Supporting Information

Palladium-Catalyzed Chemoselective Decarboxylative Coupling of Alkynyl Carboxylic Acids with Halogenated Aryl Triflates

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1. General considerations

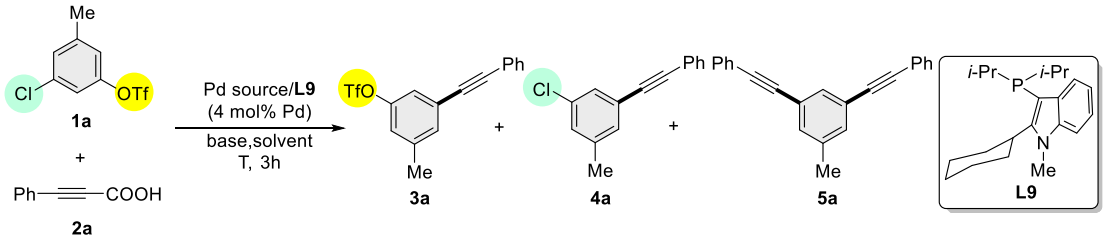
Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All decarboxylative coupling reactions were performed in a resealable screw cap Schlenk tube (approx. 20 mL volume) in the presence of a Teflon-coated magnetic stirrer bar (5 mm x 10 mm). An oil bath was used as the heating source for the reactions. 1,4-Dioxane and toluene were freshly distilled from sodium under nitrogen.[1] Ligands **L1–L8** were purchased from commercial suppliers. Ligands **L9**,[2] **L11**–**L15**,[2] and **L10**[3] were prepared according to the reported literature. A new bottle of *n*-butyllithium was used. Halogenated aryl triflates were prepared according to the literature method.[4] Propiolic acids were prepared following literature procedures.[5] Thin-layer chromatography was performed on pre-coated silica gel 60 F_{254} plates. Silica gel (Grace, 60Å, 40-63 μm) was used for column chromatography. NMR spectra were recorded on a Brüker spectrometer (400 or 600 MHz for ^{1}H, 100 or 151 MHz for ^{13}C or 565 MHz for ^{19}F) and JEOL spectrometer (470 MHz for ^{19}F). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm) as the internal standard. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS) were recorded on an HP 5977A MSD Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on the Agilent 6540 ESI-QTof-MS or APPI-QTof-MS and a Waters GCT Premier EI-ToF-MS. GC-MS analysis was conducted on a HP 7890B GC system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 7890B GC-FID system. All yields reported referring to the isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or ^{1}H NMR. Compounds described in the literature were characterized by a comparison of their ^{1}H, ^{13}C and ^{19}F NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

2. General procedure and data for initial ligand and reaction conditions screening

General Procedure A

General procedure for initial ligand and reaction conditions screening in the chemoselective decarboxylative coupling of 3-chloro-5-methylphenyl triflate: A Schlenk tube equipped with a Teflon-coated magnetic stir bar (5 mm × 10 mm) and a screw cap was charged with Pd source (0.0080 mmol, 4.0 mol% or 0.0040 mmol, 2.0 mol%), ligand (0.0080-0.032 mmol), and base (0.40 mmol). The tube was carefully evacuated and backfilled with nitrogen (three cycles). 3-Chloro-5-methylphenyl triflate (0.20 mmol), 3-phenylpropiolic acid (0.30-0.36 mmol), and freshly distilled solvent (1.0 mL) were added via syringes under nitrogen atmosphere. The tube was sealed and stirred at room temperature for 5 minutes, then transferred to a preheated oil bath at the specified temperature and stirred for 3 hours. The reaction mixture was then cooled to room temperature. Ethyl acetate (~4 mL), dodecane (45.2 µL, internal standard), and water (~2 mL) were added. The organic layer was separated and analyzed by gas chromatography (GC). GC yields were determined using a previously established calibration curve based on authentic samples and dodecane as the internal standard.

Table S1. Screening of Chemoselective C–Cl (over C–OTf) Decarboxylative Coupling Reaction[a]



					Yields (%)[b]		
Entry	Pd source	Pd:L	Base	Solvent	**3a**	**4a**	**5a**
1	$Pd(dba)_2$	1:4	K_2CO_3	THF	82	1	trace

2	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	THF	95	0	3
3	$PdCl_2(CH_3CN)_2$	1:4	K_2CO_3	THF	65	5	9
4	dichloro-(1-methylallyl)-dipalladium	1:1	K_2CO_3	THF	76	1	0
5	dichloro-(1-methylallyl)-dipalladium	1:2	K_2CO_3	THF	78	trace	0
6	dichloro-(1-methylallyl)-dipalladium	1:3	K_2CO_3	THF	81	1	5
7	dichloro-(1-methylallyl)-dipalladium	1:4	K_3PO_4	THF	77	1	0
8	dichloro-(1-methylallyl)-dipalladium	1:4	KOAc	THF	4	1	0
9	dichloro-(1-methylallyl)-dipalladium	1:4	KF	THF	23	0	0
10	dichloro-(1-methylallyl)-dipalladium	1:4	Cs_2CO_3	THF	92	0	7
11	dichloro-(1-methylallyl)-	1:4	K_2CO_3	1,4-dioxane	75	0	0

	dipalladium						
12	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	PhMe	93	0	0
13	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	CPMe	78	0	0
14[c]	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	THF	80	1	0
15[d]	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	THF	68	1	0
16[e]	dichloro-(1-methylallyl)-dipalladium	1:4	K_2CO_3	THF	80	0	0

[a] Reaction condition: 3-chloro-5-methylphenyl triflate (0.20 mmol), 3-phenylpropiolic acid (0.36 mmol), Pd source (4 mol% Pd), **L9**, base (0.40 mmol) and solvent (1.0 mL) were stirred at 100 °C for 3 h. [b] Calibrated GC yields were reported by using dodecane as an internal standard. [c] 3-phenylpropiolic acid (0.30 mmol) was used. [d] 90 °C was conducted. [e] 110 °C was conducted.

3. General procedure for palladium-catalyzed chemoselective decarboxylative coupling of chloroaryl triflates (or polyhalogenated aryl triflates)

General Procedure B

Dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), chloroaryl triflates (or polyhalogenated aryl triflates, 0.200 mmol; if liquid, added after the solvent), and K_2CO_3 (55.2 mg, 0.400 mmol) were added to a Schlenk tube equipped with a Teflon-coated magnetic stir bar (5 mm × 10 mm) and a screw cap. The tube was carefully evacuated and backfilled with nitrogen (three cycles). Alkynyl carboxylic acids (0.360 mmol) and freshly distilled THF or toluene (1.0 mL) were added via syringes under nitrogen atmosphere. The tube was sealed and stirred at room temperature for 5 minutes, then transferred to a preheated oil bath at 100 °C and stirred for 3 hours. The reaction mixture was then cooled to room temperature. Ethyl acetate (~4 mL) and water (~2 mL) were added. The aqueous layer was separated and washed with ethyl acetate. The organic layers were combined and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (230–400 mesh) to afford the desired product.

4. General procedure for one-pot sequential reaction

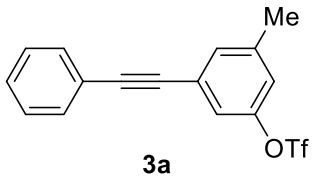
General Procedure C

Dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), chloroaryl triflates (0.200 mmol; if solid), alkynyl carboxylic acids (0.360 mmol; if solid), and K_2CO_3 (55.2 mg, 0.400 mmol) were added to a Schlenk tube equipped with a Teflon-coated magnetic stir bar (5 mm × 10 mm) and a screw cap. The tube was carefully evacuated and backfilled with nitrogen (three cycles). If the chloroaryl triflates (0.200 mmol) and/or alkynyl carboxylic acids (0.360 mmol) were liquids, they were added at this stage via syringe along with freshly distilled THF (1.0 mL) under a nitrogen atmosphere. The tube was then sealed and stirred at room temperature for 5 minutes before being transferred to a preheated oil bath at 100 °C and stirred for 3 hours. After the reaction mixture cooled to room temperature, $Pd_2(dba)_3$ (2.70 mg, 0.00300 mmol), SPhos (3.70 mg, 0.00900 mmol), 4-methoxyphenylboronic acid (60.8 mg, 0.400 mmol), and K_3PO_4 (63.6 mg, 0.300 mmol) were added under nitrogen. The sealed tube was then placed into a preheated oil bath at 110 °C and stirred for 2 hours. The reaction mixture was cooled to room temperature, followed by the addition of ethyl acetate (~4 mL) and water (~2 mL). The aqueous layer was separated and washed with ethyl acetate. The combined organic layers were concentrated under reduced pressure, and the crude product was purified by column chromatography on silica gel (230–400 mesh) to afford the desired product.

5. General procedure for competitive experiment

Dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), and K_2CO_3 (55.2 mg, 0.400 mmol) were added to a Schlenk tube equipped with a Teflon-coated magnetic stir bar (5 mm × 10 mm) and a screw cap. The tube was carefully evacuated and backfilled with nitrogen (three cycles). 3-Chloro-5-(trifluoromethyl)phenyl triflate (0.100 mmol), 3-chloro-5-methylphenyl triflate or 3-chlorophenyltriflate (0.100 mmol), 3-phenylpropiolic acid (0.200 mmol) and freshly distilled THF (1.0 mL) were then added via syringes under a nitrogen atmosphere. The tube was sealed and stirred at room temperature for 5 minutes, followed by heating in a preheated oil bath at 100 °C for 30 minutes. The reaction mixture was then cooled to room temperature. Ethyl acetate (~4 mL), dodecane (45.2 µL, internal standard), and water (~2 mL) were added. The organic layer was separated and analyzed by gas chromatography (GC). GC yields were determined using a previously established calibration curve based on authentic samples with dodecane as the internal standard.

6. Characterization data for coupling products

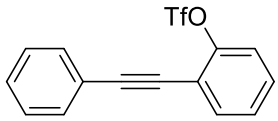


3a

3-methyl-5-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3a**):

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-5-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3a** = 93% (0.186 mmol, 63.1 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.52 (m, 2H), 7.37–7.33 (m, 4H), 7.24 (s, 1H), 7.04 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 140.9, 132.2, 131.7, 128.9, 128.5, 125.4, 122.5, 121.8, 121.2, 118.7 (q, *J* = 318.7 Hz), 91.1, 87.4, 21.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.8. The data are in agreement with those previously reported in the literature.[4]

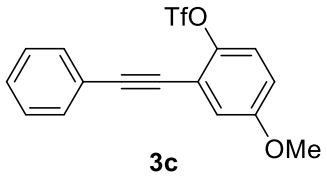


3b

2-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2/3, compound **3b**):

Followed **General Procedure B** on 0.200 mmol scale with 2-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Scheme 2; Yield of **3b** = 88% (0.176 mmol, 57.3 mg); Scheme 3, Yield of **3b** = 73% (0.146 mmol, 47.5 mg); orange liquid; For Scheme 2, the % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; For Scheme 3, the % of major product (reacting C–Br site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64–7.59 (m, 3H), 7.38 (dd, *J* = 10.8, 8.8 Hz, 5H), 7.30 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 133.7, 131.8, 129.7, 129.1, 128.4, 128.1, 122.2, 121.6, 118.7 (q, *J*=318.4 Hz), 118.4, 96.4, 82.4; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.5. The data are in agreement with those previously reported in the literature.[4]

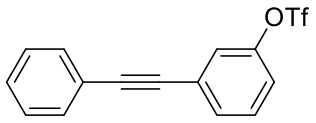


3c

4-methoxy-2-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3c**):

Followed **General Procedure B** on 0.200 mmol scale with 2-chloro-4-methoxyphenyl trifluoromethanesulfonate (58.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3c** = 85% (0.170 mmol, 60.6 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=10:1) was used for flash column chromatography Eluents; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61–7.57 (m, 2H), 7.38–7.35 (m, 3H), 7.19 (d, *J* = 9.2 Hz, 1H), 7.10 (d, *J* = 3.2 Hz, 1H), 6.88 (dd, *J* = 9.2, 3.2 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 143.4, 131.8, 129.1, 128.4, 122.5, 122.1, 119.1, 118.7 (q, *J* = 318.7 Hz), 117.6, 115.6, 96.1, 82.6, 55.8; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.5. The data are in agreement with those previously reported in the literature.[4]

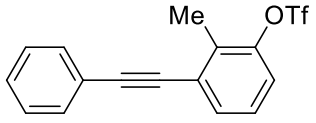


3d

3-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3d**):

Followed **General Procedure B** on 0.200 mmol scale with 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3d** = 75% (0.150 mmol, 49.2 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.53 (m, 3H), 7.42 (dd, *J* = 11.2, 5.2 Hz, 2H), 7.38–7.35 (m, 3H), 7.24 (dd, *J* = 8.0, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 131.7, 131.5, 130.2, 128.9, 128.5, 125.9, 124.2, 122.3, 121.1, 118.7 (q, *J* = 318.8 Hz), 91.6, 87.1; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6. The data are in agreement with those previously reported in the literature.[4]



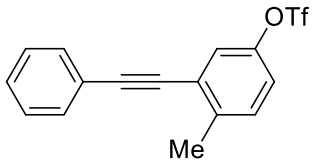
3e

2-methyl-3-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3e**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3e** = 93% (0.186 mmol, 63.5 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash

column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.55–7.50 (m, 3H), 7.37–7.34 (m, 3H), 7.23–7.22 (m, 2H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 133.1, 131.7, 131.6, 128.8, 128.5, 127.0, 126.4, 122.6, 121.2, 118.6 (q, *J* = 318.2 Hz), 95.2, 86.4, 14.7; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.6; The data are in agreement with those previously reported in the literature.[4]

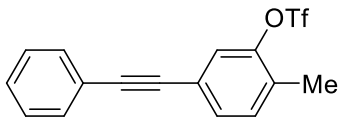


3f

4-methyl-3-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3f**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3f** = 85% (0.170 mmol, 57.8 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 6.4, 2.8 Hz, 2H), 7.39–7.32 (m, 4H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.12 (dd, *J* = 8.4, 2.8 Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 140.7, 131.6, 131.0, 128.8, 128.5, 125.3, 124.1, 122.6, 120.9, 118.7 (q, *J* = 318.9 Hz), 95.4, 86.3, 20.3; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.7; The data are in agreement with those previously reported in the literature.[4]

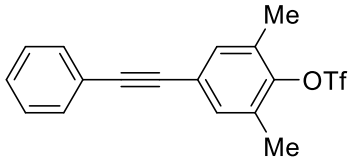


3g

2-methyl-5-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3g**)

Followed **General Procedure B** on 0.200 mmol scale with 5-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3g** = 79% (0.158 mmol, 53.8 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) = 98.4 : 1.6; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.52 (m, 2H), 7.42 (dd, *J* = 10.8, 2.8 Hz, 2H), 7.36–7.35 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 132.1, 131.7, 131.3, 131.2, 128.7, 128.4, 124.1, 123.1, 122.5, 118.6 (q, *J* = 318.1 Hz), 90.7, 87.3, 16.4; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.6; The data are in agreement with those previously reported in the literature.[4]

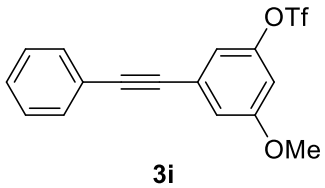


3h

2,6-dimethyl-4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3h**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloro-2,6-dimethylphenyl trifluoromethanesulfonate (57.7 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3h** = 95% (0.190 mmol, 67.4 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.36–7.34 (m, 3H), 7.29 (s, 2H), 2.38 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 132.8, 131.8, 131.6, 128.6, 128.4, 123.3, 122.7, 118.6 (q, *J* = 317.8 Hz), 90.4, 87.7, 17.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.3; The data are in agreement with those previously reported in the literature.[4]

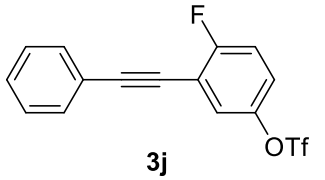


3i

3-methoxy-5-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3i**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-5-methoxyphenyl trifluoromethanesulfonate (58.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3i** = 73% (0.146 mmol, 51.9 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=10:1) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 6.8, 3.2 Hz, 2H), 7.37 (dd, *J* = 6.4, 3.6 Hz, 3H), 7.06–7.04 (m, 2H), 6.79 (t, *J* = 2.4 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 149.8, 131.7, 128.9, 128.4, 126.0, 122.3, 118.7 (q, *J* = 318.9 Hz), 116.6, 116.4, 108.2, 91.2, 87.3, 55.9; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.7; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{16}H_{11}F_3O_4S$ 356.0325, found 356.0317.

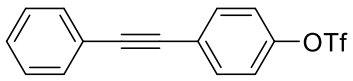


3j

4-fluoro-3-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3j**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-4-fluorophenyl trifluoromethanesulfonate (55.7 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3j** = 72% (0.144 mmol, 49.5 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58–7.55 (m, 2H), 7.44 (dd, *J* = 5.6, 3.2 Hz, 1H), 7.39–7.36 (m, 3H), 7.24–7.14 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5 (d, *J* = 252.8 Hz), 144.7 (d, *J* = 3.3 Hz), 131.8, 129.3, 128.5, 126.0, 122.7 (d, *J* = 8.5 Hz), 121.9, 118.7 (q, *J* = 318.8 Hz), 117.1 (d, *J* = 23.8 Hz), 114.2 (d, *J* = 18.6 Hz), 96.7 (d, *J* = 3.4 Hz), 80.7; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.5, -109.0; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{15}H_8F_4O_3S$ 344.0125, found 344.0138.



3k

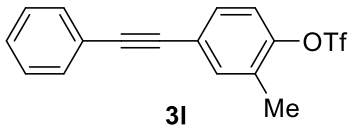
4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3k**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Followed **General Procedure B** on 1.0 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (260 mg, 1.0 mmol), 3-phenylpropiolic acid (263 mg, 1.80 mmol), dichloro-(1-methylallyl)-dipalladium (8.0 mg, 0.0200 mmol), **L9** (52.5 mg, 0.160 mmol), K_2CO_3 (276 mg, 2.0 mmol) and THF (10 mL) for 5 h;

Yield of **3k** = 80% (0.160 mmol, 52.3 mg) for 0.200 mmol scale; 70% (0.700 mmol, 227 mg) for 1.0 mmol scale; Light yellow solid, melting point 57.9–58.8 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.8 Hz, 2H), 7.53 (dd, *J* = 6.8, 2.8 Hz, 2H), 7.36 (dd, *J* = 6.8, 3.6 Hz, 3H), 7.25 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 133.4, 131.7, 128.8, 128.4, 124.0, 122.5, 121.5, 118.7 (q, *J* = 319.0 Hz), 91.2, 87.3; ^{19}F

NMR (470 MHz, $CDCl_3$) δ -72.6; The data are in agreement with those previously reported in the literature.[4]

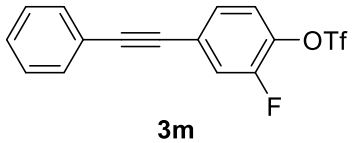


3l

2-methyl-4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3l**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3l** = 85% (0.170 mmol, 67.5 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.51 (m, 2H), 7.47 (s, 1H), 7.40 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.36–7.34 (m, 3H), 7.22 (t, *J* = 7.6 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 135.1, 131.6, 131.1, 130.8, 128.7, 128.4, 123.7, 122.6, 121.4, 118.6 (q, *J* = 318.2 Hz), 90.8, 87.5, 16.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.6; The data are in agreement with those previously reported in the literature.[4]



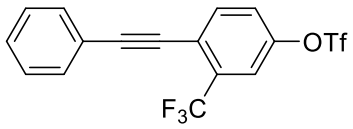
3m

2-fluoro-4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3m**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloro-2-fluorophenyl trifluoromethanesulfonate (55.7 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360

mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3m** = 82% (0.164 mmol, 56.1 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.52 (m, 2H), 7.41–7.35 (m, 4H), 7.34–7.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2 (d, *J* = 252.6 Hz), 136.5 (d, *J* = 13.5 Hz), 131.7, 129.1, 128.5, 128.3 (d, *J* = 3.6 Hz), 125.4 (d, *J* = 8.5 Hz), 123.6, 122.1, 120.4 (d, *J* = 19.5 Hz), 118.7 (q, *J* = 318.8 Hz), 92.2, 86.4 (d, *J* = 2.8 Hz); ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.0, -126.8; The data are in agreement with those previously reported in the literature.[4]

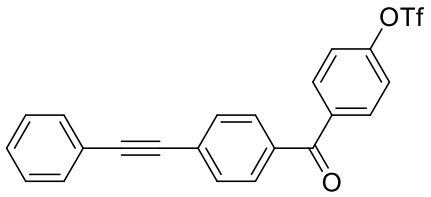


3n

4-(phenylethynyl)-3-(trifluoromethyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3n**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloro-3-(trifluoromethyl)phenyl trifluoromethanesulfonate (55.7 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3n** = 79% (0.158 mmol, 61.9 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) = 98.2 : 1.8; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.8 Hz, 1H), 7.58–7.54 (m, 3H), 7.45–7.36 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 135.6, 133.3 (q, *J* = 32 Hz), 131.8, 131.7, 129.4, 128.5, 124.6, 122.3 (q, *J* = 272.2 Hz), 122.0, 119.6 (q, *J* = 5.2 Hz), 118.7 (q, *J* = 318.9 Hz), 97.3, 83.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.9, -72.5; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{16}H_8F_6O_3S$ 394.0093, found 394.0088.

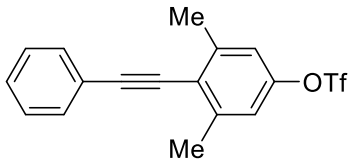


3o

4-(4-(phenylethynyl)benzoyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3o**)

Followed **General Procedure B** on 0.200 mmol scale with 4-(4-chlorobenzoyl)phenyl trifluoromethanesulfonate (72.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg , 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3o** = 63% (0.126 mmol, 54.0 mg); white solid; melting point 157.0–158.5 ^oC; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=10:1) was used for flash column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 7.91–7.89 (m, 2H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.58–7.55 (m, 2H), 7.43–7.37 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 152.0, 137.4, 135.7, 132.0, 131.8, 131.6, 130.0, 128.9, 128.5, 128.3, 122.5, 121.5, 118.7 (q, *J* = 318.9 Hz), 93.0, 88.4; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; The data are in agreement with those previously reported in the literature.[4]



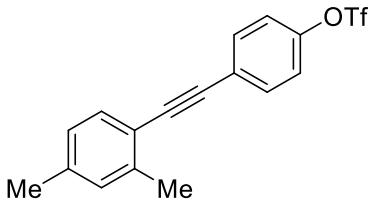
3p

3,5-dimethyl-4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3p**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate (57.7 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360

mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3p** = 76% (0.152 mmol, 53.7 mg); white solid; melting point 61.1–62.3 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.36 (dd, *J* = 6.4, 4.0 Hz, 3H), 6.99 (s, 2H), 2.53 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 142.8, 131.5, 128.6, 128.5, 123.7, 123.0, 119.4, 118.7 (q, *J* = 318.9 Hz), 99.5, 85.3, 21.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.8; The data are in agreement with those previously reported in the literature.[4]

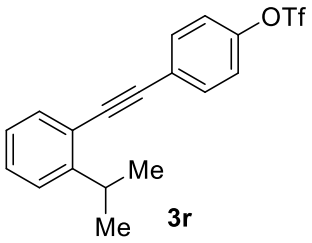


3q

4-((2,4-dimethylphenyl)ethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3q**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(2,4-dimethylphenyl)propiolic acid (62.7 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3q** = 90% (0.180 mmol, 64.0 mg); light yellow solid; melting point 41.0–41.9 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.56 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.26–7.23 (m, 2H), 7.06 (s, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 2.46 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 140.2, 139.0, 133.2, 131.8, 130.4, 126.5, 124.5, 121.4, 119.2, 118.7 (q, *J* = 319.1 Hz), 90.6, 90.5, 21.4, 20.6; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{17}H_{13}F_3O_3S$ 354.0532; found 354.0527.

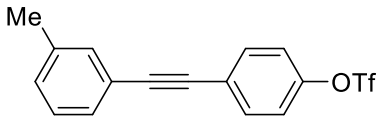


3r

4-((2-isopropylphenyl)ethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3r**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(2-isopropylphenyl)propiolic acid (67.8 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3r** = 76% (0.152 mmol, 56.0 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) = 97.5 : 2.5; Eluents (Hexane:) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.49 (m, 3H), 7.34–7.30 (m, 2H), 7.28–7.24 (m, 2H), 7.20–7.16 (m, 1H), 3.55–3.45 (m, 1H), 1.32 (s, 3H), 1.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 148.8, 133.2, 132.4, 129.2, 125.7, 125.1, 124.3, 121.5, 121.2, 118.7 (q, J = 319.0 Hz), 90.9, 90.2, 31.7, 23.1; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{18}H_{15}F_3O_3S$ 368.0689; found 368.0685.



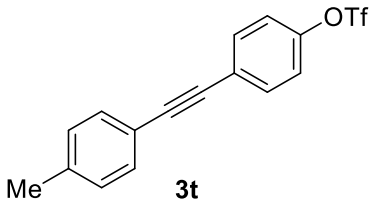
3s

4-(*m*-tolylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3s**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(*m*-tolyl)propiolic acid (57.7 mg, 0.360

mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3s** = 70% (0.140 mmol, 47.8 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) = 97.6 : 2.4; Eluents (Hexane:) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.49 (m, 2H), 7.36–7.33 (m, 2H), 7.25 (dd, *J* = 8.0, 5.2 Hz, 3H), 7.17 (d, *J* = 7.6 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 138.2, 133.4, 132.2, 131.5, 129.7, 128.8, 128.3, 124.1, 121.5, 118.7 (q, *J* = 318.9 Hz), 91.5, 87.0, 21.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{16}H_{11}F_3O_3S$ 340.0376; found 340.0364.

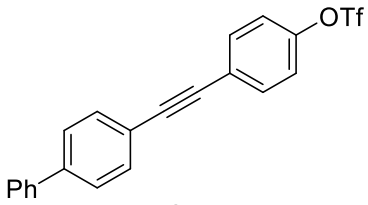


3t

4-(*p*-tolylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3t**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(*p*-tolyl)propiolic acid (57.7 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3t** = 70% (0.140 mmol, 47.4 mg); light yellow solid; melting point 68.6–70.3 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.8 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.26–7.24 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 139.0, 133.3, 131.6, 129.2, 124.2, 121.4, 119.4, 118.7 (q, *J* = 318.9 Hz), 91.5, 86.7, 21.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; The data are in agreement with those previously reported in the literature.[4]

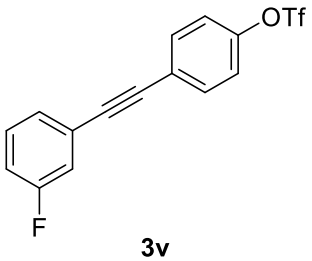


3u

4-([1,1'-biphenyl]-4-ylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3u**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-([1,1'-biphenyl]-4-yl)propiolic acid (80.0 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3u** = 76% (0.152 mmol, 61.2 mg); light yellow solid; melting point 151.1–152.3 ^{o}C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=20:1) was used for flash column chromatography; ^{1}H NMR (400 MHz, CDCl3) δ 7.56–7.53 (m, 8H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.31–7.28 (m, 1H), 7.21–7.17 (m, 2H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 141.6, 140.2, 133.4, 132.2, 128.9, 127.8, 127.2, 127.1, 126.6, 124.1, 121.6, 118.8 (q, *J* = 318.9 Hz), 91.2, 88.0, ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; The data are in agreement with those previously reported in the literature.[4]



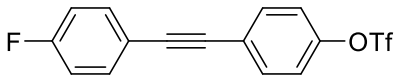
3v

4-((3-fluorophenyl)ethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3v**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(3-fluorophenyl)propiolic acid (59.1 mg,

0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3v** = 77% (0.154 mmol, 53.1 mg); light yellow solid; melting point 42.9–44.1 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) = 97.3 : 2.7; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.51 (m, 2H), 7.33–7.21 (m, 5H), 7.09–7.05 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4 (d, *J* = 245.3 Hz), 149.1, 133.5, 131.6, 130.1 (d, *J* = 8.4 Hz), 127.6 (d, *J* = 3.1 Hz), 124.4 (d, *J* = 9.4 Hz), 121.6, 118.8 (q, *J* = 319.0 Hz), 118.4 (d, *J* = 22.9 Hz), 116.1 (d, *J* = 21.2 Hz), 89.9, 88.1; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6, -112.5; The data are in agreement with those previously reported in the literature.[4]

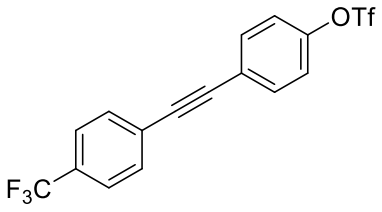


3w

4-((4-fluorophenyl)ethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3w**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(4-fluorophenyl)propiolic acid (59.1 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3w** = 78% (0.156 mmol, 53.4 mg); light yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.57 (m, 2H), 7.53–7.49 (m, 2H), 7.26 (d, *J* = 8.8 Hz, 2H), 7.08–7.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 248.9 Hz), 148.9, 133.6 (d, *J* = 8.4 Hz), 133.3, 123.8, 121.5, 118.7 (q, *J* = 319.0 Hz), 118.6 (d, *J* = 3.5 Hz), 115.8 (d, *J* = 22.0 Hz), 90.2, 87.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.7, -109.8; The data are in agreement with those previously reported in the literature.[4]

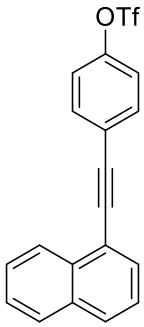


3x

4-((4-(trifluoromethyl)phenyl)ethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3x**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(4-(trifluoromethyl)phenyl)propiolic acid (77.1 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3x** = 82% (0.164 mmol, 64.8 mg); orange solid, melting point 44.1–45.5 ^{o}C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63–7.61 (m, 6H), 7.30–7.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 133.6, 131.9, 130.5 (q, *J* = 33.0 Hz), 126.5, 125.4 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 270.0 Hz), 123.3, 121.6, 118.7 (q, *J* = 318.8 Hz), 89.7, 89.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.8, -72.7; The data are in agreement with those previously reported in the literature.[4]

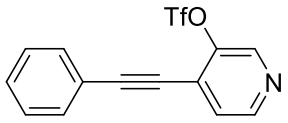


3y

4-(naphthalen-1-ylethynyl)phenyl trifluoromethanesulfonate (Scheme 2, compound **3y**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.200 mmol), 3-(naphthalen-1-yl)propiolic acid (70.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3y** = 77% (0.154 mmol, 58.2 mg); white solid; melting point 68.4–70.7 °C; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.4 Hz, 1H), 7.84 (dd, *J* = 8.4, 3.2 Hz, 2H), 7.75 (d, *J* = 6.8 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.46–7.42 (m, 1H), 7.32–7.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 138.4, 133.5, 133.3, 130.8, 129.4, 128.5, 127.1, 126.6, 126.0, 125.3, 124.2, 121.6, 118.8 (q, *J* = 318.9 Hz), 110.9, 92.2, 89.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ -72.6; The data are in agreement with those previously reported in the literature.[4]

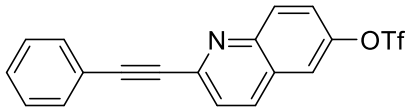


3z

4-(phenylethynyl)pyridin-3-yl trifluoromethanesulfonate (Scheme 2, compound **3z**)

Followed **General Procedure B** on 0.200 mmol scale with 4-chloropyridin-3-yl trifluoromethanesulfonate (52.3 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3z** = 70% (0.139 mmol, 45.6 mg); colourless liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=20:1) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61–8.60 (m, 2H), 7.62 (d, *J* = 6.9 Hz, 2H), 7.52 (d, *J* = 4.9 Hz, 1H), 7.46–7.39 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.2, 146.2, 143.0, 132.2, 130.1, 128.6, 126.7, 126.5, 121.0, 118.6 (q, *J* = 320.9 Hz), 101.4, 80.4; ^{19}F NMR (565 MHz, $CDCl_3$) δ -73.2; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{14}H_8F_3NO_3S$ 327.0171; found 327.0176.

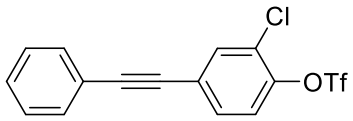


3aa

2-(phenylethynyl)quinolin-6-yl trifluoromethanesulfonate (Scheme 2, compound **3aa**)

Followed **General Procedure B** on 0.200 mmol scale with 2-chloroquinolin-6-yl trifluoromethanesulfonate (62.3 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **3aa** = 69% (0.137 mmol, 51.7 mg); white solid; melting point 116.3–117.4 ^oC; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:EA=20:1) was used for flash column chromatography; ^1H NMR (600 MHz, $CDCl_3$) δ 8.21 (d, *J* = 9.2 Hz, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.73–7.72 (m, 1H), 7.69–7.66 (m, 3H), 7.61 (dd, *J* = 9.2 Hz, 2.6 Hz, 1H), 7.43–7.37 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.2, 146.9, 145.0, 136.1, 132.3, 132.1, 129.5, 128.4, 127.0, 125.7, 123.7, 121.6, 119.0, 118.7 (q, *J* = 321.1 Hz), 91.3, 88.7; ^{19}F NMR (565 MHz, $CDCl_3$) δ -72.7; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{18}H_{10}F_3NO_3S$ 377.0328; found 377.0323.



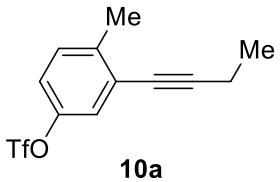
8a

2-chloro-4-(phenylethynyl)phenyl trifluoromethanesulfonate (Scheme 3, compound **8a**)

Followed **General Procedure B** on 0.200 mmol scale with 4-bromo-2-chlorophenyl trifluoromethanesulfonate (67.9 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360

mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **8a** = 77% (0.154 mmol, 55.1 mg); light yellow liquid; The % of major product (reacting C–Br site) : minor product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1: 0; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 2.0 Hz, 1H), 7.52 (dd, *J* = 6.4, 3.2 Hz, 2H), 7.46 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.37–7.33 (m, 3H), 7.31 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 133.9, 131.7, 131.3, 129.1, 128.5, 127.3, 125.1, 122.9, 122.1, 118.6 (q, *J* = 318.7 Hz), 92.3, 86.2; ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.3; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{18}H_8ClF_3O_3S$ 359.9829; found 359.9837.

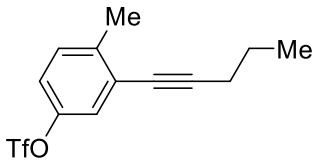


10a

3-(but-1-yn-1-yl)-4-methylphenyl trifluoromethanesulfonate (Scheme 4, compound **10a**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.8 mg, 0.200 mmol), 2-pentynoic acid (35.3 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and toluene (1.0 mL);

Yield of **10a** = 69% (0.138 mmol, 40.3 mg); colourless liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (s, 1H), 7.22 (d, *J* = 8.9 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 2.46 (q, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), 1.26 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.1, 140.5, 130.7, 126.0, 124.1, 120.1, 118.7 (q, *J* = 320.1 Hz), 98.2, 77.2, 20.2, 13.8, 13.2; ^{19}F NMR (565 MHz, $CDCl_3$) δ -72.9; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{12}H_{11}F_3O_3S$ 292.0376; found 292.0378.

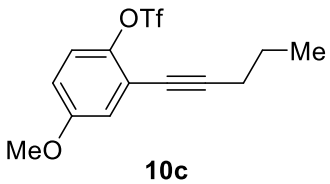


10b

4-methyl-3-(pent-1-yn-1-yl)phenyl trifluoromethanesulfonate (Scheme 4, compound **10b**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.8 mg, 0.200 mmol), 2-hexynoic acid (40.3 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and toluene (1.0 mL);

Yield of **10b** = 84% (0.168 mmol, 51.4 mg); colourless liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (s, 1H), 7.22 (d, *J* = 8.5 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 2.45–2.41 (m, 5H), 1.68–1.62 (m, 2H), 1.06 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.1, 140.5, 130.7, 126.1, 124.1, 120.1, 118.7 (q, *J* = 321.6 Hz), 96.8, 78.0, 22.1, 21.5, 20.3, 13.5; ^{19}F NMR (565 MHz, $CDCl_3$) δ -72.9; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{13}H_{13}F_3O_3S$ 306.0532; found 306.0536.

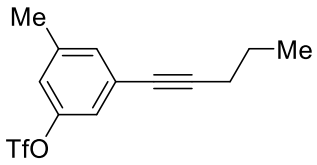


10c

4-methoxy-2-(pent-1-yn-1-yl)phenyl trifluoromethanesulfonate (Scheme 4, compound **10c**)

Followed **General Procedure B** on 0.200 mmol scale with 2-chloro-4-methoxyphenyl trifluoromethanesulfonate (58.0 mg, 0.200 mmol), 2-hexynoic acid (40.3 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL);

Yield of **10c** = 79% (0.158 mmol, 50.9 mg); yellow liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane:DCM=9:1) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (d, *J* = 9.1 Hz, 1H), 6.97 (s, 1H), 6.83 (d, *J* = 9.0 Hz, 1H), 3.80 (s, 3H), 2.43 (t, *J* = 7.0 Hz, 2H), 1.69–1.63 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.4, 143.7, 122.3, 119.8, 118.7 (q, *J* = 321.6 Hz), 117.7, 114.8, 98.1, 74.0, 55.7, 21.7, 21.5, 13.5; ^{19}F NMR (565 MHz, $CDCl_3$) δ -73.7; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{13}H_{13}F_3O_4S$ 322.0481; found 322.0486.

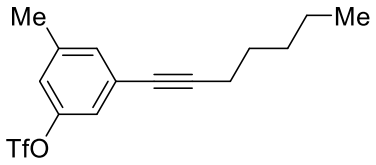


10d

3-methyl-5-(pent-1-yn-1-yl)phenyl trifluoromethanesulfonate (Scheme 4, compound **10d**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-5-methylphenyl trifluoromethanesulfonate (54.8 mg, 0.200 mmol), 2-hexynoic acid (40.3 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and toluene (1.0 mL);

Yield of **10d** = 64% (0.128 mmol, 39.2 mg); colourless liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (s, 1H), 7.10 (s, 1H), 6.98 (s, 1H), 2.39–2.35 (m, 5H), 1.66–1.60 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.1, 140.6, 132.2, 126.1, 121.2, 121.1, 118.7 (q, *J* = 320.1 Hz), 92.4, 79.0, 22.0, 21.3, 21.1, 13.5; ^{19}F NMR (565 MHz, $CDCl_3$) δ -72.9; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{13}H_{13}F_3O_3S$ 306.0532; found 306.0536.

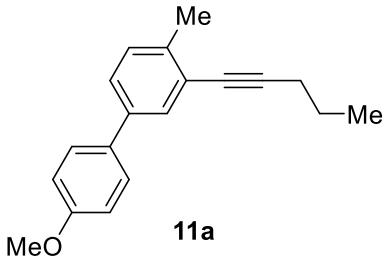


10e

3-(hept-1-yn-1-yl)-5-methylphenyl trifluoromethanesulfonate (Scheme 4, compound **10e**)

Followed **General Procedure B** on 0.200 mmol scale with 3-chloro-5-methylphenyl trifluoromethanesulfonate (54.8 mg, 0.200 mmol), 2-octynoic acid (50.4 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and toluene (1.0 mL);

Yield of **10e** = 61% (0.122 mmol, 40.8 mg); colourless liquid; The % of major product (reacting C–Cl site) : minor product (reacting C–OTf site) ≥ 99 : 1; Eluents (Hexane) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (s, 1H), 7.10 (s, 1H), 6.98 (s, 1H), 2.39 (t, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 1.63–1.58 (m, 2H), 1.45–1.34 (m, 4H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.1, 140.6, 132.2, 126.1, 121.2, 121.0, 118.7 (q, *J* = 320.1 Hz), 92.7, 78.8, 31,1, 28.2, 22.2, 21.1, 19.3, 14.0; ^{19}F NMR (565 MHz, $CDCl_3$) δ -72.9; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{15}H_{17}F_3O_3S$ 334.0845; found 334.0853.



