$ ^[2] were prepared according to their corresponding literature procedures.

2. Experimental procedures

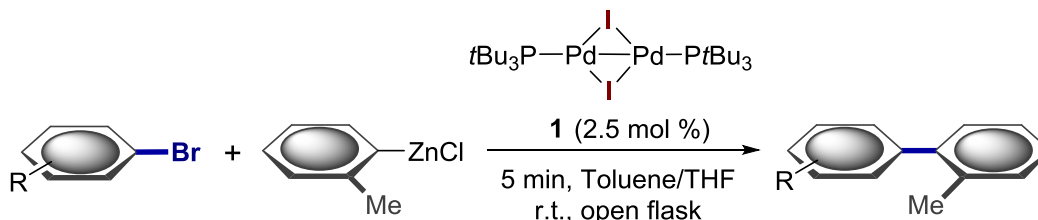
2.1. General procedure for Pd^(I)-dimer catalyzed cross-coupling reactions

2.1.1. Kumada cross-coupling reaction



To a stirred solution of aryl halide (0.2 mmol) and Pd^(I)-I-dimer (4.3 mg, 5 μmol) in 3 mL of toluene was added PhMgCl (2M in THF, 150 μL , 0.3 mmol). The reaction was stirred for 5 minutes. The reaction mixture was quenched by NH_4Cl and filtered. The filtrate was concentrated under reduced pressure and the crude material was purified by silica gel column chromatography.

2.1.2. Negishi cross-coupling reaction



To a dry 16 mL vial under Ar atmosphere were added *o*-tolyl-MgCl (1M in THF, 600 μL , 0.6 mmol) and ZnCl_2 (1M in THF, 640 μL , 0.64 mmol) and stirred for 15 minutes. Followingly, the vial was opened and a solution of aryl bromide (0.4 mmol) and Pd^(I)-I-dimer (8.7 mg, 0.01 mmol) in 1.5 mL of anhydrous toluene was added and the reaction mixture was stirred for 5 minutes. Thereafter, the reaction mixture was diluted with 3 mL of hexane and the solid residue was removed by filtration through a short plug of silica. The filtrate was concentrated under reduced pressure and the crude material was extracted with MeCN to precipitate most of the remaining Pd(I) dimer catalyst. The solution phase was filtered through a short plug of silica and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography.

Preparation of the solution of ZnCl_2 :^[3] To an oven-dried, septum-capped Schlenk flask, equipped with a stir-bar was added 2.73 g (20 mmol) of ZnCl_2 . Upon heating in vacuo at 140 $^\circ\text{C}$ for 12 hours the flask was refilled with argon and allowed to cool to room temperature. 20 mL of anhydrous THF was subsequently added and the solution stirred for 1 hour.

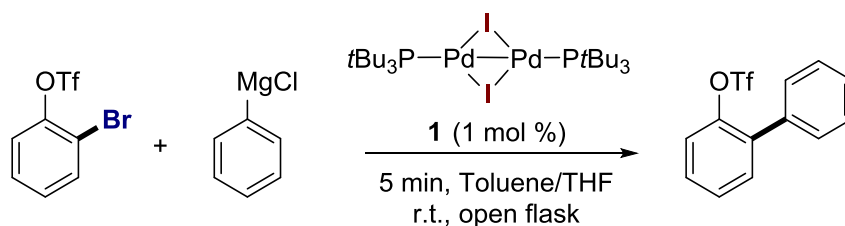
2.1.3. Coupling of a sterically challenging substrate



To a dry 4 mL vial under Ar atmosphere were added *o*-tolyl-MgCl (1M in THF, 150 μ L, 0.15 mmol) and ZnCl₂ (1M in THF, 160 μ L, 0.16 mmol) and the mixture was stirred for 15 minutes. The vial was then opened and a solution of aryl bromide (47 mg, 0.1 mmol) and Pd^(I)-I-dimer (2.2 mg, 2.5 μ mol) in 0.5 mL of anhydrous toluene was added and the reaction mixture was stirred in an open vial for 5 minutes. Conversion to the desired coupling product was thereafter determined by calibrated quantitative GC/MS analysis using mesitylene as internal standard.

2-(Adamantan-1-yl)-6-methoxy-2'-methyl-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate: Prepared using 141 mg (0.3 mmol) of 3-(Adamantan-1-yl)-4-bromo-5-methoxyphenyl trifluoromethanesulfonate. The title product was obtained after purification by column chromatography (Hexane \rightarrow 20:1 Hexane/EtOAc) as a colorless oil. 112 mg (78%). $R_f = 0.77$ (10:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 7.31 – 7.18 (m, 4H), 7.15 (s, 1H), 6.80 (s, 1H), 3.89 (s, 3H), 2.17 (s, 3H), 2.08 (br, 9H), 1.77 (br, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 158.7, 145.0, 138.7, 136.7, 135.5, 130.7, 130.0, 129.9, 128.1, 126.3, 125.5, 118.3 (q, $J = 320.2$ Hz), 104.8, 55.4, 40.5, 37.1, 37.0, 28.9, 19.9. ¹⁹F NMR (376 MHz, CDCl₃) δ -74.43. HRMS (ESI) calculated for C₂₅H₂₇F₃O₄SNa: 503.1474 [M+Na]⁺, found: 503.1456.

2.1.4. Gram-scale Kumada cross-coupling reaction

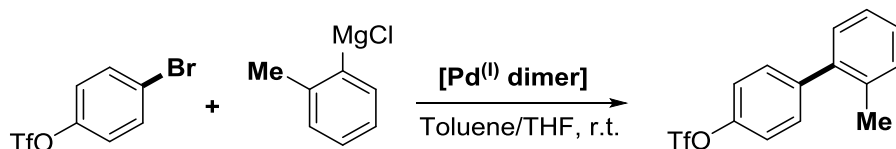


To a stirred solution of 2-Bromophenyl trifluoromethanesulfonate (1g, 3.28 mmol) and Pd^(I)-I-dimer (28 mg, 0.033 mmol) in 30 mL of toluene was added PhMgCl (1M in THF, 4.9 mL, 4.9 mmol). The reaction was stirred for 5 minutes. Thereafter, the reaction mixture was diluted with 30 mL of pentane and the solid residue was removed by filtration through a short plug of silica and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography (100% pentane) to obtain 0.940 g of 2-trifluoromethanesulfonyloxybiphenyl as a colorless oil in 95% yield.

Notes for safety:

- 1) *Organozinc and -magnesium reagents are moisture-sensitive and may react violently in air. As such, proper precautions should be taken when handling them in larger amounts.*
- 2) *Due to high rate and exothermicity of the reaction, appropriate temperature control must be considered when further scaling up the reaction.*

2.2. ReactIR studies



The ReactIR probe was immersed into a stirred solution of 4-bromophenyl triflate (61 mg, 0.2 mmol) and Pd-catalyst (Pd^(I) dimer: 4.4 mg, 5 μ mol) in 1.5 mL of anhydrous toluene. Data collection was started in the ‘rapid collect’ mode, and after 30 seconds (*o*-tolyl)MgCl (1M in THF, 300 μ L, 0.3 mmol) was added. During data acquisition, samples were also taken for GC/MS analysis, and in the end, the reaction was further analyzed by quantitative ¹⁹F NMR to determine the reaction yield.

Data analysis: Initial data treatment was undertaken using the iC IR software. The solvent background of 10:1 Toluene/THF was subtracted from the collected data. Co-addition of two spectra was used for the data obtained in the ‘rapid collect’ mode (yielding a resolution of 2 seconds per spectrum). Heights or surface areas of 2-4 peaks in the 860-720 cm^{-1} region were chosen to plot the changes in the concentrations of the starting material and the product. The raw absorption/time data were exported to MS Excel and normalized according to the obtained quantitative ¹⁹F NMR and GC/MS data to describe the changes in the reaction yield during the course of the reaction.

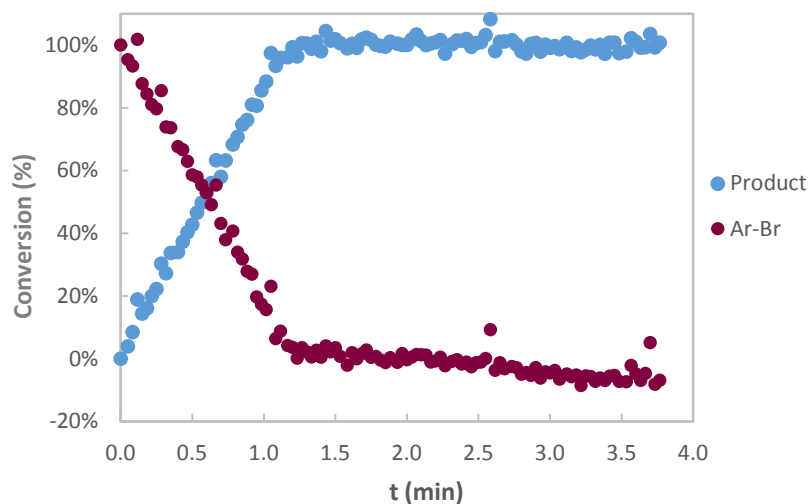
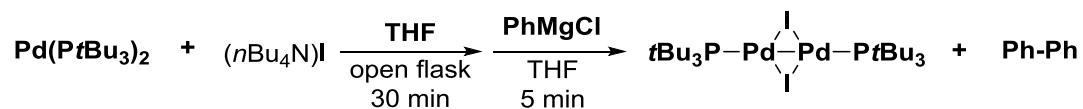


Figure S1. ReactIR traces of Pd^(I)-I dimer catalyzed Kumada cross-coupling reaction between 4-bromophenyl triflate and (*o*-tolyl)MgCl.

2.3. Mechanistic experiments

2.3.1. Oxygen-assisted formation of Pd^(I)-I dimer from Pd⁽⁰⁾



Inside an argon-filled glovebox, a mixture of Pd(PtBu₃)₂ (10 mg, 0.02 mmol) and (nBu₄N)I (74 mg, 0.2 mmol) in 1 mL of THF was prepared and taken out, to be stirred under open flask conditions. The reaction gradually turned yellow, and after 30 minutes PhMgCl (2M in THF, 20 μL, 0.04 mmol) was added, and the solution immediately turned dark brown. The mixture was subsequently qualitatively analyzed by ³¹P NMR and GC/MS.

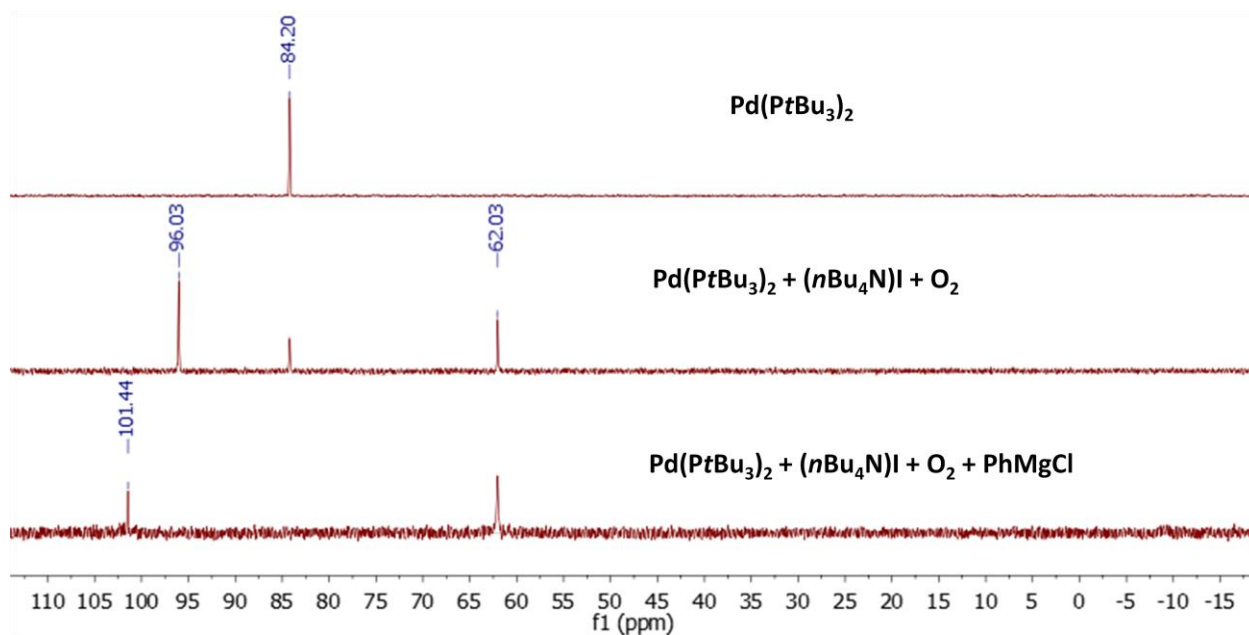
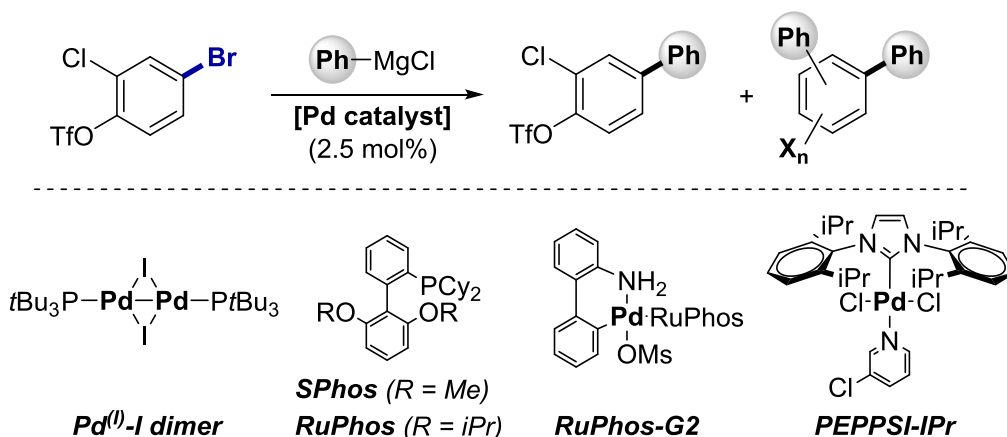


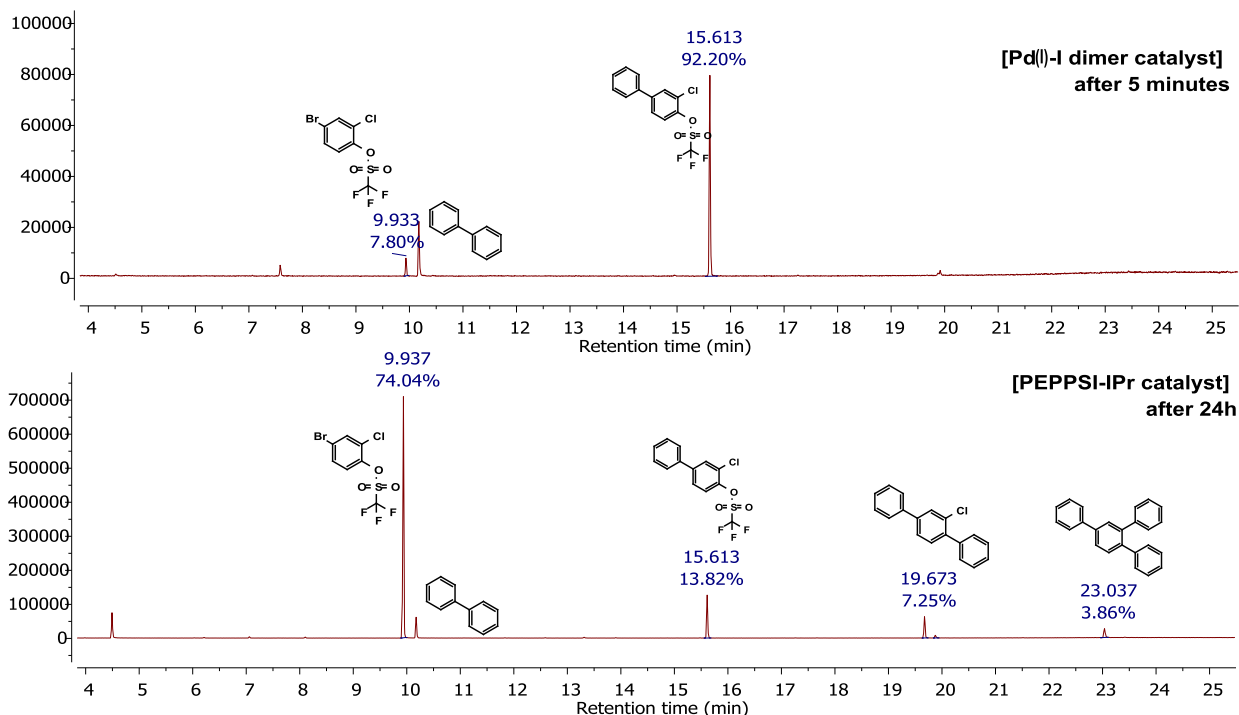
Figure S2. ³¹P NMR (121 MHz, THF) spectra of Pd(PtBu₃)₂ (top); Pd(PtBu₃)₂ + “I⁻” + PhMgCl stirred in an open flask (bottom). Signal assignments: Pd^(I)-I dimer (101.4 ppm), Pd(PtBu₃)₂ (84.2 ppm), free PtBu₃ (62.0 ppm). All shifts are reported relative to (MeO)₃PO as an internal standard (δ = 2.36 ppm). Non-quantitative ³¹P NMR.

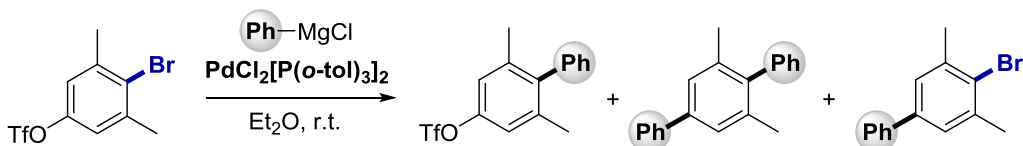
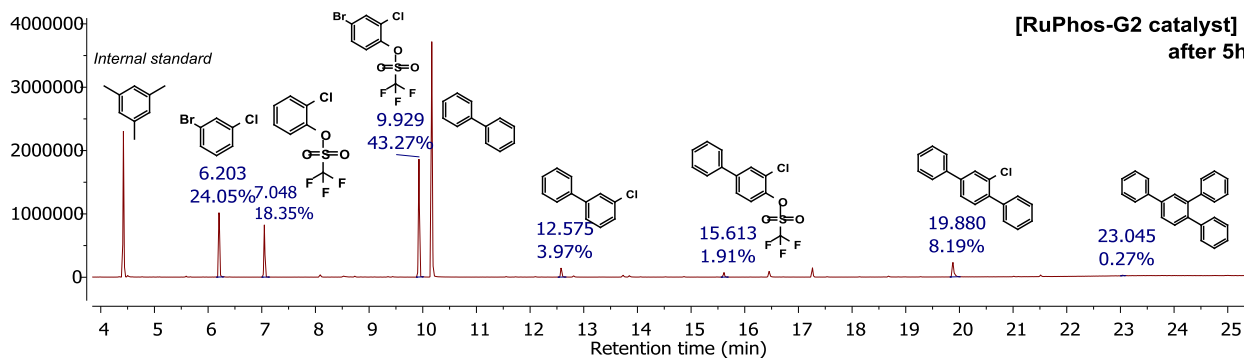
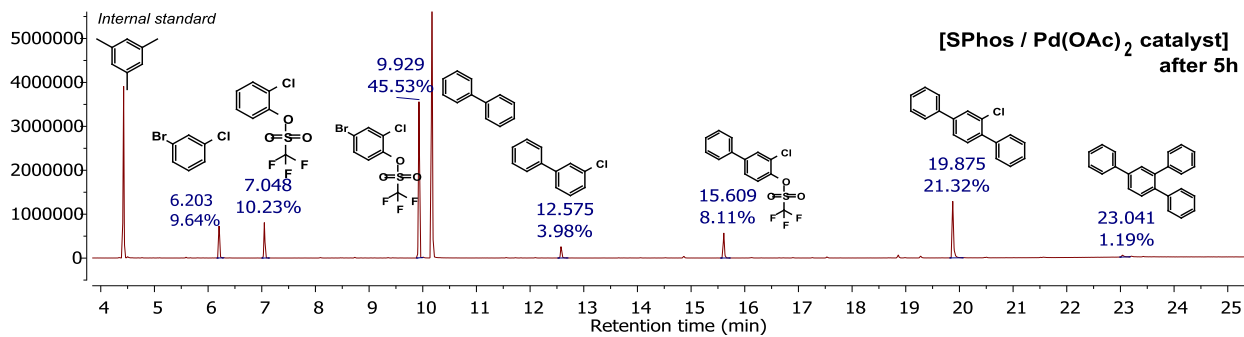
2.3.2. Performance of air-stable Pd-precatalysts



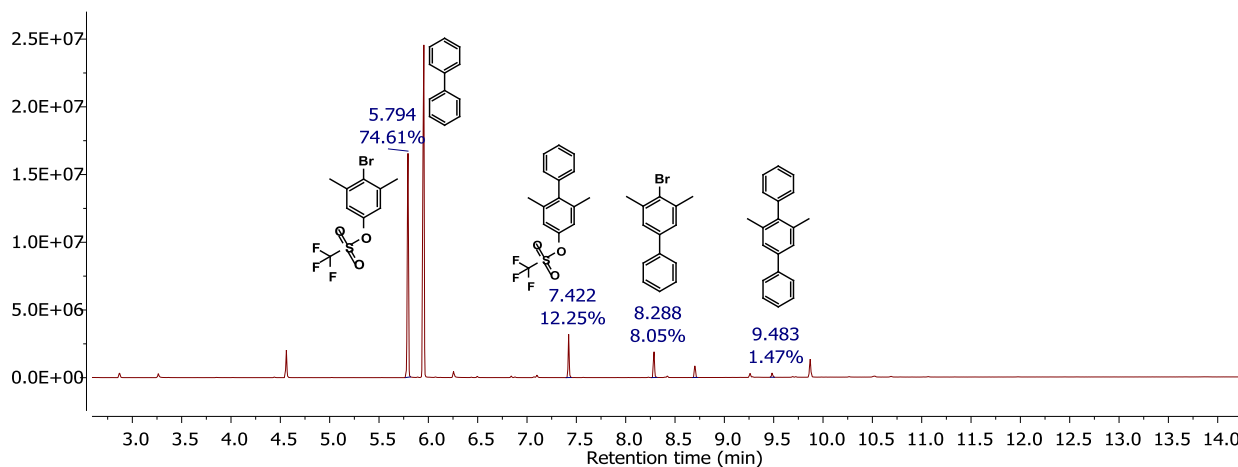
General procedure: To a solution of 4-bromo-2-chlorophenyl trifluoromethanesulfonate (34 mg, 0.1 mmol) and Pd-catalyst (2.5 μmol) in toluene (Pd^{I} -dimer) or THF (other precatalysts) was added PhMgCl (2M in THF, 75 μL , 0.15 mmol). The reactions with SPhos and RuPhos ligands were stirred under argon atmosphere and Pd^{I} -I dimer and PEPPSI-IPr catalyzed reactions were run under open flask conditions. Samples were taken at various intervals for GC/MS analysis until changes in the composition of the mixture could be not observed anymore.

As a consequence, the following chromatograms were obtained, describing the relative reactivities of the tested Pd-(pre)catalysts.





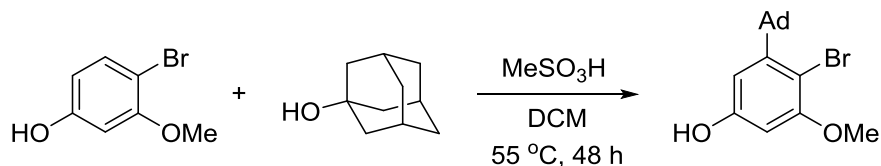
Performed following a published procedure^[4]: to a mixture of 4-bromo-3,5-dimethylphenyl trifluoromethanesulfonate (67 mg, 0.2 mmol) and PdCl₂[P(*o*-tol)₃]₂ (8 mg, 0.01 mmol) in Et₂O (0.1 mL) was added PhMgCl (1M in Et₂O, 0.4 mL, 0.4 mmol). The reaction was stirred at room temperature, under argon atmosphere for 2 hours. Thereafter, the mixture was analyzed by GC/MS and the following results were obtained:



3. Synthetic procedures

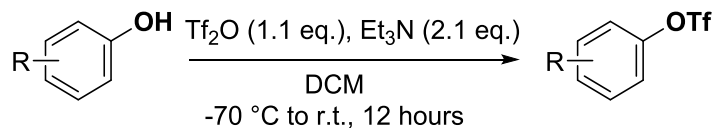
3.1. Synthesis of poly(pseudo)halogenated starting materials

3.1.1. Synthesis of 3-(adamantan-1-yl)-4-bromo-5-methoxyphenol



Performed according to a published procedure.^[5] A mixture of 4-bromo-5-methoxyphenol (950 mg, 4.68 mmol), 1-adamantanol (712 mg, 4.68 mmol) and methanesulfonic acid (200 μ L) in 3.5 mL of DCM was stirred at 55 °C for 48 hours. The resulting solution was diluted with water and extracted with EtOAc. The organic phase was washed with water, 5% aq. NaHCO₃ and brine, dried over MgSO₄ and concentrated under reduced pressure. The obtained crude material was purified by column chromatography (Hexane \rightarrow 6:1 Hexane/EtOAc) to yield the title compound as an off-white solid. 727 mg (46%). R_f = 0.21 (10:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 7.20 (s, 1H), 6.58 (s, 1H), 5.33 (s, 1H), 3.79 (s, 3H), 2.04 (br, 9H), 1.75 (br, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 159.4, 150.8, 133.0, 129.2, 100.2, 100.1, 55.2, 40.7, 37.0, 36.5, 29.0. MS (70eV, EI): *m/z* (%): 338 (84) 336 (85) [M⁺], 281 (26) 279 (26), 200 (100). These data are in agreement with those reported previously in the literature.^[5]

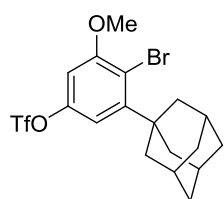
3.1.2. General procedure for the synthesis of aryl triflates



To a cooled (-70 °C) solution of a phenol derivative (9.05 mmol) and Et₃N (2.52 mL, 18.9 mmol) in DCM (20 mL) was added dropwise Tf₂O (1.74 mL, 10.3 mmol). The reaction was allowed to slowly warm to room temperature and stirred for 12 hours. Thereafter, water (or saturated aqueous NaHCO₃ in the case of basic products) was added to the mixture, followed by extraction with Et₂O. The organic layer was washed with saturated aqueous NaHCO₃ and brine, dried over Na₂SO₄ and concentrated under reduced pressure. The obtained crude material was purified by silica gel column chromatography.

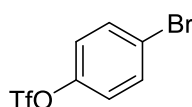
4. Characterization data

4.1. Characterization data of aryl triflates



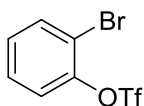
3-(Adamantan-1-yl)-4-bromo-5-methoxyphenyl trifluoromethanesulfonate:

Prepared using 500 mg (1.48 mmol) of 3-(adamantan-1-yl)-4-bromo-5-methoxyphenol. The title product was obtained after purification by column chromatography (20:1 Hexane/EtOAc) as a white solid. 494 mg (71%). $R_f = 0.36$ (Hexane). M.p. 127 - 128 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.41 (s, 1H), 6.79 (s, 1H), 3.83 (s, 3H), 2.07 (br, 3H), 2.03 (br, 6H), 1.76 (br, 6H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 158.8, 145.1, 140.7, 131.6, 118.6 (d, $J = 320.7$ Hz), 106.3, 105.5, 55.5, 40.2, 37.2, 36.8, 28.8. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -73.40. HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{20}\text{BrF}_3\text{O}_4\text{SNa}$: 491.0110 $[\text{M}+\text{Na}]^+$, found: 491.0108.



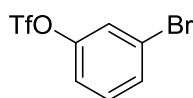
4-Bromophenyl trifluoromethanesulfonate:

Prepared using 1.57 g (9.05 mmol) of 4-bromophenol. The title product was obtained after purification by column chromatography (Hexane) as a colorless oil. 2.185 g (79%). $R_f = 0.35$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.62 - 7.54 (2H, d, $J = 9.0$ Hz), 7.21 - 7.13 (2H, d, $J = 9.0$ Hz). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 148.5, 133.4, 123.1, 122.0, 118.7 (q, $J = 321.0$ Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.79. MS (70eV, EI): m/z (%): 306 (44) 304 (42) $[\text{M}^+]$, 173 (98) 171 (100), 143 (71) 145 (69), 69 (44), 63 (47). These data are in agreement with those reported previously in the literature.^[6]



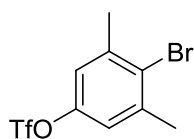
2-Bromophenyl trifluoromethanesulfonate:

Prepared using 0.80 g (4.62 mmol) of 4-bromo-2-chlorophenol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 1.13 g (80%). $R_f = 0.36$ (20:1 pentane/EtOAc). $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.73-7.67 (m, 1H), 7.44-7.33 (m, 2H), 7.31-7.22 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 147.2, 134.6, 129.6, 129.2, 123.0, 118.7 (q, $J = 321.0$ Hz), 116.1. $^{19}\text{F NMR}$ (282 MHz, CDCl_3) δ -73.40 (s). MS (70eV, EI): m/z (%): 306 (74) 304 (72) $[\text{M}^+]$, 242 (28) 240 (29) 173 (100), 171 (100) 145 (96) 143 (98), 95 (7), 92 (20), 69 (48), 63 (50). These data are in agreement with those reported previously in the literature.^[7]

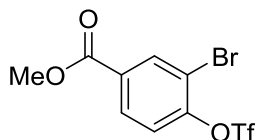


3-Bromophenyl trifluoromethanesulfonate:

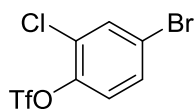
Prepared using 0.80 g (4.62 mmol) of 4-bromo-2-chlorophenol. The title product was obtained after purification by column chromatography (2:1 Pentane/EtOAc) as a colorless oil. 1.27 g (90%). $R_f = 0.35$ (2:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.55 (d, $J = 8.2$ Hz, 1H), 7.46 (d, $J = 2.2$ Hz, 1H), 7.34 (d, $J = 8.2$ Hz, 1H), 7.25 (dd, $J = 8.2, 2.2$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 149.5, 131.8, 131.2, 124.8, 123.1, 120.2, 118.6 (q, $J = 320.9$ Hz). $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -72.74. MS (70eV, EI): m/z (%): 306 (100) 304 (97) $[\text{M}^+]$, 242 (62) 240 (63) 173 (33), 171 (34) 145 (77) 143 (79), 95 (50), 92 (37), 69 (78), 63 (63). These data are in agreement with those reported previously in the literature.^[8]



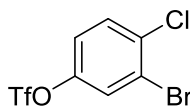
5-Bromo-4-methylpyridin-2-yl trifluoromethanesulfonate: Prepared using 0.80 g (4.00 mmol) of 4-bromo-3,5-dimethylphenol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 1.32 g (94%). $R_f = 0.42$ (2:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.01 (s, 2H), 2.45 (s, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 147.8, 141.0, 127.2, 120.7, 118.8 (q, $J = 320.8$ Hz), 24.2. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.90 (s). MS (70eV, EI): m/z (%): 334 (61), 332 (60), $[\text{M}^+]$, 201 (97) 199 (100), 173 (92), 171 (94), 92 (39), 91 (85). These data are in agreement with those reported previously in the literature.^[9]



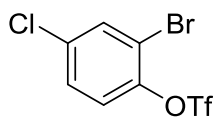
Methyl 3-bromo-4-(((trifluoromethyl)sulfonyl)oxy)benzoate: Prepared using 3.00 g (12.98 mmol) of methyl 3-bromo-4-hydroxybenzoate. The title product was obtained after purification by column chromatography (10:1 Pentane/EtOAc) as a colorless oil. 4.63 g (98%). $R_f = 0.21$ (5:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.31 (d, $J = 12.4$ Hz, 1H), 8.02 (d, $J = 8.6$ Hz, 1H), 7.40 (d, $J = 8.6$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 164.4, 150.0, 135.7, 131.4, 130.4, 122.9, 118.6 (q, $J = 320.6$ Hz), 116.1, 52.8. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.43. MS (70eV, EI): m/z (%): 369 (63), 362 (62), $[\text{M}^+]$, 333 (26) 331 (25), 269 (98), 267 (94), 269 (98), 230 (66), 229 (68), 203 (30), 201 (32), 175 (51), 173 (54). These data are in agreement with those reported previously in the literature.^[10]



4-Bromo-2-chlorophenyl trifluoromethanesulfonate: Prepared using 2.00 g (9.64 mmol) of 4-bromo-2-chlorophenol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 2.62 g (85%). $R_f = 0.25$ (5:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.70 (d, $J = 2.3$ Hz, 1H), 7.48 (dd, $J = 8.8, 2.3$ Hz, 1H), 7.24 (d, $J = 8.8$ Hz, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 145.0, 134.1, 131.7, 128.7, 124.3, 122.2, 118.7 (q, $J = 320.7$ Hz). $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.29. MS (70eV, EI): m/z (%): 340 (22), 338 (16), $[\text{M}^+]$, 207 (100) 205 (75), 179 (53), 177 (42). These data are in agreement with those reported previously in the literature.^[11]

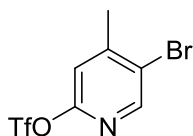


3-Bromo-4-chlorophenyl trifluoromethanesulfonate: Prepared using 900 mg (4.34 mmol) of 3-bromo-4-chlorophenol. The title product was obtained after purification by column chromatography (20:1 Hexane/EtOAc) as a colorless oil. 1038 mg (70%). $R_f = 0.47$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.58 (d, $J = 2.8$ Hz, 1H), 7.54 (d, $J = 8.9$ Hz, 1H), 7.21 (dd, $J = 8.9, 2.8$ Hz, 1H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 147.3, 135.1, 131.3, 126.7, 123.5, 121.5, 118.6 (q, $J = 320.8$ Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.65. HRMS (EI) calculated for $\text{C}_7\text{H}_3\text{BrClF}_3\text{O}_3\text{S}$: 337.8621 $[\text{M}^+]$, found: 337.8619.

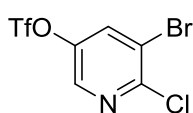


2-Bromo-4-chlorophenyl trifluoromethanesulfonate: Prepared using 1.00 g (4.82 mmol) of 2-bromo-4-chlorophenol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 1.49 g (90%). $R_f = 0.25$ (5:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.69 (d, $J = 2.4$ Hz, 1H), 7.37 (dd, J

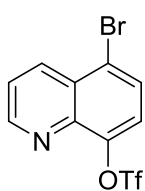
= 8.9, 2.4 Hz, 1H), 7.29 (d, $J = 8.9$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 145.6, 134.7, 134.0, 129.2, 123.6, 118.6 (q, $J = 320.6$ Hz), 116.8. ^{19}F NMR (564 MHz, CDCl_3) δ -73.31. HRMS (EI) calculated for $\text{C}_7\text{H}_3\text{BrClF}_3\text{O}_3\text{S}$: 337.8621 [M^+], found 337.8621.



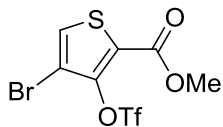
5-Bromo-4methylpyridin-2ylenyl trifluoromethanesulfonate: Prepared using 0.80 g (4.25 mmol) of 5-bromo-4-methylpyridin-2-ol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 1.32 g (94%). $R_f = 0.27$ (2:1 Pentane/EtOAc). ^1H NMR (600 MHz, CDCl_3) δ 8.42 (s, 1H), 7.08 (s, 1H), 2.48 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 154.9, 152.8, 149.8, 123.4, 118.7 (q, $J = 320.6$ Hz), 117.1, 22.9. ^{19}F NMR (564 MHz, CDCl_3) δ -73.06 (s). HRMS (ESI) calculated for $\text{C}_7\text{H}_5\text{O}_3\text{NBBrF}_3\text{SNa}$: 341.9017 [$\text{M}+\text{Na}$] $^+$, found 341.9018.



3-Bromo-5-chloropyridin-2-yl trifluoromethanesulfonate: Prepared using 0.50 g (2.40 mmol) of 5-bromo-6-chloropyridin-3-ol. The title product was obtained after purification by column chromatography (10:1 Hexane/EtOAc) as a light yellow oil. 660 mg (81%). $R_f = 0.57$ (10:1 Hexane/EtOAc). ^1H NMR (600 MHz, CDCl_3) δ 8.27 (d, $J = 2.4$ Hz, 1H), 8.08 (d, $J = 2.4$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 151.2, 145.5, 143.4, 132.3, 118.4 (q, $J = 320.9$ Hz), 111.5. ^{19}F NMR (564 MHz, CDCl_3) δ -72.88. HRMS (EI) calculated for $\text{C}_6\text{H}_2\text{BrClF}_3\text{NO}_3\text{S}$: 338.8574 [M^+], found: 338.8571.

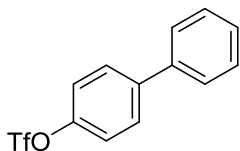


5-Bromoquinolin-8-yl trifluoromethanesulfonate: Prepared using 1.00 g (4.46 mmol) of 5-bromoquinolin-8-ol. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a white solid. 1.12 g (70%). $R_f = 0.42$ (2:1 Pentane/EtOAc). ^1H NMR (600 MHz, CDCl_3) δ 9.08 (dd, $J = 4.2, 1.4$ Hz, 1H), 8.57 (dd, $J = 8.6, 1.4$ Hz, 1H), 7.86 (d, $J = 8.3$ Hz, 1H), 7.65 (dd, $J = 8.6, 4.2$ Hz, 1H), 7.51 (d, $J = 8.3$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 152.2, 145.6, 141.6, 135.7, 129.4, 129.0, 123.7, 121.8, 121.4, 118.8 (q, $J = 320.4$ Hz). ^{19}F NMR (564 MHz, CDCl_3) δ -73.68 (s). HRMS (ESI) calculated for $\text{C}_{10}\text{H}_5\text{O}_3\text{NBBrF}_3\text{SNa}$: 377.9006 [$\text{M}+\text{Na}$] $^+$, found 377.9018. These data are in agreement with those reported previously in the literature.^[12]

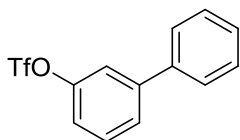


Methyl 4-bromo-3-((trifluoromethyl)sulfonyl)oxy)-2-thiophenecarboxylate: Prepared using 1.00 g (4.22 mmol) of methyl 4-bromo-3-hydroxythiophene-2-carboxylate. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 1.30 g (83%). $R_f = 0.18$ (5:1 Pentane/EtOAc). ^1H NMR (600 MHz, CDCl_3) δ 7.55 (s, 1H), 3.93 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 159.5, 143.3, 128.17, 123.5, 118.5 (q, $J = 320.9$ Hz), 106.5, 52.9. ^{19}F NMR (564 MHz, CDCl_3) δ -72.85. MS (70eV, EI): m/z (%): 370 (30), 368 (28), [M^+], 275 (53), 273 (50), 237 (38), 235 (38), 181 (42), 179 (45). These data are in agreement with those reported previously in the literature.^[13]

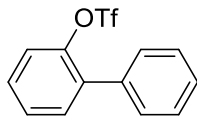
4.2. Characterization data of cross-coupling products



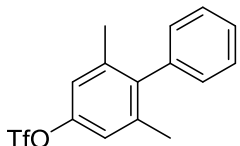
4-Trifluoromethanesulfonyloxybiphenyl: Prepared, following the Kumada cross-coupling procedure using 0.24 mmol of PhMgCl. The title product was obtained after purification by column chromatography (100% Pentane) as a white solid 49 mg (96%). $R_f = 0.19$ (20:1 Pentane/EtOAc). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.67 – 7.63 (m, 2H), 7.58–7.54 (m, 2H), 7.49–7.44 (m, 2H), 7.42–7.39 (m, 1H), 7.37–7.32 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 149.1, 141.8, 139.4, 129.1, 129.0, 128.2, 127.3, 121.8, 118.9 (q, $J = 320.7$ Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.81 (s). MS (70eV, EI): m/z (%): 302 (36) [M^+], 169 (100) 141 (52) 115 (40), 69 (13). These data are in agreement with those reported previously in the literature.^[14]



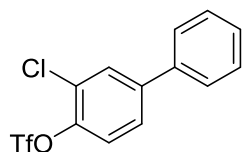
3-Trifluoromethanesulfonyloxybiphenyl: Prepared, following the Kumada cross-coupling procedure using 0.40 mmol of PhMgCl. The title product was obtained after purification by column chromatography (100% Pentane) as a colorless oil. 62 mg (85%). $R_f = 0.18$ (20:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.64 – 7.61 (m, 1H), 7.58 (dd, $J = 5.2, 3.3$ Hz, 2H), 7.52 (d, $J = 8.0$ Hz, 1H), 7.50 – 7.46 (m, 3H), 7.44 – 7.40 (m, 1H), 7.28 – 7.25 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 150.0, 143.9, 139.0, 130.5, 129.0, 128.3, 127.2, 127.0, 120.0, 119.8, 118.8 (q, $J = 320.4$ Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.85 (s). HRMS (ESI) calculated for $\text{C}_{13}\text{H}_9\text{O}_3\text{F}_3\text{SNa}$: 325.0117 [$\text{M}+\text{Na}$] $^+$, found 325.0118.



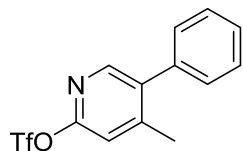
2-Trifluoromethanesulfonyloxybiphenyl: Prepared, following the Kumada cross-coupling procedure using 0.40 mmol of PhMgCl. The title product was obtained after purification by column chromatography (100% Pentane) as a colorless oil. 76 mg (93%). $R_f = 0.20$ (20:1 Pentane/EtOAc). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.50 – 7.37 (m, 9H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 146.9, 135.7, 132.1, 130.0, 129.5, 129.1, 128.6, 128.5, 128.0, 122.2, 118.5 (q, $J = 320.6$ Hz). $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -74.12 (s). MS (70eV, EI): m/z (%): 302 (36) [M^+], 169 (100) 141 (35) 115 (34), 69 (9). These data are in agreement with those reported previously in the literature.^[15]



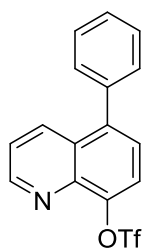
2,6-Dimethyl-1,1'-biphen-4-yl trifluoromethanesulfonate: Prepared, following the Kumada cross-coupling procedure using 0.36 mmol of PhMgCl. The title product was obtained after purification by column chromatography (100% Pentane) as a colorless oil. 68 mg (86 %). $R_f = 0.26$ (20:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.46 – 7.43 (m, 2H), 7.39 – 7.37 (m, 1H), 7.12 – 7.09 (m, 2H), 7.01 (s, 2H), 2.05 (s, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 148.1, 142.1, 139.3, 138.9, 128.72, 128.70, 127.2, 119.6, 118.9 (q, $J = 320.6$ Hz), 21.0. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.04. HRMS (EI) calculated for $\text{C}_{15}\text{H}_{13}\text{O}_3\text{F}_3\text{SNa}$: 353.0430 [M^+], found 353.0430.



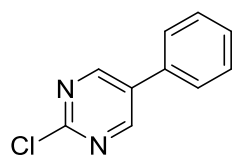
3-Chloro-1,1'-biphen-4-yl trifluoromethanesulfonate: Prepared, following the Kumada cross-coupling procedure using 0.48 mmol of PhMgCl. The title product was obtained after purification by column chromatography (100% Pentane) as a colorless oil. 54 mg (84 %). $R_f = 0.22$ (20:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.73 (d, $J = 2.2$ Hz, 1H), 7.57 – 7.52 (m, 3H), 7.50 – 7.45 (m, 2H), 7.44 – 7.40 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 144.8, 142.8, 138.1, 129.7, 129.1, 128.6, 127.4, 127.1, 126.8, 123.1, 118.6 (q, $J = 320.7$ Hz). $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.36. HRMS (EI) calculated for $\text{C}_{13}\text{H}_8\text{O}_3\text{F}_3\text{SCl}$: 335.9829 [M^+], found 335.9825.



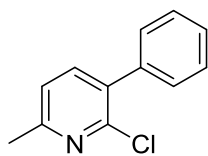
3-Chloro-1,1'-biphen-4-yl trifluoromethanesulfonate: Prepared, following the Kumada cross-coupling procedure using 0.47 mmol of PhMgCl. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a colorless oil. 51 mg (86%). $R_f = 0.22$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.20 (s, 1H), 7.50 – 7.42 (m, 3H), 7.31 – 7.28 (m, 2H), 7.09 (s, 1H), 2.36 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 155.0, 150.7, 148.3, 138.8, 136.0, 129.1, 128.7, 128.3, 118.6 (q, $J = 320.5$ Hz), 115.9, 20.4. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.20 (s). HRMS (ESI) calculated for $\text{C}_{13}\text{H}_{10}\text{O}_3\text{NF}_3\text{SNa}$: 340.0218 [$\text{M}+\text{Na}$] $^+$, found 340.0226.



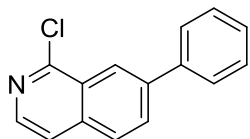
5-Phenyl-8-trifluoromethylsulfonyloxy quinoline: Prepared, following the Kumada cross-coupling procedure using 0.40 mmol of PhMgCl. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a light yellow oil. 61 mg (86 %). $R_f = 0.22$ (10:1 Pentane/EtOAc). M.p. 99 - 102 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.06 (dd, $J = 4.1, 1.6$ Hz, 1H), 8.26 (dd, $J = 8.6, 1.6$ Hz, 1H), 7.67 (d, $J = 7.9$ Hz, 1H), 7.57 – 7.47 (m, 5H), 7.46 – 7.43 (m, 2H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 151.3, 145.3, 141.23, 141.15, 138.0, 134.5, 129.9, 128.7, 128.3, 128.1, 126.3, 122.5, 120.4, 118.9 (q, $J = 320.4$ Hz), 115.2. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.81. HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{10}\text{O}_3\text{NF}_3\text{SNa}$: 376.0226 [$\text{M}+\text{Na}$] $^+$, found 376.0226.



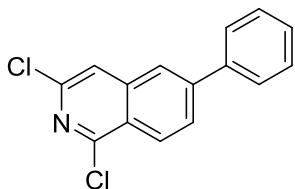
2-Chloro-5-phenylpyrimidine: Prepared, following the Kumada cross-coupling procedure using 0.39 mmol of PhMgCl. The title product was obtained after purification by preparative HPLC (9:1 Pentane/EtOAc) as a white solid. 36 mg (95 %). $R_f = 0.18$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.83 (s, 2H), 7.59–7.48 (m, 5H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 160.3, 157.6, 133.2, 133.1, 129.7, 129.5, 127.1. MS (70eV, EI): m/z (%): 192 (33), 190 (100), [M^+], 155 (14) 128 (9), 102 (55). These data are in agreement with those reported previously in the literature.^[16]



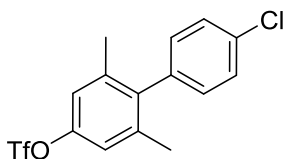
6-Chloro-5-phenyl-2-methylpyridine: Prepared, following the Kumada cross-coupling procedure using 0.29 mmol of PhMgCl. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a dark yellow oil. 38 mg (96 %). $R_f = 0.18$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.56 (d, $J = 7.7$ Hz, 1H), 7.47 – 7.38 (m, 5H), 7.15 (d, $J = 7.7$ Hz, 1H), 2.59 (s, 3H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 158.2, 148.7, 140.1, 137.7, 133.9, 129.5, 128.4, 128.2, 122.3, 24.0. HRMS (EI) calculated for $\text{C}_{12}\text{H}_{10}\text{NCl}$: 203.0496 [M^+], found 203.0495.



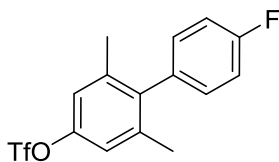
1-Chloro-4-phenylisoquinoline: Prepared, following the Kumada cross-coupling procedure using 0.30 mmol of PhMgCl. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a yellow oil. 38 mg (95 %). $R_f = 0.27$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.52 – 8.51 (m, 1H), 8.28 (d, $J = 5.6$ Hz, 1H), 8.02 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.92 (d, $J = 8.5$ Hz, 1H), 7.76 – 7.71 (m, 2H), 7.63 (d, $J = 5.6$ Hz, 1H), 7.56 – 7.50 (m, 2H), 7.47 – 7.42 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 151.7, 141.5, 141.4, 139.9, 136.8, 130.9, 129.1, 128.2, 127.5, 127.3, 124.1, 120.5. HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{11}\text{NCl}$: 240.0574 $[\text{M}+\text{H}]^+$, found 240.0575.



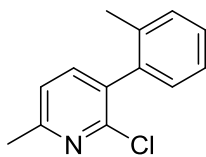
1,3-Dichloro-6-phenylisoquinoline: Prepared, following the Kumada cross-coupling procedure using 0.30 mmol of PhMgCl. The title product was obtained after purification by column chromatography (20:1 Pentane/EtOAc) as a white solid. 50 mg (92 %). $R_f = 0.30$ (10:1 Pentane/EtOAc). M.p. 103 - 107 °C. $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 8.34 (d, $J = 9.1$ Hz, 1H), 7.97 – 7.88 (m, 2H), 7.75 – 7.64 (m, 3H), 7.56 – 7.50 (m, 2H), 7.48 – 7.42 (m, 1H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 151.0, 145.1, 143.7, 139.8, 139.2, 129.3, 129.0, 128.8, 127.7, 127.3, 124.9, 123.9, 120.0. HRMS (EI) calculated for $\text{C}_{15}\text{H}_9\text{NCl}_2$: 273.0113 $[\text{M}^+]$, found 273.0107.



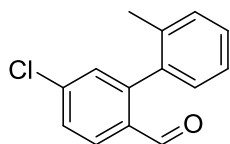
4'-Chloro-2,6-dimethyl-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate: Prepared, following the Kumada cross-coupling procedure using 0.57 mmol of (*p*-Chloro)PhMgBr. The title product was obtained after purification by column chromatography (100:1 Pentane/EtOAc) as a colorless oil. 64 mg (92 %). $R_f = 0.27$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.44 (d, $J = 8.5$ Hz, 2H), 7.06 (d, $J = 8.5$ Hz, 2H), 7.02 (s, 2H), 2.05 (s, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 148.3, 140.8, 138.9, 137.7, 133.3, 130.2, 129.0, 119.8, 118.7 (q, $J = 320.8$ Hz), 21.0. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.04 (s). HRMS (EI) calculated for $\text{C}_{15}\text{H}_{12}\text{O}_3\text{ClF}_3\text{S}$: 364.0142 $[\text{M}^+]$, found 364.0144.



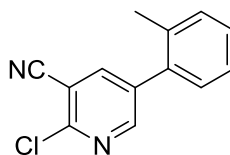
4'-Fluoro-2,6-dimethyl-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate: Prepared, following the Kumada cross-coupling procedure using 0.57 mmol of (*p*-Fluoro)PhMgBr. The title product was obtained after purification by column chromatography (100:1 Pentane/EtOAc) as a colorless oil. 55 mg (94 %). $R_f = 0.29$ (10:1 Pentane/EtOAc). $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 7.15 (d, $J = 8.7$ Hz, 2H), 7.08 (d, $J = 8.7$ Hz, 2H), 7.01 (s, 2H), 2.05 (s, 6H). $^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 162.0 (d, $J_{\text{C-F}} = 246.5$ Hz), 161.2, 148.2, 141.0, 139.1, 135.1 (d, $J_{\text{C-F}} = 3.2$ Hz), 130.4 (d, $J_{\text{C-F}} = 7.9$ Hz, 2C), 119.7, 118.7 (q, $J = 320.5$ Hz), 115.8 (d, $J_{\text{C-F}} = 21.4$ Hz, 2C), 21.0. $^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -73.05 (s, 3F), -115.09 (m, 1F). HRMS (EI) calculated for $\text{C}_{15}\text{H}_{12}\text{O}_3\text{F}_4\text{S}$: 348.0438 $[\text{M}^+]$, found 348.0435.



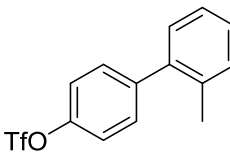
2-Chloro-6-methyl-3-(2-methylphenyl)pyridine: Prepared, following the Negishi cross-coupling procedure using 0.52 mmol of *o*-tolyl-MgCl and 0.56 mmol of ZnCl₂. The title product was obtained after purification by column chromatography (100:1 → 20:1 Hexane/EtOAc) as an orange oil. 79 mg (91%). R_f = 0.26 (20:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 7.46 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.21 (m, 3H), 7.20 – 7.08 (m, 2H), 2.60 (s, 3H), 2.14 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 158.2, 149.4, 139.8, 137.3, 136.2, 133.6, 130.0, 129.4, 128.3, 125.7, 121.8, 23.9, 19.8. HRMS (ESI) calculated for C₁₃H₁₃ClN: 218.0731 [M+H]⁺, found: 218.0728.



