Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

One pot synthesis of isocyano-containing, densely functionalised *gem*-difluoroalkenes from *α*-trifluoromethyl alkenes, alkyl halides and TosMIC

Hongtai Huang, Junyu Chen, Yubo Jiang,* and Tiebo Xiao*

Faculty of Science, Kunming University of Science and Technology, Kunming 650500, China; E-mail: xiaotb@kust.edu.cn; ybjiang@kust.edu.cn

Supporting Information

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General information

Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers and used without further purification. For chromatography, 300-400 mesh silica gel (Qingdao, China) was employed. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were measured and recorded on Brucker Avance III 600 or 500 spectrometer ($CDCl_3$, DMSO-d_6 as solvent). Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane (TMS). Coupling constants (J) were given in Hertz (Hz). Multiplicities were given as: s (singlet); d (doublet); t (triplet); q (quartet); dd (doublet of doublets); dt (doublet of triplets); m (multiplets) and etc. Exact masses (HRMS) were recorded on a high resolution magnetic mass spectrometer using electrospray ionization (ESI) techniques.

General procedure

Representative experimental procedure for the preparation of trifluoromethyl alkenes 3a-3m: To a Schlenk tube equipped with stir bar, arylboronic acid (10mmol, 1.0 equiv.) and $Pd(PPh_3)_2Cl_2$ (3 mol%, 0.3 mmol, 210.6 mg) were added. The vessel was evacuated and filled with argon (three times), and then aqueous K_2CO_3 (2.0 M, 20 mL) and THF (30 mL) were added. After addition of 2-bromo-3,3,3-trifluoropropene (20 mmol, 2.1 mL, 2.0 equiv.), the solution was stirred at 60 °C for 12 hours (TLC tracking detection). The solvent was removed under reduced pressure and the residue was purified by column chromatography to afford the corresponding trifluoromethyl alkene (petroleum ether - petroleum ether/EtOAc =100:1).

Preparation of (3-(trifluoromethyl)but-3-en-1-yl)benzene 3n:

(1) **1,1,1-Trifluoro-4-phenylbutan-2-one**: To a diethyl ether solution (100 mL) of ethyl trifluoroacetate (7.16 g, 50.4 mmol) was added phenethylmagnesium bromide (1.0 M in Et_2O, 50.0 mL, 50.0 mmol), prepared from phenethyl bromide (9.25 g, 50.0 mmol) and magnesium turning (1.32 g, 54.3 mmol), at -78 °C over 30 min. After stirring for 30 min at the same temperature, the mixture was warmed to -50 °C over 1 h, and saturated aqueous NH_4Cl was added. Organic materials were extracted three times with Et_2O. The combined extracts were washed with brine and dried over anhydrous Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by distillation under reduced pressure to give the title compound (7.47 g, 74%) as a colorless liquid.

(2) **(3-(trifluoromethyl)but-3-en-1-yl)benzene 3n:** To a diethyl ether solution (64 mL) of Ph_3PCH_3Br (6.29 g, 17.6 mmol) was added *t*-BuOK (1.97 g, 17.6 mmol) at room temperature. The reaction mixture was stirred for 30 min at room temperature and then cooled to -78 °C. To the mixture was added slowly a diethyl ether solution (16 mL) of 1,1,1-trifluoro-4-phenylbutan-2-one (3.23 g, 16.0 mmol) at -78 °C over 10 min. The mixture was then warmed to room temperature over 10 h, and aqueous HCl (1.0 M) was added. Organic materials were extracted three times with Et_2O. The combined extracts were washed with brine and dried over anhydrous Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica gel column chromatography (hexane) and further distillation under reduced pressure to give **3n** (2.65 g, 83%)

as a colorless liquid. Spectral data for this compound showed good agreement with the literature data[1].

Preparation of 2-phenylperfluoropropene 3o: Trifluoroacetophenone (12.79 g, 73.4 mmol) and triphenylphosphine (38.53 g, 146.8 mmol) were dissolved in 30 mL of dry DMF at 50 °C and placed in a 250 mL three-necked round bottom flask containing a stir bar and equipped with reflux condenser, dropping funnel and a dry nitrogeninlet. The homogeneous solution was heated to 50-55 °C (bath temperature). Sodium chloroditfuoroacetate (22.47 g, 14.7 mmol) dissolved in 30 mL of dry DMF was added dropwise into the reaction mixture over 30 min without altering the bath temperature. The reaction mixture was further heated for an additional 2 h when, practically, the conversion of TFAP into **3o** ceased. Heating was stopped and the reaction mixture was immediately quenched in an ice bath, which was then treated with dichloromethane followed by filtering off the insoluble triphenylphosphine oxide. DMF was then removed by repeatedly washing the dichloromethane extract with plenty of water. Dichloromethane was evaporated on water bath and the product 2-phenylperfluoropropene **3o** was isolated by distillation under reduced pressure[2].

Representative experimental procedure for the synthesis of *gem-difluoroalkenes* containing isocyano 4, 5: The solution of NaOH (40% in water, 2.5mL) was syringed dropwise into a vigorous stirring mixture of TosMIC **1** (0.3 mmol, 1.0 equiv.), alkyl halides **2** (0.3 mmol, 1.0 equiv.) and tetrabutylammonium iodide (0.06 mmol) in DCM (2.5 mL) at 0 ^{o}C, and the mixture was stirred for 1 hour at 0 ^{o}C. Then 1-chloro-4-(3,3,3-trifluoroprop-1-en-2-yl) benzene **3a** (0.3 mmol, 1.0 equiv.) was added to the reaction mixture and stirred for another 4 hours at 0 ^{o}C. After the reaction was completed monitored with TLC, the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired products **4**, **5**.

Representative experimental procedure for the synthesis of *gem-difluoroalkenes* containing isocyano 6, 7: The solution of NaOH (40% in water, 2.5mL) was syringed dropwise into a vigorous stirring mixture of TosMIC **1** (0.3 mmol, 1.0 equiv.),

1-chloro-4-(3,3,3-trifluoroprop-1-en-2-yl) benzene **3a** (0.6 mmol, 2.0 equiv.) and tetrabutylammonium iodide (0.06 mmol) in DCM (2.5 mL) at 0 ^{o}C, and the mixture was stirred for 5 hour at 0 ^{o}C. After the reaction was completed monitored with TLC, the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography to give desired products **6**, **7**.

Synthesis of *N*-(3-(4-chlorophenyl)-2-fluoro-5-isocyano-5-tosylhex-2-en-1-yl)aniline 8: To a 10 mL test tube equipped with a magnetic stir bar was charged with **4a** (0.2 mmol), *N*-phenylglycine (0.3 mmol), {Ir[dF(CF_3)ppy]$_2$(dtbpy)}PF_6 (0.5 mol%), NaO^{t}Bu (0.04 mol) and 2 mL of DMSO. The solution was stirred at room temperature with the irradiation of 12 W blue LEDs under argon for 12 h. Upon completion of the reaction, the resulting mixture was extracted with EtOAc. The combined organic layers were washed with water and brine and dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with petroleum ether/EtOAc=12:1 (v/v), as the eluant, giving the pure product **8** (58.8 mg, 61% yield).

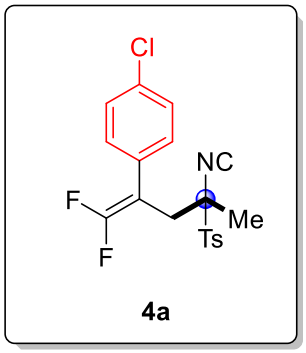
Synthesis of 1-(2-(4-chlorophenyl)-1-fluoro-4-isocyano-4-tosylpent-1-en-1-yl)-1H-pyrazole 9: To a 10 mL test tube equipped with a magnetic stir bar was charged with **4a** (0.2 mmol), pyrazole (0.2 mmol), K_3PO_4 (0.4 mmol), and DMF (1 mL). The mixture was stirred at room temperature for 12 hours. The resulting mixture was extracted with EtOAc (20 mL x3). The organic layers were combined and washed with brine, dried over Na_2SO_4. The extracts were concentrated under reduced pressure to afford the crude product, which was further purified through silica gel column chromatography (using petroleum ether/EtOAc = 8:1 as eluents) to yield the product **9** (59.4 mg, 67% yield).

Synthesis of 4-(3,3-difluoro-2-(4-methoxyphenyl)allyl)-5-phenyloxazole 10: A mixture of **7c** (0.2 mmol), benzaldehyde (0.2 mmol) and K_2CO_3 (0.4 mmol) in MeOH (1 ml) was stirred at room temperature for 3 hours. The concentration of the reaction mixture in vacuum gave a residue. The purification of the residue by using flash chromatography (eluted with petroleum ether/EtOAc= 15:1) afforded product **10**.

Synthesis of 1-(4-bromophenyl)-4-(3,3-difluoro-2-(4-methoxyphenyl)allyl)-5-tosyl-1H-imida zole 11： A Argon-purged 10 mL microwave tube was charged with **7c** (0.2 mmol), 1-bromo-4-isocyanobenzene (0.24 mmol), Ag_2CO_3 (0.02 mmol) and 1,4-dioxane (1 mL).The mixture was stirred at 80 °C for 1 hour. Upon completion of the reaction, the contents were filtered through a short path of silica gel, eluting with ethyl acetate (20 mL).The residue was subjected to column chromatography on silica-gel (petroleum ether/EtOAc = 30:1) to give **11** (69.2 mg, 62%).

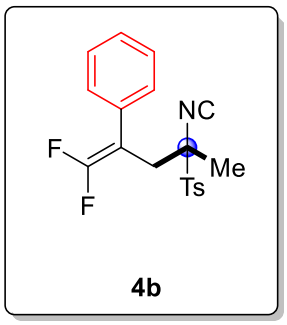
Compound characterization data

1-chloro-4-(1,1-difluoro-4-isocyano-4-tosylpent-1-en-2-yl)benzene (4a):



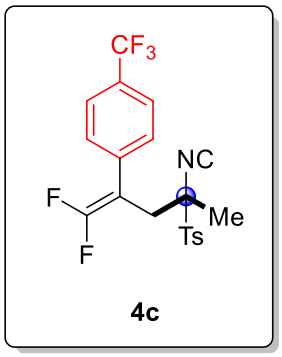
1H NMR (500 MHz, DMSO) δ 7.85 (d, J = 8.3 Hz, 2H), 7.57 (d, J = 8.1 Hz, 2H), 7.47 (d, J = 2.5 Hz, 4H), 3.16 (q, J = 14.9 Hz, 2H), 2.46 (s, 3H), 1.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.73 (s), 154.57 (t, *J* = 290.9 Hz), 147.02 (s), 132.92 (s), 131.11 (s), 130.94 (s), 130.53 (s), 130.30 (s), 128.76 (s), 128.42 (d, *J* = 25.1 Hz), 86.35 (dd, *J* = 20.4, 18.2 Hz), 77.34 (s), 32.01 (s), 21.29 (s), 20.85 (s); ^{19}F NMR (471 MHz, DMSO) δ -86.45 (d, *J* = 31.5 Hz, 1F), -87.07 (d, *J* = 31.5 Hz, 1F); HRMS (ESI): mass found: 418.0454, calculated mass for $C_{19}H_{16}ClF_2NNaO_2S^+$ [M+Na $^+$]: 418.0451.

1-((5,5-difluoro-2-isocyano-4-phenylpent-4-en-2-yl)sulfonyl)-4-methylbenzene (4b):



^{1}H NMR (500 MHz, DMSO) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.41 (dt, *J* = 15.1, 7.6 Hz, 4H), 7.33 (d, *J* = 7.0 Hz, 1H), 3.16 (q, *J* = 14.8 Hz, 2H), 2.46 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 165.05 (s), 154.99 (t, *J* = 290.3 Hz), 147.44 (s), 132.38 (s), 131.55 (s), 130.72 (s), 130.28 (s), 129.16 (s), 129.01 (s), 128.70 (d, *J* = 2.0 Hz), 87.54 (t, *J* = 18.9 Hz), 77.88 (s), 32.52 (d, *J* = 2.4 Hz), 21.71 (s), 21.19 (s); ^{19}F NMR (471 MHz, DMSO) δ -87.29 (d, *J* = 33.3 Hz, 1F), -88.02 (d, *J* = 33.3 Hz, 1F); HRMS (ESI): mass found: 380.0845, calculated mass for $C_{19}H_{17}F_2NNaO_2S^+$ [M+Na $^+$]: 380.0840..

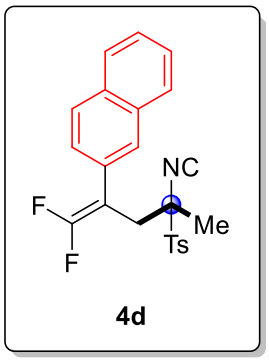
1-((5,5-difluoro-2-isocyano-4-(4-(trifluoromethyl)phenyl)pent-4-en-2-yl)sulfonyl)-4-methylbenzene (4c):



4c

^{1}H NMR (600 MHz, DMSO) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 3.23 (dd, *J* = 35.2, 15.0 Hz, 2H), 2.46 (s, 3H), 1.48 (s, 3H); ^{13}C NMR (151 MHz, DMSO) δ 164.82 (s), 154.83 (t, *J* = 243.2 Hz), 147.07 (s), 136.56 (s), 131.13 (s), 130.33 (s), 129.60 (s), 128.58 (dd, *J* = 63.9, 32.0 Hz),, 125.59 (d, *J* = 3.6 Hz), 124.98 (s), 123.18 (s), 86.51 (dd, *J* = 20.7, 17.9 Hz), 77.30 (s), 31.64 – 26.72 (m), 21.30 (s), 20.92 (s); ^{19}F NMR (471 MHz, DMSO) δ -61.18 (s, 3F), -85.22 (d, *J* = 28.8 Hz, 1F), -86.10 (d, *J* = 28.9 Hz, 1F); HRMS (ESI): mass found: 450.0720, calculated mass for $C_{20}H_{16}F_5NNaO_2S^+$ [M+Na $^+$]: 452.0714.

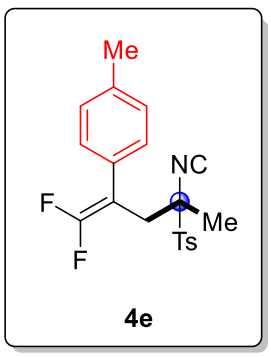
(R)-2-(1,1-difluoro-4-isocyano-4-tosylpent-1-en-2-yl)naphthalene (4d):



4d

^{1}H NMR (500 MHz, DMSO) δ 8.00 (s, 1H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.90 (dd, *J* = 5.0, 3.8 Hz, 2H), 7.86 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 3H), 7.53 (dd, *J* = 6.0, 3.5 Hz, 2H), 3.29 (q, *J* = 14.9 Hz, 2H), 2.44 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.65 (s), 154.84 (t, *J* = 290.9 Hz), 146.99 (s), 132.74 (s), 132.37 (s), 131.13 (s), 130.28 (s), 128.33 (s), 127.89 (d, *J* = 14.2 Hz), 127.61 (s), 126.65 (d, *J* = 8.4 Hz), 126.07 (s), 87.22 (dd, *J* = 19.5, 18.2 Hz), 77.54 (s), 71.18 (s), 32.13 (s), 27.24 (s), 21.27 (s), 20.88 (s), 18.87 (s), 13.56 (s); ^{1} ^{19}F NMR (471 MHz, DMSO) δ -86.50 (d, *J* = 32.0 Hz, 1F), -87.55 (d, *J* = 32.0 Hz, 1F); HRMS (ESI): mass found: 434.0999, calculated mass for $C_{23}H_{19}F_2NNaO_2S^+$ [M+Na $^+$]: 434.0997.

1-((5,5-difluoro-2-isocyano-4-(p-tolyl)pent-4-en-2-yl)sulfonyl)-4-methylbenzene (4e):

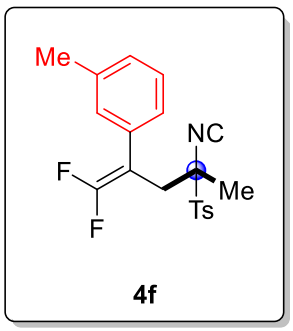


4e

^{1}H NMR (500 MHz, DMSO) δ 7.85 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 3.13 (q, *J* = 15.0 Hz 2H), 2.46 (s, 3H), 2.28 (s, 3H), 1.40 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.56 (s), 154.53 (t, *J* = 290.0 Hz), 147.02 (s), 137.66

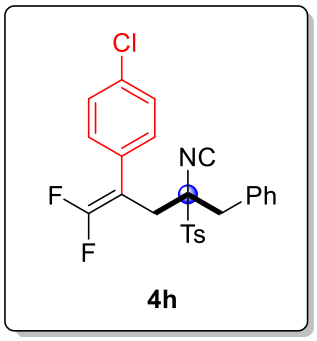
(s), 131.14 (s), 130.31 (s), 129.35 (s), 128.37 (d, *J* = 11.1 Hz), 86.96 (t, *J* = 18.8 Hz), 77.54 (s), 71.20 (s), 32.10 (s), 27.26 (s), 21.31 (s), 20.78 (s), 18.91 (s); ^{19}F NMR (471 MHz, DMSO) δ -87.61 (d, *J* = 34.3 Hz, 1F), -88.38 (d, *J* = 34.3 Hz, 1F); HRMS (ESI): mass found: 398.1011, calculated mass for $C_{20}H_{19}F_2NNaO_2S^+$ [M+Na $^+$]: 398.0997.