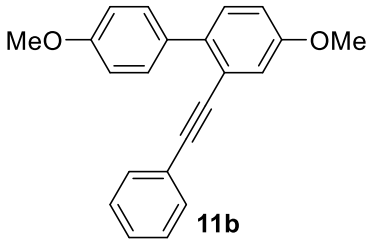
11a

4'-methoxy-4-methyl-3-(pent-1-yn-1-yl)-1,1'-biphenyl (Scheme 5, compound **11a**)

Followed **General Procedure C** on 0.200 mmol scale with 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.8 mg, 0.200 mmol), 2-hexynoic acid (40.3 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL) for the 1st step; $Pd_2(dba)_3$ (2.70 mg, 0.00300

mmol), SPhos (3.70 mg, 0.00900 mmol), 4-methoxyphenylboronic acid (60.8 mg, 0.400 mmol), and K_3PO_4 (63.6 mg, 0.300 mmol) for the 2nd step;

Yield of **11a** = 76% (0.152 mmol, 40.1 mg); light yellow liquid; Eluents (Hexane:EA=20:1) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.94 (d, *J* = 8.3 Hz, 2H), 3.82 (s, 3H), 2.46–2.44 (m, 5H), 1.69–1.63 (m, 2H), 1.07 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.0, 138.2, 138.1, 133.0, 129.9, 129.7, 127.9, 125.8, 124.1, 114.1, 94.2, 79.6, 55.3, 22.3, 21.5, 20.3, 13.6; HRMS (EI) m/z: $[M]^+$ calcd. for $C_{19}H_{20}$ 264.1509; found 264.1505.



11b

4,4'-dimethoxy-2-(phenylethynyl)-1,1'-biphenyl (Scheme 5, compound **11b**)

Followed **General Procedure C** on 0.200 mmol scale with 2-chloro-4-methoxyphenyl trifluoromethanesulfonate (58.0 mg, 0.200 mmol), 3-phenylpropiolic acid (52.6 mg, 0.360 mmol), dichloro-(1-methylallyl)-dipalladium (1.60 mg, 0.00400 mmol), **L9** (10.5 mg, 0.0320 mmol), K_2CO_3 (55.2 mg, 0.400 mmol) and THF (1.0 mL) for the 1st step; $Pd_2(dba)_3$ (2.70 mg, 0.00300 mmol), SPhos (3.70 mg, 0.00900 mmol), 4-methoxyphenylboronic acid (60.8 mg, 0.400 mmol), and K_3PO_4 (63.6 mg, 0.300 mmol) for the 2nd step;

Yield of **11b** = 75% (0.150 mmol, 47.1 mg); yellow gel; Eluents (Hexane:EA=20:1) was used for flash column chromatography; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.5 Hz, 2H), 7.38–7.36 (m, 2H), 7.31–7.27 (m, 4H), 7.14 (s, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 1H), 3.83 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.7, 158.1, 136.3, 132.7, 131.3, 130.41, 130.38, 128.2, 128.1, 123.3, 122.1, 117.0, 115.4, 113.2, 91.8, 89.6, 55.4, 55.2; The data are in agreement with those previously reported in the literature.[6]

7. Computational Details

All density functional theory (DFT) calculations were performed using the Gaussian 16 software.[7] The B3PW91[8] functional has been used in this study. This hybrid functional has been shown to perform well in modeling a range of reactions involving transition metals.[9] Geometry optimizations of all the minima and transition states were fully optimized at the B3PW91-D3(BJ) level of theory, with the SDD[10] pseudopotential for Pd and the 6-31G(d) for other atoms using the Polarizable Continuum Model (PCM) model[11] with THF as the solvent. Dispersion corrections according to Grimmes's DFT-D3 scheme,[12] including Becke–Johnson damping, were employed.[13] Vibrational frequencies were computed at the same level of theory to evaluate its zero-point vibrational energy and thermal corrections at 298.15K, and to check whether each optimized structure is an energy minimum or a transition state. Intrinsic reaction coordinates (IRC) calculations were performed to confirm whether the located transition state connect the correct reactant and product. [14] On the basis of the optimized structures, the single point energies were calculated at the PBE0-D3(BJ)/Def2-TZVP [15] level, and solvation energy corrections were calculated using the Solvation Model Based on Density (SMD) model [16] with THF as the solvent. The reported Gibbs free energies were corrected using the quasi-harmonic model[17] with a cut-off frequency of 100 cm^{-1}. The Gibbs free energies were further corrected to standard state from 1 atm to 1 mol/L, a correction of RTLn(cs/cg) (1.89 kcal/mol) was added to the energies of all species. cs is the standard molar concentration in solution (1 mol/L), cg is the standard molar concentration in the gas phase (0.0446 mol/L), and R is the gas constant. Conformational searches are conducted to ensure that the most stable conformers are located. The images of computed species were generated using CYLView. [18]

Table S2: Table of energies of minimum energy structures[a]

Structure	***ZPE***	***tcH***	***E caled***	***H***	***G***	***qh-G***	***Imaginary frequency (cm^{-1})***
12A	0.493703	0.520955	-1342.805155	-1342.284200	-1342.36802	-1342.363559	
12B	0.604775	0.647144	-2994.832840	-2994.185696	-2994.30466	-2994.295073	
12C	0.604202	0.646898	-2994.830849	-2994.183951	-2994.30564	-2994.294751	
12D-TS	0.603758	0.64597	-2994.812696	-2994.166726	-2994.28776	-2994.276972	-75.68
12E	0.606526	0.648873	-2994.864165	-2994.215292	-2994.33456	-2994.325181	

12F	0.721764	0.772228	-3030.795230	-3030.023002	-3030.16330	-3030.149744	
12G	0.722315	0.772453	-3030.796083	-3030.02363	-3030.15815	-3030.14755	
12H-TS	0.718687	0.769446	-3030.764861	-3029.995415	-3030.13368	-3030.121434	-315.57
12I	0.718778	0.770768	-3030.780613	-3030.009845	-3030.15290	-3030.138986	
12J	0.705859	0.753939	-2842.307866	-2841.553927	-2841.68857	-2841.675741	
12K-TS	0.703800	0.751821	-2842.292835	-2841.541014	-2841.67731	-2841.663225	-392.52
12L	0.706205	0.754037	-2842.349666	-2841.595629	-2841.72976	-2841.716812	
12M	0.604406	0.646842	-2994.833881	-2994.187039	-2994.30674	-2994.296663	
12N-TS	0.602784	0.645040	-2994.796762	-2994.151722	-2994.27023	-2994.260989	-377.61
12O	0.606804	0.648838	-2994.872357	-2994.223519	-2994.34088	-2994.332113	
KCl	0.000394	0.004303	-1059.916084	-1059.911781	-1059.939476	-1059.93947	
CO_2	0.011633	0.015221	-188.465070	-188.449849	-188.474152	-188.474153	
1a	0.110392	0.124805	-1651.985603	-1651.860798	-1651.918149	-1651.915470	
2a'	0.113733	0.125164	-1095.84609	-1095.720926	-1095.771666	-1095.769600	

[a]Zero-point correction(ZPE), thermal correction to enthalpy (tcH), energies(E), enthalpies (H), Gibbs free energies (G) (in Hartree), and quasi-harmonic corrected Gibbs free energy of the structures calculated at the PBE0-GD3(BJ)/Def2-TZVP-SMD(THF)//B3PW91-D3(BJ)/6-31G(d)-SDD(Pd)-PCM(THF) level of theory.

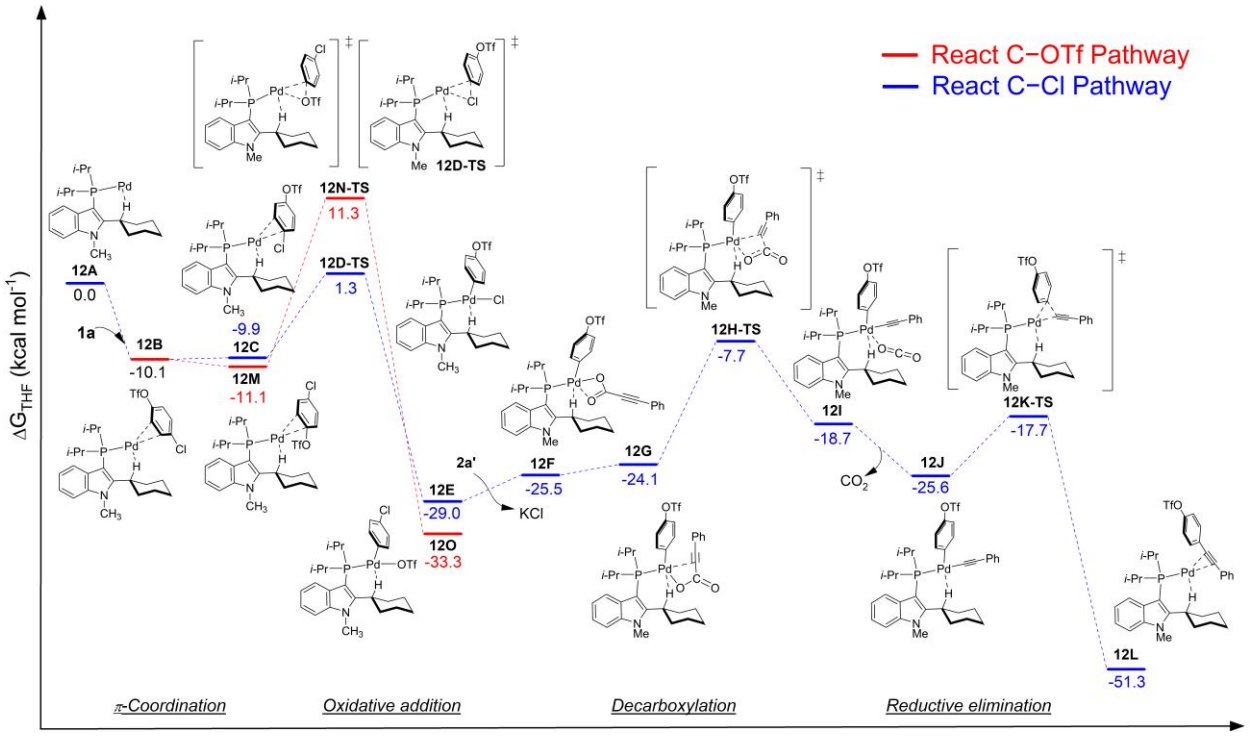


Figure S1. Free energy profiles calculated for the chemoselective Palladium/Selectphos-catalyzed decarboxylative cross-coupling reaction of chloroaryltriflate. The relative free energies are given in kcal/mol.

Cartesian Coordinates of Minimum Energy Calculated Structures

12A

Charge: 0 Multiplicity: 1

Pd	1.81660500	-1.79568800	-0.41981400
P	-0.27827600	-1.44608300	0.15914700
C	-0.90513700	0.25683600	0.01660300
C	-2.27298800	0.72738600	-0.08476800
N	-0.88033600	2.51361500	-0.18610800
C	-0.08983900	1.39028800	-0.03912200
C	1.40166800	1.44308300	0.03408400
H	1.69227900	0.38809000	0.19525600
C	-2.20795300	2.14141400	-0.21063500
C	-0.62115000	-1.90112100	1.94235100
H	-0.26463100	-2.93648300	2.02579000
C	-3.54726000	0.13350100	-0.08486500
H	-3.66538600	-0.93701800	0.02663000
C	1.97558400	2.21405600	1.23204600
H	1.78475100	3.29164400	1.14579400
H	1.48096600	1.87907800	2.15134700
C	-1.47409900	-2.47192600	-0.83344700
H	-2.47991500	-2.34185100	-0.42441300
C	-3.34017800	2.95042200	-0.32759300
H	-3.25828600	4.03025500	-0.40806700
C	-4.58101600	2.32577500	-0.32946700
H	-5.48307100	2.92453300	-0.41974000
C	2.08616300	1.82917700	-1.28728600
H	1.66933600	1.21284600	-2.09331700
H	1.89221500	2.87701000	-1.55288000
C	-1.46788100	-2.00279400	-2.28607500
H	-1.78467500	-0.95864800	-2.37159200
H	-2.14669900	-2.61927800	-2.88796600
H	-0.45869800	-2.08818200	-2.70878600
C	3.48417700	1.97959300	1.32096800
H	3.90497800	2.54487600	2.16179200
H	3.66625100	0.91471100	1.52981400
C	-4.67924500	0.92911500	-0.20829700
H	-5.65996600	0.46102100	-0.20493500
C	0.24629200	-1.02043200	2.84084700
H	1.30426300	-1.09442800	2.56393800
H	0.13709200	-1.31692700	3.89107800
H	-0.05376800	0.03038600	2.75200300
C	-2.08703000	-1.83738300	2.36066900
H	-2.47902900	-0.82038400	2.25798900
H	-2.18942500	-2.13198400	3.41277800
H	-2.71790900	-2.50902200	1.76923700
C	4.18492600	2.36233700	0.01642300
H	5.26209400	2.16856700	0.09296500
H	4.06997900	3.44401700	-0.14993200
C	-1.10028700	-3.94861700	-0.71762200
H	-0.07693000	-4.11223000	-1.07817200
H	-1.78426300	-4.55946400	-1.31970900
H	-1.15317400	-4.30646600	0.31635400
C	-0.46851100	3.89936400	-0.25487700
H	-1.00817700	4.40001000	-1.06404300
H	0.59488600	3.96498700	-0.46598000
H	-0.67803200	4.41944100	0.68659000
C	3.59451300	1.60703400	-1.17488900
H	4.09193200	1.90717800	-2.10556400
H	3.77919600	0.52864500	-1.04755600

12B

Charge: 0 Multiplicity: 1

C	2.60017100	-0.96223600	-0.02928500
C	3.61796300	-1.98765300	-0.12628300
N	4.56986700	0.02798300	-0.54331400
C	3.23304300	0.25580100	-0.28527600
C	2.61743200	1.61680900	-0.26655700
H	1.56177800	1.42473200	0.01331200
C	4.83327400	-1.32333400	-0.43994800
C	3.65293500	-3.38383600	0.02512200
H	2.75278600	-3.94321300	0.24989400
C	2.52375700	2.31826400	-1.63029500
H	3.51735200	2.59715100	-2.00558900
H	2.09280400	1.62519800	-2.36196900
C	6.04800100	-1.99412200	-0.59563900
H	6.96464600	-1.46027200	-0.82794100
C	6.04482400	-3.37451300	-0.43580300
H	6.97242000	-3.92871500	-0.54858200
C	3.15956700	2.54412000	0.83106100
H	3.16839800	2.00378800	1.78565900
H	4.19585000	2.83982000	0.62289500
C	1.65865200	3.57224100	-1.50483400
H	1.60817700	4.09302100	-2.46913500
H	0.63342000	3.26765700	-1.25211900
C	4.85662500	-4.06007900	-0.12900800
H	4.87899400	-5.14005400	-0.01103900
C	2.18499700	4.50929700	-0.41717200
H	1.53431200	5.38689400	-0.32989800
H	3.18114300	4.87743300	-0.70583000
C	5.60924300	0.99503500	-0.82613300
H	6.27358000	1.11850700	0.03633000
H	5.16972400	1.95710000	-1.07342300
H	6.19959000	0.65775100	-1.68317300
C	2.28555400	3.79336700	0.92987000
H	2.67885100	4.47091700	1.69782300
H	1.27744000	3.49392500	1.25339600
Pd	-0.30532500	0.82312600	0.89135200

C	-2.44211000	0.96314300	0.72720000
C	-1.96701000	2.23782600	1.16864600
C	-2.79280200	0.83545500	-0.64116100
H	-2.82318900	0.23924000	1.43940500
H	-1.94634600	2.48146500	2.22749900
C	-1.86211200	3.28252900	0.21364600
C	-2.68952400	1.86466500	-1.54369300
O	-3.19361500	-0.42695700	-1.12117900
C	-2.20564900	3.11681900	-1.11319500
Cl	-1.32602100	4.84690200	0.76901400
H	-2.96543200	1.70421300	-2.58032700
S	-4.72756500	-0.91876100	-0.88615800
H	-2.11352500	3.93831300	-1.81414000
O	-5.46856400	0.06103800	-0.11448900
O	-5.21360100	-1.45963000	-2.13970900
C	-4.36310700	-2.37129800	0.21499100
F	-3.45464300	-3.14754100	-0.36305000
F	-5.48810800	-3.04801900	0.39411400
F	-3.90676100	-1.94118500	1.38622700
P	0.84649700	-1.10952900	0.38719100
C	0.03965200	-1.89074600	-1.10207200
C	0.78627400	-2.38810500	1.73362500
H	-1.01723900	-1.96397200	-0.81866000
C	0.14820300	-0.90921100	-2.26886400
C	0.55431900	-3.27342800	-1.48630600
H	1.23674300	-3.31746800	1.37187200
C	1.59040900	-1.88398300	2.93016200
C	-0.66764000	-2.66331600	2.11057800
H	-0.25330000	0.07372800	-1.99780600
H	-0.40876500	-1.28381300	-3.13575400
H	1.19547900	-0.77906200	-2.56620500
H	1.60947400	-3.23218300	-1.77460900
H	-0.01329800	-3.65899200	-2.34250800
H	0.44894100	-3.99611900	-0.67011300
H	2.64115200	-1.72455700	2.66823200
H	1.54621300	-2.60914200	3.75162300
H	1.18078100	-0.93214400	3.29225900
H	-1.15439100	-1.74187500	2.45154400
H	-0.71512000	-3.39814800	2.92338400
H	-1.24543500	-3.05701300	1.26924200

12C

Charge: 0 Multiplicity: 1

Pd	0.03712700	0.41575900	1.10933500
P	1.57778200	-1.19099600	0.51817500
C	3.13315600	-0.61945300	-0.20387100
C	-2.07177300	2.17453300	0.42548700
C	4.38467900	-1.32576600	-0.37864200
N	4.63775000	0.80303400	-1.11797600
C	3.33860300	0.68204100	-0.66750900
C	2.35010800	1.80303000	-0.69059900
H	1.43977000	1.36408200	-0.23517400
C	5.29822700	-0.39662900	-0.94250700
C	0.81379000	-2.31963200	-0.75493800
H	-0.11026900	-2.66833300	-0.27418500
C	4.84651500	-2.62678600	-0.11910700
H	4.18729600	-3.38071900	0.29410100
C	-2.74185300	-0.53464400	0.82944800
C	1.90465000	2.24872300	-2.09220900
H	2.72280000	2.74522600	-2.63040000
H	1.62935900	1.36683200	-2.68161300
C	2.07186000	-2.28070900	1.93877400
H	2.69943400	-3.09758300	1.56973900
C	-2.74086900	1.47221800	-0.56034500
H	-3.00599700	1.94625400	-1.49789200
C	-3.08431100	0.13239000	-0.32533900
C	-2.01677300	0.14744600	1.83870400
H	-1.94313900	-0.29299100	2.82794400
C	6.62472800	-0.71824300	-1.23714200
H	7.30497900	0.01423600	-1.66125300
C	7.04771100	-2.01316600	-0.96290300
H	8.07359400	-2.29824200	-1.17866100
C	2.70797900	2.99440600	0.21063200
H	2.97792900	2.62248700	1.20654900
H	3.58139200	3.53472000	-0.17608500
C	-1.71009900	1.53011400	1.63989700
C	2.87487100	-1.45246900	2.93979100
H	3.79190200	-1.05911400	2.49002600
H	3.15118600	-2.06556200	3.80592900
H	2.27876600	-0.60328600	3.29778200
C	0.71924600	3.20630100	-1.97740800
H	0.41530700	3.54985900	-2.97389600
H	-0.13277500	2.65618800	-1.55535800
C	6.16415400	-2.95663700	-0.41041800
H	6.51750100	-3.96418000	-0.20858400
C	0.42616900	-1.47491500	-1.96876400
H	-0.21521600	-0.63492300	-1.67760200
H	-0.11200500	-2.08492100	-2.70386600
H	1.32032200	-1.06756200	-2.45524400
C	1.66114400	-3.52214400	-1.15649400
H	2.59800400	-3.20090200	-1.62313000
H	1.11796000	-4.13923800	-1.88300500
H	1.90568800	-4.15998800	-0.30047300
C	1.04706800	4.40000600	-1.07907600
H	0.17051800	5.05336000	-0.98453200
H	1.83747400	5.00139400	-1.55252400
C	0.82092900	-2.87829600	2.58153400
H	0.15429100	-2.08178600	2.93332400
H	1.09947100	-3.49992600	3.44093600
H	0.25741100	-3.50598300	1.88291100
C	5.30234400	1.97273100	-1.65287700
H	6.03344400	2.36508800	-0.93751300
H	4.57633800	2.74906800	-1.87522100
H	5.81918300	1.70991900	-2.58077100
C	1.51916800	3.95067300	0.30448600

H	1.78265600	4.81948600	0.92007600
H	0.69694000	3.43485600	0.82039000
H	-1.83662900	3.22485900	0.29151900
H	-3.03040500	-1.56978100	0.97351500
Cl	-1.31643000	2.54084400	3.03793500
O	-3.72621700	-0.60402400	-1.34341200
S	-5.31156200	-0.36713700	-1.60961400
O	-5.68357800	1.01706900	-1.38772200
O	-5.59709400	-1.06872900	-2.84366600
C	-6.04728800	-1.36497000	-0.21756500
F	-7.33447400	-1.54660300	-0.47761000
F	-5.43108500	-2.53791800	-0.14115300
F	-5.90540500	-0.70655800	0.92511100

12D-TS

Charge: 0 Multiplicity: 1

Pd	0.50787300	1.27362400	1.15360200
P	1.33092900	-0.80936200	0.71811500
C	2.97646600	-0.93688700	-0.01961700
C	-1.81637300	1.72442600	-0.55864700
C	3.84797600	-2.08813700	-0.12517900
N	4.87164600	-0.30712000	-1.08473600
C	3.64950700	0.13200800	-0.61736500
C	3.17570400	1.54266900	-0.74140000
H	2.20542800	1.53634100	-0.20776200
C	5.02438100	-1.64641700	-0.78733900
C	0.18432100	-1.67519500	-0.47303700
H	-0.81375000	-1.46792700	-0.06653000
C	3.78211900	-3.43501000	0.26876000
H	2.90439100	-3.82835000	0.76762600
C	-3.17431100	-0.13326200	1.04919100
C	2.82997900	2.00313200	-2.16528900
H	3.73245400	2.12070300	-2.78060300
H	2.21161100	1.24169200	-2.65352600
C	1.38666500	-1.87750300	2.23646500
H	1.62346700	-2.90576900	1.94681300
C	-2.64283200	0.77555700	-1.14687700
H	-2.77478700	0.74876500	-2.22241900
C	-3.30080100	-0.14391400	-0.33820900
C	-2.34978400	0.80635600	1.64875200
H	-2.23590100	0.83753400	2.72581100
C	6.10808500	-2.48631600	-1.05154300
H	7.00023500	-2.12052800	-1.55103100
C	6.00821600	-3.81163800	-0.64571700
H	6.83311800	-4.49296000	-0.83451600
C	4.02326100	2.58008500	0.01041500
H	4.21550900	2.21845500	1.02808800
H	5.00091300	2.72227400	-0.46819500
C	-1.60760600	1.68333300	0.83305900
C	2.47670000	-1.36551500	3.17498500
H	3.46563300	-1.42248000	2.70953300
H	2.49446100	-1.95959700	4.09662000
H	2.28657900	-0.31882200	3.44540800
C	2.08779000	3.33833500	-2.10072500
H	1.84565900	3.68757500	-3.11207100
H	1.13232900	3.18267800	-1.57722200
C	4.85444000	-4.27876000	0.00725200
H	4.79932400	-5.31980600	0.31377500
C	0.29628200	-0.99155400	-1.83457900
H	0.16514200	0.09136100	-1.74718800
H	-0.47309000	-1.37444500	-2.51536300
H	1.27805500	-1.18406200	-2.28197400
C	0.37678500	-3.18310400	-0.59889800
H	1.36722800	-3.41902700	-1.00129800
H	-0.37072800	-3.59637200	-1.28759200
H	0.26162800	-3.70037100	0.35923700
C	2.90256900	4.39309900	-1.35040200
H	2.34137100	5.33395900	-1.29189100
H	3.82099400	4.60788900	-1.91706300
C	0.01455400	-1.86162700	2.90861700
H	-0.24664200	-0.83980600	3.20764800
H	0.02409600	-2.49538400	3.80360600
H	-0.77683800	-2.22524200	2.24432300
C	5.90428100	0.46201000	-1.74564100
H	6.73913800	0.66500100	-1.06576000
H	5.49815900	1.40578000	-2.09886900
H	6.27755200	-0.09479000	-2.61003700
C	3.27808600	3.91501500	0.05301300
H	3.88566100	4.67120300	0.56544200
H	2.36101200	3.78348800	0.64709400
H	-1.29970700	2.45928600	-1.16513900
H	-3.71496300	-0.85797400	1.64814500
Cl	-0.92378100	3.22050900	1.62691400
O	-4.08255800	-1.16146100	-0.92001800
S	-5.55442100	-0.79609900	-1.50950400
O	-5.57605100	0.53591600	-2.08311100
O	-5.97080000	-1.97389800	-2.24187400
C	-6.55363600	-0.73393600	0.06235500
F	-7.83812900	-0.74801300	-0.26499500
F	-6.26523900	-1.79119400	0.81081800
F	-6.26763700	0.37857100	0.72559800

12E

Charge: 0 Multiplicity: 1

Pd	0.46238100	-0.01968700	1.61398600
P	1.65878200	-1.25870600	0.11625900
C	3.19910700	-0.44571500	-0.33676700
C	-1.62876500	1.02830500	-0.06442700
C	4.47549000	-1.06025500	-0.64475400
N	4.69284500	1.19615600	-0.75138100
C	3.37772800	0.93902900	-0.43540300
C	2.34342100	2.01183300	-0.28416300
H	1.39944100	1.46930700	-0.12928300
C	5.37877200	0.00472900	-0.89299300

C	0.87140200	-1.80807800	-1.46979200
H	-0.10913800	-2.20566600	-1.18462700
C	4.96280200	-2.37356200	-0.75420200
H	4.31651200	-3.22876600	-0.60084200
C	-3.08033800	-1.34315400	-0.31692100
C	2.14251900	2.86156500	-1.55213100
H	3.04124400	3.44862400	-1.77378000
H	1.97963700	2.20116500	-2.41129000
C	2.12936300	-2.79340300	1.04773200
H	2.70162800	-3.43709900	0.37481400
C	-2.80259200	1.01845200	-0.81573700
H	-3.16493200	1.91898300	-1.29899800
C	-3.50710700	-0.17265800	-0.92757200
C	-1.89596200	-1.32595200	0.42041700
H	-1.55974800	-2.24019800	0.89598100
C	6.71819000	-0.19730400	-1.23121100
H	7.38508400	0.63616800	-1.42849200
C	7.16781100	-1.50839900	-1.32006100
H	8.20386800	-1.70259900	-1.58193400
C	2.51378700	2.88518100	0.97221400
H	2.59717200	2.23576900	1.85209300
H	3.43987800	3.47171900	0.92459700
C	-1.16106900	-0.14386500	0.53838900
C	3.00351200	-2.42790100	2.24734800
H	3.92366000	-1.92310400	1.94037100
H	3.27648800	-3.33659500	2.79564300
H	2.46640600	-1.77010000	2.94207800
C	0.96119200	3.81530700	-1.37827000
H	0.86024500	4.44496100	-2.27059800
H	0.03438600	3.23022600	-1.30444600
C	6.29480300	-2.58410300	-1.08586100
H	6.66571800	-3.60158900	-1.17137500
C	0.66155900	-0.59313300	-2.37221200
H	0.07365200	0.18524600	-1.87856400
H	0.12758400	-0.89560100	-3.27975400
H	1.62492700	-0.16607300	-2.67066700
C	1.67783100	-2.89227600	-2.18234600
H	2.68626100	-2.53934800	-2.42270200
H	1.18195900	-3.15346900	-3.12438900
H	1.76225800	-3.80859900	-1.59026100
C	1.11937900	4.68235300	-0.12866800
H	0.24411200	5.33173800	-0.00630100
H	1.98802700	5.34470100	-0.25978300
C	0.87250800	-3.55058500	1.47538400
H	0.27320400	-2.94775100	2.16731200
H	1.15768700	-4.47430900	1.99126200
H	0.24471500	-3.82761000	0.62190200
C	5.34200800	2.47515500	-0.96161300
H	6.31066000	2.47199800	-0.45487300
H	4.74440900	3.27774600	-0.54036600
H	5.49776100	2.66386900	-2.02901500
C	1.32271000	3.82964600	1.12386900
H	1.46643500	4.46911700	2.00303900
H	0.42335100	3.23063800	1.32215500
H	-1.08280900	1.95793200	0.04824400
H	-3.66262700	-2.25284900	-0.41963500
Cl	-0.54428500	1.17243100	3.37021500
O	-4.66462300	-0.23824700	-1.73310900
S	-6.04498800	0.42825000	-1.19691100
O	-5.79236000	1.65413100	-0.46466300
O	-6.95533100	0.35996700	-2.32096000
C	-6.58893300	-0.85114500	0.04444700
F	-7.85704000	-0.61425900	0.34973500
F	-6.47036200	-2.06121000	-0.48821800
F	-5.83658400	-0.76186800	1.13220800

12F

Charge: 0 Multiplicity: 1

P	-0.73975600	-2.08292500	-1.01066200
S	6.61023100	0.61878900	0.94515600
C	-2.19946100	-2.58350400	-0.08337000
O	5.66742200	-0.68948200	0.76404300
C	1.61847800	-0.31125800	-0.25816200
C	-3.19433300	-3.56856200	-0.46059900
N	-3.74593300	-2.69186400	1.55814400
F	7.93591400	1.92702800	-0.87037300
C	-2.57066200	-2.08790300	1.17170200
C	-1.84180700	-1.09337500	2.02137500
H	-0.91478800	-0.88408600	1.46732300
C	-4.14126400	-3.60012600	0.59529400
O	5.88123100	1.71965900	1.54508100
C	0.55082400	-3.36716400	-0.65047600
H	1.46436400	-3.00559200	-1.13476800
C	-3.39747700	-4.43429800	-1.54871700
H	-2.70196100	-4.46978200	-2.37778600
C	4.30646400	-0.51386700	0.42631000
C	-1.39983500	-1.63298200	3.39313500
H	-2.26919500	-1.83720400	4.02888600
H	-0.87415800	-2.58565200	3.26376900
C	-1.15700500	-2.24303600	-2.81090500
H	-1.35305100	-3.30042900	-3.00831900
C	2.56581700	-0.72226800	-1.20453400
H	2.26412500	-0.96212800	-2.21845700
O	7.85459600	0.11469300	1.48824400
C	3.91612700	-0.82157300	-0.86900100
H	4.65581900	-1.13379300	-1.59902100
C	3.39890800	-0.10381700	1.39317600
H	3.73568000	0.13023800	2.39719400
C	-5.25262800	-4.44515300	0.59590000
H	-5.95396900	-4.45784200	1.42433400
C	-5.42463800	-5.28252200	-0.49861800
H	-6.27777600	-5.95400500	-0.53074700
F	7.22879800	-0.02018200	-1.52333800
C	-2.54793400	0.26837500	2.14825800
H	-2.82386200	0.62307100	1.15105400

H	-3.47483800	0.17889700	2.72912600
C	2.05537400	0.00198700	1.03739500
H	1.34450400	0.33925000	1.78524200
C	-2.40404300	-1.42797000	-3.14965500
H	-3.27168800	-1.75445100	-2.56970900
H	-2.63820300	-1.54615100	-4.21391400
H	-2.24257100	-0.36451100	-2.94719400
F	5.83722800	1.63751900	-1.34731400
C	-0.49868500	-0.61804200	4.09721800
H	-0.23016300	-0.98975500	5.09363100
H	0.44163500	-0.52578300	3.53678500
C	-4.50256200	-5.27532300	-1.55867500
H	-4.65239500	-5.94383700	-2.40182200
C	0.79326900	-3.43298100	0.85614200
H	1.06726800	-2.45765500	1.26725100
H	1.61075000	-4.13120000	1.06748800
H	-0.10270300	-3.79142400	1.37383200
C	0.18485000	-4.74142700	-1.20916000
H	-0.76568900	-5.09594800	-0.79686100
H	0.96036400	-5.46372000	-0.92908200
H	0.11277600	-4.74434100	-2.30091500
C	-1.16589900	0.75452000	4.20395900
H	-0.47977400	1.47113300	4.67170700
H	-2.04089700	0.67679700	4.86631800
C	0.03999600	-1.81782000	-3.66080000
H	0.27878800	-0.76148100	-3.49192300
H	-0.20072400	-1.94611500	-4.72210600
H	0.93298600	-2.41542300	-3.44924400
C	-4.50311500	-2.49966400	2.77894400
H	-4.21880100	-1.56774300	3.25808100
H	-4.33978500	-3.32847700	3.47589500
H	-5.56711900	-2.44366500	2.53457300
C	-1.62041300	1.26825200	2.83715800
H	-2.12489700	2.23673700	2.93954400
H	-0.74609200	1.43989400	2.19341100
C	6.92220900	1.07302800	-0.83540200
Pd	-0.25793200	0.09223000	-0.67961800
O	-0.26265600	2.29251000	-0.46386500
C	-1.50592800	2.32634500	-0.73939400
O	-2.14639500	1.27072000	-1.04255100
C	-2.20105100	3.58488900	-0.68941900
C	-2.79587300	4.64358800	-0.63214000
C	-3.48953600	5.88190800	-0.56494000
C	-4.86235300	5.94177700	-0.86568200
C	-2.80794900	7.05581600	-0.19605300
C	-5.53612600	7.15572900	-0.79745100
H	-5.38411800	5.03333200	-1.15008300
C	-3.49150500	8.26444700	-0.13058800
H	-1.74853900	7.00472500	0.03495500
C	-4.85390300	8.31708600	-0.43046100
H	-6.59603700	7.19716500	-1.03094400
H	-2.96097400	9.16820000	0.15471600
H	-5.38425100	9.26371800	-0.37837400

12G

Charge: 0 Multiplicity: 1

P	-1.94894700	-1.32692900	-0.50550400
S	5.84201500	-1.08012600	1.39445800
C	-3.46764300	-0.82255900	0.31646700
O	4.36735500	-1.74274000	1.45565400
C	0.89940400	-0.25172300	-0.36985700
C	-4.74420300	-1.50932500	0.32226800
N	-4.91828600	0.39336700	1.54639400
F	7.71909300	-1.42653000	-0.37230300
C	-3.61820200	0.32710000	1.09993700
C	-2.56941600	1.32814400	1.47494400
H	-1.63920200	0.92570800	1.04799200
C	-5.62018000	-0.71005200	1.10131600
O	5.77890400	0.36630300	1.32464500
C	-1.13422400	-2.53957500	0.64521700
H	-0.14435100	-2.72850100	0.21644400
C	-5.25275000	-2.70267100	-0.21842500
H	-4.63087300	-3.36314200	-0.80971800
C	3.26645700	-1.15115000	0.79363000
C	-2.32209600	1.44786800	2.98948200
H	-3.19082800	1.89247800	3.48867500
H	-2.18562000	0.45140600	3.42393000
C	-2.42686300	-2.30320900	-2.00984100
H	-2.92362800	-3.20700900	-1.64528100
C	1.62750700	-1.30293700	-0.94393200
H	1.26688300	-1.79465200	-1.84094100
O	6.61398600	-1.78077700	2.39967600
C	2.81222700	-1.76020500	-0.36672400
H	3.35978500	-2.59466600	-0.79265300
C	2.60243400	-0.07771600	1.37043700
H	2.99024800	0.38941300	2.26900300
C	-6.95072500	-1.05539800	1.34523800
H	-7.59524200	-0.43032600	1.95531900
C	-7.42076100	-2.23811500	0.78947200
H	-8.45057400	-2.53825000	0.96019300
F	6.22538100	-3.00460400	-0.34047100
C	-2.73714800	2.71150100	0.82348200
H	-2.90328100	2.58157300	-0.24935400
H	-3.61241700	3.23663600	1.22650800
C	1.42119100	0.36444500	0.77676300
H	0.90421400	1.20837800	1.22218200
C	-3.38741300	-1.53091000	-2.91000200
H	-4.30228800	-1.24946600	-2.38219800
H	-3.66273200	-2.15984900	-3.76467000
H	-2.92252700	-0.61428700	-3.28143300
F	5.75537600	-1.08537700	-1.23464700
C	-1.09530200	2.31946300	3.26077300
H	-0.95980700	2.44259400	4.34219100
H	-0.19983000	1.79947900	2.89417500
C	-6.57580400	-3.05267900	0.01709100

H	-6.96213800	-3.97738000	-0.40234400
C	-0.95810200	-1.90002300	2.02084700
H	-0.41325200	-0.95459000	1.96540300
H	-0.39121500	-2.57643700	2.67005300
H	-1.93233100	-1.71677800	2.48572100
C	-1.90763500	-3.85332000	0.75545700
H	-2.93740600	-3.68101500	1.08660500
H	-1.42203600	-4.49441000	1.50033900
H	-1.93223000	-4.40785000	-0.18709800
C	-1.20480500	3.68495000	2.57993700
H	-0.28583500	4.26133300	2.74380000
H	-2.02205000	4.25464300	3.04608100
C	-1.17134500	-2.73150800	-2.76883300
H	-0.64000800	-1.85621200	-3.15968900
H	-1.45660700	-3.36158300	-3.61874600
H	-0.48120700	-3.30791600	-2.14409400
C	-5.53623000	1.40669000	2.37809800
H	-4.94416400	2.31698200	2.36644000
H	-5.64181000	1.05704400	3.41055600
H	-6.52584300	1.64217100	1.97805800
C	-1.48486900	3.54643800	1.08339400
H	-1.58526300	4.53383500	0.61656100
H	-0.63341900	3.05352700	0.59344700
C	6.42616700	-1.69603700	-0.26236600
Pd	-0.74989100	0.46302700	-1.21485500
O	-2.40037700	1.44657100	-2.32023900
C	-1.79940700	2.47009400	-2.82075900
O	-2.24784600	3.33584900	-3.56041100
C	-0.38658900	2.52452800	-2.35460900
C	0.73751300	2.56835500	-1.86298300
C	2.01947800	2.71462500	-1.26619200
C	2.19159400	3.65199300	-0.23480600
C	3.08557000	1.88509200	-1.64876300
C	3.41933600	3.74787500	0.41088600
H	1.36155200	4.28895000	0.05303900
C	4.30610700	1.99297900	-0.99790600
H	2.93448600	1.14917500	-2.43111800
C	4.47373400	2.91723900	0.03435900
H	3.55031800	4.46882600	1.21261400
H	5.12489500	1.34059400	-1.27633600
H	5.42571000	2.97804700	0.55131800