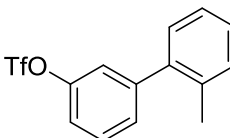
4-Chloro-2-(2-methylphenyl)benzaldehyde: Prepared, following the Negishi cross-coupling procedure using 0.52 mmol of *o*-tolyl-MgCl and 0.56 mmol of ZnCl₂. The title product was obtained after purification by column chromatography (100:1 → 50:1 → 30:1 Hexane/EtOAc) as a dark yellow oil. 64 mg (70%). R_f = 0.70 (5:1 Hexane/EtOAc). ¹H NMR (600 MHz, CDCl₃) δ 9.68 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.48 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.37 – 7.34 (m, 1H), 7.32 (d, *J* = 2.1 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.18 (d, *J* = 7.5 Hz, 1H), 2.12 (s, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 191.0, 147.0, 140.0, 136.0, 136.0, 132.2, 130.7, 130.2, 129.9, 128.7, 128.6, 128.3, 125.8, 20.2. HRMS (ESI) calculated for C₁₄H₁₁ClONa: 253.0391 [M+Na]⁺, found: 253.0389.



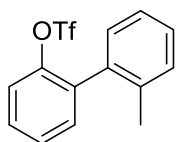
2-Chloro-3-cyano-5-(2-methylphenyl)pyridine: The title product was obtained after purification by column chromatography (100:1 → 20:1 Hexane/EtOAc; 100% DCM) as a white solid. 65 mg (71%). R_f = 0.19 (20:1 Hexane/EtOAc). M.p. 132 - 134 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.56 (d, *J* = 2.4 Hz, 1H), 7.96 (d, *J* = 2.4 Hz, 1H), 7.40 – 7.29 (m, 3H), 7.18 (m, 1H), 2.28 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 152.8, 151.0, 142.6, 136.6, 135.4, 134.4, 131.0, 129.6, 129.4, 126.6, 114.6, 110.3, 20.2. HRMS (ESI) calculated for C₁₃H₉ClN₂Na: 251.0347 [M+Na]⁺, found: 251.0337.



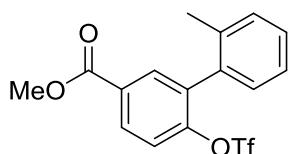
2'-Methyl-[1,1'-biphenyl]-4-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (30:1 Hexane/EtOAc) as a colorless oil. 122 mg (97%). R_f = 0.13 (Hexane). ¹H NMR (400 MHz, CDCl₃) δ 7.40 (d, *J* = 8.9 Hz, 2H), 7.36 – 7.24 (m, 5H), 7.21 (d, *J* = 7.2 Hz, 1H), 2.27 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 148.5, 142.4, 139.9, 135.2, 131.0, 130.5, 129.6, 127.9, 126.0, 121.0, 118.8 (d, *J* = 320.8 Hz), 20.3. ¹⁹F NMR (376 MHz, CDCl₃) δ -72.88. MS (70eV, EI): *m/z* (%): 316 (60) [M⁺], 183 (100), 153 (24), 128 (15), 69 (10). These data are in agreement with those reported previously in the literature.^[17]



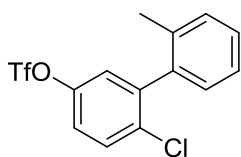
2'-Methyl-[1,1'-biphenyl]-3-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (100:1 Hexane/EtOAc) as a colorless oil. 119 mg (94%). R_f = 0.19 (Hexane). ¹H NMR (400 MHz, CDCl₃) δ 7.56 – 7.46 (m, 1H), 7.37 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.35 – 7.24 (m, 5H), 7.22 (d, *J* = 7.2 Hz, 1H), 2.28 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 149.3, 144.5, 139.6, 135.2, 130.6, 129.9, 129.6, 129.2, 128.1, 126.0, 122.1, 119.6, 118.8 (q, *J* = 320.8 Hz), 20.2. ¹⁹F NMR (376 MHz, CDCl₃) δ -72.86. HRMS (ESI) calculated for C₁₄H₁₁F₃O₃SNa: 339.0273 [M+Na]⁺, found: 339.0262.



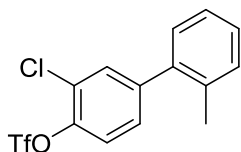
2'-Methyl-[1,1'-biphenyl]-2-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (100:1 Hexane/EtOAc) as a colorless oil. 119 mg (94%). $R_f = 0.21$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.49 – 7.42 (m, 1H), 7.41 – 7.35 (m, 2H), 7.37 – 7.23 (m, 3H), 7.22 (m, 1H), 2.18 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 147.0, 136.4, 135.5, 134.9, 132.3, 130.3, 130.1, 129.1, 128.6, 128.2, 125.6, 121.6, 118.3 (q, $J = 320.4$ Hz), 19.8. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -74.42. HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{11}\text{F}_3\text{O}_3\text{SNa}$: 339.0273 $[\text{M}+\text{Na}]^+$, found: 339.0265.



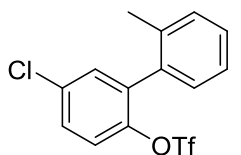
Methyl 2'-methyl-6-(trifluoromethylsulfonyloxy)-[1,1'-biphenyl]-3-carboxylate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (Hexane \rightarrow 100:1 \rightarrow 20:1 Hexane/EtOAc) as a orange oil. 135 mg (91%). $R_f = 0.25$ (20:1 Hexane/EtOAc). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.14 (dd, $J = 8.6, 2.2$ Hz, 1H), 8.09 (d, $J = 2.2$ Hz, 1H), 7.46 (d, $J = 8.6$ Hz, 1H), 7.40 – 7.25 (m, 3H), 7.21 (m, 1H), 3.94 (s, 3H), 2.16 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 165.5, 149.9, 136.3, 135.7, 134.0, 133.7, 130.5, 130.2, 130.2, 130.2, 128.9, 125.8, 121.8, 118.2 (q, $J = 320.5$ Hz), 52.5, 19.7. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -74.25. HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{14}\text{F}_3\text{O}_5\text{S}$: 375.0509 $[\text{M}+\text{H}]^+$, found: 375.0493.



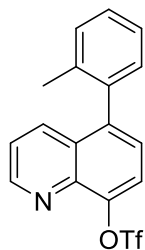
4-Chloro-3-(2-methylphenyl)phenyl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (50:1 Hexane/EtOAc) as a colorless oil. 129 mg (92%). $R_f = 0.16$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.56 (d, $J = 8.8$ Hz, 1H), 7.40 – 7.23 (m, 4H), 7.20 (d, $J = 2.9$ Hz, 1H), 7.14 (d, $J = 7.5$ Hz, 1H), 2.13 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 147.6, 142.8, 137.4, 135.9, 133.6, 131.0, 130.1, 129.1, 128.7, 125.8, 123.9, 121.4, 118.7 (q, $J = 321.0$ Hz), 19.6. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -72.68. HRMS (EI) calculated for $\text{C}_{14}\text{H}_{10}\text{ClF}_3\text{O}_3\text{S}$: 349.9986 $[\text{M}^+]$, found: 349.9981.



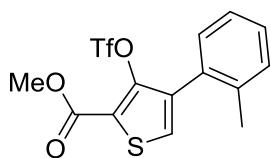
2-Chloro-4-(2-methylphenyl)phenyl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (100:1 Hexane/EtOAc) as a colorless oil. 133 mg (95%). $R_f = 0.21$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.43 (dd, $J = 8.8, 2.6$ Hz, 1H), 7.38 (d, $J = 2.6$ Hz, 1H), 7.30 (m, 4H), 7.19 (m, 1H), 2.18 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.4, 137.2, 136.3, 133.9, 133.7, 132.1, 130.2, 130.1, 129.1, 129.0, 125.8, 122.9, 118.2 (q, $J = 320.4$ Hz), 19.7. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -74.24. HRMS (EI) calculated for $\text{C}_{14}\text{H}_{10}\text{ClF}_3\text{O}_3\text{S}$: 349.9986 $[\text{M}^+]$, found: 349.9989.



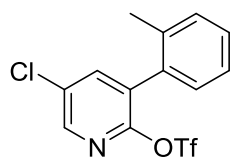
4-Chloro-2-(2-methylphenyl)phenyl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (50:1 Hexane/EtOAc) as a colorless oil. 137 mg (98%). $R_f = 0.16$ (Hexane). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.50 (d, $J = 2.1$ Hz, 1H), 7.41 (d, $J = 8.5$ Hz, 1H), 7.34 – 7.27 (m, 4H), 7.20 (m, 1H), 2.28 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 144.5, 143.5, 138.7, 135.1, 131.8, 130.6, 129.5, 129.1, 128.4, 126.8, 126.1, 122.5, 118.6 (q, $J = 320.6$ Hz), 20.3. $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -73.43. HRMS (EI) calculated for $\text{C}_{14}\text{H}_{10}\text{ClF}_3\text{O}_3\text{S}$: 349.9986 $[\text{M}^+]$, found: 349.9990.



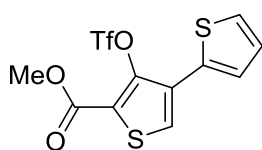
5-(2-Methylphenyl)quinolin-8-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure using 0.44 mmol of *o*-tolyl-MgCl and 0.48 mmol of ZnCl₂. The title product was obtained after purification by column chromatography (20:1 → 10:1 Hexane/EtOAc) as an orange oil. 114 mg (78%). R_f = 0.40 (5:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 9.05 (dd, *J* = 4.2, 1.7 Hz, 1H), 7.83 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.30 (m, 5H), 7.21 (m, 1H), 2.01 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 151.4, 145.3, 141.0, 140.8, 137.3, 136.5, 134.5, 130.3, 130.2, 128.6, 128.5, 126.3, 125.9, 122.5, 120.4, 118.9 (q, *J* = 320.8 Hz), 20.1. ¹⁹F NMR (376 MHz, CDCl₃) δ -73.81. HRMS (ESI) calculated for C₁₇H₁₃F₃NO₃S: 368.0563 [M+H]⁺, found: 368.0549.



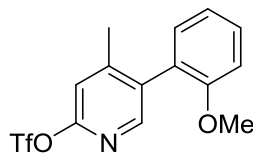
Methyl 4-(2-methylphenyl)-3-(trifluoromethylsulfonyloxy)thiophene-2-carboxylate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (50:1 Hexane/EtOAc) as a white solid. 125 mg (82%). R_f = 0.37 (10:1 Hexane/EtOAc). M.p. 81 - 83 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.43 (s, 1H), 7.36 – 7.27 (m, 2H), 7.25 – 7.18 (m, 2H), 3.96 (s, 3H), 2.24 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.3, 143.4, 136.8, 136.7, 131.0, 130.6, 130.3, 129.1, 128.2, 125.8, 122.9, 117.9 (q, *J* = 320.9 Hz), 52.5, 19.8. ¹⁹F NMR (376 MHz, CDCl₃) δ -74.50. HRMS (ESI) calculated for C₁₄H₁₁F₃O₅S₂Na: 402.9892 [M+Na]⁺, found: 402.9872.



5-Chloro-3-(2-methylphenyl)pyridin-2-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure. The title product was obtained after purification by column chromatography (50:1 Hexane/EtOAc) as a colorless oil. 127 mg (91%). R_f = 0.39 (20:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 2.6 Hz, 1H), 7.77 (d, *J* = 2.6 Hz, 1H), 7.44 – 7.27 (m, 3H), 7.17 (d, *J* = 7.5 Hz, 1H), 2.18 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 151.5, 145.9, 141.5, 136.1, 131.9, 131.8, 130.6, 130.5, 129.7, 129.6, 126.1, 118.2 (q, *J* = 320.6 Hz), 19.7. ¹⁹F NMR (376 MHz, CDCl₃) δ -73.70. HRMS (ESI) calculated for C₁₃H₁₀ClF₃NO₃S: 352.0017 [M+H]⁺, found: 352.0008.



Methyl 4'-(trifluoromethylsulfonyloxy)-[2,3'-bithiophene]-5'-carboxylate: Prepared, following the Negishi cross-coupling procedure using 0.6 mmol of (2-thienyl)MgBr and 0.64 mmol of ZnCl₂. The title product was obtained after purification by column chromatography (50:1 → 20:1 → 10:1 Hexane/EtOAc) as a light orange solid. 128 mg (86%). R_f = 0.31 (10:1 Hexane/EtOAc). M.p. 83 - 85 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.53 (s, 1H), 7.39 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.23 (dd, *J* = 3.6, 0.9 Hz, 2H), 7.11 (dd, *J* = 5.1, 3.6 Hz, 1H), 3.96 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.2, 142.4, 132.2, 130.0, 127.8, 127.0, 126.7, 123.9, 118.1 (q, *J* = 320.9 Hz), 52.6. ¹⁹F NMR (376 MHz, CDCl₃) δ -74.38. HRMS (ESI) calculated for C₁₁H₇O₅F₃S₃: 371.9402 [M]⁺, found: 371.9403.



5-(2-methoxyphenyl)-4-methylpyridin-2-yl trifluoromethanesulfonate: Prepared, following the Negishi cross-coupling procedure using 0.8 mmol of (2-methoxyphenyl)MgBr and 0.88 mmol of ZnCl₂. The title product was obtained after purification by column chromatography (50:1 → 20:1 → 10:1 Hexane/EtOAc) as a yellow oil. 119 mg (86%). R_f = 0.29 (10:1 Hexane/EtOAc). ¹H NMR (400 MHz, CDCl₃) δ 8.13 (s, 1H), 7.47 – 7.38 (m, 1H), 7.18 – 7.11 (m, 1H), 7.09 – 7.03 (m, 2H), 7.00 (d, *J* = 8.3 Hz, 1H), 3.78 (s, 3H), 2.23 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 156.7, 155.1, 152.3, 148.6, 135.9, 130.9, 130.1, 124.8, 120.8, 118.6 (q, *J* = 320.5 Hz), 115.2, 110.8, 55.3, 19.9. ¹⁹F NMR (376 MHz, CDCl₃) δ -73.30. HRMS (ESI) calculated for C₁₄H₁₂O₄NF₃S: 347.0434 [M]⁺, found: 347.0431.

5. Computational details

All calculations were performed using Gaussian 09 software.^[18] Structural optimizations and frequency calculations were performed with ω B97XD method along with 6-31G(d) basis set and the SDD ECP on Pd. Single point energy calculations were performed with M06 and def2-TZVP basis set. Solvent effects of toluene were included using the CPCM solvation model. Frequency calculations were performed to confirm whether the structure is a minimum or a transition state and IRC calculations were performed to confirm whether the located transition state connect the correct minima.

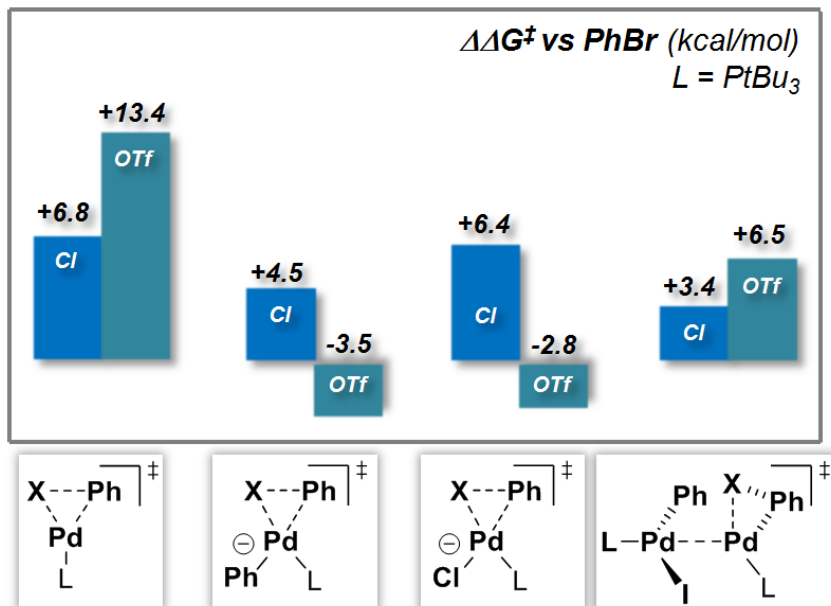


Figure S3. Comparison of C-Br vs C-Cl vs C-OTf oxidative addition selectivity with PtBu₃-ligated Pd⁽⁰⁾ and Pd^(I) complexes. Calculated at the CPCM (Toluene) M06/def2-TZVP // ω B97XD/6-31G(d) SDD level of theory.

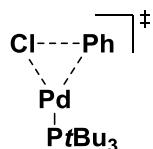
Cartesian coordinates of computed structures

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C	-2.733483000000	0.093138000000	-0.009290000000
Br	-2.251556000000	-2.084967000000	0.000282000000
C	-3.172870000000	0.618221000000	1.215404000000
C	-3.199207000000	0.607233000000	-1.228572000000
C	-4.023964000000	1.720380000000	1.205725000000
C	2.179176000000	1.706636000000	-0.991070000000
C	2.231028000000	0.338398000000	1.806060000000
C	2.456276000000	-1.389373000000	-0.776696000000
C	-4.462883000000	2.265914000000	0.000097000000
C	-4.049967000000	1.709866000000	-1.209743000000
C	1.418927000000	-0.637396000000	2.685327000000
C	1.864057000000	1.742935000000	2.320130000000
C	3.613607000000	2.195269000000	-0.738006000000
C	2.014461000000	1.429402000000	-2.497010000000

C	3.940157000000	-1.241543000000	-1.146310000000
C	1.657483000000	-1.792560000000	-2.034983000000
C	2.303702000000	-2.574793000000	0.194420000000
C	1.191643000000	2.853343000000	-0.683072000000
C	3.730324000000	0.105530000000	2.046750000000
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H	-2.901587000000	0.144694000000	-2.163741000000
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H	2.026574000000	1.770574000000	3.404715000000
H	2.480114000000	2.532637000000	1.885170000000
H	0.808602000000	1.973538000000	2.138586000000
H	4.360623000000	1.420330000000	-0.926570000000
H	3.831333000000	3.032974000000	-1.413244000000
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H	2.139034000000	2.374492000000	-3.039761000000
H	2.760220000000	0.733911000000	-2.887282000000
H	1.015136000000	1.044192000000	-2.726849000000
H	4.317199000000	-2.207276000000	-1.507208000000
H	4.097604000000	-0.516753000000	-1.949148000000
H	4.558405000000	-0.944794000000	-0.295365000000
H	1.711730000000	-1.059526000000	-2.839321000000
H	2.070251000000	-2.732767000000	-2.423192000000
H	0.602107000000	-1.958849000000	-1.795695000000
H	2.597873000000	-3.492090000000	-0.330362000000
H	2.944746000000	-2.491110000000	1.074686000000
H	1.264246000000	-2.698596000000	0.516399000000
H	1.428881000000	3.705033000000	-1.333766000000
H	1.240564000000	3.208708000000	0.345686000000
H	0.157927000000	2.550506000000	-0.886803000000
H	4.361112000000	0.757628000000	1.437437000000
H	4.025075000000	-0.929047000000	1.854751000000
H	3.959568000000	0.314080000000	3.099868000000
H	-4.402194000000	2.127632000000	-2.148627000000

Zero-point correction=	0.469825 (Hartree/Particle)
Thermal correction to Energy=	0.495695
Thermal correction to Enthalpy=	0.496640
Thermal correction to Gibbs Free Energy=	0.414737
Sum of electronic and zero-point Energies=	-3745.232217
Sum of electronic and thermal Energies=	-3745.206347
Sum of electronic and thermal Enthalpies=	-3745.205403
Sum of electronic and thermal Free Energies=	-3745.287305

CPCM (Toluene) M06/def2TZVP E = -3748.27105597

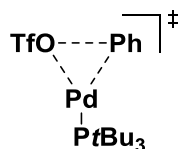


C	-2.877727000000	0.340982000000	-0.006453000000
C	-3.410266000000	-0.085151000000	-1.228713000000
C	-3.396419000000	-0.099554000000	1.216938000000
Pd	-0.895957000000	0.313863000000	-0.019355000000
H	-3.040915000000	0.331374000000	-2.160154000000
C	-4.421929000000	-1.042886000000	-1.213711000000
H	-3.016978000000	0.307022000000	2.148838000000
C	-4.408580000000	-1.056496000000	1.202650000000
P	1.447284000000	-0.125852000000	-0.005098000000
C	-4.918808000000	-1.529826000000	-0.005512000000
H	-4.831741000000	-1.400732000000	-2.153989000000
H	-4.808098000000	-1.424657000000	2.143395000000
C	1.966534000000	-0.733630000000	1.736732000000

C	1.867998000000	-1.493205000000	-1.280581000000
C	2.453700000000	1.447617000000	-0.433697000000
C	3.472769000000	-0.715460000000	2.039893000000
C	1.227090000000	0.122518000000	2.788237000000
C	1.444445000000	-2.166884000000	1.951611000000
C	0.757688000000	-2.564483000000	-1.221096000000
C	1.784005000000	-0.902856000000	-2.700196000000
C	3.236463000000	-2.171778000000	-1.114491000000
C	2.383015000000	2.422544000000	0.756332000000
C	3.928468000000	1.220291000000	-0.799846000000
C	1.748176000000	2.178543000000	-1.596240000000
H	4.054668000000	-1.290281000000	1.315054000000
H	3.879116000000	0.298206000000	2.075888000000
H	3.642775000000	-1.163744000000	3.027418000000
H	0.142902000000	0.077221000000	2.636454000000
H	1.448376000000	-0.279031000000	3.785602000000
H	1.519562000000	1.171616000000	2.785367000000
H	1.574639000000	-2.427179000000	3.009307000000
H	0.376221000000	-2.247044000000	1.722331000000
H	1.988955000000	-2.913405000000	1.369808000000
H	0.728100000000	-3.113453000000	-0.280576000000
H	-0.230033000000	-2.116140000000	-1.380716000000
H	0.929684000000	-3.296299000000	-2.021006000000
H	2.610173000000	-0.227383000000	-2.930963000000
H	1.829835000000	-1.726378000000	-3.423541000000
H	0.838448000000	-0.374077000000	-2.861219000000
H	3.387233000000	-2.882238000000	-1.937592000000
H	4.062996000000	-1.457317000000	-1.140663000000
H	3.308817000000	-2.740264000000	-0.184131000000
H	1.348801000000	2.593715000000	1.073573000000
H	2.972238000000	2.092763000000	1.614663000000
H	2.794102000000	3.388019000000	0.437100000000
H	4.043485000000	0.672434000000	-1.738726000000
H	4.415465000000	2.194471000000	-0.936445000000
H	4.478694000000	0.684210000000	-0.022591000000
H	1.778363000000	1.631290000000	-2.537952000000
H	0.700709000000	2.387999000000	-1.356161000000
H	2.255706000000	3.137476000000	-1.761966000000
Cl	-2.175380000000	2.400410000000	0.006146000000
H	-5.715786000000	-2.266793000000	-0.005220000000

Zero-point correction=	0.469693 (Hartree/Particle)
Thermal correction to Energy=	0.495563
Thermal correction to Enthalpy=	0.496508
Thermal correction to Gibbs Free Energy=	0.415082
Sum of electronic and zero-point Energies=	-1633.964516
Sum of electronic and thermal Energies=	-1633.938646
Sum of electronic and thermal Enthalpies=	-1633.937702
Sum of electronic and thermal Free Energies=	-1634.019127

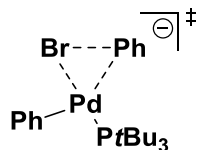
CPCM (Toluene) M06/def2TZVP E = -1634.38828698



C	1.328587000000	4.436856000000	-0.446967000000
C	1.770645000000	2.162080000000	-1.157635000000
C	1.670018000000	1.782096000000	0.188984000000
C	1.512700000000	2.700063000000	1.236315000000
H	1.559258000000	2.373620000000	2.269541000000
Pd	0.181300000000	0.553674000000	0.193856000000
H	2.038796000000	1.438743000000	-1.919731000000
C	1.308765000000	4.034636000000	0.890604000000
C	1.563323000000	3.510258000000	-1.460523000000
H	1.149510000000	4.767505000000	1.676180000000

H	1.613471000000	3.834237000000	-2.496037000000
O	3.159244000000	0.565987000000	0.654822000000
S	2.897979000000	-0.901608000000	0.861884000000
O	3.656319000000	-1.515947000000	1.931878000000
O	1.444148000000	-1.215155000000	0.815107000000
C	3.514455000000	-1.631056000000	-0.717170000000
F	3.289778000000	-2.940122000000	-0.733650000000
F	4.812814000000	-1.406311000000	-0.863877000000
F	2.863511000000	-1.076633000000	-1.749824000000
H	-1.681607000000	2.512179000000	-0.829194000000
C	-2.750970000000	2.306633000000	-0.702450000000
C	-3.093141000000	0.853635000000	-1.101089000000
H	-3.305181000000	2.988211000000	-1.360448000000
H	-3.019955000000	2.554220000000	0.323498000000
C	-4.614735000000	0.652199000000	-1.022122000000
P	-2.043504000000	-0.332763000000	-0.024849000000
C	-2.658673000000	0.730066000000	-2.573549000000
H	-4.915626000000	-0.367690000000	-1.274572000000
H	-5.014701000000	0.889193000000	-0.033138000000
H	-5.103279000000	1.327040000000	-1.736624000000
C	-1.995112000000	-2.056621000000	-0.854065000000
C	-2.853468000000	-0.489963000000	1.699887000000
H	-3.131741000000	1.540379000000	-3.141977000000
H	-1.574576000000	0.840512000000	-2.685975000000
H	-2.968903000000	-0.209245000000	-3.035419000000
C	-0.944599000000	-2.014473000000	-1.985266000000
C	-1.459607000000	-3.094945000000	0.150898000000
C	-3.333466000000	-2.560714000000	-1.414985000000
C	-3.202888000000	0.912361000000	2.231938000000
C	-4.113859000000	-1.366576000000	1.765311000000
C	-1.794372000000	-1.040784000000	2.679574000000
H	-1.190607000000	-1.321030000000	-2.788966000000
H	0.042991000000	-1.751820000000	-1.593356000000
H	-0.870324000000	-3.015435000000	-2.429157000000
H	-2.174468000000	-3.329883000000	0.942394000000
H	-1.268014000000	-4.028591000000	-0.392384000000
H	-0.513414000000	-2.776601000000	0.598944000000
H	-3.197177000000	-3.579611000000	-1.799208000000
H	-4.117021000000	-2.598068000000	-0.653989000000
H	-3.695197000000	-1.951058000000	-2.246776000000
H	-2.344778000000	1.591156000000	2.174937000000
H	-4.050784000000	1.369012000000	1.716981000000
H	-3.479590000000	0.820492000000	3.289321000000
H	-3.898809000000	-2.418795000000	1.565004000000
H	-4.536313000000	-1.311153000000	2.776803000000
H	-4.888715000000	-1.039191000000	1.067810000000
H	-1.447742000000	-2.043795000000	2.437296000000
H	-0.915069000000	-0.388972000000	2.719855000000
H	-2.234812000000	-1.076947000000	3.684159000000
H	1.185261000000	5.483592000000	-0.694990000000

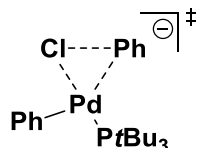
Zero-point correction=	0.496990 (Hartree/Particle)
Thermal correction to Energy=	0.529880
Thermal correction to Enthalpy=	0.530824
Thermal correction to Gibbs Free Energy=	0.432605
Sum of electronic and zero-point Energies=	-2134.981452
Sum of electronic and thermal Energies=	-2134.948562
Sum of electronic and thermal Enthalpies=	-2134.947618
Sum of electronic and thermal Free Energies=	-2135.045838
CPCM (Toluene) M06/def2TZVP E =	-2135.68378565



C	-3.442037000000	2.163036000000	2.255249000000
C	-2.907579000000	-0.105311000000	1.548838000000
C	-2.228334000000	0.406255000000	0.421829000000
C	-2.275042000000	1.804683000000	0.161453000000
H	-2.068125000000	2.189285000000	-0.835865000000
Pd	-0.297200000000	0.727898000000	0.029814000000
Br	-3.163930000000	-0.626568000000	-1.780449000000
H	-2.939873000000	-1.175523000000	1.724093000000
C	-2.870287000000	2.670439000000	1.106839000000
C	-3.466302000000	0.767640000000	2.461597000000
H	-2.923758000000	3.735055000000	0.890122000000
H	-3.913902000000	0.369441000000	3.370737000000
C	0.836155000000	-4.200971000000	0.210649000000
C	0.114209000000	-2.923666000000	-0.257321000000
H	0.823495000000	-4.303210000000	1.299718000000
H	0.297897000000	-5.068143000000	-0.195648000000
H	1.871381000000	-4.274300000000	-0.126518000000
P	0.990410000000	-1.252230000000	0.148358000000
C	-1.295643000000	-2.932657000000	0.362053000000
C	-0.124668000000	-3.013106000000	-1.777032000000
C	2.539464000000	-1.162842000000	-0.999453000000
C	1.626670000000	-1.392993000000	1.960378000000
H	-1.921472000000	-2.160533000000	-0.088473000000
H	-1.758238000000	-3.903741000000	0.137012000000
H	-1.296872000000	-2.815473000000	1.444725000000
H	-0.798393000000	-3.858588000000	-1.967272000000
H	-0.630867000000	-2.117695000000	-2.152594000000
H	0.790589000000	-3.194116000000	-2.346023000000
C	2.063584000000	-0.623149000000	-2.363922000000
C	3.548374000000	-0.124748000000	-0.471922000000
C	3.308723000000	-2.474817000000	-1.232414000000
C	0.486193000000	-1.863135000000	2.882936000000
C	2.836806000000	-2.315338000000	2.185404000000
C	1.986793000000	0.018798000000	2.459432000000
H	1.345510000000	-1.273237000000	-2.862863000000
H	1.605950000000	0.359490000000	-2.245105000000
H	2.935927000000	-0.516904000000	-3.023834000000
H	4.069447000000	-0.456771000000	0.429960000000
H	4.312663000000	0.031260000000	-1.245431000000
H	3.073144000000	0.839146000000	-0.280237000000
H	4.188930000000	-2.253004000000	-1.851725000000
H	3.670998000000	-2.924855000000	-0.304128000000
H	2.719963000000	-3.220410000000	-1.771173000000
H	-0.428270000000	-1.283333000000	2.719757000000
H	0.799075000000	-1.706561000000	3.924297000000
H	3.743659000000	-1.930644000000	1.713367000000
H	3.036363000000	-2.377504000000	3.264363000000
H	2.670339000000	-3.332037000000	1.824440000000
H	2.728155000000	0.525745000000	1.843896000000
H	1.094894000000	0.651742000000	2.485164000000
H	2.387190000000	-0.060806000000	3.480429000000
H	0.259775000000	-2.925927000000	2.770706000000
C	1.125998000000	2.273176000000	-0.261331000000
C	1.766845000000	3.001897000000	0.760919000000
C	1.281695000000	2.821212000000	-1.553177000000
C	2.526569000000	4.148154000000	0.521287000000
C	2.033243000000	3.967768000000	-1.814045000000
C	2.672959000000	4.637827000000	-0.774080000000
H	1.671049000000	2.670658000000	1.793722000000
H	0.788644000000	2.341014000000	-2.399498000000
H	3.003154000000	4.664139000000	1.354270000000
H	2.117042000000	4.340783000000	-2.834109000000

H 3.264386000000 5.530141000000 -0.968239000000
H -3.903609000000 2.826536000000 2.981867000000

Zero-point correction= 0.558884 (Hartree/Particle)
Thermal correction to Energy= 0.590252
Thermal correction to Enthalpy= 0.591196
Thermal correction to Gibbs Free Energy= 0.498364
Sum of electronic and zero-point Energies= -3976.714783
Sum of electronic and thermal Energies= -3976.683415
Sum of electronic and thermal Enthalpies= -3976.682471
Sum of electronic and thermal Free Energies= -3976.775303
CPCM (Toluene) M06/def2TZVP E = -3979.86060938

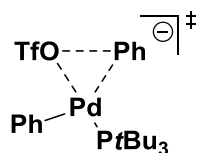


C -3.442037000000 2.163036000000 2.255249000000
C -3.331262000000 -3.106739000000 1.420668000000
C -0.952131000000 -3.169607000000 0.906799000000
C -1.144201000000 -2.192322000000 -0.091259000000
C -2.463004000000 -1.766113000000 -0.399854000000
H -2.673759000000 -1.274191000000 -1.348932000000
Pd -0.813438000000 -0.229113000000 -0.142759000000
Cl -0.345718000000 -3.095406000000 -2.315201000000
H 0.042599000000 -3.553994000000 1.106668000000
C -3.545784000000 -2.220438000000 0.384165000000
C -2.028550000000 -3.585553000000 1.667142000000
H -4.555832000000 -1.909787000000 0.126106000000
H -1.861828000000 -4.281799000000 2.487510000000
C 4.192086000000 -0.843373000000 0.034552000000
C 2.753543000000 -1.021951000000 -0.485866000000
H 4.268812000000 -1.050331000000 1.105985000000
H 4.833751000000 -1.573839000000 -0.476570000000
H 4.613125000000 0.145851000000 -0.152313000000
P 1.473206000000 0.291416000000 0.108790000000
C 2.284223000000 -2.432959000000 -0.083886000000
C 2.774869000000 -1.043682000000 -2.026479000000
C 1.925453000000 1.937403000000 -0.793308000000
C 1.787628000000 0.560334000000 1.988662000000
H 1.356869000000 -2.692646000000 -0.598745000000
H 3.051482000000 -3.147655000000 -0.412652000000
H 2.159035000000 -2.564082000000 0.990219000000
H 3.347472000000 -1.924042000000 -2.345419000000
H 1.765783000000 -1.163374000000 -2.435143000000
H 3.260057000000 -0.167325000000 -2.463576000000
C 1.283380000000 1.882782000000 -2.194504000000
C 1.274535000000 3.139781000000 -0.083927000000
C 3.422810000000 2.250136000000 -0.952545000000
C 1.831230000000 -0.799530000000 2.710327000000
C 3.057523000000 1.344808000000 2.359949000000
C 0.568483000000 1.288505000000 2.583846000000
H 1.686077000000 1.093152000000 -2.828183000000
H 0.205977000000 1.736641000000 -2.113574000000
H 1.460197000000 2.842481000000 -2.699859000000
H 1.747985000000 3.376650000000 0.872382000000
H 1.393600000000 4.021249000000 -0.728198000000
H 0.205058000000 2.987196000000 0.070618000000
H 3.521643000000 3.236040000000 -1.427419000000
H 3.949016000000 2.295963000000 0.004647000000
H 3.937318000000 1.533267000000 -1.595912000000
H 0.982236000000 -1.429910000000 2.425887000000
H 1.765090000000 -0.617894000000 3.791712000000
H 3.007552000000 2.388699000000 2.041583000000
H 3.162712000000 1.346937000000 3.453910000000

H	3.966677000000	0.905575000000	1.944604000000
H	0.354424000000	2.245851000000	2.110687000000
H	-0.326315000000	0.667503000000	2.485537000000
H	0.752379000000	1.468280000000	3.652804000000
H	2.758837000000	-1.348174000000	2.531092000000
C	-1.795848000000	1.650790000000	-0.139901000000
C	-2.303341000000	2.299569000000	1.003998000000
C	-2.224199000000	2.208401000000	-1.364255000000
C	-3.126784000000	3.424900000000	0.942917000000
C	-3.048795000000	3.331152000000	-1.447653000000
C	-3.500282000000	3.957141000000	-0.288518000000
H	-2.054224000000	1.914457000000	1.991358000000
H	-1.910206000000	1.746013000000	-2.300733000000
H	-3.483204000000	3.885279000000	1.863764000000
H	-3.341396000000	3.716922000000	-2.423444000000
H	-4.138909000000	4.836268000000	-0.343630000000
H	-4.162344000000	-3.461990000000	2.024299000000

Zero-point correction=	0.560413 (Hartree/Particle)
Thermal correction to Energy=	0.591182
Thermal correction to Enthalpy=	0.592126
Thermal correction to Gibbs Free Energy=	0.501656
Sum of electronic and zero-point Energies=	-1865.452518
Sum of electronic and thermal Energies=	-1865.421749
Sum of electronic and thermal Enthalpies=	-1865.420805
Sum of electronic and thermal Free Energies=	-1865.511275

CPCM (Toluene) M06/def2TZVP E = -1865.98455186

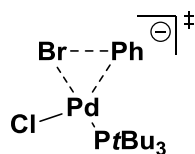


C	-1.073146000000	2.819971000000	3.118062000000
C	-1.416910000000	0.428540000000	2.802974000000
C	-1.422522000000	0.624157000000	1.389167000000
C	-1.387670000000	1.961230000000	0.855448000000
H	-1.842584000000	2.184947000000	-0.105244000000
H	-1.545386000000	-0.575972000000	3.195586000000
C	-1.217827000000	3.044416000000	1.776469000000
C	-1.177725000000	1.493217000000	3.629008000000
H	-1.239090000000	4.058436000000	1.384928000000
H	-1.063974000000	1.323274000000	4.697836000000
O	-2.888955000000	-0.392980000000	0.892302000000
S	-3.999631000000	-0.022111000000	-0.067854000000
O	-5.180060000000	-0.843907000000	0.148540000000
O	-4.174218000000	1.407374000000	-0.273365000000
C	-3.320048000000	-0.632305000000	-1.672438000000
F	-4.181991000000	-0.388105000000	-2.662730000000
F	-3.104231000000	-1.950365000000	-1.624731000000
F	-2.163018000000	-0.032530000000	-1.973915000000
H	2.163206000000	-4.381205000000	-0.131831000000
C	1.248989000000	-4.222730000000	0.443564000000
C	0.489955000000	-2.944884000000	0.046034000000
H	1.508695000000	-4.232777000000	1.505437000000
H	0.594777000000	-5.087686000000	0.267079000000
P	1.491443000000	-1.300360000000	0.088569000000
C	-0.737393000000	-2.807175000000	0.966772000000
C	-0.089390000000	-3.142843000000	-1.366540000000
C	2.713500000000	-1.364468000000	-1.404175000000
C	2.556816000000	-1.336460000000	1.694599000000
H	-1.394049000000	-1.999220000000	0.645085000000
H	-1.307072000000	-3.745950000000	0.925065000000
H	-0.480738000000	-2.627887000000	2.010682000000
H	-0.859432000000	-3.923229000000	-1.321965000000

H	-0.572224000000	-2.233804000000	-1.732774000000
H	0.659310000000	-3.467255000000	-2.093115000000
C	1.934937000000	-0.933695000000	-2.664124000000
C	3.818515000000	-0.305214000000	-1.224785000000
C	3.395136000000	-2.713620000000	-1.689323000000
C	1.682868000000	-1.712025000000	2.905450000000
C	3.777720000000	-2.271260000000	1.684331000000
C	3.030240000000	0.103397000000	1.978608000000
H	1.169067000000	-1.647945000000	-2.966223000000
H	1.464196000000	0.038453000000	-2.511041000000
H	2.644199000000	-0.838482000000	-3.497830000000
H	4.533725000000	-0.562160000000	-0.439718000000
H	4.383612000000	-0.238392000000	-2.164209000000
H	3.398899000000	0.682460000000	-1.022619000000
H	4.112171000000	-2.575718000000	-2.510512000000
H	3.952649000000	-3.098247000000	-0.831758000000
H	2.687891000000	-3.482176000000	-2.010498000000
H	0.781263000000	-1.094879000000	2.952574000000
H	1.398445000000	-2.766772000000	2.920006000000
H	2.261974000000	-1.521220000000	3.819350000000
H	4.534765000000	-1.962067000000	0.960450000000
H	4.250448000000	-2.242793000000	2.675877000000
H	3.513412000000	-3.311392000000	1.478135000000
H	3.600397000000	0.546834000000	1.163273000000
H	2.170544000000	0.753817000000	2.168286000000
H	3.665664000000	0.095511000000	2.875953000000
Pd	0.213980000000	0.697692000000	0.207131000000
C	1.447669000000	2.150924000000	-0.705724000000
C	1.240893000000	2.538261000000	-2.046154000000
C	2.381272000000	2.940643000000	-0.004533000000
C	1.929893000000	3.589404000000	-2.652825000000
C	3.082618000000	3.994162000000	-0.593182000000
C	2.867907000000	4.322255000000	-1.929942000000
H	0.504781000000	2.003587000000	-2.647784000000
H	2.570203000000	2.733029000000	1.048142000000
H	1.730300000000	3.837952000000	-3.694492000000
H	3.796578000000	4.566434000000	-0.001620000000
H	3.411859000000	5.141412000000	-2.395566000000
H	-0.927894000000	3.648119000000	3.806289000000

Zero-point correction=	0.588592 (Hartree/Particle)
Thermal correction to Energy=	0.626071
Thermal correction to Enthalpy=	0.627015
Thermal correction to Gibbs Free Energy=	0.521457
Sum of electronic and zero-point Energies=	-2366.496160
Sum of electronic and thermal Energies=	-2366.458682
Sum of electronic and thermal Enthalpies=	-2366.457738
Sum of electronic and thermal Free Energies=	-2366.563296

CPCM (Toluene) M06/def2TZVP E = -2367.3053651

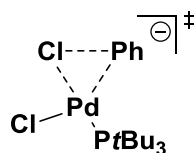


C	4.067924000000	-1.676878000000	1.576572000000
C	2.528015000000	0.203606000000	1.695839000000
C	2.201438000000	-0.007033000000	0.343530000000
C	2.890686000000	-0.974214000000	-0.422221000000
H	2.846750000000	-0.962533000000	-1.508414000000
Pd	0.578320000000	-0.854276000000	-0.452764000000
Br	2.467477000000	2.212876000000	-0.983587000000
H	2.042347000000	0.987678000000	2.263543000000
C	3.806549000000	-1.826721000000	0.228035000000
C	3.432173000000	-0.650323000000	2.299707000000
H	4.340499000000	-2.570186000000	-0.358180000000

H	3.635777000000	-0.535555000000	3.362463000000
Cl	-0.071115000000	-2.859194000000	-1.750087000000
C	-2.687181000000	2.522808000000	1.466480000000
C	-1.458140000000	2.021824000000	0.686544000000
H	-2.734304000000	2.093791000000	2.471567000000
H	-2.596747000000	3.610753000000	1.589039000000
H	-3.637777000000	2.328092000000	0.967086000000
P	-1.471953000000	0.162218000000	0.186650000000
C	-0.212081000000	2.316603000000	1.542781000000
C	-1.271612000000	2.887312000000	-0.575358000000
C	-2.773487000000	-0.015927000000	-1.224207000000
C	-2.108580000000	-0.839064000000	1.700205000000
H	0.698104000000	2.165858000000	0.960257000000
H	-0.241520000000	3.376270000000	1.832323000000
H	-0.161301000000	1.730300000000	2.459812000000
H	-1.090019000000	3.921265000000	-0.253829000000
H	-0.389247000000	2.573841000000	-1.142489000000
H	-2.145716000000	2.901520000000	-1.229670000000
C	-2.046715000000	0.319877000000	-2.545053000000
C	-3.247486000000	-1.474236000000	-1.374266000000
C	-4.036299000000	0.854017000000	-1.095317000000
C	-1.295845000000	-0.450575000000	2.949493000000
C	-3.603293000000	-0.688357000000	2.029970000000
C	-1.803742000000	-2.332894000000	1.462695000000
H	-1.603215000000	1.315898000000	-2.560655000000
H	-1.253100000000	-0.408619000000	-2.735752000000
H	-2.772829000000	0.261146000000	-3.368004000000
H	-3.905302000000	-1.794711000000	-0.561871000000
H	-3.830905000000	-1.540189000000	-2.302985000000
H	-2.407140000000	-2.166808000000	-1.466418000000
H	-4.707333000000	0.611262000000	-1.930463000000
H	-4.585745000000	0.655251000000	-0.170104000000
H	-3.831696000000	1.924915000000	-1.150472000000
H	-0.219002000000	-0.477527000000	2.750979000000
H	-1.507654000000	-1.182248000000	3.740756000000
H	-4.244230000000	-1.088622000000	1.241447000000
H	-3.822196000000	-1.257083000000	2.944595000000
H	-3.895290000000	0.347951000000	2.211317000000
H	-2.291484000000	-2.746234000000	0.581449000000
H	-0.730191000000	-2.502025000000	1.338301000000
H	-2.147651000000	-2.898842000000	2.340316000000
H	-1.562057000000	0.534489000000	3.341152000000
H	4.780067000000	-2.328970000000	2.074719000000

Zero-point correction=	0.468625 (Hartree/Particle)
Thermal correction to Energy=	0.496857
Thermal correction to Enthalpy=	0.497801
Thermal correction to Gibbs Free Energy=	0.411327
Sum of electronic and zero-point Energies=	-4205.502680
Sum of electronic and thermal Energies=	-4205.474447
Sum of electronic and thermal Enthalpies=	-4205.473503
Sum of electronic and thermal Free Energies=	-4205.559977

CPCM (Toluene) M06/def2TZVP E = -4208.60414359

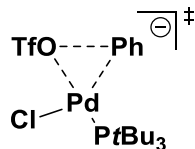


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C	2.350349000000	0.670946000000	-0.091403000000
C	3.075120000000	-0.412425000000	-0.656759000000
H	3.010455000000	-0.632959000000	-1.718147000000
Pd	0.880278000000	-0.635129000000	-0.336325000000
Cl	2.177563000000	2.378957000000	-1.718985000000
H	2.241636000000	2.131540000000	1.513100000000

C	4.112012000000	-0.996416000000	0.115293000000
C	3.754041000000	0.641831000000	1.853329000000
H	4.675876000000	-1.822539000000	-0.309776000000
H	4.013181000000	1.034110000000	2.834666000000
Cl	0.572208000000	-3.063296000000	-0.825779000000
C	-2.893737000000	2.571715000000	0.695948000000
C	-1.602014000000	2.044098000000	0.047318000000
H	-2.875137000000	2.465134000000	1.784665000000
H	-2.977366000000	3.646085000000	0.481975000000
H	-3.799842000000	2.092303000000	0.321374000000
P	-1.325289000000	0.140648000000	0.121603000000
C	-0.413008000000	2.762254000000	0.714289000000
C	-1.553912000000	2.498764000000	-1.424705000000
C	-2.587822000000	-0.650057000000	-1.102578000000
C	-1.790958000000	-0.438203000000	1.894196000000
H	0.505717000000	2.575062000000	0.157944000000
H	-0.603892000000	3.843857000000	0.676459000000
H	-0.264277000000	2.493603000000	1.759533000000
H	-1.511480000000	3.595766000000	-1.444126000000
H	-0.646723000000	2.137710000000	-1.919175000000
H	-2.432713000000	2.198204000000	-1.999704000000
C	-1.936223000000	-0.616879000000	-2.502457000000
C	-2.801558000000	-2.143302000000	-0.788834000000
C	-3.978549000000	0.004491000000	-1.169949000000
C	-1.057732000000	0.434875000000	2.929739000000
C	-3.290125000000	-0.433166000000	2.238286000000
C	-1.239207000000	-1.864389000000	2.101431000000
H	-1.690224000000	0.388220000000	-2.846558000000
H	-1.019457000000	-1.214375000000	-2.508829000000
H	-2.637826000000	-1.056800000000	-3.225414000000
H	-3.384195000000	-2.308508000000	0.121239000000
H	-3.372765000000	-2.581261000000	-1.619056000000
H	-1.850875000000	-2.679908000000	-0.722463000000
H	-4.604378000000	-0.584967000000	-1.854050000000
H	-4.481307000000	0.014690000000	-0.198235000000
H	-3.955932000000	1.025429000000	-1.557136000000
H	0.009131000000	0.521133000000	2.697837000000
H	-1.148258000000	-0.046313000000	3.912965000000
H	-3.854513000000	-1.153155000000	1.641740000000
H	-3.412333000000	-0.720351000000	3.292101000000
H	-3.752820000000	0.548047000000	2.110967000000
H	-1.645050000000	-2.598069000000	1.406978000000
H	-0.152134000000	-1.890003000000	1.983534000000
H	-1.487750000000	-2.186350000000	3.123161000000
H	-1.485872000000	1.436643000000	3.021104000000
H	5.229502000000	-0.944936000000	1.942132000000

Zero-point correction=	0.469559 (Hartree/Particle)
Thermal correction to Energy=	0.497328
Thermal correction to Enthalpy=	0.498272
Thermal correction to Gibbs Free Energy=	0.413597
Sum of electronic and zero-point Energies=	-2094.238088
Sum of electronic and thermal Energies=	-2094.210318
Sum of electronic and thermal Enthalpies=	-2094.209374
Sum of electronic and thermal Free Energies=	-2094.294049

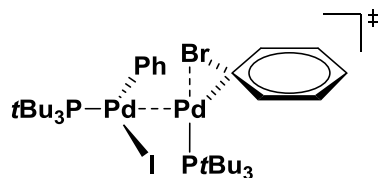
CPCM (Toluene) M06/def2TZVP E = -2094.72397397



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C	-1.272902000000	1.214641000000	0.215883000000
C	-1.192008000000	2.420362000000	-0.544881000000
H	-1.252482000000	2.395243000000	-1.629235000000

H	-1.847462000000	0.305555000000	2.110777000000
C	-1.419500000000	3.649050000000	0.139325000000
C	-1.869940000000	2.449291000000	2.187977000000
H	-1.371259000000	4.572684000000	-0.430307000000
H	-2.116853000000	2.474580000000	3.246814000000
O	-2.056486000000	-0.096122000000	-0.681334000000
S	-3.584230000000	-0.149907000000	-0.856830000000
O	-3.930630000000	-0.554065000000	-2.206933000000
O	-4.288070000000	0.951925000000	-0.230306000000
C	-3.972845000000	-1.629933000000	0.179315000000
F	-3.311148000000	-2.702932000000	-0.255652000000
F	-5.280605000000	-1.888928000000	0.124024000000
F	-3.641827000000	-1.423079000000	1.456652000000
Cl	2.336074000000	2.896907000000	-1.187597000000
H	2.552804000000	-3.786969000000	0.388309000000
C	1.650166000000	-3.520992000000	0.941010000000
C	0.899349000000	-2.312473000000	0.355830000000
H	1.926517000000	-3.357138000000	1.986892000000
H	0.980996000000	-4.392281000000	0.920151000000
P	1.925736000000	-0.700848000000	0.095077000000
C	-0.298147000000	-2.018438000000	1.279474000000
C	0.256825000000	-2.714357000000	-0.986524000000
C	3.108164000000	-1.035823000000	-1.388660000000
C	3.006217000000	-0.453146000000	1.663258000000
H	-0.953928000000	-1.283977000000	0.819811000000
H	-0.874270000000	-2.944804000000	1.405065000000
H	-0.019074000000	-1.667341000000	2.272063000000
H	-0.486537000000	-3.498846000000	-0.795258000000
H	-0.274796000000	-1.869759000000	-1.435712000000
H	0.973017000000	-3.113800000000	-1.707657000000
C	2.312883000000	-0.728501000000	-2.677009000000
C	4.281770000000	-0.037444000000	-1.390667000000
C	3.706930000000	-2.449247000000	-1.483548000000
C	2.113454000000	-0.540801000000	2.915084000000
C	4.182935000000	-1.426487000000	1.841839000000
C	3.549114000000	0.990804000000	1.650241000000
H	1.419062000000	-1.341922000000	-2.796186000000
H	2.012322000000	0.323677000000	-2.695570000000
H	2.963660000000	-0.914356000000	-3.543056000000
H	5.012868000000	-0.238323000000	-0.603023000000
H	4.807542000000	-0.142319000000	-2.349682000000
H	3.930757000000	0.996079000000	-1.316191000000
H	4.400589000000	-2.475717000000	-2.335051000000
H	4.278453000000	-2.720217000000	-0.590544000000
H	2.955544000000	-3.222695000000	-1.658310000000
H	1.217929000000	0.081485000000	2.812137000000
H	1.812293000000	-1.565117000000	3.150395000000
H	2.683378000000	-0.165798000000	3.775592000000
H	4.940139000000	-1.308469000000	1.063288000000
H	4.673834000000	-1.217971000000	2.802902000000
H	3.870267000000	-2.473179000000	1.854442000000
H	4.198387000000	1.208253000000	0.803959000000
H	2.735779000000	1.720888000000	1.614382000000
H	4.125493000000	1.151581000000	2.572662000000
Pd	0.652081000000	1.275715000000	-0.301999000000
H	-1.887017000000	4.611854000000	1.988937000000

Zero-point correction=	0.497940 (Hartree/Particle)
Thermal correction to Energy=	0.532469
Thermal correction to Enthalpy=	0.533413
Thermal correction to Gibbs Free Energy=	0.432975
Sum of electronic and zero-point Energies=	-2595.279029
Sum of electronic and thermal Energies=	-2595.244501
Sum of electronic and thermal Enthalpies=	-2595.243557
Sum of electronic and thermal Free Energies=	-2595.343995
CPCM (Toluene) M06/def2TZVP E = -2596.04636679	