1-(1,1-difluoro-4-isocyano-4-tosylpent-1-en-2-yl)-3-methylbenzene (4f):



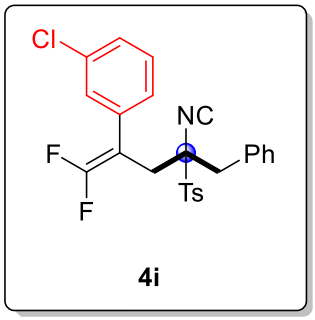
^{1}H NMR (500 MHz, DMSO) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.23 – 7.18 (m, 2H), 7.14 (d, *J* = 7.4 Hz, 1H), 3.14 (q, *J* = 14.8 Hz, 2H), 2.46 (s, 3H), 2.29 (s, 3H), 1.41 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.63 (d, *J* = 2.3 Hz), 154.56 (t, *J* = 290.4 Hz), 146.99 (s), 137.95 (s), 131.89 (s), 131.14 (s), 130.28 (s), 128.98 (s), 128.91 (s), 128.61 (s), 128.32 (s), 125.67 (s), 87.11 (t, *J* = 18.8 Hz), 77.51 (s), 32.09 (d, *J* = 2.4 Hz), 21.28 (s), 20.95 (s), 20.78 (s); ^{19}F NMR (471 MHz, DMSO) δ -87.32 (d, *J* = 33.5 Hz, 1F), -87.93 (d, *J* = 33.4 Hz, 1F); HRMS (ESI): mass found: 398.0999, calculated mass for $C_{20}H_{19}F_2NNaO_2S^+$ [M+Na $^+$]: 398.0997.

1-chloro-4-(1,1-difluoro-4-isocyano-5-phenyl-4-tosylpent-1-en-2-yl)benzene (4g):



^{1}H NMR (600 MHz, DMSO) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.29 (m, 4H), 7.28 – 7.18 (m, 3H), 7.05 (d, *J* = 8.0 Hz, 2H), 3.27 (dd, *J* = 27.4, 16.4 Hz, 2H), 3.00 (dd, *J* = 47.4, 14.8 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.06 (s), 153.82 (t, *J* = 289.8 Hz), 146.90 (s), 132.56 (s), 131.99 (s), 131.06 (s), 130.90 (s), 130.61 (s), 130.35 (s), 130.25 (s), 129.58 (s), 128.34 (s), 128.28 (s), 128.20 (s), 127.97 (s), 86.82 (t, *J* = 18.9 Hz), 79.82 (s), 31.07 (s), 21.29 (s).; ^{19}F NMR (471 MHz, DMSO) δ -85.15 (d, *J* = 30.6 Hz, 1F), -87.74 (d, *J* = 30.5 Hz, 1F); HRMS (ESI): mass found: 494.0768, calculated mass for $C_{25}H_{20}ClF_2NNaO_2S^+$ [M+Na $^+$]: 494.0764.

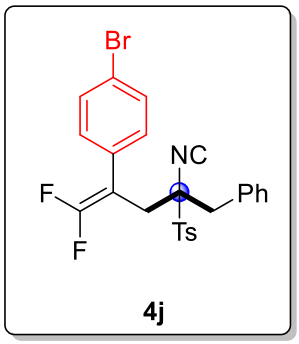
1-chloro-3-(1,1-difluoro-4-isocyano-5-phenyl-4-tosylpent-1-en-2-yl)benzene (4h):



4i

^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.35 – 7.27 (m, 5H), 7.21 (dd, *J* = 7.1, 2.3 Hz, 2H), 7.03 – 6.93 (m, 2H), 3.31 (d, *J* = 14.1 Hz, 2H), 3.04 (dd, *J* = 25.5, 14.8 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.17 (s), 153.87 (t, *J* = 290.8 Hz), 146.90 (s), 133.75 (s), 132.91 (s), 132.62 (s), 131.96 (s), 131.05 (d, *J* = 7.6 Hz), 130.87 (d, *J* = 6.6 Hz), 130.25 (s), 130.04 (s), 129.57 (s), 128.22 (d, *J* = 7.4 Hz), 127.99 (s), 127.85 (s), 127.73 (s), 127.24 (s), 86.81 (dd, *J* = 19.9, 18.7 Hz), 79.80 (s), 30.97 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -84.69 (d, *J* = 29.5 Hz, 1F), -87.20 (d, *J* = 29.5 Hz, 1F); HRMS (ESI): mass found: 494.0767, calculated mass for $C_{25}H_{20}ClF_2NNaO_2S^+$ [M+Na $^+$]: 494.0764.

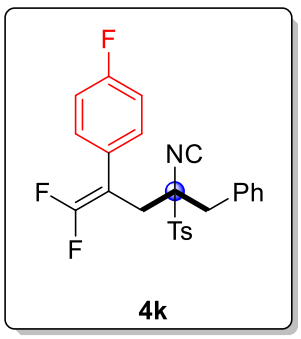
1-bromo-4-(1,1-difluoro-4-isocyano-5-phenyl-4-tosylpent-1-en-2-yl)benzene (4i):



4j

^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.31 (dd, *J* = 4.9, 2.3 Hz, 3H), 7.19 (dd, *J* = 7.2, 2.0 Hz, 2H), 6.99 (d, *J* = 7.8 Hz, 2H), 3.28 (dt, *J* = 7.4, 4.8 Hz, 2H), 3.00 (dd, *J* = 36.1, 14.8 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.07 (s), 153.78 (t, *J* = 290.1 Hz), 146.93 (s), 132.64 (s), 131.99 (s), 131.28 (s), 130.98 (dd, *J* = 20.7, 3.8 Hz), 130.65 (s), 130.23 (d, *J* = 9.4 Hz), 129.58 (s), 128.27 (d, *J* = 10.8 Hz), 127.99 (s), 127.76 (s), 121.17 (s), 86.90 (dd, *J* = 19.5, 19.0 Hz), 81.69 (s), 79.86 (s), 31.04 (s), 21.32 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.00 (d, *J* = 30.2 Hz, 1F), -87.65 (d, *J* = 30.2 Hz, 1F); HRMS (ESI): mass found: 538.0260, calculated mass for $C_{25}H_{20}BrF_2NNaO_2S^+$ [M+Na $^+$]: 538.0258.

1-((5,5-difluoro-4-(4-fluorophenyl)-2-isocyano-1-phenylpent-4-en-2-yl)sulfonyl)-4-methylben zene (4j):

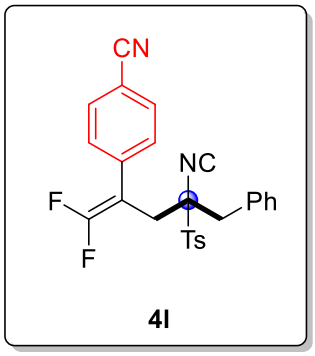


4k

^{1}H NMR (500 MHz, DMSO) δ 7.83 (dd, *J* = 8.3, 5.7 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.29 (ddd, *J* = 25.3, 5.0, 2.0 Hz, 4H), 7.22 – 7.00 (m, 5H), 3.31 – 2.93 (m, 4H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO)

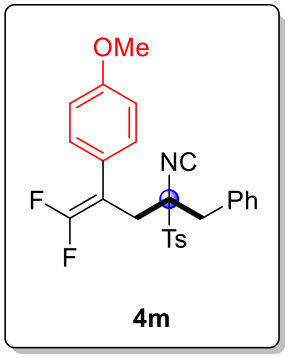
δ 166.42 (d, *J* = 137.3 Hz), 161.58 (d, *J* = 245.0 Hz), 153.80 (t, *J* = 289.9 Hz), 146.76 (d, *J* = 29.1 Hz), 132.63 (s), 132.04 (s), 131.20 – 130.46 (m), 130.22 (d, *J* = 8.1 Hz), 129.86 (d, *J* = 6.5 Hz), 129.60 (s), 128.23 (d, *J* = 6.1 Hz), 127.85 (d, *J* = 25.9 Hz), 115.75 (d, *J* = 21.7 Hz), 115.27 (d, *J* = 21.7 Hz), 86.80 (t, *J* = 19.4 Hz), 81.68 (s), 79.82 (s), 31.42 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -86.02 (d, *J* = 32.2 Hz, 1F), -88.42 (d, *J* = 32.3 Hz, 1F), -113.81 – -114.03 (m, 1F); HRMS (ESI): mass found: 478.1063, calculated mass for $C_{25}H_{20}F_3NNaO_2S^+$ [M+Na $^+$]: 478.1059.

4-(1,1-difluoro-4-isocyano-5-phenyl-4-tosylpent-1-en-2-yl)benzonitrile (4k):



^{1}H NMR (500 MHz, DMSO) δ 7.78 (dd, *J* = 42.1, 8.3 Hz, 4H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.24 (m, 5H), 7.20 (dd, *J* = 7.2, 1.9 Hz, 2H), 3.31 (dd, *J* = 33.2, 19.4 Hz, 2H), 3.01 (dd, *J* = 74.0, 14.8 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.15 (s), 154.02 (t, *J* = 291.9 Hz), 146.97 (s), 136.98 (s), 132.02 (d, *J* = 35.0 Hz), 130.98 (d, *J* = 21.1 Hz), 130.26 (d, *J* = 7.5 Hz), 129.76 (s), 129.73 – 129.37 (m), 128.61 (s), 128.35 (s), 128.12 (d, *J* = 20.5 Hz), 118.54 (s), 110.49 (s), 87.17 (dd, *J* = 20.3, 18.1 Hz), 79.81 (s), 72.25 (s), 33.64 (s), 30.63 (s), 21.30 (s); ^{19}F NMR (471 MHz, DMSO) δ -83.35 (d, *J* = 26.3 Hz, 1F), -86.22 (d, *J* = 26.4 Hz, 1F); HRMS (ESI): mass found: 485.1106, calculated mass for $C_{26}H_{20}F_2N_2NaO_2S^+$ [M+Na $^+$]: 485.1111.

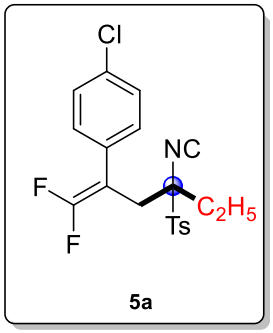
1-((5,5-difluoro-2-isocyano-4-(4-methoxyphenyl)-1-phenylpent-4-en-2-yl)sulfonyl)-4-methylbenzene (4l):



^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.30 (dd, *J* = 8.3, 3.1 Hz, 3H), 7.19 – 7.16 (m, 2H), 6.98 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.70 (s, 3H), 3.22 (dd, *J* = 20.1, 14.8 Hz, 2H), 3.03 (t, *J* = 14.1 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 166.90 (s), 158.81 (s), 153.85 (t, *J* = 289.8 Hz), 146.83 (s), 132.22 (s), 131.07 (s), 130.93 (s), 130.23 (s), 129.73 (s), 129.61 (s), 128.64 (s), 128.21 (s), 127.90 (s), 123.55 (s), 113.81 (s), 87.04 (t, *J* = 19.1 Hz), 80.00 (s), 55.08 (s), 31.71 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -86.84 (d, *J* = 34.5 Hz, 1F), -89.23 (d, *J* = 34.4 Hz, 1F); HRMS (ESI): mass found: 490.1260, calculated mass for

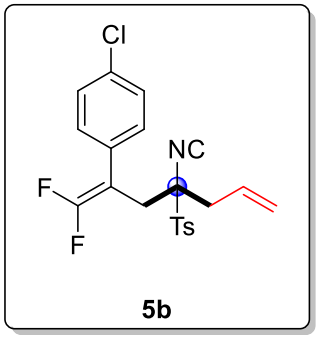
$C_{26}H_{23}F_2NNaO_3S^+$ [M+Na $^+$]: 490.1259.

1-chloro-4-(1,1-difluoro-4-isocyano-4-tosylhex-1-en-2-yl)benzene (5a):



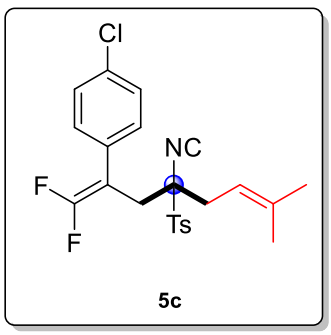
^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.44 (dt, *J* = 19.2, 5.1 Hz, 4H), 3.17 (dd, *J* = 37.3, 15.3 Hz, 2H), 2.45 (s, 3H), 1.81 (ddt, *J* = 32.6, 14.9, 7.4 Hz, 2H), 0.85 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, DMSO) δ 165.80 (s), 154.69 (t, *J* = 290.6 Hz), 147.30 (s), 133.27 (s), 131.29 (s), 131.01 (s), 130.70 (s), 129.94 (s), 129.04 (s), 87.12 (t, *J* = 19.2 Hz), 81.20 (s), 31.24 (s), 27.61 (s), 26.11 (s), 21.69 (s), 8.54 (s); ^{19}F NMR (471 MHz, DMSO) δ -86.00 (d, *J* = 31.3 Hz), -87.45 (d, *J* = 31.2 Hz); HRMS (ESI): mass found: 432.0611, calculated mass for $C_{20}H_{18}ClF_2NNaO_2S$+ [M+Na $^+$]: 432.0607.

1-chloro-4-(1,1-difluoro-4-isocyano-4-tosylhepta-1,6-dien-2-yl)benzene (5b):



^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 5.63 (ddt, *J* = 17.1, 10.2, 7.1 Hz, 1H), 5.11 (ddd, *J* = 18.3, 13.6, 1.2 Hz, 2H), 3.19 (s, 2H), 2.66 – 2.52 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 165.92 (s), 154.12 (t, *J* = 290.6 Hz), 147.01 (s), 132.83 (s), 131.00 (s), 130.72 (s), 130.65 (s), 130.28 (s), 129.24 (s), 128.97 (s), 128.58 (s), 121.48 (s), 86.57 (t, *J* = 18.9 Hz), 79.66 (s), 38.13 (s), 31.05 (s), 21.28 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.67 (d, *J* = 30.6 Hz, 1F), -87.37 (d, *J* = 30.5 Hz, 1F); HRMS (ESI): mass found: 440.0610, calculated mass for $C_{21}H_{18}ClF_2NNaO_2S^+$ [M+Na $^+$]: 444.0607.

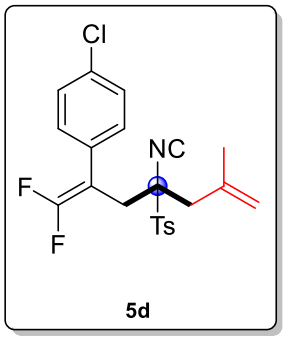
1-chloro-4-(1,1-difluoro-4-isocyano-7-methyl-4-tosylocta-1,6-dien-2-yl)benzene (5c):



^{1}H NMR (500 MHz, DMSO) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.42 (dd, *J* = 27.4, 8.4 Hz, 4H), 4.89 (t, *J* = 6.3 Hz, 1H), 3.25 – 3.17 (m, 1H), 2.44 (s, 3H), 1.57 (s, 3H), 1.35 (s, 3H);

^{13}C NMR (126 MHz, DMSO) δ 166.23 (s), 154.73 (t, *J* = 290.8 Hz), 147.28 (s), 137.59 (s), 133.22 (s), 131.40 (s), 130.97 (s), 130.56 (s), 129.86 (s), 128.98 (s), 114.93 (s), 87.13 (dd, *J* = 19.9, 18.5 Hz), 80.39 (s), 33.20 (s), 31.36 (s), 26.02 (s), 21.66 (s), 18.17 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.67 (d, *J* = 30.6 Hz), -87.51 (d, *J* = 30.6 Hz); HRMS (ESI): mass found: 472.0922, calculated mass for $C_{23}H_{22}ClF_2NNaO_2S^+$ [M+Na $^+$]: 472.0920.

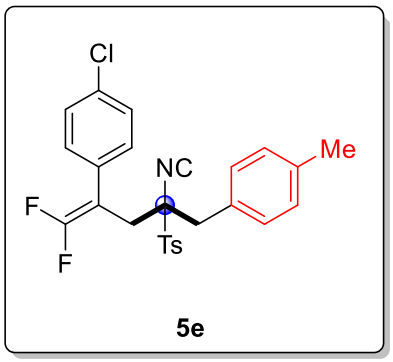
1-chloro-4-(1,1-difluoro-4-isocyano-6-methyl-4-tosylhepta-1,6-dien-2-yl)benzene (5d):



5d

^{1}H NMR (500 MHz, DMSO) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 2H), 5.00 (s, 1H), 4.87 (s, 1H), 3.17 (s, 2H), 2.69 (d, *J* = 14.1 Hz, 1H), 2.45 (s, 3H), 2.32 (d, *J* = 14.1 Hz, 1H), 1.66 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.47 (s), 154.34 (t, *J* = 291.1 Hz), 147.33 (s), 137.67 (s), 133.08 (s), 131.51 (s), 131.07 (s), 130.65 (s), 130.04 (s), 128.87 (s), 119.48 (s), 87.37 (t, *J* = 18.9 Hz), 79.09 (s), 42.52 (s), 31.70 (s), 31.68 (s), 23.43 (s), 21.70 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.43 (d, *J* = 30.8 Hz), -87.91 (d, *J* = 30.8 Hz); HRMS (ESI): mass found: 458.0770, calculated mass for $C_{22}H_{20}ClF_2NNaO_2S^+$ [M+Na $^+$]: 458.0764.