12H-TS

Charge: 0 Multiplicity: 1

P	-2.25576300	-0.98146900	-0.91966300
S	5.44469000	-1.93193000	1.43135600
C	-3.79521800	-0.59279400	-0.06879500
O	4.01578300	-2.66728200	1.21117300
C	0.73815900	-0.46071000	-0.19322300
C	-5.13309900	-1.05370900	-0.37943300
N	-5.22388700	0.31909800	1.42462100
F	7.31575700	-1.41663000	-0.29553600
C	-3.89898300	0.23057400	1.05667400
C	-2.78897600	0.89864400	1.80751500
H	-1.87107200	0.55504600	1.30704000
C	-5.99291100	-0.45601100	0.57814400
O	5.27609300	-0.58602200	1.94763300
C	-1.73546500	-2.64740900	-0.28317100
H	-0.73747300	-2.81314900	-0.70553700
C	-5.70848100	-1.90186300	-1.34062700
H	-5.10085800	-2.39931600	-2.08641900
C	2.91944100	-1.90186000	0.75008700
C	-2.66364400	0.45713500	3.27652300
H	-3.53057800	0.79505000	3.85625000
H	-2.65430400	-0.63703000	3.33351200
C	-2.67869800	-1.22132500	-2.71115600
H	-3.34429800	-2.08529400	-2.78770600
C	1.40428300	-1.36739700	-1.02556900
H	1.08735200	-1.50707000	-2.05368000
O	6.28155200	-2.91664200	2.08489000
C	2.50309700	-2.09012800	-0.55931600
H	3.03559300	-2.78197000	-1.20398600
C	2.27232900	-1.02614000	1.61112600
H	2.62162700	-0.89955000	2.62999000
C	-7.37182300	-0.67433100	0.60177800
H	-8.00601200	-0.21529400	1.35379200
C	-7.90682200	-1.51349400	-0.36720900
H	-8.97573900	-1.70627600	-0.37746900
F	5.91110100	-2.94513600	-0.93978500
C	-2.76260000	2.43145200	1.67985400
H	-2.85657500	2.70614900	0.62520800
H	-3.61305000	2.88686200	2.20305900
C	1.18954800	-0.29780200	1.12305200
H	0.70922200	0.42286200	1.77559600
C	-3.39250600	0.00976600	-3.26618400
H	-4.31702500	0.22232900	-2.72200900
H	-3.64521500	-0.15693700	-4.31973100
H	-2.75098600	0.89444500	-3.20654200
F	5.32866600	-0.85410400	-0.96323600
C	-1.39306900	1.03404700	3.90199800
H	-1.34823300	0.76439300	4.96425200
H	-0.51903700	0.56817300	3.42806800
C	-7.07976000	-2.12123100	-1.32704600
H	-7.51942800	-2.77986800	-2.07083600
C	-1.61148400	-2.58277200	1.23822600
H	-0.94176800	-1.77962700	1.55748300
H	-1.20884400	-3.52858900	1.61777800
H	-2.59282200	-2.42124700	1.69690700
C	-2.66870200	-3.77811300	-0.71025700
H	-3.68997400	-3.60057900	-0.35675700
H	-2.32308200	-4.72173800	-0.27177400
H	-2.69596700	-3.91155200	-1.79598100
C	-1.31212900	2.55277100	3.73631000
H	-0.36408100	2.92483300	4.14344900
H	-2.11419400	3.02135100	4.32571700

C	-1.40379300	-1.53205700	-3.49568500
H	-0.70320300	-0.69029400	-3.44183600
H	-1.65063900	-1.70272100	-4.54978200
H	-0.89596800	-2.42802200	-3.12331200
C	-5.80673300	1.04835700	2.53289300
H	-5.12227000	1.81586200	2.88180300
H	-6.04766400	0.37578100	3.36305400
H	-6.72272100	1.54047200	2.19559700
C	-1.46278100	2.97203300	2.27316800
H	-1.43281900	4.06440100	2.18249300
H	-0.61767200	2.58504000	1.68466300
C	6.03895300	-1.77474800	-0.32765600
Pd	-0.68165700	0.72524400	-0.86161300
O	-1.81667300	2.61601400	-1.62851500
C	-0.97154500	3.43349700	-1.32433900
O	-0.66035800	4.55747000	-1.13654900
C	0.69226600	2.23765900	-0.96532900
C	1.89988300	2.50250200	-0.97253100
C	3.29772700	2.74076600	-0.93358100
C	4.08812200	2.04488400	0.00185900
C	3.91443900	3.63232300	-1.83089700
C	5.46443800	2.23596500	0.02930700
H	3.61438000	1.34413900	0.68151200
C	5.28984200	3.82961800	-1.78046600
H	3.30517500	4.16478700	-2.55491300
C	6.06817300	3.13160000	-0.85484300
H	6.06344300	1.67957300	0.74346700
H	5.75824600	4.52554900	-2.47089800
H	7.14361100	3.28338900	-0.82565700

12I

Charge: 0 Multiplicity: 1

P	-2.25859600	-1.13202900	-0.73872600
S	5.52742800	-2.04210500	1.39123700
C	-3.79614000	-0.63099500	0.05731200
O	4.11858200	-2.81287200	1.15887800
C	0.81447700	-0.61905100	-0.19074300
C	-5.09817500	-1.25719900	-0.04874000
N	-5.22098800	0.44900100	1.43976600
F	7.39128400	-1.46905500	-0.32463900
C	-3.92221900	0.41444700	0.97723400
C	-2.87283700	1.38987400	1.40999000
H	-1.98988200	1.12923900	0.80077100
C	-5.95905700	-0.54281300	0.82393700
O	5.32492200	-0.71258900	1.93694200
C	-1.70678800	-2.66758400	0.15874300
H	-0.68328900	-2.83406100	-0.19831500
C	-5.64323700	-2.32381900	-0.78318500
H	-5.03297000	-2.90806300	-1.46108500
C	3.00197100	-2.06405500	0.71826900
C	-2.39669100	1.24751600	2.86577900
H	-3.19374500	1.51446900	3.57168100
H	-2.13978500	0.20178200	3.06536600
C	-2.70967400	-1.68163800	-2.45435500
H	-3.34785800	-2.56546500	-2.36877800
C	1.49936300	-1.48281500	-1.05245800
H	1.20164300	-1.57574200	-2.09089800
O	6.39387400	-3.01864800	2.01828300
C	2.60103800	-2.21021300	-0.60159900
H	3.15235800	-2.86543500	-1.26816700
C	2.32514300	-1.24106100	1.60775200
H	2.66163500	-1.14992300	2.63465900
C	-7.31331400	-0.84912500	0.97335100
H	-7.95427800	-0.27851000	1.63830200
C	-7.81788100	-1.90999100	0.23197600
H	-8.86721200	-2.17551900	0.32332800
F	5.97953300	-2.96668700	-1.02200000
C	-3.19799400	2.85347400	1.06481200
H	-3.52186500	2.91629100	0.02069500
H	-4.03159900	3.22250100	1.67444800
C	1.23455100	-0.51165300	1.13942300
H	0.73194500	0.16788300	1.81815700
C	-3.48048900	-0.58845100	-3.18999000
H	-4.39431200	-0.30964200	-2.65711400
H	-3.75957300	-0.94220400	-4.18934500
H	-2.86613800	0.30944800	-3.30914800
F	5.40300800	-0.87415600	-0.95977900
C	-1.18978300	2.15466800	3.11030200
H	-0.86086700	2.06762400	4.15282500
H	-0.35446000	1.81492000	2.48218800
C	-6.98794500	-2.63899100	-0.63685100
H	-7.40541700	-3.46421000	-1.20702800
C	-1.65110600	-2.36465800	1.65483400
H	-1.04899300	-1.47665200	1.86338700
H	-1.20136300	-3.20873000	2.18986600
H	-2.65782700	-2.20037800	2.05382400
C	-2.54561000	-3.91265500	-0.11492200
H	-3.58076800	-3.77286500	0.21206400
H	-2.13126800	-4.75901500	0.44599900
H	-2.54994700	-4.19304200	-1.17278700
C	-1.49590700	3.61094300	2.76095100
H	-0.60598700	4.23145100	2.92041300
H	-2.27592000	3.99241600	3.43650200
C	-1.43989200	-2.07759800	-3.20742600
H	-0.78231700	-1.20937300	-3.33253200
H	-1.69895500	-2.45508700	-4.20334000
H	-0.87646900	-2.86012800	-2.68819200
C	-5.81805400	1.37534100	2.37992700
H	-5.04726700	1.86828600	2.96505600
H	-6.46441400	0.82307000	3.06721000
H	-6.41437200	2.13332500	1.86067500
C	-1.97458600	3.73506100	1.31443100
H	-2.20738000	4.77930100	1.07286500
H	-1.15784800	3.42302700	0.64719300
C	6.11327200	-1.82192100	-0.36427700

Pd	-0.61234100	0.54691100	-0.88380600
O	-2.03009600	2.21273800	-1.92288900
C	-1.48054800	3.21527600	-2.19924300
O	-0.98358600	4.22245900	-2.48985400
C	0.89185200	1.84246300	-0.96594500
C	1.98162700	2.40450900	-0.86917800
C	3.30404400	2.89986200	-0.68353600
C	4.23653600	2.08712000	-0.00733900
C	3.71920100	4.15672200	-1.15714700
C	5.54397100	2.51932700	0.18042200
H	3.91849300	1.11784900	0.36274400
C	5.02995600	4.58350100	-0.96173600
H	3.00630900	4.78886500	-1.67891000
C	5.94711100	3.76904200	-0.29548500
H	6.24793200	1.87494000	0.70003700
H	5.33808300	5.55734600	-1.33350100
H	6.96951200	4.10644000	-0.14811700

12J

Charge: 0 Multiplicity: 1

P	2.11556100	-1.08352300	0.86749800
S	-5.38862100	-2.46135400	-1.51688800
C	3.66789100	-0.60012400	0.09246300
O	-3.90985400	-3.01766100	-1.14863500
C	-0.93782200	-0.46940200	0.32366800
C	4.98236700	-1.17889100	0.27584700
N	5.13179200	0.54193800	-1.19477900
F	-7.42224000	-2.07092200	0.05484500
C	3.80585500	0.44150200	-0.82859100
C	2.73123600	1.32475100	-1.38316700
H	1.79372000	0.92516100	-0.96207700
C	5.86559500	-0.43394900	-0.54771600
O	-5.32577400	-1.15454800	-2.14280000
C	1.56671100	-2.63159100	-0.00064900
H	0.53892700	-2.79120500	0.34785800
C	5.51848700	-2.23458100	1.03201000
H	4.88919900	-2.84542100	1.66802900
C	-2.93566700	-2.11656400	-0.66142900
C	2.56378800	1.23157900	-2.90926900
H	3.45494900	1.60452300	-3.42759800
H	2.45168700	0.17907700	-3.19478700
C	2.54461500	-1.55274600	2.61011400
H	3.23305100	-2.40179500	2.58843500
C	-1.59725500	-1.36102100	1.17581700
H	-1.33504900	-1.41965400	2.22584100
O	-6.07203400	-3.58578100	-2.12223400
C	-2.60135900	-2.19428700	0.68310800
H	-3.11853400	-2.89320100	1.33226000
C	-2.30876000	-1.23175500	-1.52755200
H	-2.59713700	-1.19013200	-2.57200300
C	7.23124000	-0.71031900	-0.63960700
H	7.88432100	-0.13552500	-1.28897700
C	7.72760200	-1.75932300	0.12411600
H	8.78519200	-2.00245200	0.07587500
F	-5.84819700	-3.28323300	0.93261000
C	2.80224200	2.77993000	-0.88453100
H	2.82722600	2.77314600	0.21343700
H	3.72809300	3.26725600	-1.21551900
C	-1.31622300	-0.39444700	-1.02063300
H	-0.83660500	0.31581900	-1.68545800
C	3.23211700	-0.37307300	3.29597300
H	4.16653500	-0.10340400	2.79527900
H	3.45934900	-0.62556700	4.33810900
H	2.57777100	0.50822100	3.29991600
F	-5.58685600	-1.13561500	0.74138800
C	1.35321000	2.04610100	-3.36404700
H	1.25874600	1.99408400	-4.45549200
H	0.43914000	1.60037800	-2.94667800
C	6.87687100	-2.51271200	0.95095100
H	7.28751200	-3.33194900	1.53454300
C	1.53129800	-2.35332300	-1.50361800
H	0.94036600	-1.46357000	-1.73787200
H	1.08173800	-3.20304200	-2.02963300
H	2.54480400	-2.20485600	-1.89157600
C	2.40842000	-3.86569400	0.31100400
H	3.44492400	-3.72721100	-0.01328000
H	2.00379600	-4.73073500	-0.22801400
H	2.40916600	-4.11380700	1.37711400
C	1.45502000	3.49882500	-2.90012800
H	0.57265900	4.06270000	-3.22663400
H	2.32697500	3.96983700	-3.37850600
C	1.27816700	-1.97255800	3.35518200
H	0.58736500	-1.12584700	3.44003000
H	1.53425200	-2.30466000	4.36780200
H	0.75312100	-2.79332500	2.85513700
C	5.74286100	1.45879400	-2.13592000
H	5.10132000	2.32035600	-2.29707000
H	5.93308600	0.96786400	-3.09641500
H	6.69099300	1.81502900	-1.72463600
C	1.59830000	3.58060700	-1.38091000
H	1.69263300	4.62530500	-1.05921600
H	0.69037000	3.18528700	-0.90565100
C	-6.11066600	-2.21835300	0.18450500
Pd	0.52615400	0.65404800	0.98210400
C	-0.79460200	2.11881100	1.10225100
C	-1.60199700	3.04775700	1.10051900
C	-2.49873000	4.15472700	1.08420600
C	-2.30259600	5.21919500	0.18295700
C	-3.59788800	4.21018500	1.96221700
C	-3.17727100	6.30039800	0.16410500
H	-1.45667700	5.18242000	-0.49740300
C	-4.46903300	5.29446700	1.93718300
H	-3.75646700	3.39264500	2.65951200
C	-4.26349800	6.34380500	1.03999300

H	-3.01136300	7.11369800	-0.53761100
H	-5.31304700	5.32127100	2.62145000
H	-4.94540400	7.18956000	1.02311800

12K-TS

Charge: 0 Multiplicity: 1

P	2.17674000	-1.00582800	0.82040300
S	-5.36319900	-2.57629400	-1.49101400
C	3.78766600	-0.64597600	0.09590300
O	-3.87622200	-2.95132800	-0.95872600
C	-1.21971100	0.02193500	0.32578400
C	5.02218200	-1.39342800	0.19497400
N	5.37636700	0.43988400	-1.09194000
F	-7.54548200	-2.23899100	-0.11692300
C	4.05439700	0.47141600	-0.69932200
C	3.09987200	1.55446500	-1.08726400
H	2.15896900	1.27165800	-0.58118500
C	5.99016000	-0.67449700	-0.55411400
O	-5.36158000	-1.33505300	-2.24154500
C	1.47473700	-2.43325400	-0.14874100
H	0.43902800	-2.50528500	0.21024400
C	5.42726300	-2.57562900	0.83582900
H	4.72543600	-3.16619800	1.41309800
C	-3.01416300	-1.91323200	-0.54108400
C	2.72408500	1.59732400	-2.57693200
H	3.57053400	1.92898700	-3.19271600
H	2.46459200	0.58762600	-2.91445000
C	2.51873000	-1.64230300	2.52862100
H	3.13029700	-2.54740600	2.46391900
C	-1.89982000	-0.78709900	1.25501800
H	-1.72392900	-0.65747600	2.31698400
O	-5.89629800	-3.81283000	-2.02479600
C	-2.79360900	-1.76039900	0.82255200
H	-3.31320200	-2.39761500	1.53064000
C	-2.37149500	-1.12158100	-1.48493600
H	-2.56607200	-1.26575900	-2.54205300
C	7.31790300	-1.08949700	-0.67346500
H	8.04153200	-0.51765300	-1.24649500
C	7.68406100	-2.26350700	-0.02612600
H	8.70906700	-2.61627300	-0.09739000
F	-5.94168500	-3.19487600	0.99293900
C	3.44241200	2.94870900	-0.53850800
H	3.66846400	2.86998300	0.53211700
H	4.33959500	3.35482100	-1.02289600
C	-1.48435600	-0.14563200	-1.04591700
H	-0.99010600	0.49102900	-1.77156800
C	3.28712600	-0.57998600	3.31221300
H	4.25444900	-0.36105900	2.84963500
H	3.46476900	-0.92068500	4.33903200
H	2.71173200	0.35370900	3.36037100
F	-5.86533300	-1.06154300	0.59428100
C	1.54810300	2.55296000	-2.78075900
H	1.28090300	2.60135200	-3.84345500
H	0.67265100	2.15421800	-2.24727700
C	6.74580800	-2.99765400	0.72019900
H	7.05734700	-3.91280500	1.21623000
C	1.44181800	-2.03564800	-1.62392700
H	0.94276100	-1.07244300	-1.76605800
H	0.89765500	-2.78792000	-2.20643600
H	2.45853000	-1.95809600	-2.02499200
C	2.17813000	-3.77222100	0.04763400
H	3.21198600	-3.72656400	-0.30960900
H	1.66100200	-4.55084900	-0.52658700
H	2.18908000	-4.08919800	1.09561100
C	1.86409400	3.94898500	-2.24234200
H	0.99837800	4.60953100	-2.37436100
H	2.68710700	4.38409800	-2.82885000
C	1.19317600	-1.99009300	3.20587800
H	0.56502200	-1.09575000	3.29308200
H	1.37563000	-2.38213700	4.21342000
H	0.62641100	-2.74304800	2.64796900
C	6.09864500	1.40334100	-1.89592300
H	5.40498600	2.09502900	-2.36497800
H	6.65143200	0.88347700	-2.68409400
H	6.80515600	1.97096000	-1.28064100
C	2.26563400	3.89857800	-0.76759200
H	2.51694400	4.90251500	-0.40393800
H	1.40731800	3.54832900	-0.17567000
C	-6.24046600	-2.24109400	0.11920000
Pd	0.58991700	0.73943000	0.86931800
C	-1.00497600	1.87211700	0.82646500
C	-1.82024500	2.79850400	0.85779400
C	-2.75415300	3.86428500	0.87064200
C	-2.91893600	4.68232300	-0.26586900
C	-3.53823700	4.12476700	2.01270500
C	-3.83894500	5.72409800	-0.25570400
H	-2.31619000	4.48597800	-1.14768200
C	-4.45553800	5.16917200	2.01306400
H	-3.41515200	3.49810200	2.89106800
C	-4.61010200	5.97259100	0.88159000
H	-3.95575600	6.34644400	-1.13880100
H	-5.05363000	5.35851600	2.90034800
H	-5.32759200	6.78835200	0.88617000

12L

Charge: 0 Multiplicity: 1

P	1.59798800	-1.46740100	0.43103600
S	-7.20635100	-0.57381100	-0.84171700
C	3.34142400	-1.63420100	-0.02839900
O	-5.75850300	-0.96655500	-1.46884900
C	-2.24141500	0.89432100	-0.18934700
C	4.17406400	-2.81908000	-0.06188200
N	5.40794900	-1.04102500	-0.73788300
F	-8.36494300	-1.53227600	1.28018200

C	4.14827100	-0.56820800	-0.43380900
C	3.78025500	0.87804300	-0.49725200
H	2.75058000	0.90378700	-0.08534600
C	5.45747400	-2.40098000	-0.50388700
O	-7.27543700	0.83820800	-0.51929700
C	0.63600200	-2.30201800	-0.93439900
H	-0.41076400	-2.16709200	-0.63243700
C	3.99696900	-4.17842200	0.24610700
H	3.03786000	-4.55426300	0.58120100
C	-4.60224300	-0.30681600	-1.00799500
C	3.62039800	1.47096500	-1.90522700
H	4.59550700	1.58112200	-2.39927100
H	3.02507100	0.78770000	-2.52129300
C	1.40579000	-2.54275100	1.93373500
H	1.71615700	-3.56410600	1.69329100
C	-2.54291900	-0.42171300	0.19737300
H	-1.83350200	-0.95435700	0.82048300
O	-8.17545100	-1.23526100	-1.68955900
C	-3.72605300	-1.02653100	-0.20462000
H	-3.97023000	-2.04128900	0.09045000
C	-4.33479100	0.99426400	-1.41862400
H	-5.03900500	1.52117500	-2.05238700
C	6.53620200	-3.27705900	-0.64152200
H	7.51063400	-2.92968800	-0.97140200
C	6.32307600	-4.61397700	-0.32920900
H	7.14125000	-5.32255600	-0.42279000
F	-6.71502200	-2.74206900	0.54943900
C	4.60080400	1.80014900	0.41513300
H	4.69309500	1.34520900	1.40889000
H	5.61887000	1.93142100	0.02706000
C	-3.15365200	1.59454700	-1.00046000
H	-2.92385900	2.60950500	-1.30831000
C	2.31037800	-1.99974400	3.03841100
H	3.36335000	-2.02256100	2.74026100
H	2.19740400	-2.59644500	3.95139300
H	2.04462400	-0.96111800	3.27428700
F	-6.31656700	-0.88663900	1.60460400
C	2.93580400	2.83509900	-1.80594700
H	2.83936800	3.28308500	-2.80281600
H	1.91743200	2.68245100	-1.42260100
C	5.06411700	-5.05729600	0.11141800
H	4.92206900	-6.10737400	0.35197000
C	0.85673800	-1.51436500	-2.22552500
H	0.61367200	-0.45482900	-2.08651600
H	0.22656900	-1.91509500	-3.02833400
H	1.90281700	-1.58463200	-2.54625100
C	0.90709900	-3.78883200	-1.13538400
H	1.93762400	-3.95881000	-1.46171800
H	0.23999200	-4.18663400	-1.91030400
H	0.73455100	-4.37024900	-0.22338500
C	3.68529500	3.78293600	-0.86799000
H	3.12570000	4.71986600	-0.76190300
H	4.65936800	4.03750500	-1.31242900
C	-0.05759600	-2.56427400	2.36982200
H	-0.40487900	-1.54750300	2.59083700
H	-0.17427500	-3.16923800	3.27692600
H	-0.71077200	-2.99082500	1.60037500
C	6.55830900	-0.28566700	-1.18720300
H	6.23844300	0.65372200	-1.63124500
H	7.08813200	-0.85869700	-1.95273000
H	7.24525300	-0.07674900	-0.35971900
C	3.90954300	3.15902100	0.51009500
H	4.49016300	3.83862000	1.14627700
H	2.93637500	3.02149200	0.99872500
C	-7.14160900	-1.50551300	0.77086900
Pd	0.82494800	0.71643000	0.64371300
C	-1.01067400	1.51536600	0.21285600
C	-0.25464500	2.50224900	0.47593900
C	0.13239700	3.88166600	0.55855200
C	-0.13328200	4.75304900	-0.51360400
C	0.82202500	4.37471700	1.67940000
C	0.28695100	6.07801900	-0.46321100
H	-0.65532300	4.37331600	-1.38690900
C	1.22748100	5.70390000	1.72894900
H	1.03408600	3.69983000	2.50379800
C	0.96792200	6.55919400	0.65663800
H	0.08225200	6.73842000	-1.30159200
H	1.75664000	6.07204300	2.60362700
H	1.29468900	7.59460800	0.69298400

12M

Charge: 0 Multiplicity: 1

Pd	-0.74312700	0.35898400	0.60211600
P	1.17352200	1.18766800	-0.36229100
C	2.62567700	0.11002100	-0.34846300
C	-3.54559700	0.19003200	0.60274600
C	3.83429500	0.17569100	-1.14111100
N	3.96808200	-1.61374200	0.24430000
C	2.74886600	-1.00920600	0.47903600
C	1.75043700	-1.52090200	1.46653600
H	0.87712200	-0.85236100	1.32542300
C	4.63974900	-0.92558800	-0.74666800
C	1.71345300	2.76729700	0.46957500
H	0.81369100	3.39585700	0.43816500
C	4.32454500	1.02439300	-2.14721700
H	3.75329900	1.88437000	-2.47624800
C	-2.50714300	2.59430500	1.44196400
C	2.14043300	-1.34054000	2.94155700
H	2.96855800	-2.00631200	3.22078600
H	2.49168500	-0.31521000	3.10122100
C	0.89540500	1.63819400	-2.14360500
H	1.77088600	2.16557900	-2.53540500
C	-4.00073200	1.35424600	0.02353800
H	-4.74342800	1.31516200	-0.76517900
C	-3.48745100	2.58721500	0.47066600

H	-3.83763300	3.51497500	0.03273400
C	-2.02104500	1.40555500	2.04749100
H	-1.45174300	1.48069500	2.96844100
C	5.88394800	-1.19776600	-1.31940000
H	6.47725200	-2.05267200	-1.00904400
C	6.33677500	-0.33763400	-2.31265900
H	7.30003900	-0.52091300	-2.78054500
C	1.21444900	-2.93189200	1.18039900
H	0.91235100	-2.99628600	0.12856500
H	1.98892300	-3.69298600	1.34027400
C	-2.60238300	0.15894000	1.65954100
H	-2.52148900	-0.72658800	2.28445600
C	0.68386500	0.36002700	-2.95257400
H	1.57002400	-0.28171500	-2.92490900
H	0.46773800	0.60417000	-3.99977600
H	-0.16268300	-0.21125200	-2.55436100
C	0.93321300	-1.63759100	3.83098700
H	1.20455200	-1.52529500	4.88804200
H	0.15209100	-0.89187800	3.61910800
C	5.56247400	0.76253400	-2.72065000
H	5.93898100	1.42068800	-3.49906300
C	2.02352000	2.45944700	1.93339400
H	1.18035100	1.95366100	2.41659200
H	2.23616500	3.38409700	2.48296700
H	2.90172700	1.80778900	2.01173400
C	2.86960100	3.50262700	-0.19991500
H	3.77672200	2.88952800	-0.19692300
H	3.08937000	4.43045200	0.34314600
H	2.64344200	3.77461600	-1.23626000
C	0.37770300	-3.03742000	3.56541600
H	-0.50271300	-3.22132000	4.19403100
H	1.13260400	-3.78411100	3.85413600
C	-0.31539200	2.56839100	-2.23069500
H	-1.19809800	2.09125300	-1.78744000
H	-0.53671200	2.80528800	-3.27860900
H	-0.14670200	3.51264100	-1.70190000
C	4.50332500	-2.81118700	0.85638600
H	3.98787700	-3.01622100	1.79098300
H	5.56360900	-2.66168900	1.07834200
H	4.39757800	-3.67641000	0.19248600
C	0.02089400	-3.22425600	2.09047100
H	-0.34899200	-4.24133200	1.91063000
H	-0.79397200	-2.53835300	1.82178200
Cl	-1.81816600	4.11120100	1.96487200
O	-1.85597300	-1.96947300	-0.55961600
S	-3.28800500	-2.02882800	-0.79198000
O	-4.02725000	-3.27356500	-0.76185700
O	-4.11615500	-1.03056000	0.18998800
C	-3.59960500	-1.22645400	-2.44510100
F	-4.88943000	-0.94333800	-2.56294700
F	-3.23233900	-2.08219000	-3.38802400
F	-2.88442700	-0.11238900	-2.54465200

12N-TS

Charge: 0 Multiplicity: 1

Pd	-0.83197900	-0.36043300	0.26913500
P	1.00436900	-0.49886100	-1.11363900
C	2.55275500	-0.42437000	-0.18077400
C	-2.28274400	0.76083800	-0.66587900
C	3.84475000	-0.98695900	-0.51442400
N	4.00113600	0.07177900	1.48504100
C	2.70227800	0.22833800	1.04758500
C	1.66863000	1.00276200	1.80429100
H	0.78177900	0.98428700	1.14771100
C	4.71718700	-0.65563600	0.55531200
C	1.16666400	0.82218000	-2.40680300
H	0.21918200	0.78644300	-2.95635900
C	4.37253000	-1.72290000	-1.58869700
H	3.75872900	-1.98699300	-2.44106400
C	-2.05063100	3.34135300	-1.65784300
C	1.98726500	2.49360700	2.00095700
H	2.83282900	2.63130300	2.68634500
H	2.28297000	2.93417300	1.04259300
C	1.00962800	-2.11070500	-2.03270100
H	1.85921200	-2.12857900	-2.72136100
C	-2.21204900	0.96982100	-2.05694900
H	-2.22975100	0.12016200	-2.72946600
C	-2.06020400	2.25957700	-2.54173300
H	-1.94100000	2.42532200	-3.60773000
C	-2.24514300	3.15008300	-0.29147300
H	-2.28184800	4.00044200	0.38177400
C	6.06242200	-1.02896000	0.58231900
H	6.71132900	-0.75182600	1.40751900
C	6.54766100	-1.76231600	-0.49318600
H	7.58957600	-2.06949400	-0.50520200
C	1.20682400	0.33668900	3.11275700
H	0.94182900	-0.70821700	2.90696400
H	2.01518100	0.31729200	3.85491000
C	-2.42432600	1.86441000	0.20942300
H	-2.62949900	1.71478700	1.26395900
C	1.13994300	-3.26745100	-1.04487800
H	2.08271800	-3.22088000	-0.49152100
H	1.10069900	-4.22458800	-1.57818000
H	0.31690300	-3.24549900	-0.32016600
C	0.76220500	3.21245200	2.56600300
H	0.98719100	4.27547400	2.71597800
H	-0.05181700	3.15898800	1.82882200
C	5.70826300	-2.10294600	-1.56792500
H	6.11259800	-2.66980900	-2.40204300
C	1.26104600	2.17523400	-1.70561900
H	0.44832600	2.31354600	-0.98603300
H	1.20621100	2.98785200	-2.43853300
H	2.21395200	2.26113000	-1.17157300
C	2.32725400	0.61060800	-3.37458100

H	3.28310900	0.58552100	-2.84071100
H	2.36567700	1.43770600	-4.09404200
H	2.22834300	-0.31799500	-3.94578000
C	0.30131400	2.57319700	3.87651600
H	-0.58780900	3.08950600	4.25900300
H	1.08918300	2.69752700	4.63440900
C	-0.27526400	-2.21487200	-2.85500000
H	-1.15402900	-2.16154100	-2.20274600
H	-0.30098600	-3.17245900	-3.38819400
H	-0.35270000	-1.41662800	-3.60101700
C	4.61866100	0.60200900	2.68303100
H	3.85833000	0.92045900	3.38998500
H	5.26593300	1.45341200	2.44601700
H	5.21866700	-0.17951500	3.15750800
C	0.00600000	1.08431200	3.69418800
H	-0.28893900	0.63061200	4.64831500
H	-0.84857100	0.96692500	3.01378300
Cl	-1.81844600	4.95864000	-2.28034800
O	-2.48766500	-0.93341700	1.76107500
S	-3.70372000	-1.10877900	0.93146000
O	-4.99276000	-0.83034000	1.54631300
O	-3.51966000	-0.41650900	-0.44255000
C	-3.72793800	-2.90141500	0.44156300
F	-4.75701300	-3.12189700	-0.36685500
F	-3.85058300	-3.63746300	1.54058400
F	-2.59707500	-3.22357300	-0.18081800

12O

Charge: 0 Multiplicity: 1

Pd	-0.75341700	-0.36713700	-0.25799300
P	1.02447700	0.72146600	-1.13156800
C	2.52900900	0.27604700	-0.25340200
C	-1.80925100	1.27409200	-0.16606700
C	3.87392000	0.17375900	-0.78530000
N	3.90358300	-0.35978800	1.42081200
C	2.60236300	-0.04085100	1.10844800
C	1.49396300	-0.02984500	2.11547600
H	0.62682800	0.37072600	1.56933500
C	4.69816200	-0.22715800	0.29721000
C	0.99670300	2.57111100	-1.22603300
H	0.02191900	2.82493000	-1.65708900
C	4.48451500	0.38502800	-2.03299400
H	3.91351200	0.71285500	-2.89261700
C	-3.48986100	3.46582100	0.12456900
C	1.71780800	0.92737600	3.29888000
H	2.55971600	0.59595700	3.91701700
H	1.97823100	1.92185000	2.91904100
C	1.20286000	0.07835700	-2.86005100
H	2.07081300	0.56623900	-3.31043300
C	-2.34541100	1.89537200	-1.29305400
H	-2.12332300	1.53113100	-2.28889900
C	-3.19059900	2.99750800	-1.15098700
H	-3.61089200	3.48144300	-2.02677300
C	-2.97838100	2.84338700	1.25974500
H	-3.23084700	3.20915500	2.24980600
C	6.07529400	-0.42007100	0.17304800
H	6.68594100	-0.71199200	1.02157300
C	6.64355400	-0.21010400	-1.07658800
H	7.71254700	-0.34932100	-1.20876200
C	1.06224900	-1.43190300	2.58263600
H	0.88016500	-2.06683900	1.70579500
H	1.86159800	-1.91781600	3.15648900
C	-2.13845500	1.74030600	1.10763800
H	-1.75412100	1.24615500	1.99371900
C	1.43334900	-1.43136300	-2.82324000
H	2.31516600	-1.69781400	-2.23356400
H	1.57370100	-1.80926600	-3.84205200
H	0.56063600	-1.93933900	-2.39737900
C	0.46384700	0.99783400	4.17041100
H	0.65098900	1.64559200	5.03531100
H	-0.34599800	1.47079600	3.59819800
C	5.85291300	0.19045600	-2.16673100
H	6.32049000	0.35818800	-3.13278900
C	1.07223200	3.14730000	0.18704900
H	0.27284900	2.76360900	0.82657900
H	0.97655000	4.23775500	0.14481200
H	2.03538800	2.90712300	0.64987300
C	2.11180700	3.12477700	-2.11151300
H	3.09757600	2.83117200	-1.73566200
H	2.06592300	4.21979100	-2.10825500
H	2.02311300	2.79514700	-3.15114400
C	0.01927800	-0.39101600	4.63124400
H	-0.89992100	-0.31520400	5.22439900
H	0.78953500	-0.81206900	5.29434300
C	-0.03152500	0.42913500	-3.68942400
H	-0.91993500	-0.07304700	-3.29082200
H	0.11313200	0.08693900	-4.72013200
H	-0.22147700	1.50689500	-3.72136100
C	4.45576400	-0.74545000	2.70482500
H	3.67117100	-1.11234600	3.36019600
H	4.96180700	0.09908700	3.18413900
H	5.17557000	-1.55375100	2.55417700
C	-0.19350600	-1.33555400	3.44763700
H	-0.47850100	-2.33366300	3.80115200
H	-1.02670500	-0.97675500	2.82808900
Cl	-4.53547500	4.85738400	0.30573800
O	-2.37500300	-1.46330900	0.58483100
S	-3.25070900	-2.26200900	-0.36065300
O	-4.50476300	-2.67420100	0.27076200
O	-3.31142500	-1.71953400	-1.72281300
C	-2.25514800	-3.81359300	-0.52128000
F	-2.85190400	-4.67278900	-1.34524300
F	-2.09239900	-4.39116400	0.66980000
F	-1.03780800	-3.52494000	-1.01600300

CO_2

Charge: 0 Multiplicity: 1

C	-1.57129400	0.10989000	-0.02056900
O	-2.73875000	0.10989000	-0.02056900
O	-0.40383800	0.10989000	-0.02056900

KCl

Charge: 0 Multiplicity: 1

K	0.00000000	0.00000000	1.39559900
Cl	0.00000000	0.00000000	-1.55978700

1a

Charge: 0 Multiplicity: 1

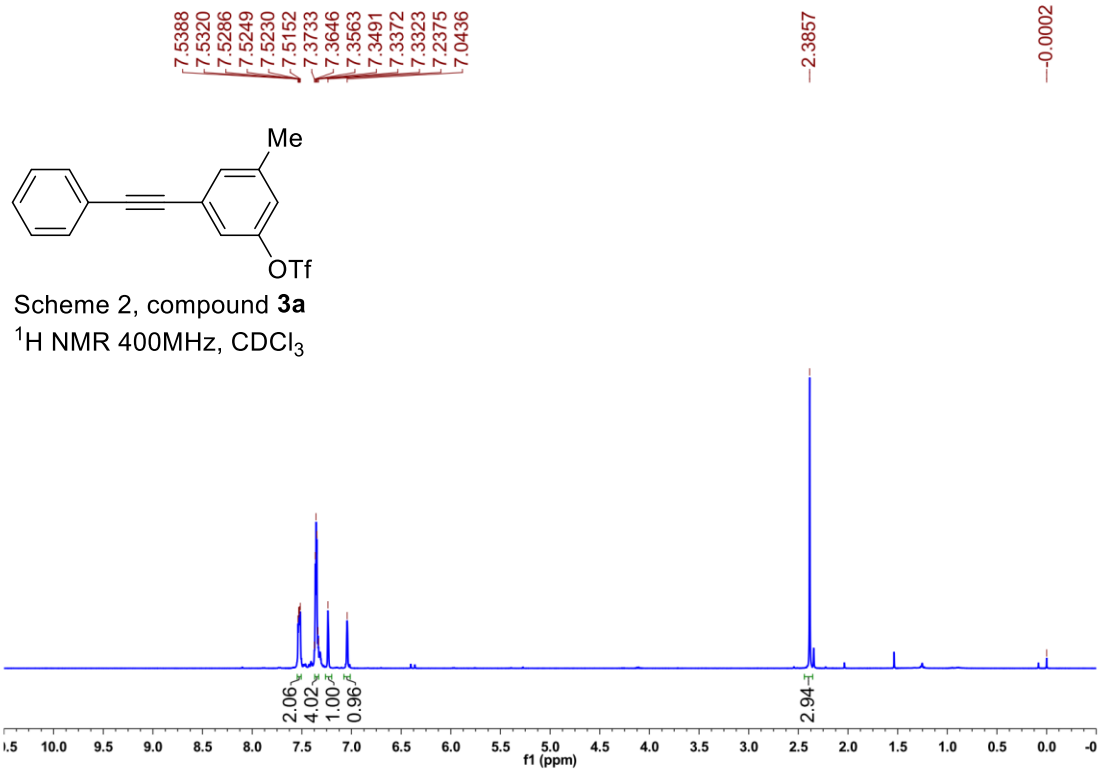
C	-2.02601500	0.74331300	0.53114200
C	-1.69256600	1.97674700	1.08162900
C	-2.66508900	0.70822700	-0.70093800
H	-1.79034400	-0.18030600	1.04795400
H	-1.19086300	2.03216400	2.04119000
C	-2.01325600	3.13986800	0.38450800
C	-2.97950200	1.86182500	-1.40693900
O	-2.92536600	-0.55306400	-1.26600700
C	-2.65256800	3.09571800	-0.85288600
Cl	-1.60053400	4.68731600	1.07491800
H	-3.47092500	1.79767500	-2.37068200
S	-4.45620500	-1.10917100	-1.31727900
H	-2.88842800	4.01283500	-1.38092700
O	-5.40246500	-0.02036300	-1.46317600
O	-4.41427900	-2.24343500	-2.21471700
C	-4.63017100	-1.76915400	0.41953200
F	-3.57314300	-2.51301900	0.71539500
F	-5.73216400	-2.50195400	0.47524500
F	-4.71669500	-0.75228100	1.26712900

2a'