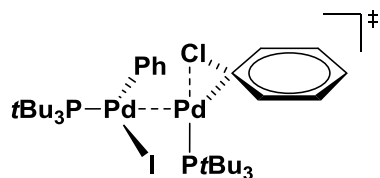


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C	3.042994000000	-1.878174000000	-2.555556000000
C	2.278932000000	-2.161217000000	-1.417535000000
C	2.680914000000	-3.145826000000	-0.507514000000
H	2.039373000000	-3.405509000000	0.328743000000
H	2.685048000000	-1.160930000000	-3.284825000000
C	3.916454000000	-3.763615000000	-0.688929000000
C	4.265243000000	-2.517363000000	-2.723798000000
H	4.248147000000	-4.502636000000	0.034386000000
H	4.871915000000	-2.281425000000	-3.593458000000
Pd	1.509022000000	-0.498015000000	-0.282129000000
Pd	-1.310706000000	0.062309000000	0.098210000000
Br	0.165549000000	-2.021637000000	-1.723219000000
H	5.663597000000	-3.954100000000	-1.932932000000
H	2.630648000000	3.825791000000	-2.040856000000
C	2.429534000000	3.312427000000	-1.092199000000
C	3.570120000000	2.315814000000	-0.823253000000
H	1.469722000000	2.800437000000	-1.199282000000
H	2.336536000000	4.083097000000	-0.324084000000
P	3.049376000000	1.130393000000	0.595102000000
C	4.875211000000	3.098916000000	-0.610991000000
C	3.683908000000	1.494236000000	-2.123851000000
C	2.386920000000	2.199537000000	2.046821000000
C	4.618300000000	0.223826000000	1.229661000000
H	5.754491000000	2.449796000000	-0.609253000000
H	5.000406000000	3.808098000000	-1.439819000000
H	4.876425000000	3.676864000000	0.315759000000
H	4.411617000000	0.684451000000	-2.074443000000
H	2.712927000000	1.059808000000	-2.380914000000
H	3.985387000000	2.168885000000	-2.936321000000
C	3.176759000000	3.486278000000	2.340510000000
C	0.927179000000	2.576907000000	1.739363000000
C	2.329537000000	1.364581000000	3.339124000000
C	4.174749000000	-0.993253000000	2.068744000000
C	5.386589000000	-0.353752000000	0.028749000000
C	5.597180000000	1.066404000000	2.063616000000
H	4.233408000000	3.298104000000	2.542823000000
H	3.109272000000	4.215070000000	1.529593000000
H	2.750840000000	3.959377000000	3.234768000000
H	0.309957000000	1.679645000000	1.623215000000
H	0.524862000000	3.150808000000	2.585197000000
H	0.816500000000	3.182885000000	0.842558000000
H	1.752135000000	1.929002000000	4.082199000000
H	1.814954000000	0.412299000000	3.186828000000
H	3.314344000000	1.181135000000	3.773606000000
H	3.679963000000	-0.723196000000	3.000359000000
H	3.497323000000	-1.638236000000	1.504717000000
H	5.066551000000	-1.580009000000	2.326068000000
H	5.888374000000	0.413909000000	-0.564930000000
H	6.163687000000	-1.031128000000	0.404358000000
H	4.736247000000	-0.937693000000	-0.624988000000
H	6.476810000000	0.451747000000	2.296065000000
H	5.950618000000	1.954378000000	1.534556000000
H	5.169496000000	1.383600000000	3.017033000000
P	-3.708288000000	0.044124000000	0.043476000000
C	-4.431988000000	1.090317000000	1.478754000000
C	-4.579827000000	0.597311000000	-1.589541000000
C	-4.203189000000	-1.810863000000	0.337549000000
C	-5.855348000000	0.696174000000	1.915143000000
C	-3.481435000000	0.974190000000	2.685769000000
C	-4.477127000000	2.582099000000	1.101902000000

C	-4.116758000000	1.977247000000	-2.112271000000
C	-4.203607000000	-0.399800000000	-2.702011000000
C	-6.115811000000	0.693555000000	-1.473554000000
C	-4.029337000000	-2.222787000000	1.811577000000
C	-5.646101000000	-2.184648000000	-0.048480000000
C	-3.232422000000	-2.700085000000	-0.467819000000
H	-6.580470000000	0.757770000000	1.101438000000
H	-5.909194000000	-0.303000000000	2.346768000000
H	-6.179699000000	1.398817000000	2.693050000000
H	-2.488991000000	1.373704000000	2.453347000000
H	-3.899520000000	1.558970000000	3.515112000000
H	-3.341538000000	-0.048464000000	3.035174000000
H	-4.695419000000	3.154462000000	2.011916000000
H	-3.526394000000	2.943577000000	0.707133000000
H	-5.264422000000	2.811714000000	0.380471000000
H	-4.093301000000	2.760792000000	-1.359284000000
H	-3.136489000000	1.928803000000	-2.578203000000
H	-4.832239000000	2.285543000000	-2.885113000000
H	-4.675652000000	-1.377091000000	-2.589421000000
H	-4.537532000000	0.014200000000	-3.661383000000
H	-3.118409000000	-0.536074000000	-2.762524000000
H	-6.526762000000	0.802866000000	-2.484939000000
H	-6.593845000000	-0.171660000000	-1.021795000000
H	-6.416398000000	1.582671000000	-0.912757000000
H	-3.039498000000	-1.987767000000	2.199498000000
H	-4.784978000000	-1.794974000000	2.472241000000
H	-4.139190000000	-3.312967000000	1.864415000000
H	-5.844326000000	-2.105764000000	-1.118627000000
H	-5.797828000000	-3.235799000000	0.224910000000
H	-6.393627000000	-1.601517000000	0.495131000000
H	-3.563713000000	-3.742140000000	-0.377069000000
H	-3.191291000000	-2.459285000000	-1.531015000000
H	-2.219322000000	-2.642397000000	-0.063665000000
C	-1.164237000000	1.534387000000	-1.210659000000
C	-1.279787000000	2.843620000000	-0.735440000000
C	-0.770458000000	1.338972000000	-2.539400000000
C	-1.037724000000	3.934155000000	-1.569279000000
C	-0.522005000000	2.431089000000	-3.371405000000
C	-0.668026000000	3.732163000000	-2.895904000000
H	-1.551332000000	3.024095000000	0.300078000000
H	-0.656496000000	0.336687000000	-2.936325000000
H	-1.139374000000	4.942207000000	-1.175806000000
H	-0.219831000000	2.257638000000	-4.400882000000
H	-0.483239000000	4.579184000000	-3.549840000000
I	-0.368757000000	-1.479765000000	2.242025000000

Zero-point correction=	0.942936 (Hartree/Particle)
Thermal correction to Energy=	0.996906
Thermal correction to Enthalpy=	0.997850
Thermal correction to Gibbs Free Energy=	0.858335
Sum of electronic and zero-point Energies=	-4930.517759
Sum of electronic and thermal Energies=	-4930.463790
Sum of electronic and thermal Enthalpies=	-4930.462846
Sum of electronic and thermal Free Energies=	-4930.602361

CPCM (Toluene) M06/def2TZVP E = -5220.28706631



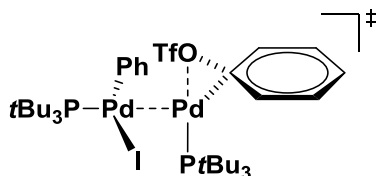
C	4.527298000000	-3.310358000000	-2.480059000000
C	2.985395000000	-1.494316000000	-2.910027000000
C	2.221996000000	-1.911324000000	-1.814991000000

C	2.548651000000	-3.071356000000	-1.105174000000
H	1.896166000000	-3.422490000000	-0.311745000000
H	2.675445000000	-0.635129000000	-3.493294000000
C	3.724589000000	-3.744371000000	-1.427575000000
C	4.146726000000	-2.192012000000	-3.222941000000
H	4.001611000000	-4.625719000000	-0.856288000000
H	4.757329000000	-1.856921000000	-4.056698000000
Pd	1.500131000000	-0.467187000000	-0.446148000000
Pd	-1.333702000000	0.003255000000	0.087203000000
Cl	0.195852000000	-1.643286000000	-2.080642000000
H	5.434395000000	-3.849808000000	-2.733670000000
H	2.667106000000	4.054016000000	-1.417890000000
C	2.478732000000	3.372911000000	-0.578575000000
C	3.616846000000	2.339515000000	-0.522154000000
H	1.513654000000	2.892633000000	-0.760817000000
H	2.404896000000	3.986352000000	0.321816000000
P	3.115756000000	0.916811000000	0.665153000000
C	4.934070000000	3.063727000000	-0.203034000000
C	3.694966000000	1.767564000000	-1.952407000000
C	2.487104000000	1.703756000000	2.301443000000
C	4.684530000000	-0.104778000000	1.087184000000
H	5.805001000000	2.416073000000	-0.330149000000
H	5.052356000000	3.902055000000	-0.901991000000
H	4.959891000000	3.475236000000	0.808206000000
H	4.416593000000	0.958995000000	-2.067798000000
H	2.714297000000	1.391243000000	-2.259198000000
H	3.983189000000	2.576126000000	-2.637371000000
C	3.296804000000	2.908329000000	2.809993000000
C	1.025897000000	2.142890000000	2.096031000000
C	2.441968000000	0.645473000000	3.418642000000
C	4.241364000000	-1.450206000000	1.698941000000
C	5.423905000000	-0.460970000000	-0.214121000000
C	5.687283000000	0.566013000000	2.040639000000
H	4.352596000000	2.675116000000	2.965318000000
H	3.232792000000	3.769724000000	2.141397000000
H	2.884421000000	3.221587000000	3.777938000000
H	0.396801000000	1.288423000000	1.824308000000
H	0.642651000000	2.549536000000	3.041781000000
H	0.904481000000	2.908279000000	1.332311000000
H	1.888630000000	1.068865000000	4.266145000000
H	1.910878000000	-0.257010000000	3.104227000000
H	3.432420000000	0.374063000000	3.789704000000
H	3.765974000000	-1.350114000000	2.673150000000
H	3.548544000000	-1.976822000000	1.039371000000
H	5.130470000000	-2.081387000000	1.827708000000
H	5.915782000000	0.399643000000	-0.673703000000
H	6.206224000000	-1.192884000000	0.021808000000
H	4.757939000000	-0.922173000000	-0.946334000000
H	6.565409000000	-0.085814000000	2.136833000000
H	6.038075000000	1.534212000000	1.675649000000
H	5.281483000000	0.704676000000	3.044992000000
P	-3.712952000000	-0.016592000000	-0.026589000000
C	-4.459436000000	0.674985000000	1.599361000000
C	-4.576353000000	0.878708000000	-1.506517000000
C	-4.172490000000	-1.896313000000	-0.162701000000
C	-5.886123000000	0.187794000000	1.911580000000
C	-3.528508000000	0.293185000000	2.765950000000
C	-4.500670000000	2.213202000000	1.563272000000
C	-4.122064000000	2.343531000000	-1.704975000000
C	-4.187230000000	0.155578000000	-2.810000000000
C	-6.114250000000	0.933759000000	-1.385414000000
C	-4.008160000000	-2.624855000000	1.184033000000
C	-5.605598000000	-2.190549000000	-0.643394000000
C	-3.174951000000	-2.564456000000	-1.132634000000
H	-6.600142000000	0.436506000000	1.124669000000
H	-5.939832000000	-0.885027000000	2.096293000000
H	-6.224533000000	0.687839000000	2.827733000000
H	-2.531635000000	0.726937000000	2.638435000000
H	-3.958194000000	0.689098000000	3.694984000000
H	-3.397698000000	-0.781422000000	2.889569000000

H	-4.731822000000	2.571197000000	2.573959000000
H	-3.542218000000	2.648297000000	1.273118000000
H	-5.276575000000	2.599986000000	0.898984000000
H	-4.110904000000	2.940023000000	-0.796130000000
H	-3.138566000000	2.407367000000	-2.162359000000
H	-4.835240000000	2.810513000000	-2.396058000000
H	-4.650519000000	-0.826224000000	-2.919567000000
H	-4.522417000000	0.769612000000	-3.654926000000
H	-3.101622000000	0.044589000000	-2.896289000000
H	-6.517020000000	1.267681000000	-2.349788000000
H	-6.587706000000	-0.016361000000	-1.149980000000
H	-6.429157000000	1.669178000000	-0.640328000000
H	-3.024332000000	-2.473296000000	1.626234000000
H	-4.775256000000	-2.361951000000	1.914165000000
H	-4.106290000000	-3.699839000000	0.989710000000
H	-5.793048000000	-1.879202000000	-1.672215000000
H	-5.747743000000	-3.277526000000	-0.610379000000
H	-6.366440000000	-1.748939000000	0.005052000000
H	-3.493896000000	-3.601930000000	-1.293669000000
H	-3.116031000000	-2.082491000000	-2.108943000000
H	-2.168859000000	-2.592876000000	-0.708018000000
C	-1.176397000000	1.692238000000	-0.916176000000
C	-1.267508000000	2.898291000000	-0.216458000000
C	-0.784758000000	1.720425000000	-2.259440000000
C	-1.004152000000	4.111919000000	-0.850011000000
C	-0.515446000000	2.935677000000	-2.889263000000
C	-0.639003000000	4.136206000000	-2.193370000000
H	-1.538164000000	2.899980000000	0.835220000000
H	-0.690244000000	0.797048000000	-2.819866000000
H	-1.086624000000	5.039544000000	-0.289781000000
H	-0.215115000000	2.939495000000	-3.933782000000
H	-0.440992000000	5.081251000000	-2.690138000000
I	-0.361814000000	-1.904435000000	1.875630000000

Zero-point correction=	0.942265 (Hartree/Particle)
Thermal correction to Energy=	0.996232
Thermal correction to Enthalpy=	0.997176
Thermal correction to Gibbs Free Energy=	0.857717
Sum of electronic and zero-point Energies=	-2819.252426
Sum of electronic and thermal Energies=	-2819.198458
Sum of electronic and thermal Enthalpies=	-2819.197514
Sum of electronic and thermal Free Energies=	-2819.336973

CPCM (Toluene) M06/def2TZVP E = -3106.40888343

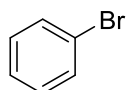


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C	-1.632796000000	3.109521000000	-1.251876000000
C	-1.130590000000	2.267774000000	-0.245183000000
C	-1.475650000000	2.392058000000	1.113661000000
H	-0.876304000000	1.922631000000	1.888018000000
H	-1.278815000000	3.012759000000	-2.271263000000
C	-2.460665000000	3.348174000000	1.443201000000
C	-2.620228000000	4.003950000000	-0.882623000000
H	-2.726924000000	3.491298000000	2.486790000000
H	-3.082743000000	4.621087000000	-1.647754000000
Pd	-1.750633000000	0.413974000000	-0.223646000000
Pd	1.493373000000	-0.094795000000	-0.084338000000
O	0.803299000000	2.106158000000	-0.297417000000
H	-3.790165000000	4.864252000000	0.718174000000
H	-4.855103000000	-1.396458000000	-3.380873000000

C	-4.282309000000	-1.717983000000	-2.502073000000
C	-4.785201000000	-0.922525000000	-1.282517000000
H	-3.225893000000	-1.522814000000	-2.709826000000
H	-4.433359000000	-2.794693000000	-2.398803000000
P	-3.575853000000	-1.156525000000	0.189520000000
C	-6.246332000000	-1.321942000000	-1.019636000000
C	-4.737363000000	0.559148000000	-1.719939000000
C	-3.195446000000	-3.029702000000	0.357310000000
C	-4.471447000000	-0.590543000000	1.793455000000
H	-6.734055000000	-0.673159000000	-0.288545000000
H	-6.809211000000	-1.229224000000	-1.957329000000
H	-6.346582000000	-2.355450000000	-0.679218000000
H	-5.001693000000	1.265072000000	-0.932905000000
H	-3.742166000000	0.827684000000	-2.088565000000
H	-5.449087000000	0.700165000000	-2.544066000000
C	-4.397528000000	-3.979008000000	0.226662000000
C	-2.145811000000	-3.411903000000	-0.704115000000
C	-2.524386000000	-3.288027000000	1.718738000000
C	-3.412068000000	-0.373078000000	2.894777000000
C	-5.101780000000	0.795198000000	1.556610000000
C	-5.557394000000	-1.532193000000	2.338964000000
H	-5.190257000000	-3.761033000000	0.945534000000
H	-4.831995000000	-3.961280000000	-0.775327000000
H	-4.057351000000	-5.006450000000	0.411215000000
H	-1.268411000000	-2.765392000000	-0.649686000000
H	-1.823846000000	-4.446085000000	-0.523455000000
H	-2.521585000000	-3.360082000000	-1.725227000000
H	-2.099554000000	-4.299505000000	1.714895000000
H	-1.703559000000	-2.589575000000	1.905951000000
H	-3.225115000000	-3.236197000000	2.554837000000
H	-2.932410000000	-1.295155000000	3.223250000000
H	-2.631545000000	0.317619000000	2.565498000000
H	-3.903747000000	0.067173000000	3.772204000000
H	-5.970498000000	0.764097000000	0.896018000000
H	-5.447112000000	1.188364000000	2.521376000000
H	-4.375105000000	1.507894000000	1.154726000000
H	-6.040927000000	-1.052535000000	3.199997000000
H	-6.337096000000	-1.750697000000	1.605991000000
H	-5.145987000000	-2.480572000000	2.693662000000
P	3.141311000000	-1.741150000000	0.094075000000
C	2.342241000000	-3.481165000000	0.063758000000
C	4.248550000000	-1.524071000000	-1.462113000000
C	4.310653000000	-1.612671000000	1.612381000000
C	3.274301000000	-4.644272000000	0.441690000000
C	1.146745000000	-3.462404000000	1.033009000000
C	1.748220000000	-3.772810000000	-1.326295000000
C	3.390047000000	-1.174278000000	-2.693015000000
C	5.191100000000	-0.319201000000	-1.273364000000
C	5.087428000000	-2.769376000000	-1.806692000000
C	3.588829000000	-2.080954000000	2.891606000000
C	5.603059000000	-2.447373000000	1.502270000000
C	4.716293000000	-0.121802000000	1.803791000000
H	4.165821000000	-4.694968000000	-0.187401000000
H	3.588916000000	-4.609446000000	1.487055000000
H	2.723769000000	-5.583146000000	0.303924000000
H	0.404114000000	-2.734721000000	0.698735000000
H	0.670683000000	-4.450853000000	1.026164000000
H	1.417813000000	-3.228334000000	2.063667000000
H	1.146573000000	-4.687362000000	-1.252636000000
H	1.085219000000	-2.973412000000	-1.665882000000
H	2.509277000000	-3.948901000000	-2.088897000000
H	2.614466000000	-1.906653000000	-2.915564000000
H	2.914975000000	-0.195956000000	-2.585801000000
H	4.056201000000	-1.119561000000	-3.563109000000
H	5.948728000000	-0.472809000000	-0.503532000000
H	5.719392000000	-0.161689000000	-2.221384000000
H	4.639869000000	0.599908000000	-1.056174000000
H	5.752806000000	-2.508891000000	-2.638866000000
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H	4.470500000000	-3.605979000000	-2.141428000000

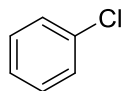
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H	3.398010000000	-3.156854000000	2.898278000000
H	4.244325000000	-1.867581000000	3.744366000000
H	6.272475000000	-2.086500000000	0.719957000000
H	6.142863000000	-2.348932000000	2.452077000000
H	5.421295000000	-3.510739000000	1.339656000000
H	5.798924000000	0.000222000000	1.702423000000
H	4.246318000000	0.556979000000	1.092038000000
H	4.433727000000	0.220835000000	2.802469000000
S	1.783476000000	3.033903000000	-1.029378000000
C	1.707899000000	4.555242000000	0.020577000000
F	2.062490000000	4.283605000000	1.276382000000
F	2.543632000000	5.464558000000	-0.471173000000
F	0.476175000000	5.055291000000	0.027140000000
O	3.143868000000	2.533512000000	-0.873312000000
O	1.316191000000	3.445906000000	-2.337729000000
I	-0.233682000000	-0.456314000000	-2.368445000000
C	1.401314000000	0.270579000000	1.850804000000
C	0.416514000000	-0.413575000000	2.566820000000
C	2.000227000000	1.393659000000	2.419548000000
C	0.045747000000	0.011719000000	3.843664000000
C	1.623821000000	1.818961000000	3.692278000000
C	0.651211000000	1.127885000000	4.412664000000
H	-0.084158000000	-1.270766000000	2.132584000000
H	2.731992000000	1.964958000000	1.862080000000
H	-0.725610000000	-0.530748000000	4.383836000000
H	2.087098000000	2.706585000000	4.113903000000
H	0.363532000000	1.462002000000	5.405132000000

Zero-point correction=	0.971511 (Hartree/Particle)
Thermal correction to Energy=	1.031750
Thermal correction to Enthalpy=	1.032694
Thermal correction to Gibbs Free Energy=	0.879383
Sum of electronic and zero-point Energies=	-3320.284351
Sum of electronic and thermal Energies=	-3320.224112
Sum of electronic and thermal Enthalpies=	-3320.223168
Sum of electronic and thermal Free Energies=	-3320.376478
CPCM (Toluene) M06/def2TZVP E =	-3607.71396346



C	0.000000000000	0.000000000000	-0.097553000000
C	0.000000000000	1.212437000000	-0.778143000000
C	0.000000000000	-1.212437000000	-0.778143000000
H	0.000000000000	2.146853000000	-0.228040000000
H	0.000000000000	-2.146853000000	-0.228040000000
C	0.000000000000	1.204632000000	-2.170589000000
C	0.000000000000	-1.204632000000	-2.170589000000
H	0.000000000000	2.147876000000	-2.708280000000
H	0.000000000000	-2.147876000000	-2.708280000000
C	0.000000000000	0.000000000000	-2.868384000000
H	0.000000000000	0.000000000000	-3.953939000000
Br	0.000000000000	0.000000000000	1.800200000000

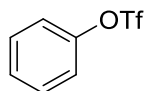
Zero-point correction=	0.092044 (Hartree/Particle)
Thermal correction to Energy=	0.097668
Thermal correction to Enthalpy=	0.098613
Thermal correction to Gibbs Free Energy=	0.061883
Sum of electronic and zero-point Energies=	-2802.899628
Sum of electronic and thermal Energies=	-2802.894003
Sum of electronic and thermal Enthalpies=	-2802.893059
Sum of electronic and thermal Free Energies=	-2802.929789
CPCM (Toluene) M06/def2TZVP E =	-2805.6085239



C	0.000000000000	0.000000000000	-2.266574000000
C	0.000000000000	1.204595000000	-1.568458000000
C	0.000000000000	-1.204595000000	-1.568458000000
H	0.000000000000	2.147716000000	-2.106331000000
H	0.000000000000	-2.147716000000	-2.106331000000
C	0.000000000000	1.213006000000	-0.176135000000
C	0.000000000000	-1.213006000000	-0.176135000000
H	0.000000000000	2.146386000000	0.376165000000
H	0.000000000000	-2.146386000000	0.376165000000
C	0.000000000000	0.000000000000	0.503964000000
H	0.000000000000	0.000000000000	-3.352096000000
Cl	0.000000000000	0.000000000000	2.254306000000

Zero-point correction=	0.092364 (Hartree/Particle)
Thermal correction to Energy=	0.097805
Thermal correction to Enthalpy=	0.098749
Thermal correction to Gibbs Free Energy=	0.063274
Sum of electronic and zero-point Energies=	-691.647479
Sum of electronic and thermal Energies=	-691.642038
Sum of electronic and thermal Enthalpies=	-691.641094
Sum of electronic and thermal Free Energies=	-691.676568

CPCM (Toluene) M06/def2TZVP E = -691.7377127

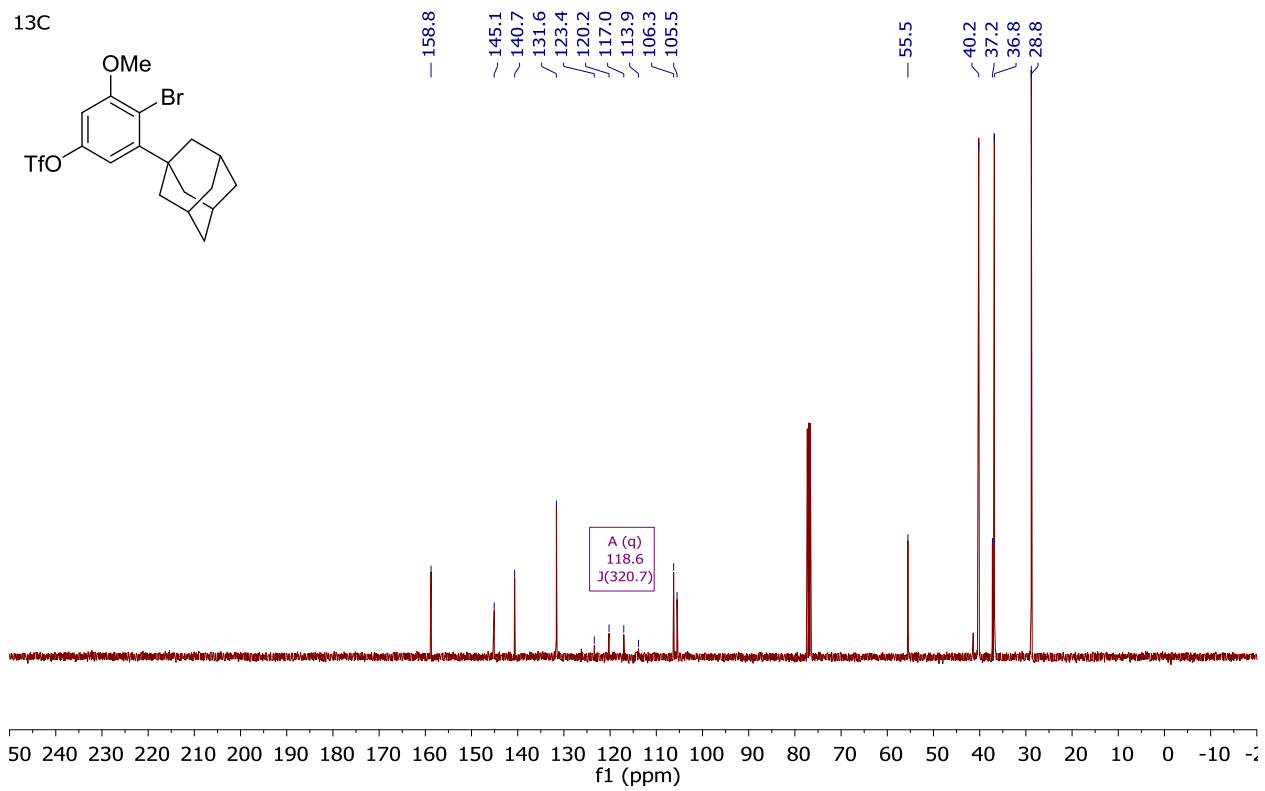
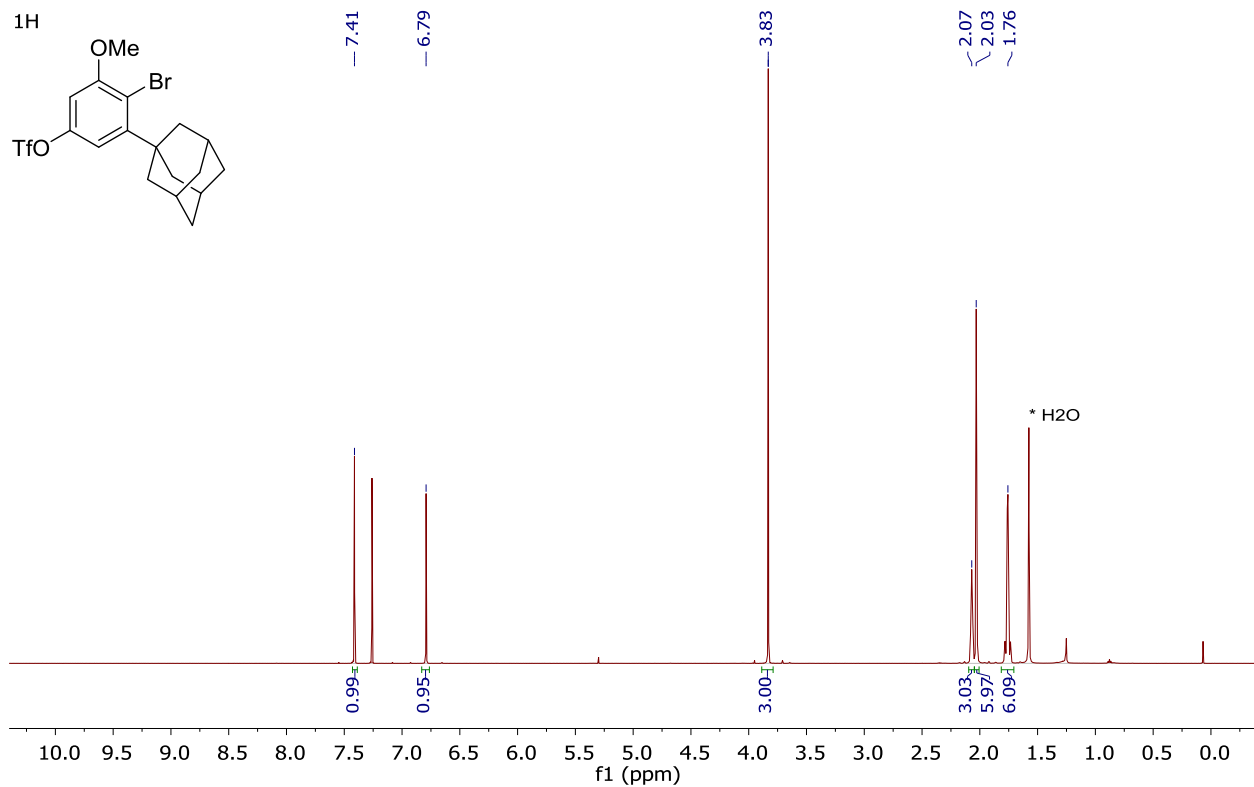


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C	2.100280000000	1.279201000000	-0.116290000000
C	2.131244000000	-1.130081000000	-0.456697000000
C	3.476826000000	1.260109000000	0.087590000000
C	3.507258000000	-1.132350000000	-0.245632000000
C	4.178589000000	0.058199000000	0.023409000000
H	1.527070000000	2.198106000000	-0.066867000000
H	1.584087000000	-2.041763000000	-0.668794000000
H	3.999085000000	2.187647000000	0.298897000000
H	4.053408000000	-2.068899000000	-0.294202000000
H	5.252053000000	0.049335000000	0.183990000000
O	0.075940000000	0.109912000000	-0.656288000000
S	-0.901221000000	-0.254069000000	0.584302000000
O	-0.730845000000	0.699228000000	1.653688000000
O	-0.894649000000	-1.676236000000	0.828532000000
C	-2.446829000000	0.169817000000	-0.342943000000
F	-2.535221000000	-0.568345000000	-1.436672000000
F	-3.470788000000	-0.089140000000	0.457678000000
F	-2.441805000000	1.453279000000	-0.662432000000

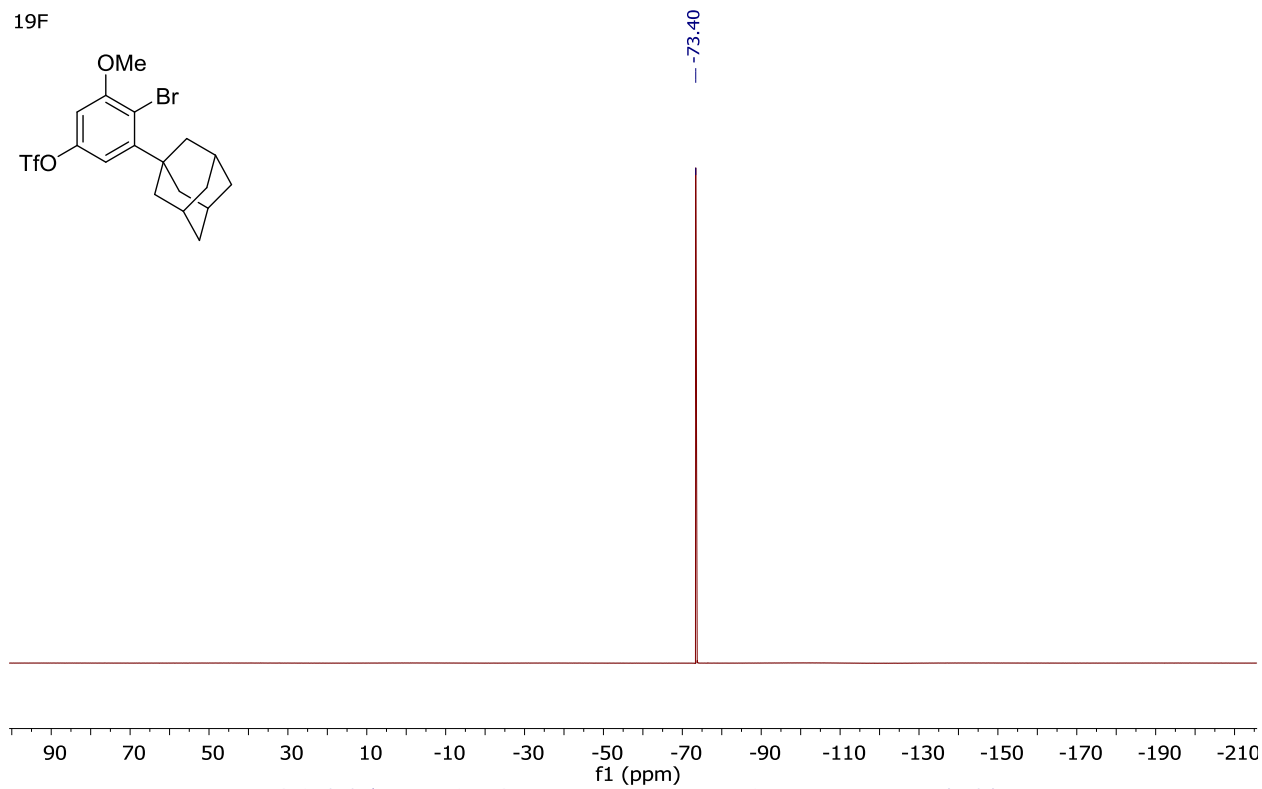
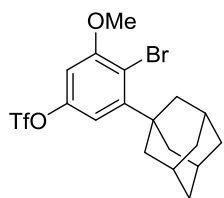
Zero-point correction=	0.121749 (Hartree/Particle)
Thermal correction to Energy=	0.133927
Thermal correction to Enthalpy=	0.134871
Thermal correction to Gibbs Free Energy=	0.080229
Sum of electronic and zero-point Energies=	-1192.663489
Sum of electronic and thermal Energies=	-1192.651312
Sum of electronic and thermal Enthalpies=	-1192.650368
Sum of electronic and thermal Free Energies=	-1192.705010

CPCM (Toluene) M06/def2TZVP E = -1193.04300917

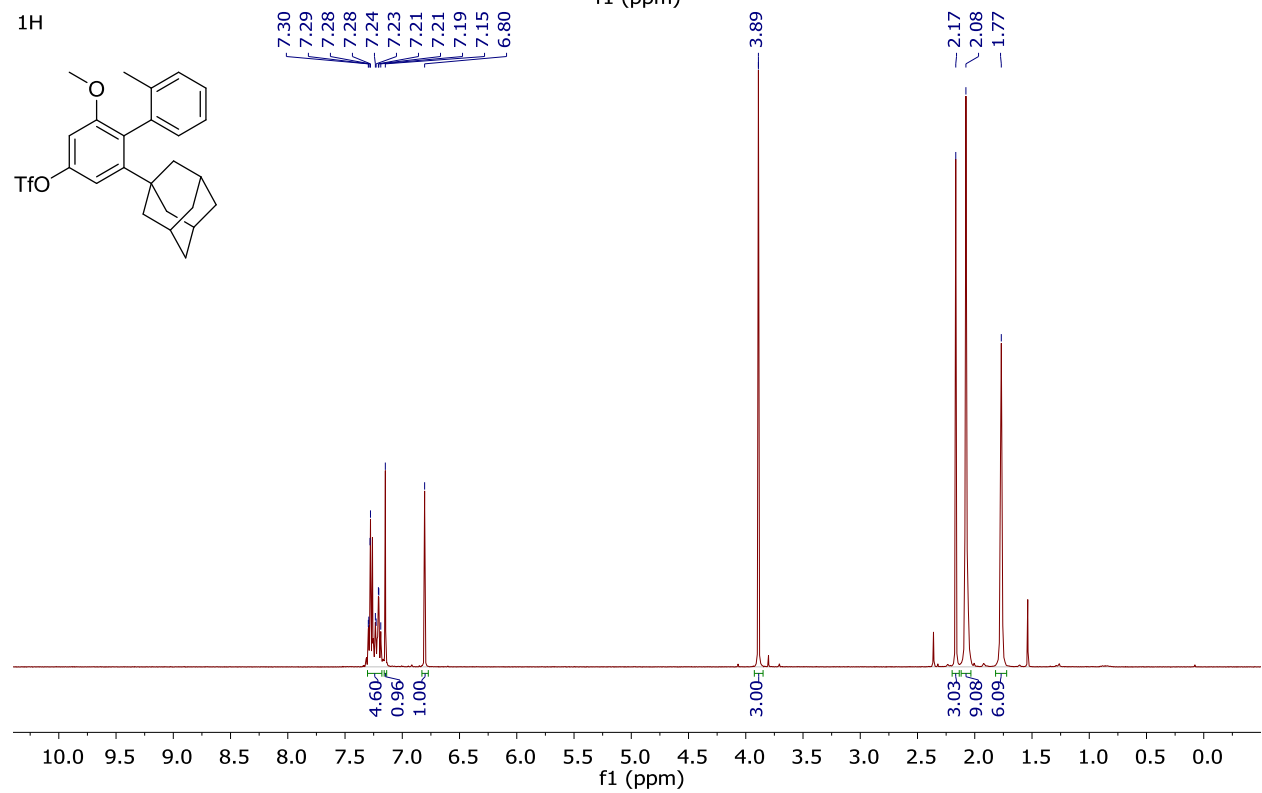
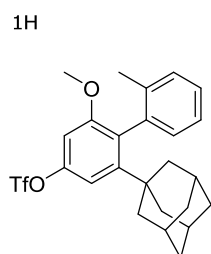
6. NMR spectra



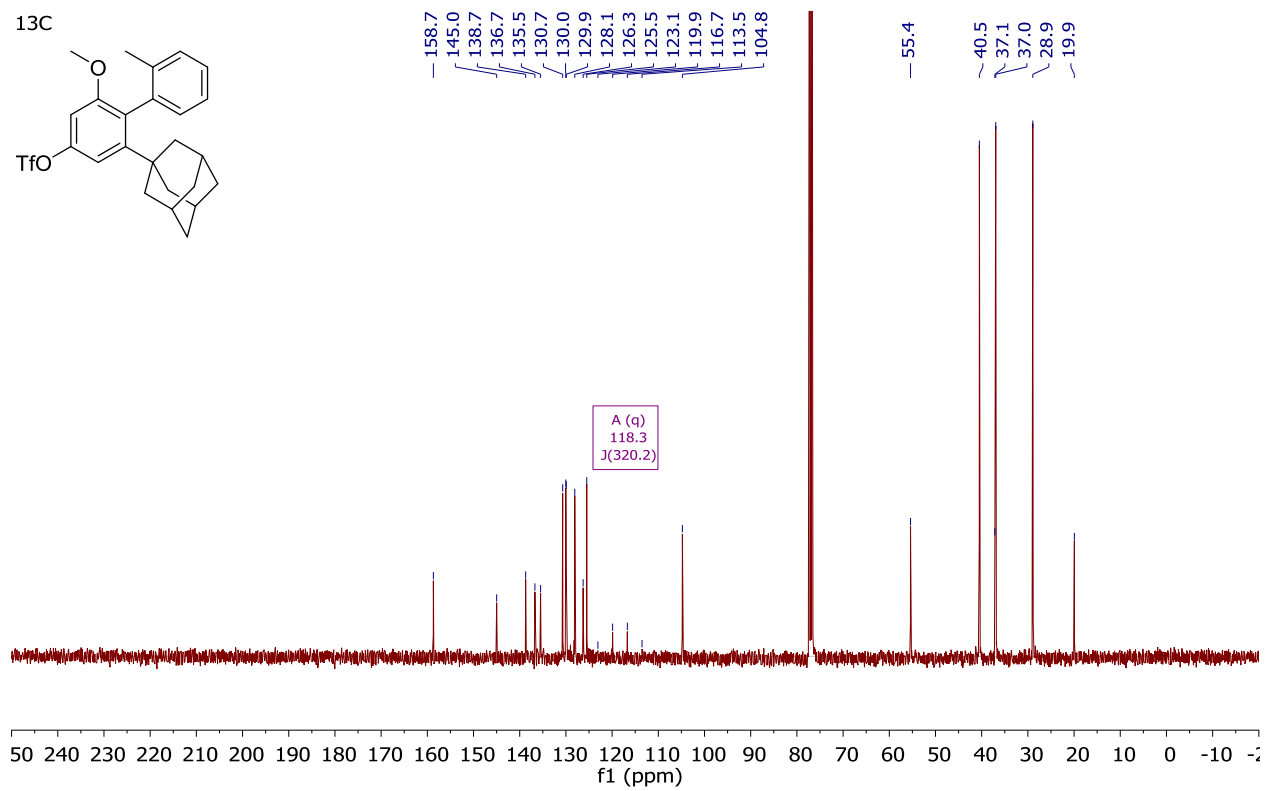
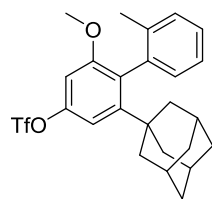
19F



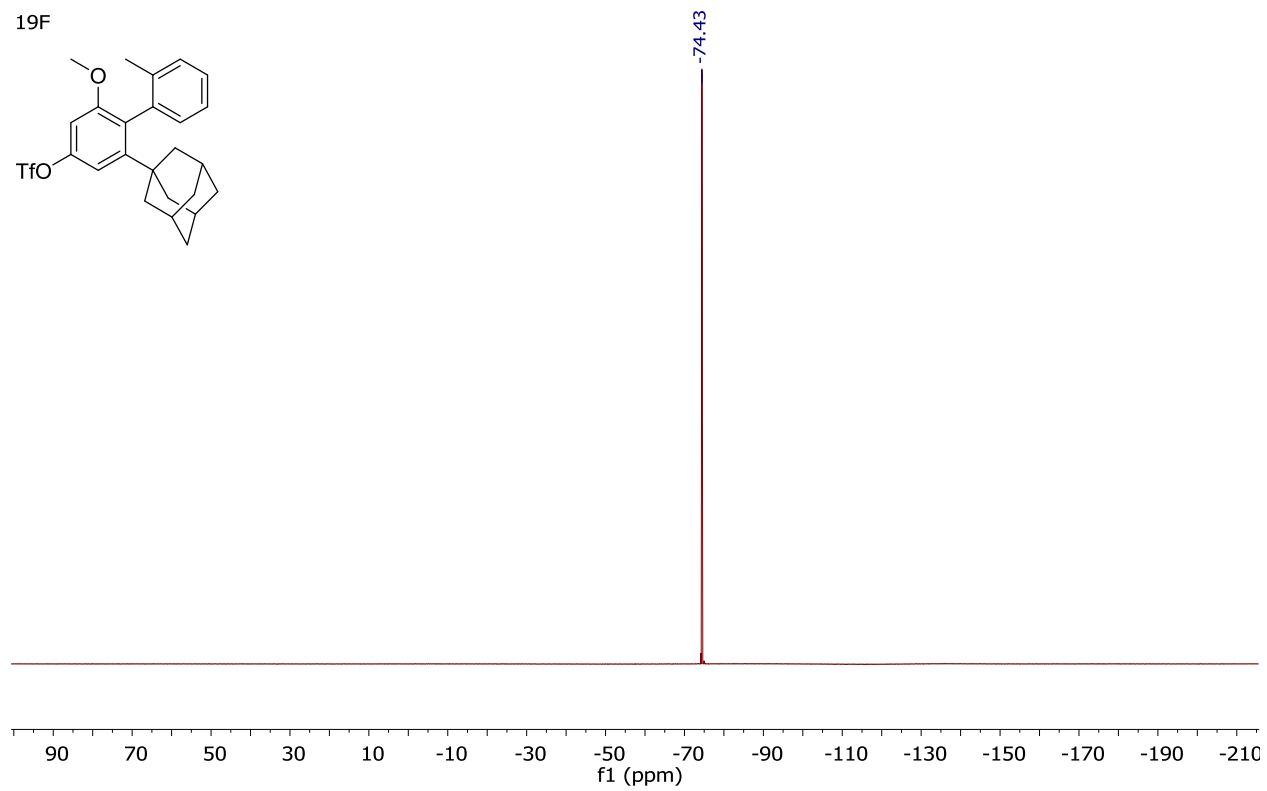
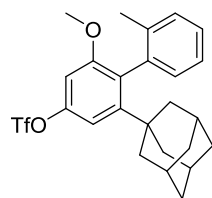
1H



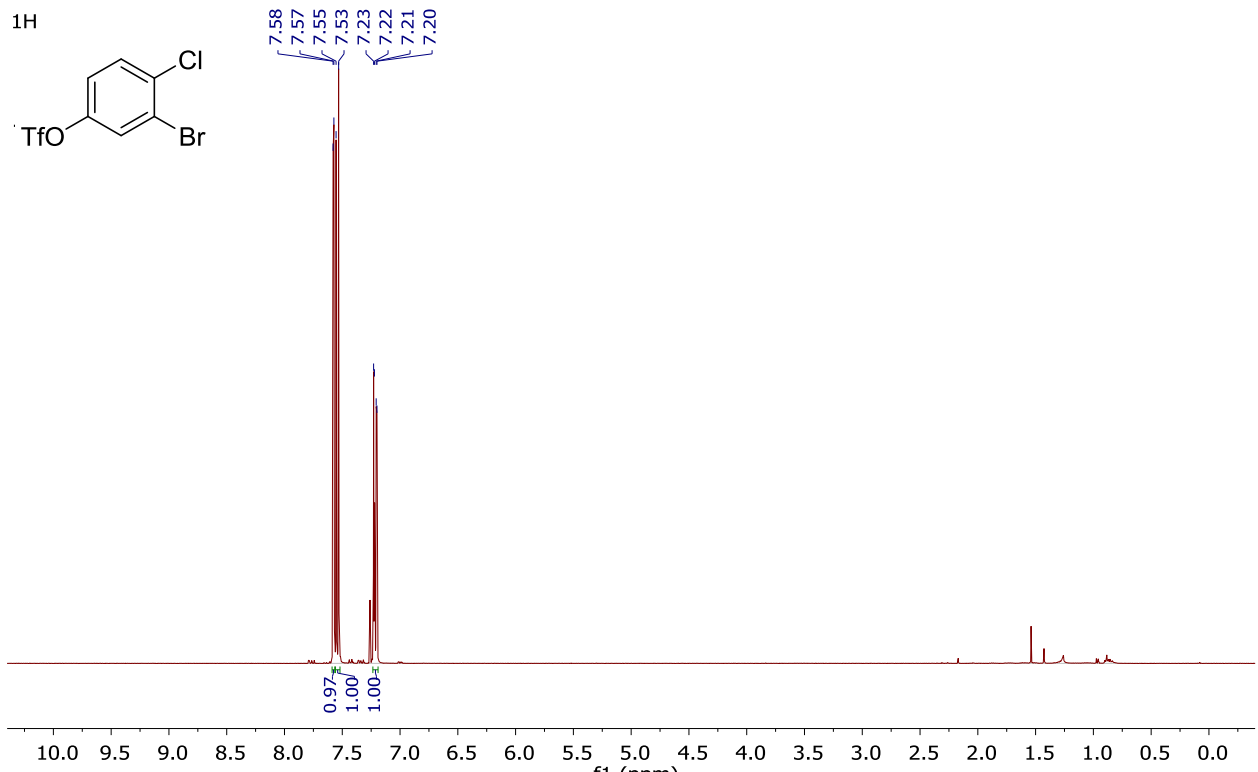
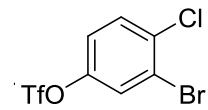
13C



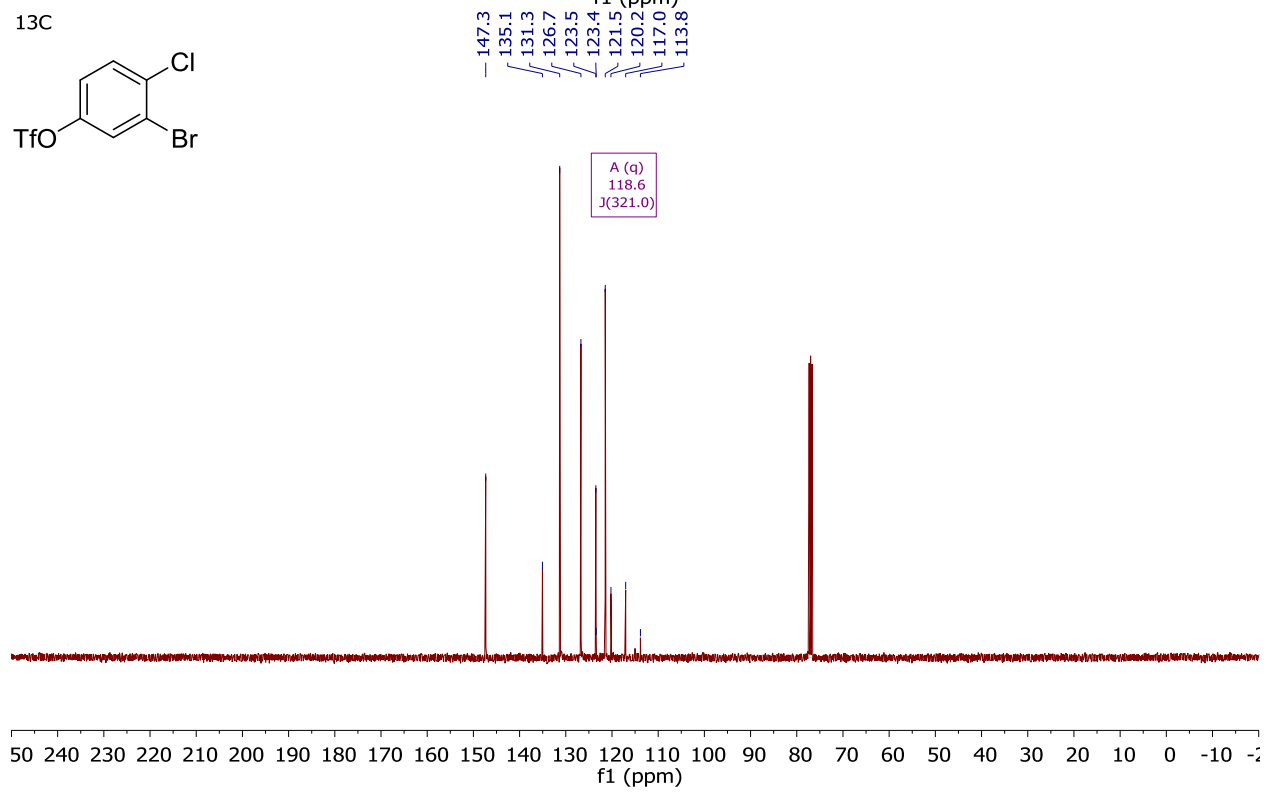
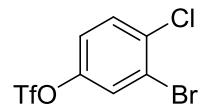
19F



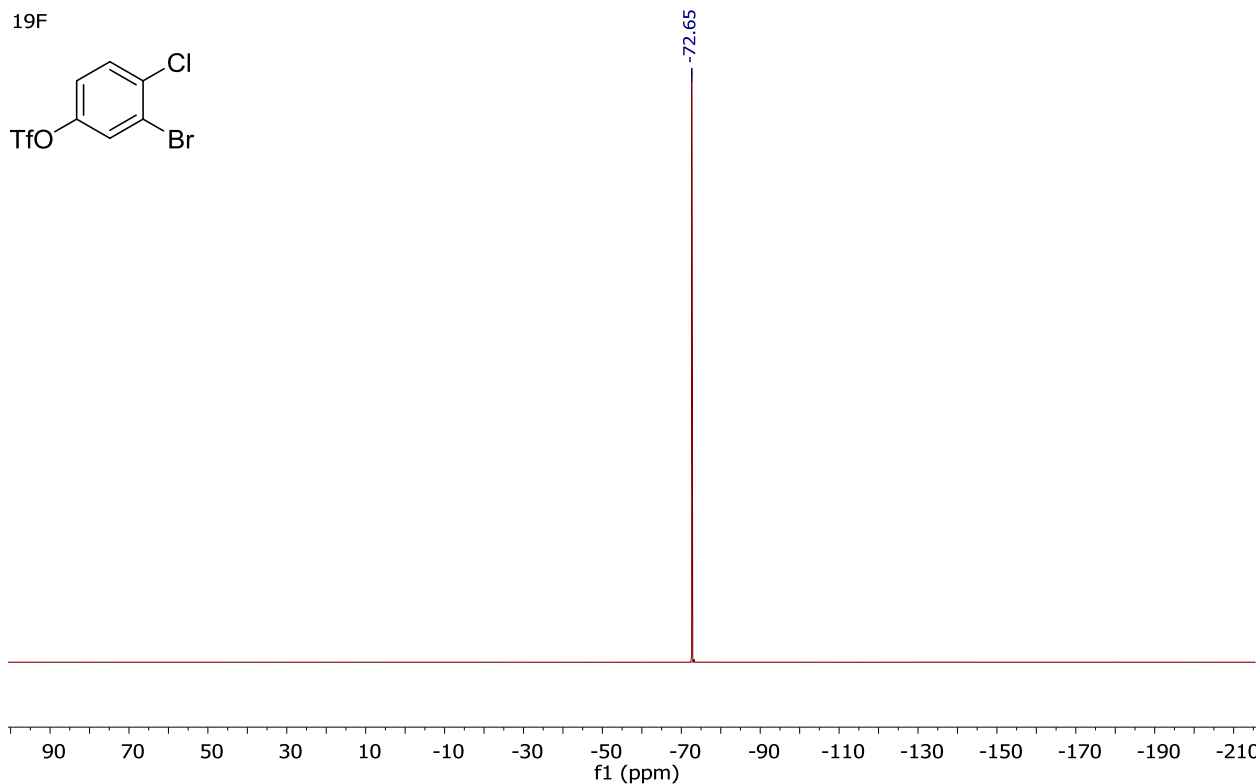
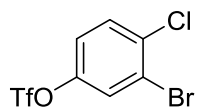
¹H