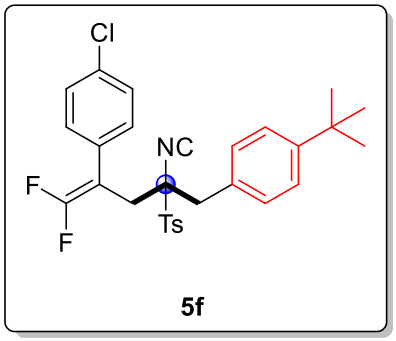
1-chloro-4-(1,1-difluoro-4-isocyano-5-(p-tolyl)-4-tosylpent-1-en-2-yl)benzene (5e):



5e

^{1}H NMR (500 MHz, DMSO) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.07 (q, *J* = 8.4 Hz, 6H), 3.26 (dd, *J* = 26.9, 14.8 Hz, 2H), 2.97 (dd, *J* = 63.4, 14.8 Hz, 2H), 2.45 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 166.86 (s), 153.85 (t, *J* = 290.1 Hz), 146.85 (s), 137.22 (s), 132.53 (s), 131.03 (s), 130.72 (s), 130.39 (s), 130.23 (s), 129.65 (s), 128.83 (d, *J* = 7.0 Hz), 128.32 (s), 125.55 (s), 86.88 (t, *J* = 18.9 Hz), 79.95 (s), 71.17 (s), 31.06 (s), 21.28 (s), 20.71 (s), 18.88 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.23 (d, *J* = 30.6 Hz, 1F), -87.81 (d, *J* = 30.6 Hz, 1F); HRMS (ESI): mass found: 508.0923, calculated mass for $C_{26}H_{22}ClF_2NNaO_2S^+$ [M+Na $^+$]: 508.0920.

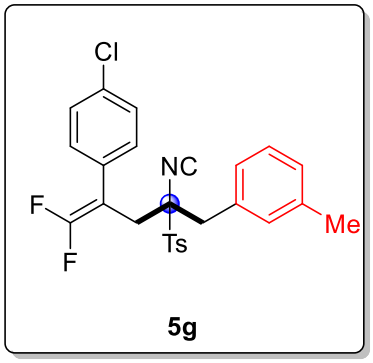
1-(tert-butyl)-4-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)benzene (5f):



5f

^{1}H NMR (500 MHz, DMSO) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 4H), 7.11 (d, *J* = 8.3 Hz, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 3.25 (dd, *J* = 26.1, 14.9 Hz, 2H), 3.02 (dd, *J* = 60.9, 14.8 Hz, 2H), 2.46 (s, 3H), 1.27 (s, 9H); ^{13}C NMR (126 MHz, DMSO) δ 166.97 (s), 153.78 (t, *J* = 286.0 Hz), 150.36 (s), 146.81 (s), 132.50 (s), 131.06 (s), 130.55 (s), 130.32 (s), 130.20 (s), 129.48 (s), 128.89 (s), 128.29 (s), 125.00 (s), 86.83 (t, *J* = 17.6 Hz), 79.87 (s), 34.27 (s), 31.09 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.01 (d, *J* = 30.5 Hz, 1F), -87.75 (d, *J* = 30.5 Hz, 1F); HRMS (ESI): mass found: 550.1395, calculated mass for $C_{29}H_{28}ClF_2NNaO_2S^+$ [M+Na $^+$]: 550.1390.

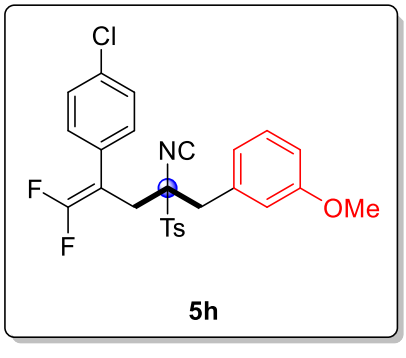
1-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)-3-methylbenzene (5g):



5g

^{1}H NMR (500 MHz, DMSO) δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 6.99 – 6.92 (m, 2H), 3.31 – 3.19 (m, 2H), 2.98 (dd, *J* = 70.0, 14.8 Hz, 2H), 2.46 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.35 (s), 153.06 (dd, *J* = 289.7, 1.7 Hz), 147.31 (s), 137.81 (s), 132.97 (s), 132.25 (s), 131.89 (s), 131.50 (s), 130.82 (s), 130.67 (s), 129.96 (s), 129.01 (s), 128.75 (s), 128.61 (s), 128.32 (s), 87.29 (t, *J* = 19.2 Hz), 80.27 (s), 31.41 (s), 21.72 (s), 21.34 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.17 (d, *J* = 30.7 Hz, 1F), -87.87 (d, *J* = 30.7 Hz, 1F); HRMS (ESI): mass found: 508.0922, calculated mass for $C_{26}H_{22}ClF_2NNaO_2S^+$ [M+Na $^+$]: 508.0920.

1-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)-3-methoxybenzene (5h):

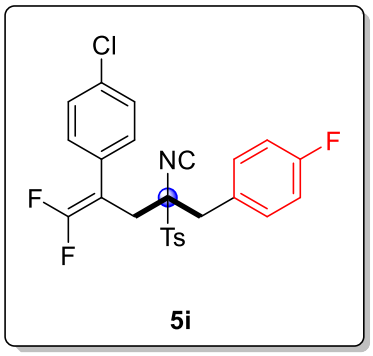


5h

^{1}H NMR (500 MHz, DMSO) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.22 (t, *J*

= 8.1 Hz, 1H), 7.07 (d, *J* = 8.2 Hz, 2H), 6.89 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.75 (d, *J* = 5.8 Hz, 2H), 3.70 (s, 3H), 3.31 – 3.23 (m, 2H), 2.98 (dd, *J* = 57.5, 14.8 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.41 (s), 159.38 (s), 154.23 (t, *J* = 290.4 Hz), 147.35 (s), 133.79 (s), 132.95 (s), 131.48 (s), 131.02 (s), 130.82 (s), 130.80 (s), 130.69 (s), 129.96 (s), 129.77 (s), 128.74 (s), 123.41 (s), 116.86 (s), 113.90 (s), 87.30 (t, *J* = 19.1 Hz), 80.24 (s), 55.42 (s), 31.37 (s), 21.72 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.07 (d, *J* = 30.5 Hz), -87.82 (d, *J* = 30.5 Hz); HRMS (ESI): mass found: 524.0869, calculated mass for $C_{26}H_{22}ClF_2NNaO_3S^+$ [M+Na $^+$]: 524.0869.

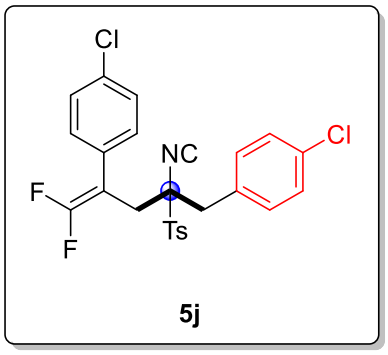
1-chloro-4-(1,1-difluoro-5-(4-fluorophenyl)-4-isocyano-4-tosylpent-1-en-2-yl)benzene (5i):



5i

^{1}H NMR (500 MHz, DMSO) δ 7.83 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.25 (dd, *J* = 8.3, 5.7 Hz, 2H), 7.11 (dt, *J* = 17.4, 8.5 Hz, 4H), 3.29 (dd, *J* = 32.3, 15.0 Hz, 2H), 3.03 (dd, *J* = 20.4, 15.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.21 (s), 161.92 (dd, *J* = 244.6, 17.3 Hz), 153.98 (t, *J* = 290.7 Hz), 146.85 (s), 132.77 (dd, *J* = 19.9, 9.3 Hz), 130.99 (d, *J* = 5.9 Hz), 130.22 (t, *J* = 12.8 Hz), 129.66 (s), 128.21 (dd, *J* = 16.9, 13.9 Hz), 125.63 (s), 115.02 (dd, *J* = 21.4, 5.8 Hz), 86.69 (dd, *J* = 32.8, 13.5 Hz), 81.53 (s), 79.88 (s), 59.76 (s), 38.66 (s), 37.95 (s), 31.26 (s), 21.22 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.12 (d, *J* = 30.3 Hz, 1F), -87.60 (d, *J* = 30.3 Hz, 1F), -114.33 (d, *J* = 7.5 Hz, 1F); HRMS (ESI): mass found: 512.0672, calculated mass for $C_{25}H_{19}ClF_3NNaO_2S^+$ [M+Na $^+$]: 512.0669.

4,4'-(5,5-difluoro-2-isocyano-2-tosylpent-4-ene-1,4-diyl)bis(chlorobenzene) (5j):

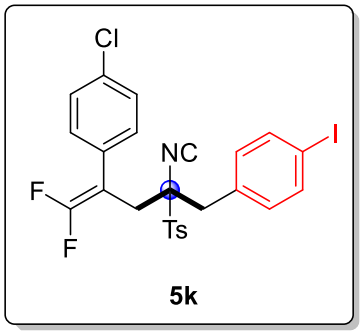


5j

^{1}H NMR (500 MHz, DMSO) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 7.35 (dd, *J* = 8.6, 2.7 Hz, 4H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 7.9 Hz, 2H), 3.29 (dd, *J* = 34.8, 15.1 Hz, 2H), 3.03 (dd, *J* = 19.3, 14.9 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.11 (s), 153.97 (t, *J* = 290.6 Hz), 146.93 (s), 132.87 (s), 132.67 (d, *J* = 8.8 Hz), 131.04 (d, *J* = 7.0 Hz), 130.59 (s), 130.32 (d, *J* = 17.0 Hz), 129.56 (s), 128.39 (s), 128.17 (s), 86.72 (t, *J* = 19.3 Hz), 79.83 (s), 71.16 (s), 38.62 (s), 31.48 (s), 27.23 (s), 21.29 (s), 18.87 (s); ^{19}F

NMR (471 MHz, DMSO) δ -85.19 (d, *J* = 30.3 Hz, 1F), -87.55 (d, *J* = 30.3 Hz, 1F); HRMS (ESI): mass found: 528.0377, calculated mass for $C_{25}H_{19}ClF_3NNaO_2S^+$ [M+Na $^+$]: 528.0374.

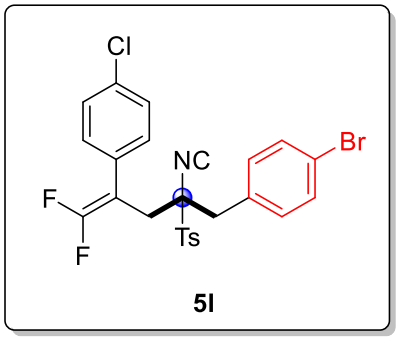
1-chloro-4-(1,1-difluoro-5-(4-iodophenyl)-4-isocyano-4-tosylpent-1-en-2-yl)benzene (5k):



5k

^{1}H NMR (500 MHz, DMSO) δ 7.80 (dd, *J* = 8.3, 6.5 Hz, 2H), 7.65 – 7.52 (m, 4H), 7.35 (d, *J* = 8.6 Hz, 1H), 7.06 (dd, *J* = 72.7, 8.1 Hz, 3H), 6.93 (d, *J* = 8.3 Hz, 1H), 3.25 (dd, *J* = 26.2, 13.9 Hz, 2H), 3.00 (dd, *J* = 44.1, 14.8 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.06 (s), 153.95 (t, *J* = 292.3 Hz), 146.88 (s), 136.94 (s), 133.06 (d, *J* = 4.0 Hz), 132.60 (s), 132.20 (s), 131.78 (s), 130.93 (d, *J* = 11.2 Hz), 130.25 (t, *J* = 12.7 Hz), 129.53 (s), 128.37 (s), 94.49 (s), 94.31 (s), 86.69 (t, *J* = 19.3 Hz), 81.17 (s), 79.74 (s), 31.46 (s), 21.30 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.14 (d, *J* = 30.3 Hz, 1F), -87.47 (d, *J* = 30.2 Hz, 1F); HRMS (ESI): mass found: 619.9730, calculated mass for $C_{25}H_{19}ClF_2INNaO_2S^+$ [M+Na $^+$]: 619.9730.

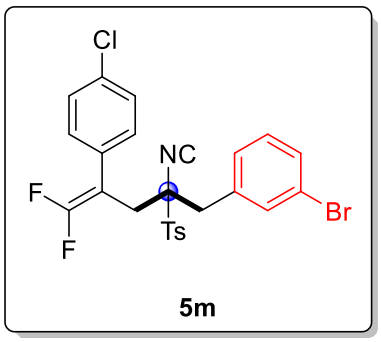
1-bromo-4-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)benzene (5l):



5l

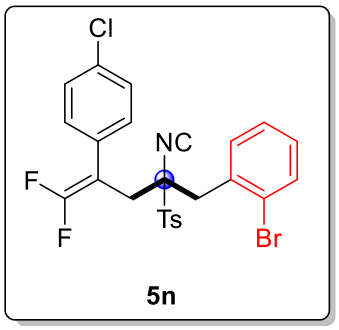
^{1}H NMR (500 MHz, DMSO) δ 7.87 – 7.79 (m, 2H), 7.52 (t, *J* = 8.9 Hz, 2H), 7.48 – 7.07 (m, 8H), 3.34 – 2.96 (m, 4H), 2.44 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 166.72 (d, *J* = 107.1 Hz), 164.23 (s), 153.99 (t, *J* = 290.7 Hz), 146.67 (d, *J* = 11.6 Hz), 132.87 (t, *J* = 22.7 Hz), 131.67 (d, *J* = 52.4 Hz), 131.28 – 130.69 (m), 130.24 (dd, *J* = 16.3, 10.1 Hz), 129.68 (d, *J* = 32.7 Hz), 128.59 (d, *J* = 53.2 Hz), 121.50 (s), 121.33 (s), 86.69 (t, *J* = 19.4 Hz), 81.21 (s), 79.77 (s), 69.43 (s), 31.48 (s), 27.25 (s), 21.27 (d, *J* = 4.9 Hz); ^{19}F NMR (471 MHz, DMSO) δ -85.09 (d, *J* = 30.2 Hz, 1F), -87.46 (d, *J* = 30.5 Hz, 1F); HRMS (ESI): mass found: 571.9810, calculated mass for $C_{25}H_{19}BrF_2NNaO_2S^+$ [M+Na $^+$]: 571.9869.

1-bromo-3-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)benzene (5m):



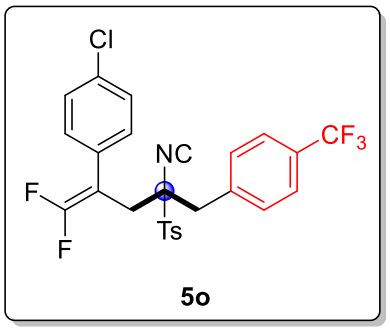
^{1}H NMR (500 MHz, DMSO) δ 7.82 (dd, *J* = 12.8, 8.3 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.47 (dd, *J* = 21.1, 8.0 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.30 – 7.16 (m, 3H), 7.11 (dd, *J* = 24.1, 8.0 Hz, 2H), 3.30 (dd, *J* = 19.3, 12.5 Hz, 2H), 3.10 (dd, *J* = 61.3, 47.8 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.21 (s), 166.32 (s), 153.96 (t, *J* = 290.7 Hz), 146.96 (s), 135.13 (s), 134.81 (s), 133.47 (d, *J* = 8.3 Hz), 132.66 (s), 131.02 (s), 130.78 (s), 130.70 (s), 130.29 (t, *J* = 10.3 Hz), 129.94 (d, *J* = 13.1 Hz), 129.46 (s), 128.42 (s), 121.36 (s), 86.65 (t, *J* = 19.3 Hz), 81.30 (s), 79.81 (s), 31.55 (s), 21.31 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.07 (d, *J* = 30.2 Hz, 1F), -87.42 (d, *J* = 30.2 Hz, 1F); HRMS (ESI): mass found: 571.9871, calculated mass for $C_{25}H_{19}BrF_2NNaO_2S^+$ [M+Na $^+$]: 571.9869.