Charge: 0 Multiplicity: 1

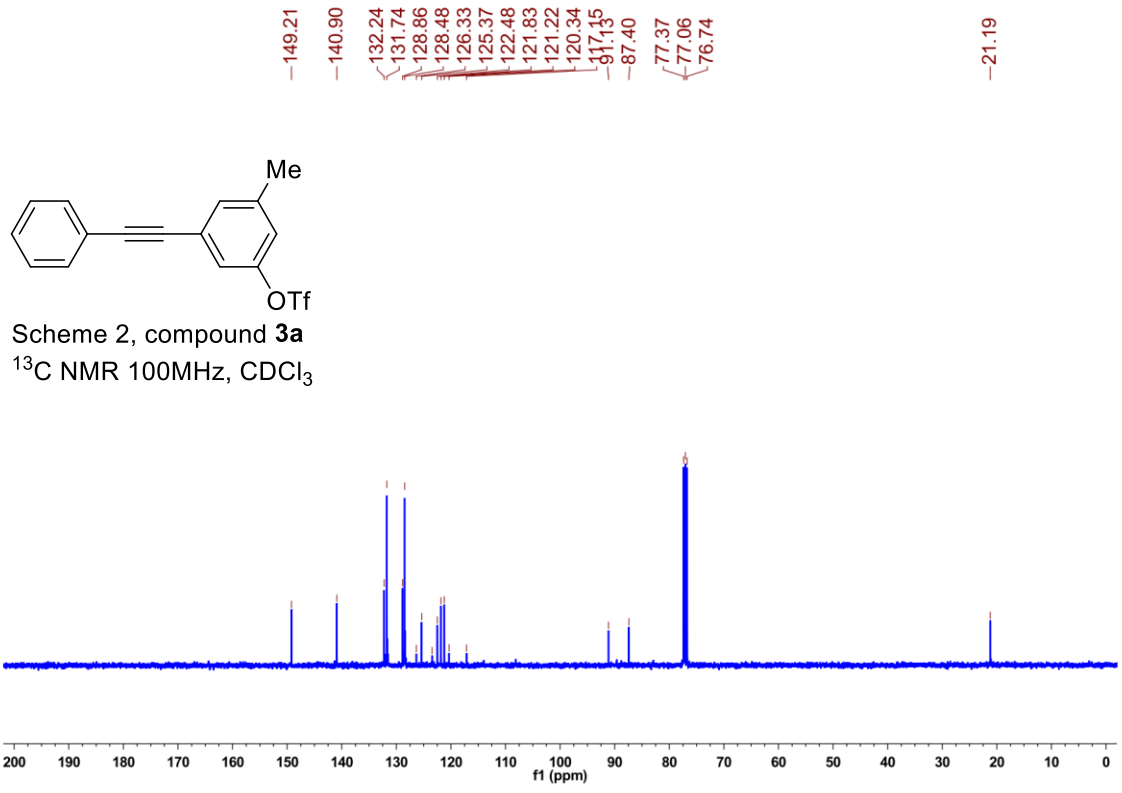
O	1.08753600	0.34448300	2.74251500
C	0.10822300	0.97167600	3.22379600
O	0.01746800	1.49001000	4.36710300
C	-1.06937200	1.11985800	2.34359900
C	-2.03700700	1.24679500	1.61651100
C	-3.16909500	1.39677200	0.76475600
C	-4.19941000	0.43961800	0.77072400
C	-3.27286600	2.50488200	-0.09500900
C	-5.30219200	0.59115600	-0.06299500
H	-4.12330200	-0.41743600	1.43304200
C	-4.37969500	2.64750000	-0.92486600
H	-2.47952300	3.24620100	-0.10274500
C	-5.39764100	1.69340800	-0.91304300
H	-6.09143600	-0.15559200	-0.04877600
H	-4.44764100	3.50836300	-1.58444800
H	-6.26069300	1.80827000	-1.56280300
K	2.52631400	0.75287900	4.97081900

8. ^{1}H, ^{13}C, ^{19}F NMR and HRMS spectra



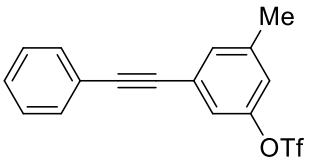
Scheme 2, compound **3a**

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



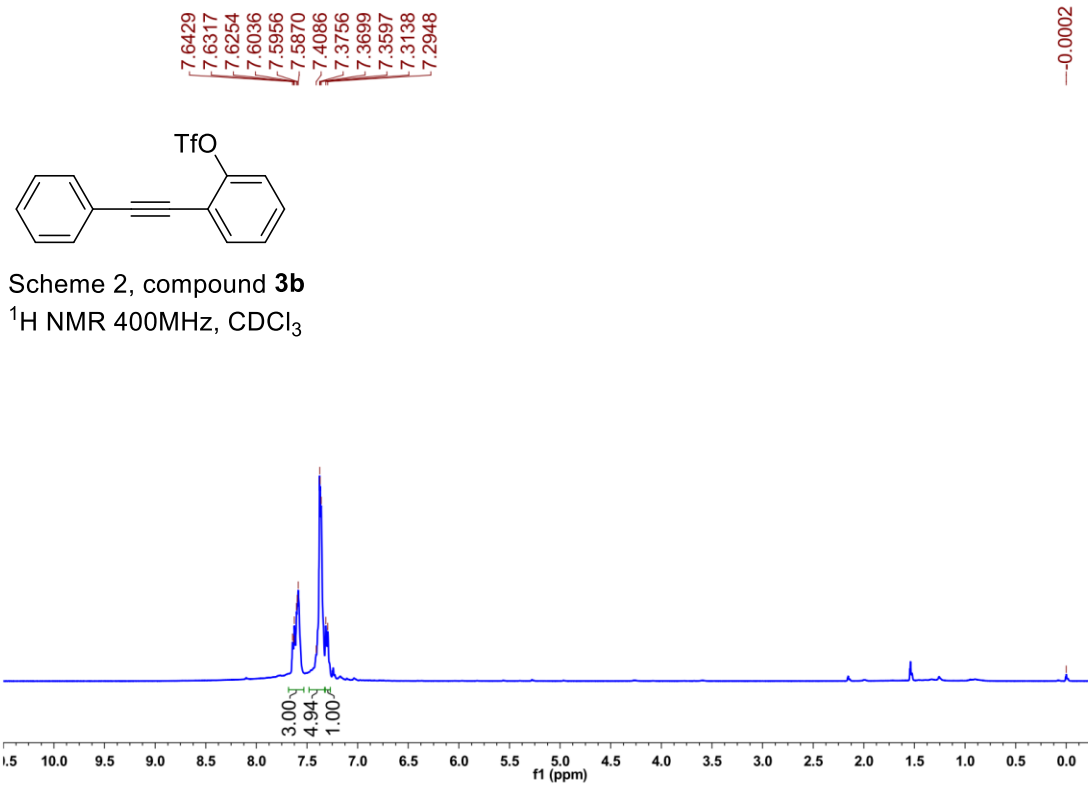
Scheme 2, compound **3a**

^{13}C NMR 100MHz, $CDCl_3$



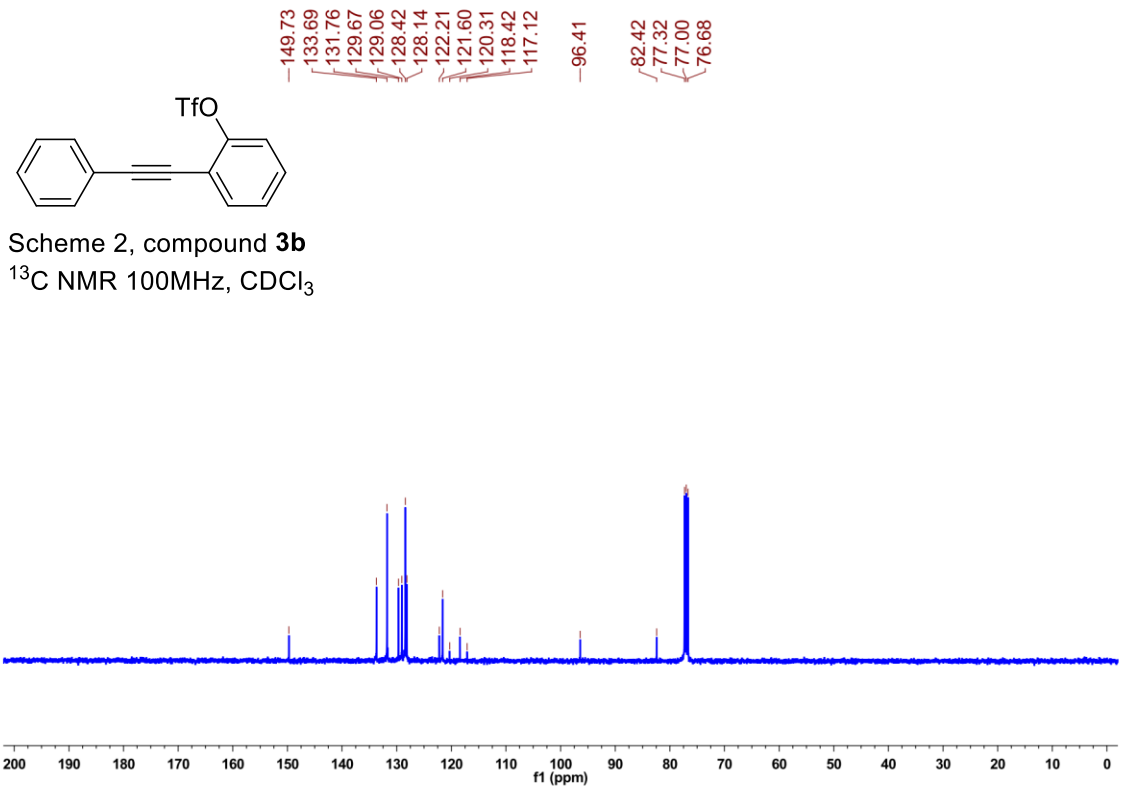
Scheme 2, compound **3a**

^{19}F NMR 470MHz, $CDCl_3$



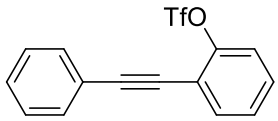
Scheme 2, compound **3b**

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



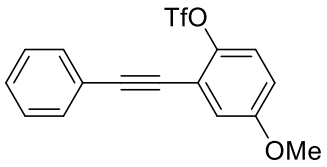
Scheme 2, compound **3b**

^{13}C NMR 100MHz, $CDCl_3$



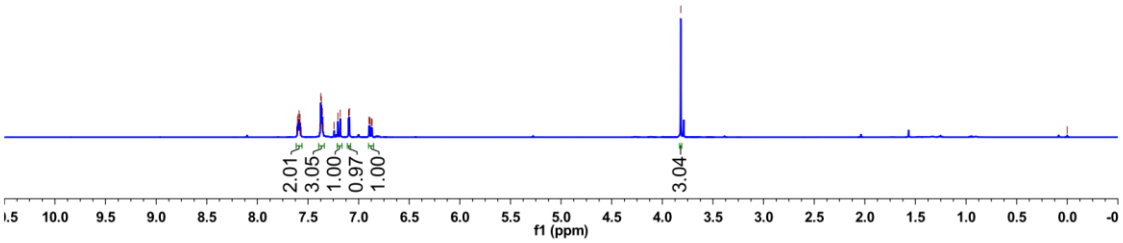
Scheme 2, compound **3b**

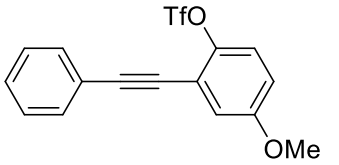
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3c**

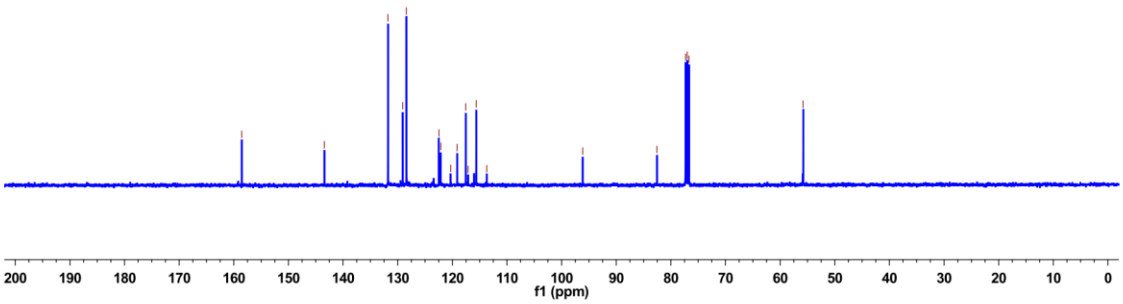
^{1}H NMR 400MHz, $CDCl_3$

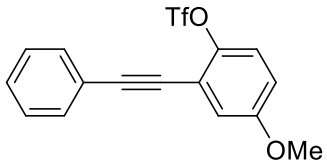




Scheme 2, compound **3c**

^{13}C NMR 100MHz, $CDCl_3$



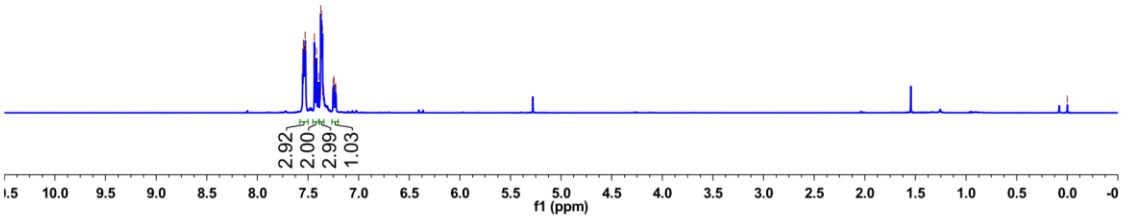


Scheme 2, compound **3c**

^{19}F NMR 470MHz, $CDCl_3$

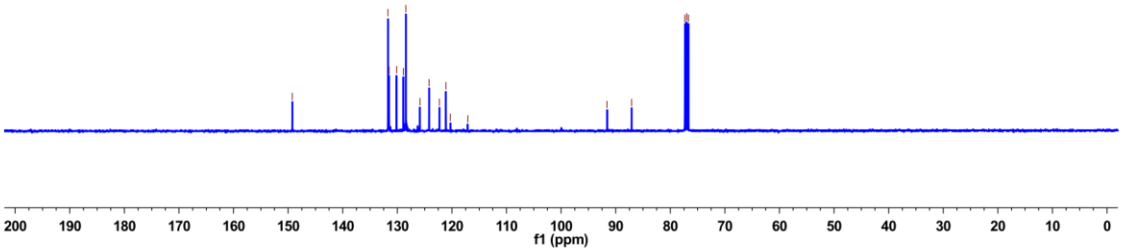
Scheme 2, compound **3d**

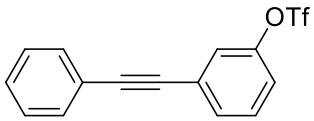
^{1}H NMR 400MHz, $CDCl_3$



Scheme 2, compound **3d**

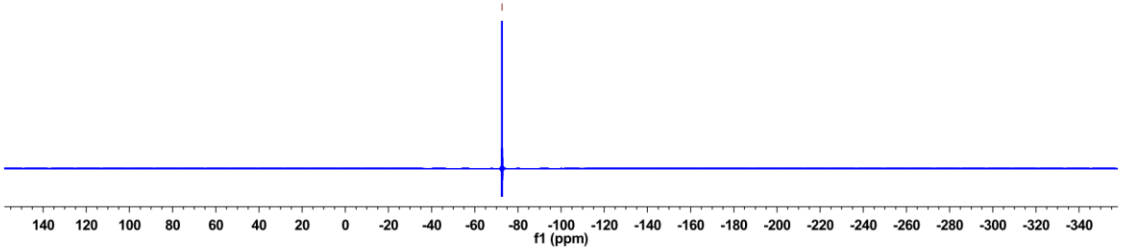
^{13}C NMR 100MHz, $CDCl_3$

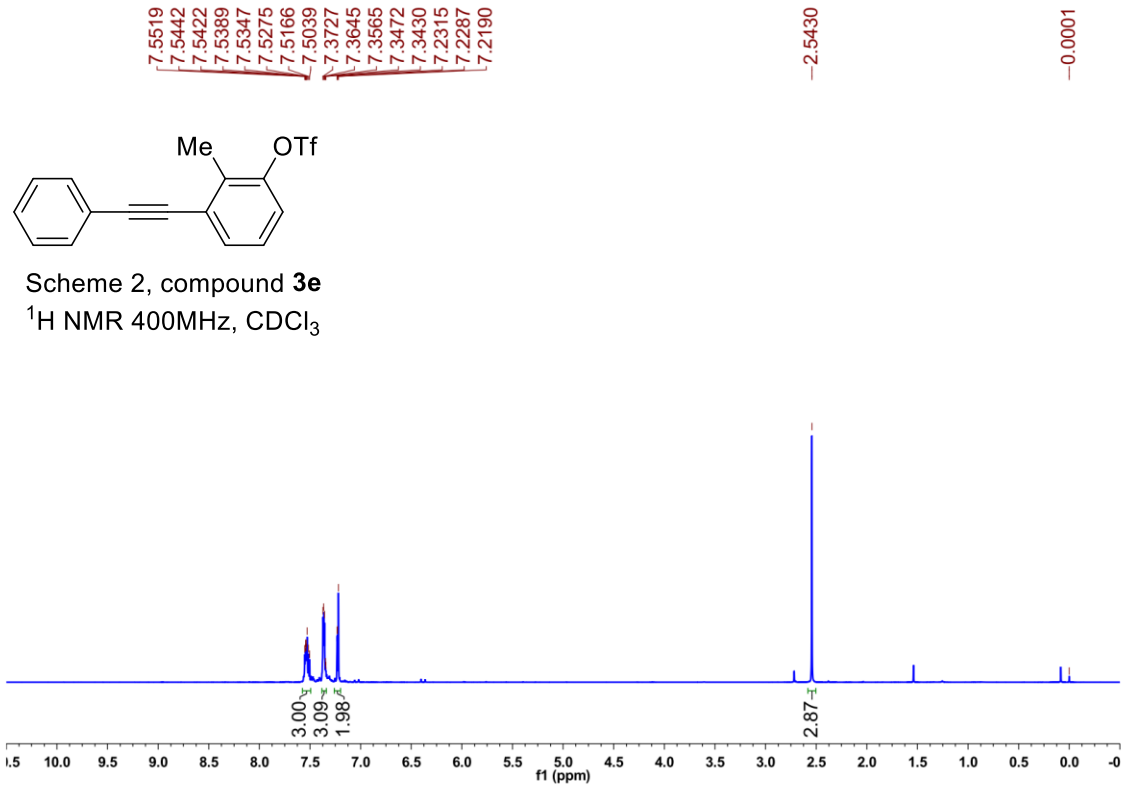




Scheme 2, compound **3d**

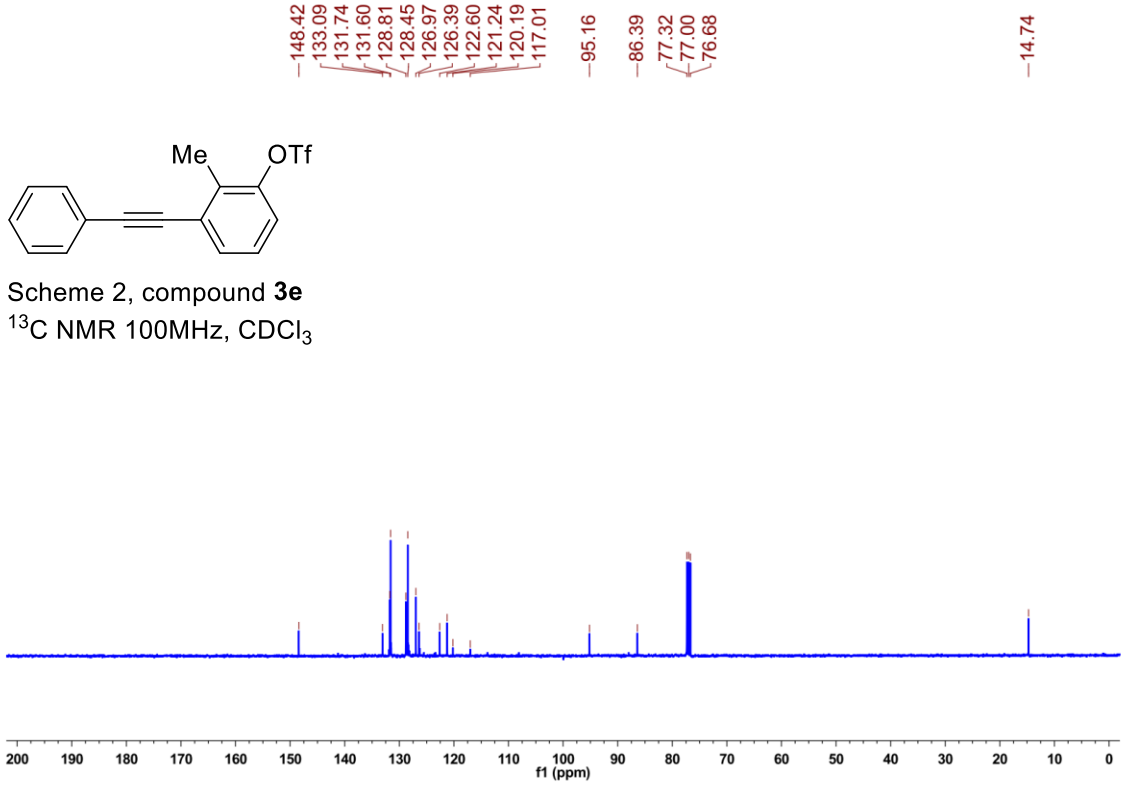
^{19}F NMR 470MHz, $CDCl_3$





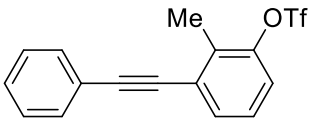
Scheme 2, compound **3e**

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



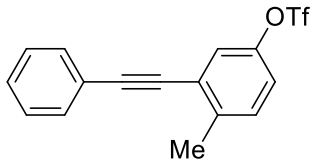
Scheme 2, compound **3e**

^{13}C NMR 100MHz, $CDCl_3$



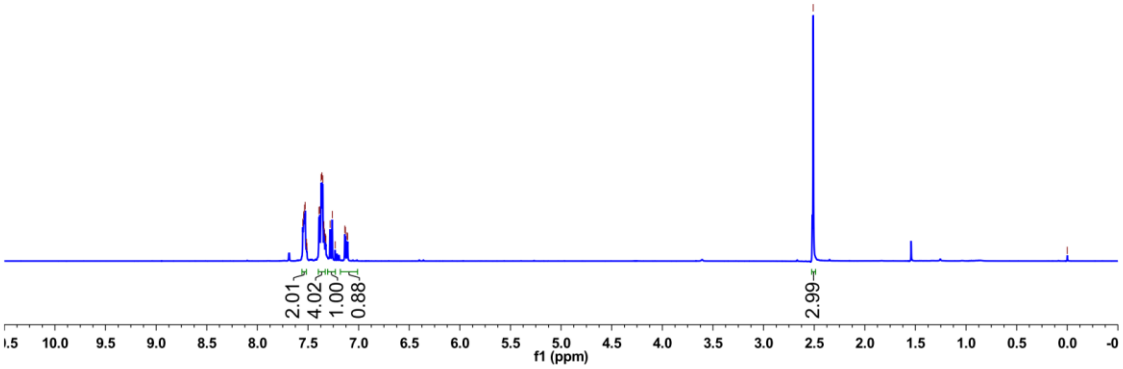
Scheme 2, compound **3e**

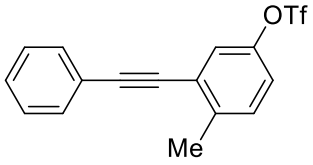
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3f**

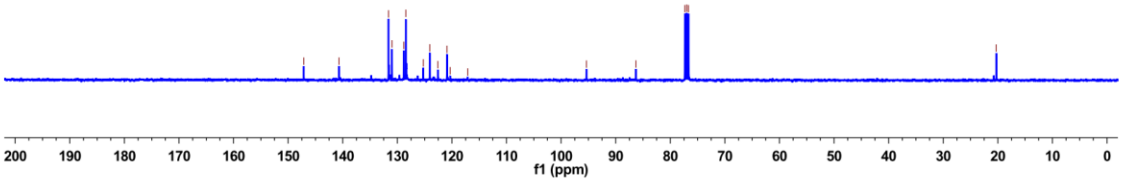
^{1}H NMR 400MHz, $CDCl_3$

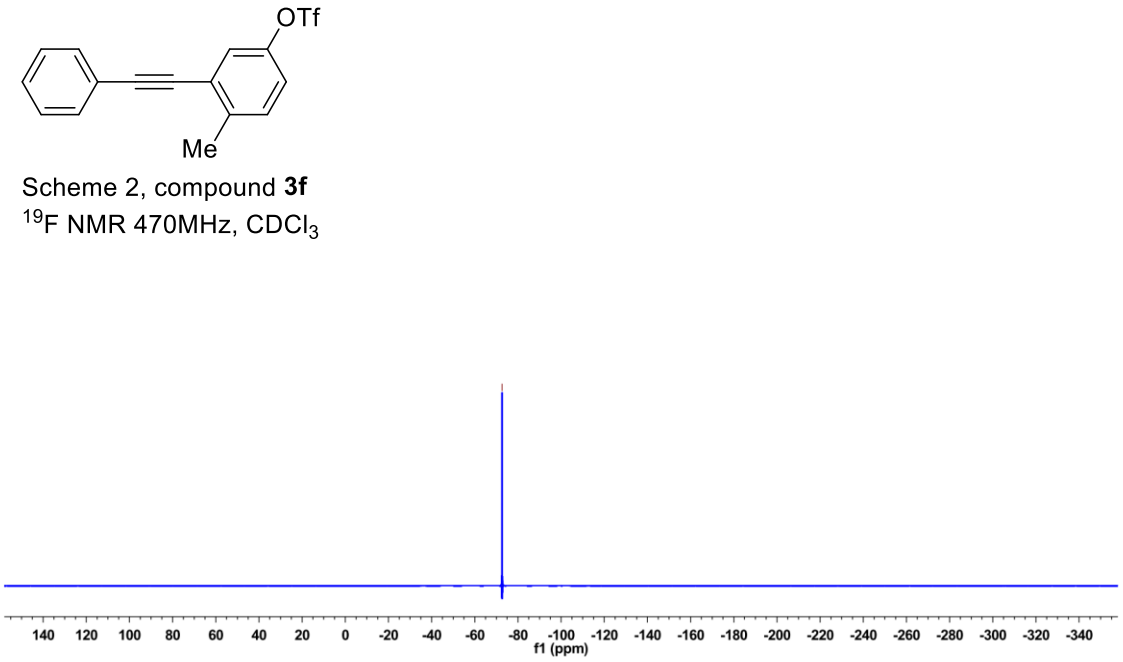




Scheme 2, compound **3f**

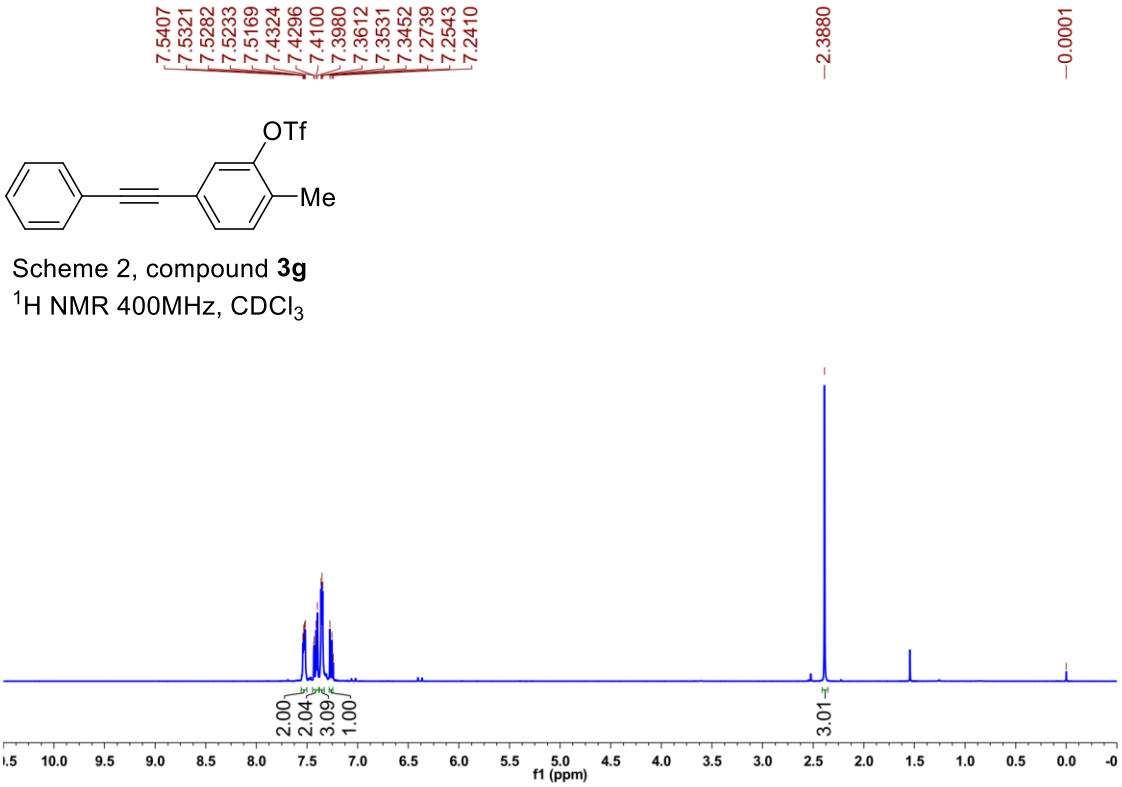
^{13}C NMR 100MHz, $CDCl_3$



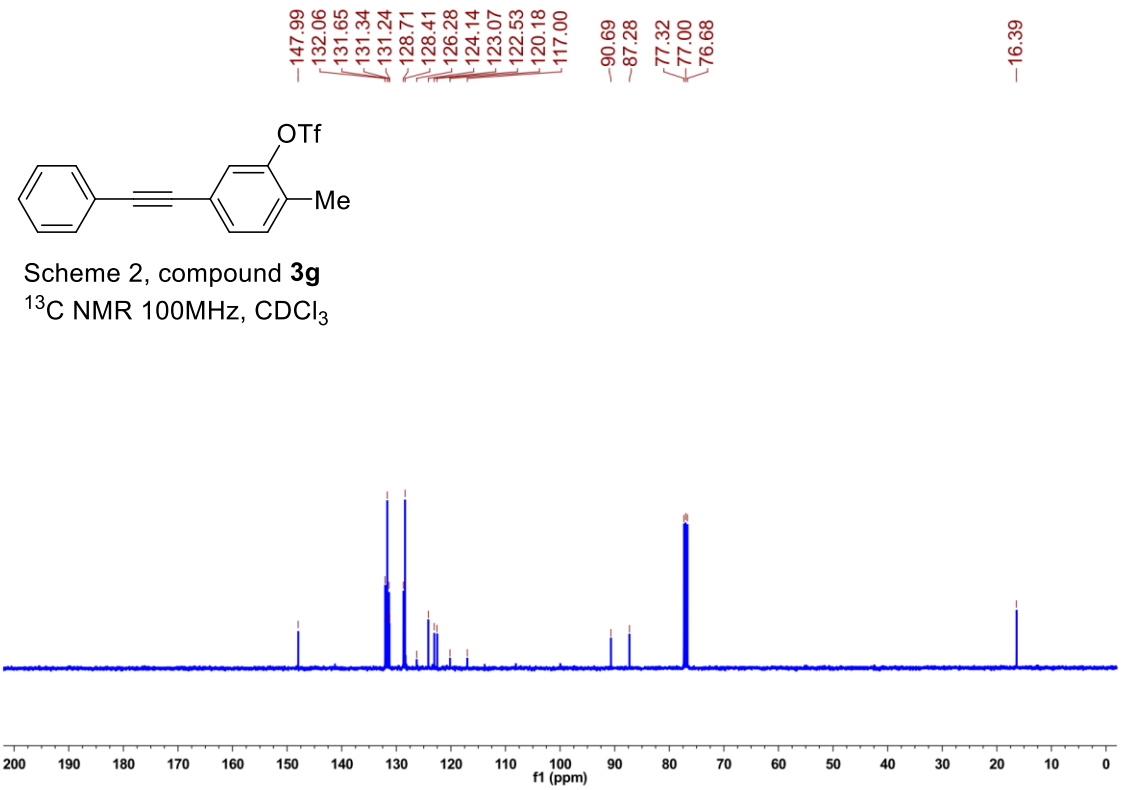


Scheme 2, compound **3f**

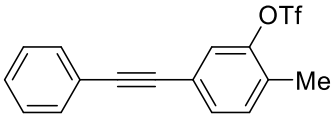
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3g**
^{1}H NMR 400MHz, $CDCl_3$

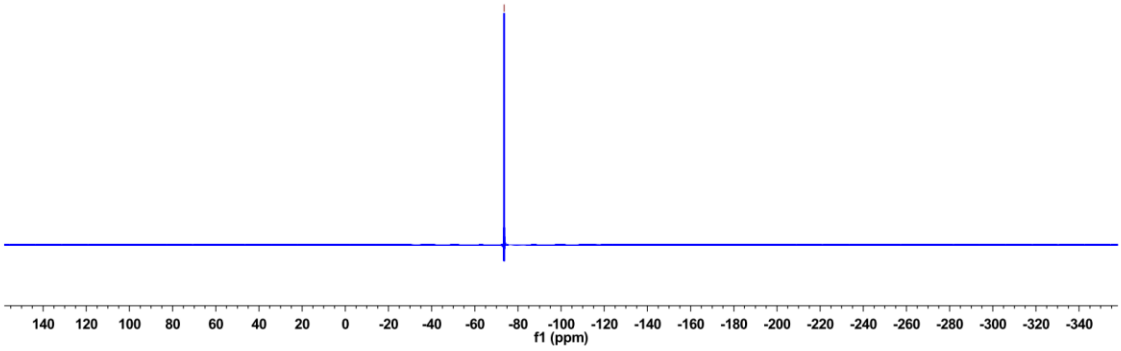


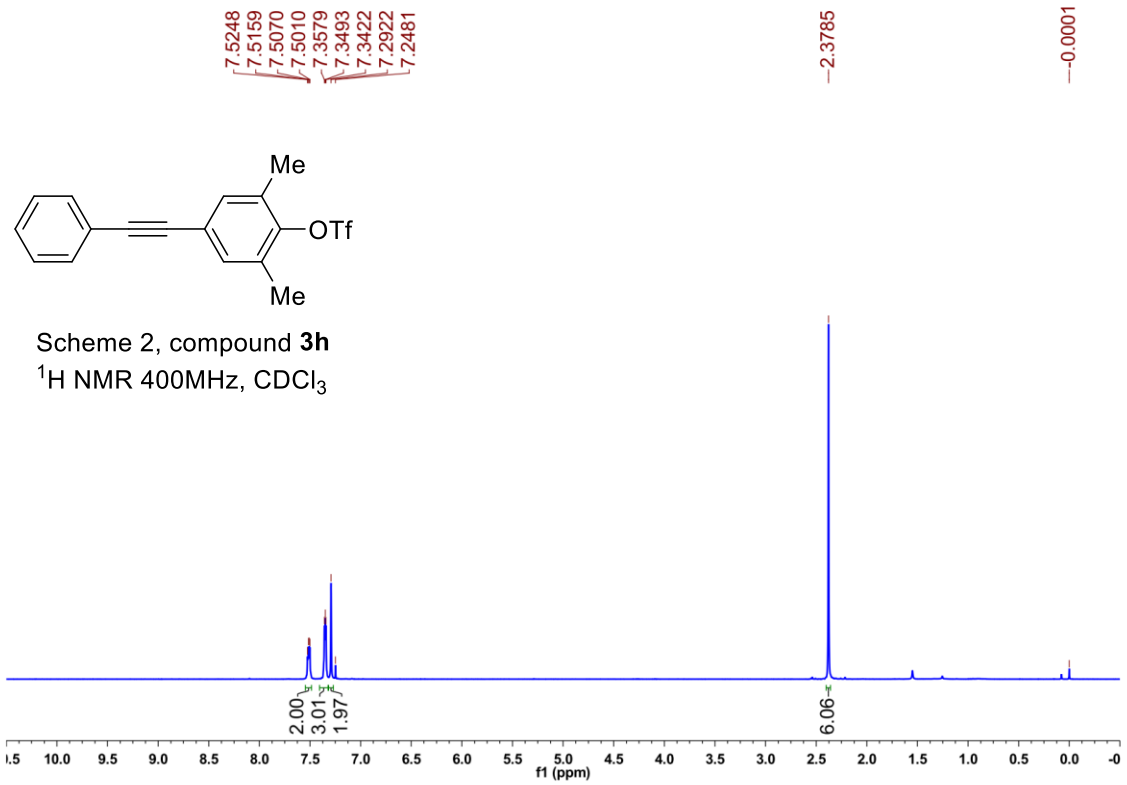
Scheme 2, compound **3g**
^{13}C NMR 100MHz, $CDCl_3$