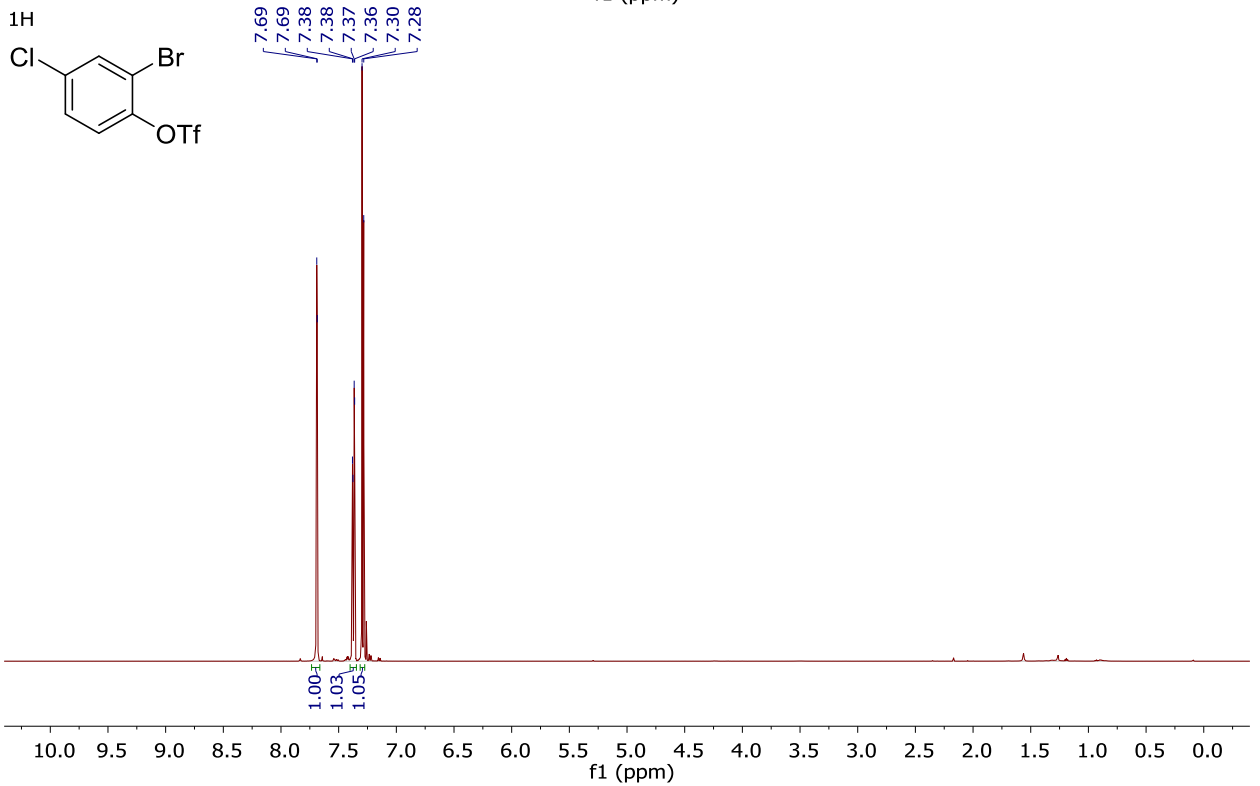
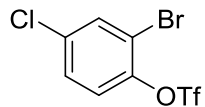
¹³C

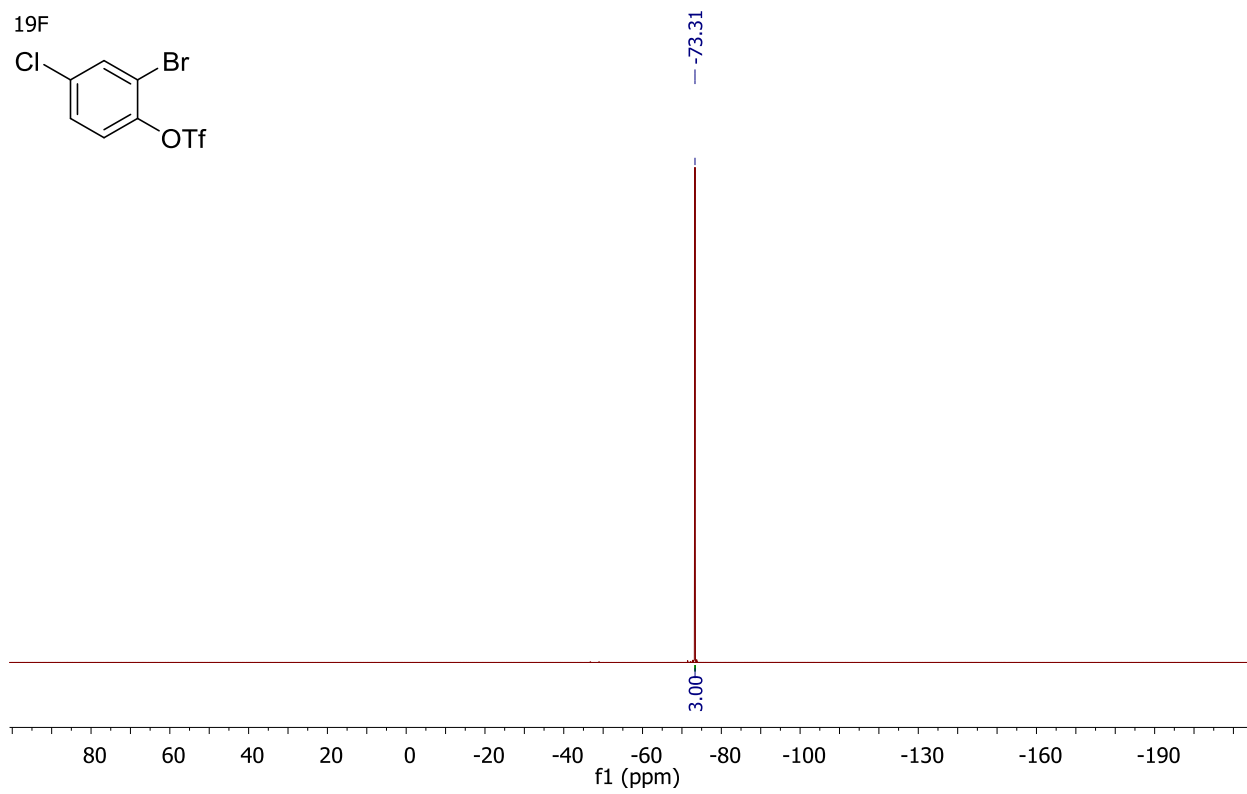
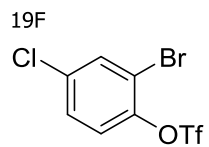
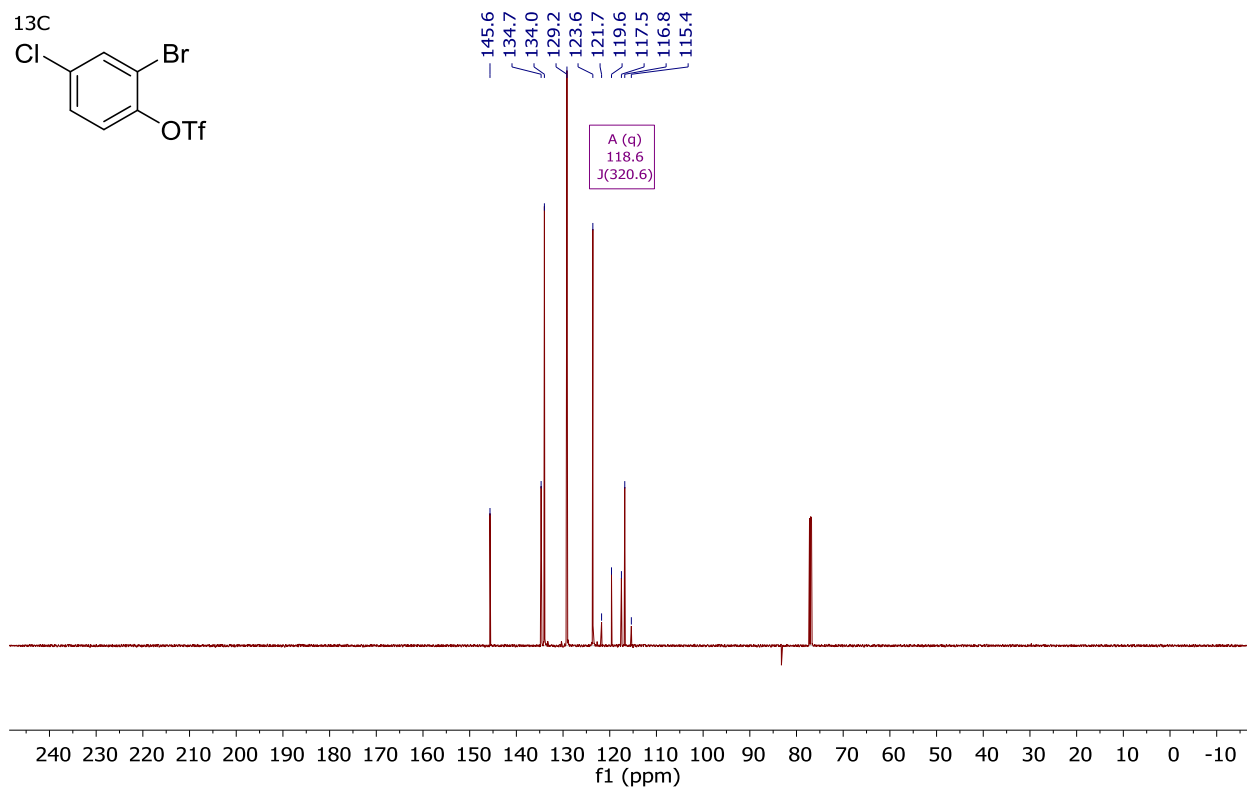
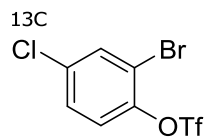


19F

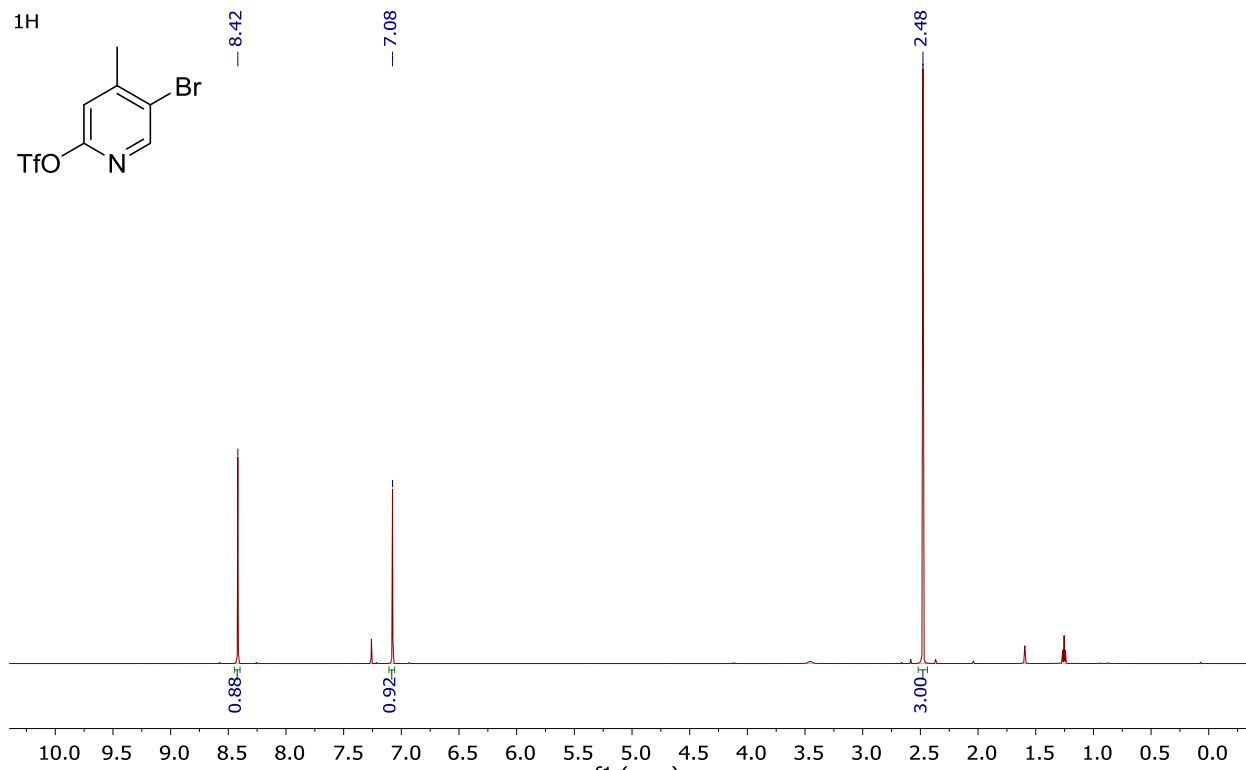
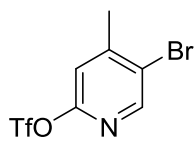


1H

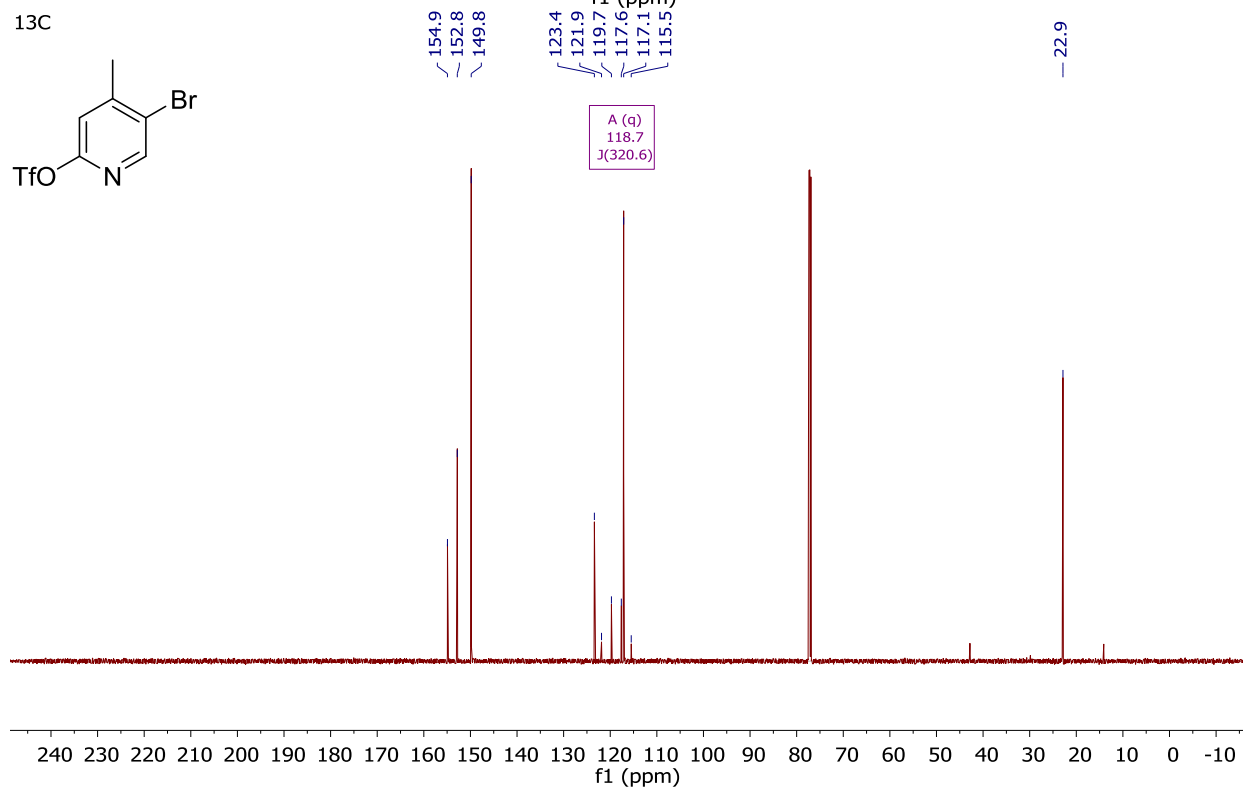
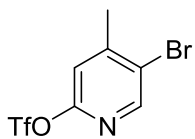




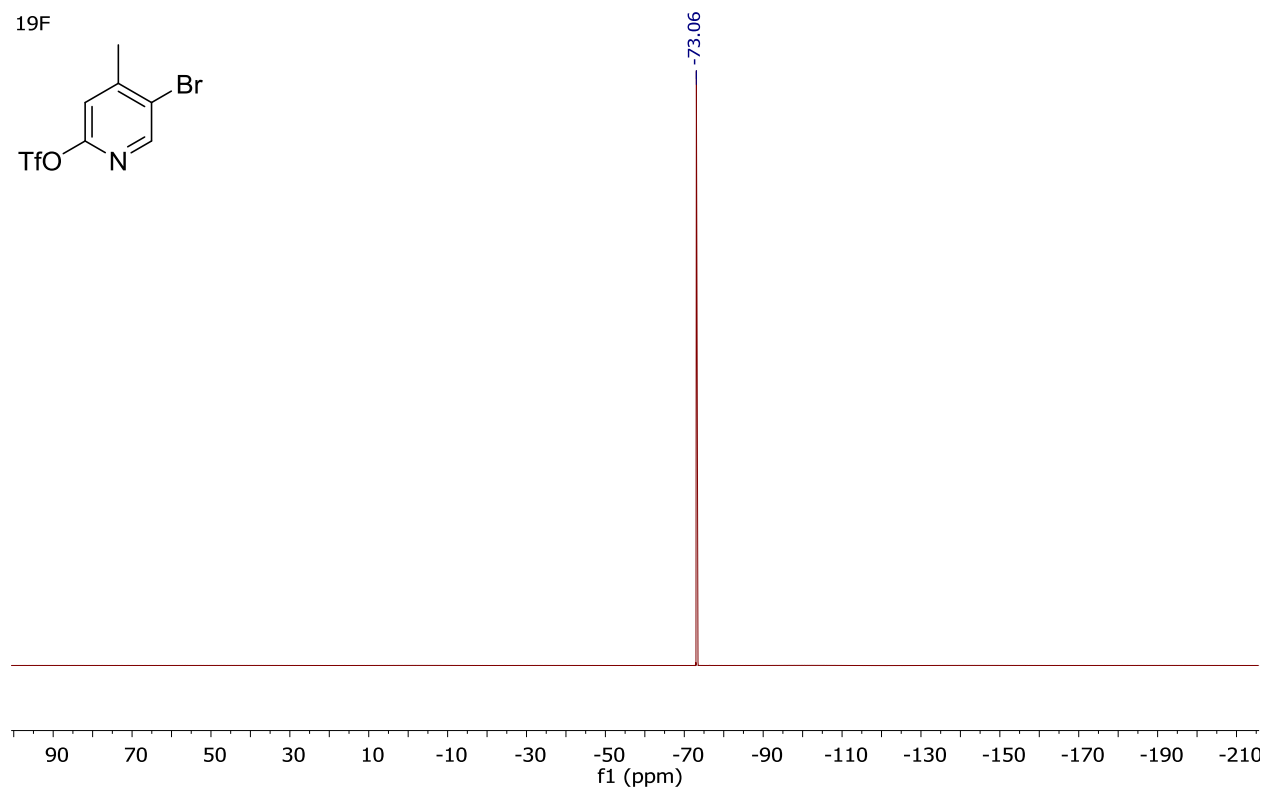
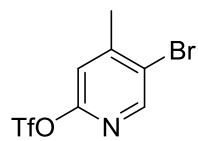
1H



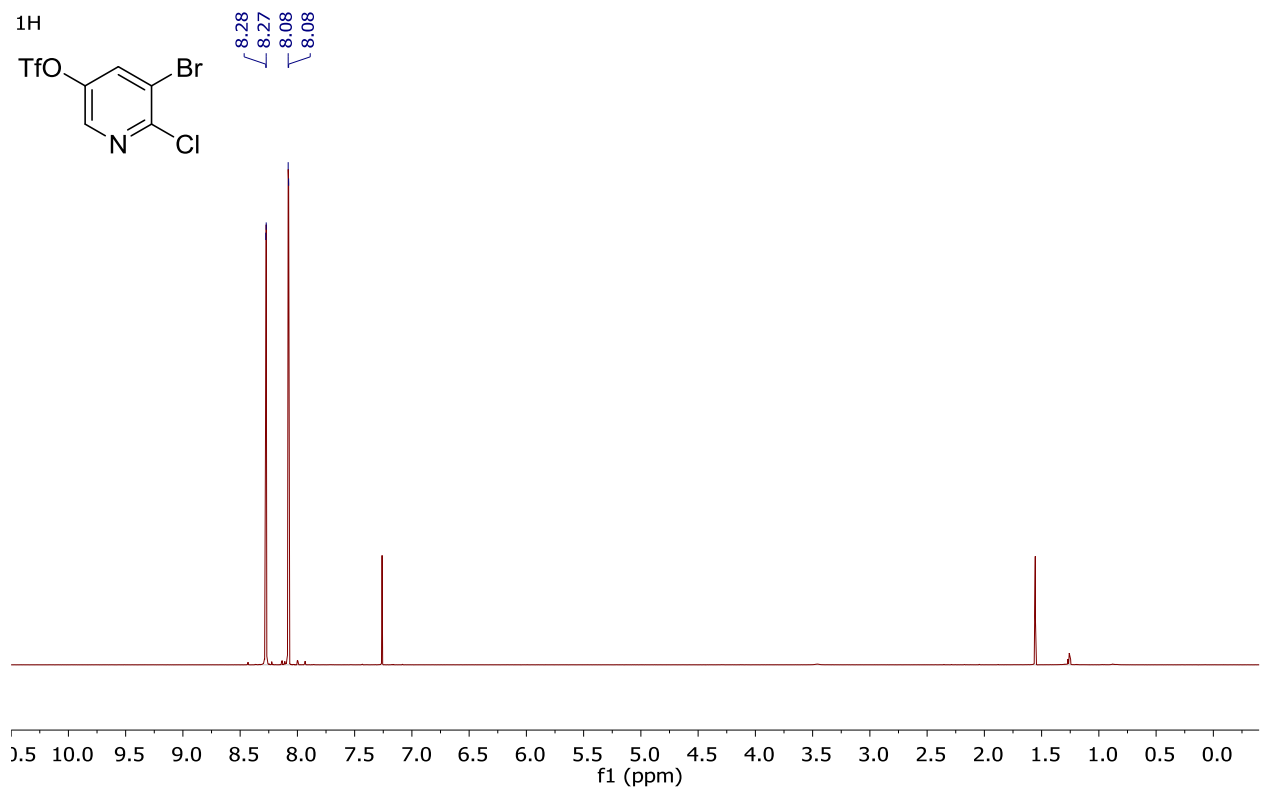
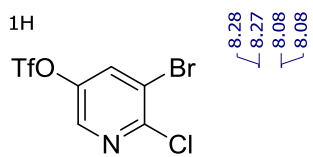
13C



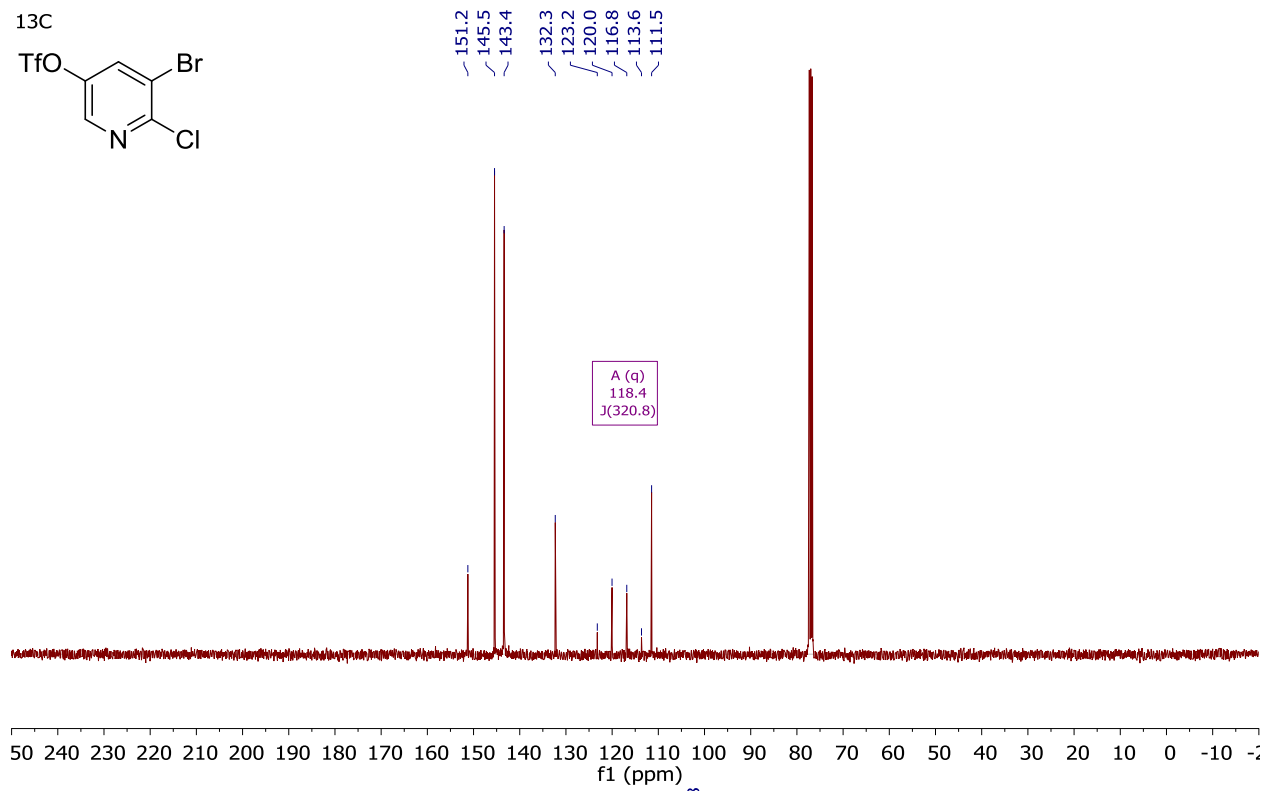
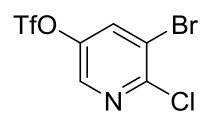
19F



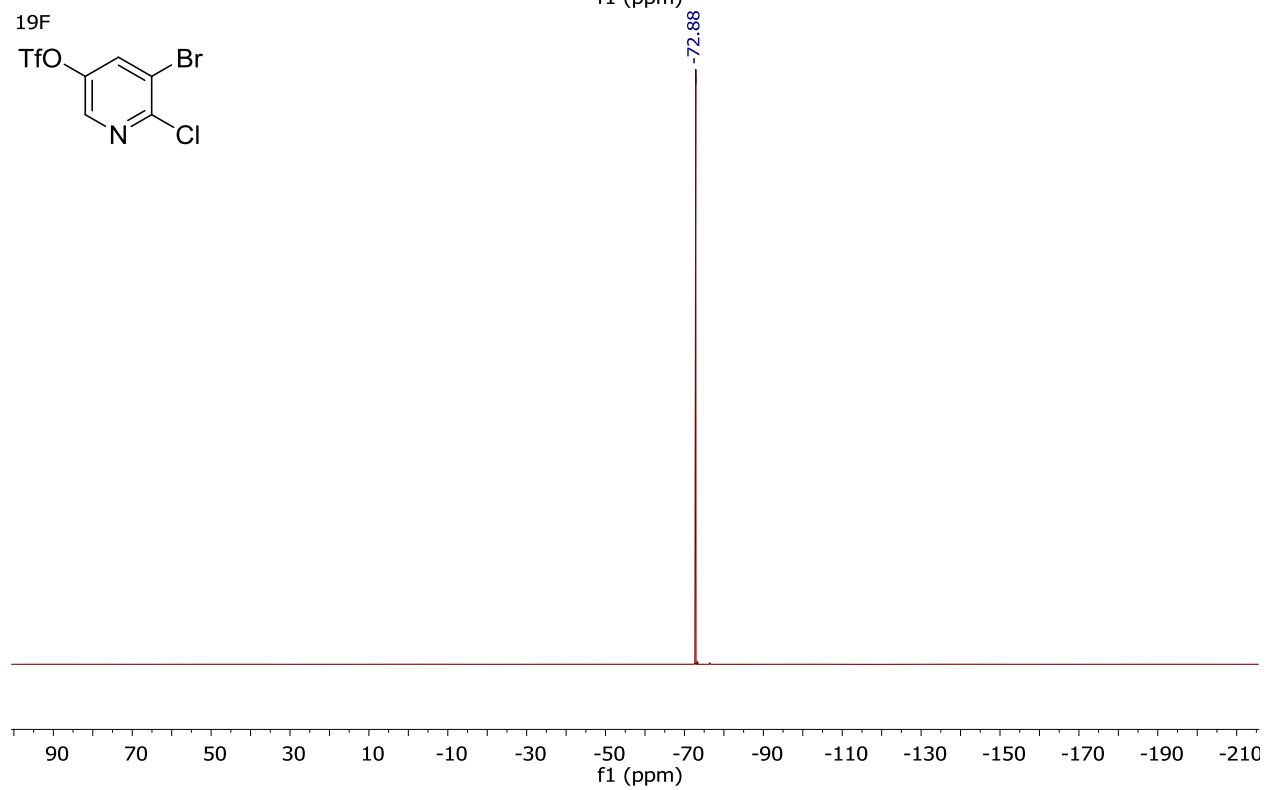
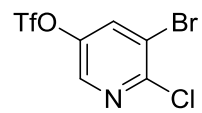
1H



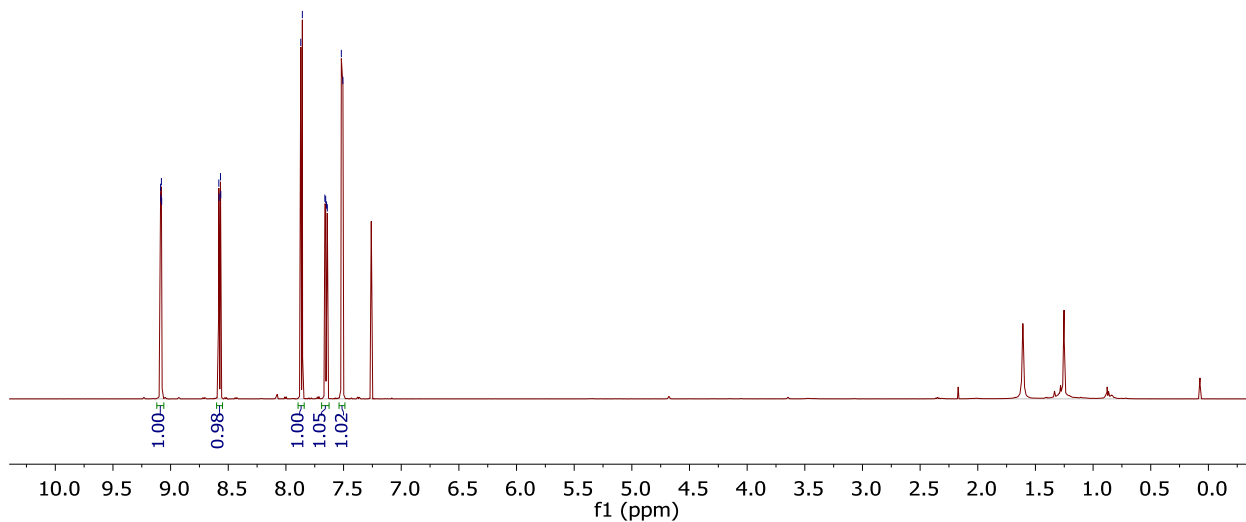
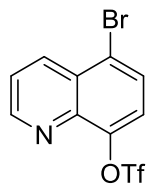
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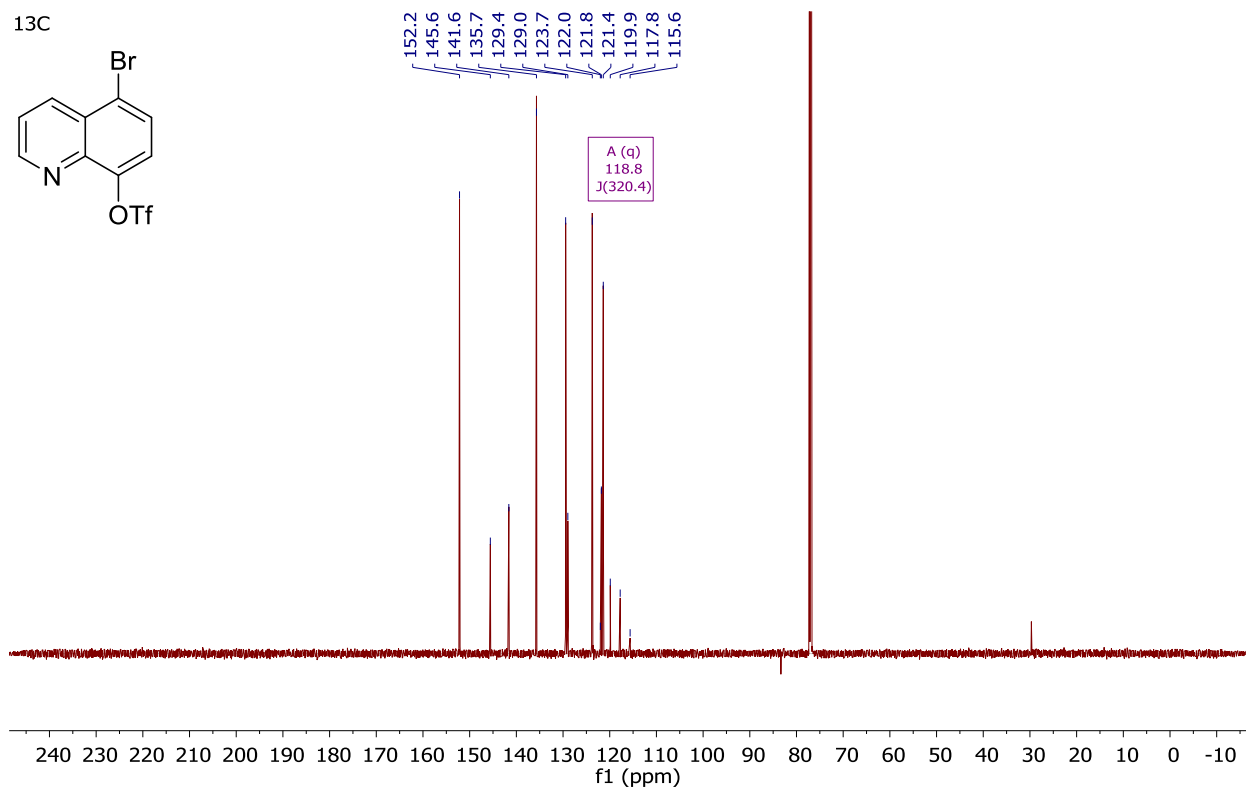
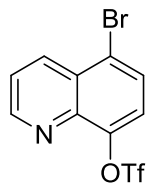
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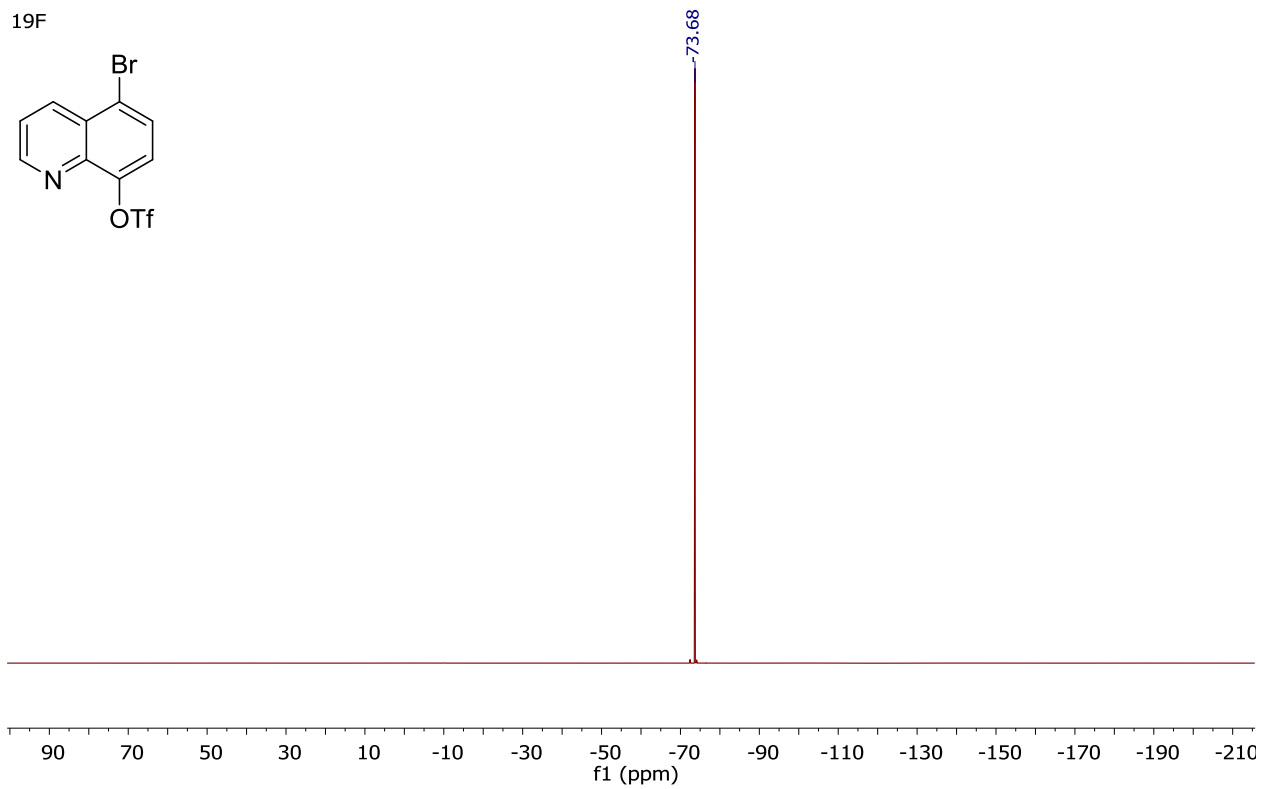
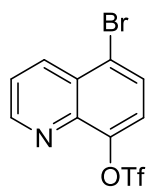
¹H
9.09
9.08
9.08
9.08
8.58
8.58
8.57
8.57
7.87
7.86
7.66
7.66
7.66
7.65
7.64
7.52
7.51



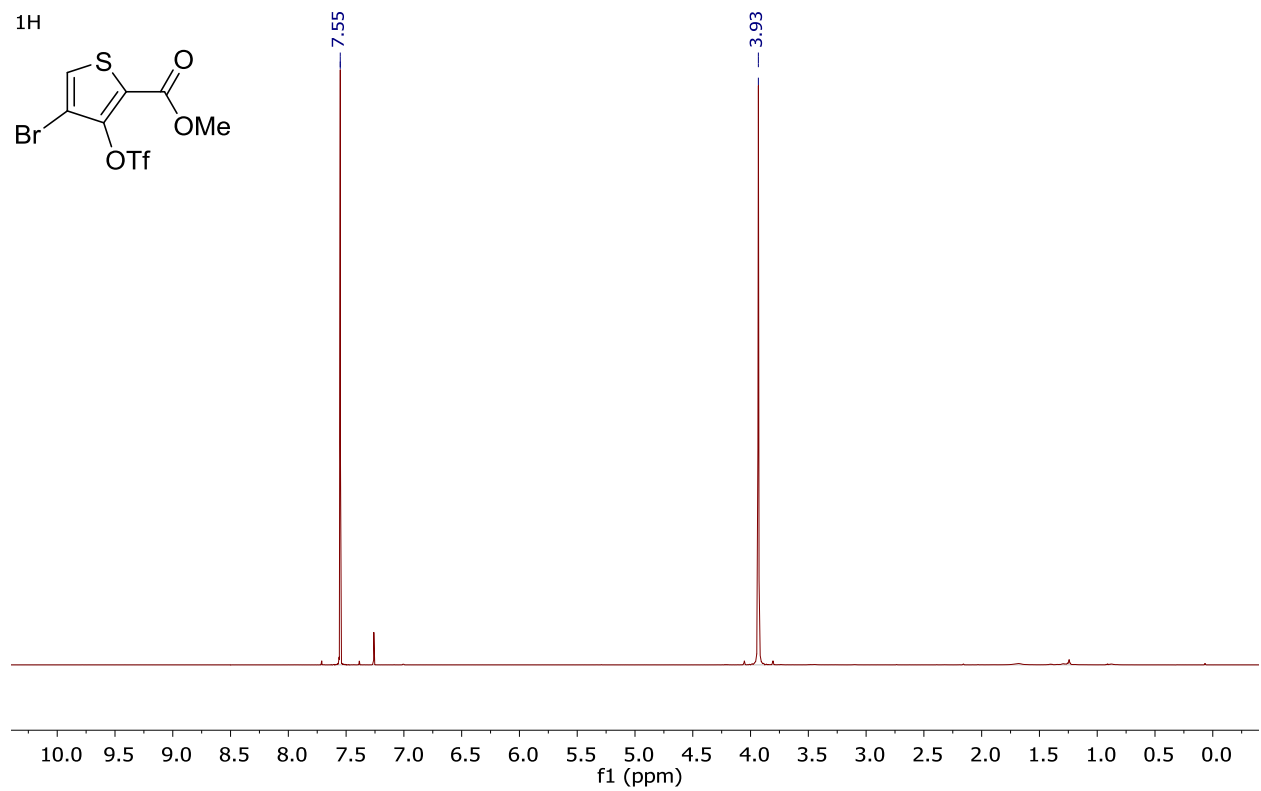
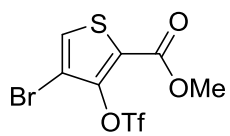
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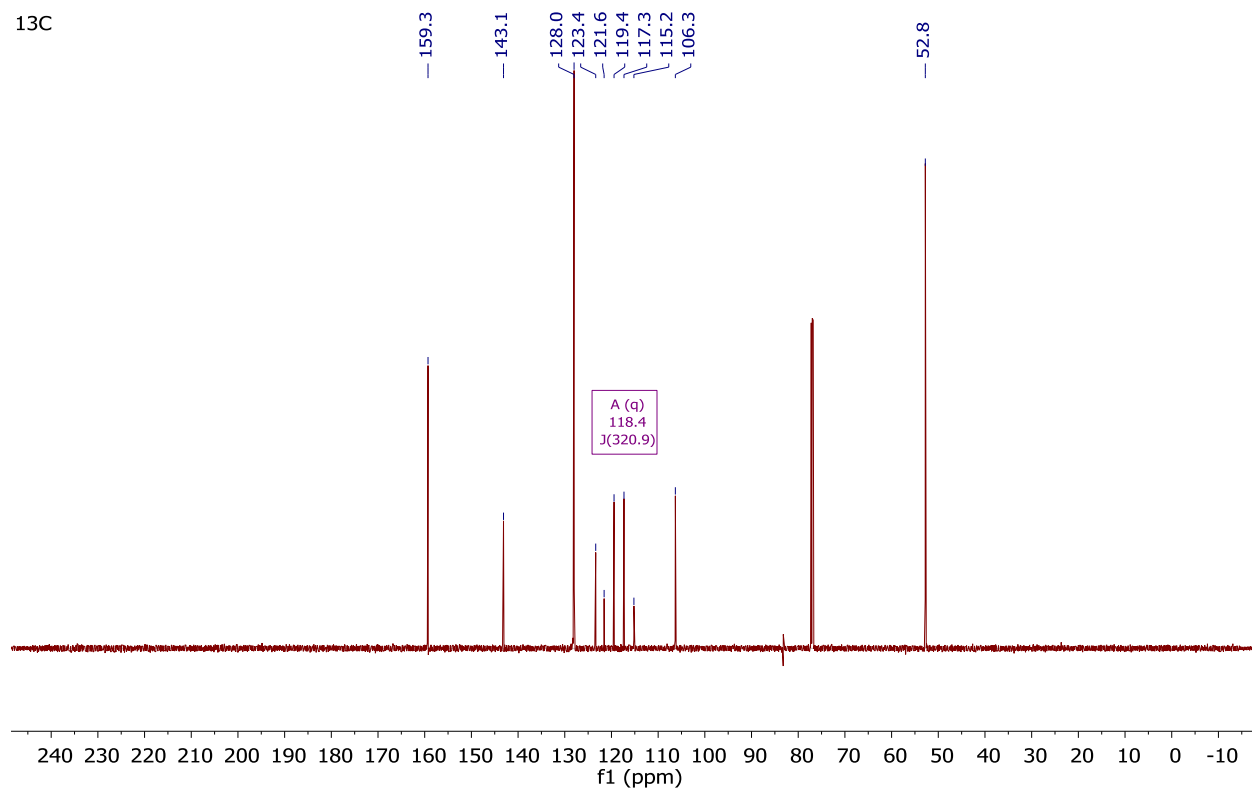
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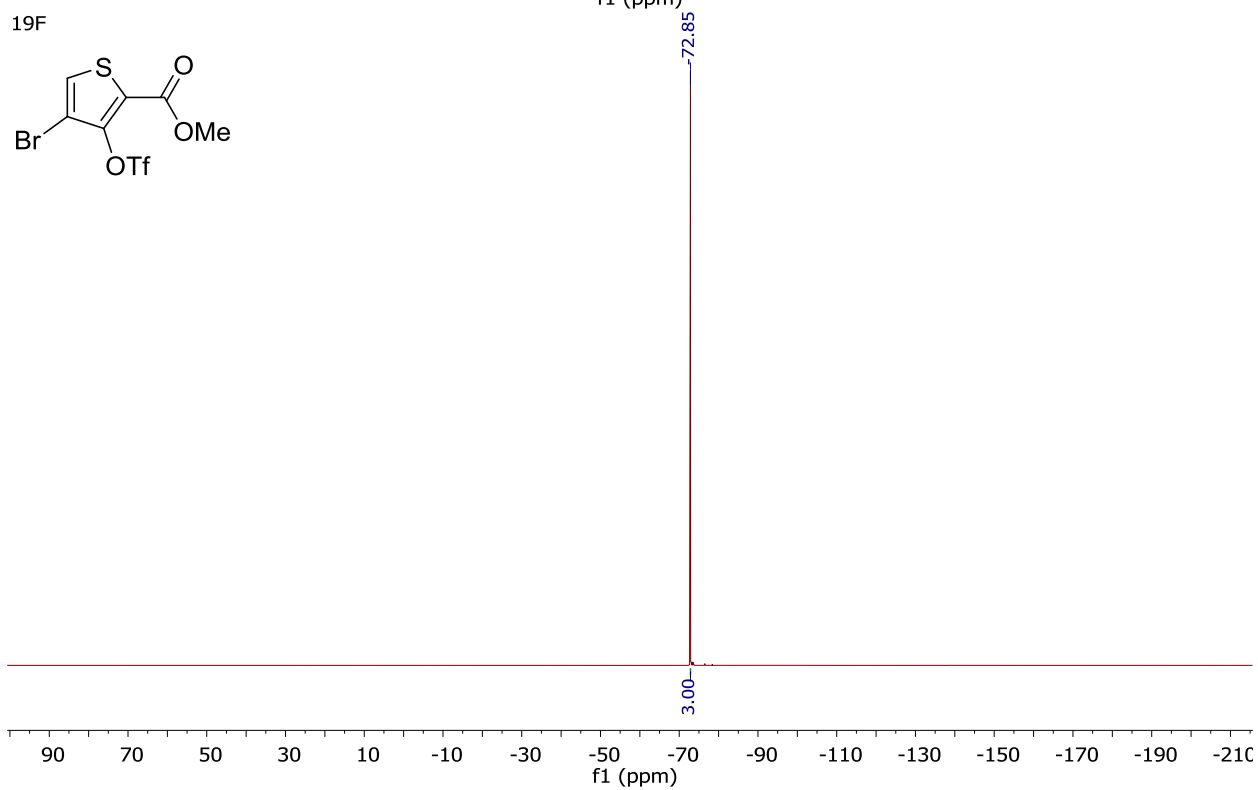
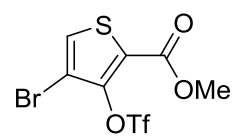
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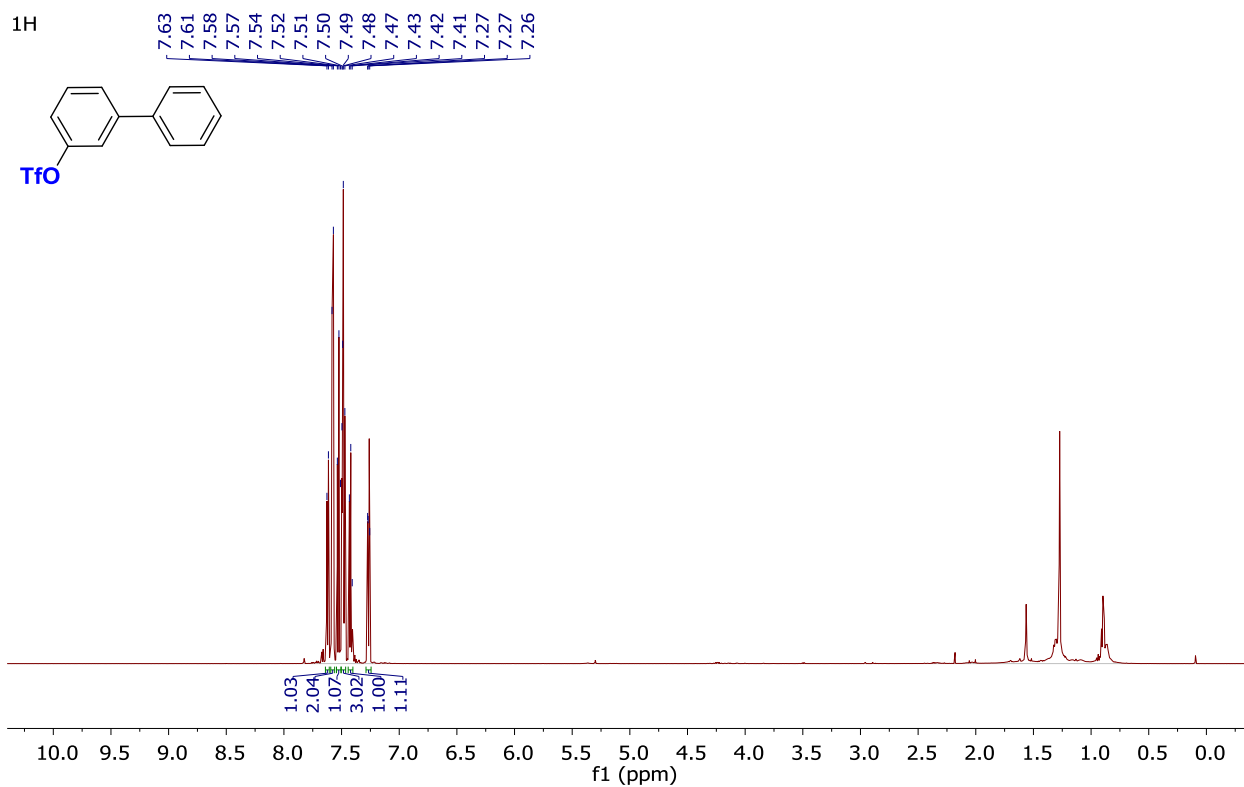
13C