1-bromo-2-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)benzene (5n):



^{1}H NMR (500 MHz, DMSO) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.58 (dd, *J* = 22.2, 7.8 Hz, 3H), 7.35 (dd, *J* = 20.2, 5.1 Hz, 4H), 7.25 (td, *J* = 7.8, 1.6 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 2H), 3.56 – 3.40 (m, 2H), 3.15 (dd, *J* = 56.4, 15.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.02 (s), 154.03 (t, *J* = 290.8 Hz), 147.01 (s), 133.16 (s), 132.82 (s), 132.51 (s), 131.69 (s), 131.19 (s), 130.36 (s), 130.31 (s), 130.20 (s), 129.44 (s), 128.33 (s), 127.75 (s), 125.74 (s), 86.89 (t, *J* = 19.2 Hz), 79.43 (s), 38.75 (s), 30.89 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -84.96 (d, *J* = 30.0 Hz, 1F), -87.69 (d, *J* = 29.9 Hz, 1F); HRMS (ESI): mass found: 571.9872, calculated mass for $C_{25}H_{19}BrF_2NNaO_2S^+$ [M+Na $^+$]: 571.9869.

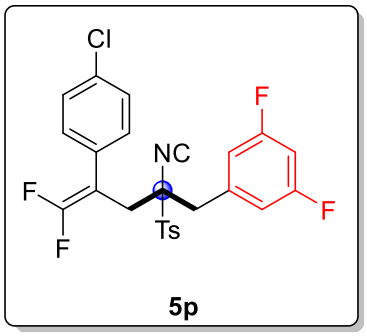
1-chloro-4-(1,1-difluoro-4-isocyano-4-tosyl-5-(4-(trifluoromethyl)phenyl)pent-1-en-2-yl)benzene (5o):



^{1}H NMR (500 MHz, DMSO) δ 7.82 (dd, *J* = 8.2, 5.7 Hz, 2H), 7.65 – 7.30 (m, 9H), 7.15 (d, *J* = 8.0 Hz, 1H), 3.45 – 3.37 (m,

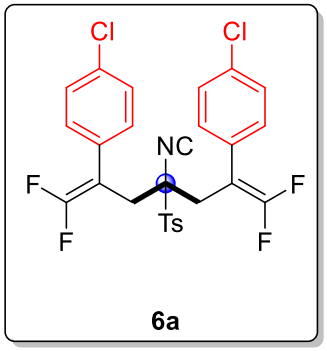
3H), 3.36 – 3.08 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.13 (d, *J* = 74.1 Hz), 154.13 (t, *J* = 290.7 Hz), 146.87 (d, *J* = 18.0 Hz), 137.07 (d, *J* = 26.8 Hz), 132.71 (s), 131.72 (d, *J* = 13.5 Hz), 131.04 (s), 130.23 (dd, *J* = 15.9, 10.6 Hz), 129.84 (s), 129.57 (d, *J* = 16.9 Hz), 129.06 – 128.19 (m), 125.24 (d, *J* = 6.1 Hz), 124.89 (s), 123.08 (d, *J* = 6.1 Hz), 120.90 (s), 86.62 (t, *J* = 19.4 Hz), 81.12 (s), 79.85 (s), 31.78 (s), 21.21 (d, *J* = 2.7 Hz); ^{19}F NMR (471 MHz, DMSO) δ -61.25 (s, 3F), -85.09 (d, *J* = 30.1 Hz, 1F), -87.39 (d, *J* = 30.0 Hz, 1F); HRMS (ESI): mass found: 562.0636, calculated mass for $C_{26}H_{19}ClF_5NNaO_2S^+$ [M+Na $^+$]: 562.0637.

1-(4-(4-chlorophenyl)-5,5-difluoro-2-isocyano-2-tosylpent-4-en-1-yl)-3,5-difluorobenzene (5p):



^{1}H NMR (500 MHz, DMSO) δ 7.83 (dd, *J* = 12.7, 8.3 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.28 – 7.09 (m, 3H), 6.90 (dd, *J* = 41.0, 6.3 Hz, 3H), 3.37 – 2.94 (m, 4H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.34 (s), 162.84 (d, *J* = 13.4 Hz), 160.88 (dd, *J* = 13.4, 3.0 Hz), 154.03 (t, *J* = 290.7 Hz), 147.05 (s), 136.46 (dt, *J* = 36.3, 9.8 Hz), 132.71 (s), 131.05 (s), 130.38 (d, *J* = 14.4 Hz), 129.50 (s), 128.47 (d, *J* = 11.8 Hz), 114.54 – 113.88 (m), 103.49 (td, *J* = 25.6, 13.8 Hz), 86.66 (t, *J* = 19.4 Hz), 80.90 (s), 79.74 (s), 38.08 (s), 31.62 (s), 21.29 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.16 (d, *J* = 30.1 Hz, 1F), -87.48 (d, *J* = 30.2 Hz, 1F), -110.14 (t, *J* = 8.5 Hz, 1F), -110.28 (t, *J* = 8.6 Hz, 1F); HRMS (ESI): mass found: 530.0580, calculated mass for $C_{25}H_{18}ClF_4NNaO_2S^+$ [M+Na $^+$]: 530.0575.

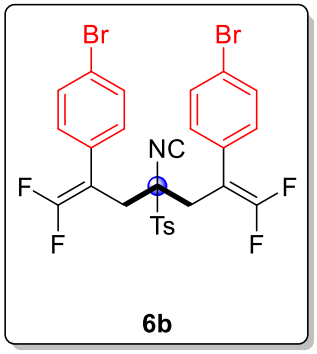
4,4'-(1,1,7,7-tetrafluoro-4-isocyano-4-tosylhepta-1,6-diene-2,6-diyl)bis(chlorobenzene) (6a):



^{1}H NMR (500 MHz, DMSO) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.39 (m, 4H), 7.25 (d, *J* = 7.8 Hz, 4H), 3.20 (d, *J* = 15.5 Hz, 2H), 2.97 (d, *J* = 15.4 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.14 (s), 154.05 (t, *J* = 290.5 Hz), 147.14 (s), 132.80 (s), 131.02 (s), 130.54 (s), 130.33 (d, *J* = 6.5 Hz), 129.53 (s), 128.52 (s), 86.56 (t, *J* = 19.4 Hz), 78.02 (s), 32.20 (s), 21.30 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.67 (d, *J* = 30.8 Hz, 2F), -87.37 (d, *J* = 30.7 Hz,

2F); HRMS (ESI): mass found: 590.0381, calculated mass for $C_{27}H_{19}Cl_2F_4NNaO_2S^+$ [M+Na $^+$]: 590.0342.

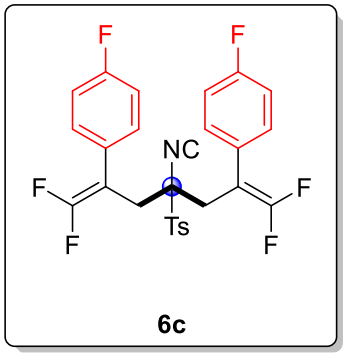
4,4'-(1,1,7,7-tetrafluoro-4-isocyano-4-tosylhepta-1,6-diene-2,6-diyl)bis(bromobenzene) (6b):



6b

^{1}H NMR (500 MHz, DMSO) δ 7.80 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 6H), 7.19 (d, *J* = 7.9 Hz, 4H), 3.19 (d, *J* = 15.5 Hz, 2H), 2.97 (d, *J* = 15.4 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.14 (s), 153.97 (t, *J* = 290.7 Hz), 147.10 (s), 131.42 (s), 130.99 (s), 130.75 (s), 130.27 (s), 129.50 (s), 121.39 (s), 86.60 (t, *J* = 18.9 Hz), 78.06 (s), 32.13 (s), 21.28 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.48 (d, *J* = 30.4 Hz, 2F), -87.26 (d, *J* = 30.3 Hz, 2F); HRMS (ESI): mass found: 677.9330, calculated mass for $C_{27}H_{19}Br_2F_4NNaO_2S^+$ [M+Na $^+$]: 677.9332.

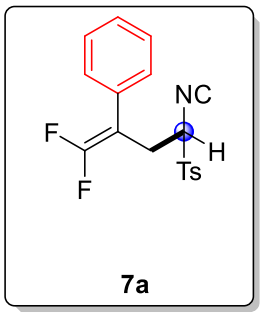
4,4'-(1,1,7,7-tetrafluoro-4-isocyano-4-tosylhepta-1,6-diene-2,6-diyl)bis(fluorobenzene) (6c):



6c

^{1}H NMR (500 MHz, DMSO) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.27 (dd, *J* = 8.1, 5.6 Hz, 4H), 7.18 (t, *J* = 8.8 Hz, 4H), 3.20 (d, *J* = 15.5 Hz, 2H), 2.97 (d, *J* = 15.6 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 168.06 (s), 162.71 (s), 160.76 (s), 154.01 (t, *J* = 289.8 Hz), 147.06 (s), 131.20 – 130.63 (m), 130.27 (s), 129.61 (s), 127.68 (s), 115.40 (d, *J* = 21.7 Hz), 86.57 (t, *J* = 19.5 Hz), 77.95 (s), 32.41 (s), 21.25 (s); ^{19}F NMR (471 MHz, DMSO) δ -86.68 (d, *J* = 32.6 Hz, 2F), -88.17 (d, *J* = 32.6 Hz, 2F), -113.57 – -113.68 (m, 2F); HRMS (ESI): mass found: 558.0950, calculated mass for $C_{27}H_{19}F_6NNaO_2S^+$ [M+Na $^+$]: 558.0933.

1-((4,4-difluoro-1-isocyano-3-phenylbut-3-en-1-yl)sulfonyl)-4-methylbenzene (7a):

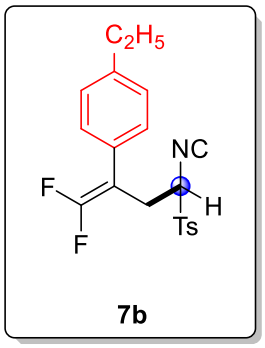


7a

^{1}H NMR (500 MHz, DMSO) δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.38 (dd, *J* = 21.9, 6.9 Hz, 5H), 5.56 (dd, *J* = 10.6, 3.7 Hz, 1H), 3.22 (dd, *J* = 14.7, 3.0 Hz, 1H), 3.00 – 2.92 (m, 1H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.58 (s), 154.65 (t, *J* = 290.0 Hz), 147.09

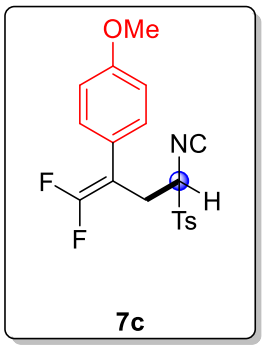
(s), 131.17 (s), 130.63 (s), 130.29 (s), 129.22 (s), 128.87 (t, *J* = 2.8 Hz), 128.76 (s), 88.11 (dd, *J* = 19.4, 18.2 Hz), 69.99 (s), 27.82 (s), 21.69 (s), 19.33 (s); ^{19}F NMR (471 MHz, DMSO) δ -88.11 (d, *J* = 35.5 Hz, 1F), -88.42 (dd, *J* = 35.5, 2.6 Hz, 1F); HRMS (ESI): mass found: 370.0688, calculated mass for $C_{18}H_{15}F_2NNaO_2S^+$ [M+Na $^+$]: 370.0684.

1-(1,1-difluoro-4-isocyano-4-tosylbut-1-en-2-yl)-4-ethylbenzene (7b):



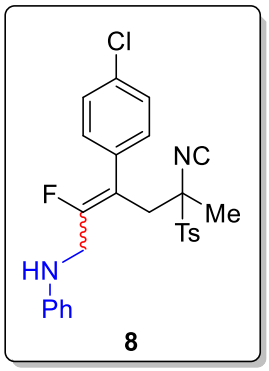
^{1}H NMR (500 MHz, DMSO) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.29 – 7.22 (m, 4H), 5.54 (dd, *J* = 10.7, 3.8 Hz, 1H), 3.19 (ddd, *J* = 14.6, 6.5, 3.4 Hz, 1H), 2.94 (ddd, *J* = 14.7, 10.7, 1.8 Hz, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 2.45 (s, 3H), 1.17 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.06 (s), 154.21 (t, *J* = 289.7 Hz), 146.66 (s), 143.94 (s), 130.75 (s), 130.19 (s), 129.88 (s), 128.32 (t, *J* = 2.8 Hz), 128.20 (s), 127.96 (s), 87.49 (dd, *J* = 19.1, 18.4 Hz), 69.57 (s), 27.86 (s), 27.40 (s), 21.27 (s), 15.37 (s); ^{19}F NMR (471 MHz, DMSO) δ -88.49 (d, *J* = 36.5 Hz, 1F), -88.68 (dd, *J* = 36.5, 3.1 Hz, 1F); HRMS (ESI): mass found: 398.0998, calculated mass for $C_{20}H_{19}F_2NNaO_2S^+$ [M+Na $^+$]: 398.0997.

1-((4,4-difluoro-1-isocyano-3-(4-methoxyphenyl)but-3-en-1-yl)sulfonyl)-4-methylbenzene (7c):



^{1}H NMR (500 MHz, DMSO) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.6 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 5.51 (dd, *J* = 10.6, 3.7 Hz, 1H), 3.76 (s, 3H), 3.18 (dd, *J* = 14.7, 3.3 Hz, 1H), 2.98 – 2.88 (m, 1H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.05 (s), 159.11 (s), 154.08 (t, J = 289.2 Hz), 146.65 (s), 130.78 (s), 130.19 (s), 129.86 (s), 129.72 (t, J = 2.8 Hz), 122.58 (s), 114.24 (s), 87.23 (t, J = 19.0 Hz), 69.59 (s), 55.17 (s), 27.53 (s), 21.26 (s); ^{19}F NMR (471 MHz, DMSO) δ -89.31 (d, *J* = 38.2 Hz, 1F), -89.42 (dd, *J* = 38.3, 2.7 Hz, 1F); HRMS (ESI): mass found: 400.0793, calculated mass for $C_{19}H_{17}F_2NNaO_3S^+$ [M+Na $^+$]: 400.0789.

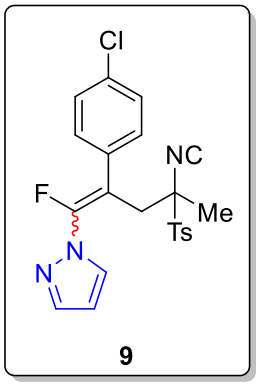
***N*-(3-(4-chlorophenyl)-2-fluoro-5-isocyano-5-tosylhex-2-en-1-yl)aniline (8):**



8

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.36 (m, 4H), 7.18 – 7.15 (m, 2H), 7.14 – 7.10 (m, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.40 (d, *J* = 7.7 Hz, 2H), 3.92 (d, *J* = 18.9 Hz, 2H), 3.22 – 3.14 (m, 2H), 2.48 (s, 3H), 1.49 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.16 (s), 159.16 (s), 157.08 (s), 146.72 (d, *J* = 13.0 Hz), 134.65 (d, *J* = 7.6 Hz), 131.48 (s), 130.52 (d, *J* = 2.6 Hz), 130.06 (s), 129.30 (d, *J* = 3.4 Hz), 128.92 (s), 118.72 (s), 114.14 (d, *J* = 17.0 Hz), 113.58 (s), 77.72 (s), 42.34 (s), 42.12 (s), 34.03 (d, *J* = 5.8 Hz), 21.94 (s), 21.23 (s); ^{19}F NMR (471 MHz, $CDCl_3$) δ -105.38 (t, *J* = 18.9 Hz, 1F); HRMS (ESI): mass found: 505.1129, calculated mass for $C_{26}H_{24}ClFN_2NaO_2S^+$ [M+Na $^+$]: 505.1123.

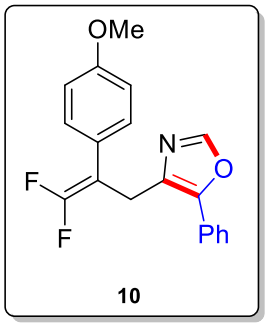
1-(2-(4-chlorophenyl)-1-fluoro-4-isocyano-4-tosylpent-1-en-1-yl)-1H-pyrazole (9):



9

^{1}H NMR (500 MHz, DMSO) δ 7.88 (d, *J* = 8.3 Hz, 2H), 7.70 (dd, *J* = 10.9, 2.0 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 7.33 – 7.28 (m, 2H), 7.16 – 7.13 (m, 2H), 6.33 (dd, *J* = 2.4, 1.9 Hz, 1H), 3.38 (d, *J* = 2.1 Hz, 2H), 2.47 (s, 3H), 1.53 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 164.87 (s), 148.47 (s), 147.05 (s), 146.35 (s), 142.58 (s), 133.03 (dd, *J* = 12.6, 9.3 Hz), 131.18 (s), 130.33 (s), 130.14 (d, *J* = 2.9 Hz), 128.57 (s), 128.21 (s), 109.10 (d, *J* = 25.4 Hz), 107.84 (s), 77.13 (d, *J* = 3.3 Hz), 33.62 (s), 21.31 (s), 20.93 (s); ^{19}F NMR (471 MHz, DMSO) δ -85.49 (s, 1F); HRMS (ESI): mass found: 466.0766, calculated mass for $C_{22}H_{19}ClFN_3NaO_2S^+$ [M+Na $^+$]: 466.0763.