Scheme 2, compound **3g**

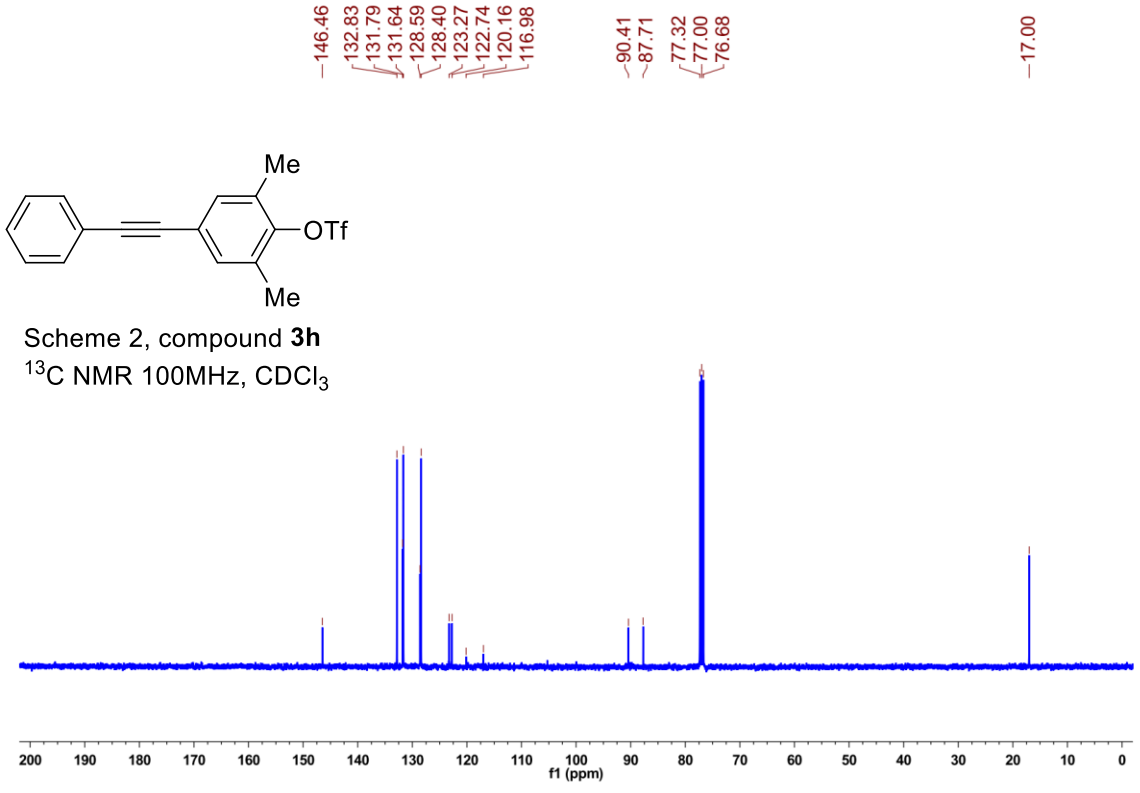
^{19}F NMR 470MHz, $CDCl_3$





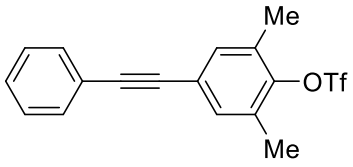
Scheme 2, compound **3h**

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



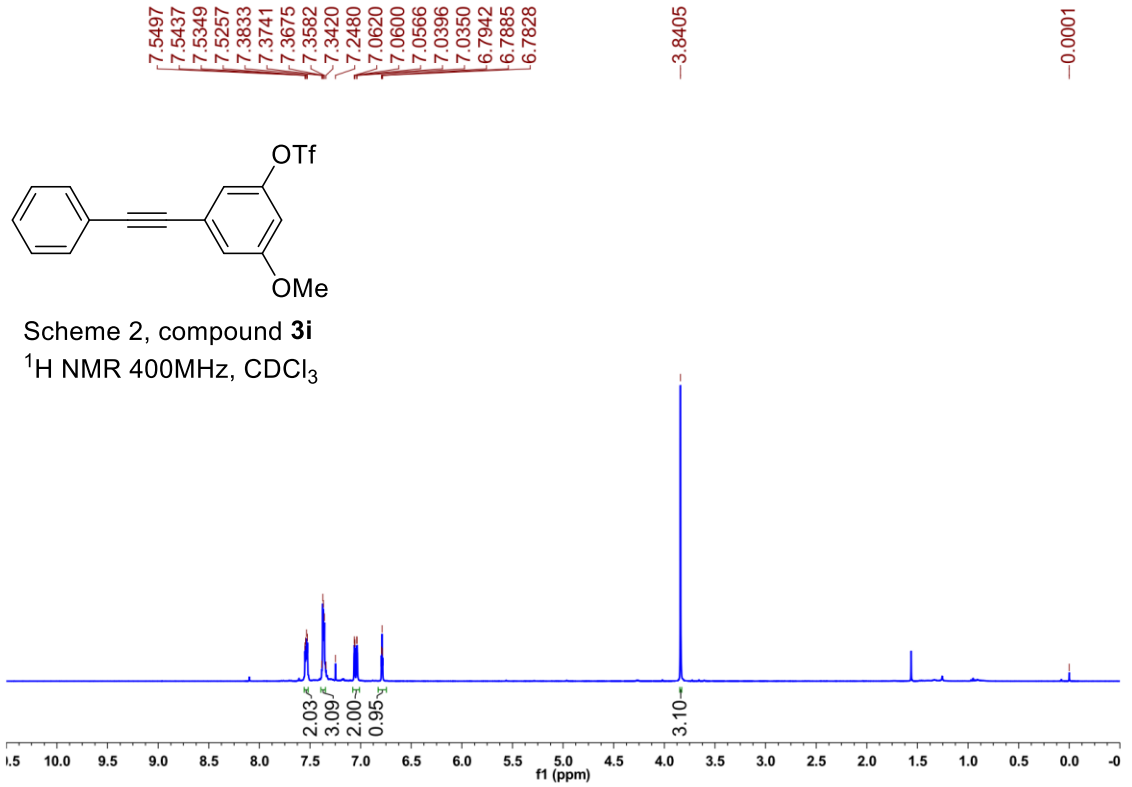
Scheme 2, compound **3h**

^{13}C NMR 100MHz, $CDCl_3$



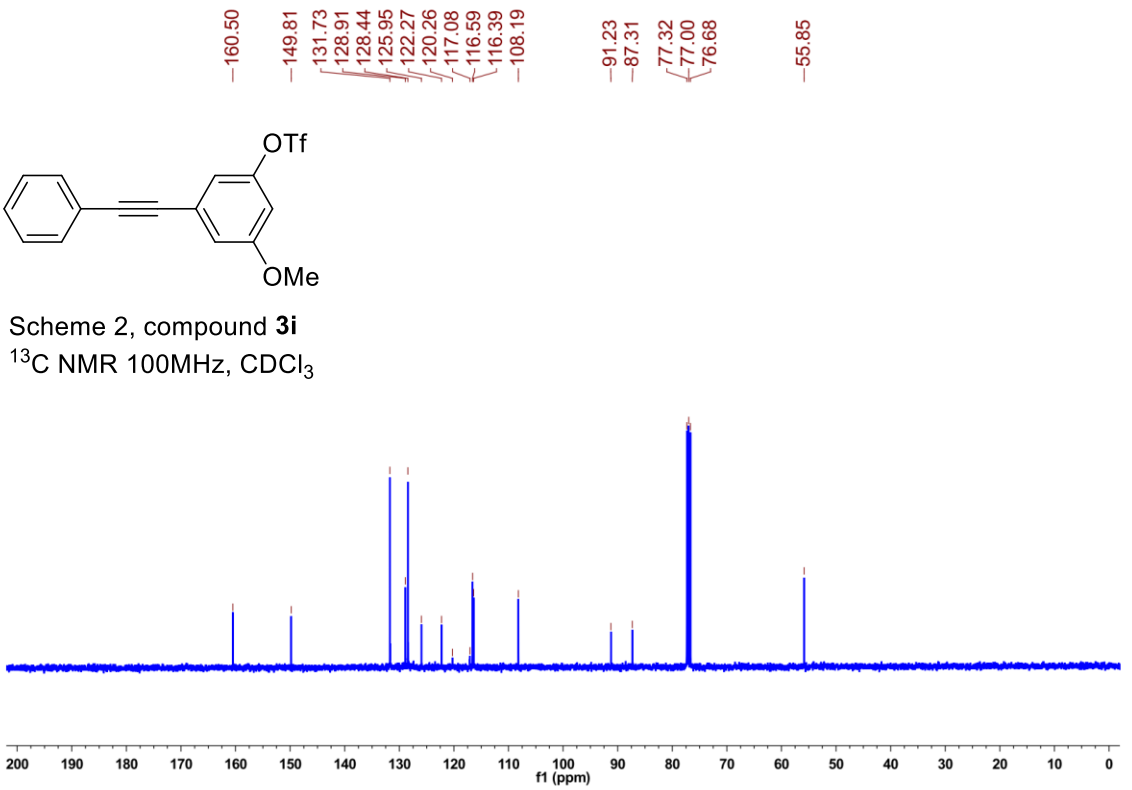
Scheme 2, compound **3h**

^{19}F NMR 470MHz, $CDCl_3$



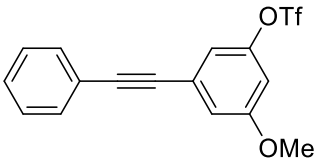
Scheme 2, compound **3i**

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



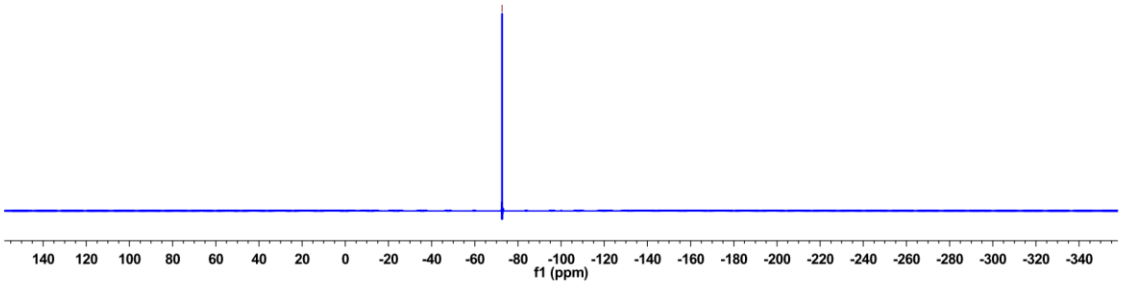
Scheme 2, compound **3i**

^{13}C NMR 100MHz, $CDCl_3$



Scheme 2, compound **3i**

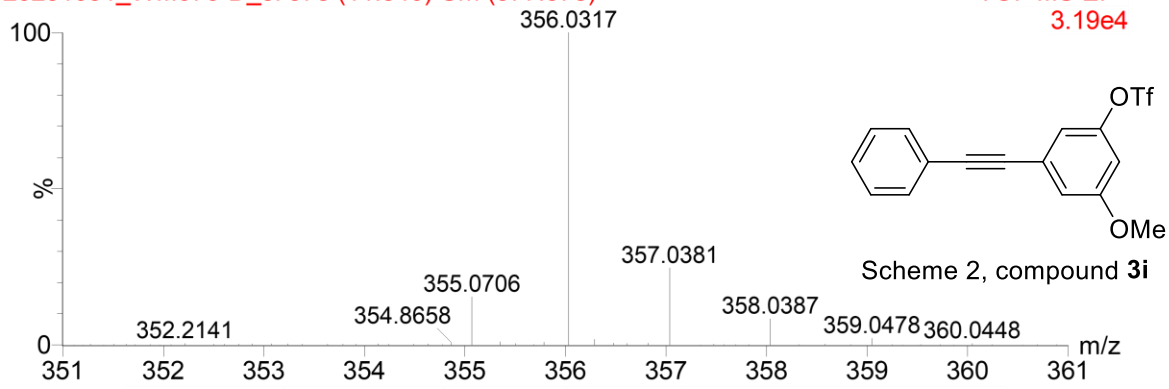
^{19}F NMR 470MHz, $CDCl_3$



20231031_WM676-D_3i

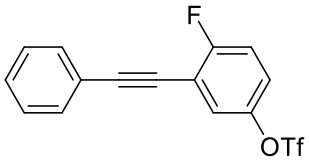
20231031_WM676-D_3i 578 (11.540) Cm (577:578)

TOF MS EI+
3.19e4



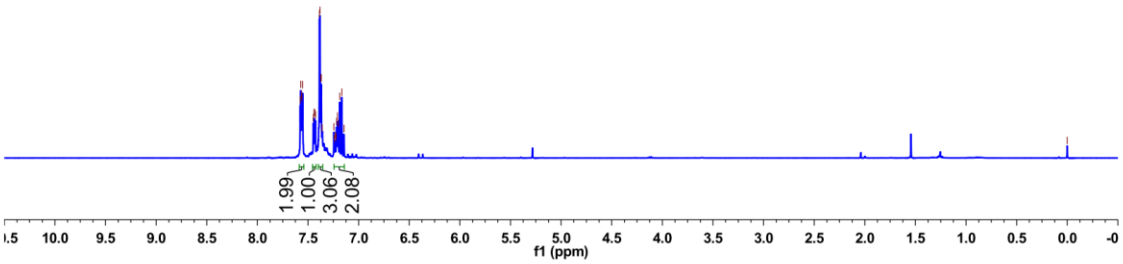
Scheme 2, compound **3i**

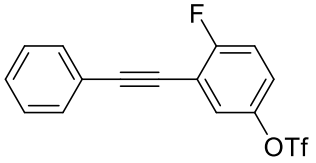
Mass	Calc. Mass	mDa	PPM	Formula
356.0317	356.0325	0.77	2.15	C16 H11 F3 O4 S



Scheme 2, compound **3j**

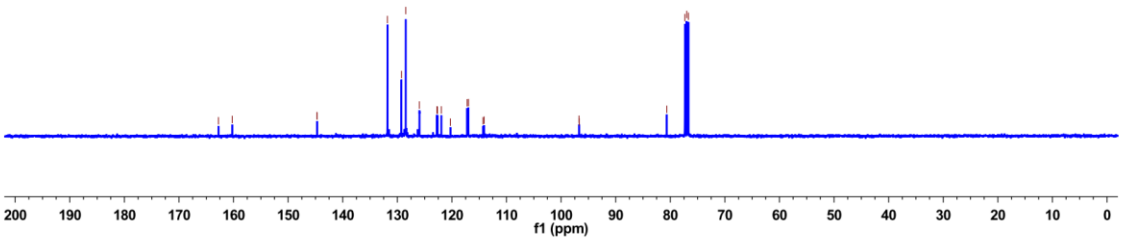
^{1}H NMR 400MHz, $CDCl_3$

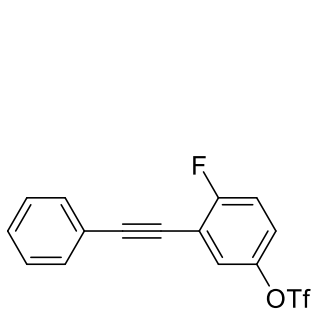




Scheme 2, compound **3j**

^{13}C NMR 100MHz, $CDCl_3$





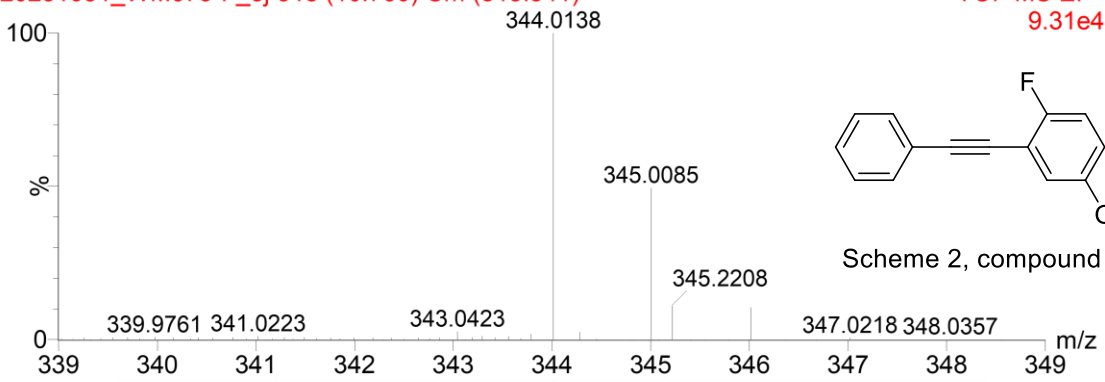
Scheme 2, compound **3j**

^{19}F NMR 470MHz, $CDCl_3$

20231031_WM673-F_3j

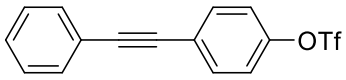
20231031_WM673-F_3j 518 (10.760) Cm (515:541)

TOF MS EI+
9.31e4



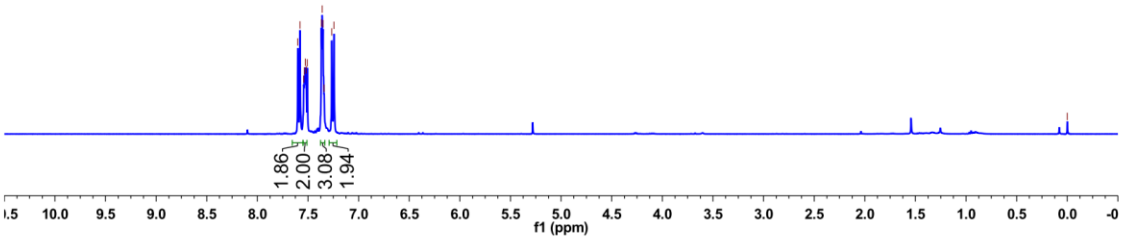
Scheme 2, compound **3j**

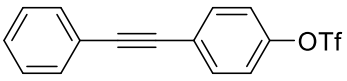
Mass	Calc. Mass	mDa	PPM	Formula
344.0138	344.0125	-1.32	-3.84	C15 H8 F4 O3 S



Scheme 2, compound **3k**

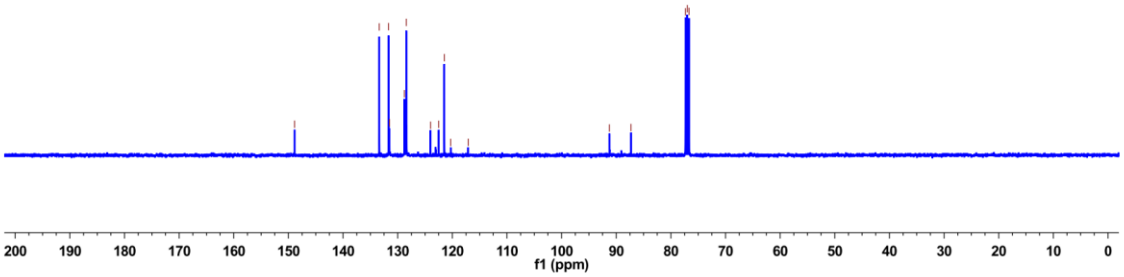
^{1}H NMR 400MHz, $CDCl_3$

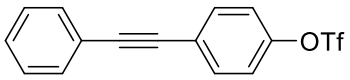




Scheme 2, compound **3k**

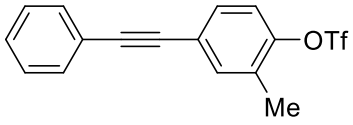
^{13}C NMR 100MHz, $CDCl_3$





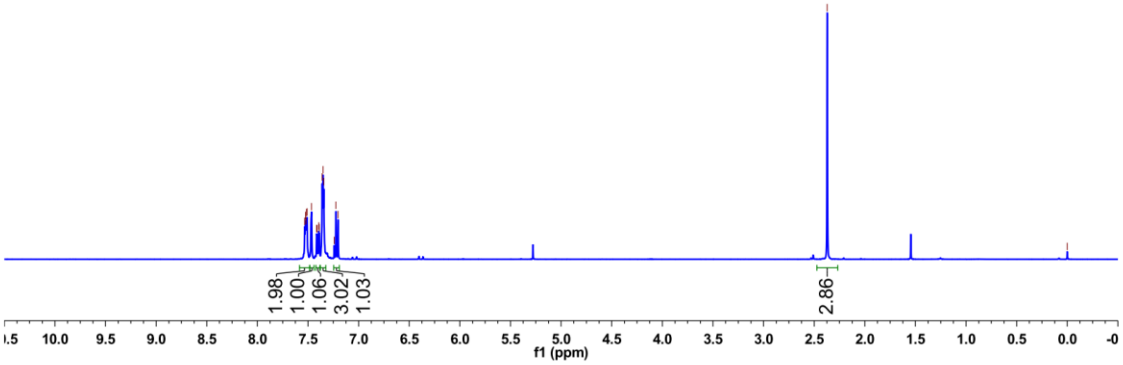
Scheme 2, compound **3k**

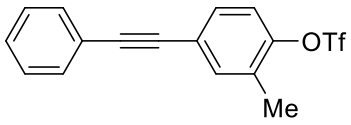
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3l**

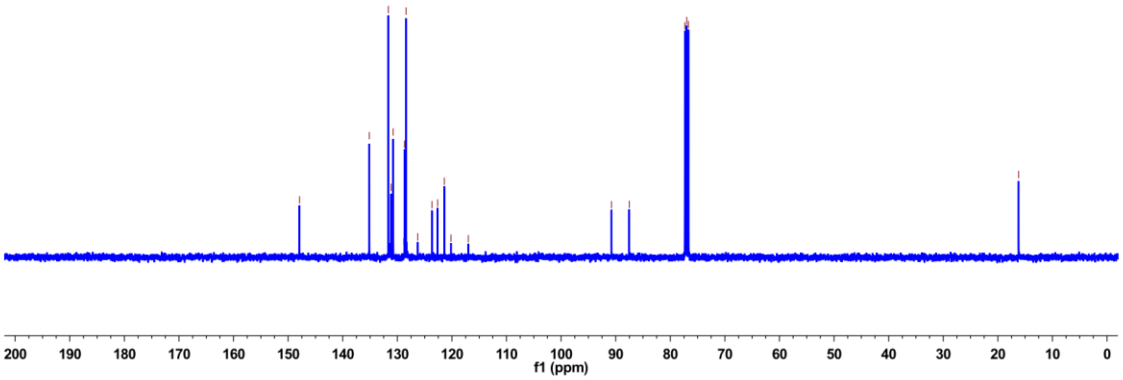
^{1}H NMR 400MHz, $CDCl_3$

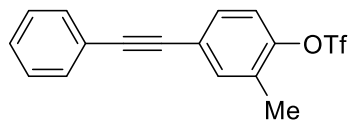




Scheme 2, compound **3l**

^{13}C NMR 100MHz, $CDCl_3$



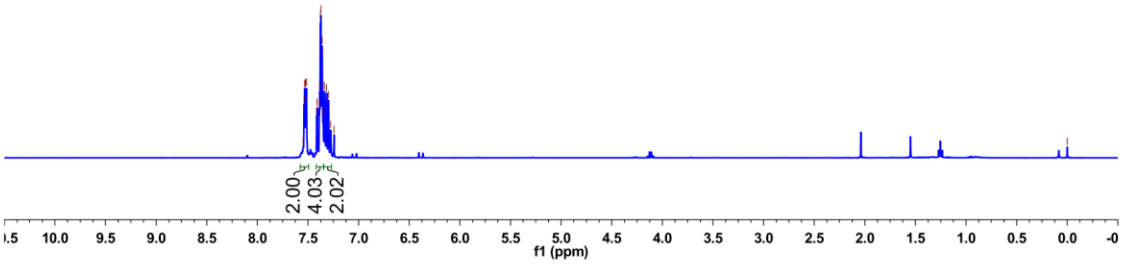


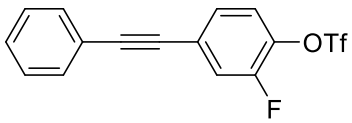
Scheme 2, compound **3l**

^{19}F NMR 470MHz, $CDCl_3$

Scheme 2, compound **3m**

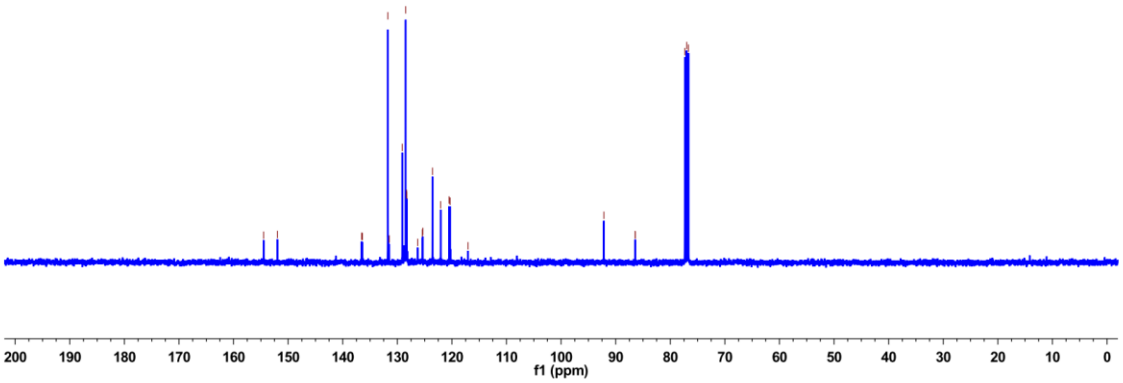
^{1}H NMR 400MHz, $CDCl_3$

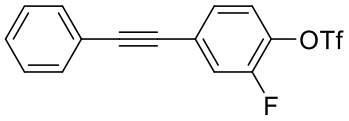




Scheme 2, compound **3m**

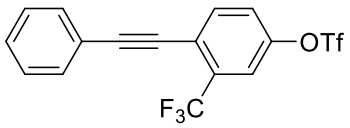
^{13}C NMR 100MHz, $CDCl_3$





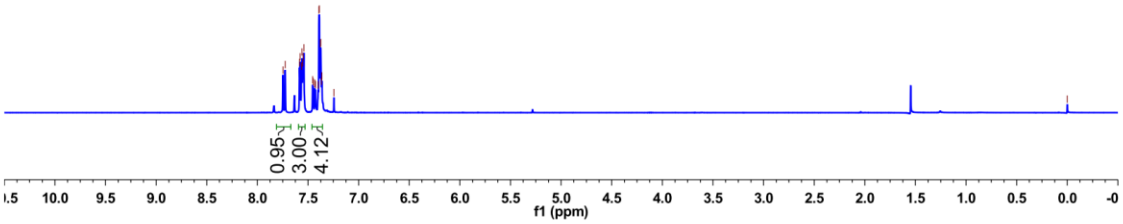
Scheme 2, compound **3m**

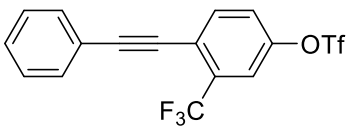
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3n**

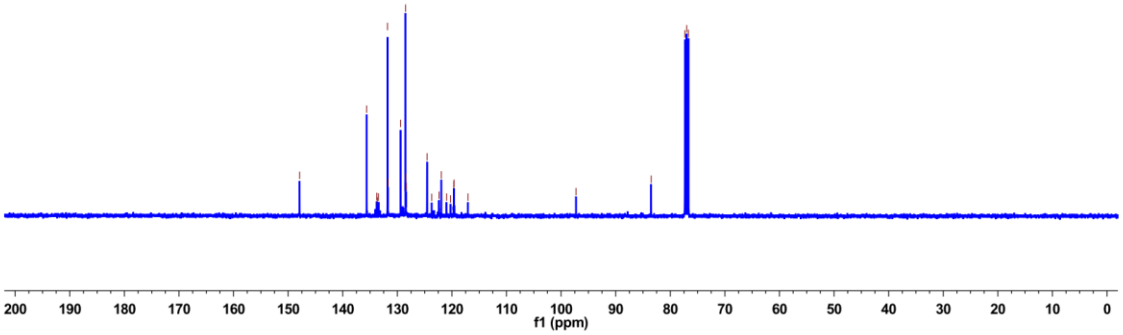
^{1}H NMR 400MHz, $CDCl_3$

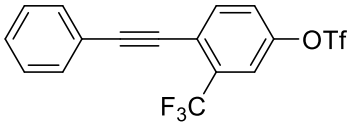




Scheme 2, compound **3n**

^{13}C NMR 100MHz, $CDCl_3$





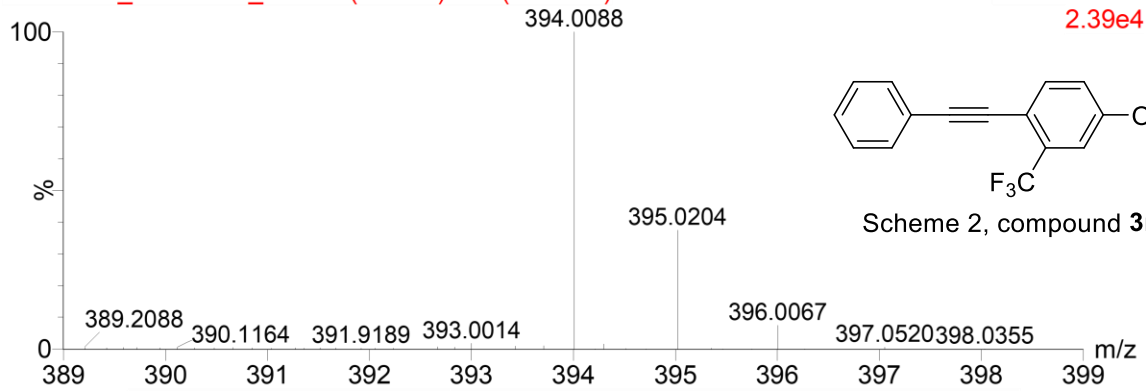
Scheme 2, compound **3n**

^{19}F NMR 470MHz, $CDCl_3$

20231031_WM675-E_3n

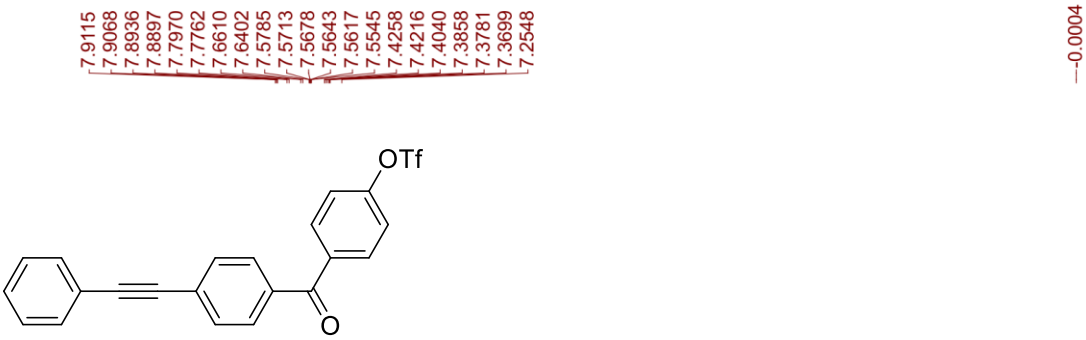
20231031_WM675-E_3n 468 (10.060) Cm (468:474)

TOF MS EI+
2.39e4



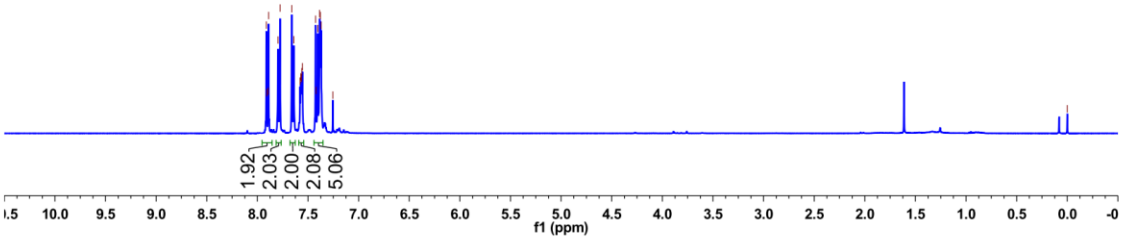
Scheme 2, compound **3n**

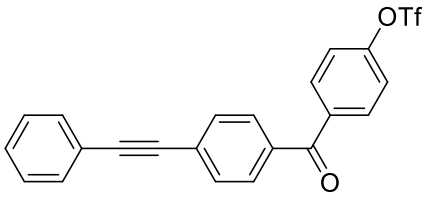
Mass	Calc. Mass	mDa	PPM	Formula
394.0088	394.0093	0.49	1.23	C16 H8 F6 O3 S