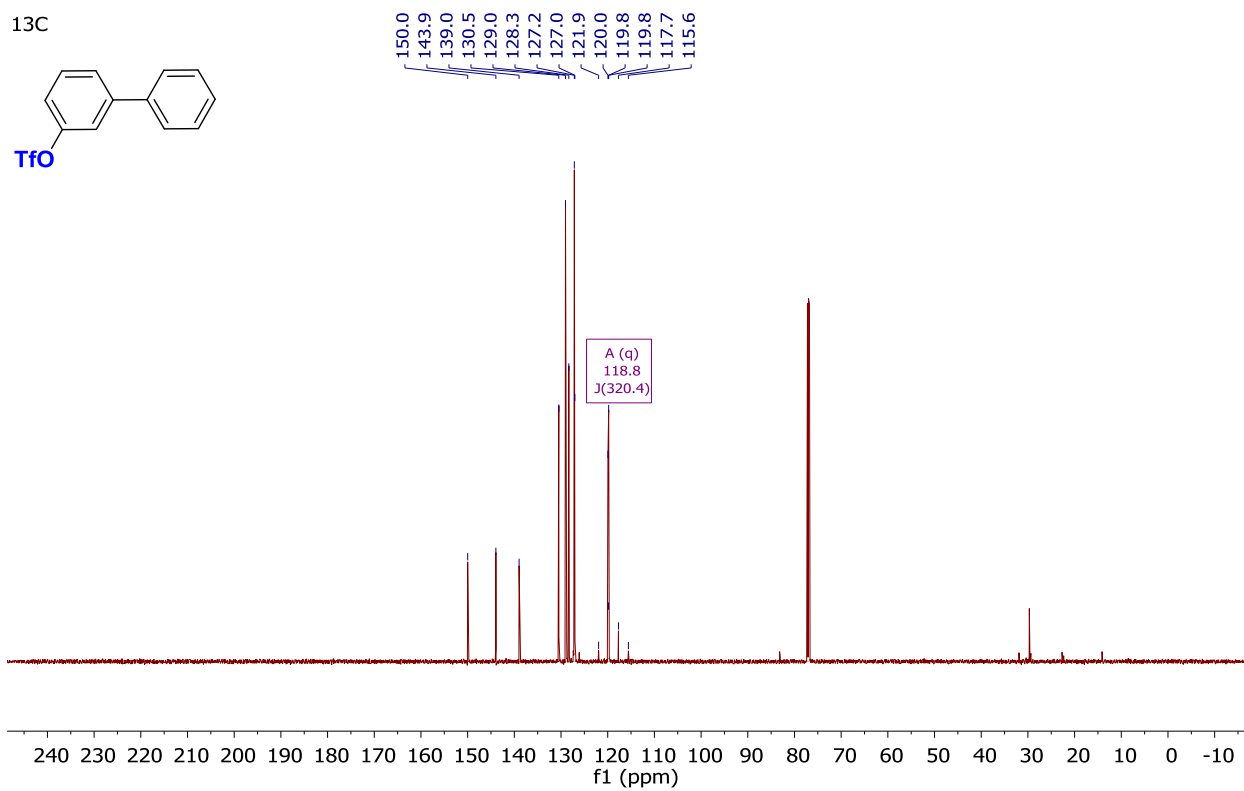
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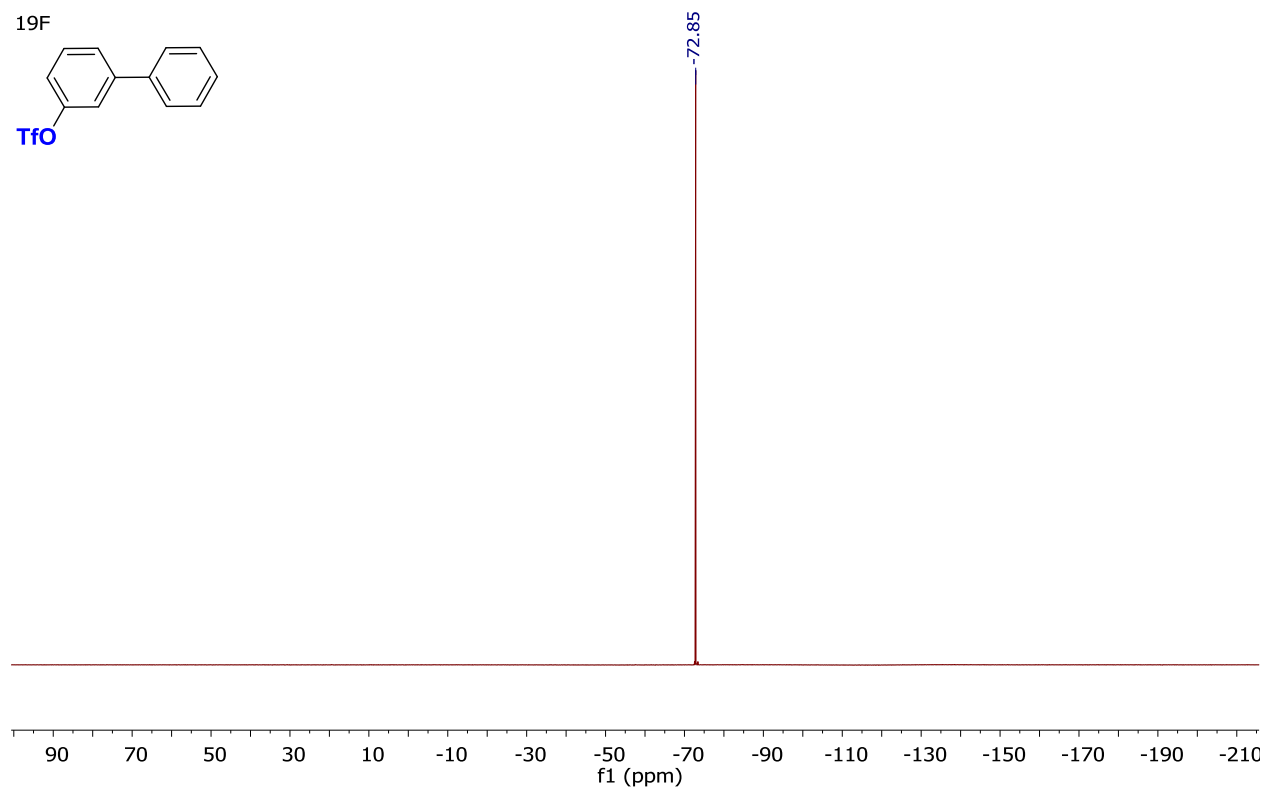
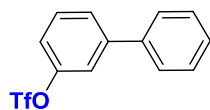
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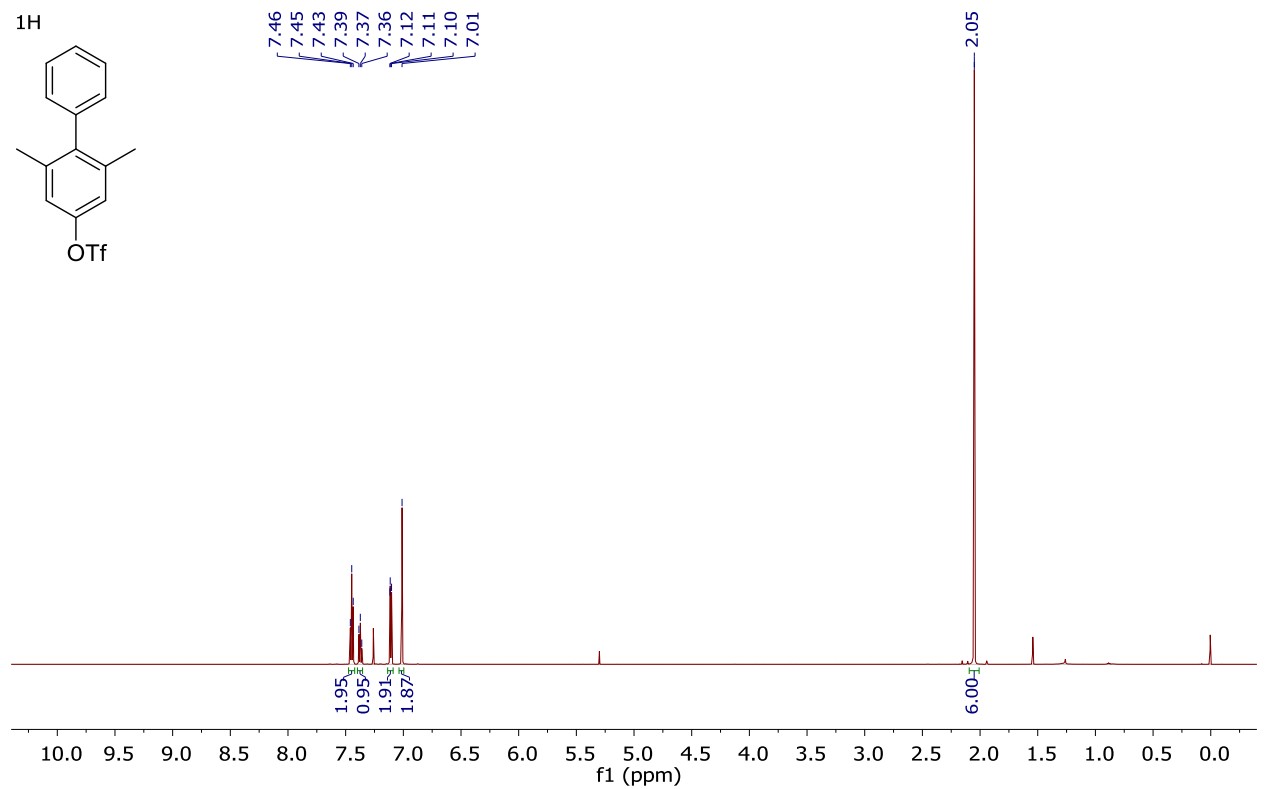
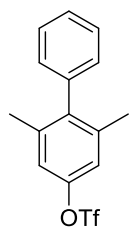
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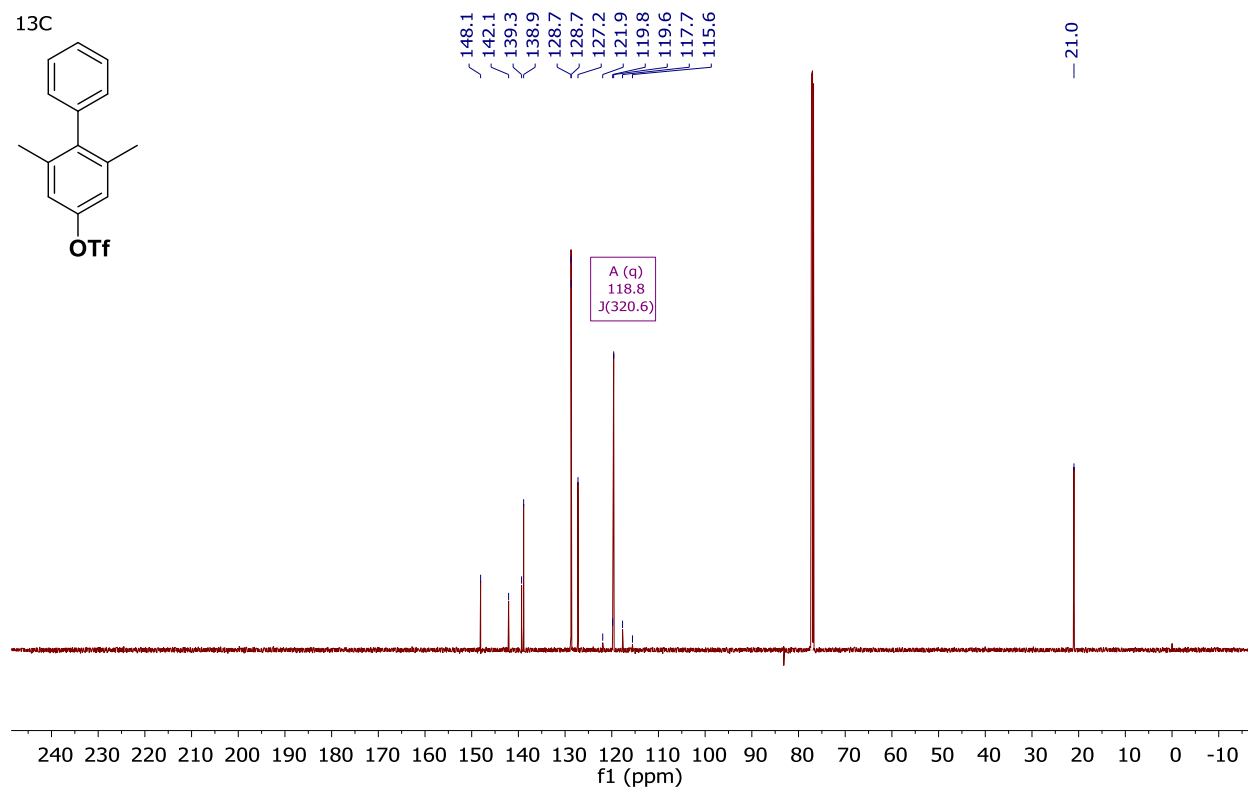
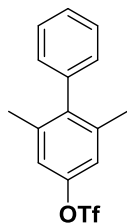
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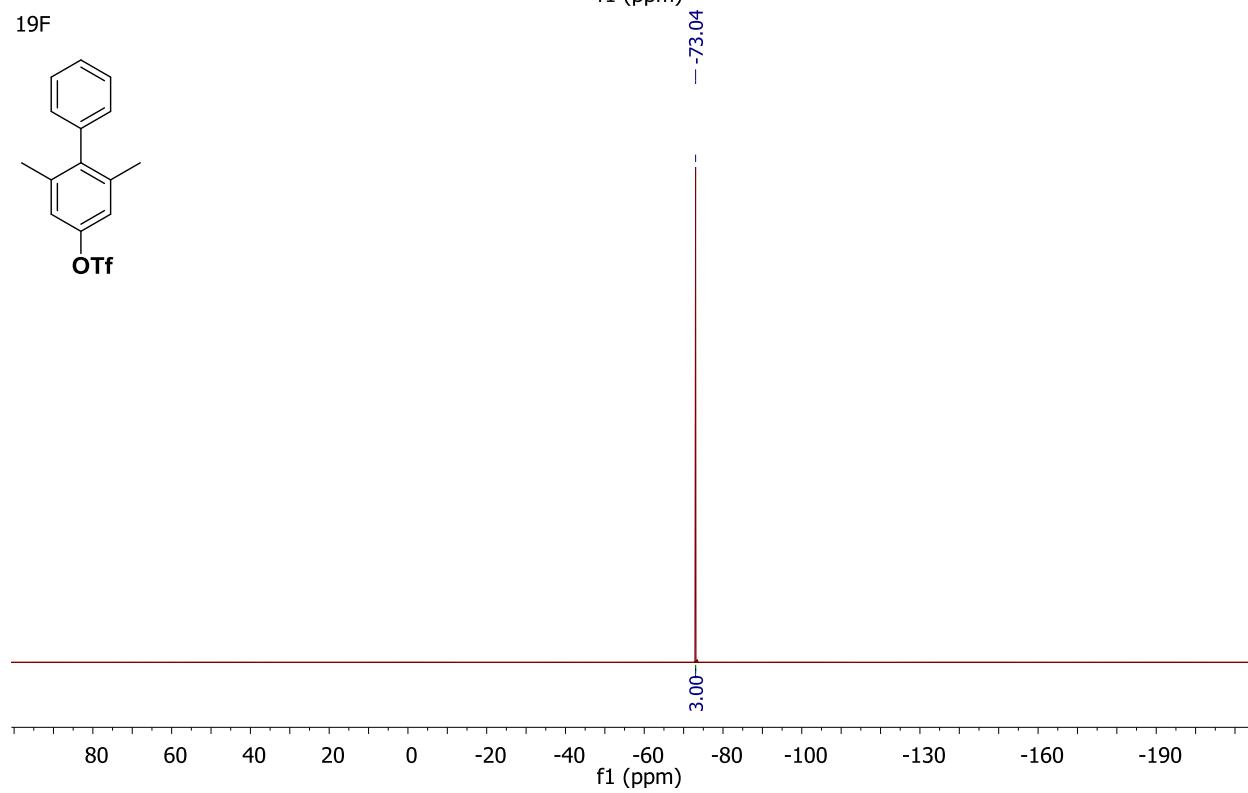
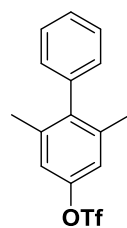
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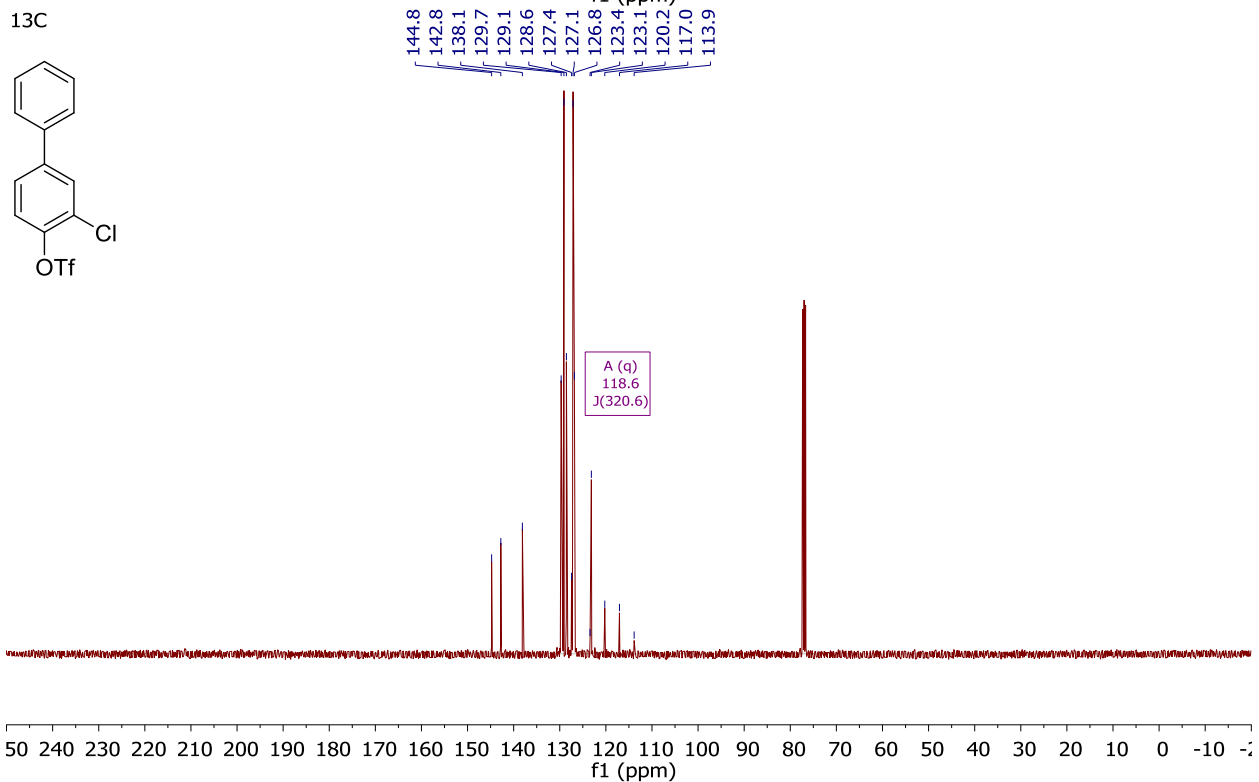
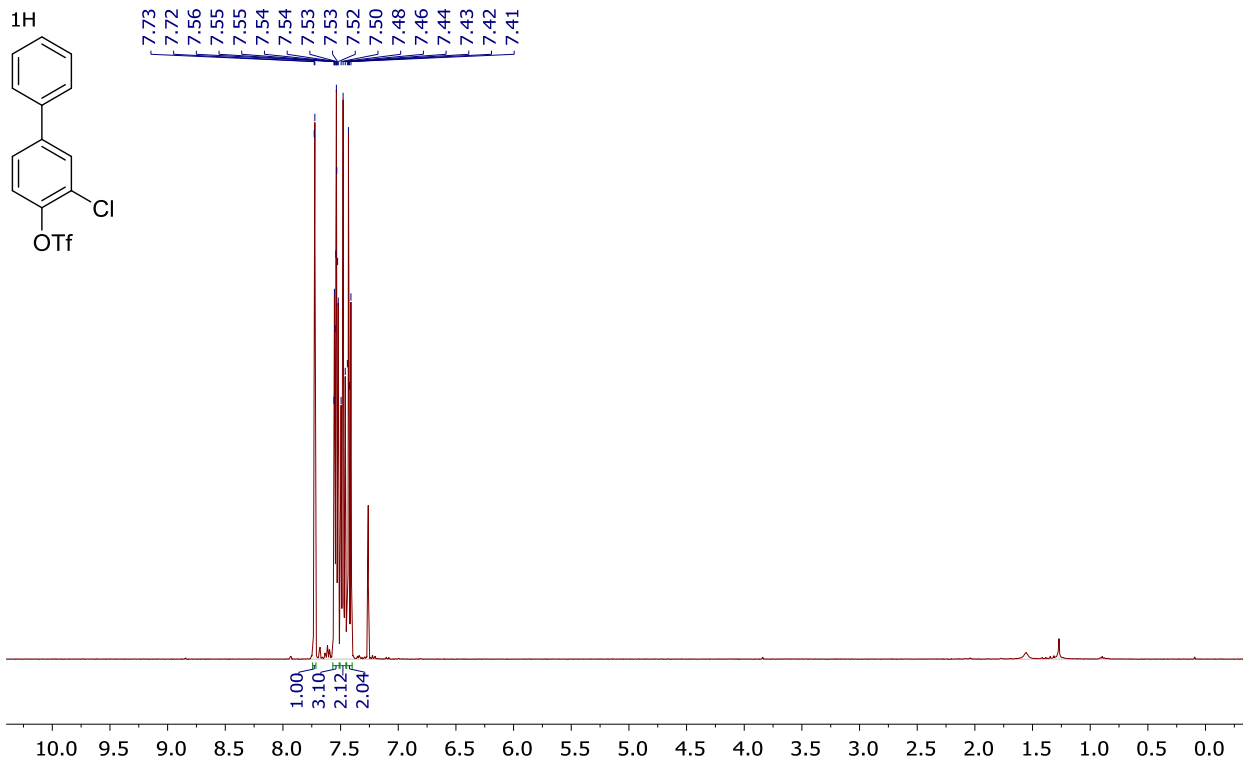


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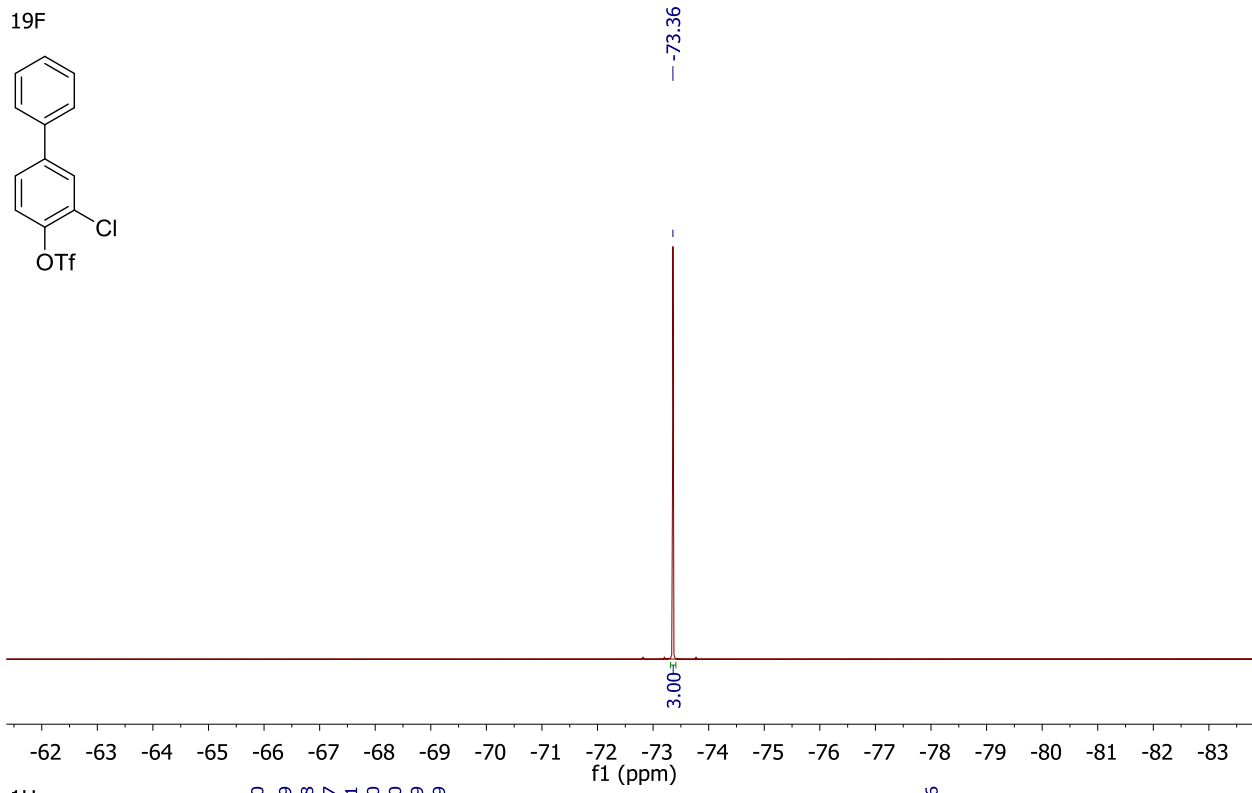
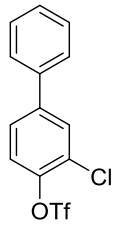


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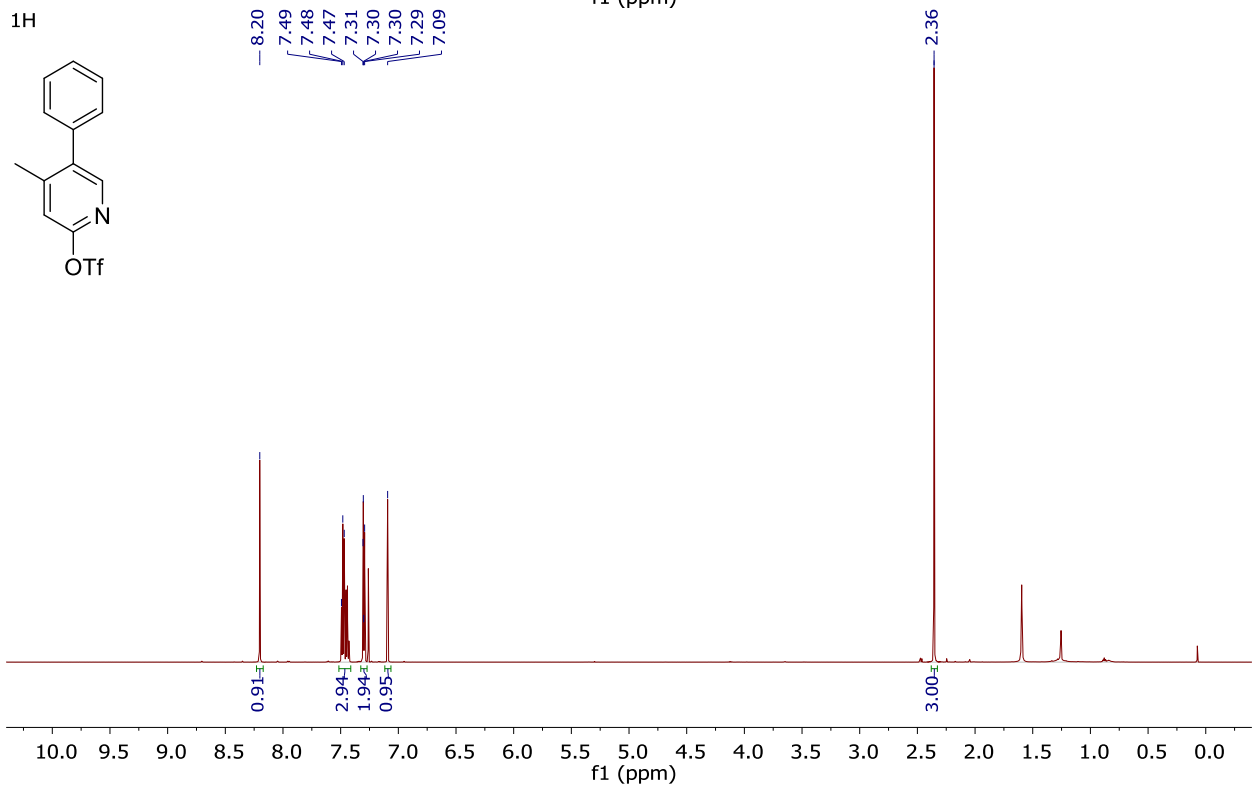
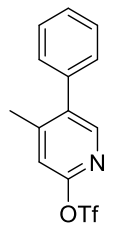




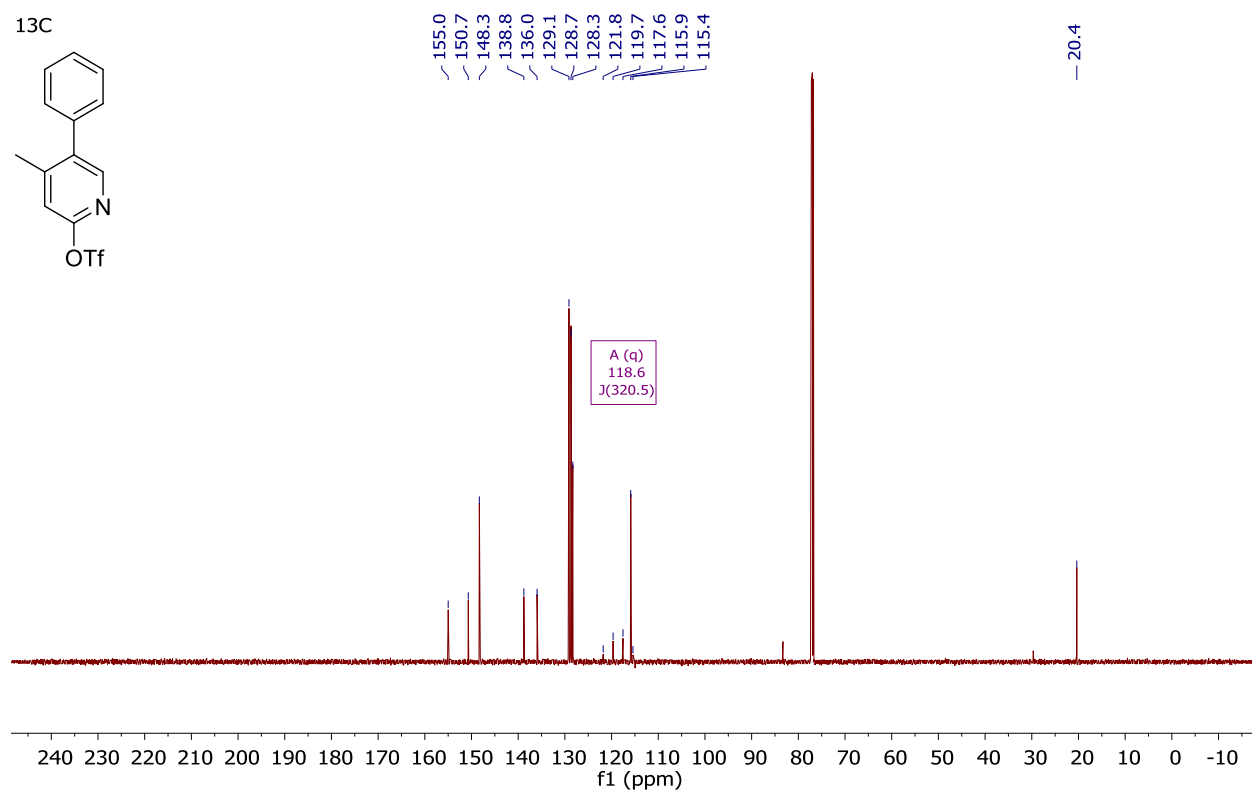
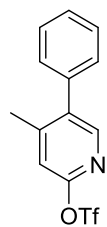
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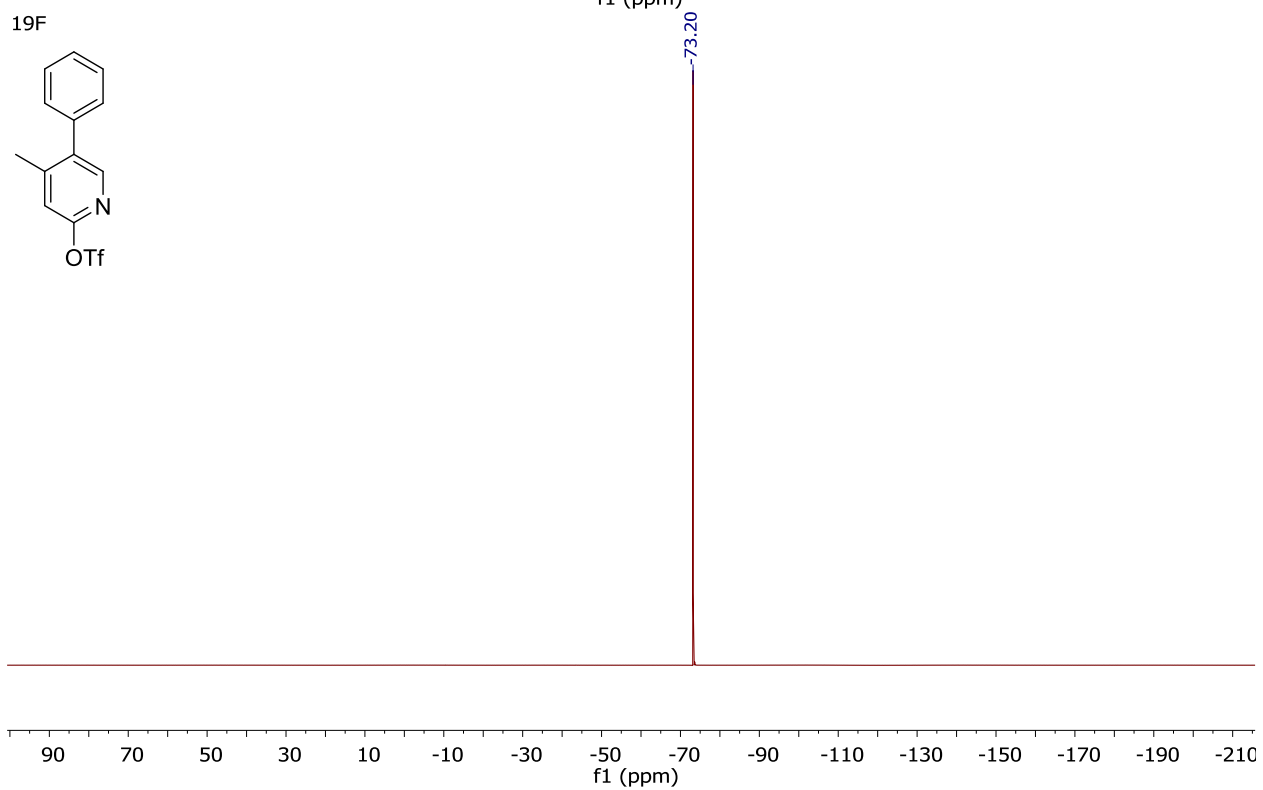
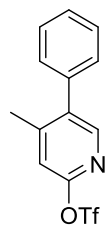
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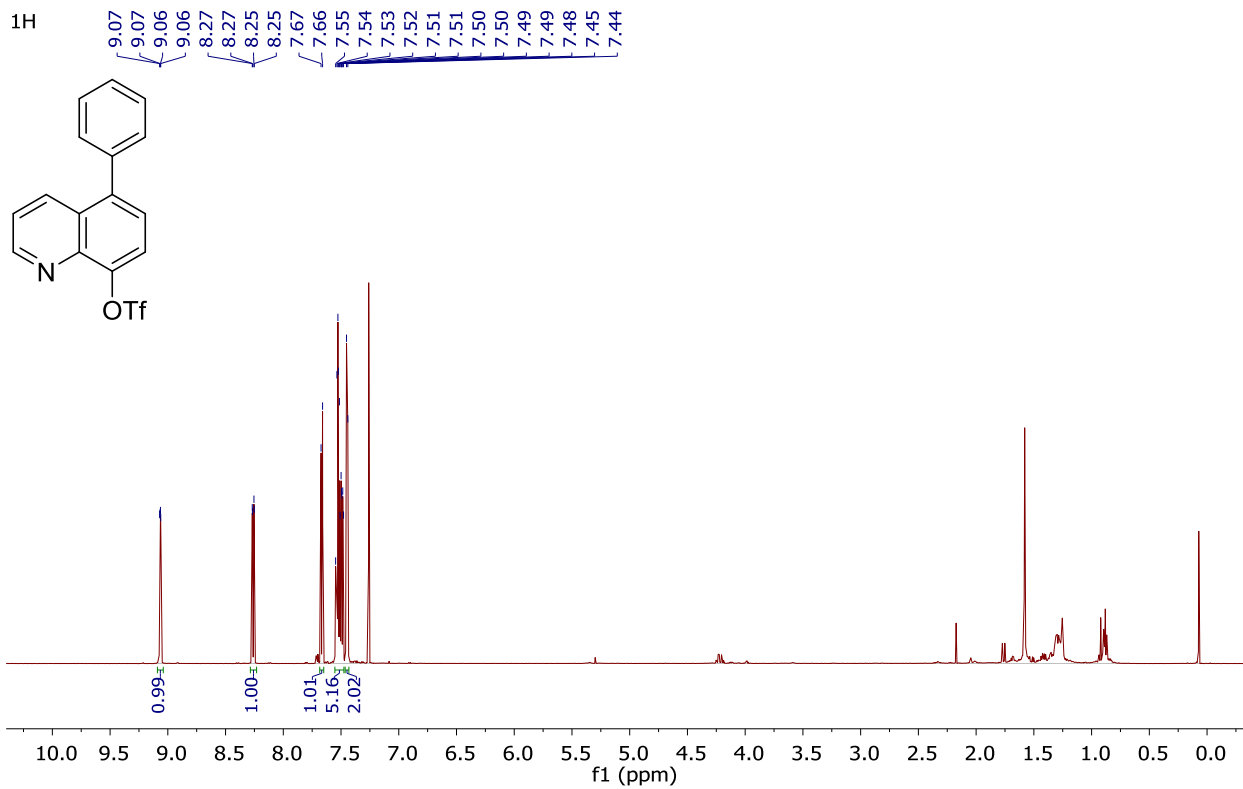
13C



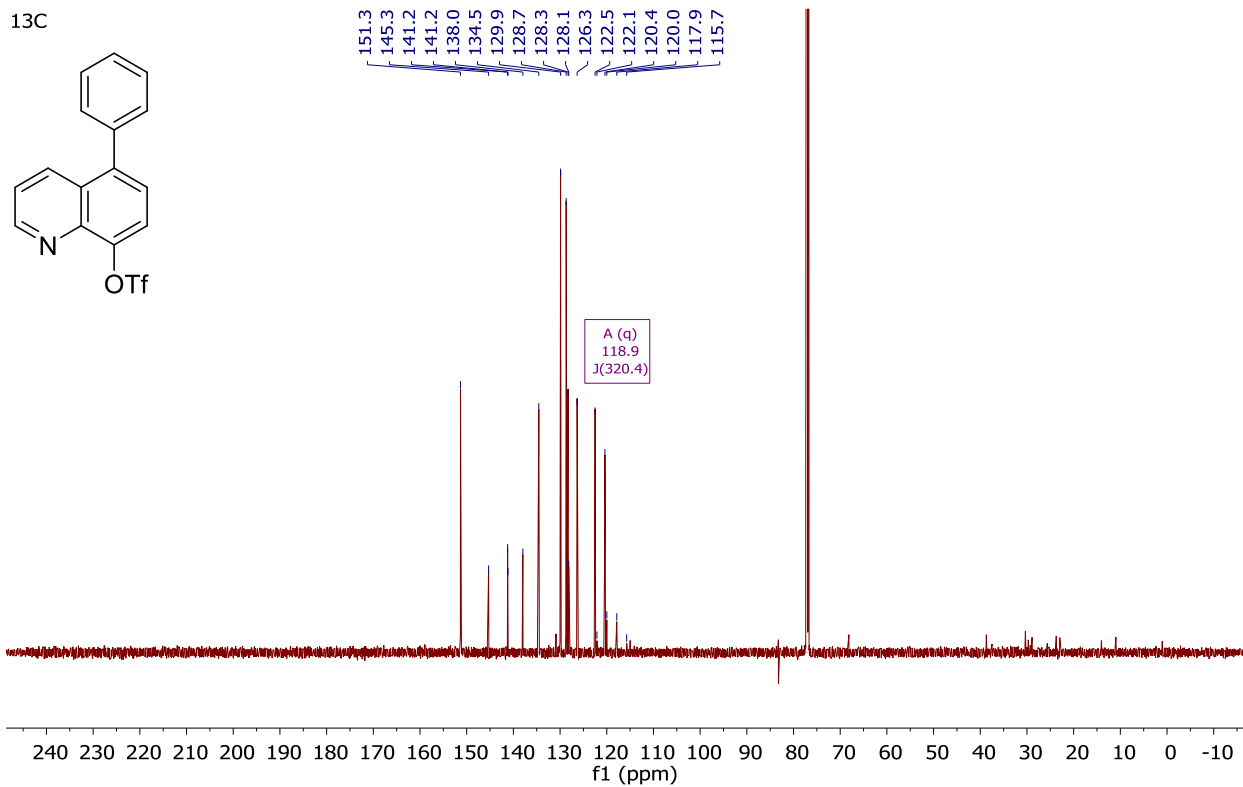
19F



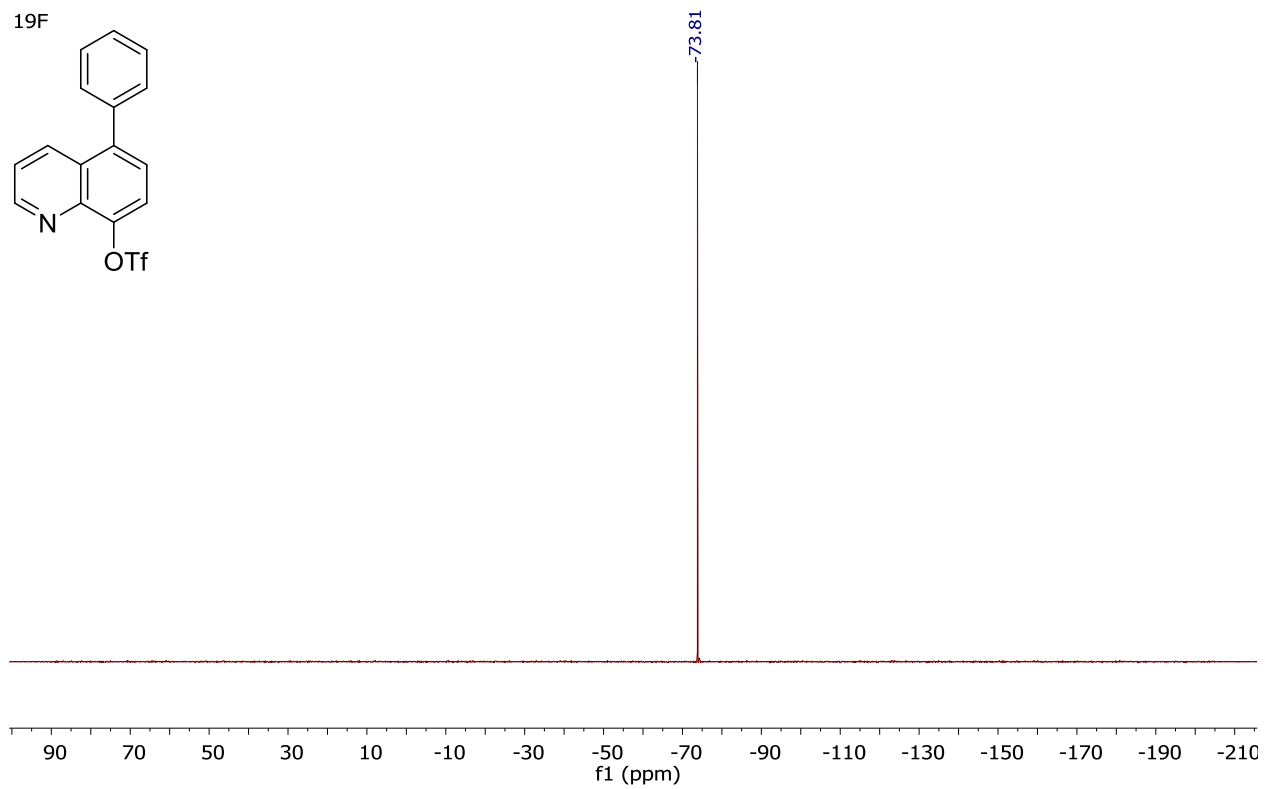
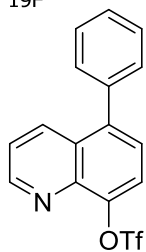
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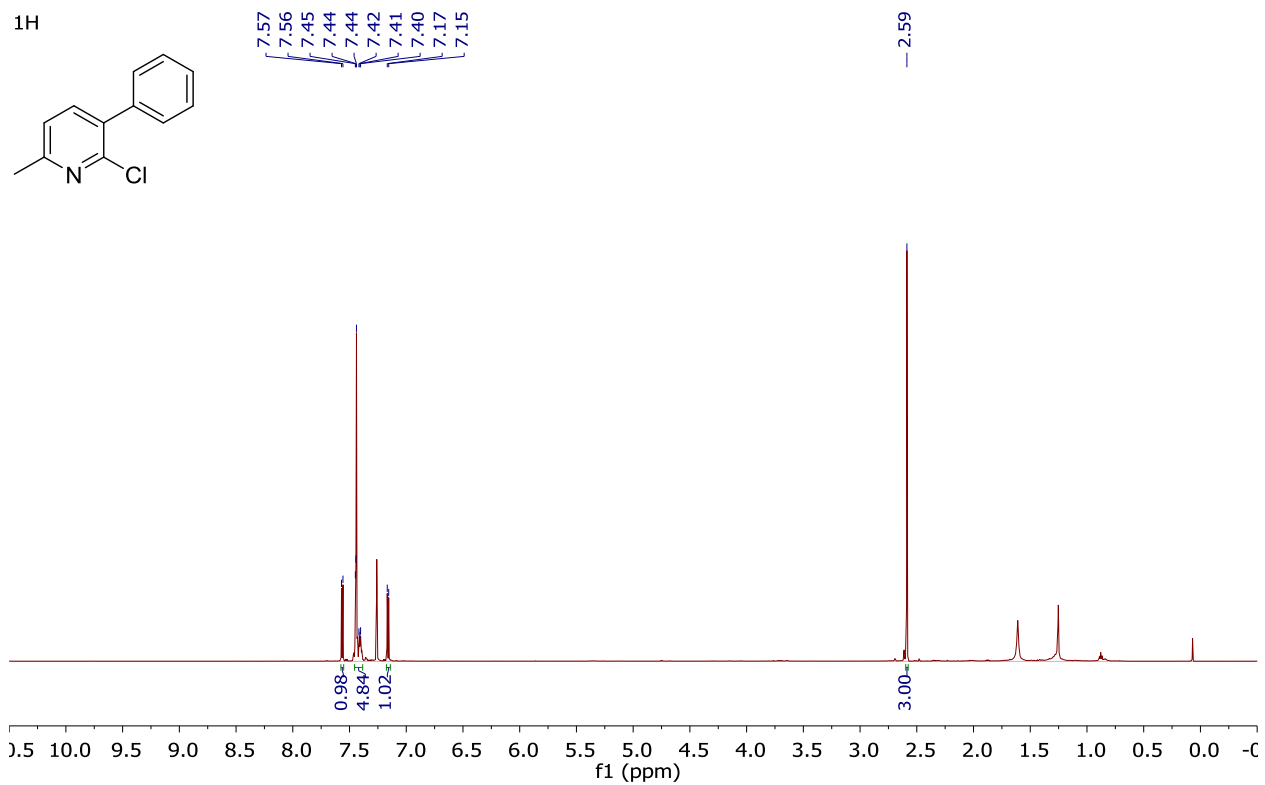
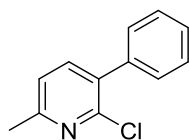
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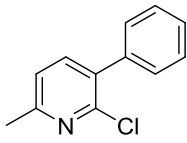
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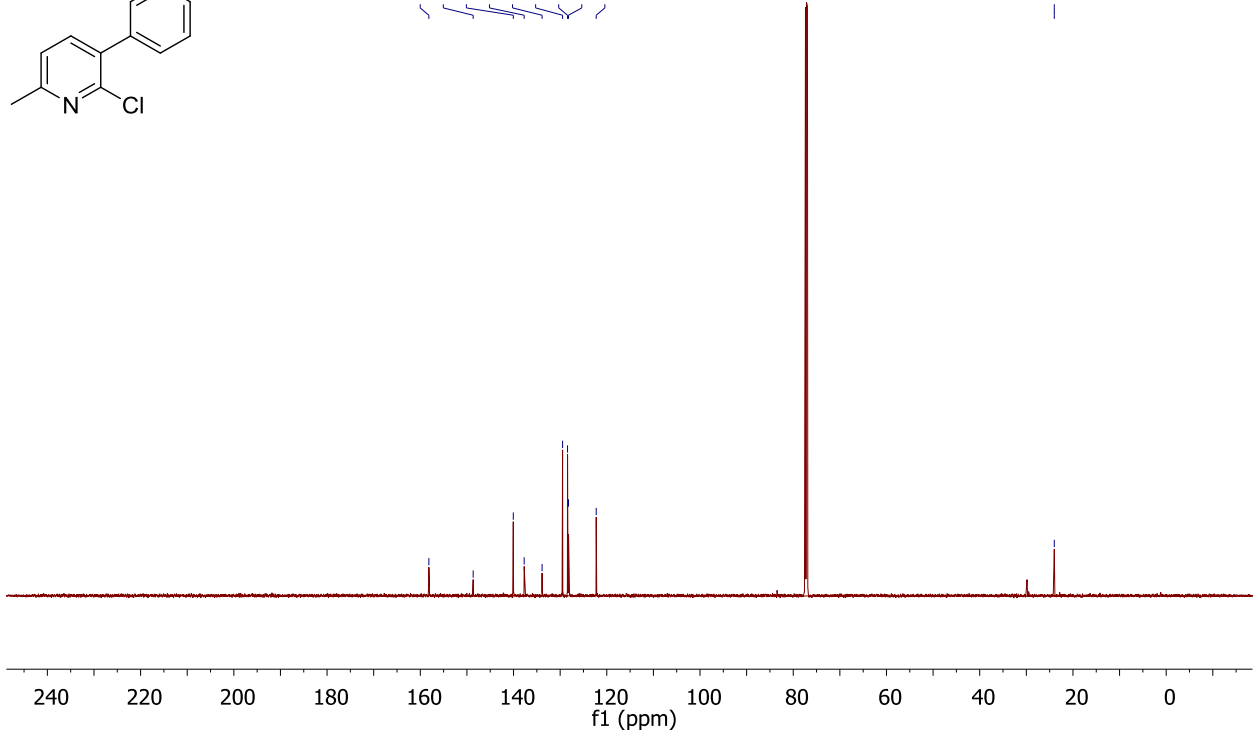


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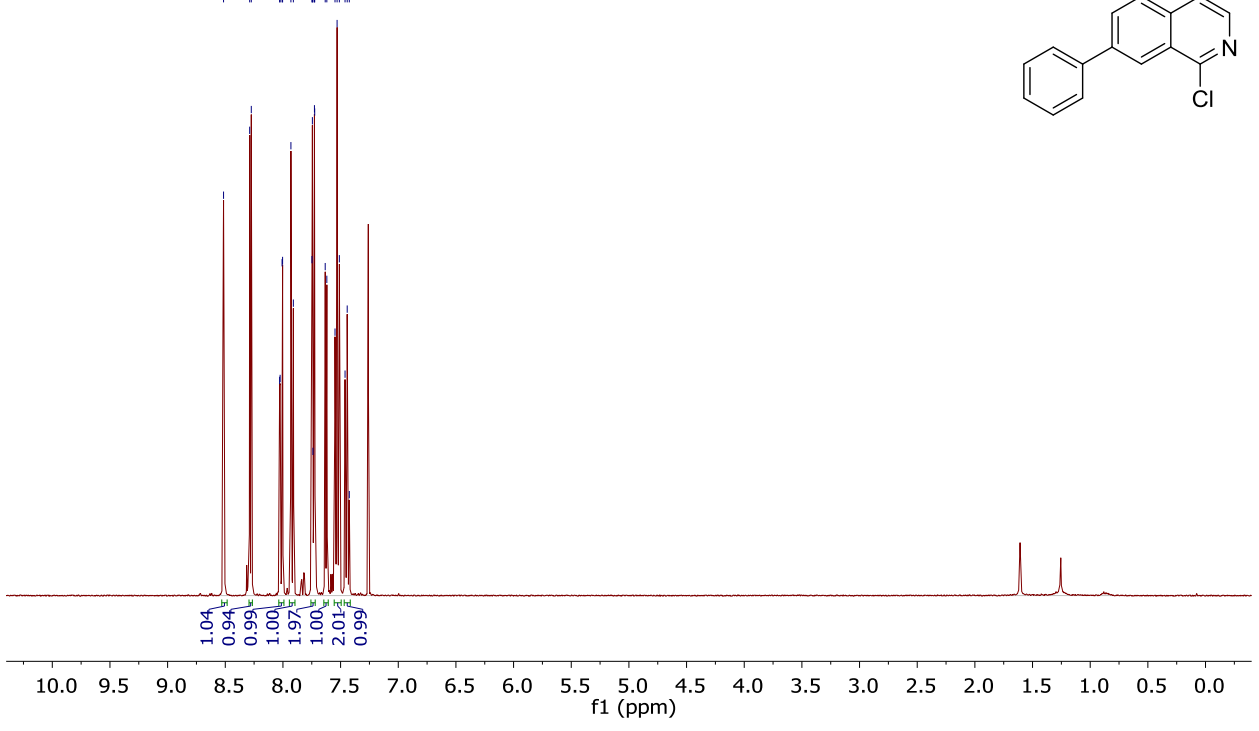
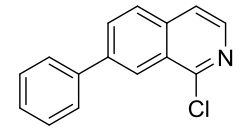