4-(3,3-difluoro-2-(4-methoxyphenyl)allyl)-5-phenyloxazole (10):

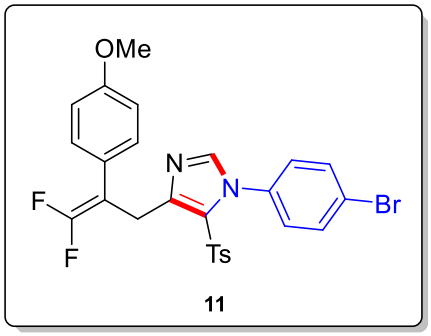


10

^{1}H NMR (500 MHz, DMSO) δ 8.31 (s, 1H), 7.55 – 7.52 (m, 2H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.14 (d, *J* = 8.1 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 2H), 3.68 (s, 3H); ^{13}C NMR (126 MHz,

DMSO) δ 158.93 (s), 153.84 (t, *J* = 287.0 Hz), 151.21 (s), 145.93 (s), 132.07 (s), 129.86 (t, *J* = 3.0 Hz), 129.42 (s), 128.90 (s), 128.23 (s), 126.21 (s), 125.14 – 124.85 (m), 114.20 (s), 90.55 (dd, *J* = 20.4, 15.3 Hz), 55.44 (s), 26.01 (s); ^{19}F NMR (471 MHz, DMSO) δ -91.84 (d, *J* = 44.1 Hz), -92.43 (d, *J* = 44.1 Hz); HRMS (ESI): mass found: 350.0966, calculated mass for $C_{19}H_{15}F_2NNaO_2^+$ [M+Na$^+$]: 350.0963.

1-(4-bromophenyl)-4-(3,3-difluoro-2-(4-methoxyphenyl)allyl)-5-tosyl-1H-imidazole (11):



11

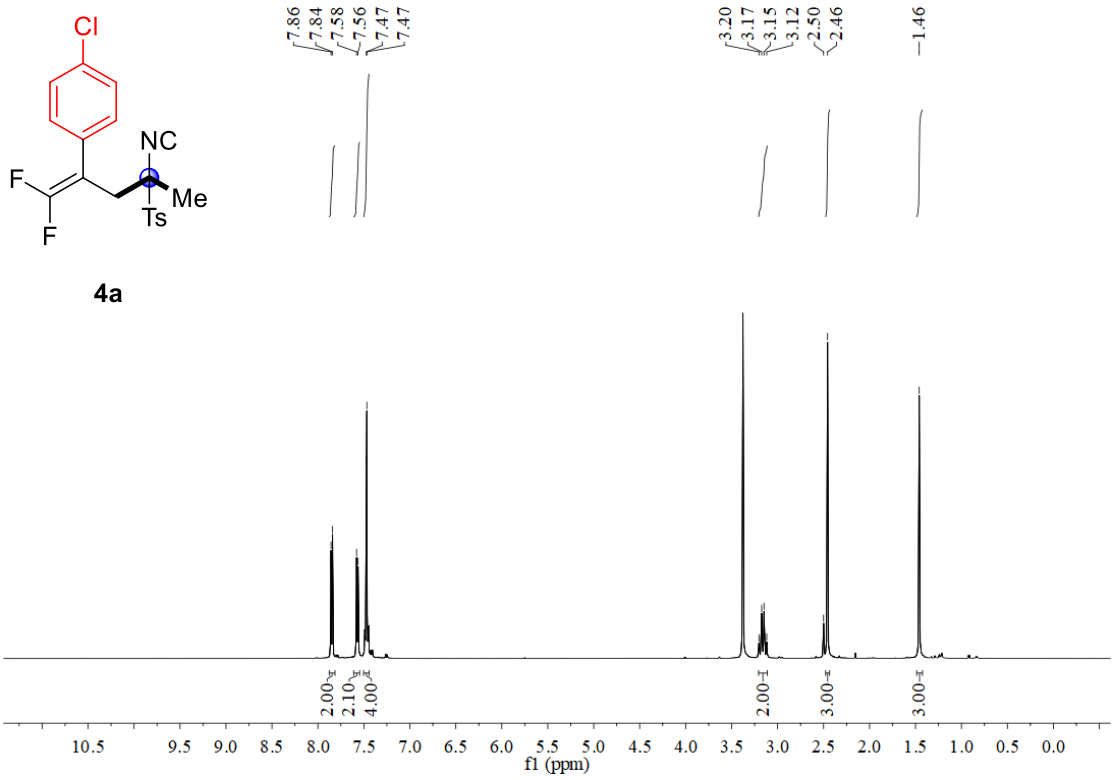
^{1}H NMR (500 MHz, DMSO) δ 7.98 (s, 1H), 7.59 (d, *J* = 8.7 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.10 (s, 2H), 3.76 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 159.01 (s), 154.14 (t, *J* = 286.8 Hz), 146.54 (s), 145.00 (s), 142.87 (s), 138.30 (s), 134.01 (s), 132.04 (d, *J* = 13.6 Hz), 130.36 (s), 130.11 (dd, *J* = 6.7, 3.7 Hz), 127.04 (s), 126.09 (s), 125.31 (s), 123.44 (s), 120.69 (s), 114.33 (s), 90.59 (dd, *J* = 20.8, 15.8 Hz), 55.54 (s), 27.16 (s), 21.52 (s); ^{19}F NMR (471 MHz, DMSO) δ -91.67 (dd, *J* = 43.4, 1.3 Hz), -92.47 (d, *J* = 43.3 Hz); HRMS (ESI): mass found: 581.0320, calculated mass for $C_{26}H_{21}BrF_2N_2NaO_3S^+$ [M+Na$^+$]: 581.0317.

References:

1. T. Ichitsuka, T. Fujita and J. Ichikawa, Nickel-Catalyzed C (sp^3)-F Bond Activation of Trifluoromethyl Groups via *β*-Fluorine Elimination: Synthesis of Difluoro-1,4-dienes, *ACS Catal.*, 2015, **5**, 5947.

2. P. S. Bhadury, B. P. Pant, M. Palit and D. K. Jaiswa, Synthesis of 2-phenylperfluoropropene and 1,1,1,3,3,3-hexafluoro-2-phenylpropane, *J. Fluor. Chem.*, 1997, **85**, 115.

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



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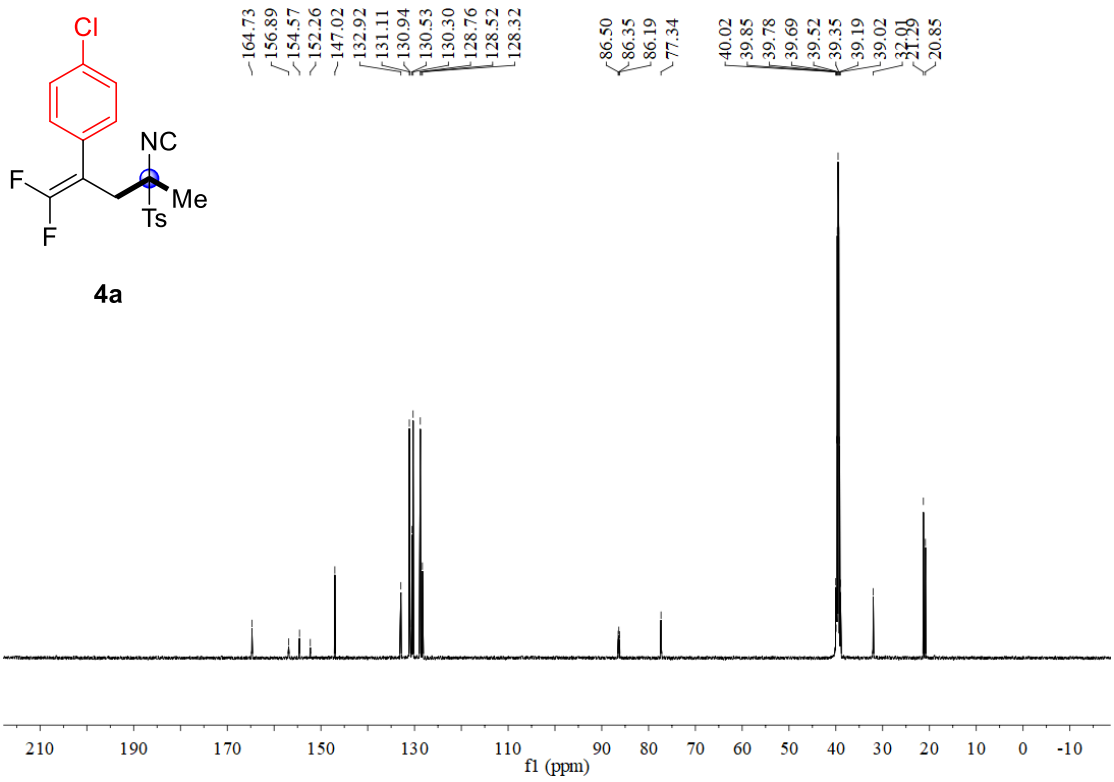

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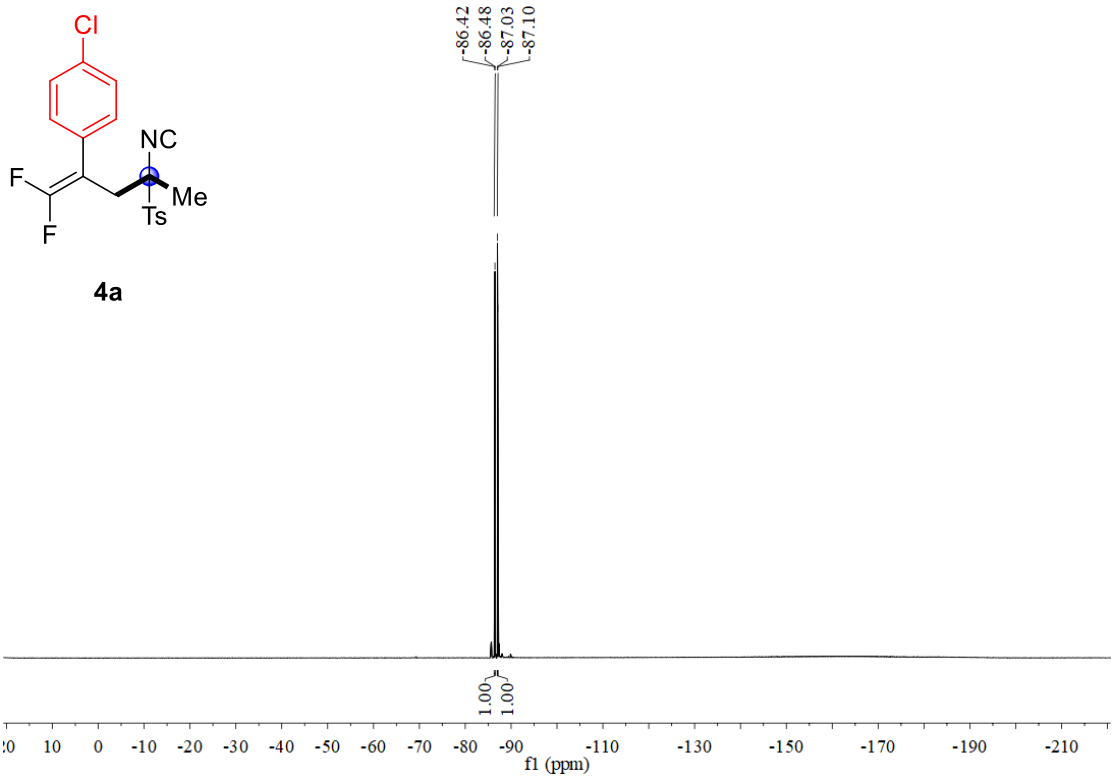
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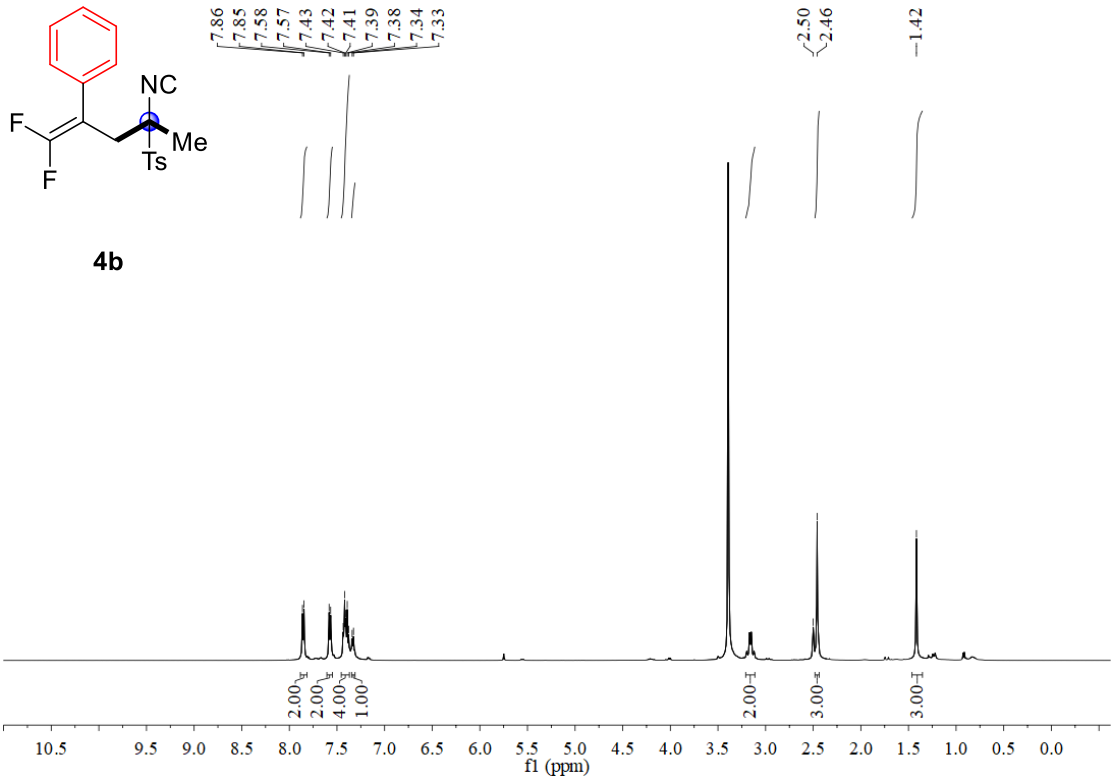
f1 (ppm)

4a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F
Me
Ts
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7.42
7.41
7.39
7.38
7.34
7.33
2.50
2.46
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2.00
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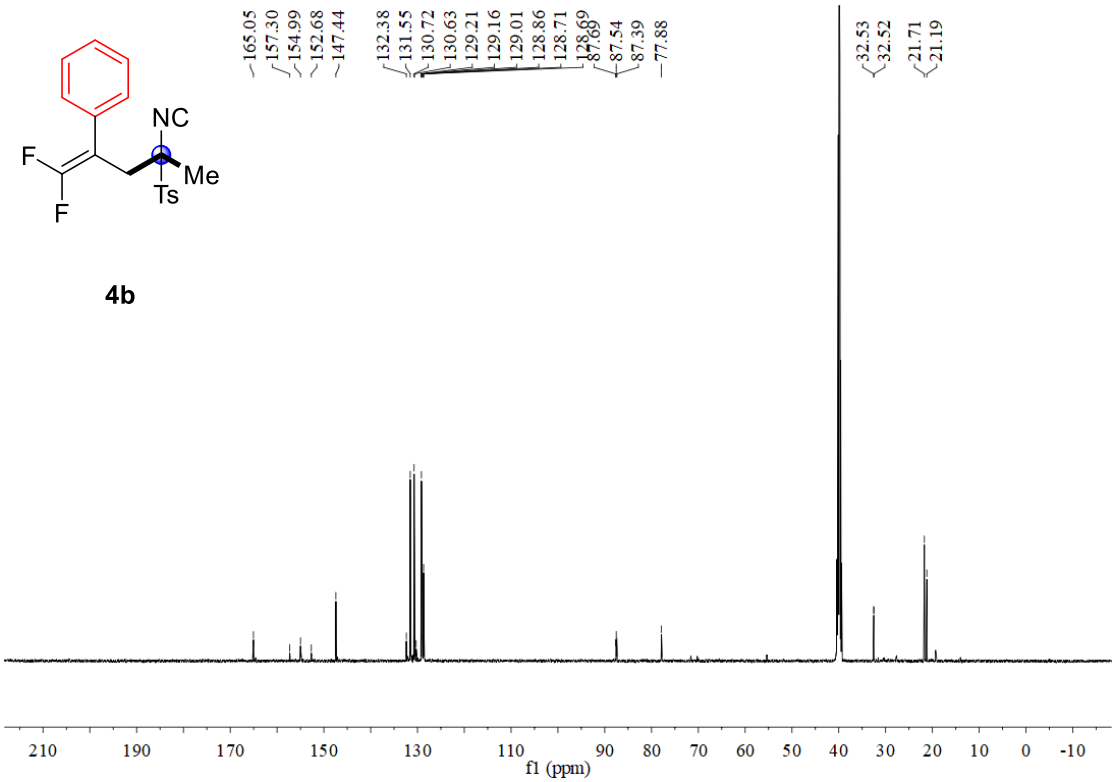
f1 (ppm)