Scheme 2, compound **3o**

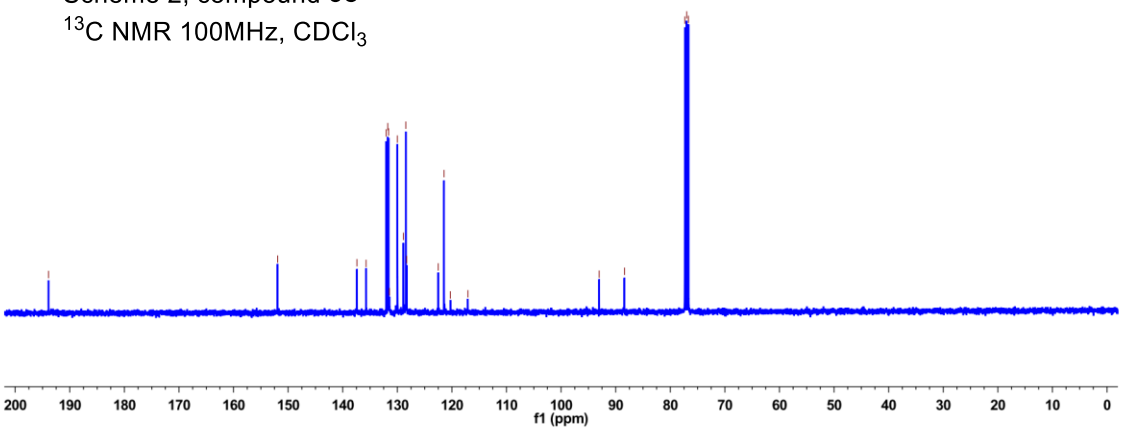
^{1}H NMR 400MHz, $CDCl_3$

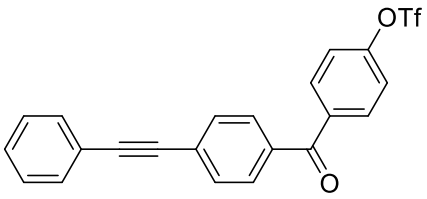




Scheme 2, compound **3o**

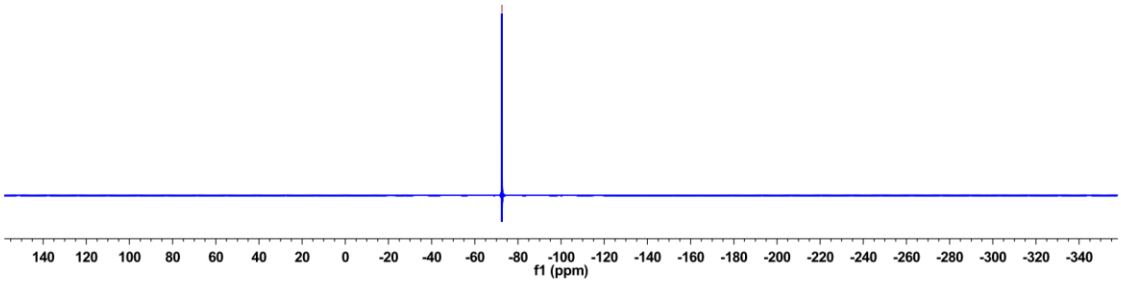
^{13}C NMR 100MHz, $CDCl_3$

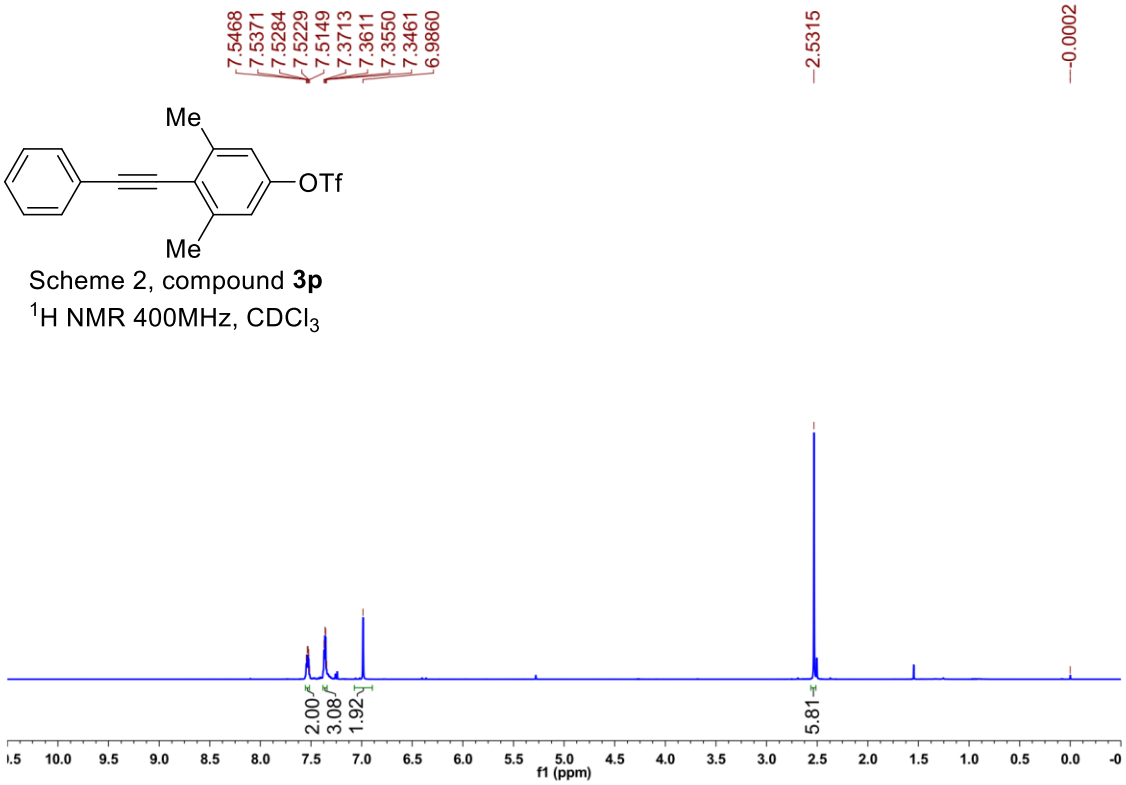




Scheme 2, compound **3o**

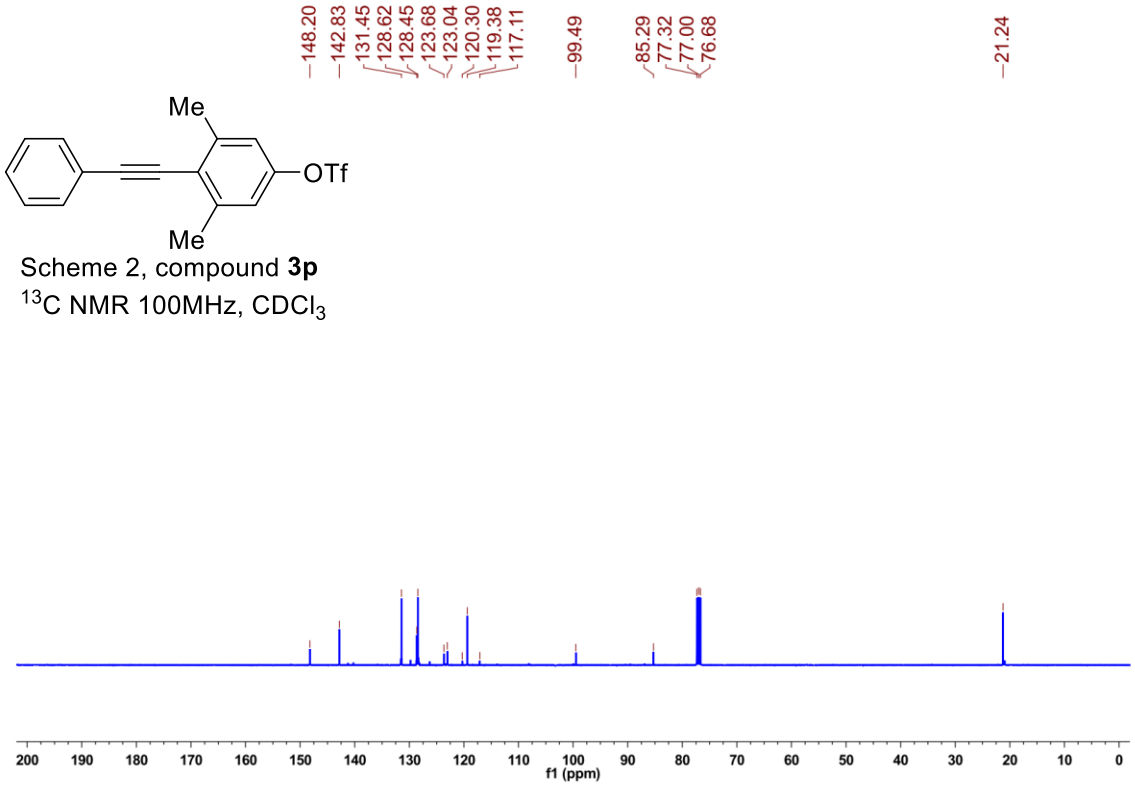
^{19}F NMR 470MHz, $CDCl_3$





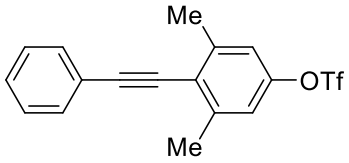
Scheme 2, compound **3p**

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



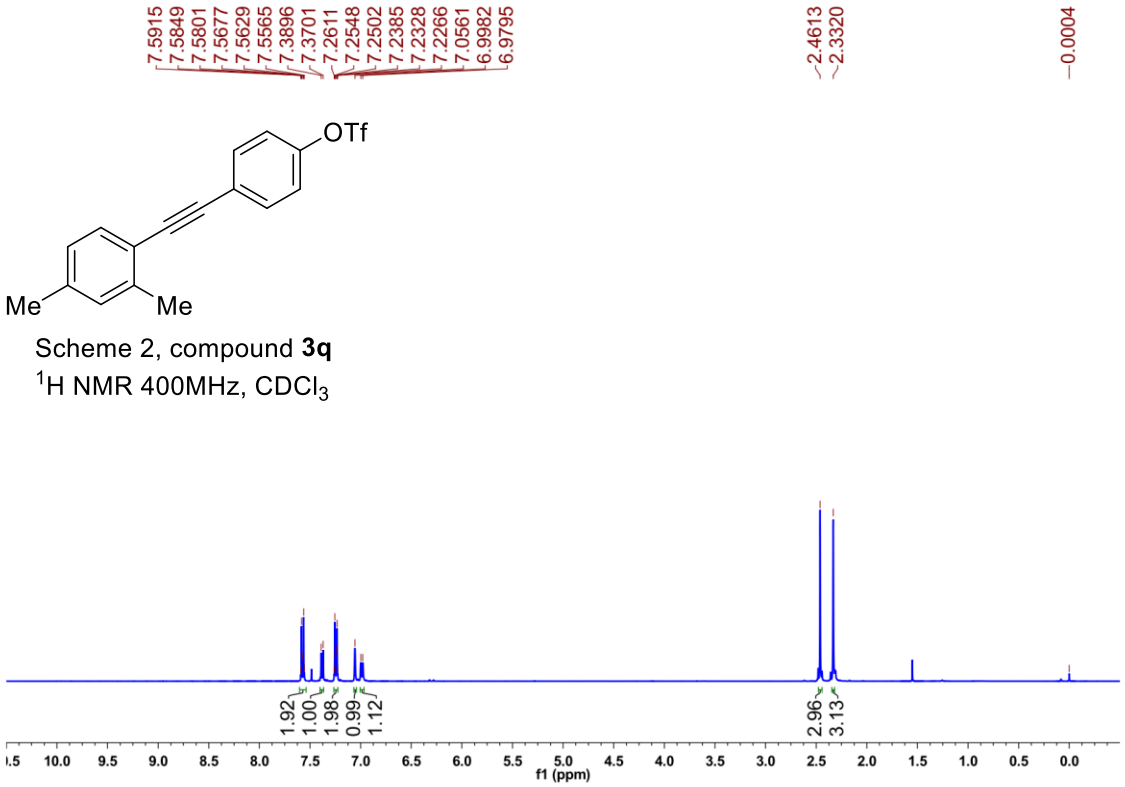
Scheme 2, compound **3p**

^{13}C NMR 100MHz, $CDCl_3$



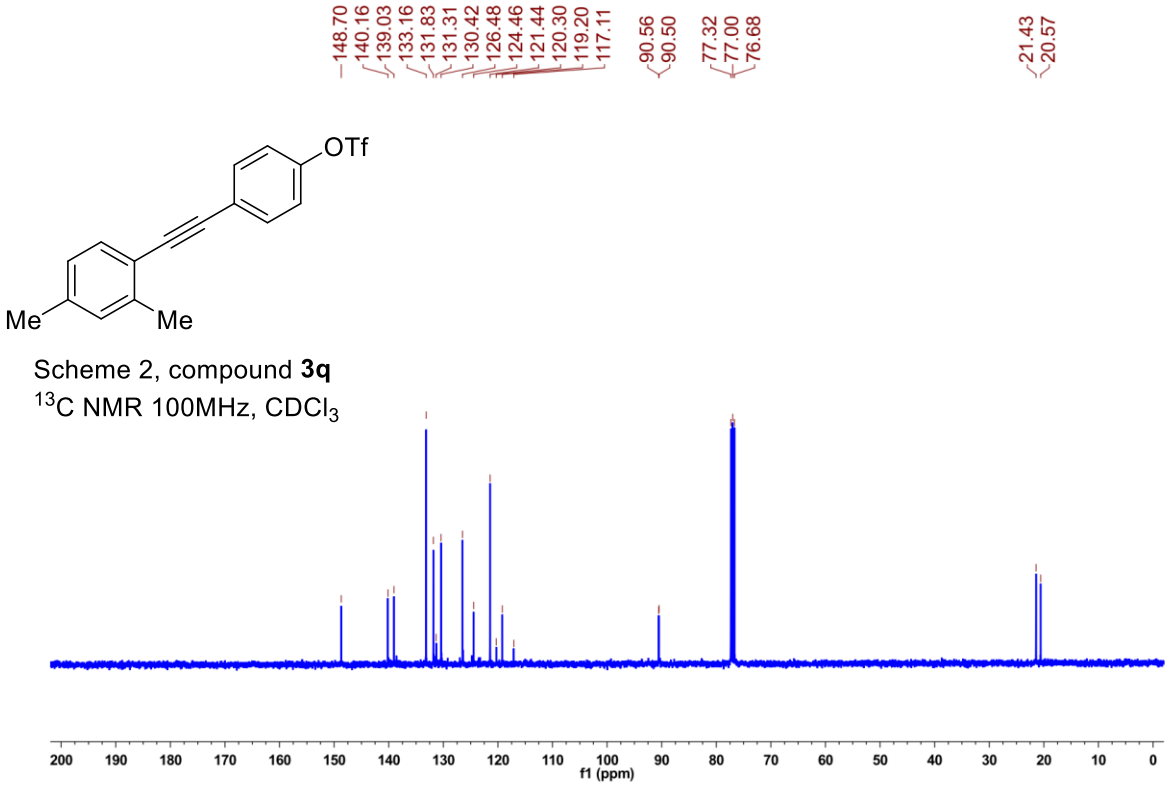
Scheme 2, compound **3p**

^{19}F NMR 470MHz, $CDCl_3$



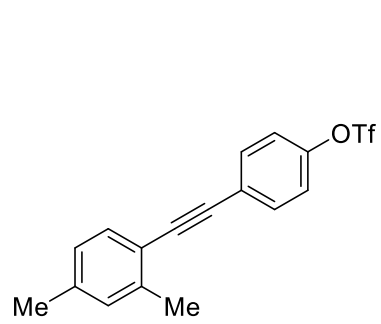
Scheme 2, compound **3q**

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



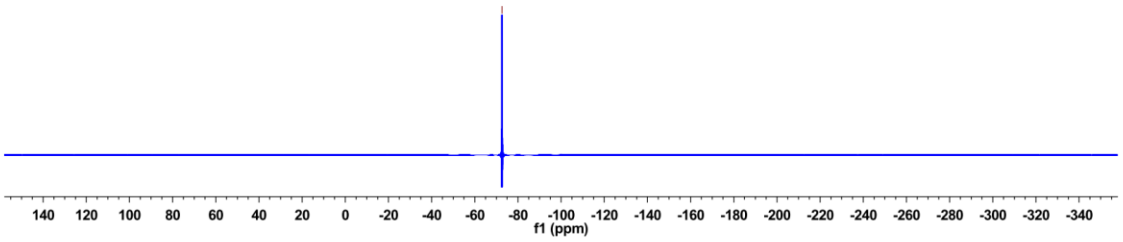
Scheme 2, compound **3q**

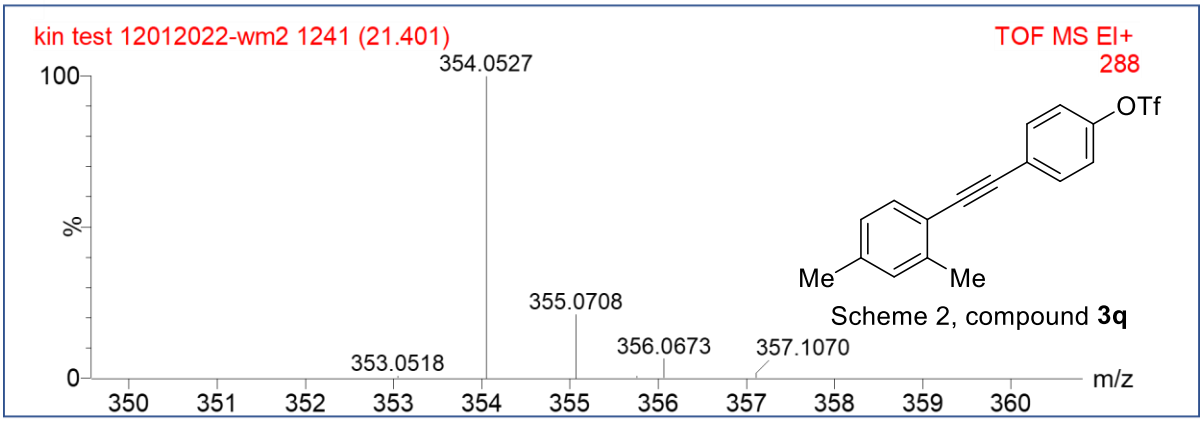
^{13}C NMR 100MHz, $CDCl_3$



Scheme 2, compound **3q**

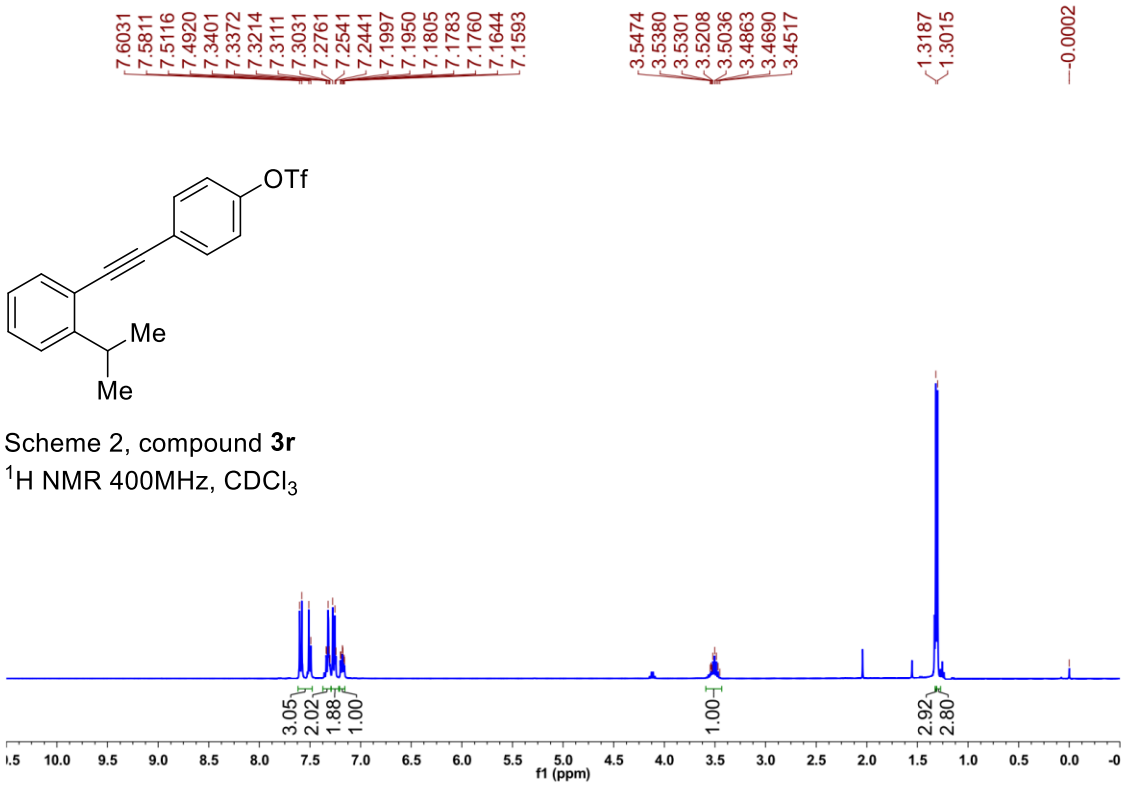
^{19}F NMR 470MHz, $CDCl_3$





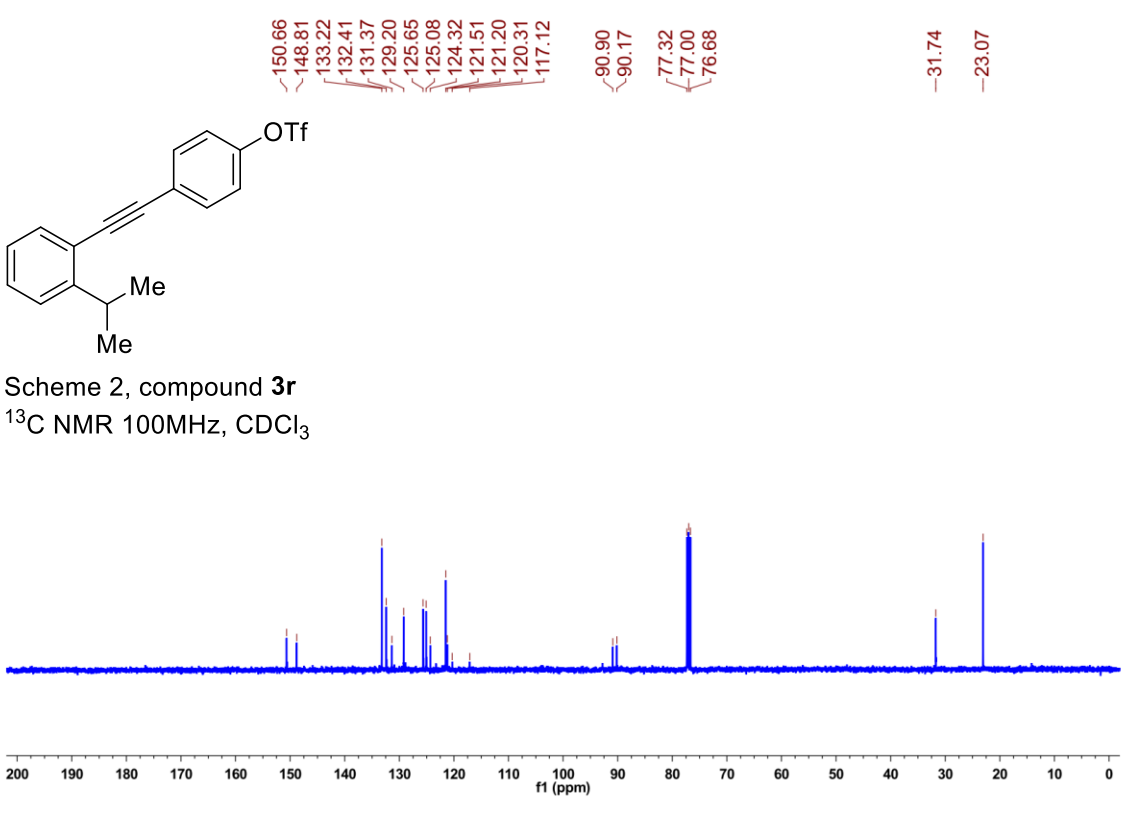
Scheme 2, compound **3q**

Mass	m/z (Calc)	Diff (mDa)	Diff (ppm)	Formula
354.0527	354.0532	0.5	1.42	C17 H13 F3 O3 S



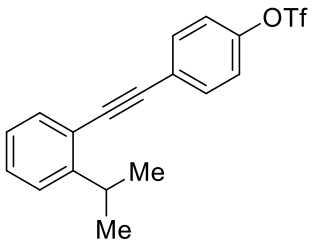
Scheme 2, compound **3r**

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



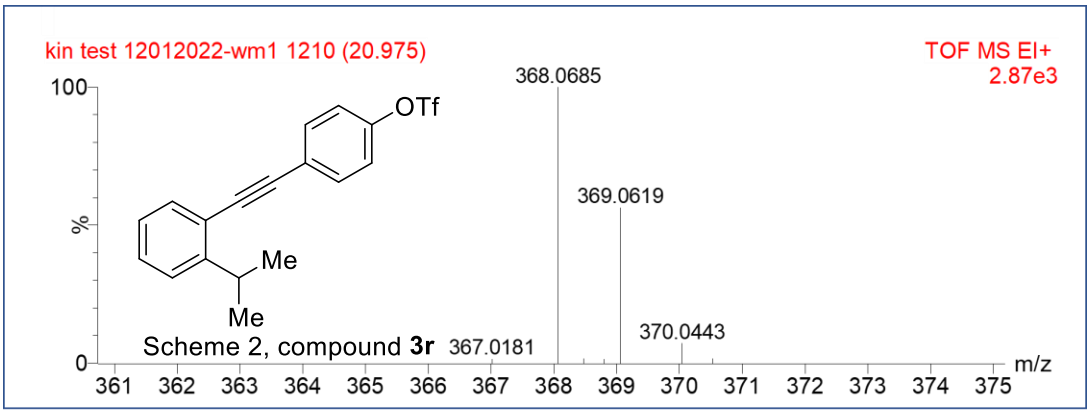
Scheme 2, compound **3r**

^{13}C NMR 100MHz, $CDCl_3$



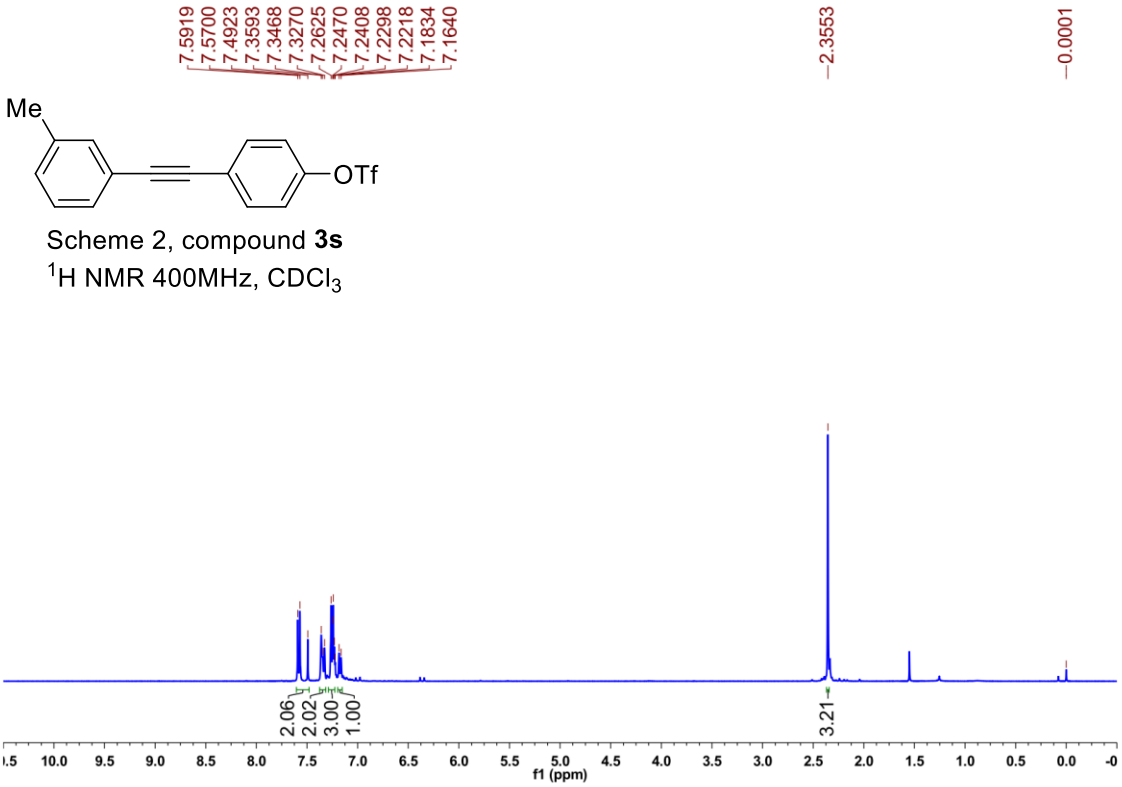
Scheme 2, compound **3r**

^{19}F NMR 470MHz, $CDCl_3$



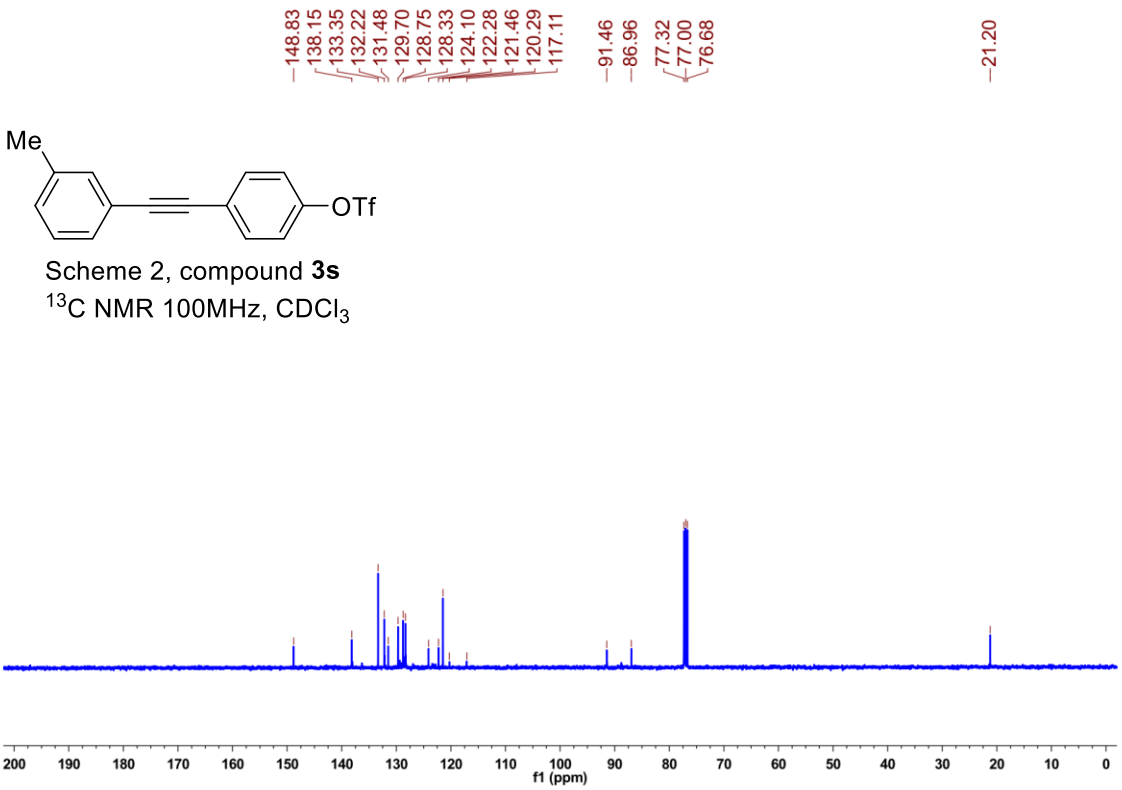
Scheme 2, compound **3r**

Mass	m/z (Calc)	Diff (mDa)	Diff (ppm)	Formula
368.0685	368.0689	0.35	0.95	C18 H15 F3 O3 S



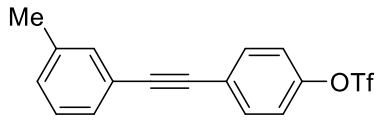
Scheme 2, compound **3s**

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



Scheme 2, compound **3s**

^{13}C NMR 100MHz, $CDCl_3$



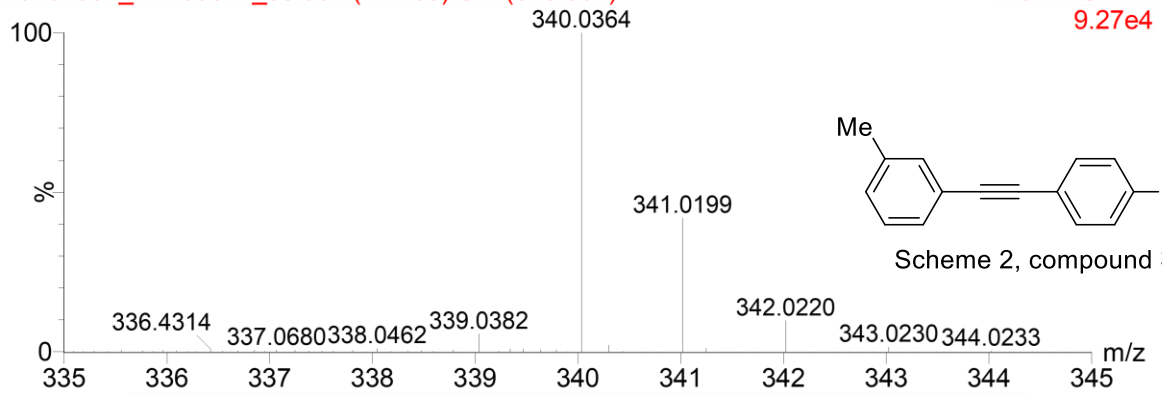
Scheme 2, compound **3s**

^{19}F NMR 470MHz, $CDCl_3$

20231031_WM690-D_3s

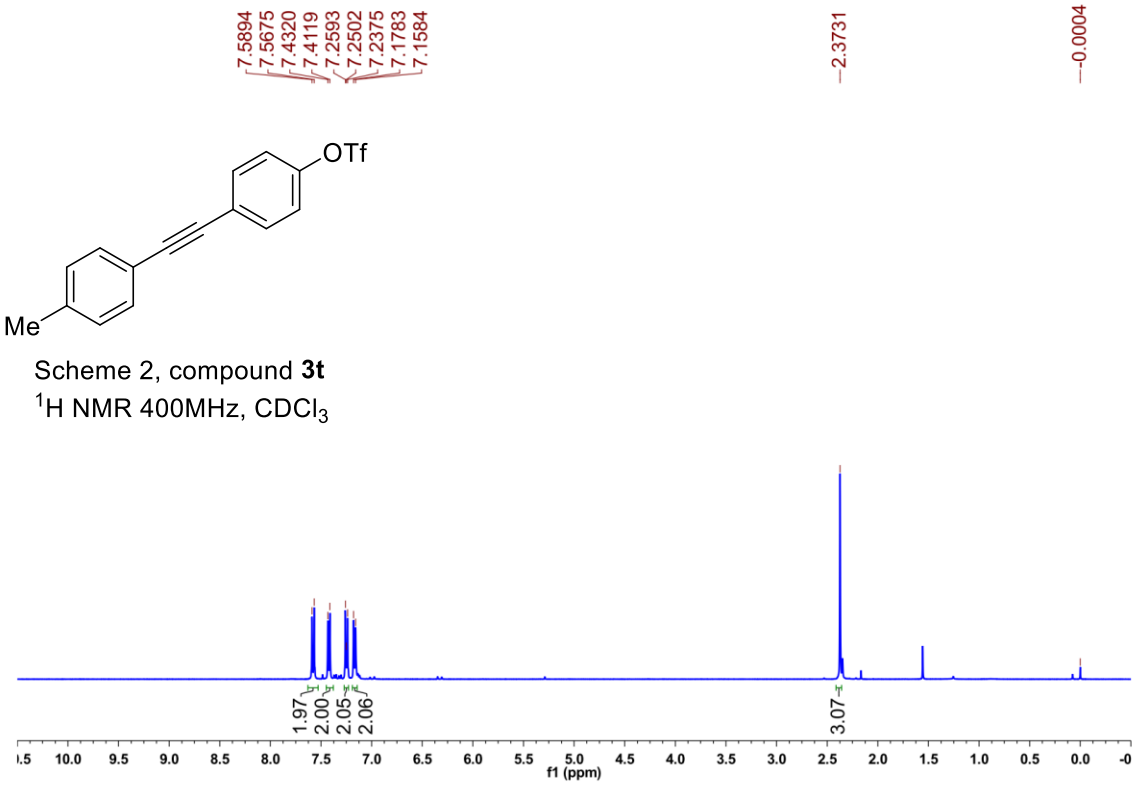
20231031_WM690-D_3s 551 (11.200) Cm (548:561)