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140.1
137.7
133.9
129.5
128.4
128.2
122.3

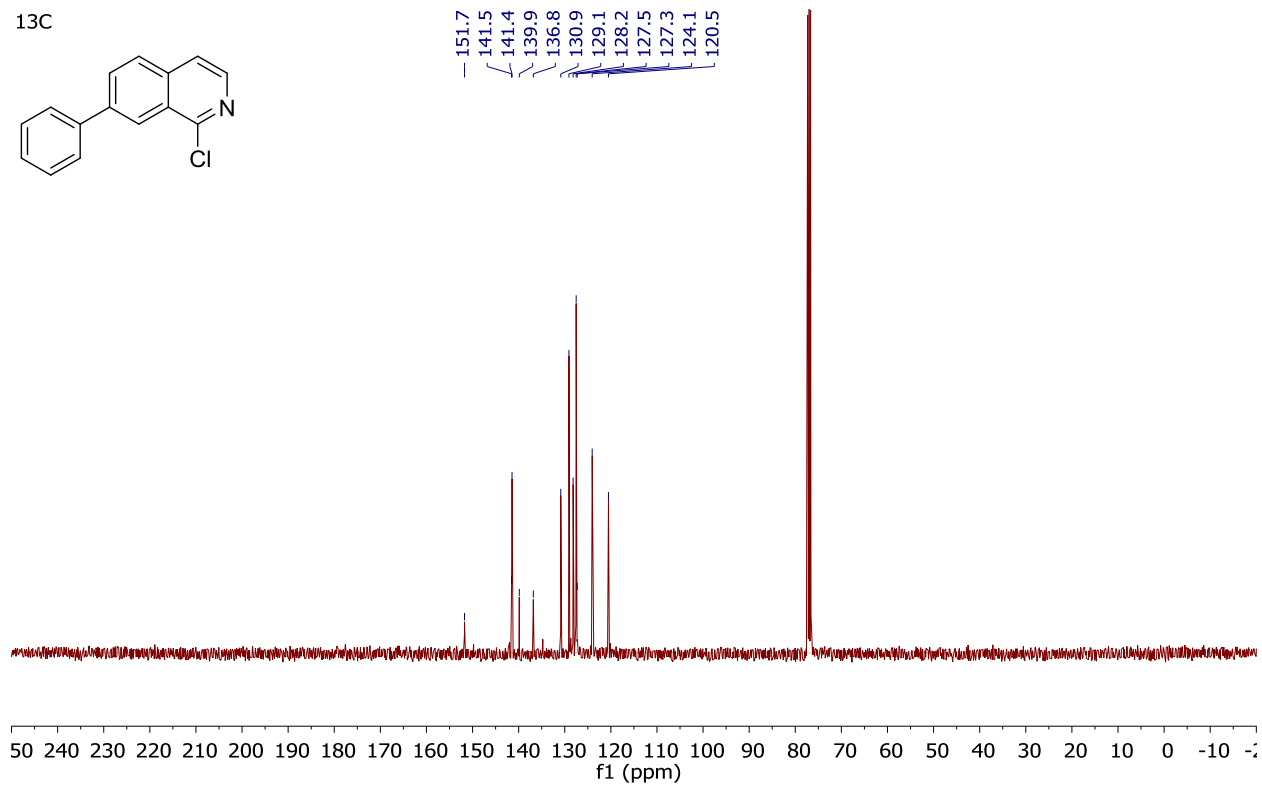
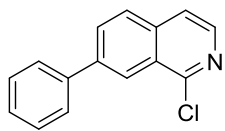
24.0



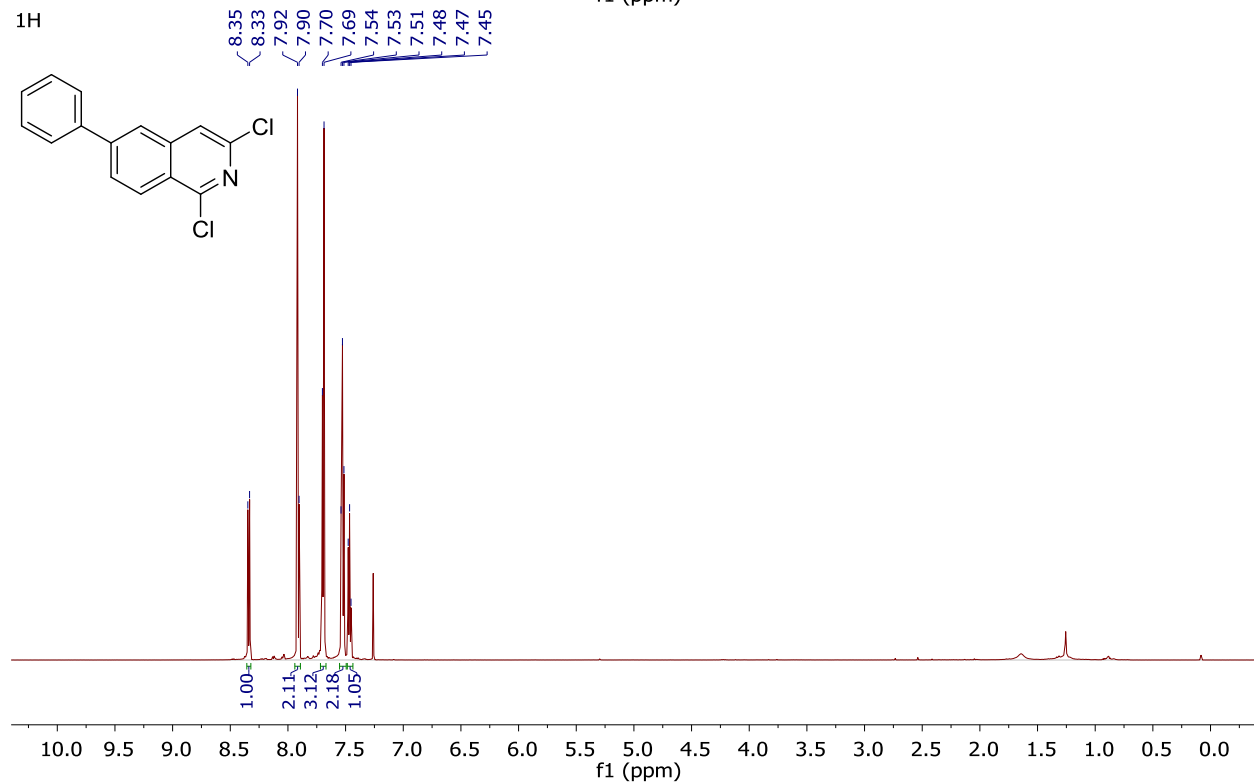
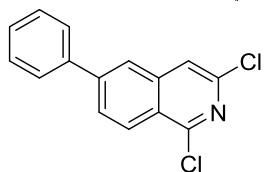
1H
8.51
8.29
8.27
8.03
8.02
8.01
8.00
7.93
7.91
7.75
7.74
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7.62
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7.53
7.51
7.46
7.44
7.42



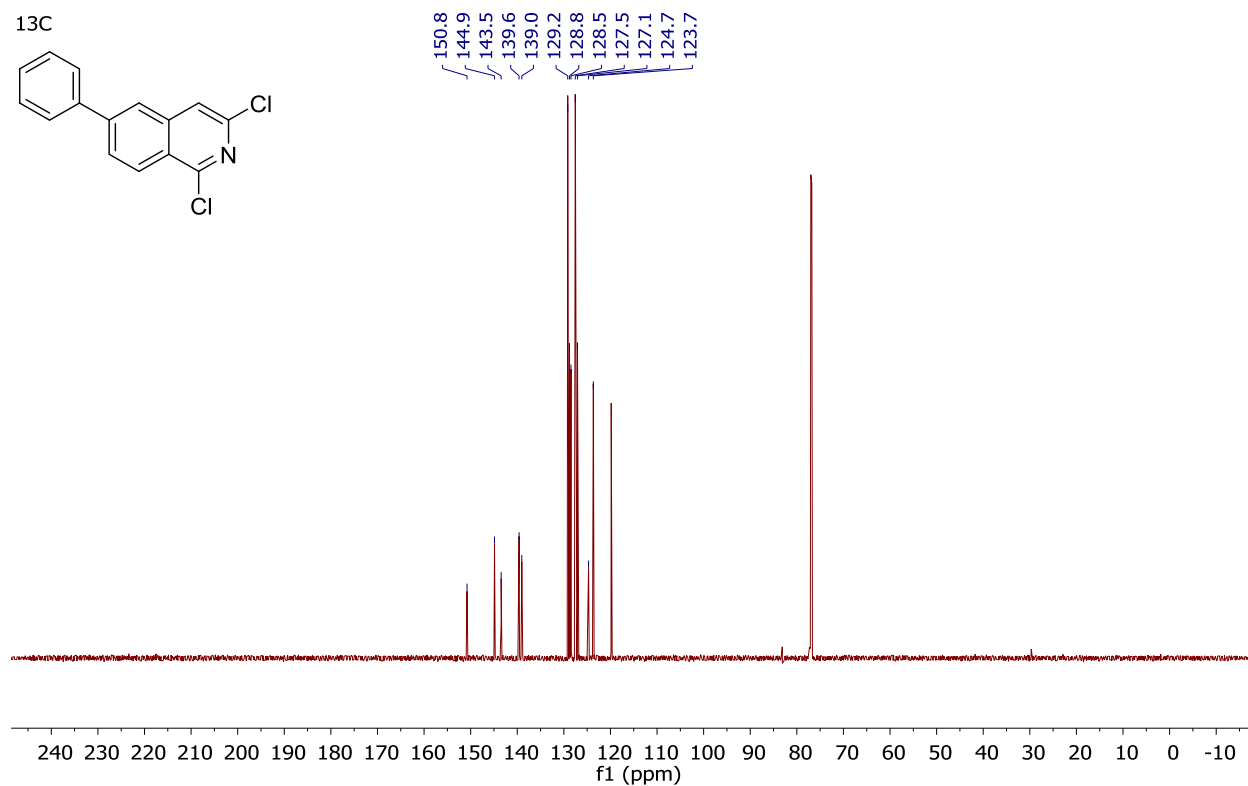
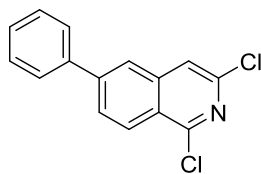
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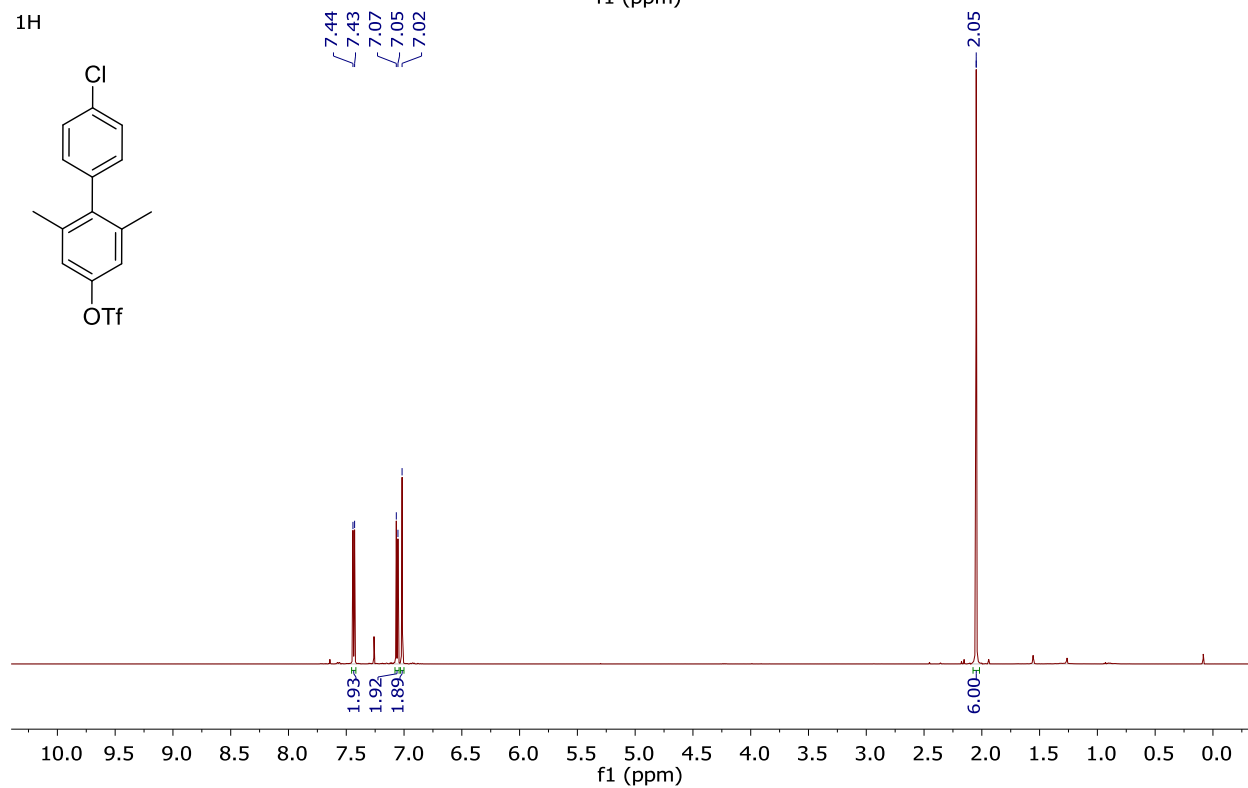
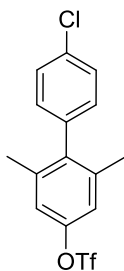
¹H



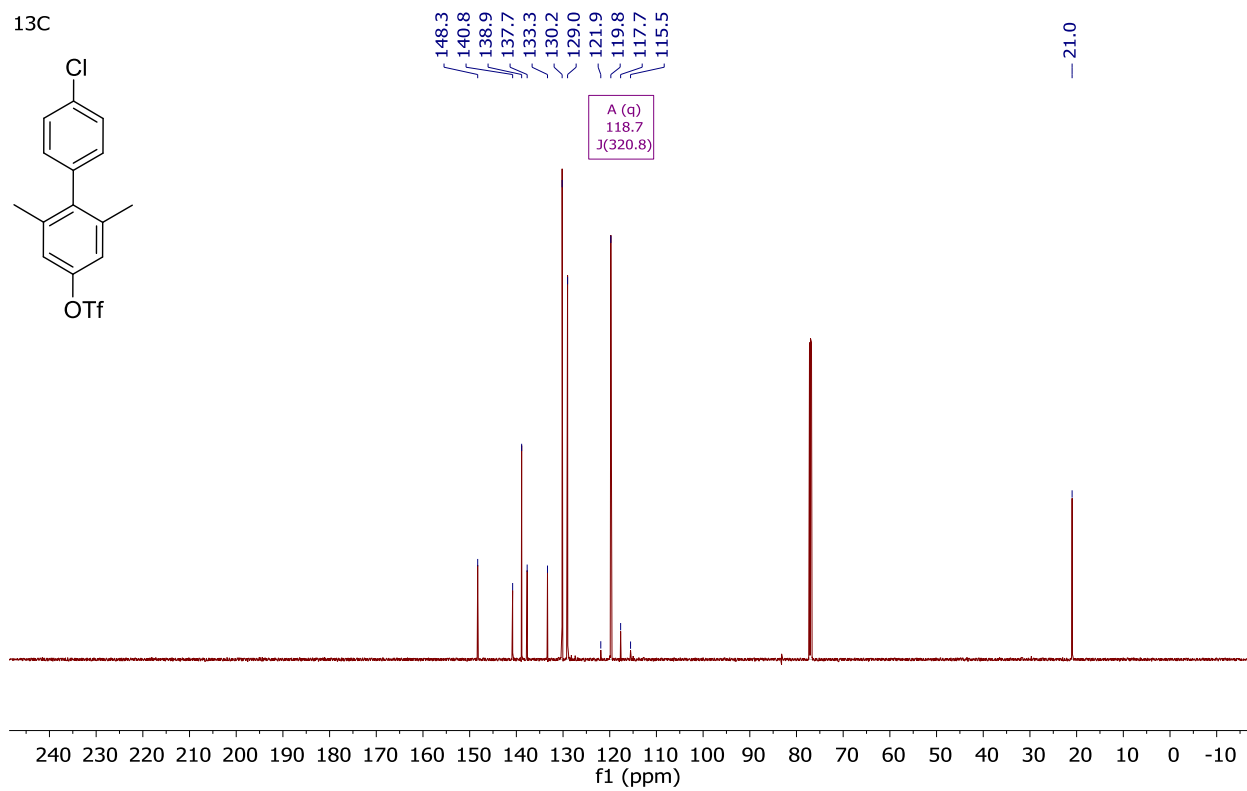
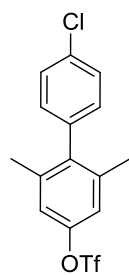
13C



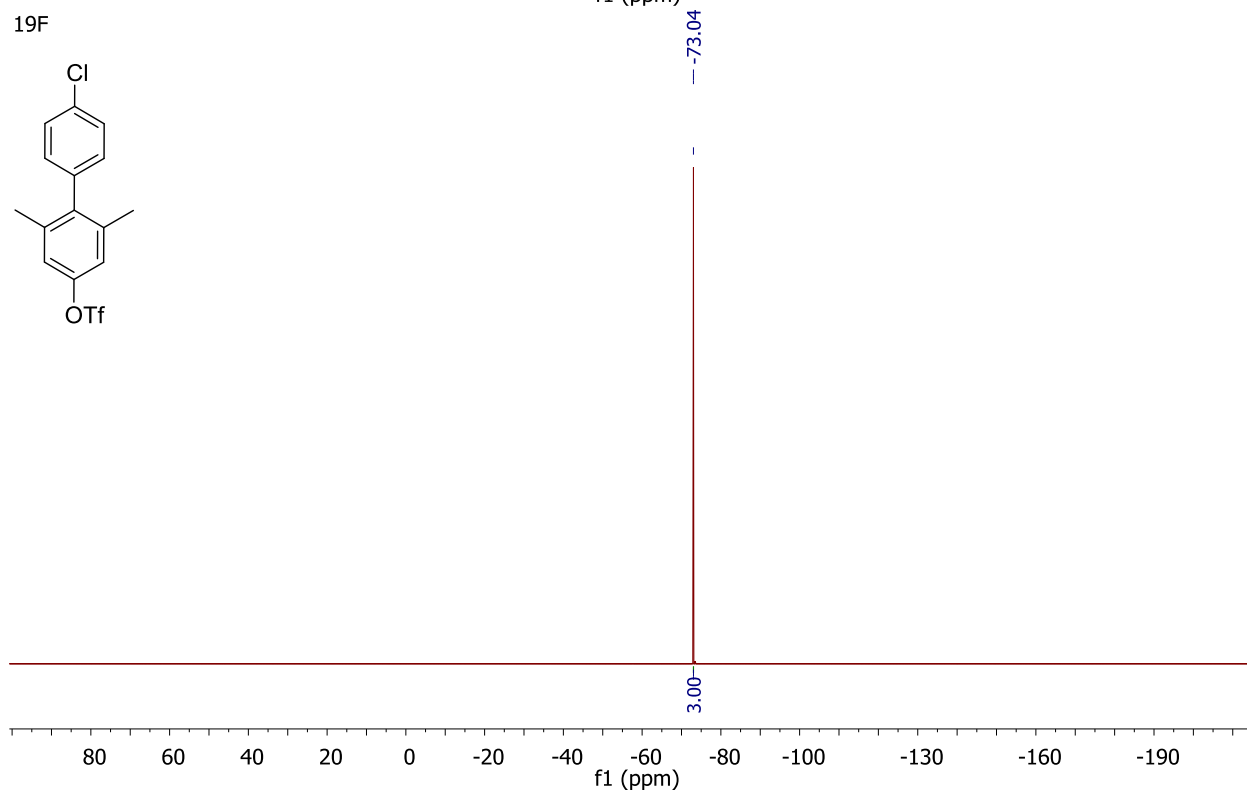
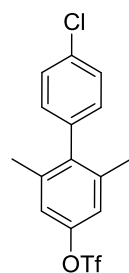
1H



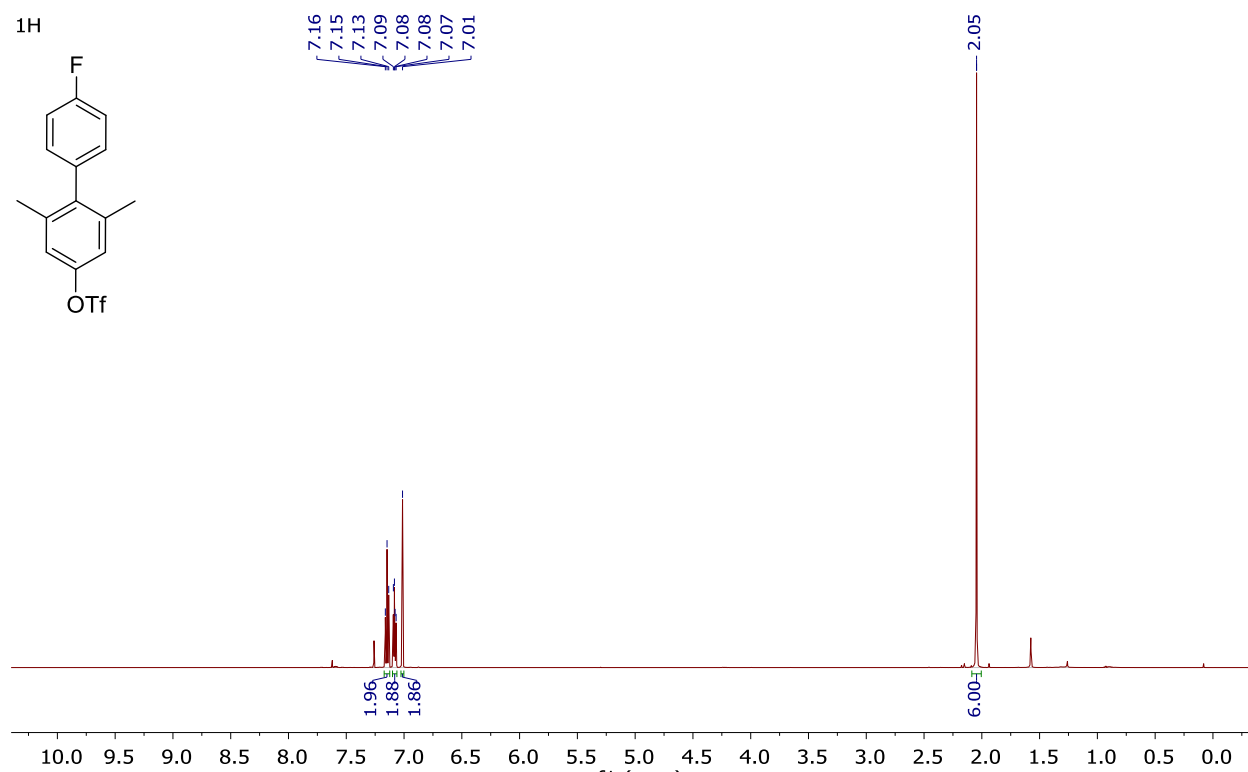
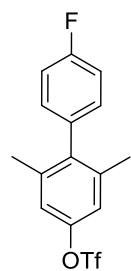
13C



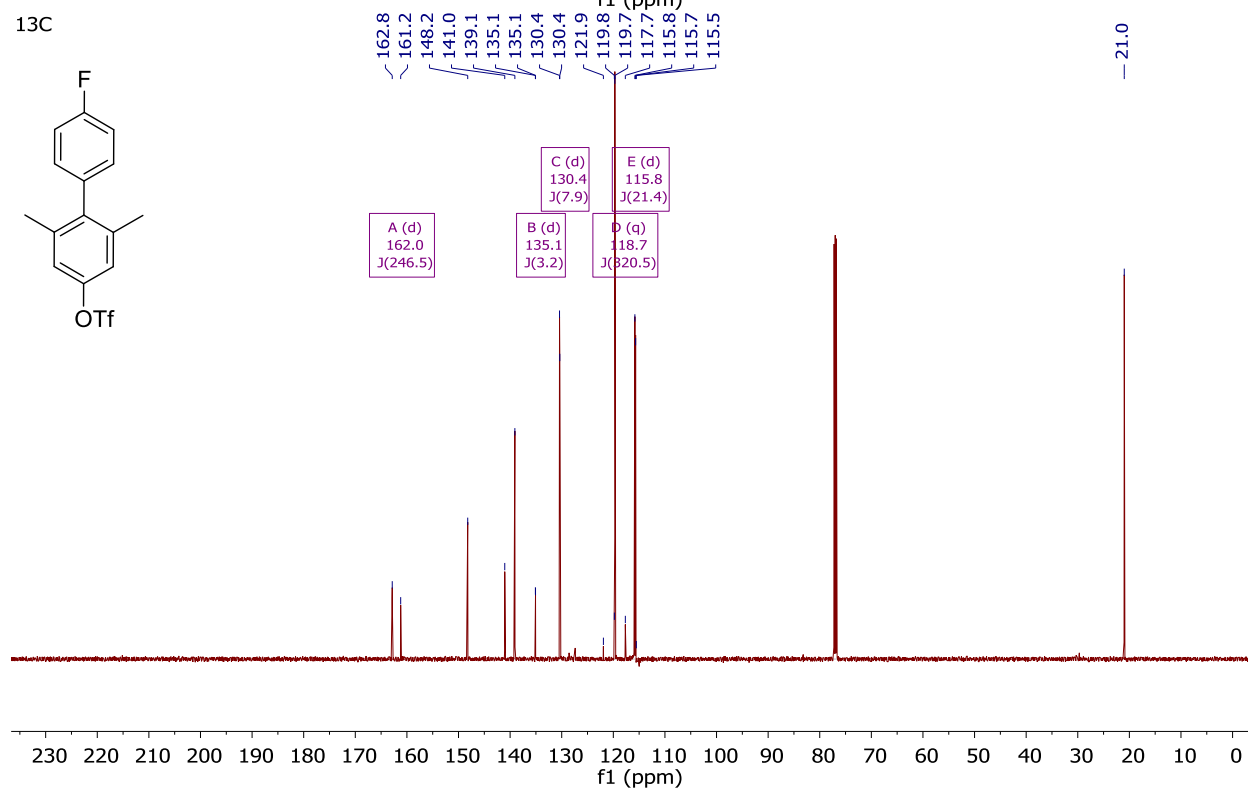
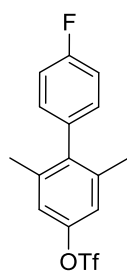
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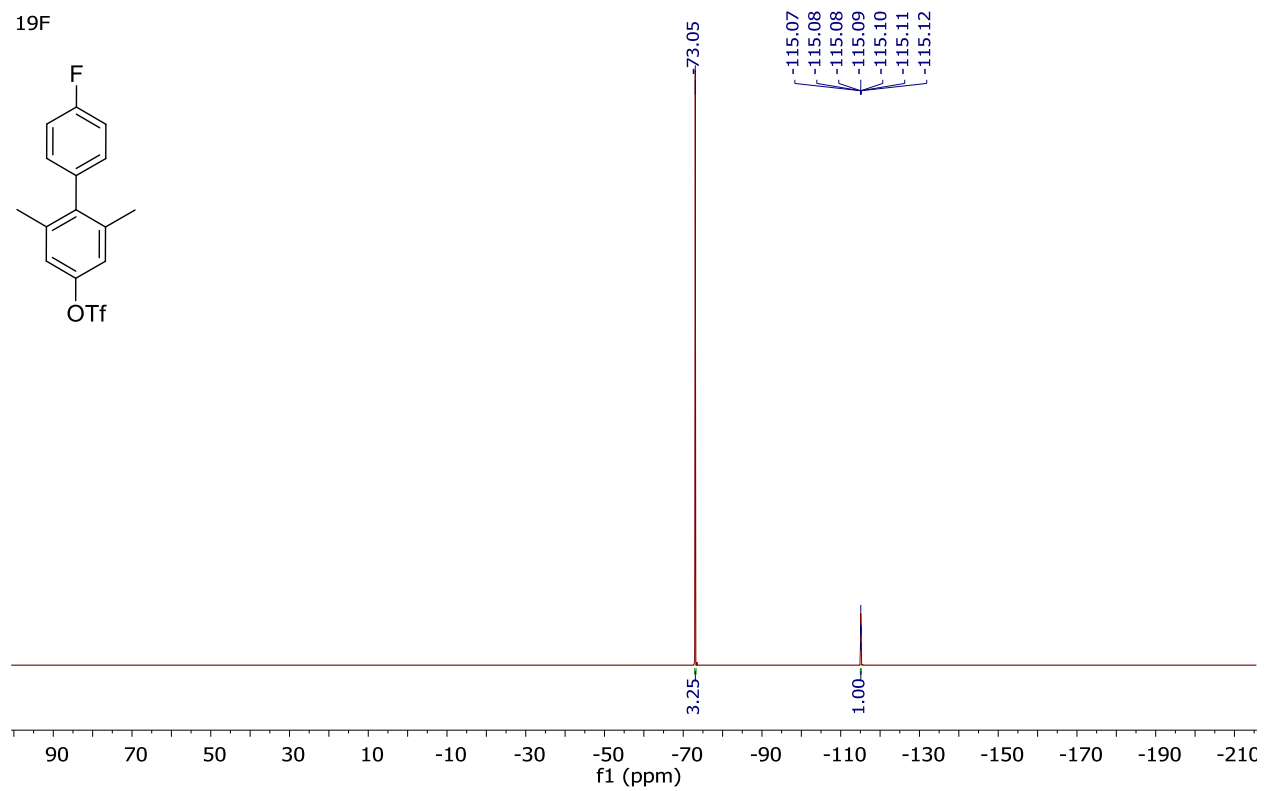
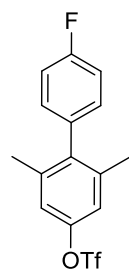
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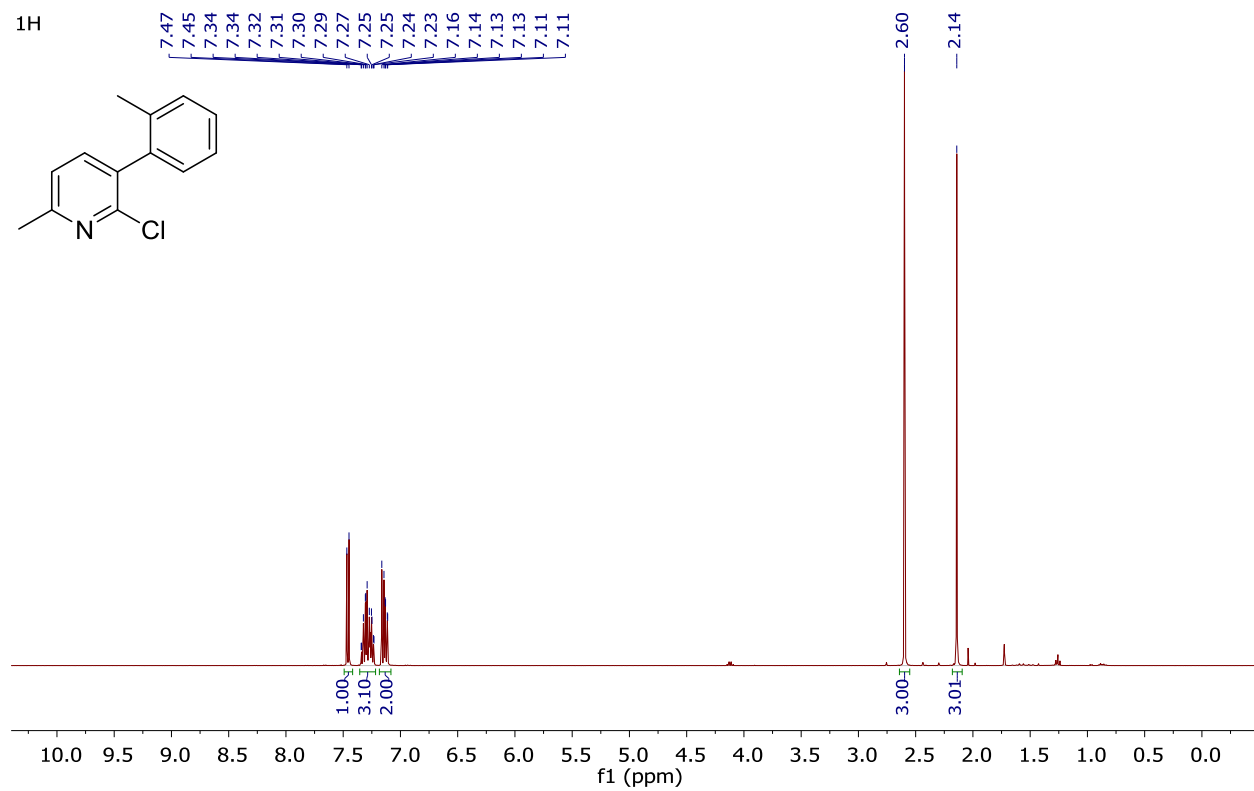
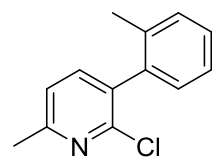
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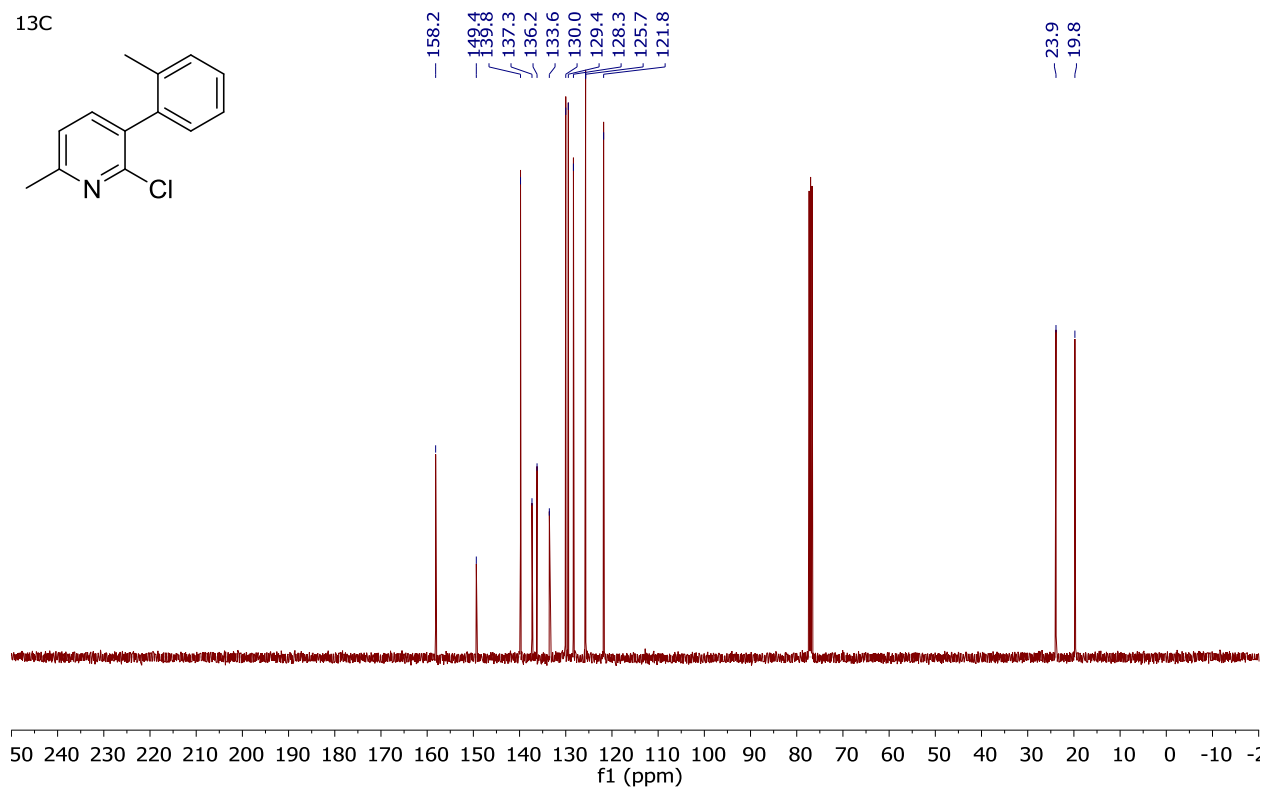
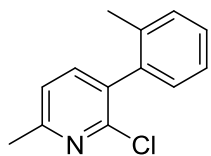
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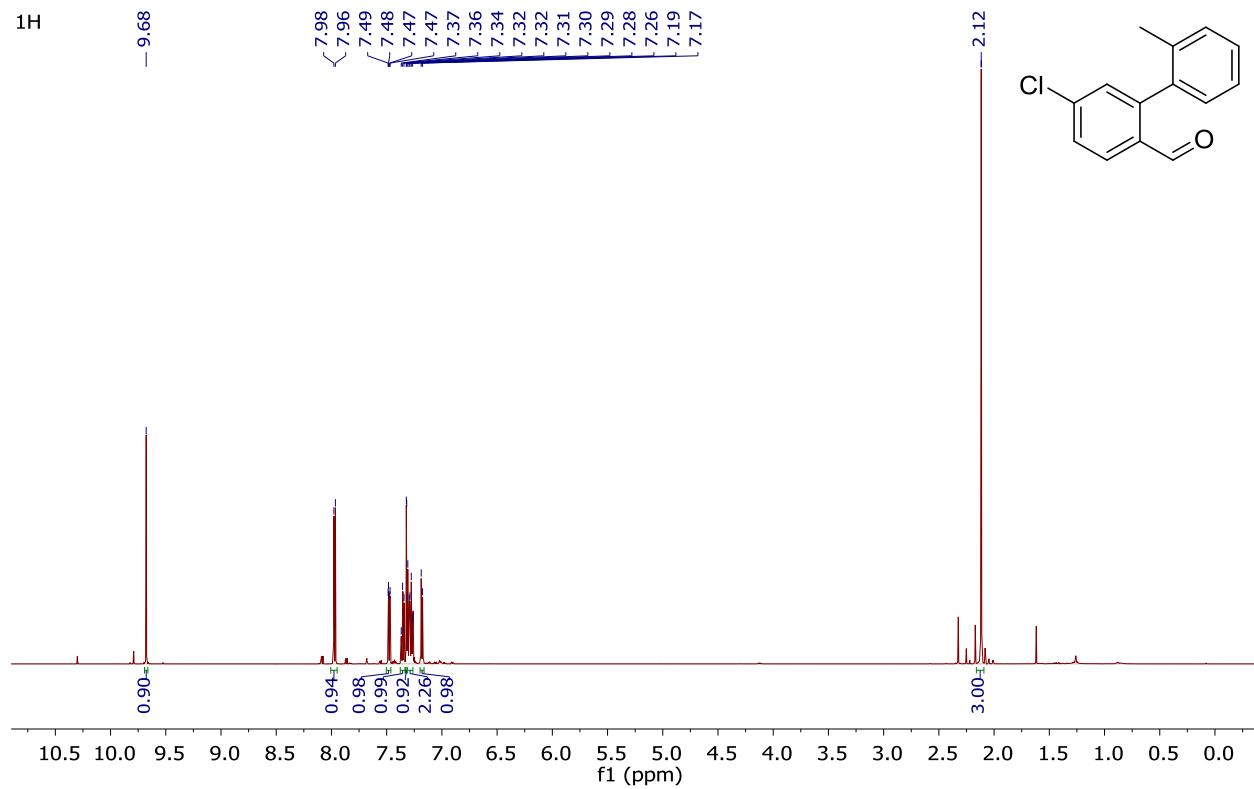
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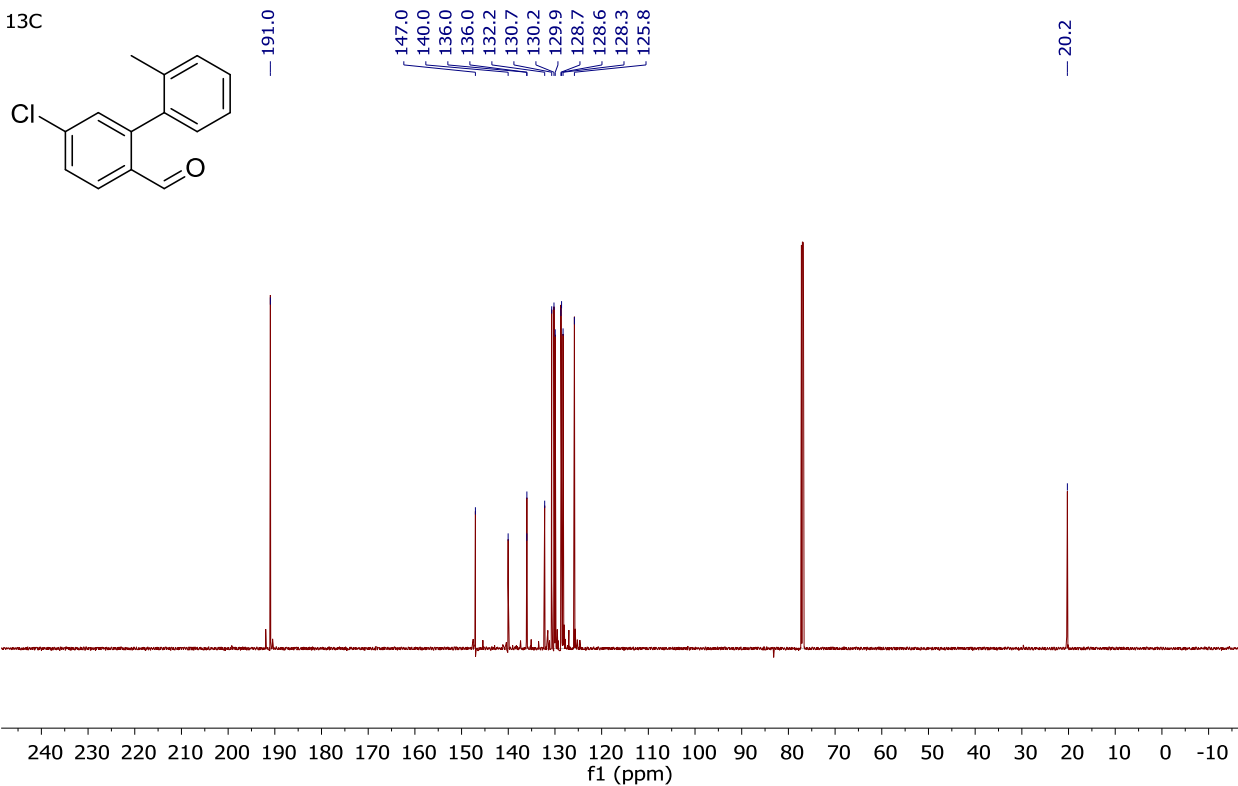
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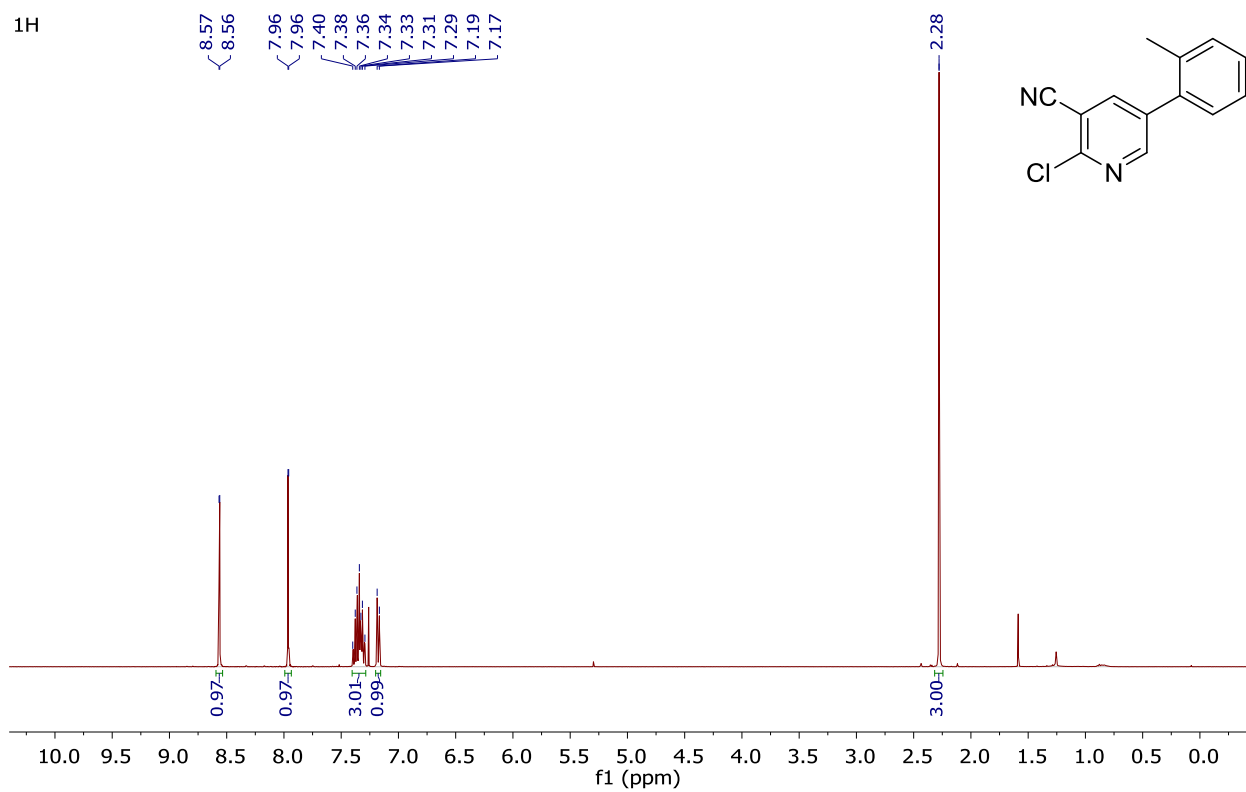
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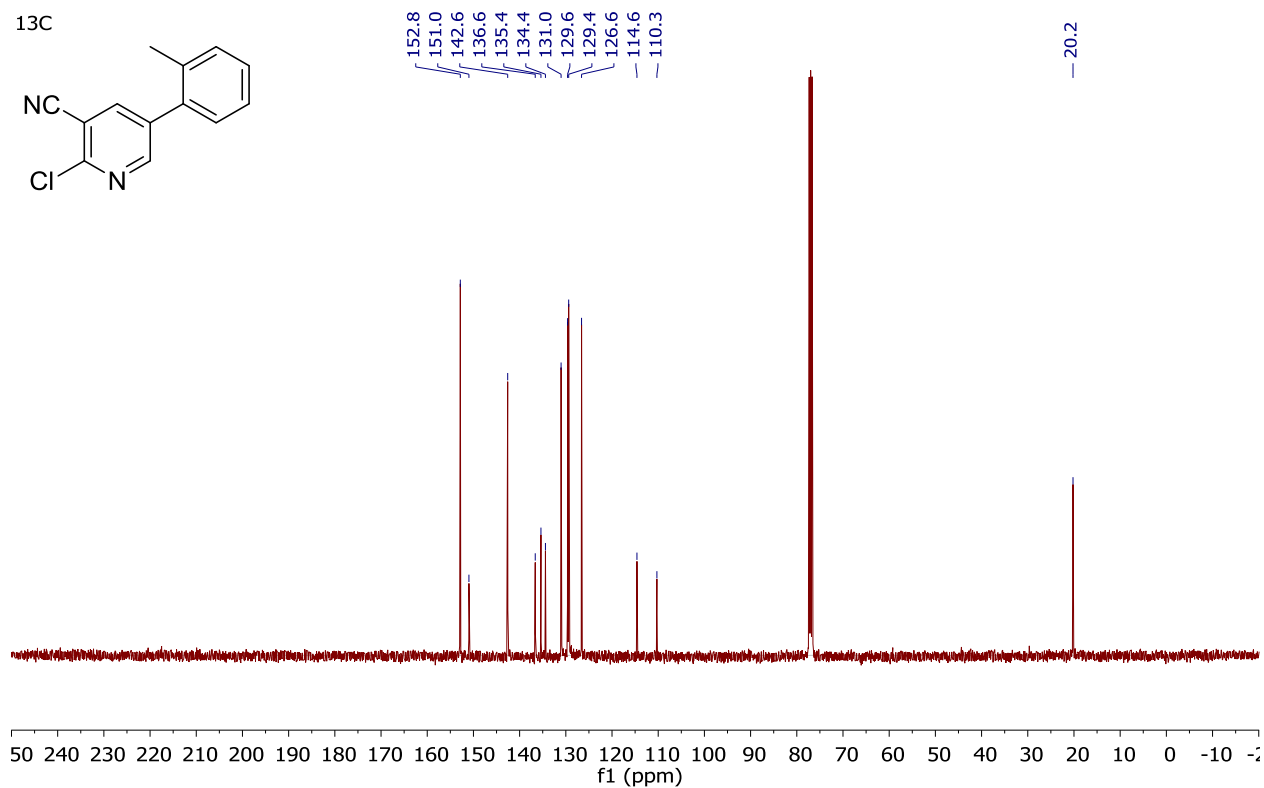
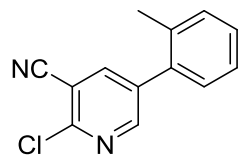
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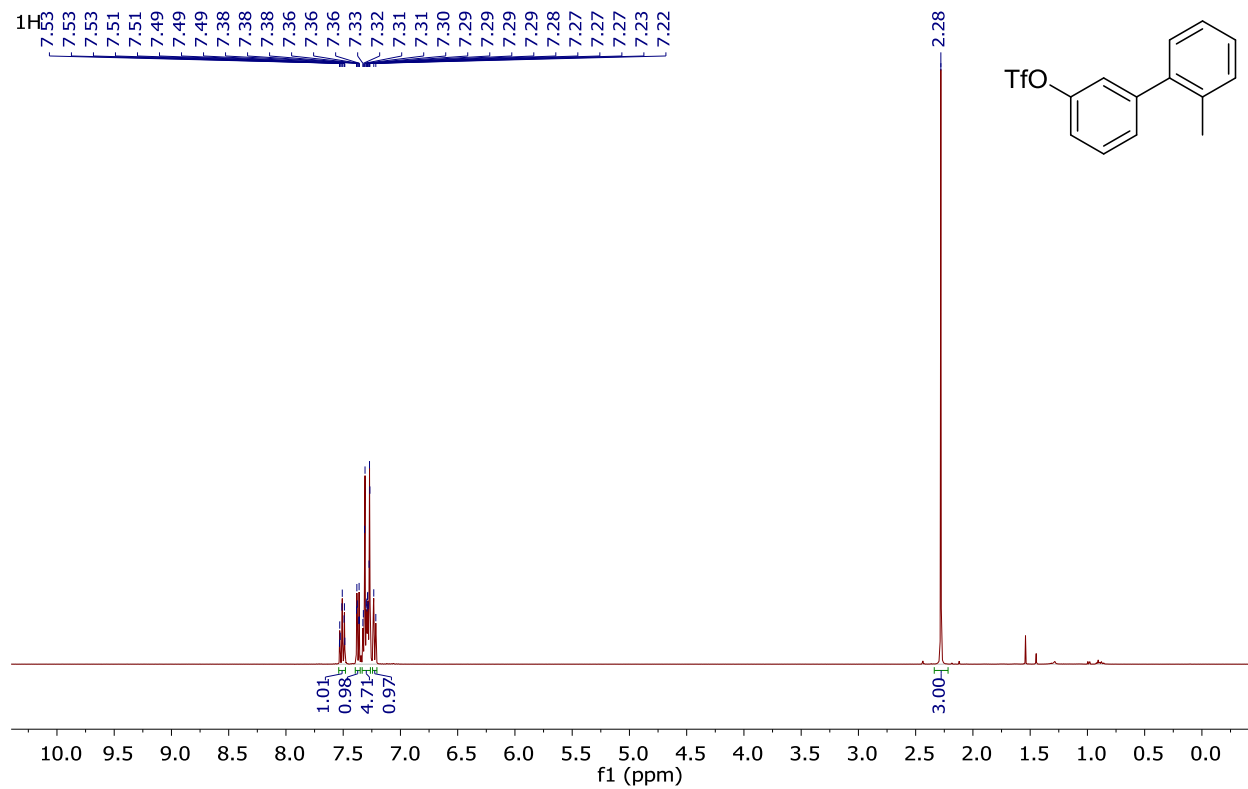
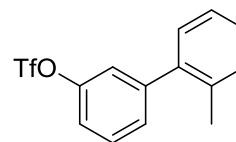
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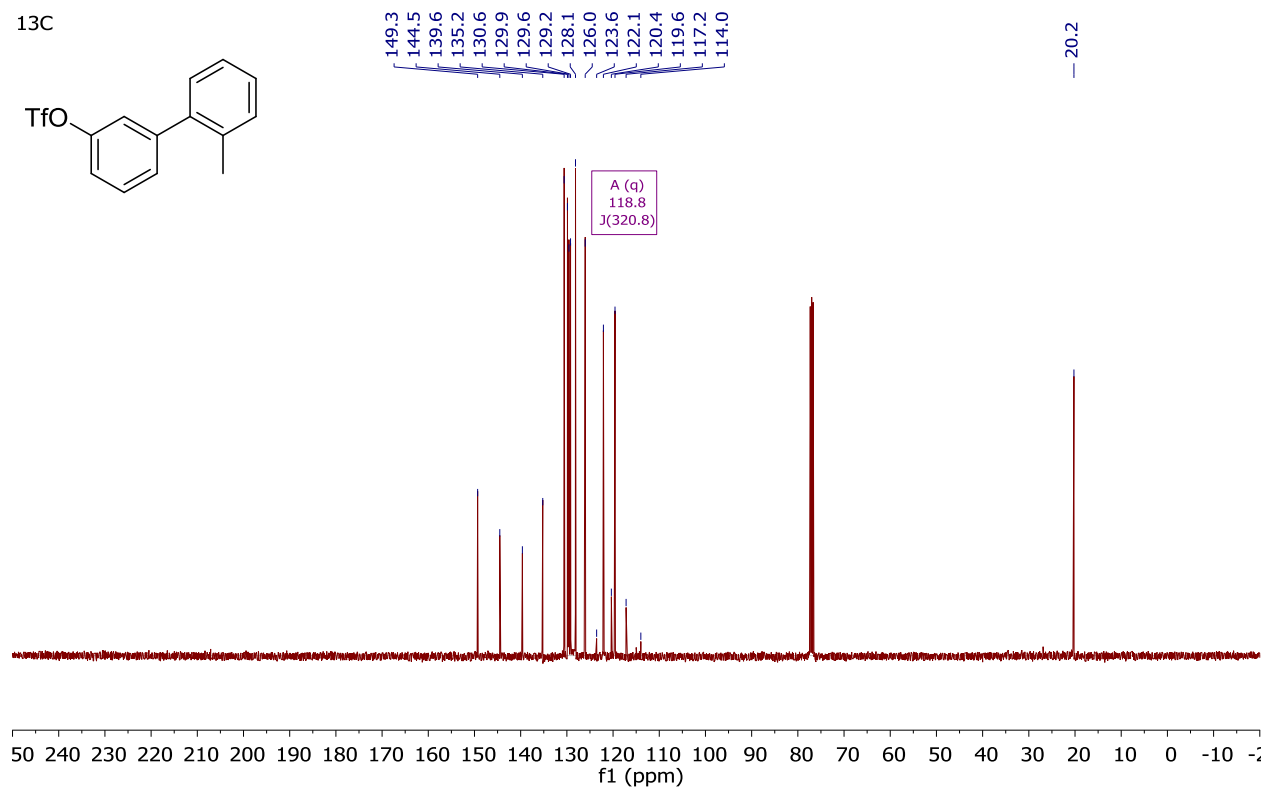
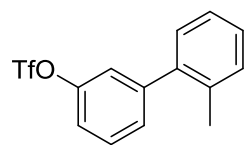
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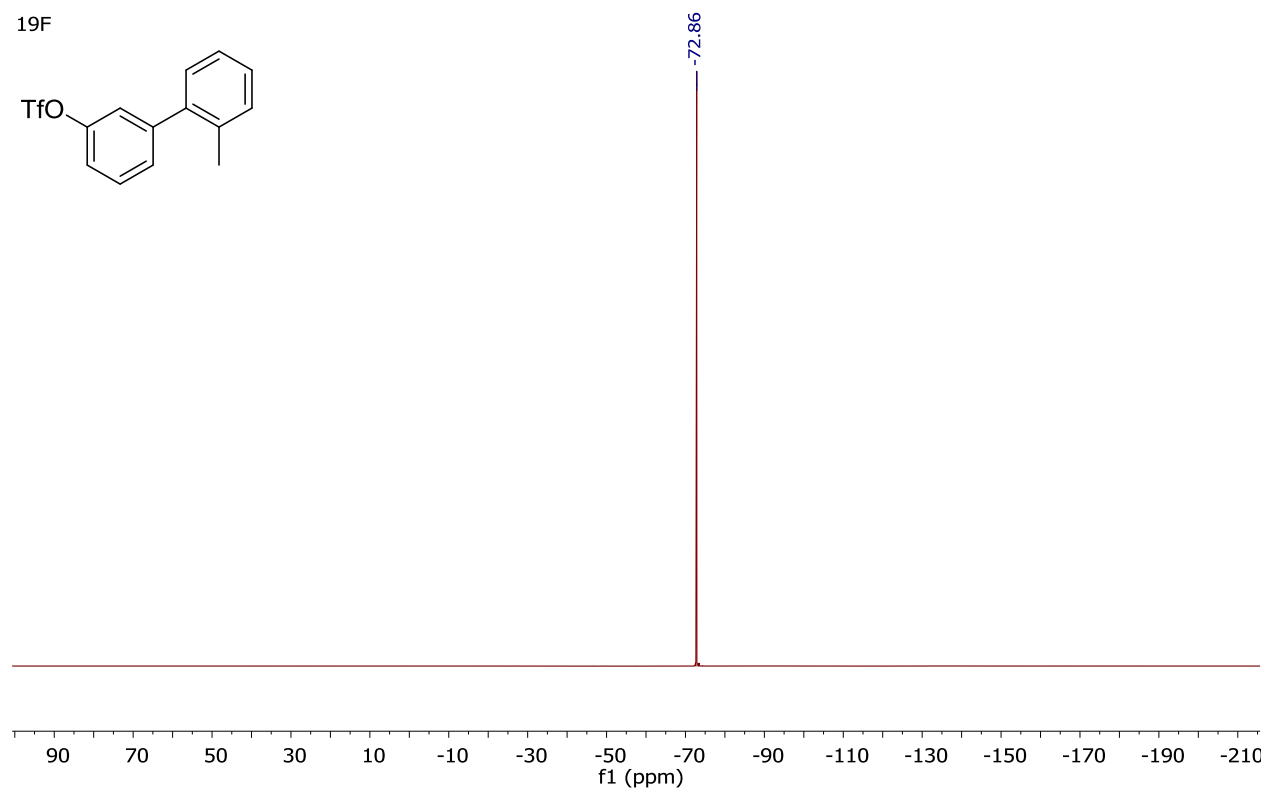
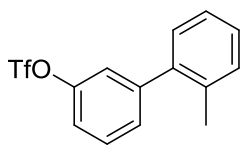
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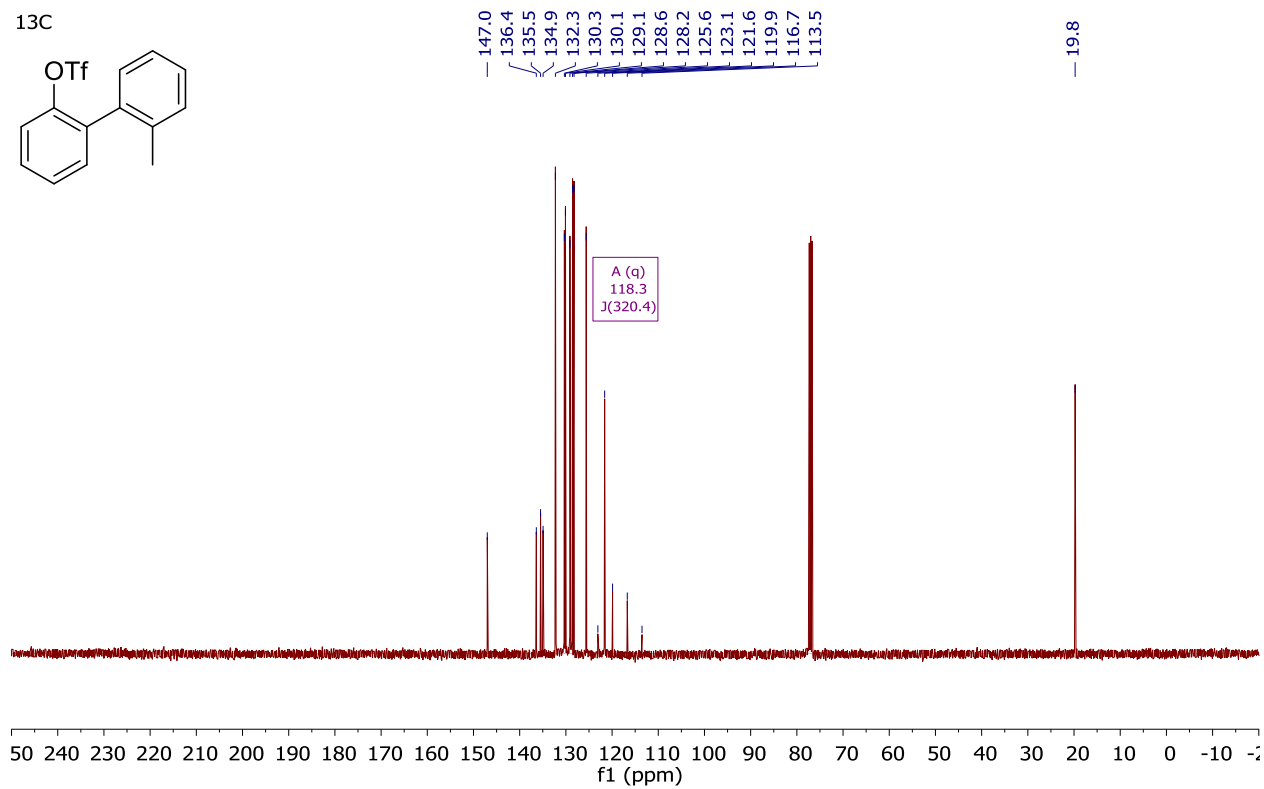
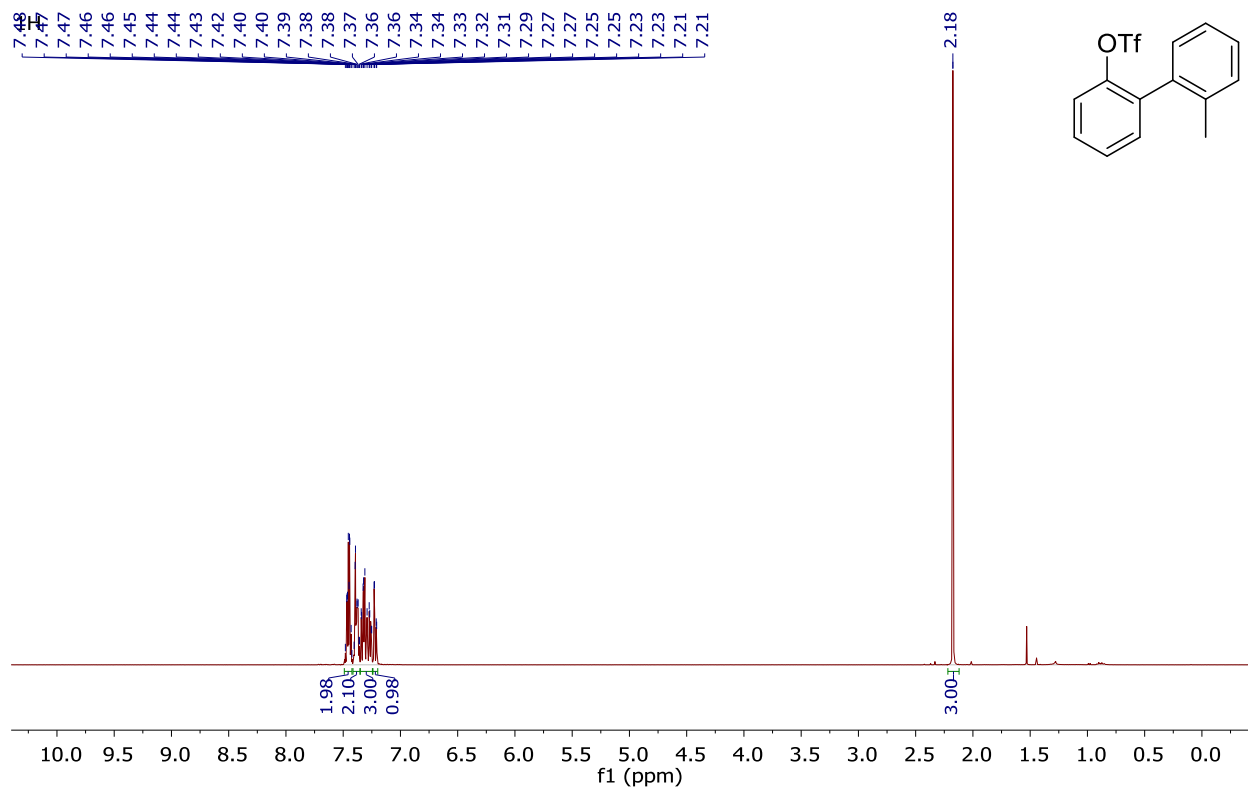