4b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Ts
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129.21
129.16
129.01
128.86
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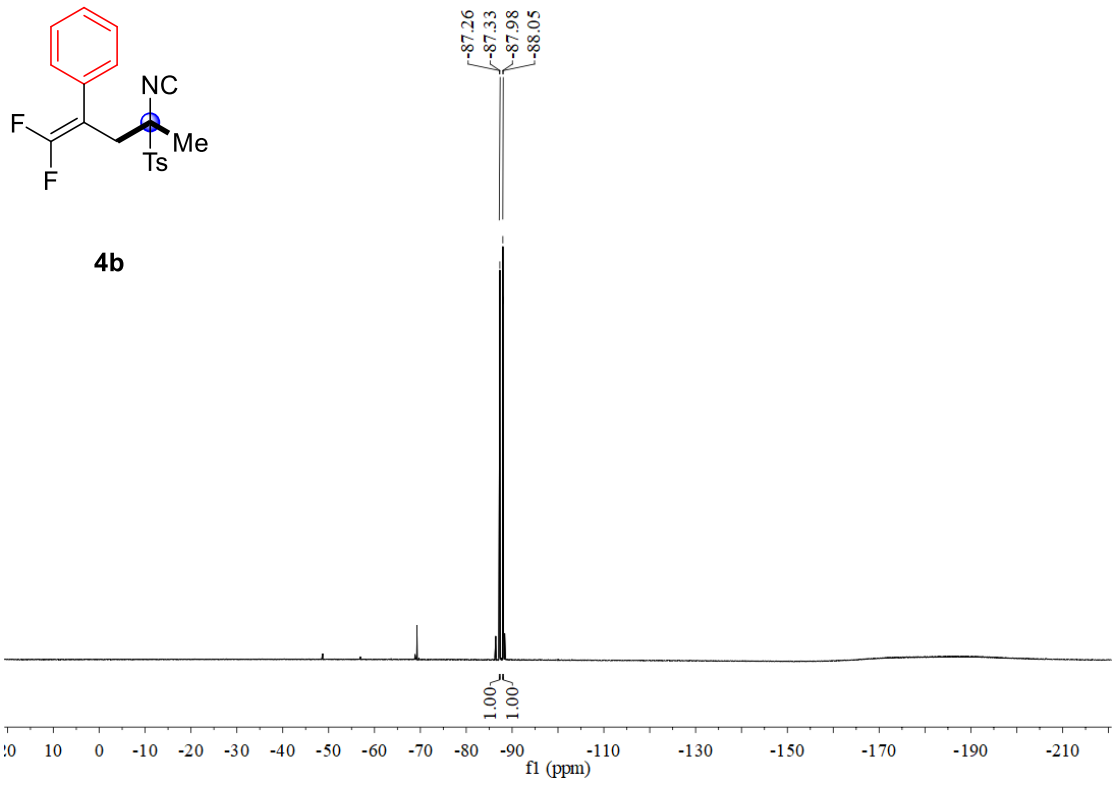
21.19
f1 (ppm)

4b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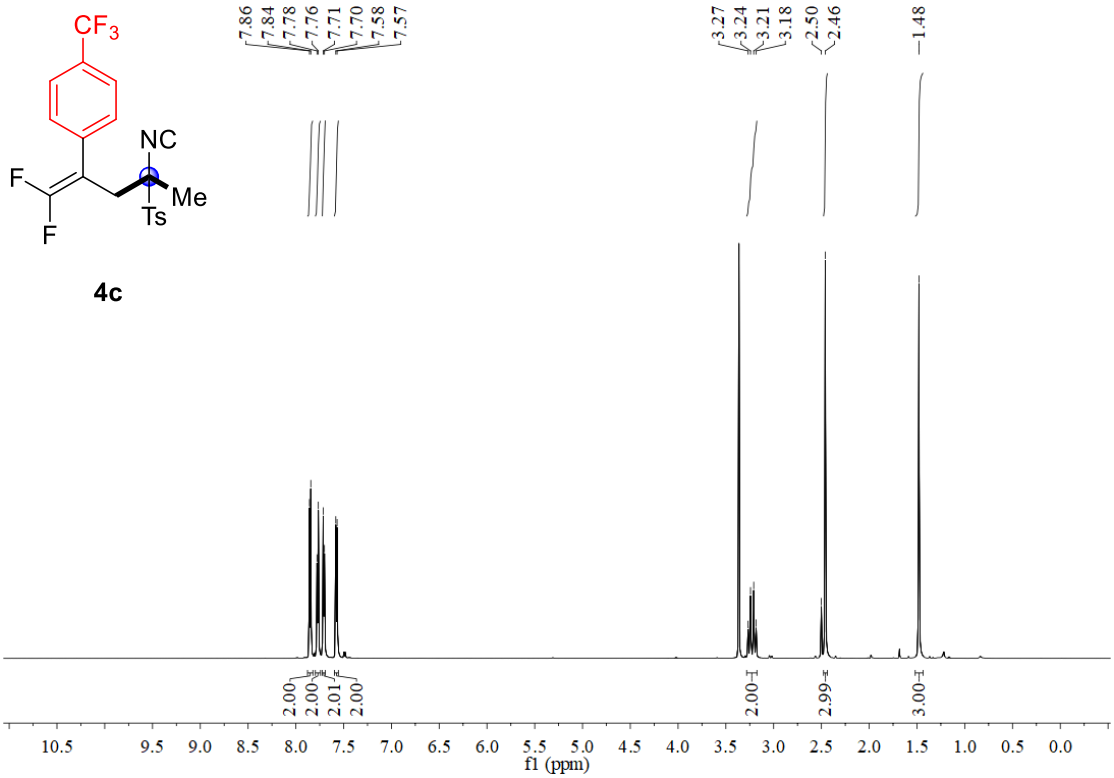
4b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Me
Ts
F
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7.70
7.58
7.57
3.27
3.24
3.21
3.18
2.50
2.46
1.48
2.00
2.00
2.01
2.00
2.00
2.99
3.00
10.5
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7.5
7.0
6.5
6.0
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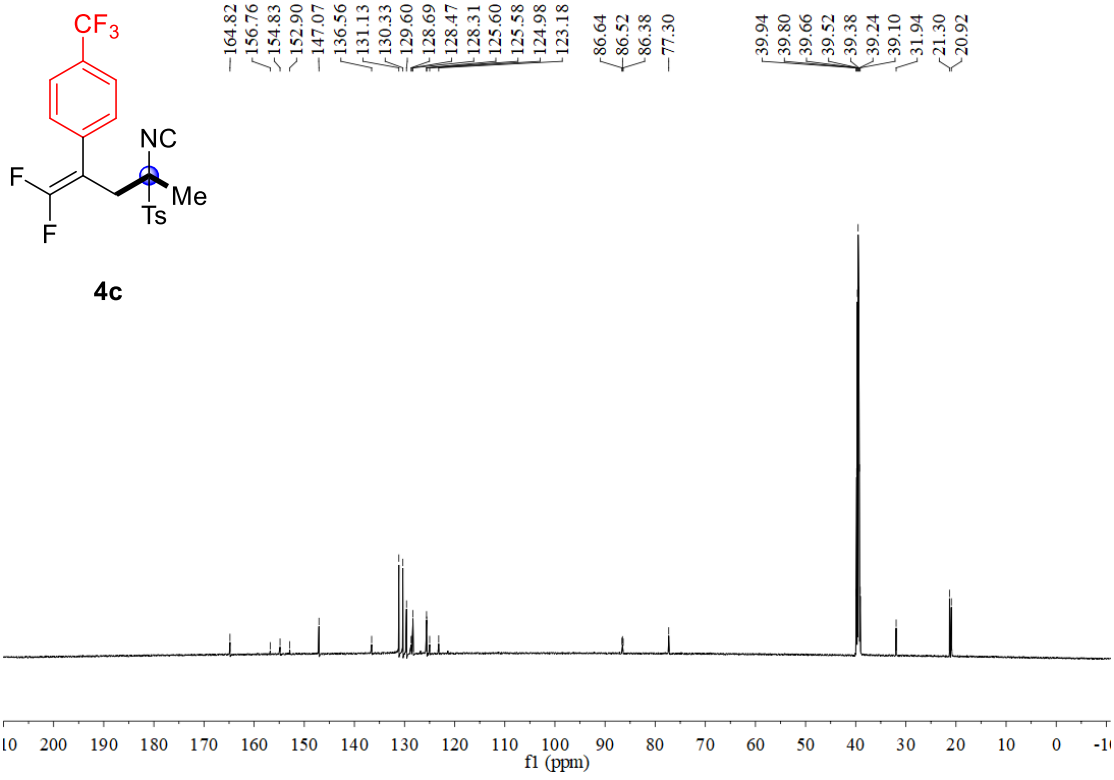
f1 (ppm)

4c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Me
Ts
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129.60
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128.47
128.31
125.60
125.58
124.98
123.18
86.64
86.52
86.38
77.30
39.94
39.80
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39.10
31.94
21.30
20.92
200
190
180
170
160
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140
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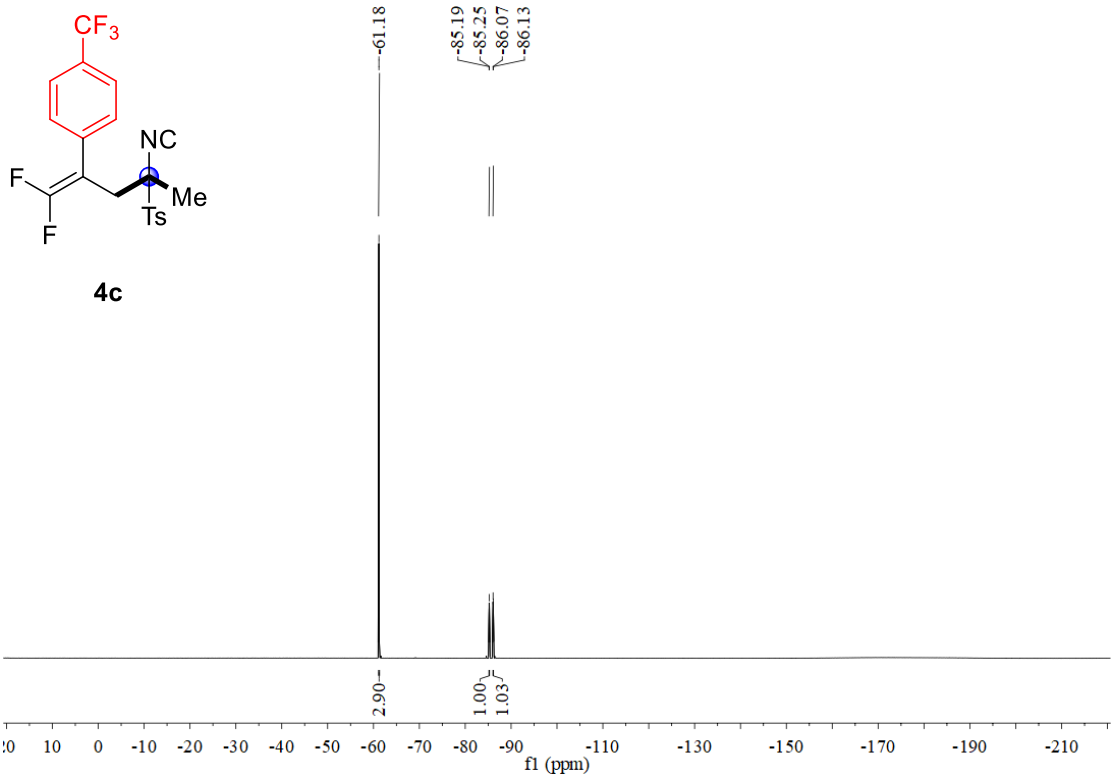
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4c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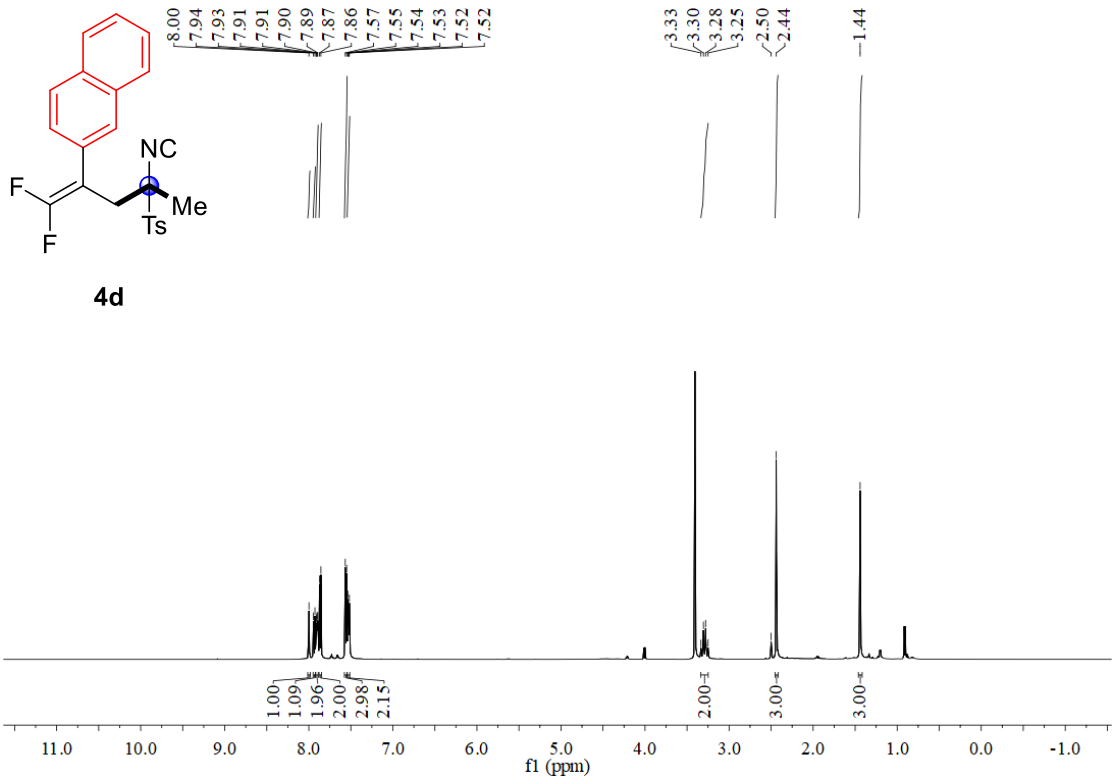
f1 (ppm)

4c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7.54
7.53
7.52
7.52
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3.30
3.28
3.25
2.50
2.44
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1.96
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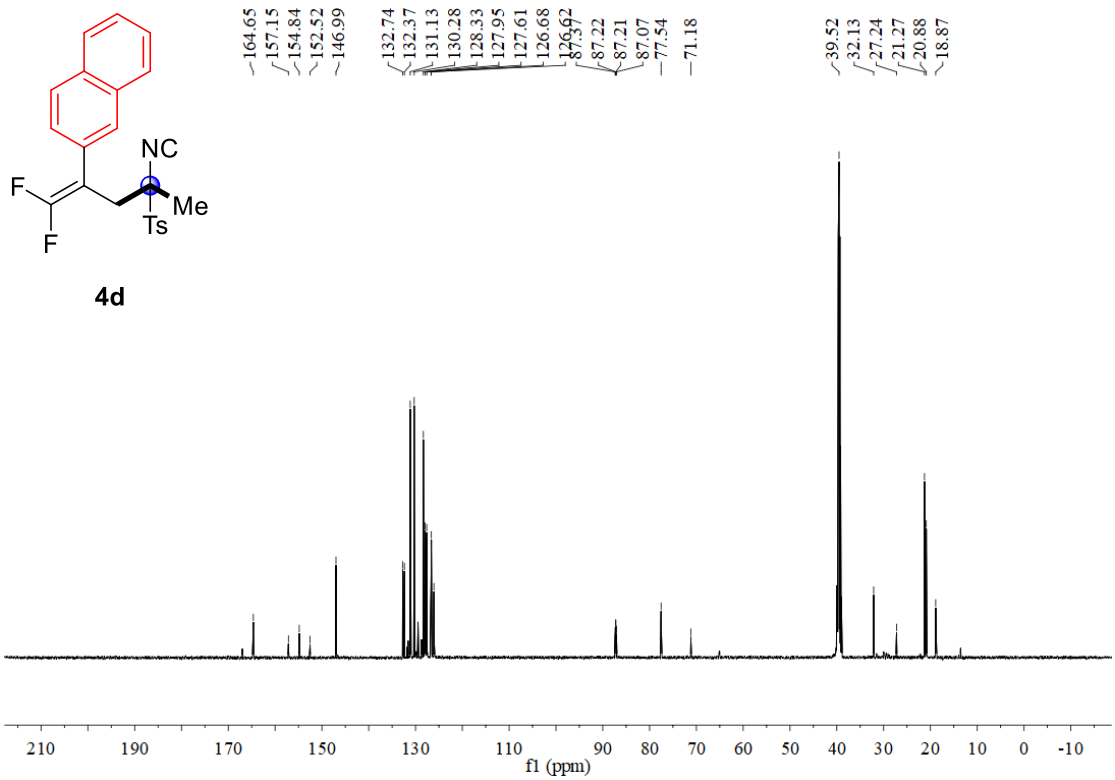
2.00
3.00
3.00
f1 (ppm)