TOF MS EI+
9.27e4



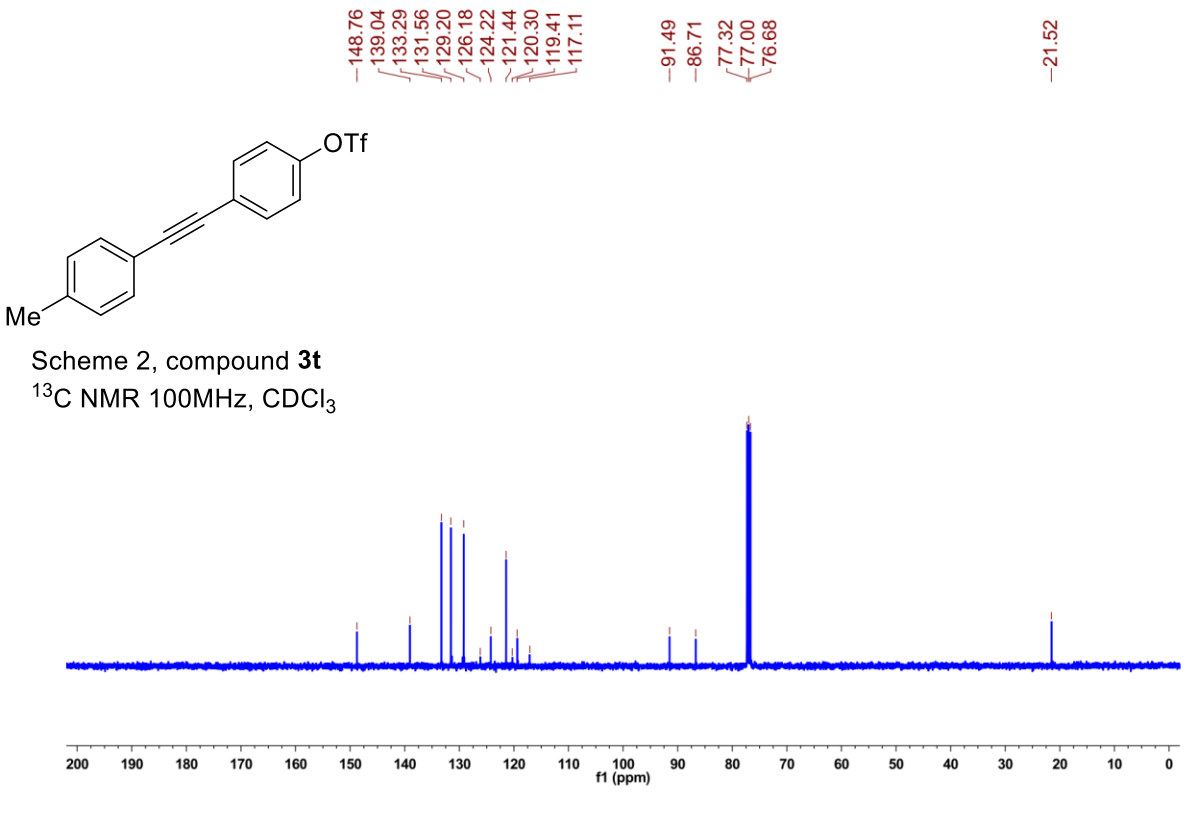
Scheme 2, compound **3s**

Mass	Calc. Mass	mDa	PPM	Formula
340.0364	340.0376	1.15	3.38	C16 H11 F3 O3 S



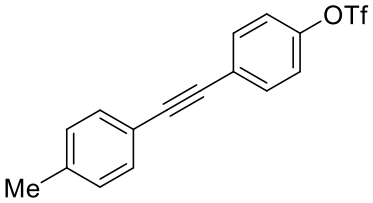
Scheme 2, compound **3t**

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



Scheme 2, compound **3t**

^{13}C NMR 100MHz, $CDCl_3$

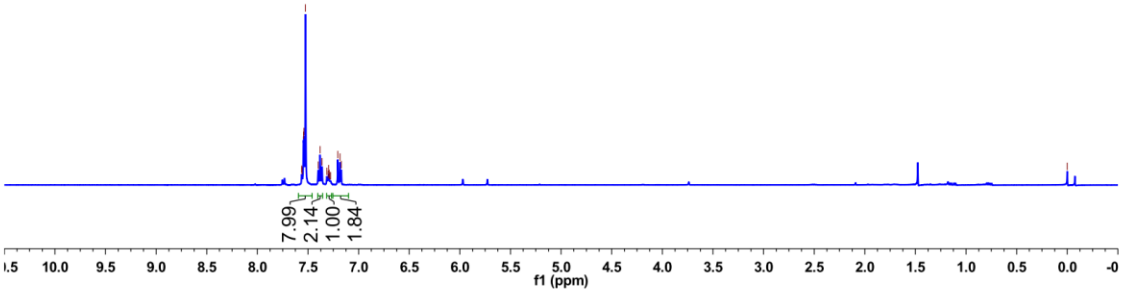


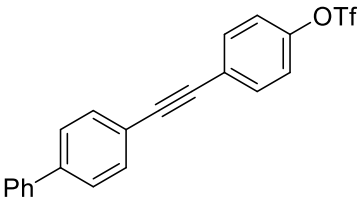
Scheme 2, compound **3t**

^{19}F NMR 470MHz, $CDCl_3$

Scheme 2, compound **3u**

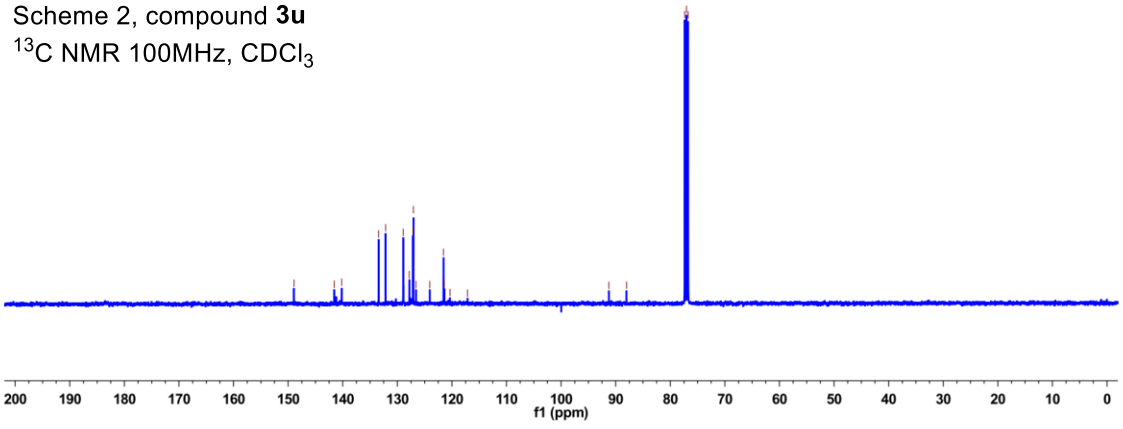
^{1}H NMR 400MHz, $CDCl_3$

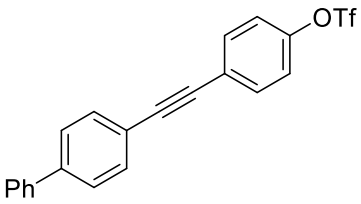




Scheme 2, compound **3u**

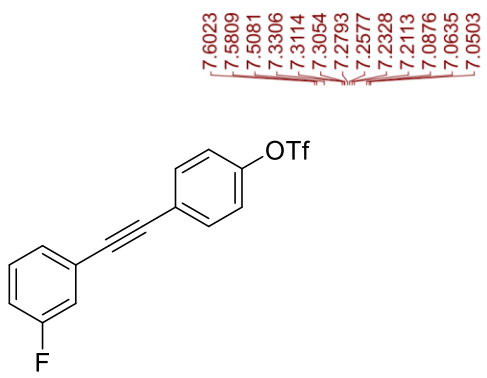
^{13}C NMR 100MHz, $CDCl_3$





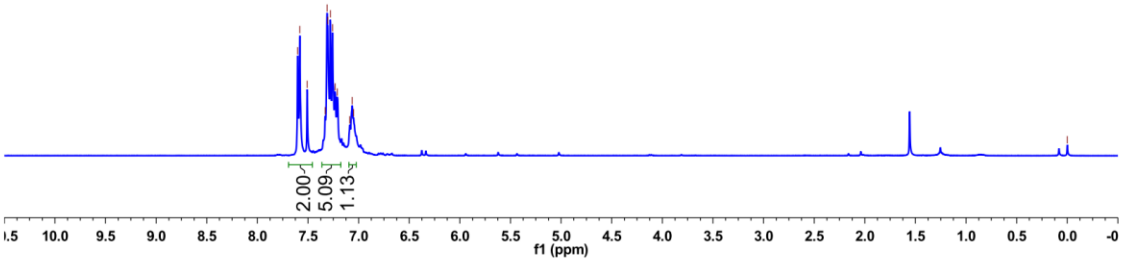
Scheme 2, compound **3u**

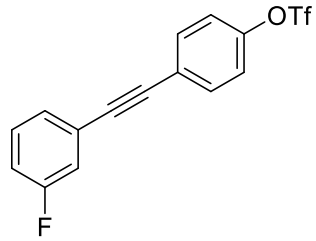
^{19}F NMR 470MHz, $CDCl_3$



Scheme 2, compound **3v**

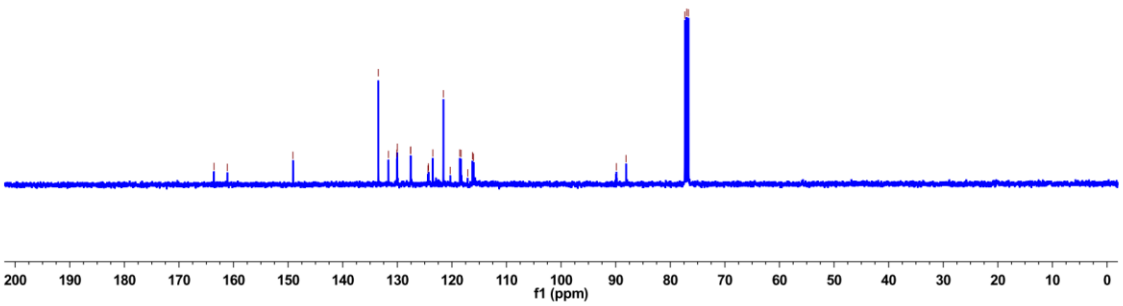
^{1}H NMR 400MHz, $CDCl_3$

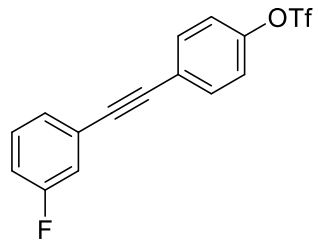




Scheme 2, compound **3v**

^{13}C NMR 100MHz, $CDCl_3$



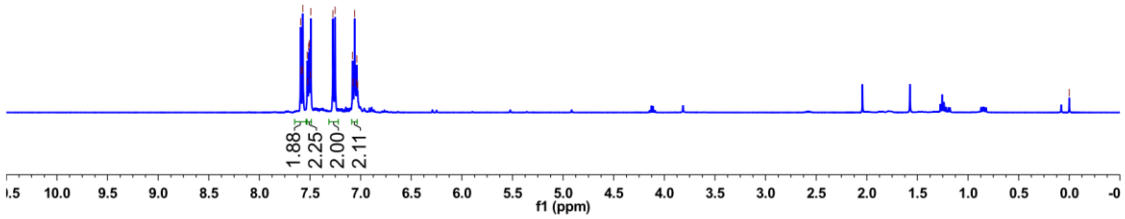


Scheme 2, compound **3v**

^{19}F NMR 470MHz, $CDCl_3$

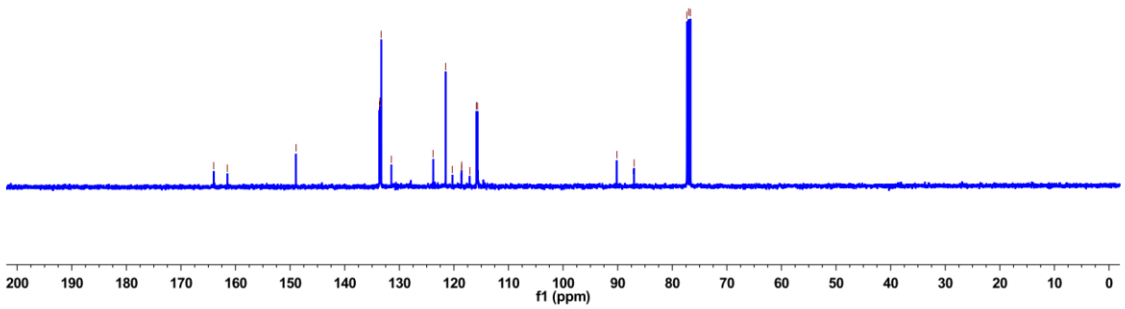
Scheme 2, compound **3w**

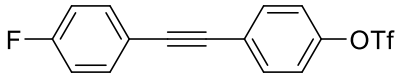
^{1}H NMR 400MHz, $CDCl_3$



Scheme 2, compound **3w**

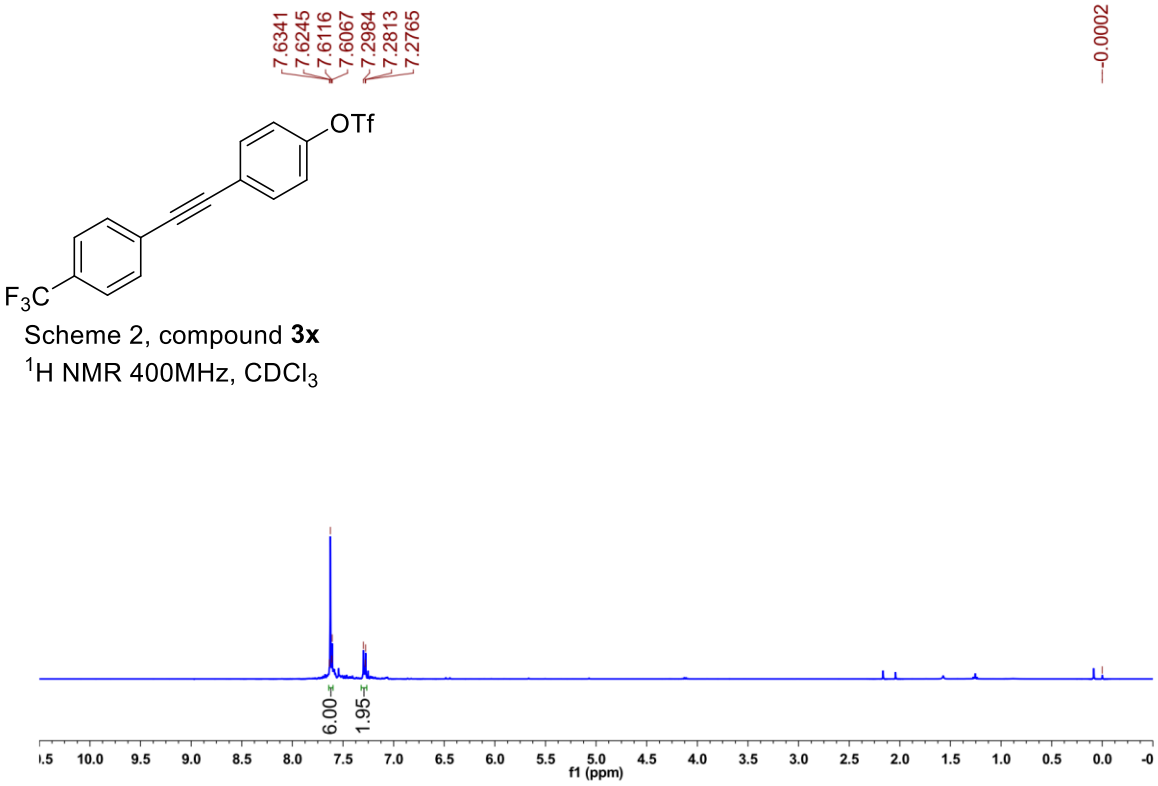
^{13}C NMR 100MHz, $CDCl_3$





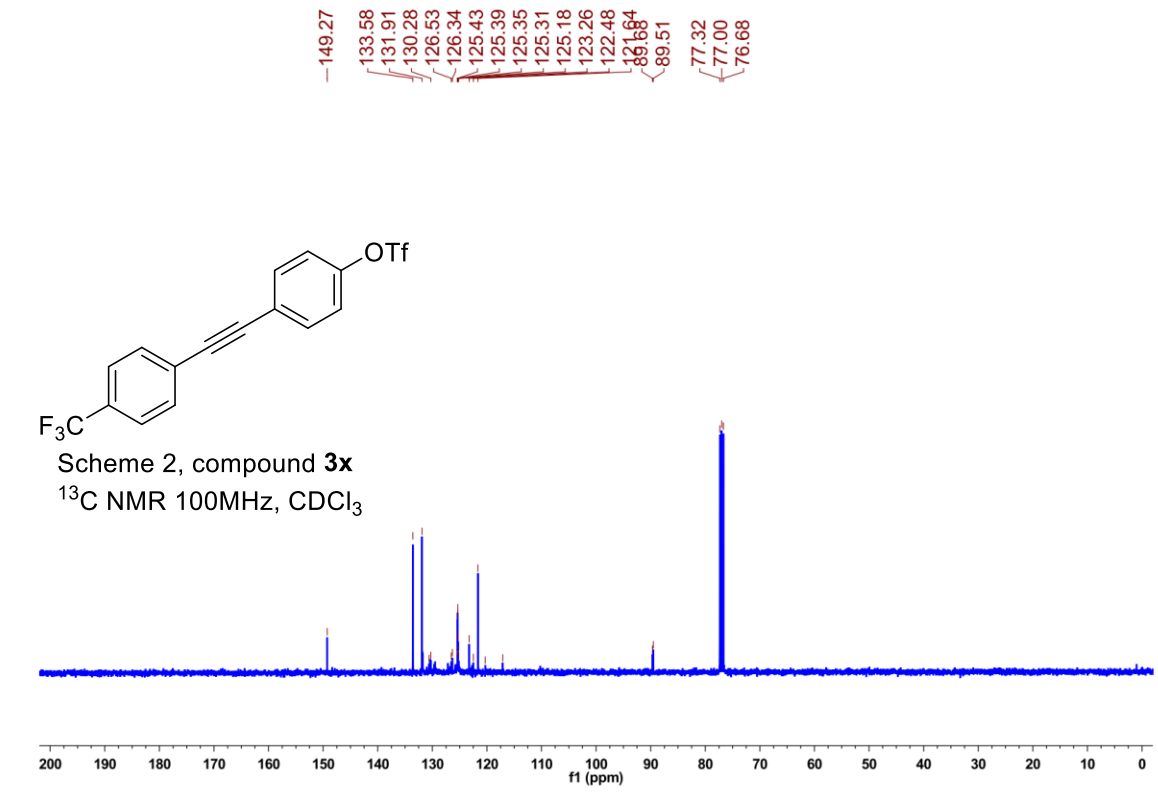
Scheme 2, compound **3w**

^{19}F NMR 470MHz, $CDCl_3$



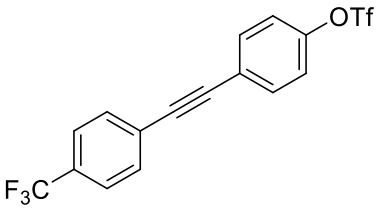
Scheme 2, compound **3x**

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



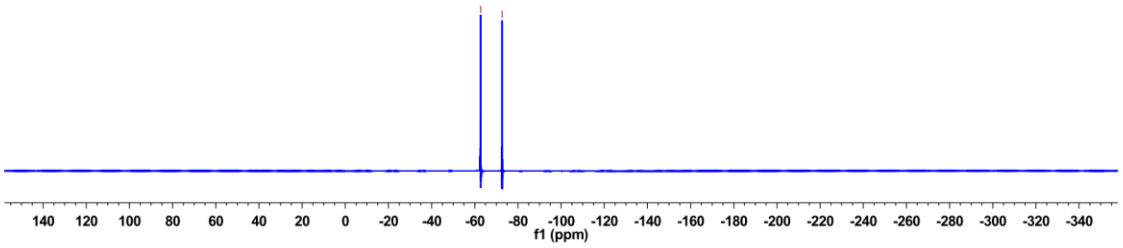
Scheme 2, compound **3x**

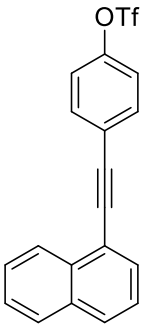
^{13}C NMR 100MHz, $CDCl_3$



Scheme 2, compound **3x**

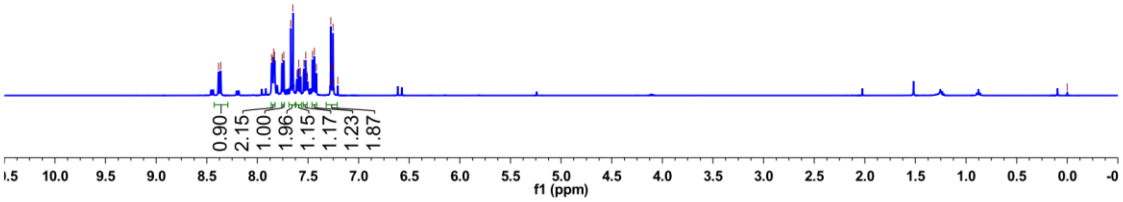
^{19}F NMR 470MHz, $CDCl_3$

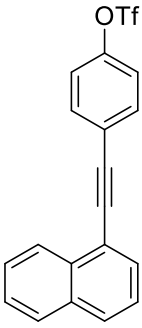




Scheme 2, compound **3y**

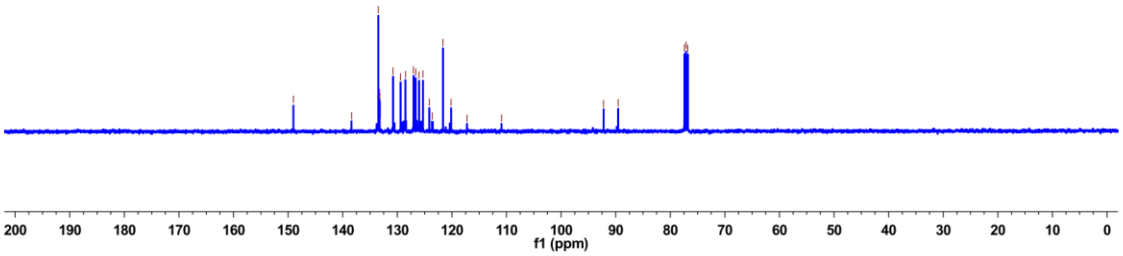
^{1}H NMR 400MHz, $CDCl_3$

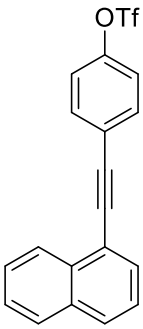




Scheme 2, compound **3y**

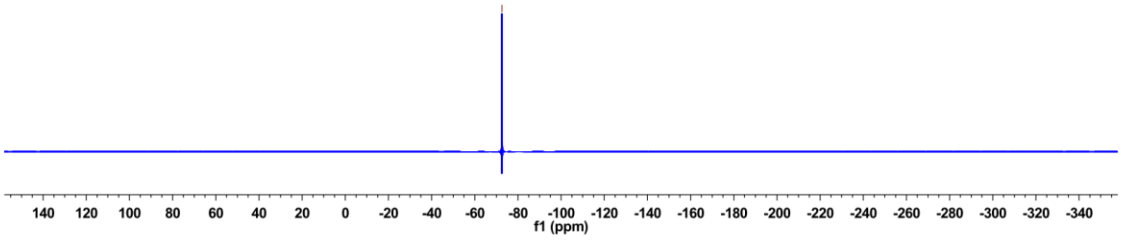
^{13}C NMR 100MHz, $CDCl_3$

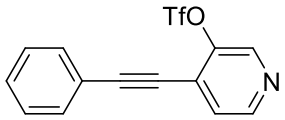




Scheme 2, compound **3y**

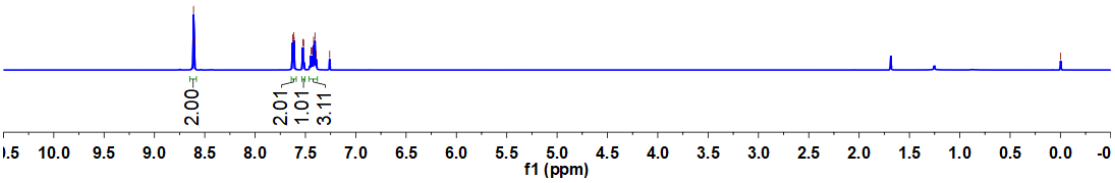
^{19}F NMR 470MHz, $CDCl_3$

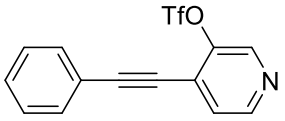




Scheme 2, compound **3z**

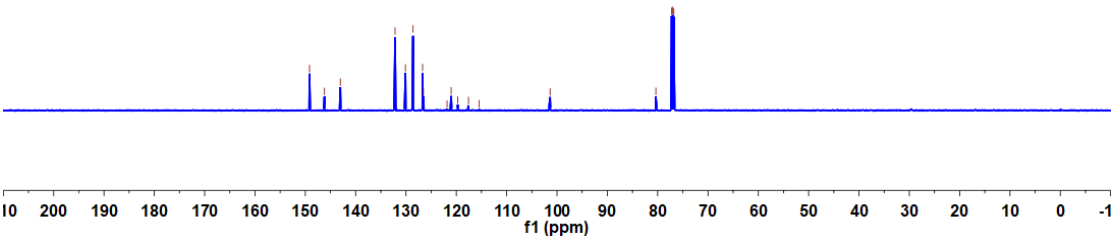
^{1}H NMR 600MHz, $CDCl_3$

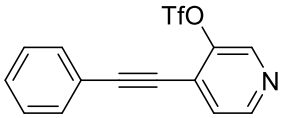




Scheme 2, compound **3z**

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





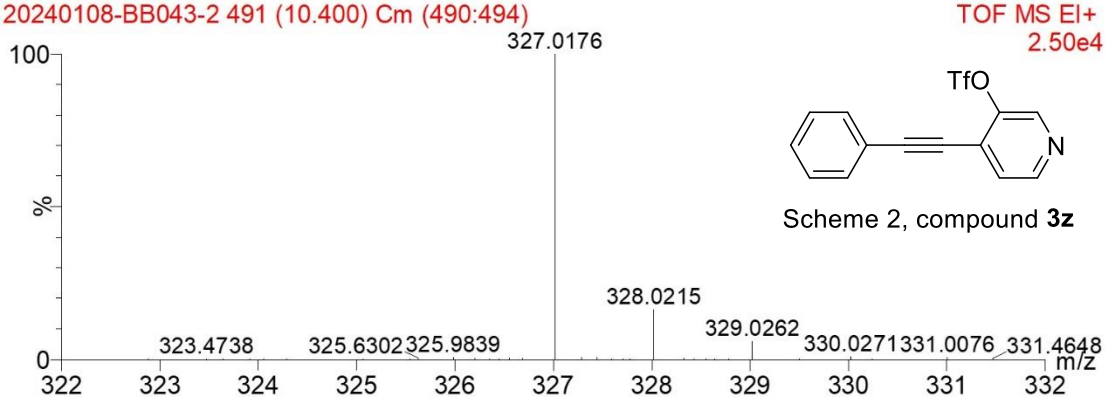
Scheme 2, compound **3z**

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

20240108-BB043-2

20240108-BB043-2 491 (10.400) Cm (490:494)

TOF MS EI+
2.50e4

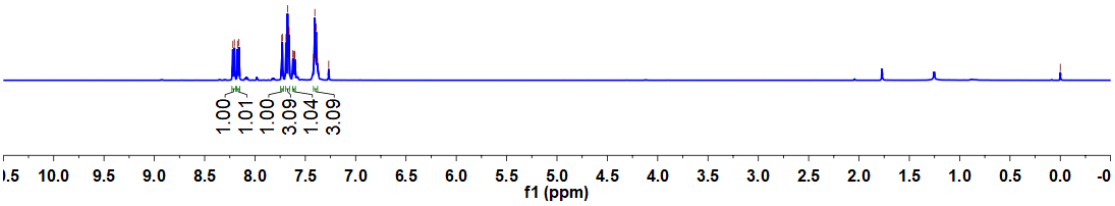


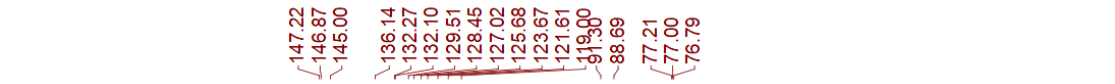
Scheme 2, compound **3z**

Mass	Calc. Mass	mDa	PPM	Formula
327.0176	327.0171	-0.45	-1.38	C14 H8 F3 N O3 S

Scheme 2, compound **3aa**

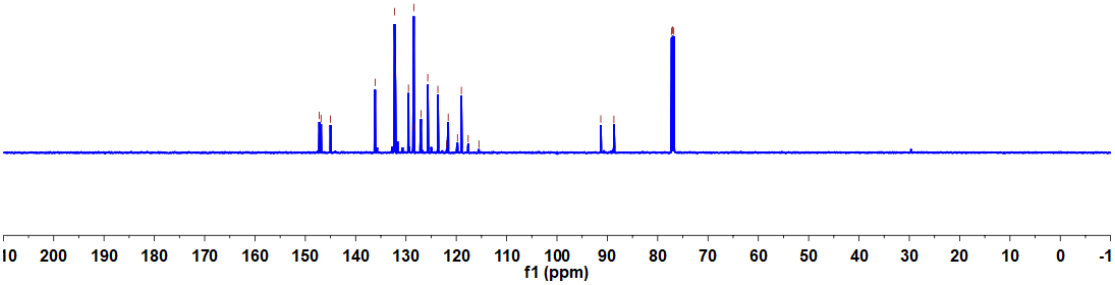
^{1}H NMR 600MHz, $CDCl_3$

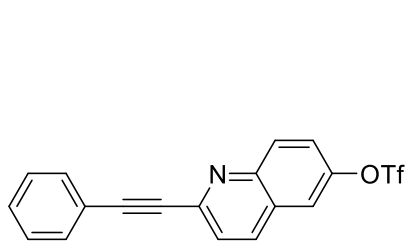




Scheme 2, compound **3aa**

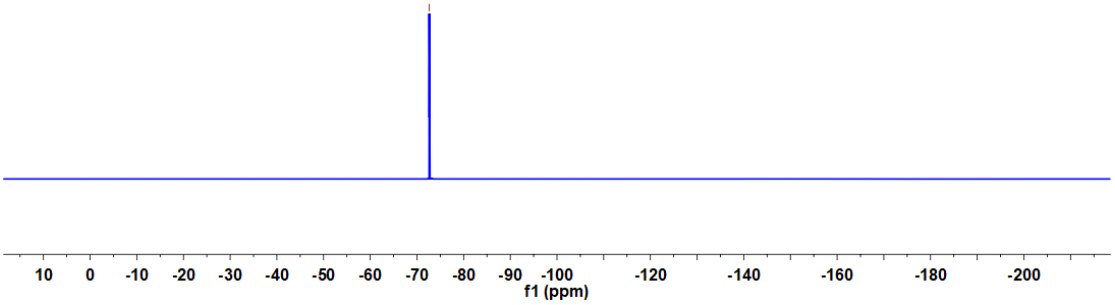
^{13}C NMR 151MHz, $CDCl_3$





Scheme 2, compound **3aa**

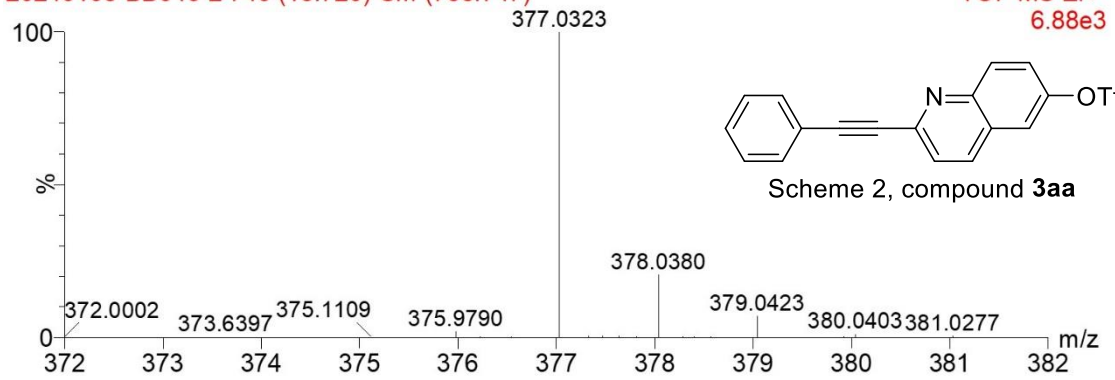
^{19}F NMR 565MHz, $CDCl_3$



20240108-BB046-2

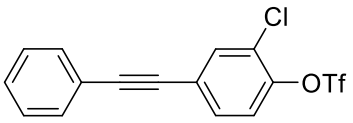
20240108-BB046-2 740 (13.720) Cm (738:747)

TOF MS EI+
6.88e3

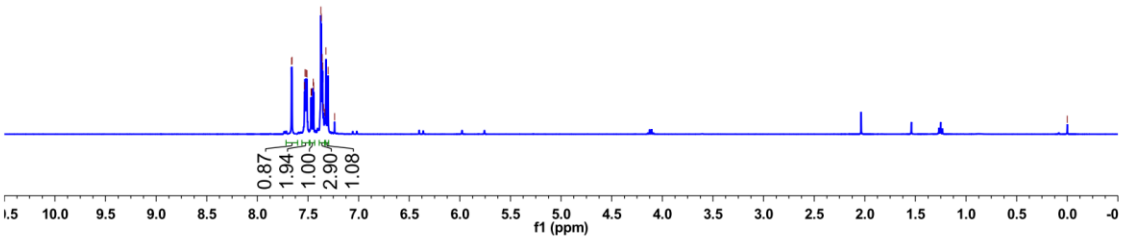


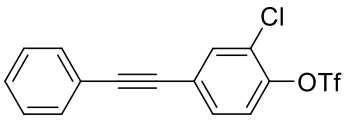
Scheme 2, compound **3aa**

Mass	Calc. Mass	mDa	PPM	Formula
377.0323	377.0328	0.50	1.33	C18 H10 F3 N O3 S

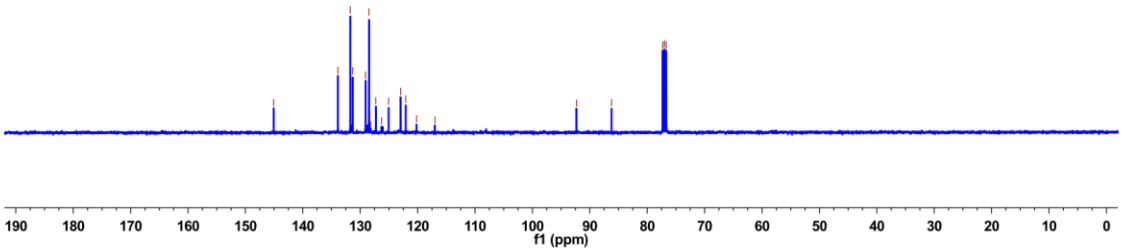


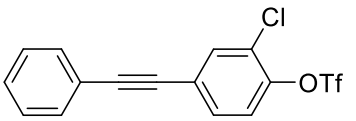
Scheme 3, compound **8a**
^{1}H NMR 400MHz, $CDCl_3$





Scheme 3, compound **8a**
^{13}C NMR 100MHz, $CDCl_3$





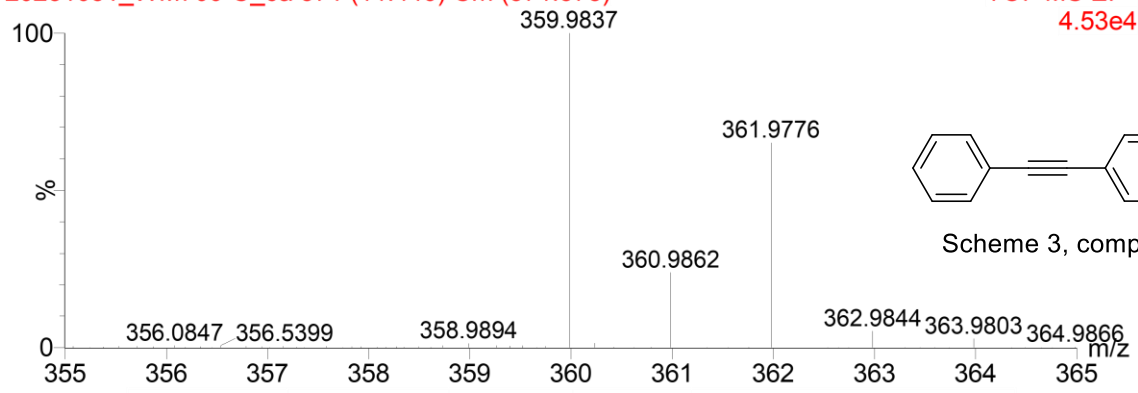
Scheme 3, compound **8a**

^{19}F NMR 470MHz, $CDCl_3$

20231031_WM700-C_6a

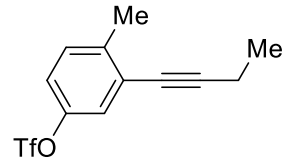
20231031_WM700-C_6a 571 (11.446) Cm (571:578)

TOF MS EI+
4.53e4



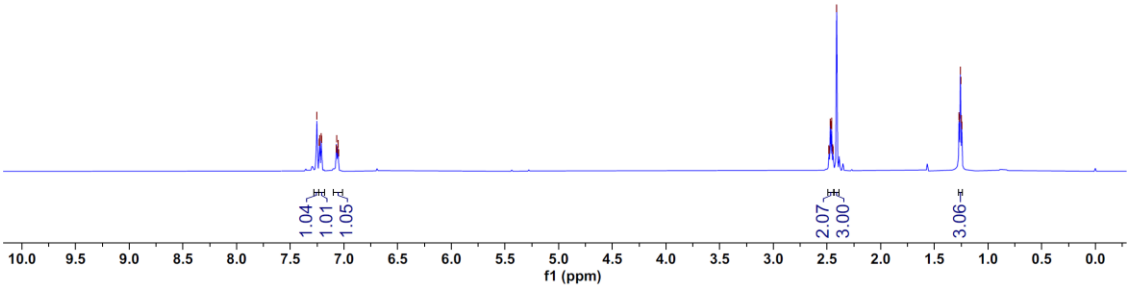
Scheme 3, compound **8a**

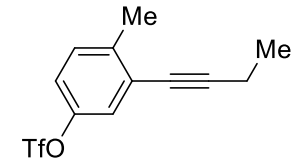
Mass	Calc. Mass	mDa	PPM	Formula
359.9837	359.9829	-0.77	-2.14	C15 H8 Cl F3 O3 S



Scheme 4, compound **10a**

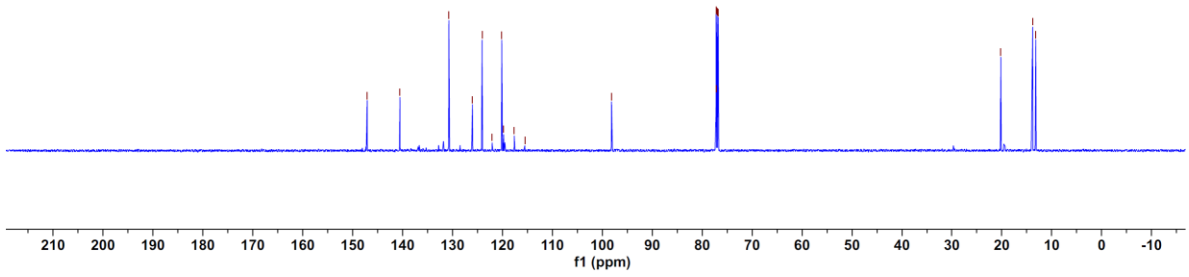
^{1}H NMR 600MHz, $CDCl_3$

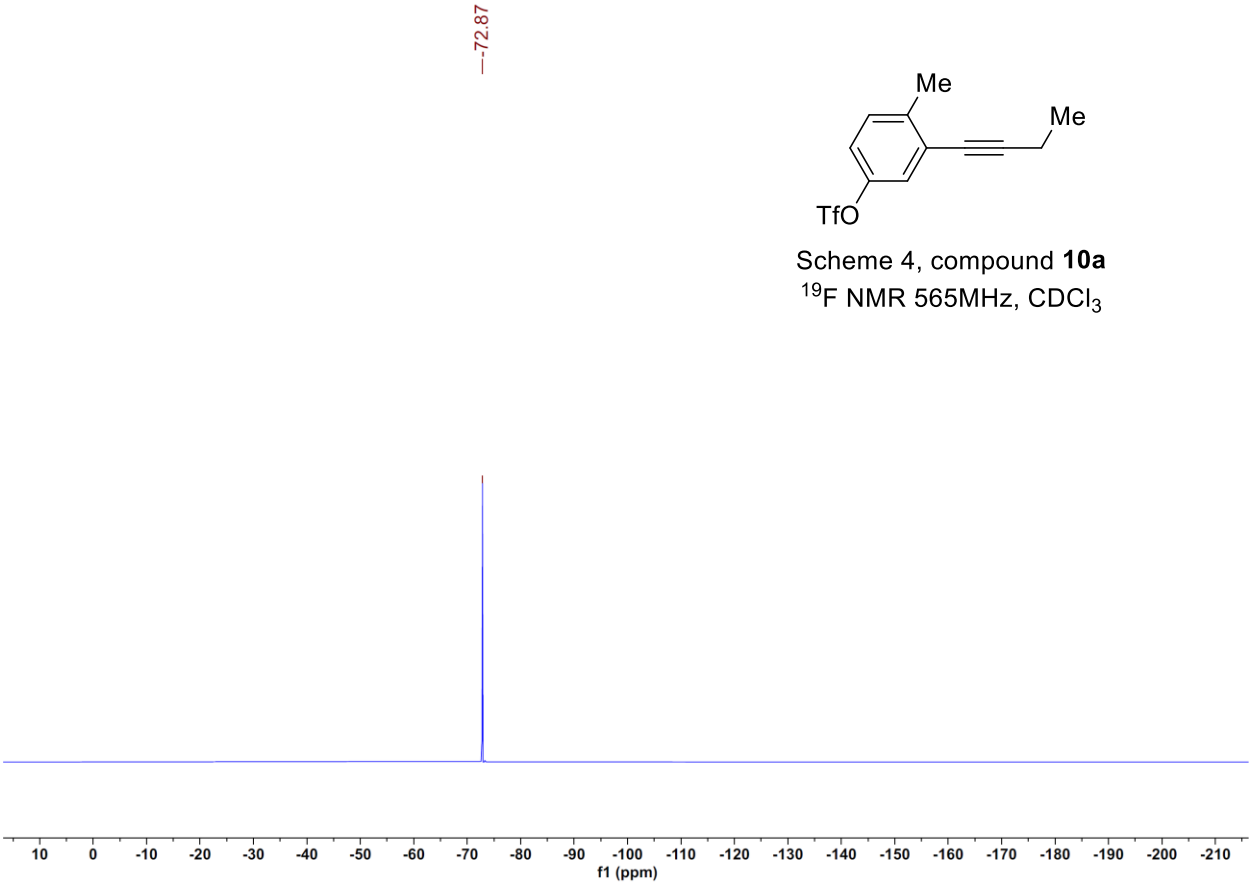




Scheme 4, compound **10a**

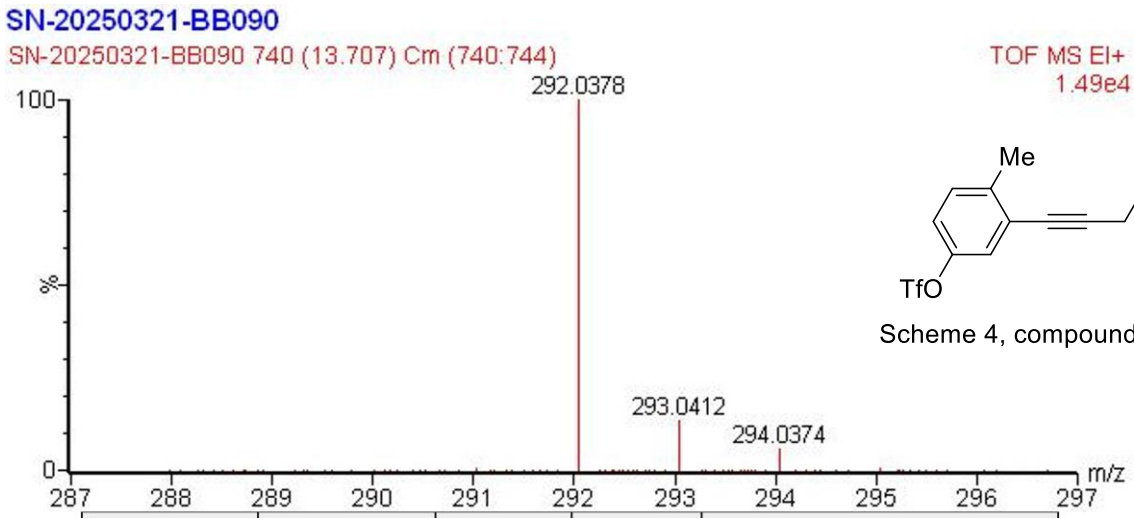
^{13}C NMR 151MHz, $CDCl_3$





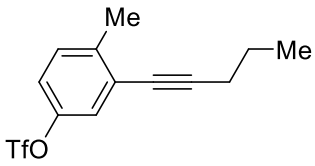
Scheme 4, compound **10a**

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



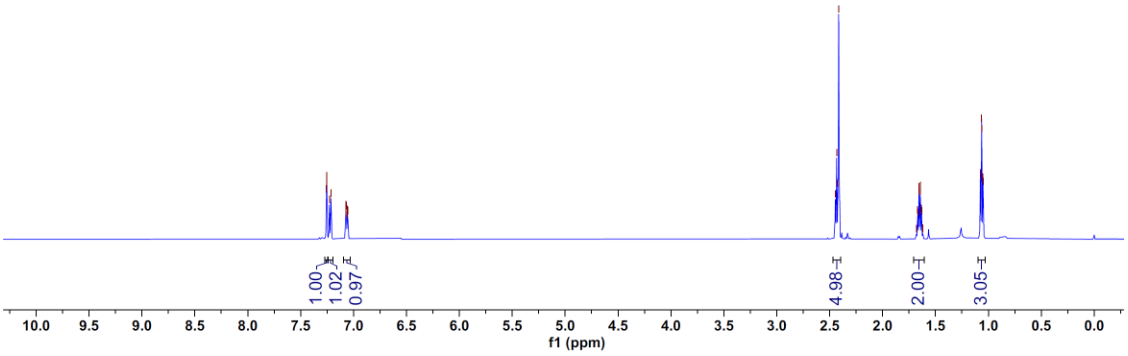
Scheme 4, compound **10a**

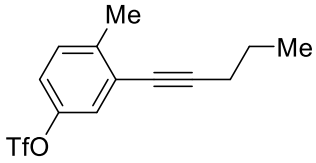
Mass	Calc. Mass	mDa	PPM	Formula
292.0378	292.0376	-0.25	-0.85	C12 H11 F3 O3 S