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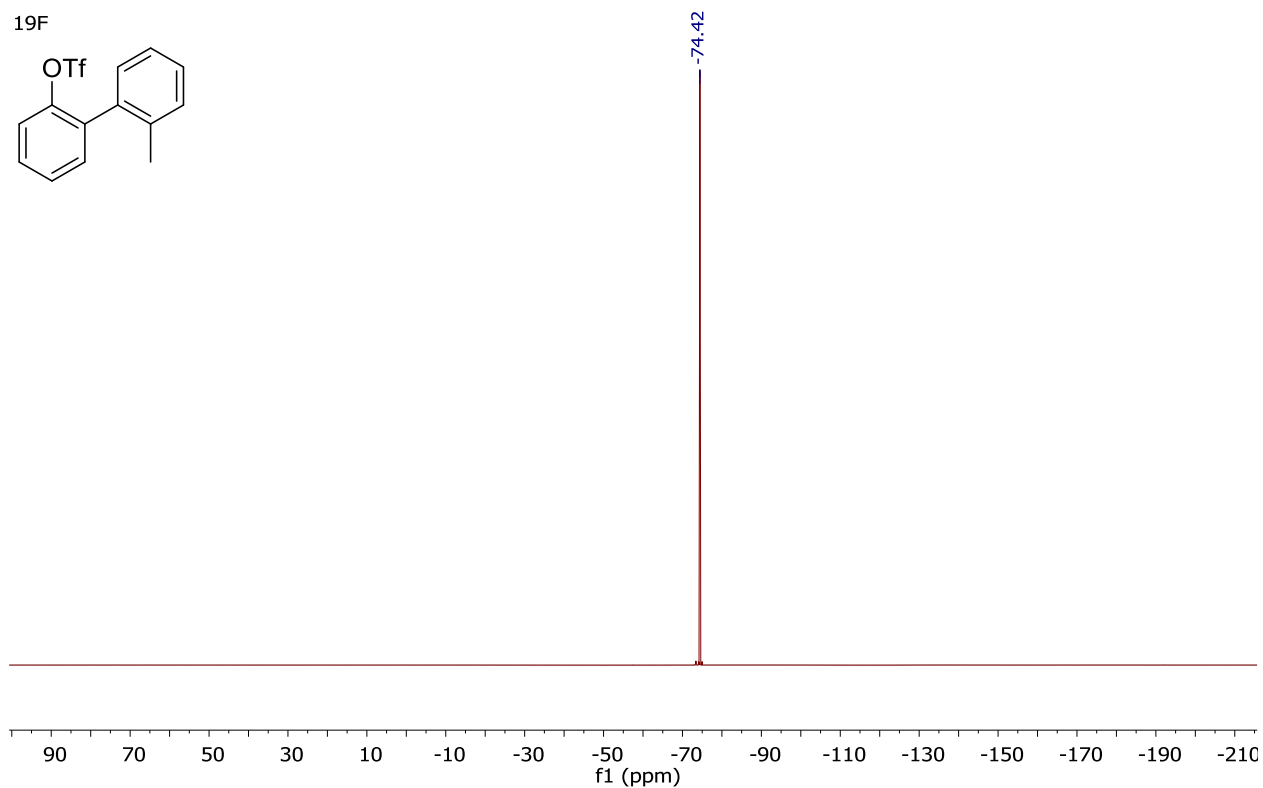
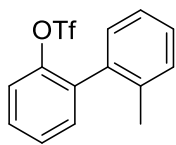


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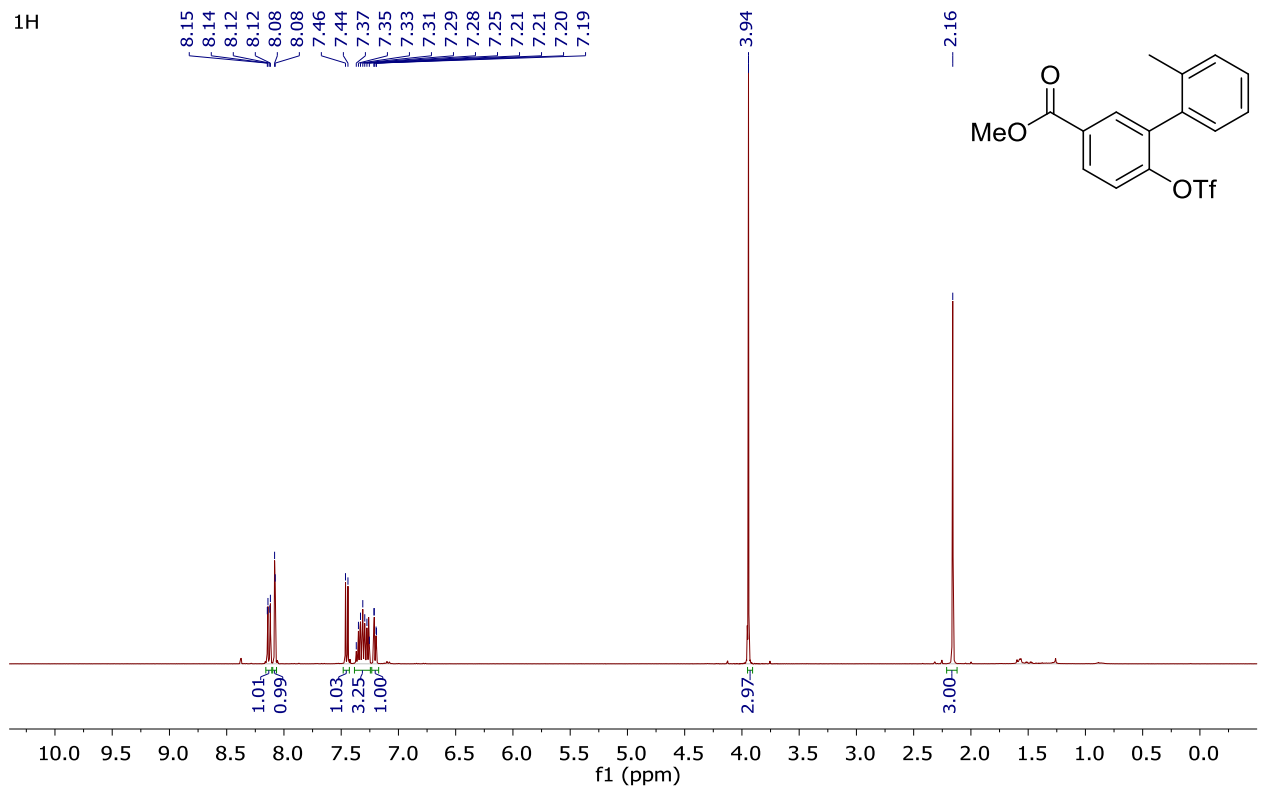
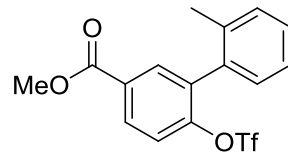


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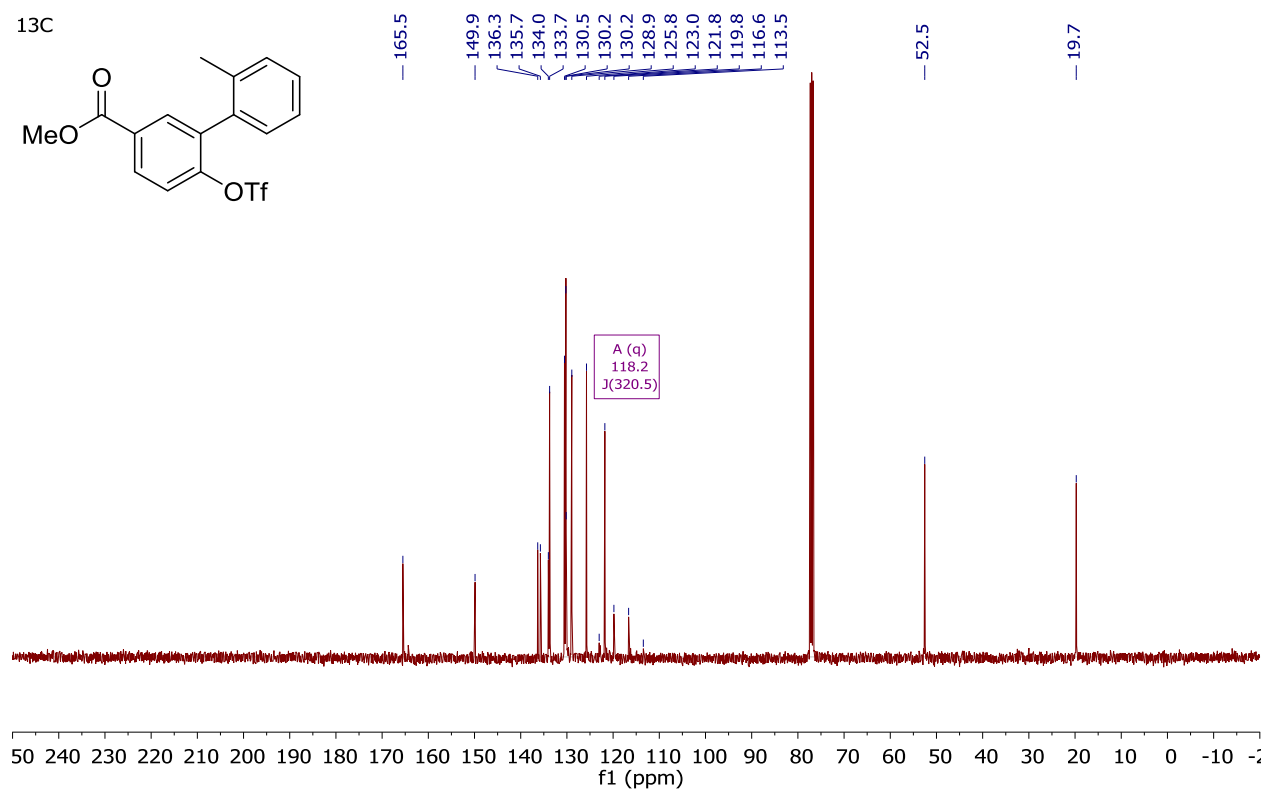
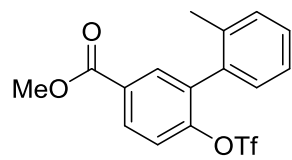


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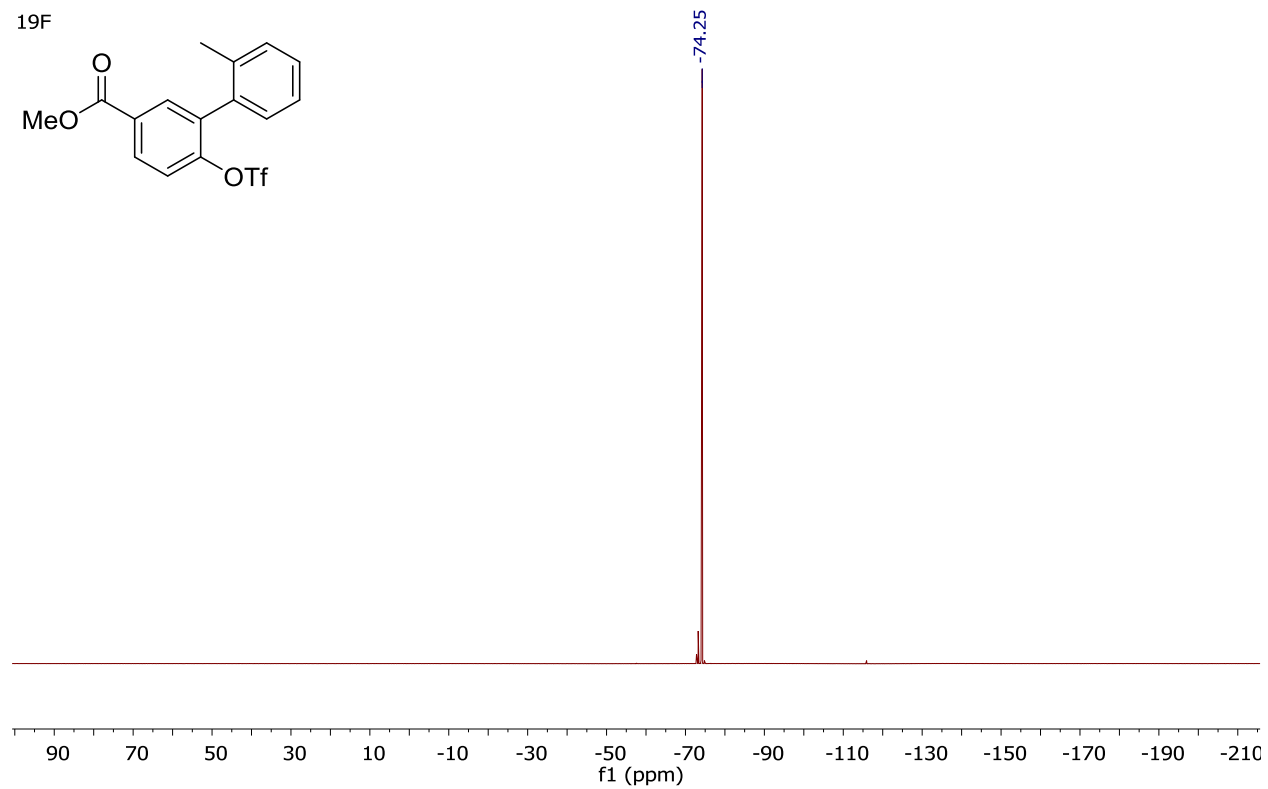
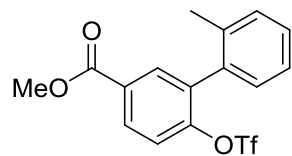
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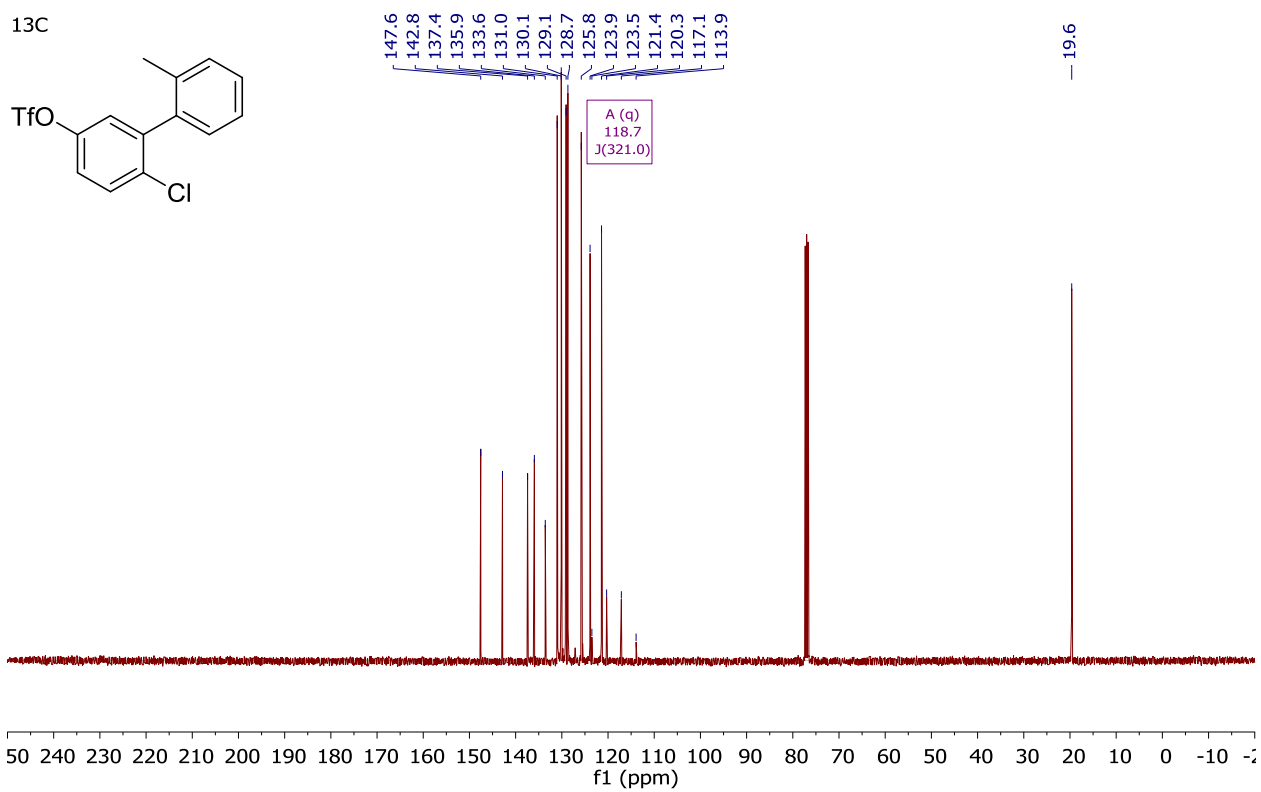
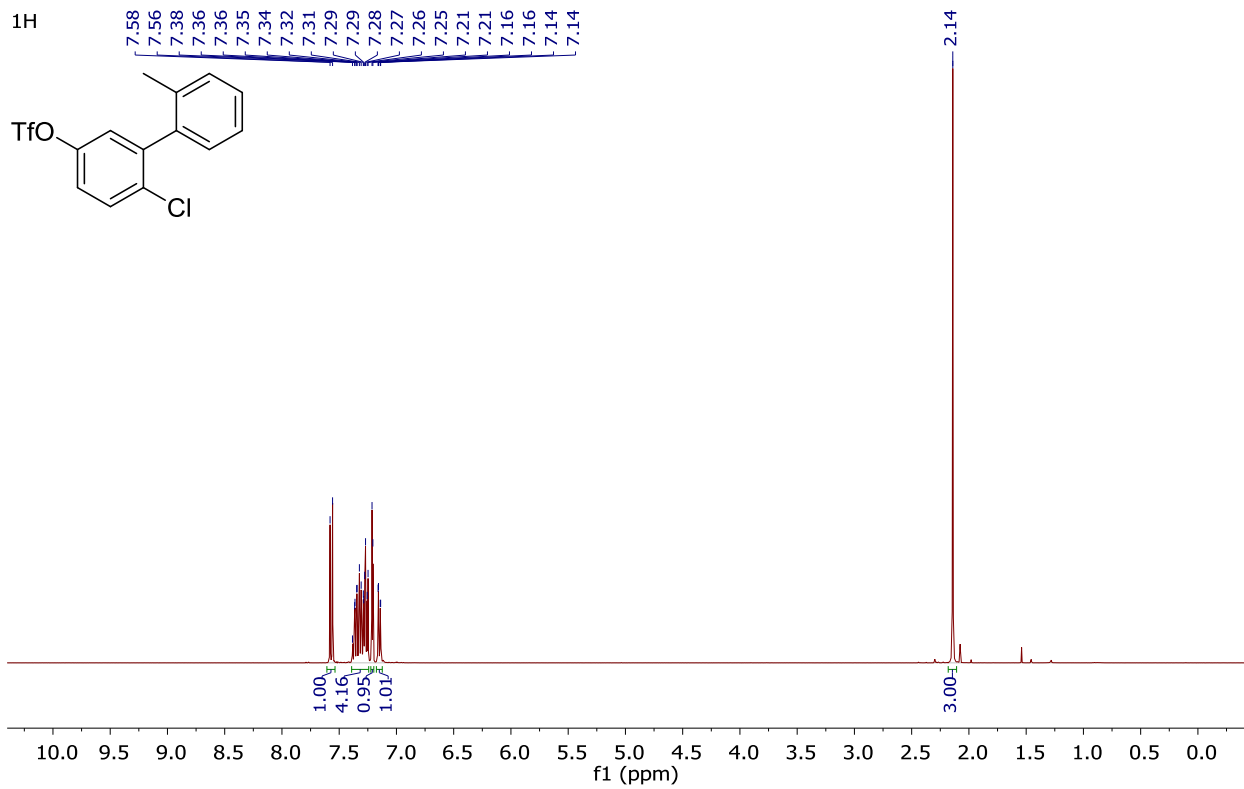


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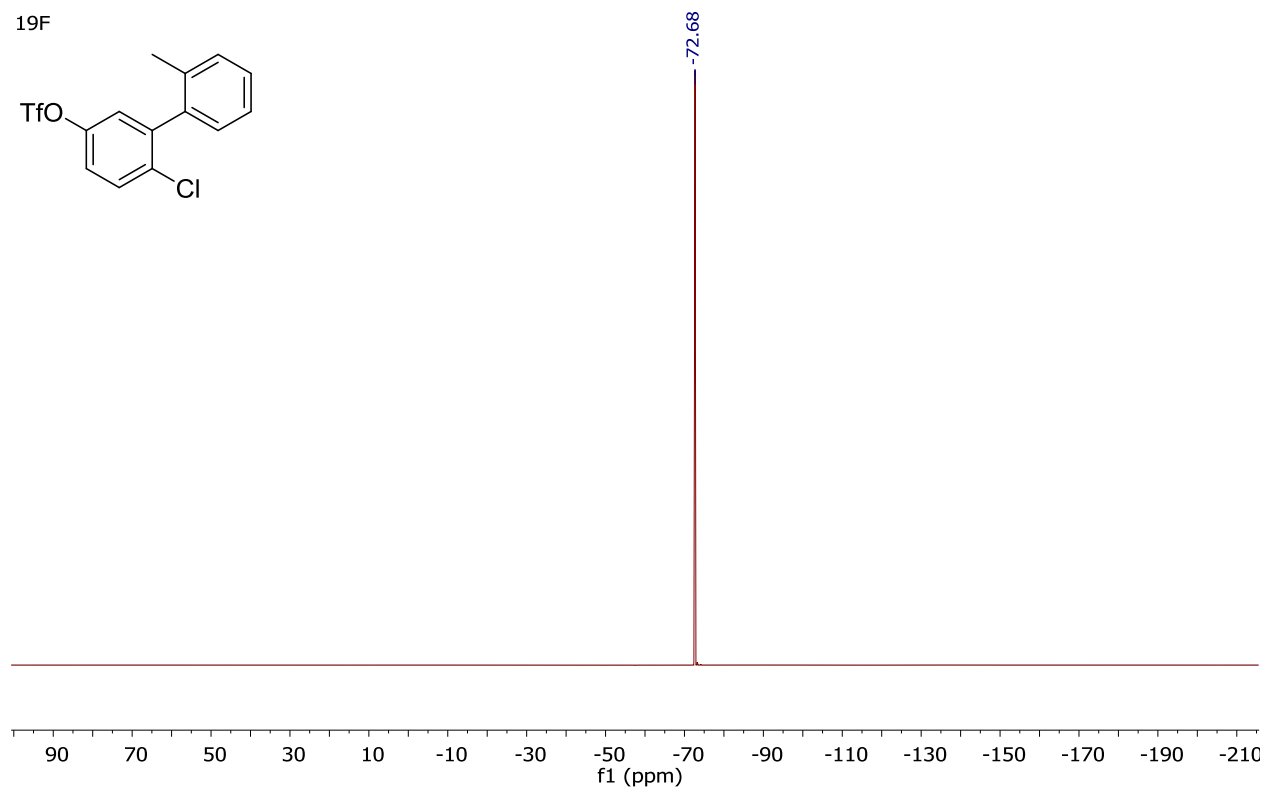
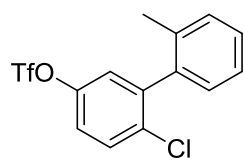


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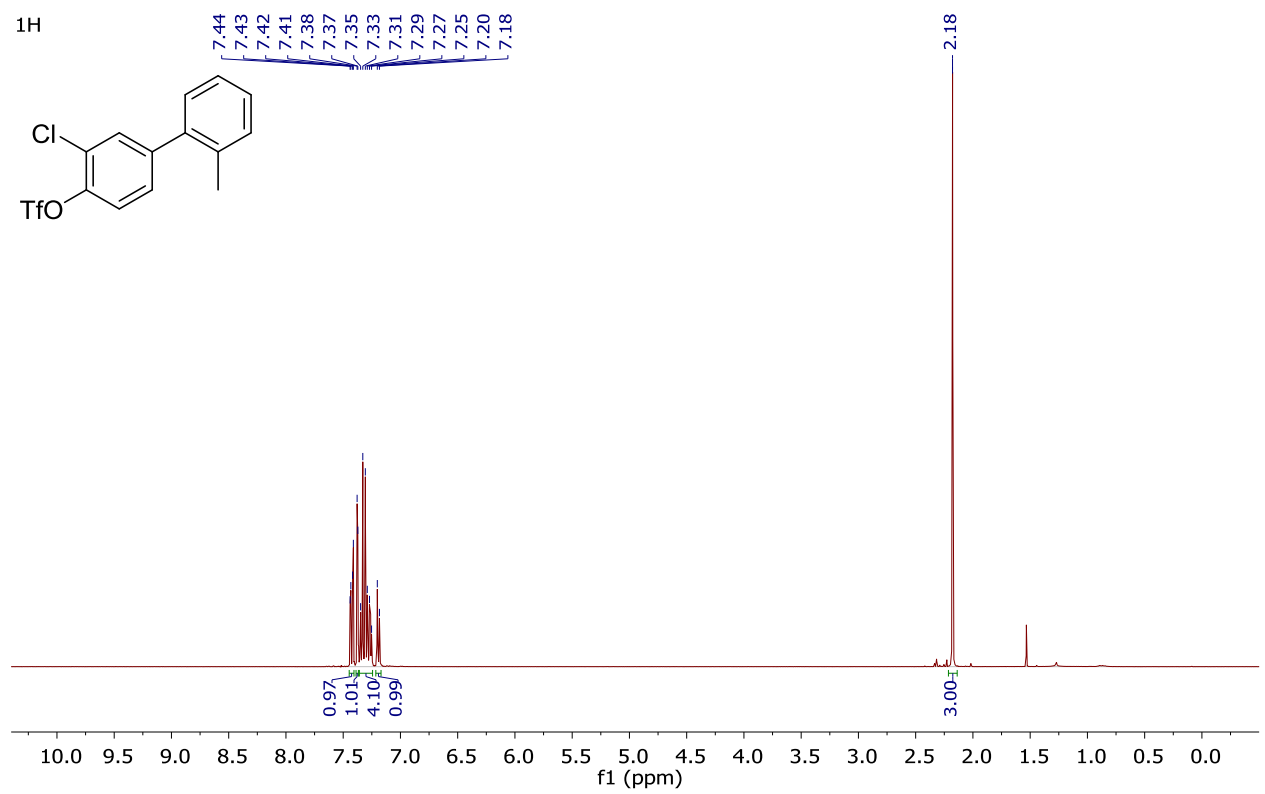
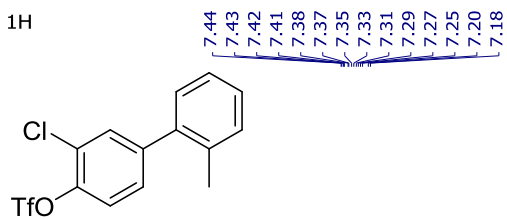




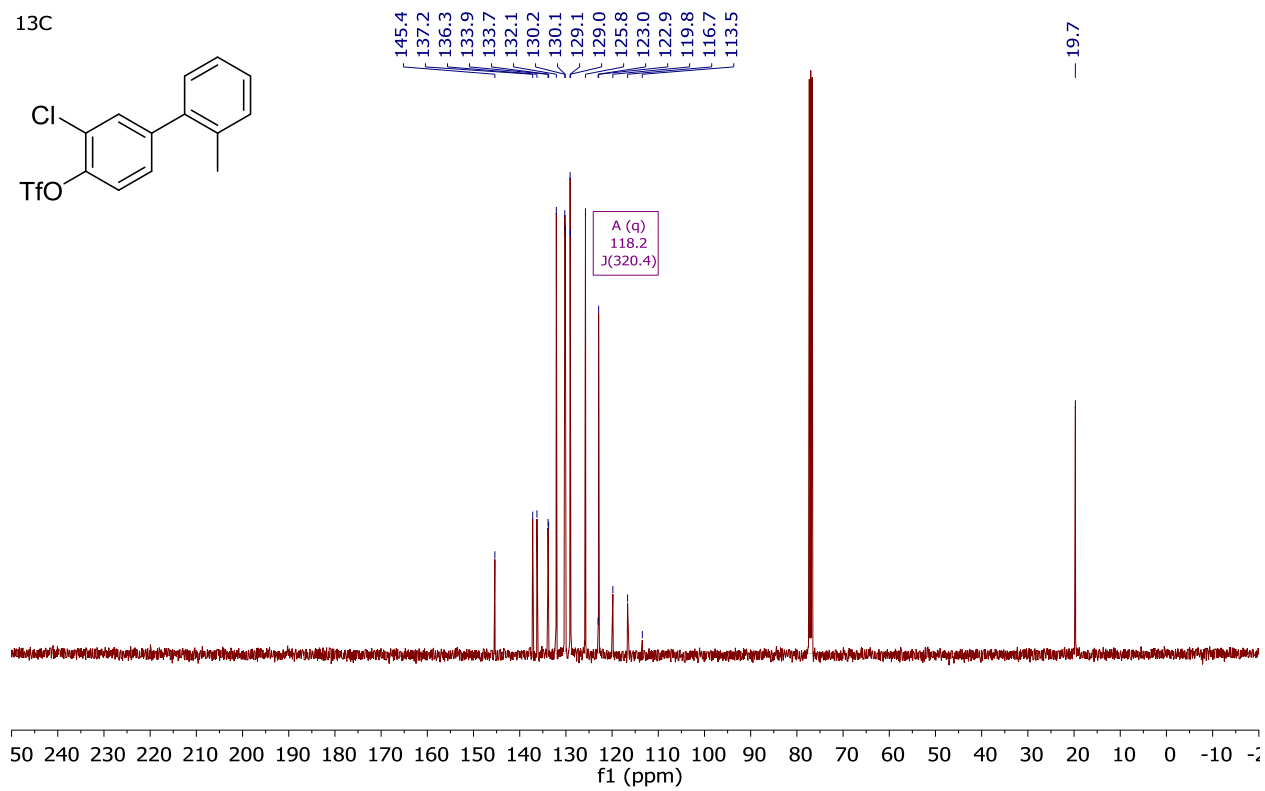
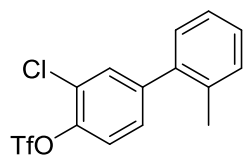
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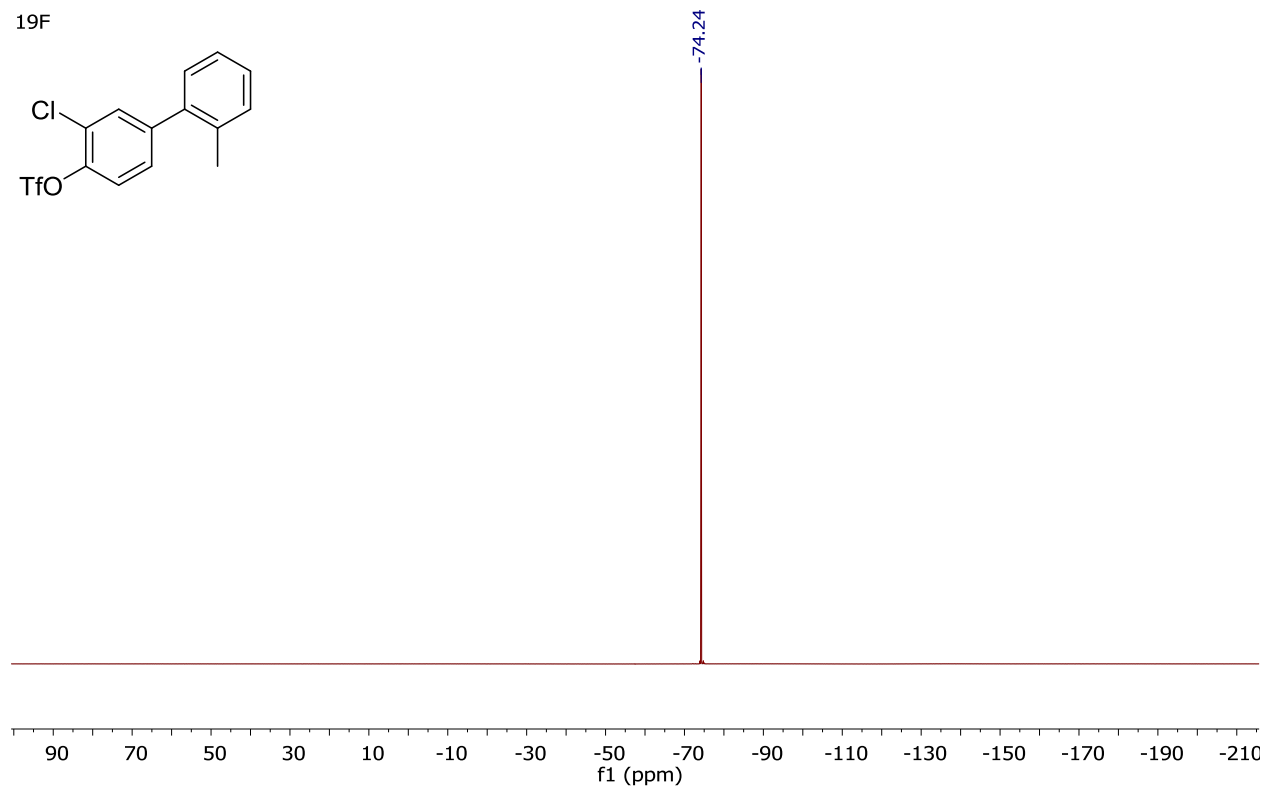
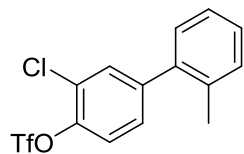
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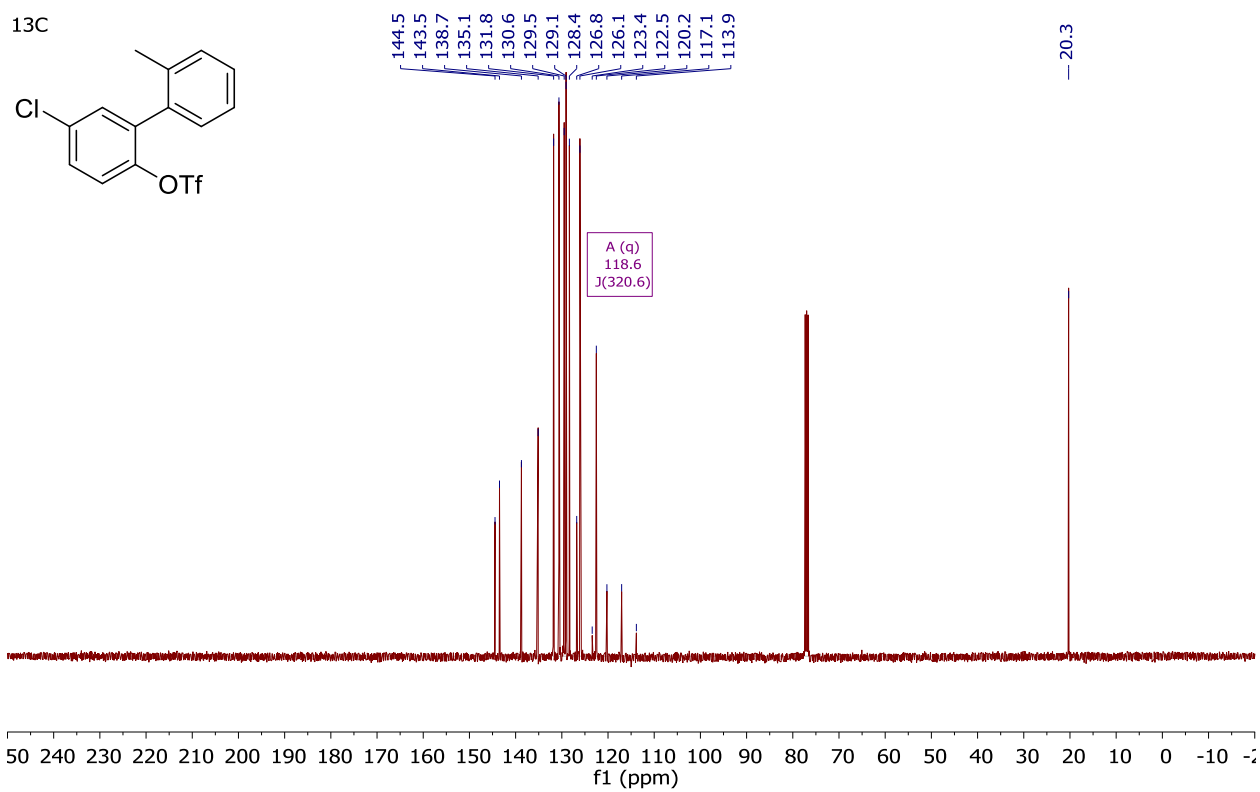
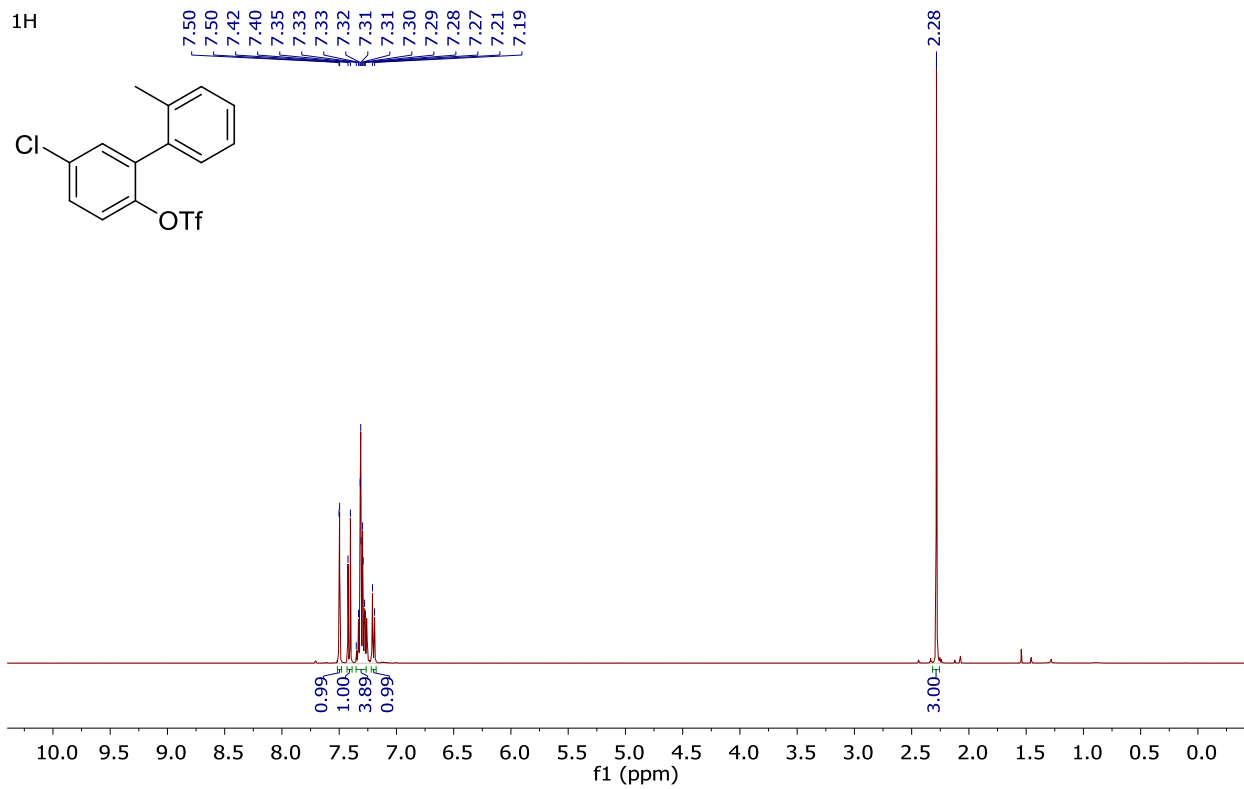