4d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Ts
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126.68
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87.21
87.07
77.54
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39.52
32.13
27.24
21.27
20.88
18.87
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20
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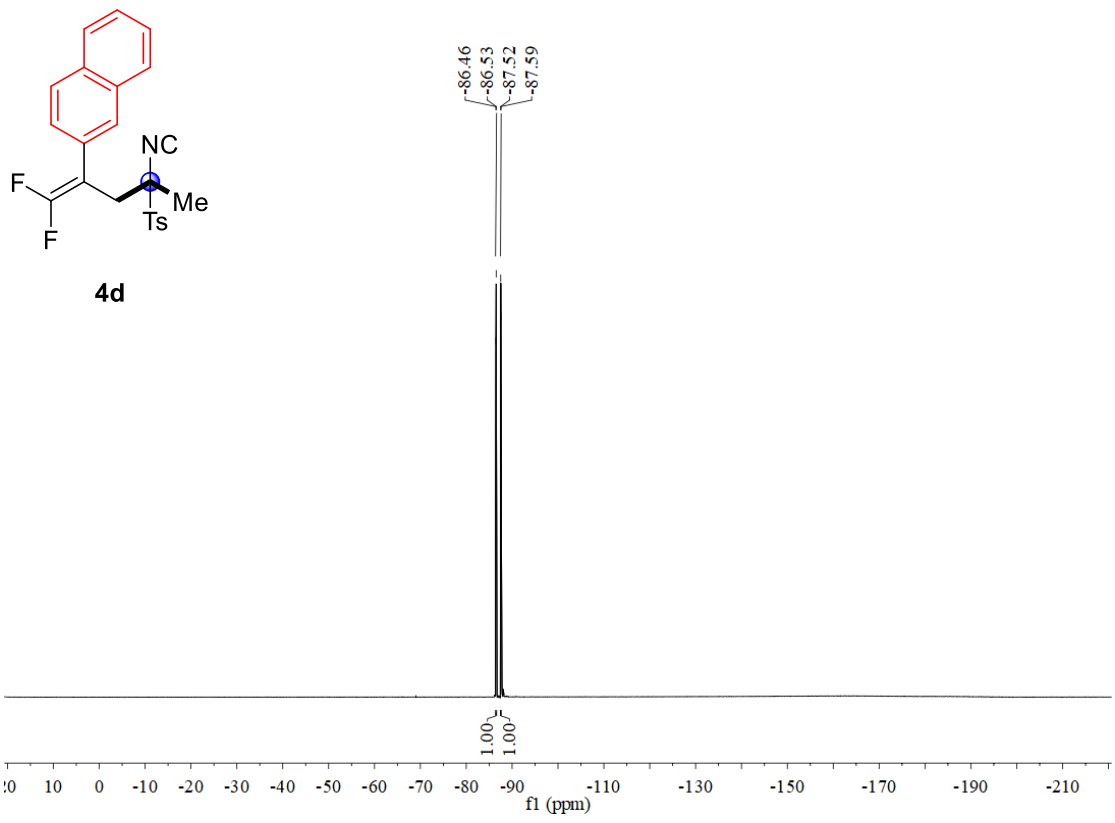
f1 (ppm)

4d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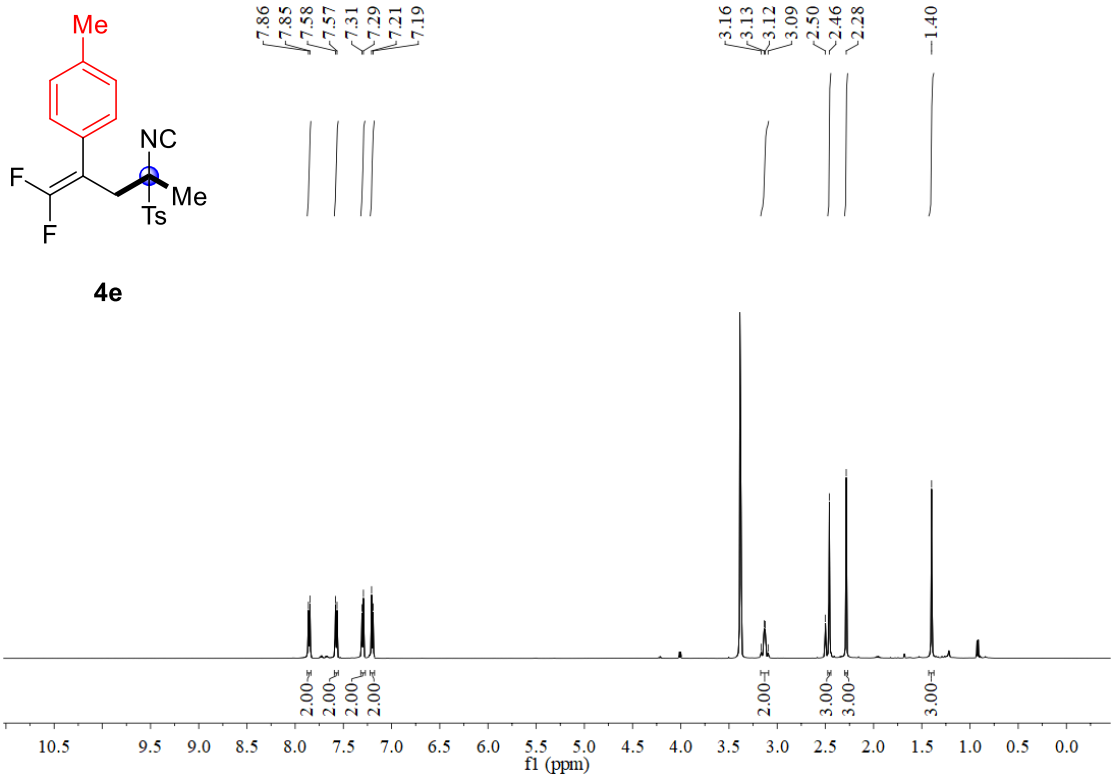
-170
-190
-210
f1 (ppm)

4d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Me
Ts
F
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3.16
3.13
3.12
3.09
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2.00
2.00
3.00
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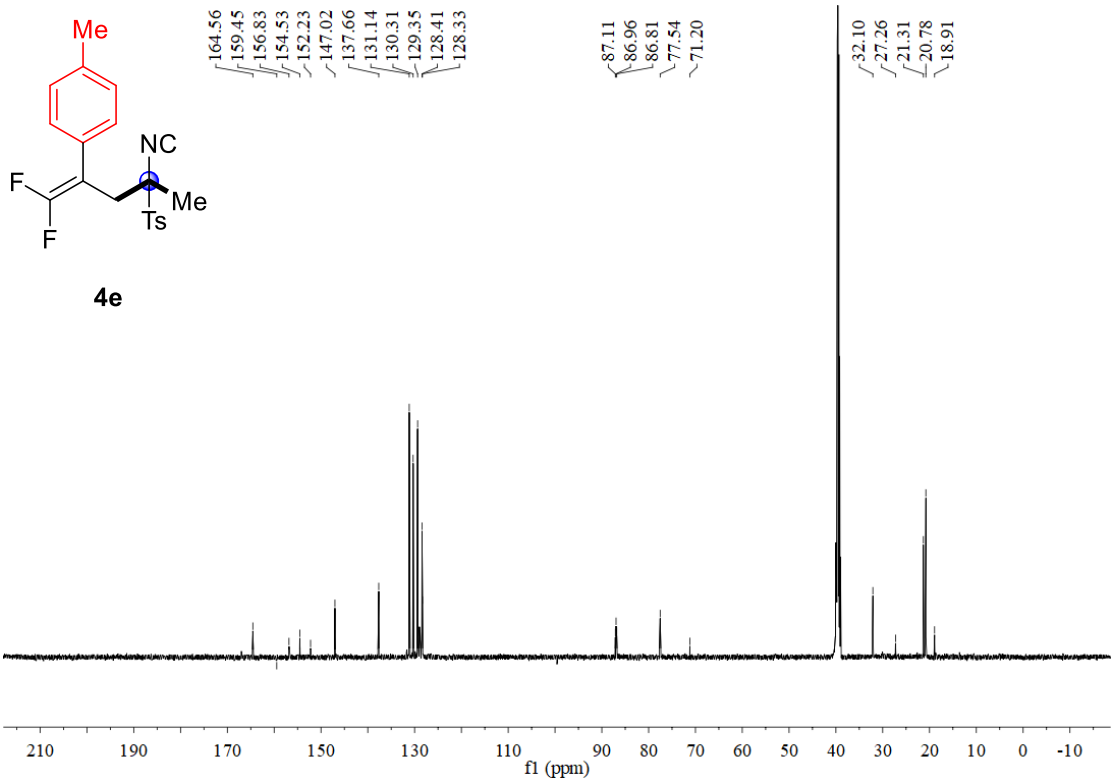
3.00
f1 (ppm)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Ts
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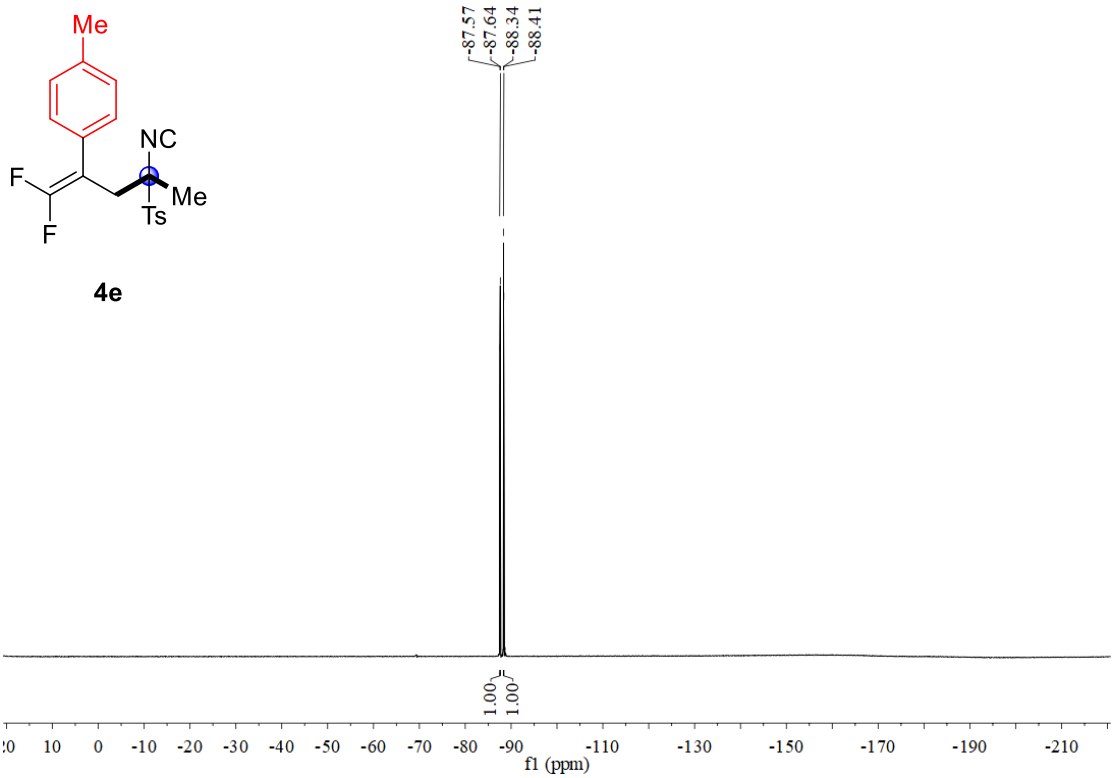
f1 (ppm)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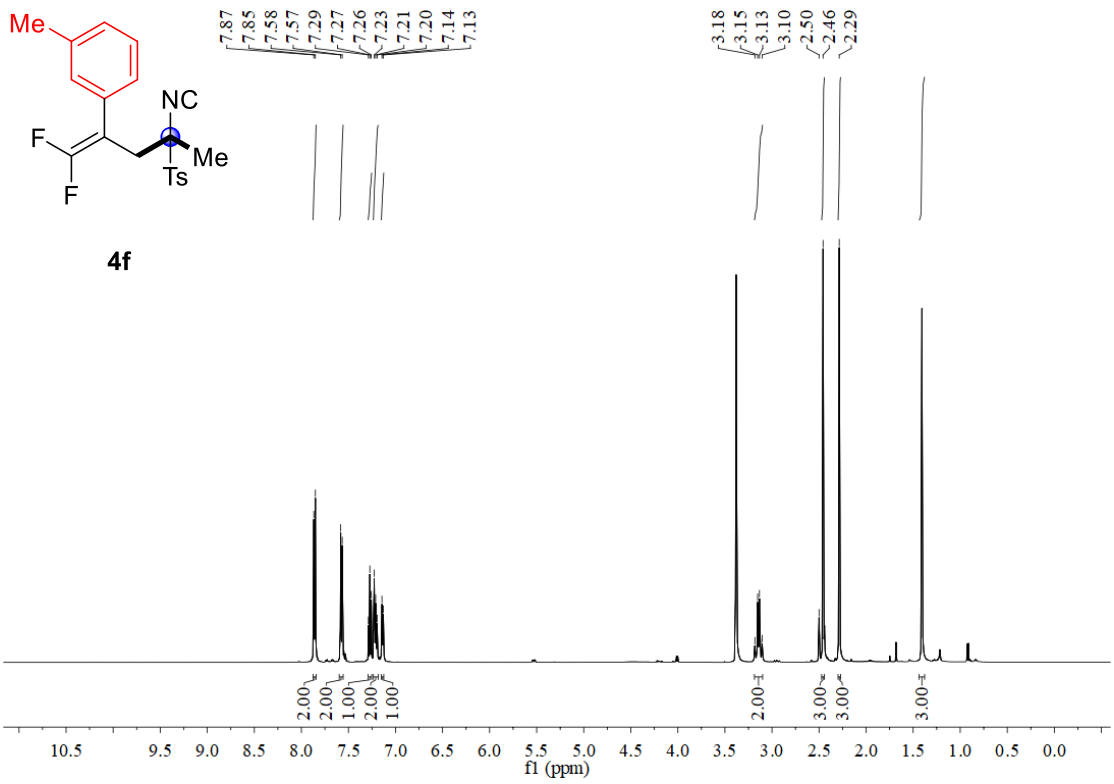
f1 (ppm)

4e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7.20
7.14
7.13
3.18
3.15
3.13
3.10
2.50
2.46
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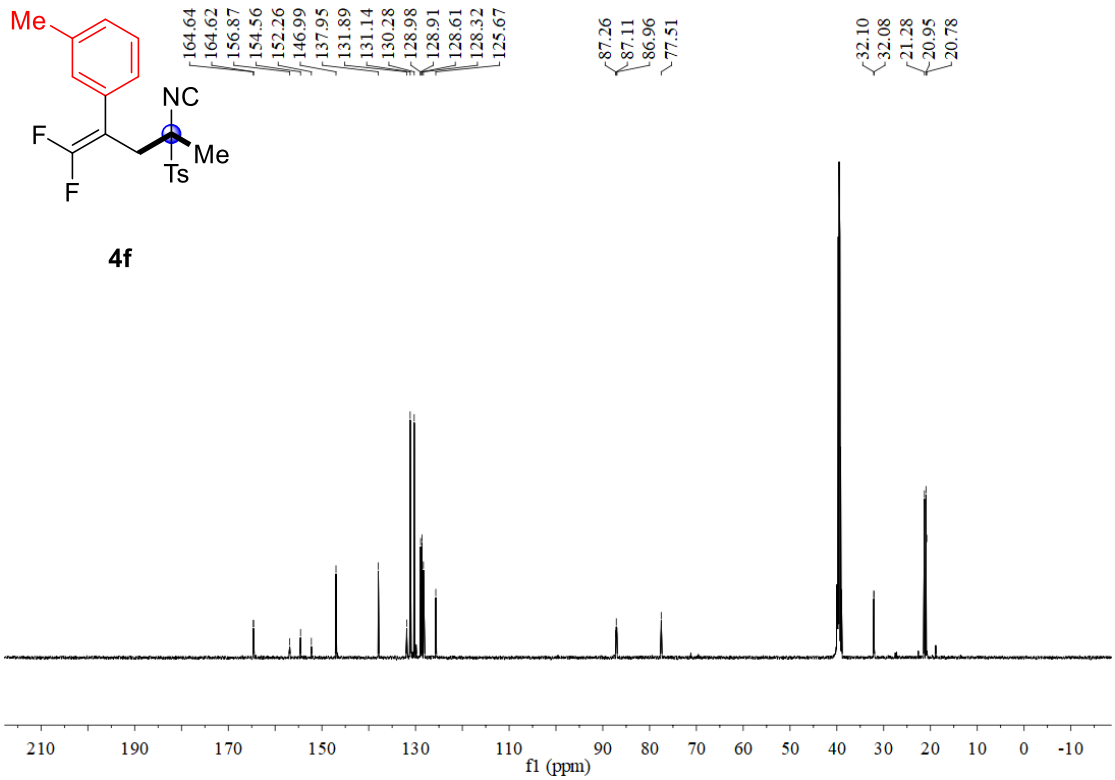
2.00
3.00
3.00
3.00
f1 (ppm)