Scheme 4, compound **10b**

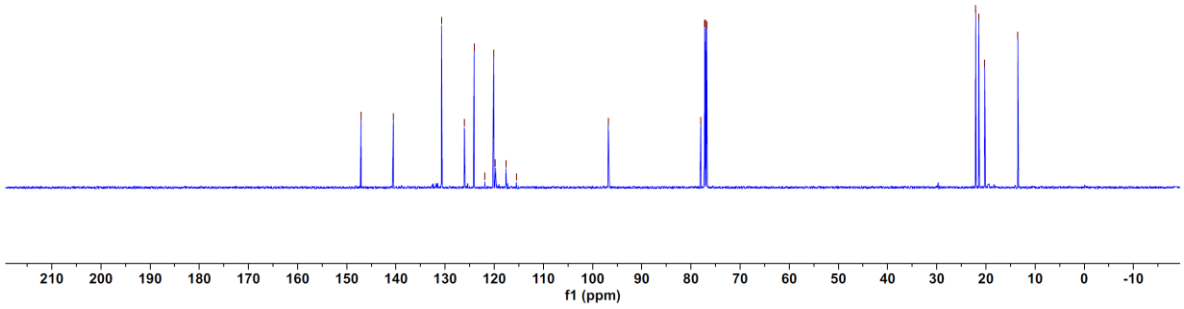
^{1}H NMR 600MHz, $CDCl_3$

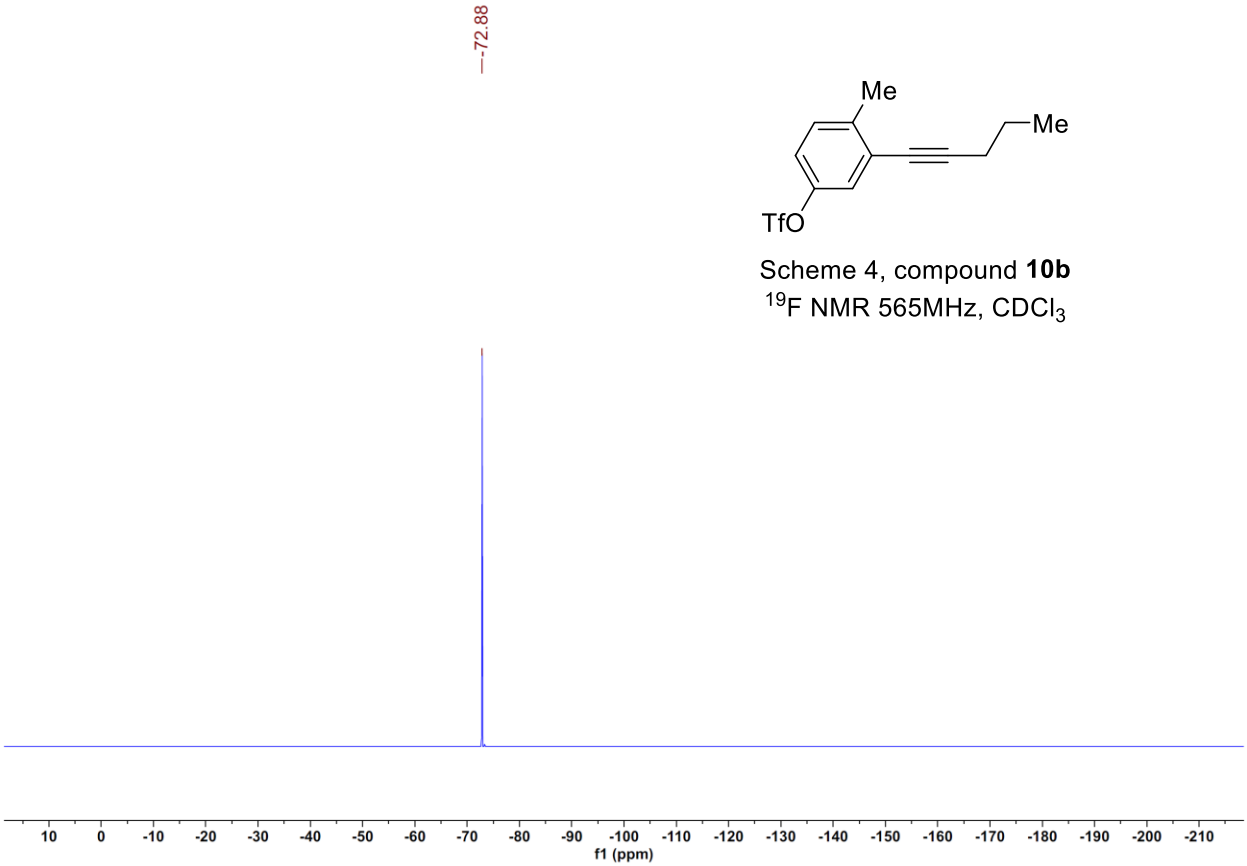




Scheme 4, compound **10b**

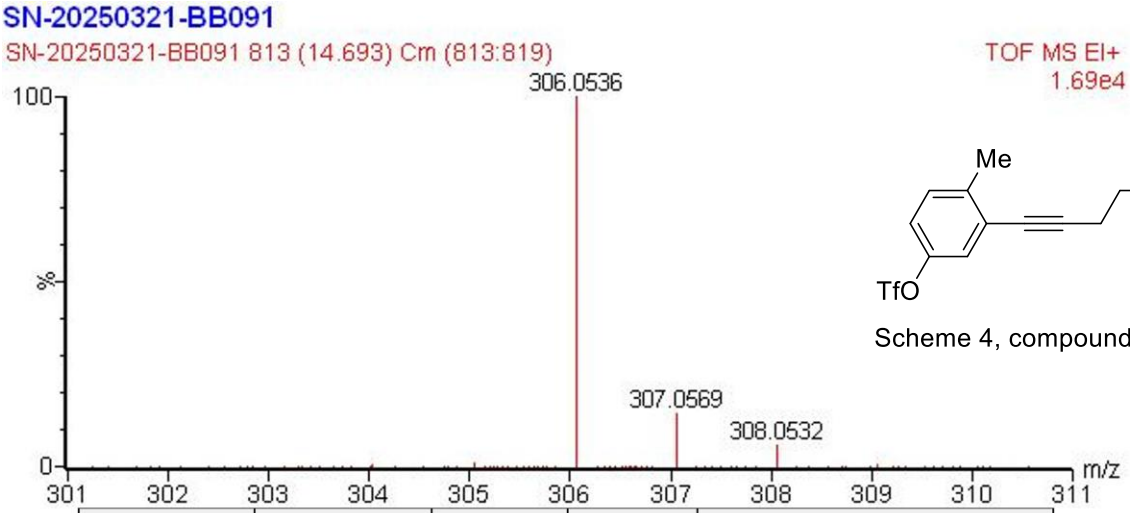
^{13}C NMR 151MHz, $CDCl_3$





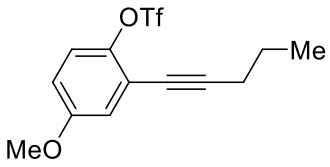
Scheme 4, compound **10b**

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



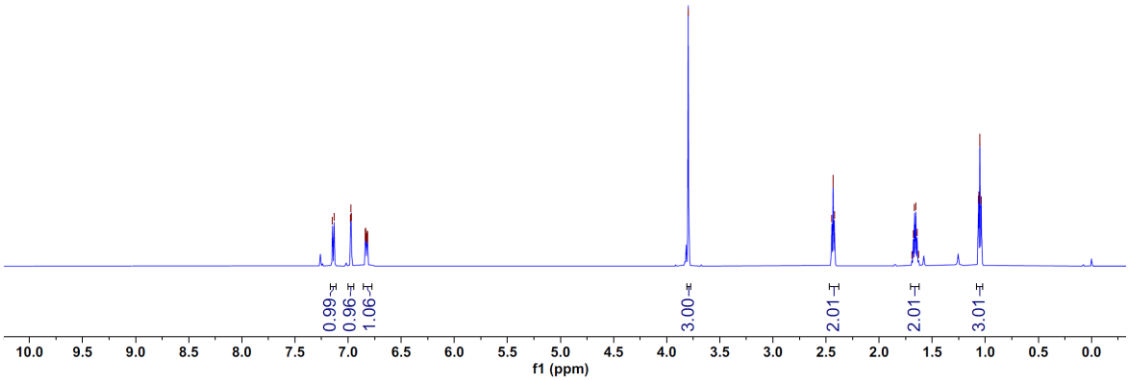
Scheme 4, compound **10b**

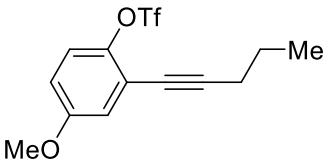
Mass	Calc. Mass	mDa	PPM	Formula
306.0536	306.0532	-0.40	-1.30	C13 H13 F3 O3 S



Scheme 4, compound **10c**

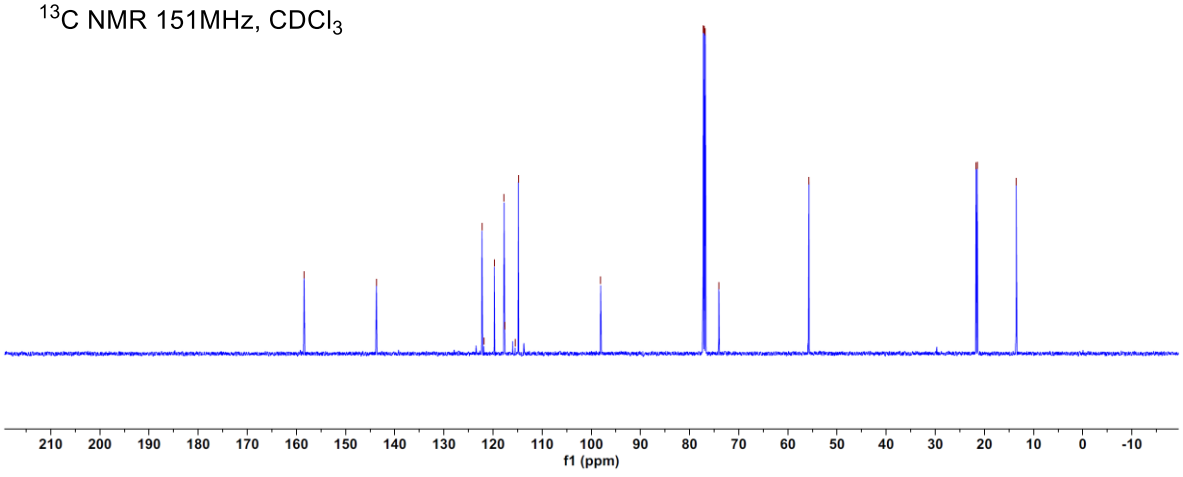
^{1}H NMR 600MHz, $CDCl_3$

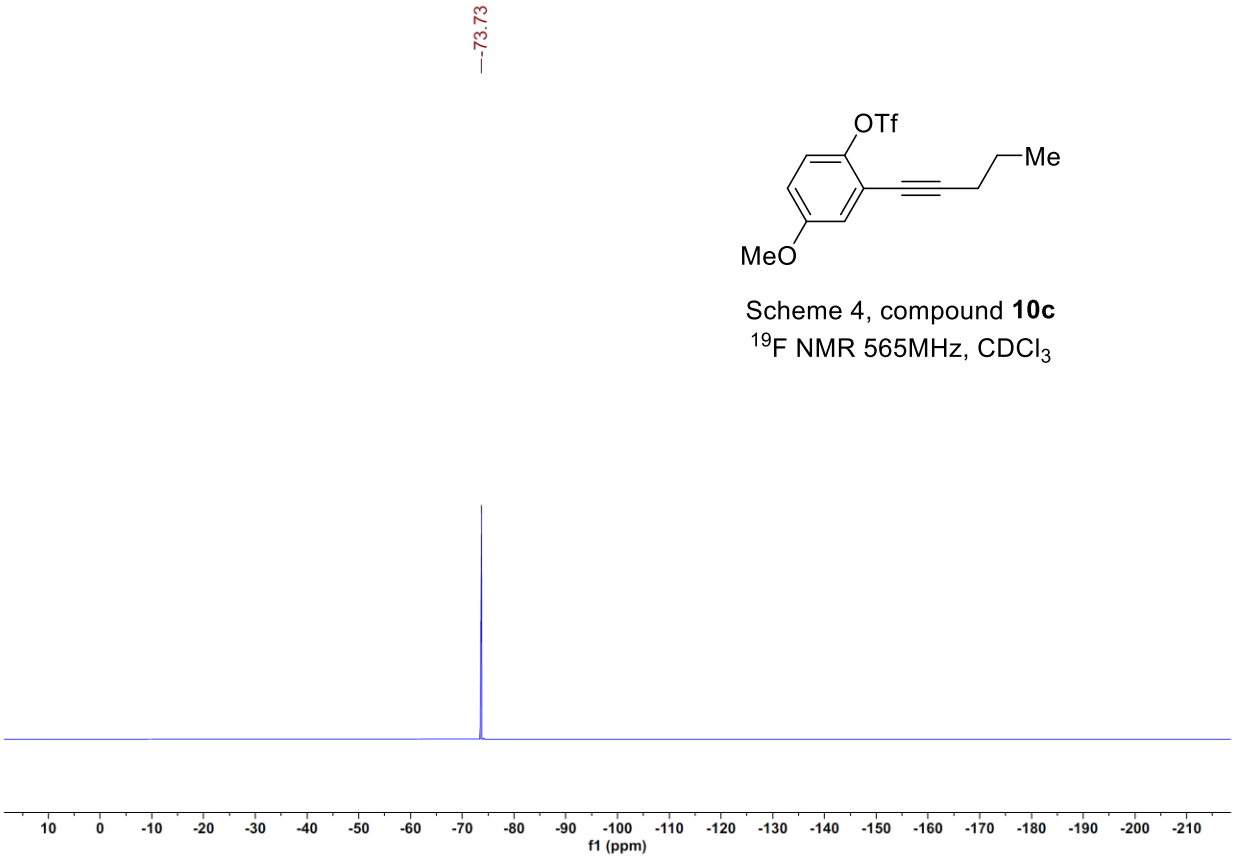




Scheme 4, compound **10c**

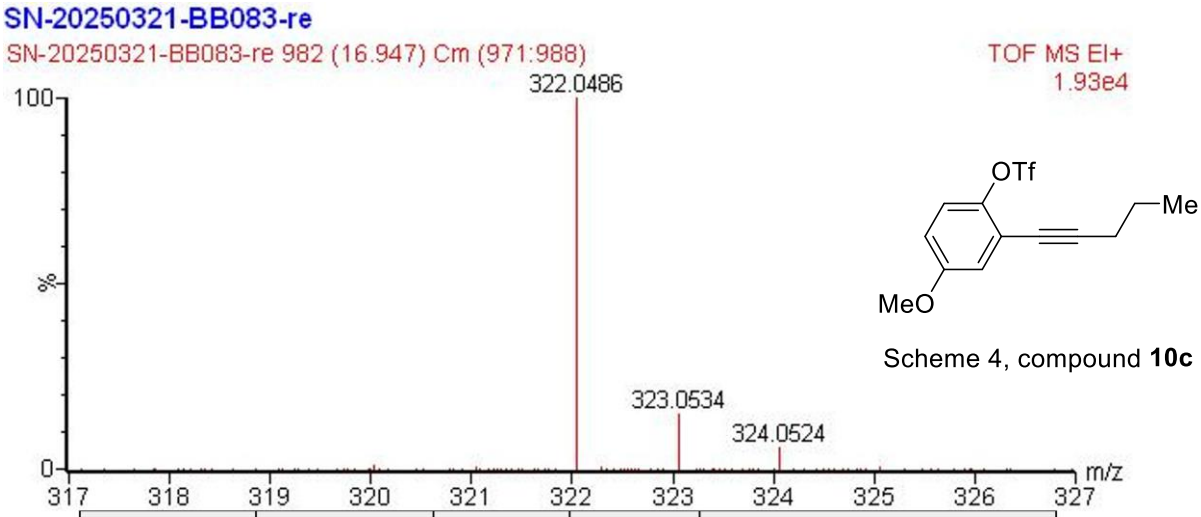
^{13}C NMR 151MHz, $CDCl_3$





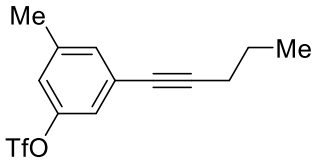
Scheme 4, compound **10c**

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



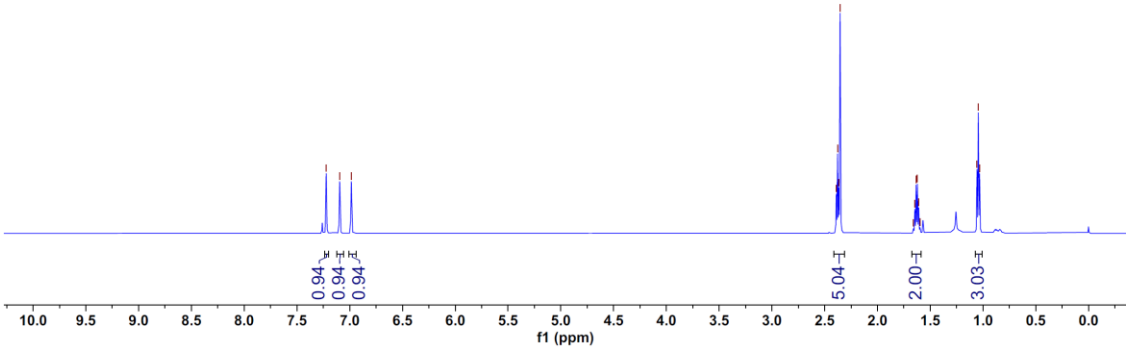
Scheme 4, compound **10c**

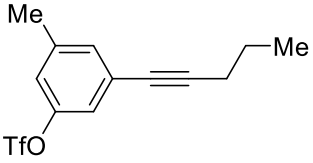
Mass	Calc. Mass	mDa	PPM	Formula
322.0486	322.0481	-0.48	-1.50	C13 H13 F3 O4 S



Scheme 4, compound **10d**

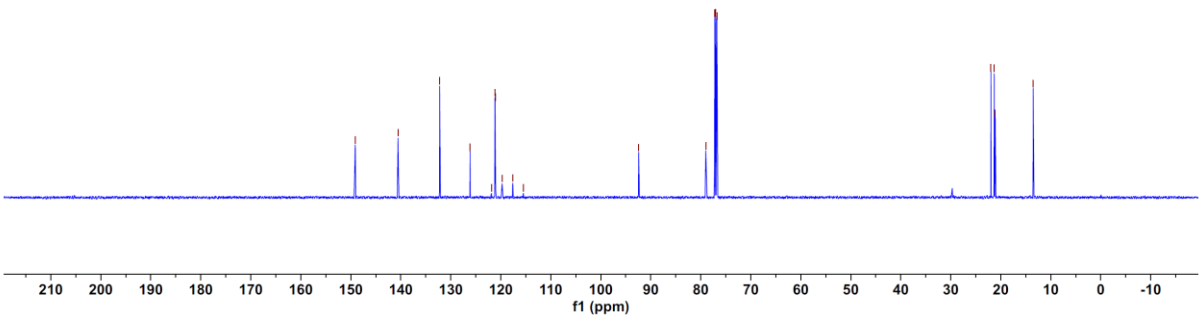
^{1}H NMR 600MHz, $CDCl_3$

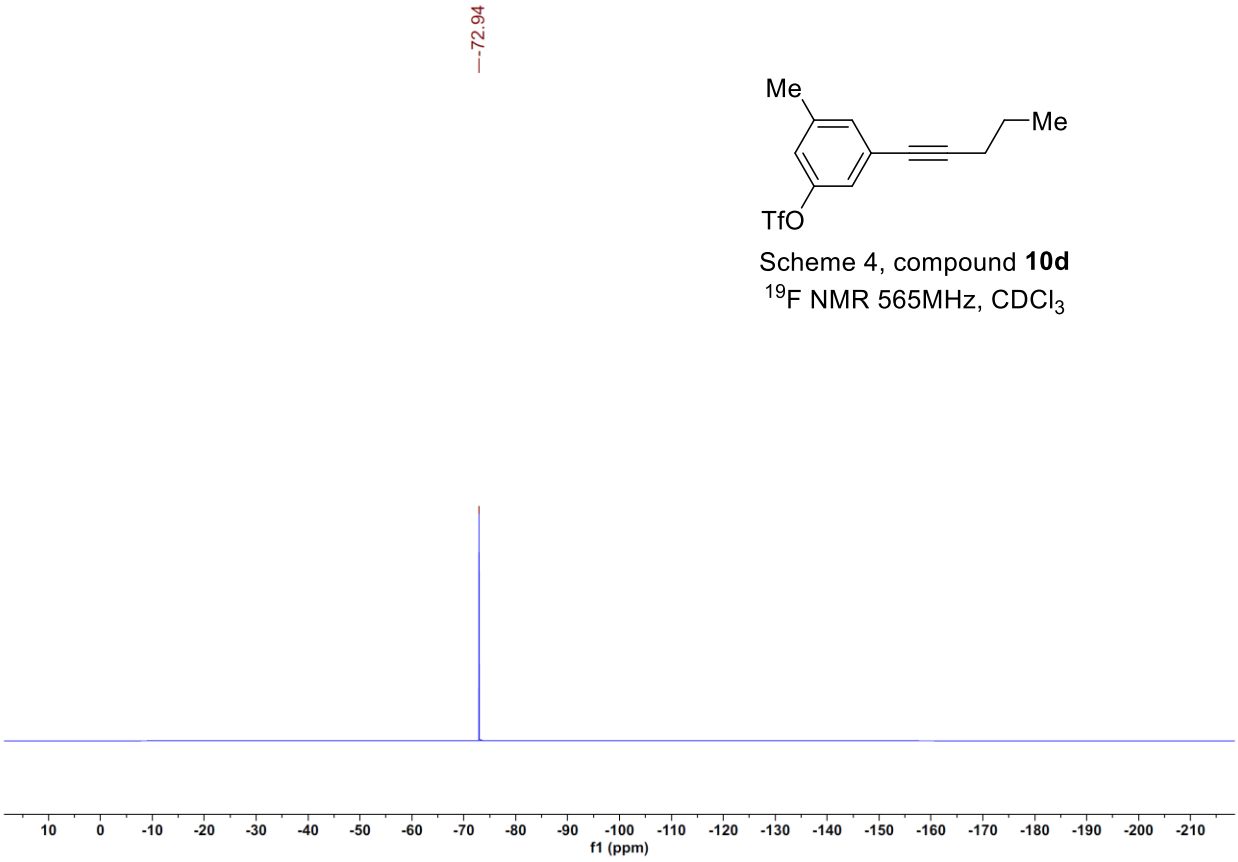




Scheme 4, compound **10d**

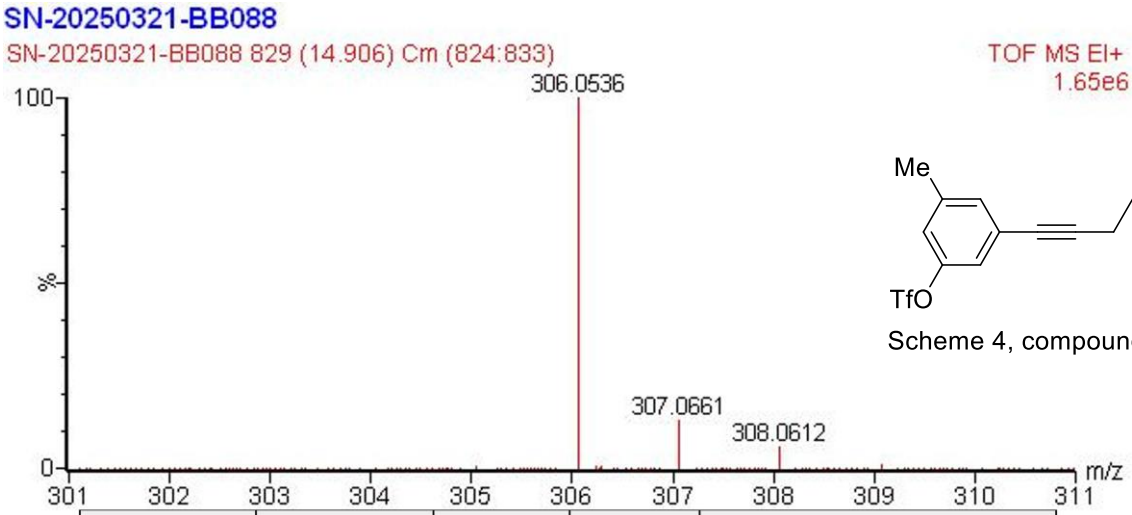
^{13}C NMR 151MHz, $CDCl_3$





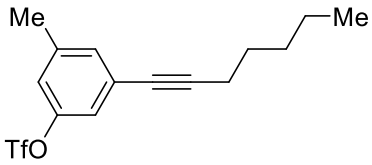
Scheme 4, compound **10d**

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



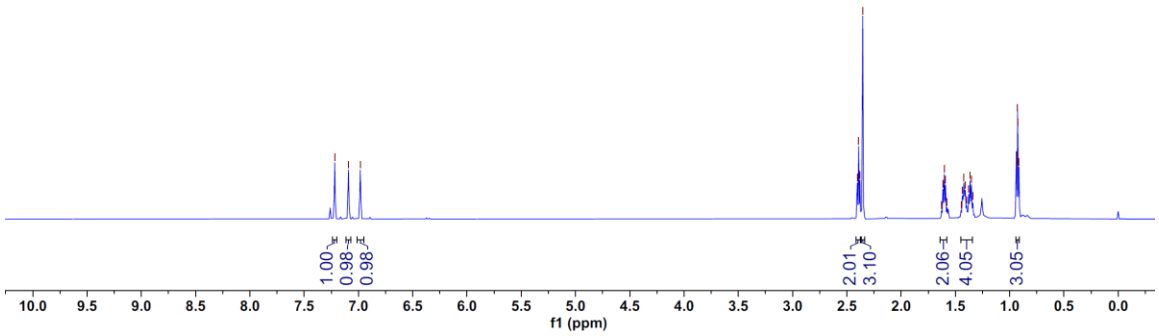
Scheme 4, compound **10d**

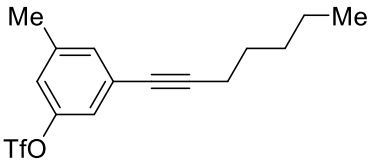
Mass	Calc. Mass	mDa	PPM	Formula
306.0536	306.0532	-0.40	-1.30	C13 H13 F3 O3 S



Scheme 4, compound **10e**

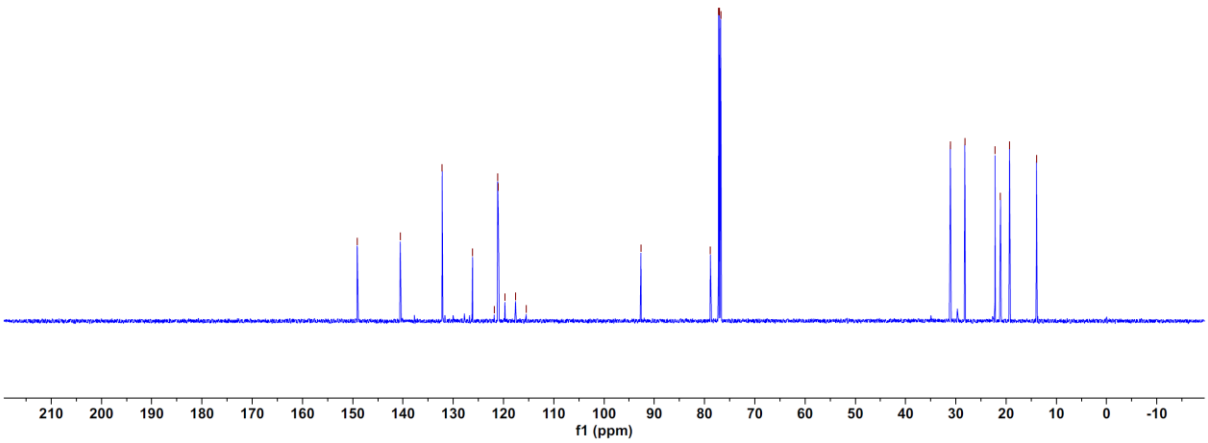
^{1}H NMR 600MHz, $CDCl_3$

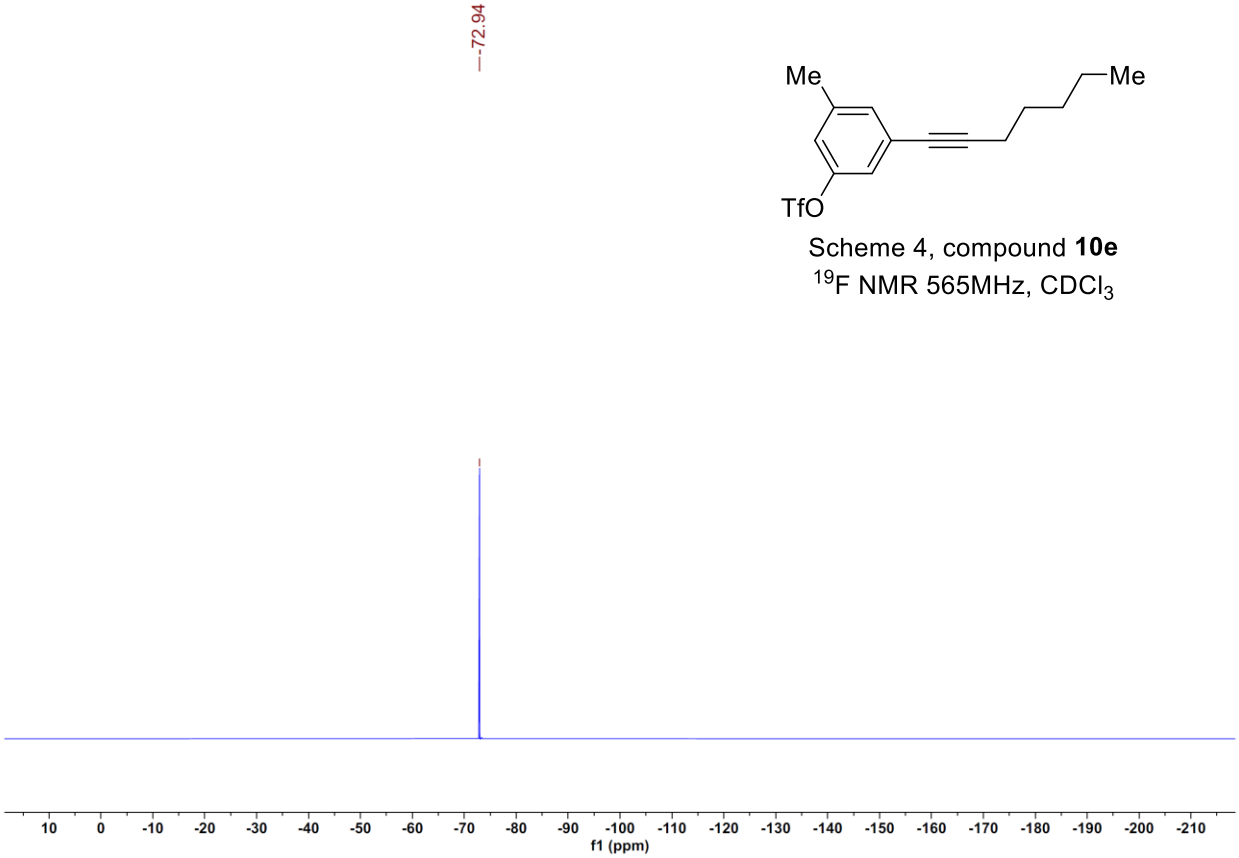




Scheme 4, compound **10e**

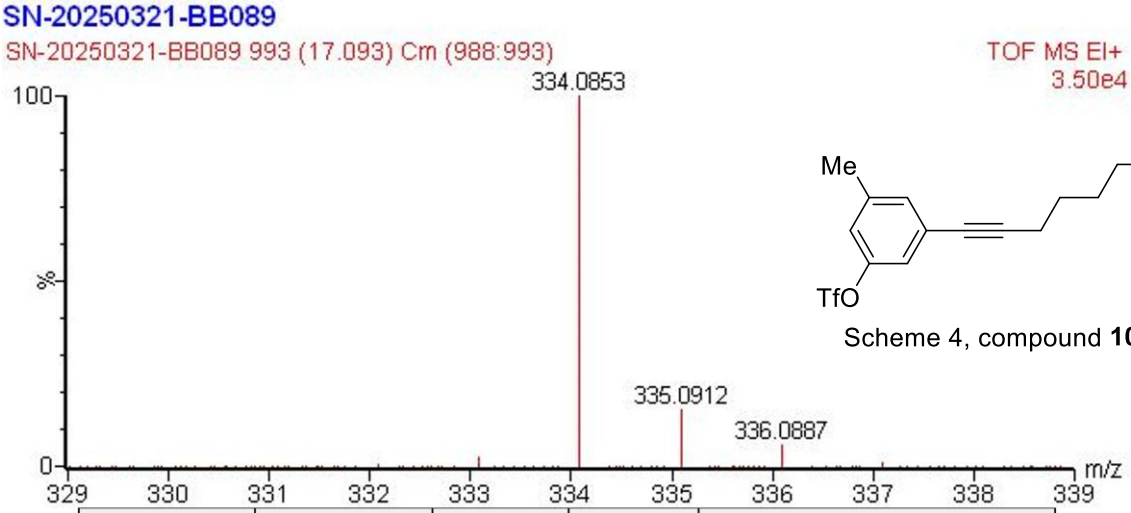
^{13}C NMR 151MHz, $CDCl_3$





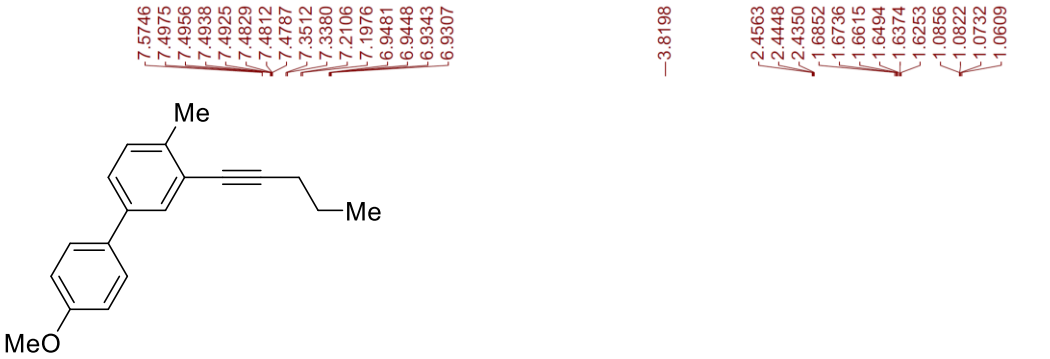
Scheme 4, compound **10e**

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



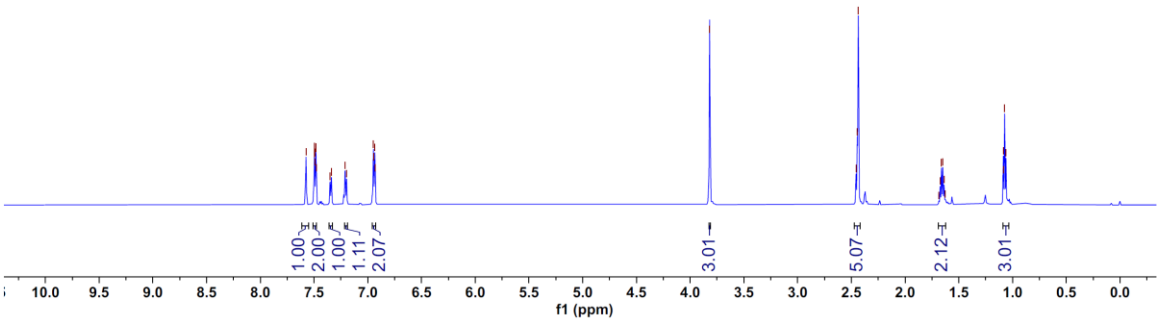
Scheme 4, compound **10e**

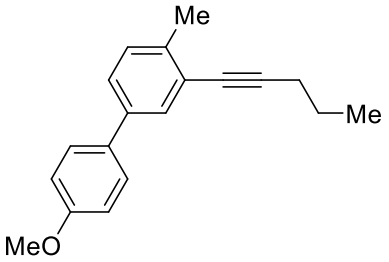
Mass	Calc. Mass	mDa	PPM	Formula
334.0853	334.0845	-0.80	-2.39	C15 H17 F3 O3 S



Scheme 5, compound **11a**

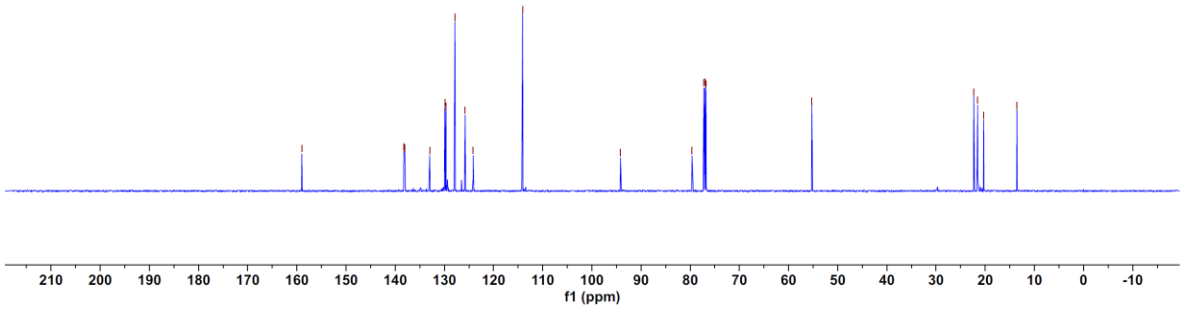
^{1}H NMR 600MHz, $CDCl_3$



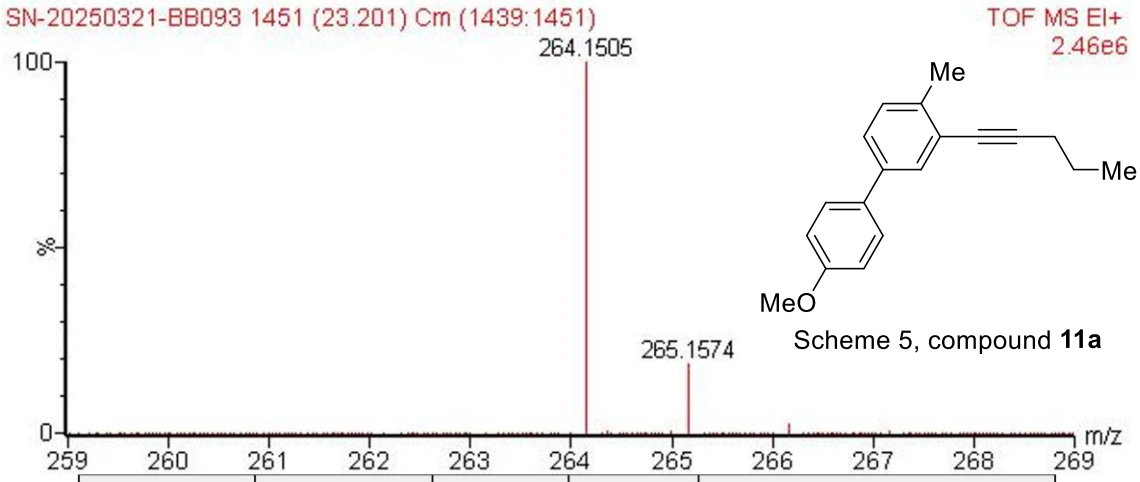


Scheme 5, compound **11a**

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

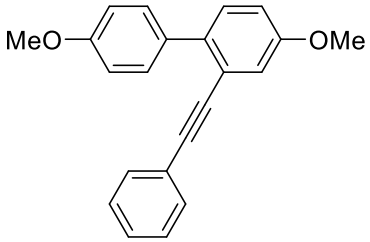


SN-20250321-BB093



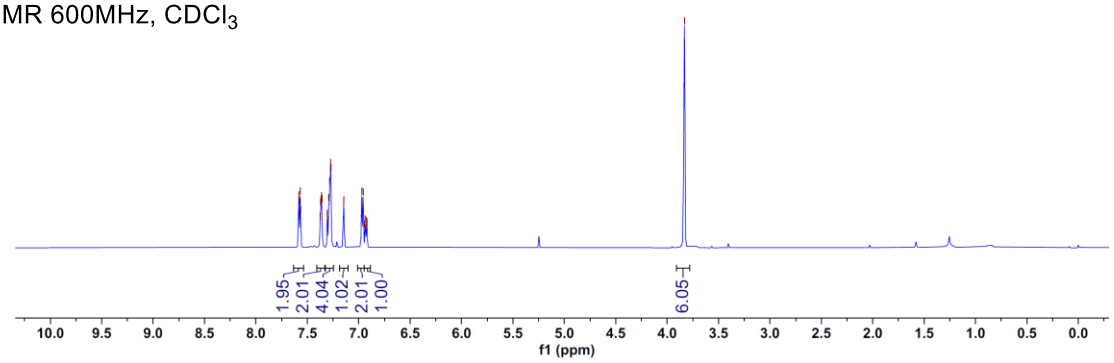
Scheme 5, compound **11a**

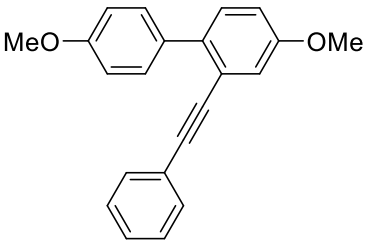
Mass	Calc. Mass	mDa	PPM	Formula
264.1505	264.1509	0.37	1.39	C19 H20 O



Scheme 5, compound **11b**

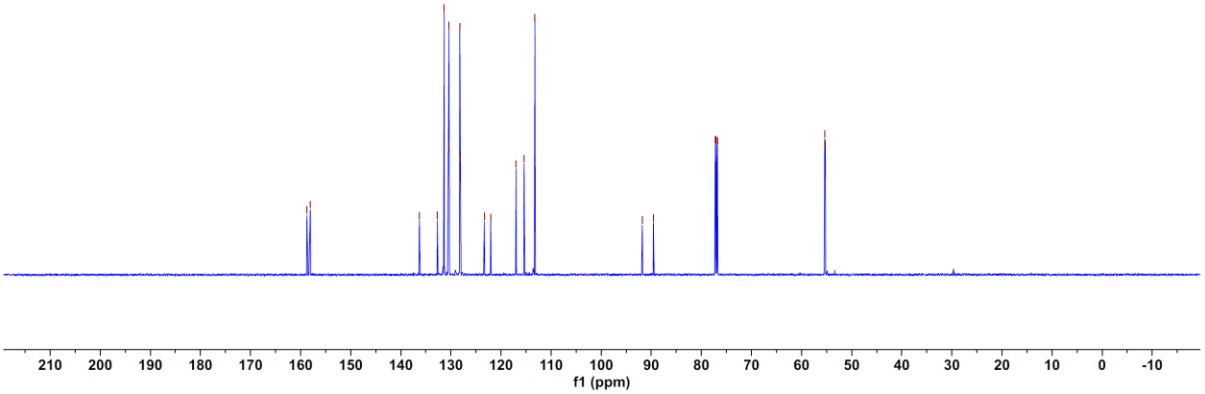
^{1}H NMR 600MHz, $CDCl_3$





Scheme 5, compound **11b**

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



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