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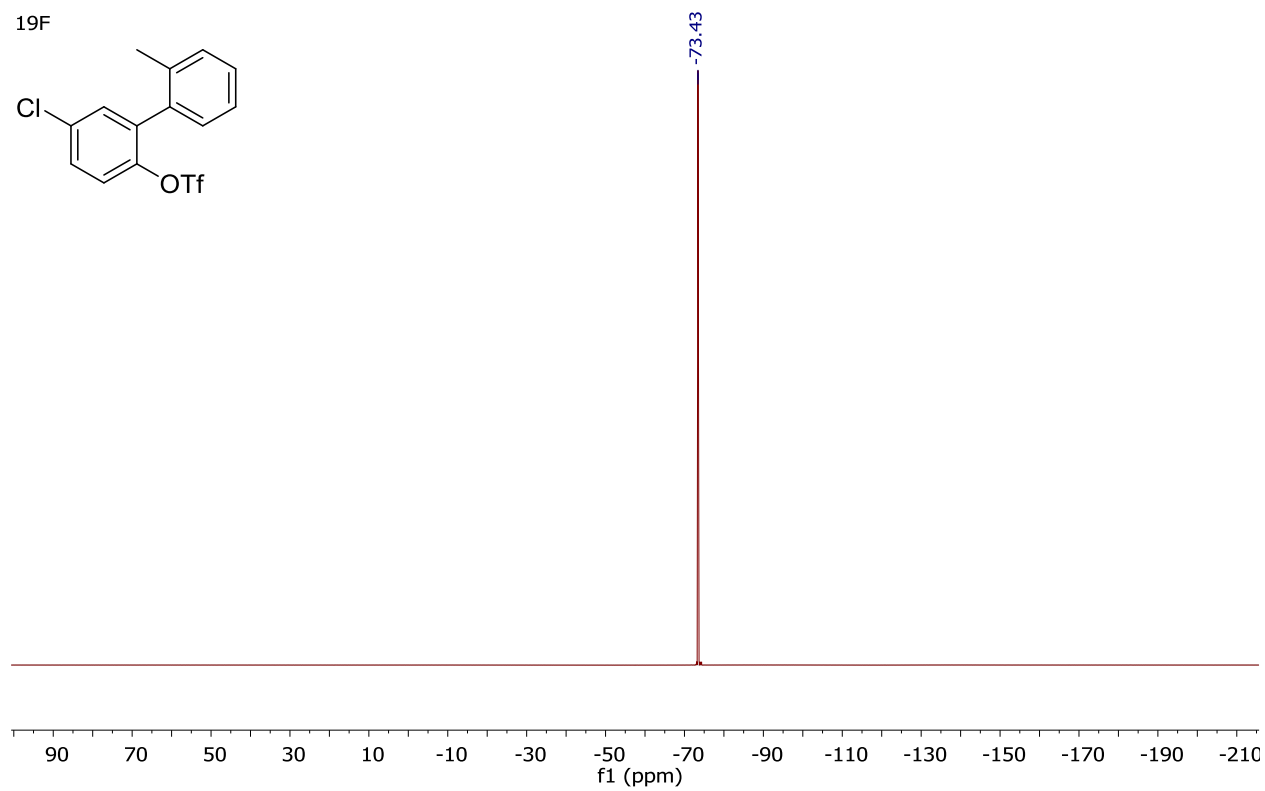
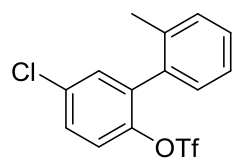


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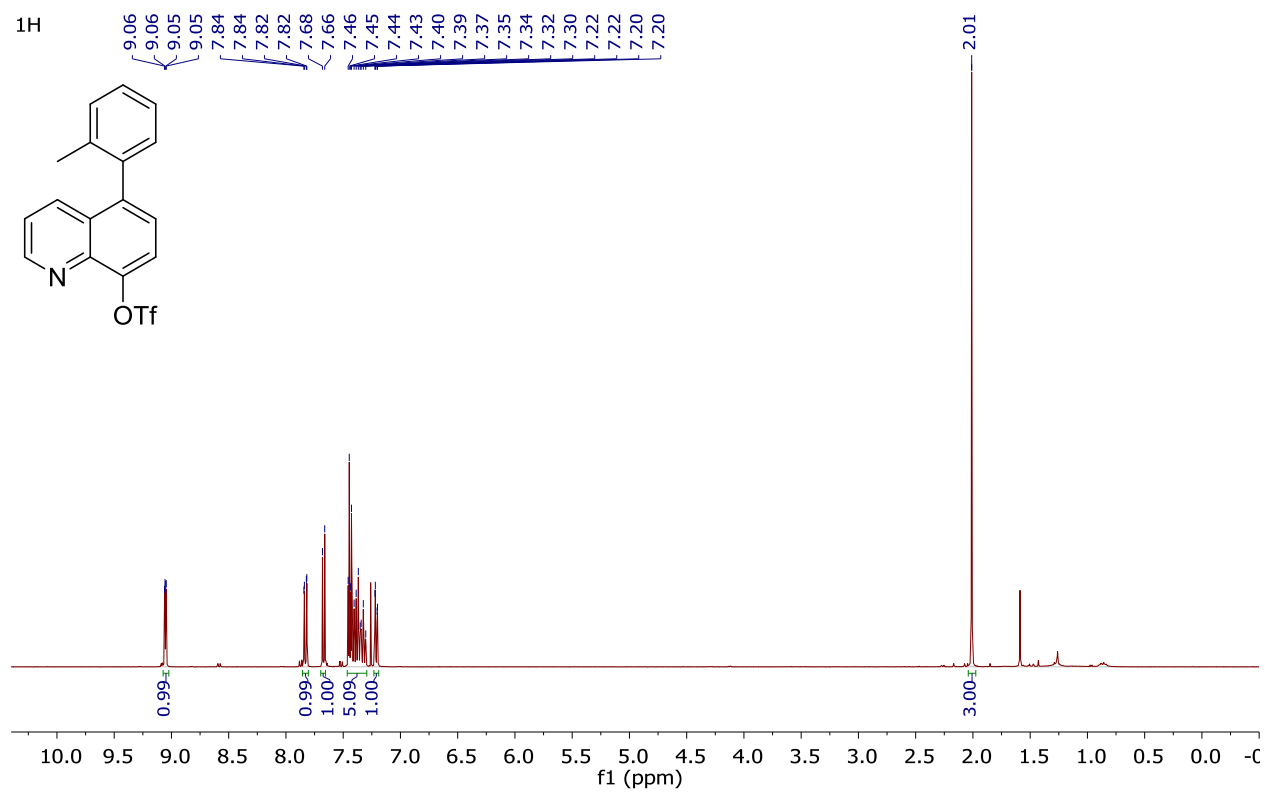
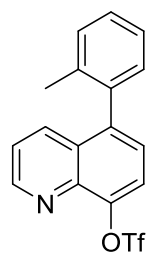




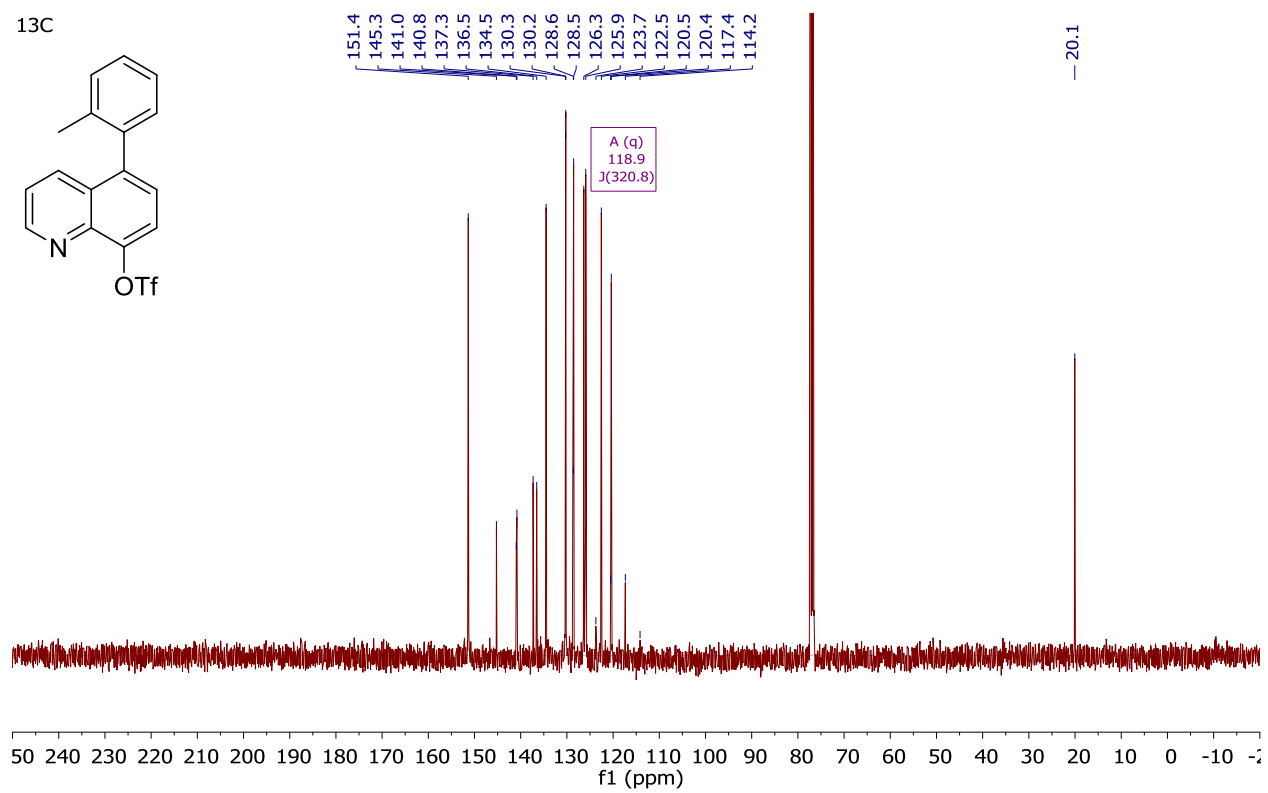
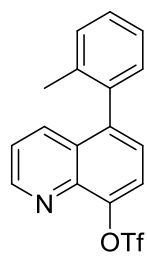
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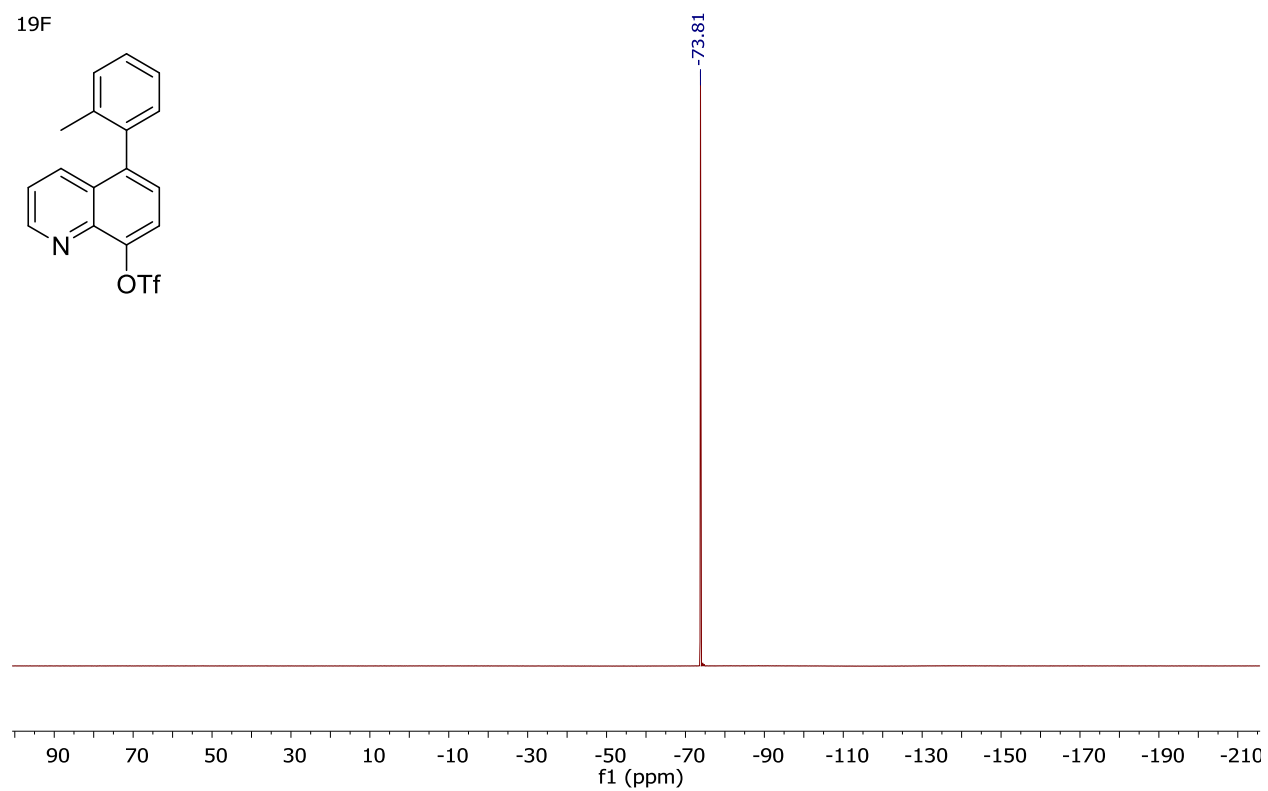
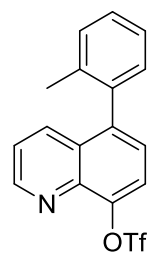
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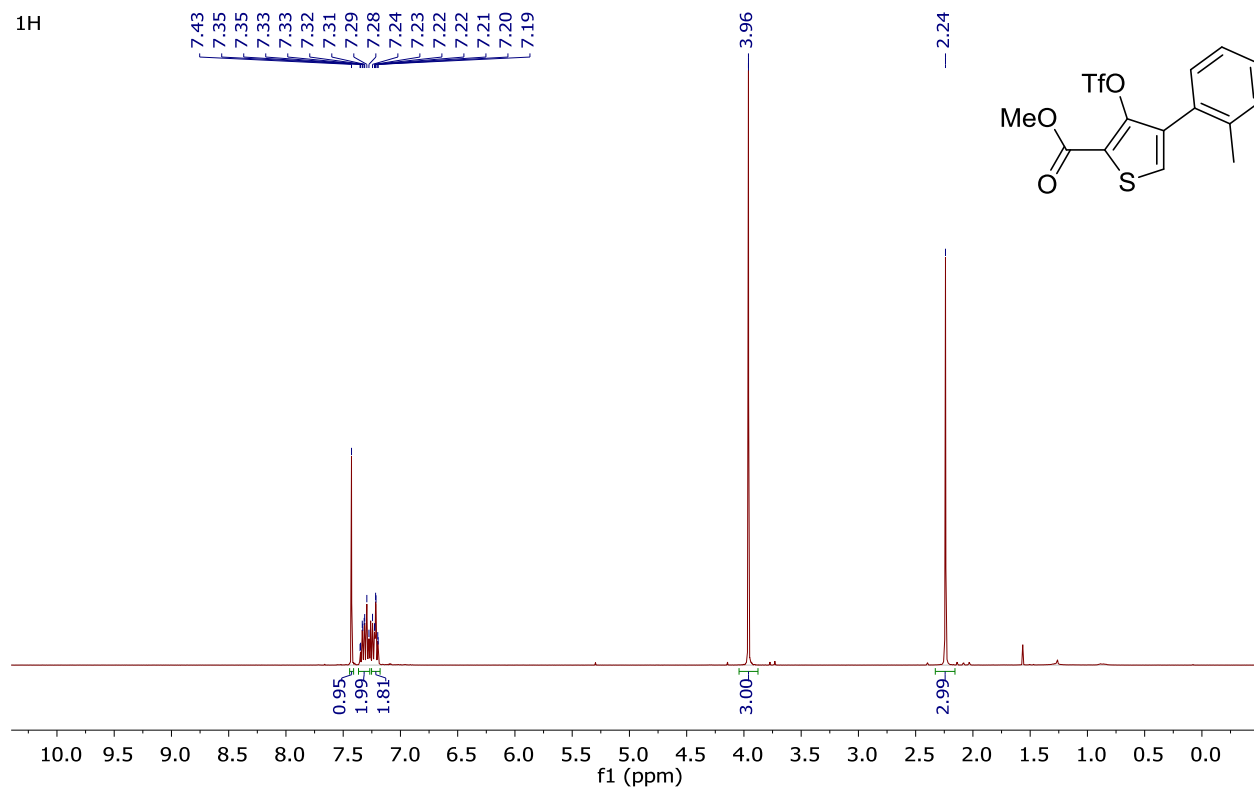
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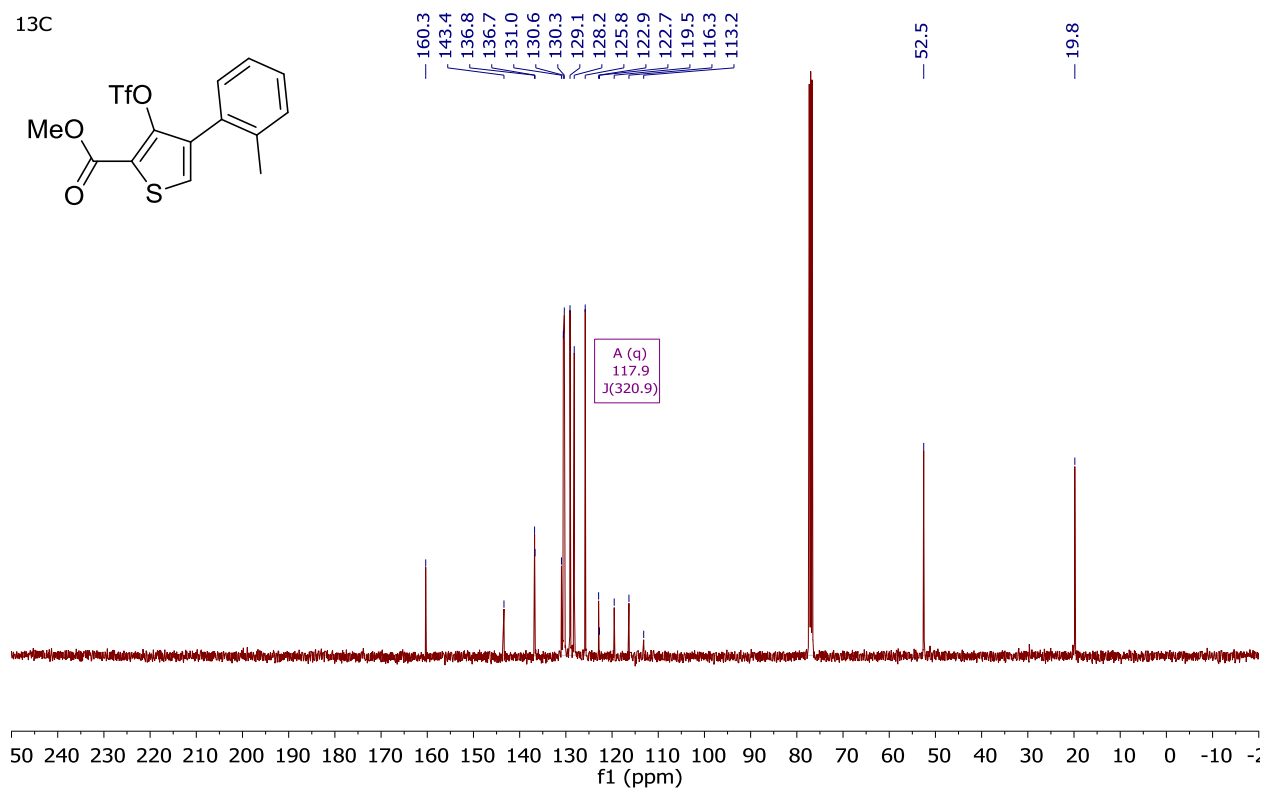
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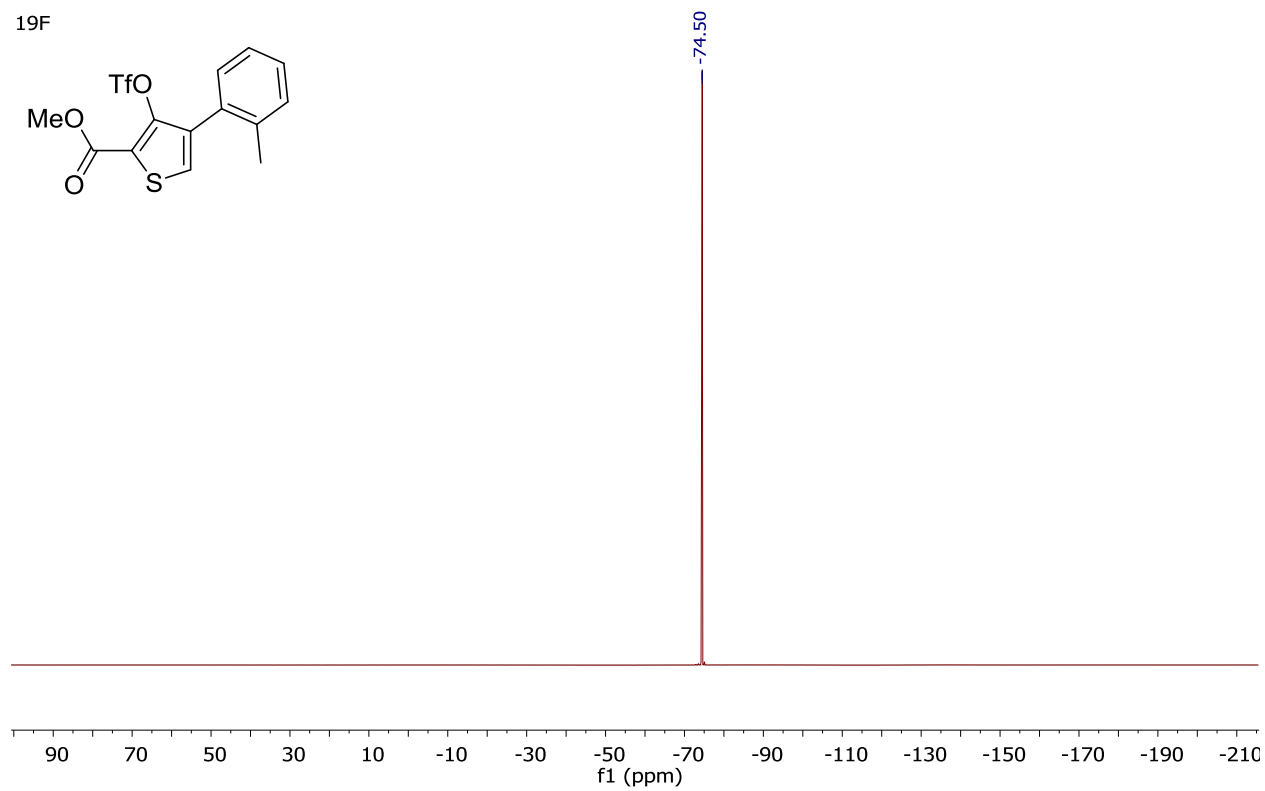
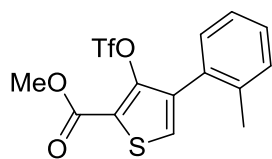
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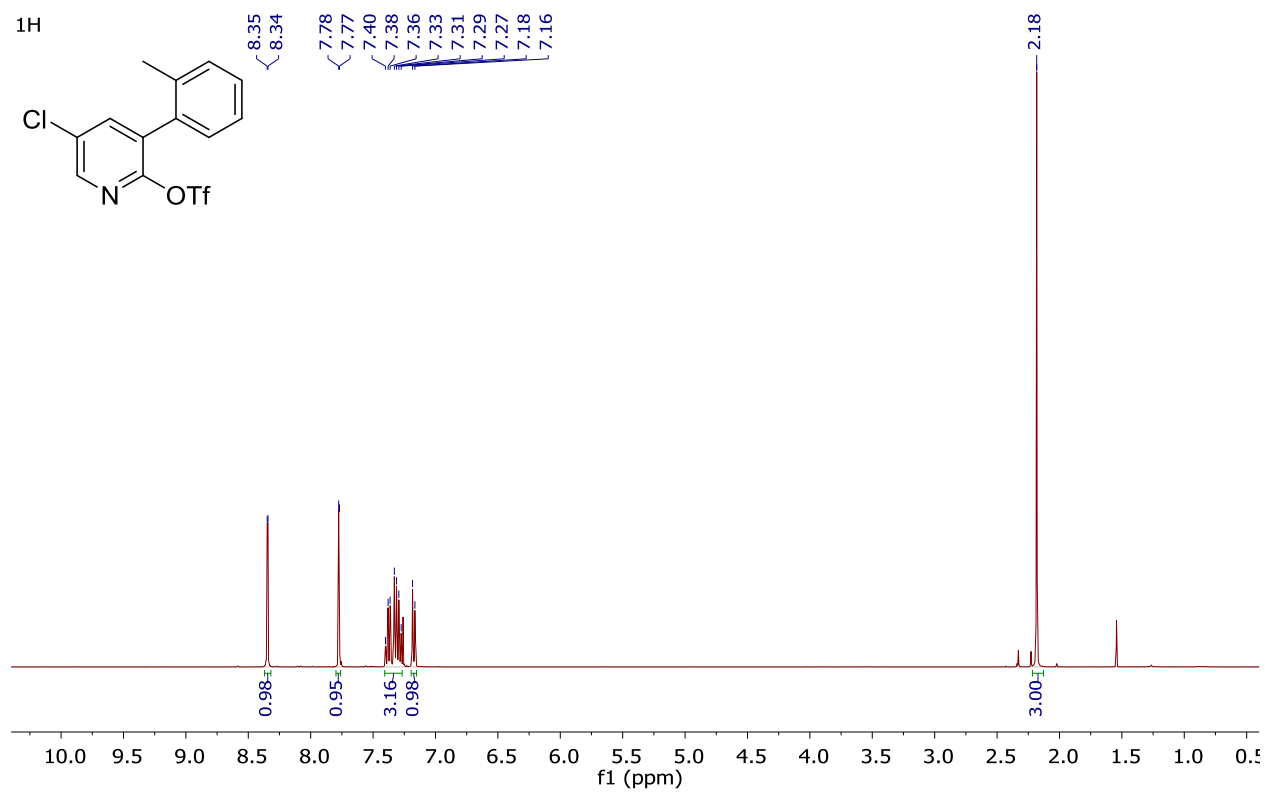
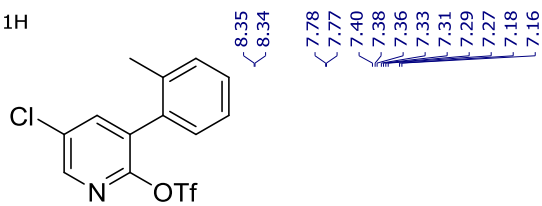
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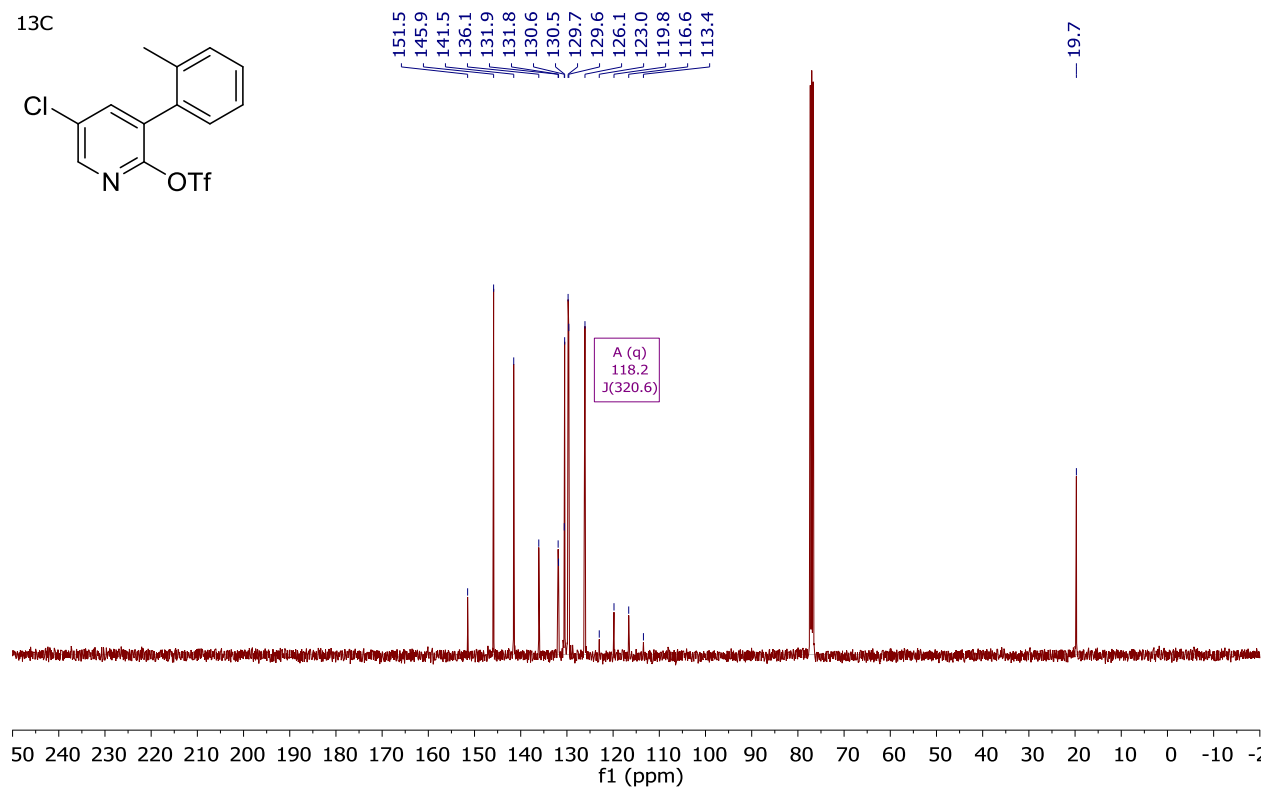
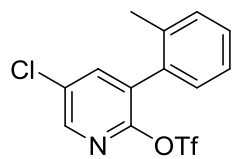
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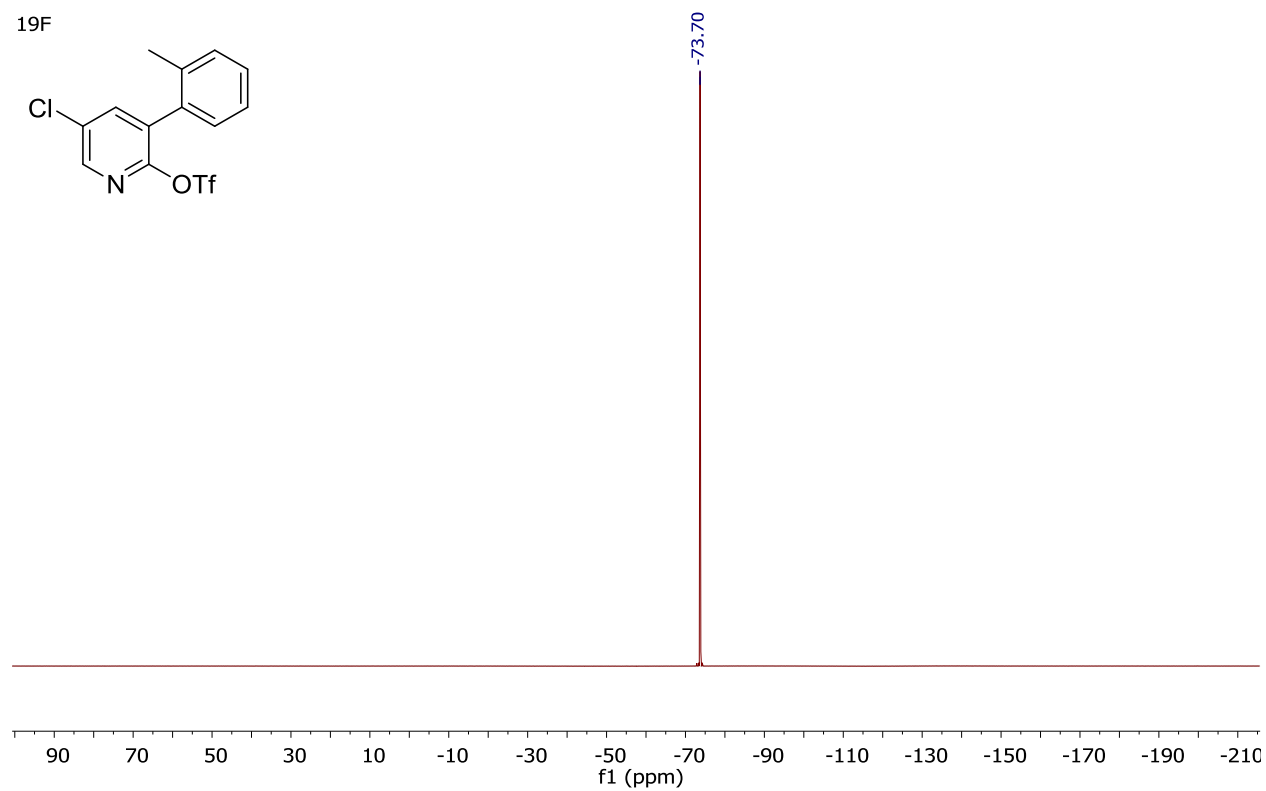
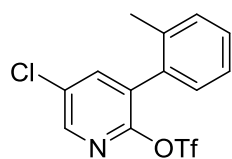
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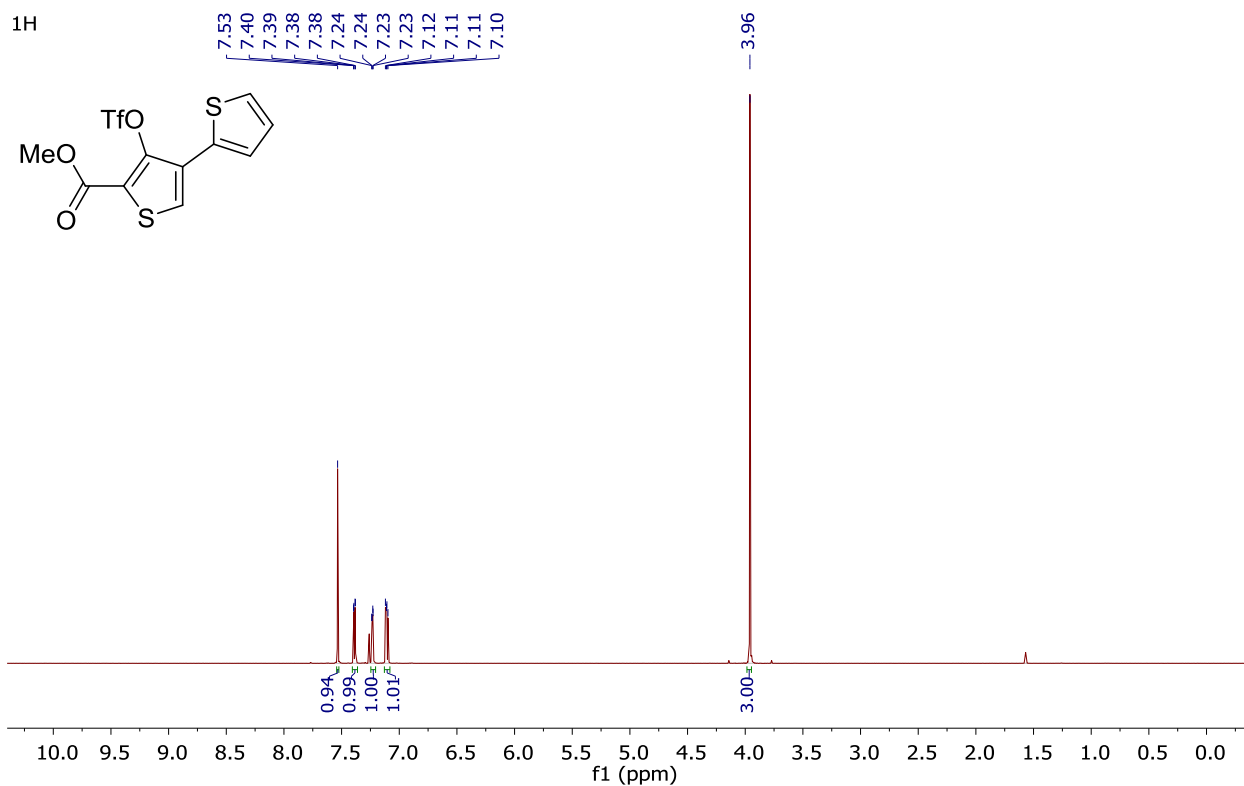
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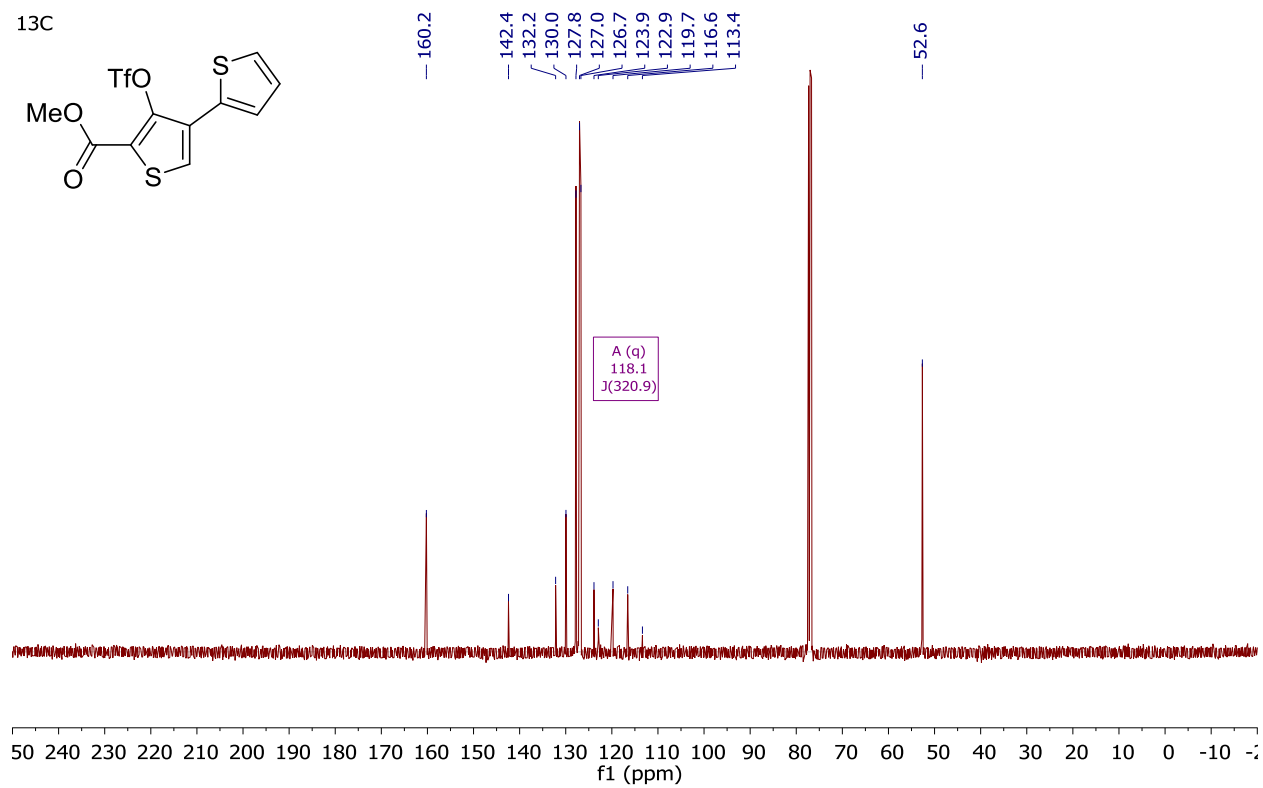
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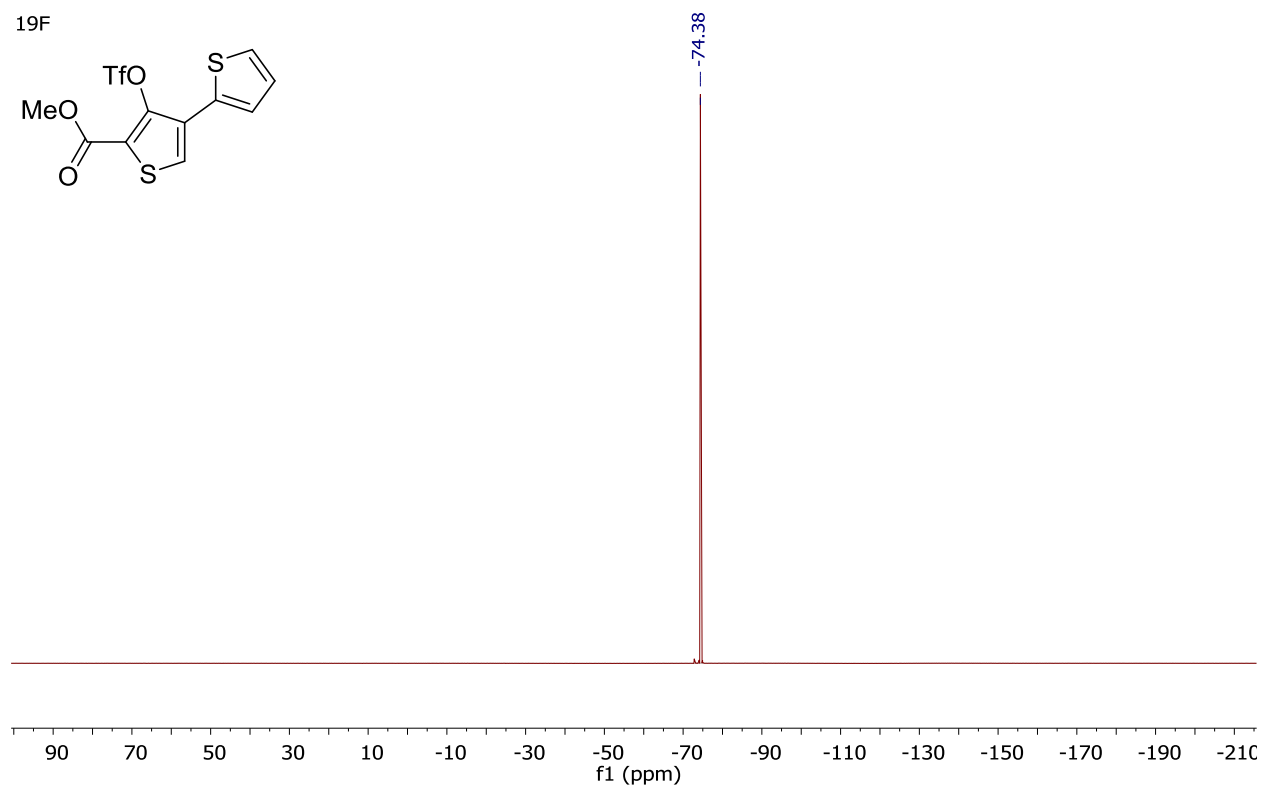
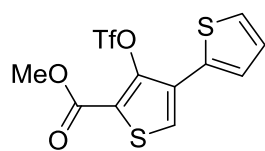
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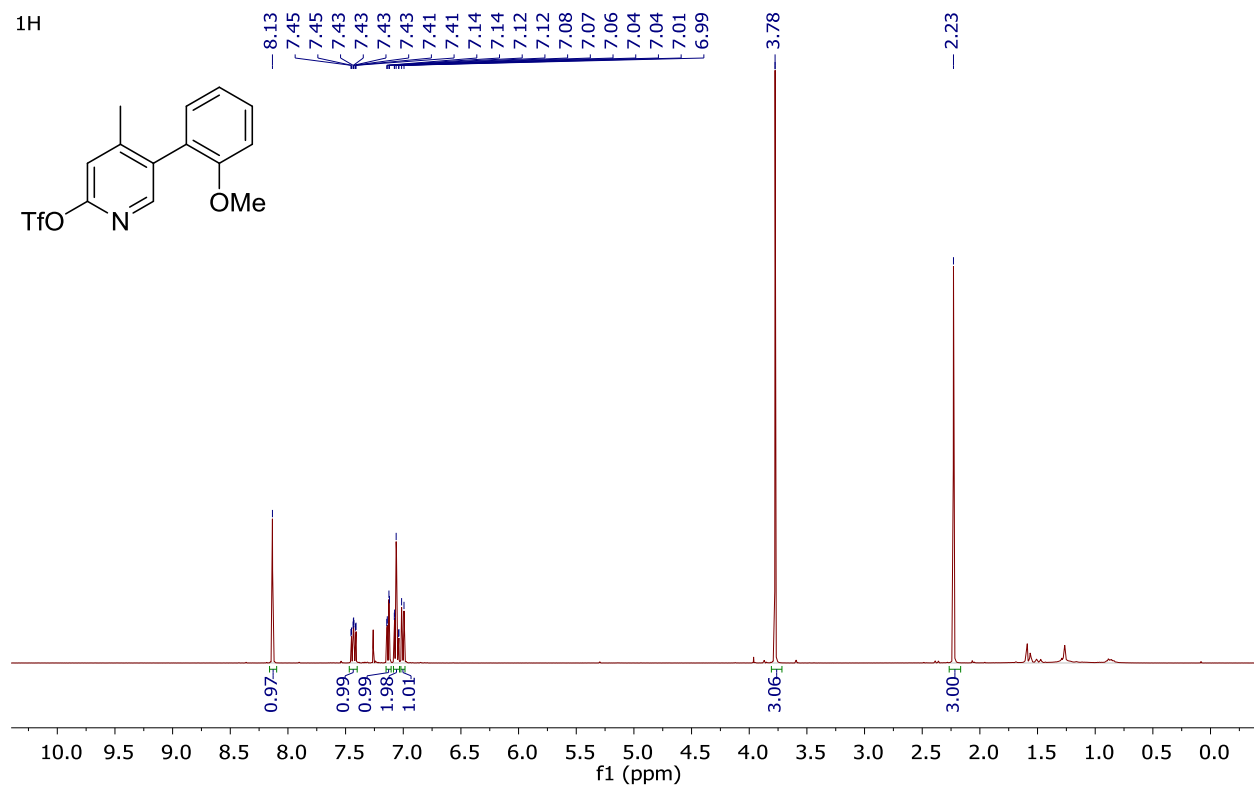
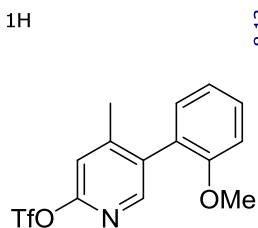
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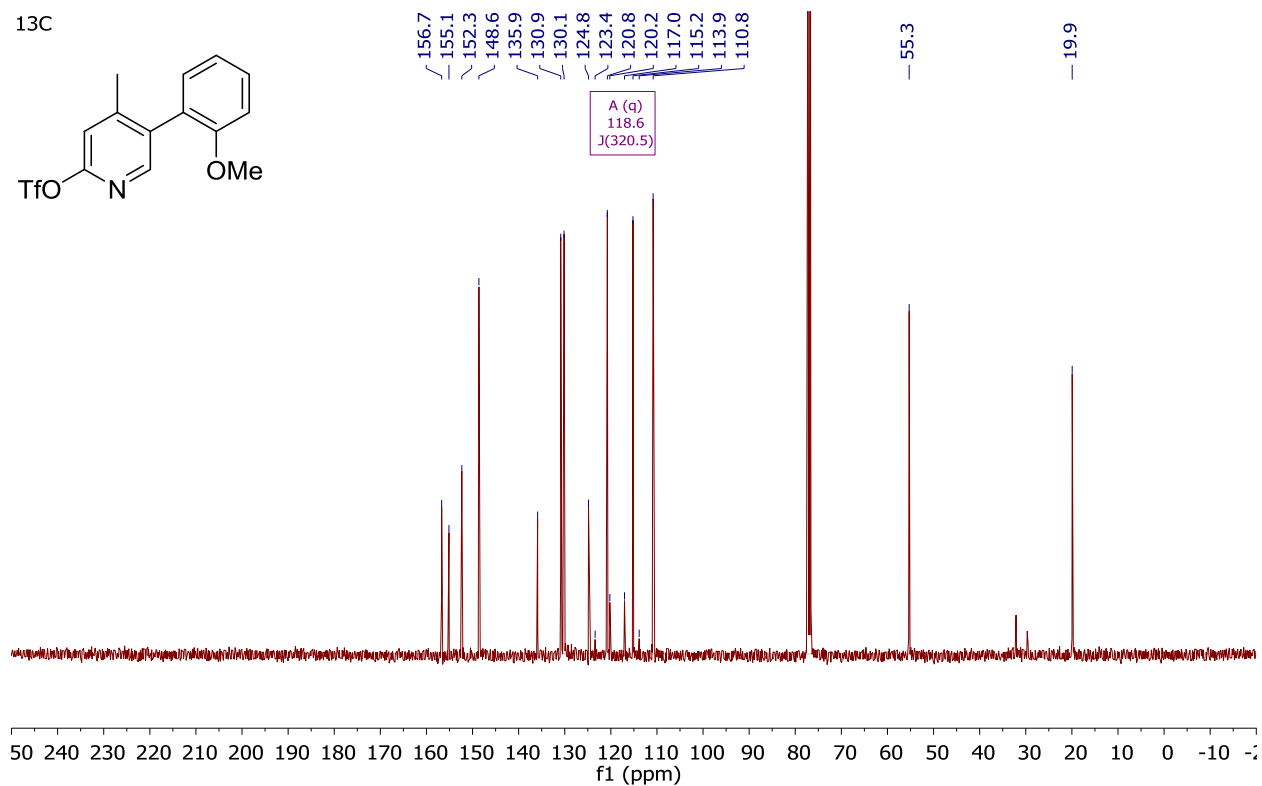
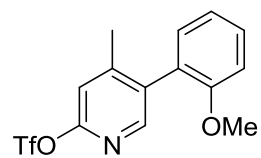
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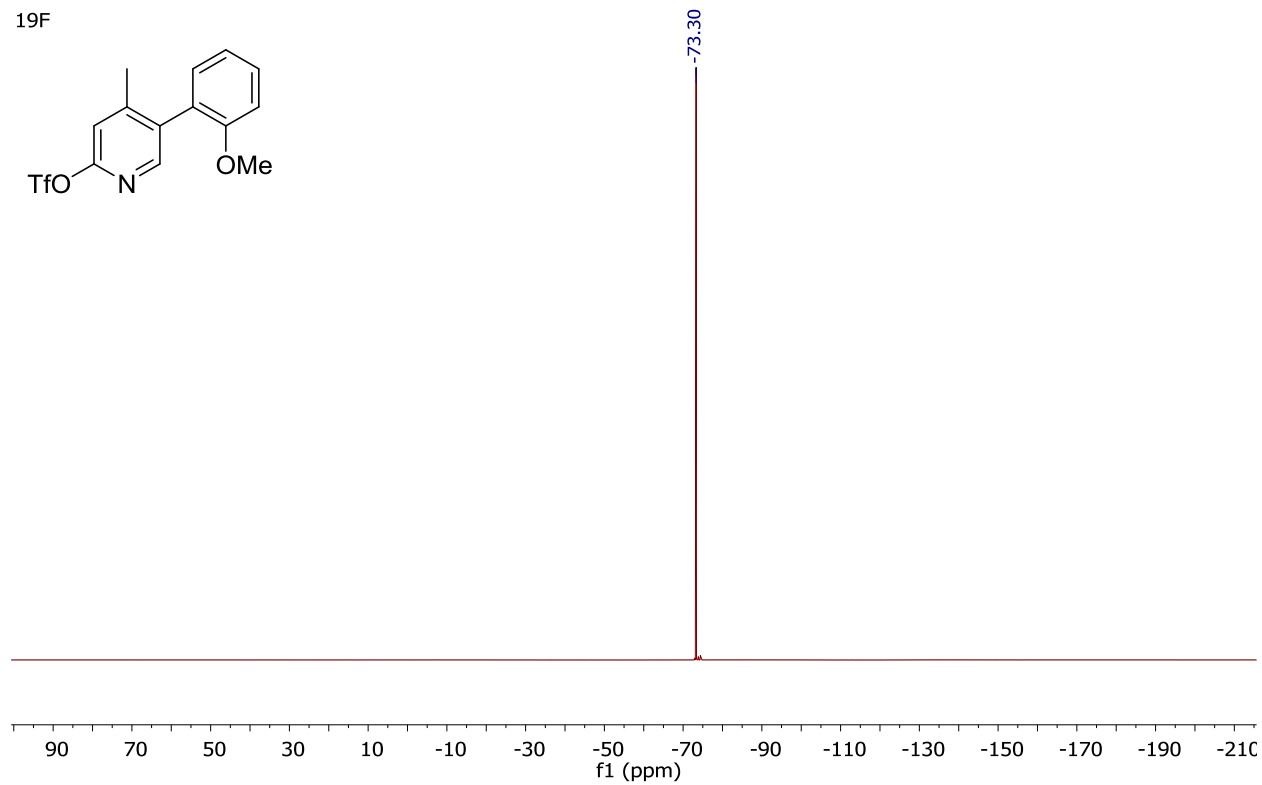
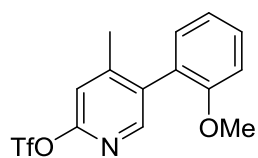
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