4f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87.11
86.96
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32.08
21.28
20.95
20.78
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110
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60
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20
10
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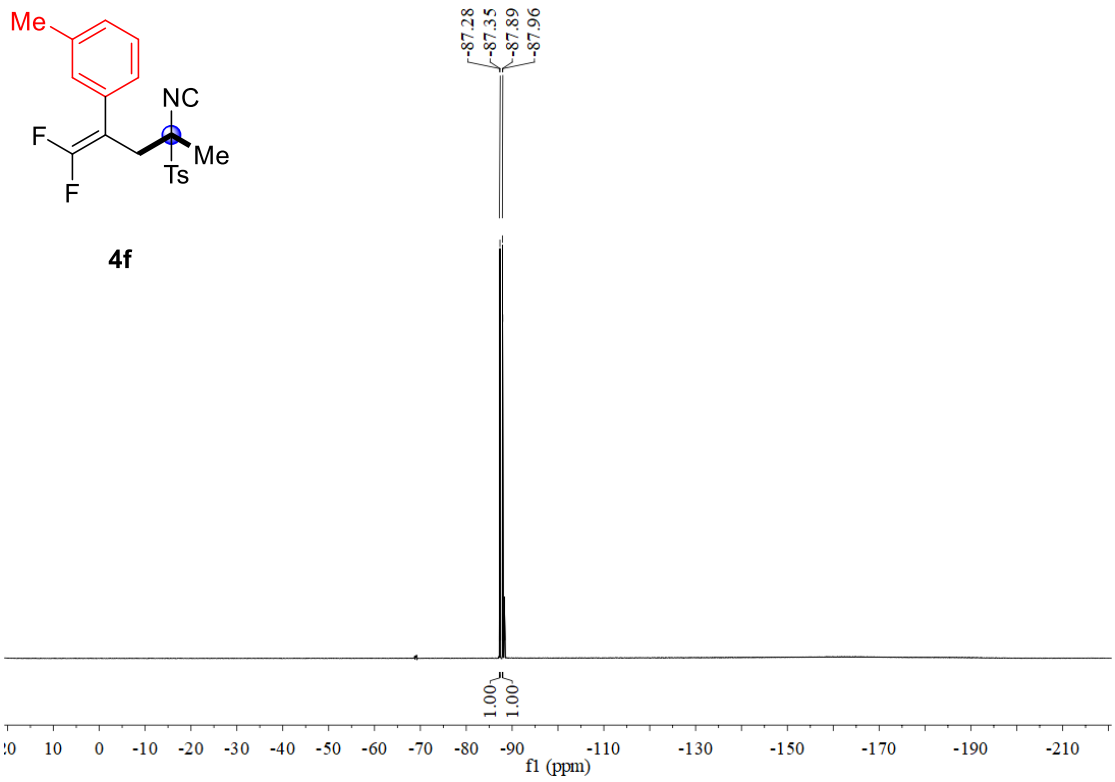
-10
f1 (ppm)

4f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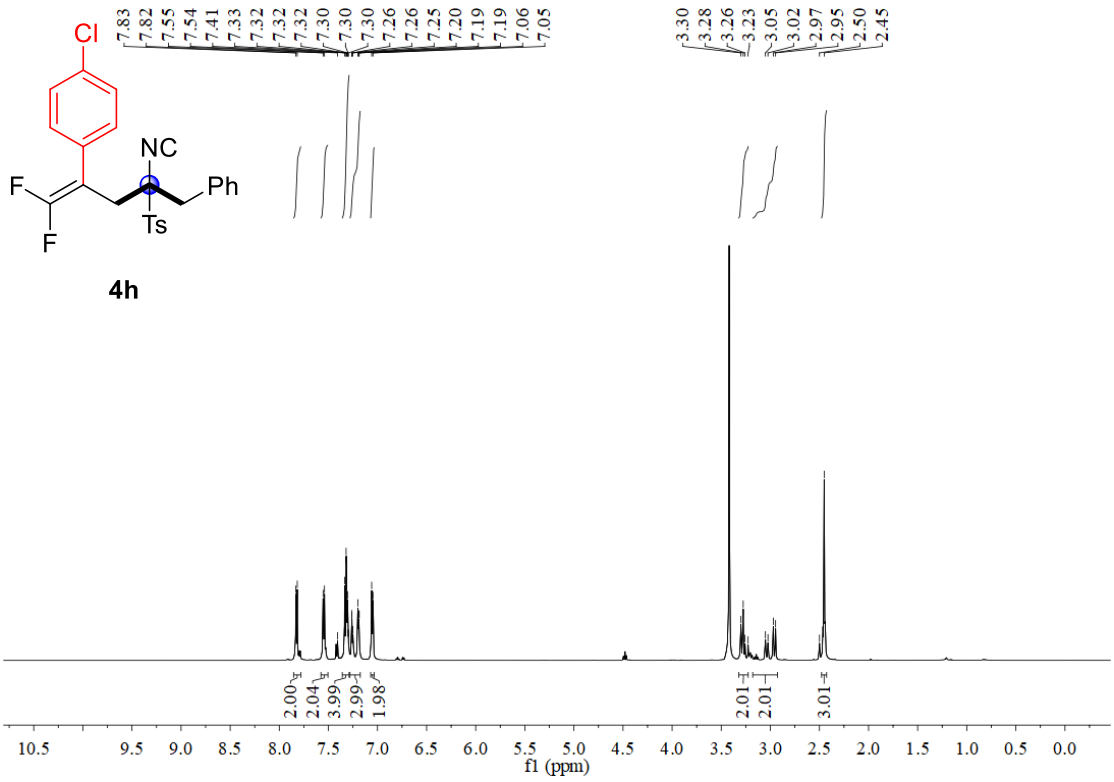
f1 (ppm)

4f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3.26
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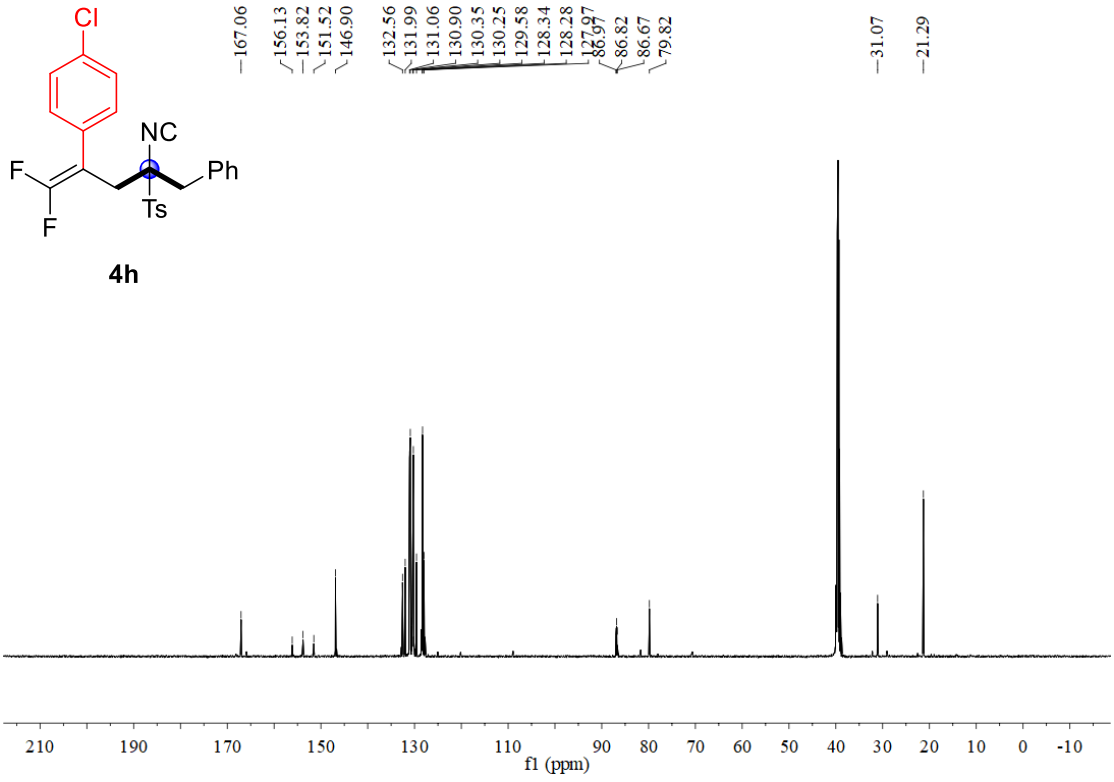
3.01
f1 (ppm)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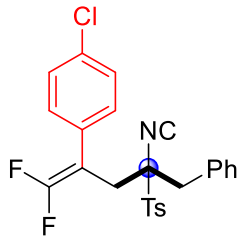
f1 (ppm)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4h

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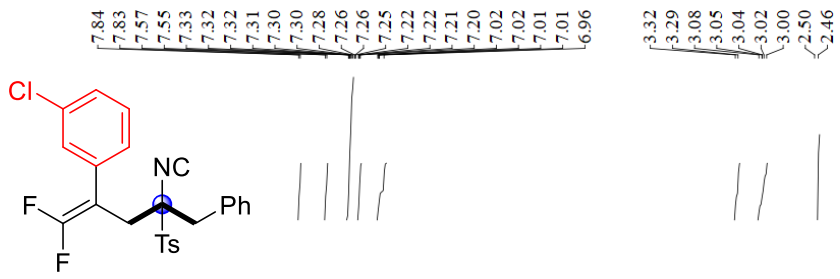
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7.01
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3.32
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Cl
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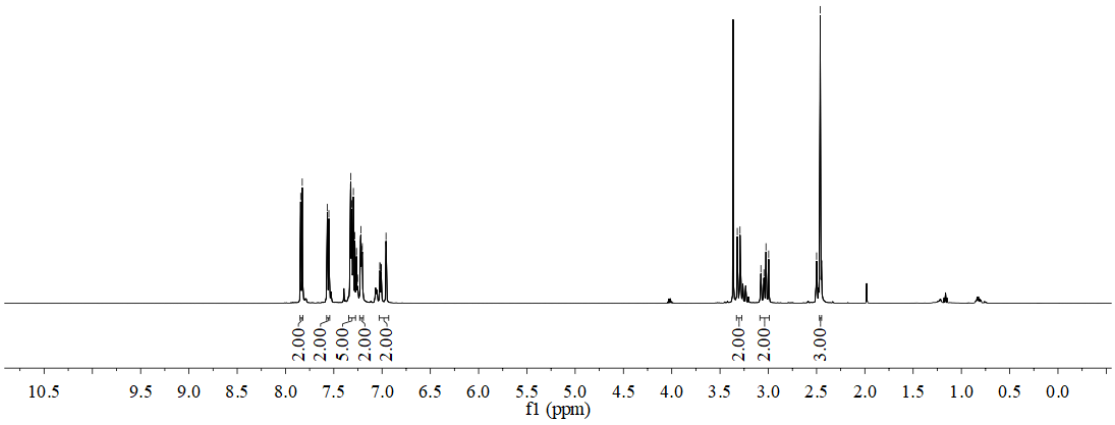
Ph
F
Ts

4i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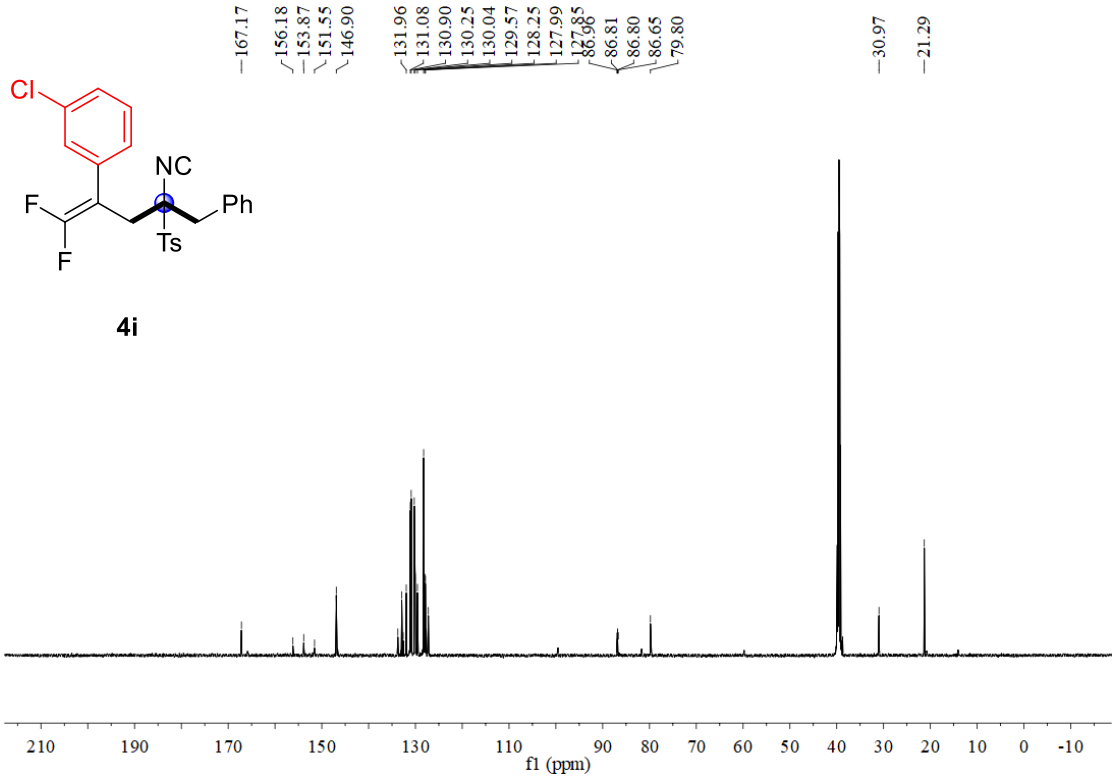
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30.97
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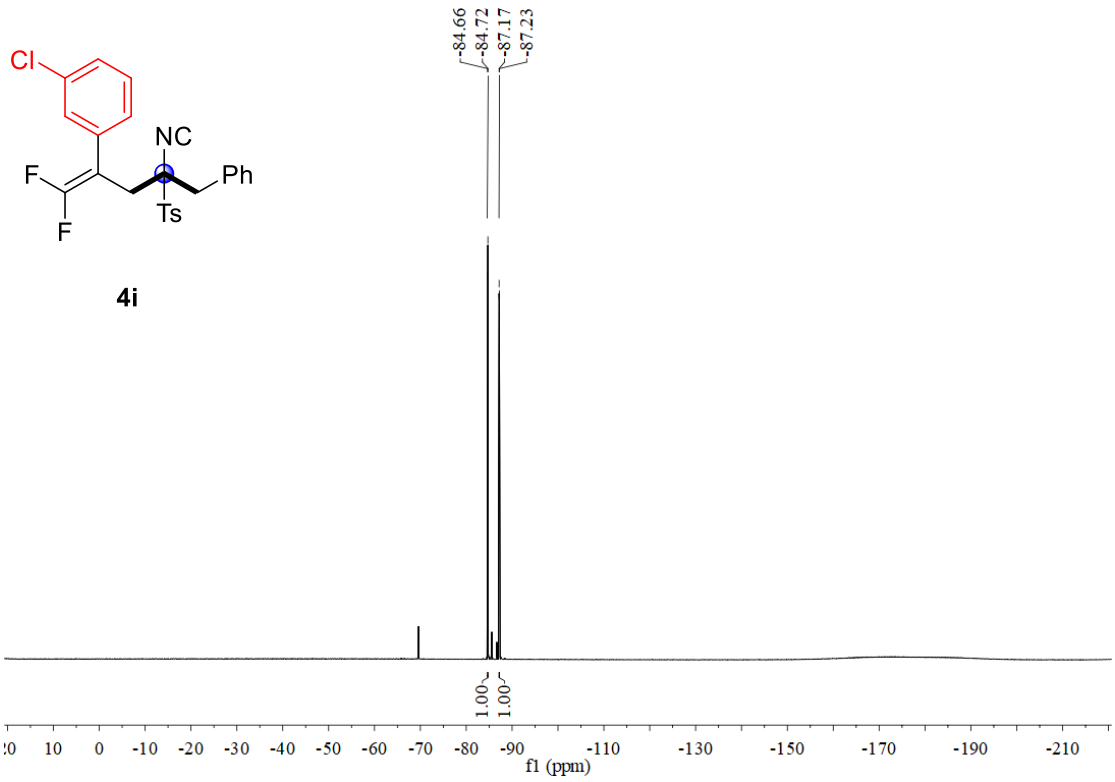
f1 (ppm)

4i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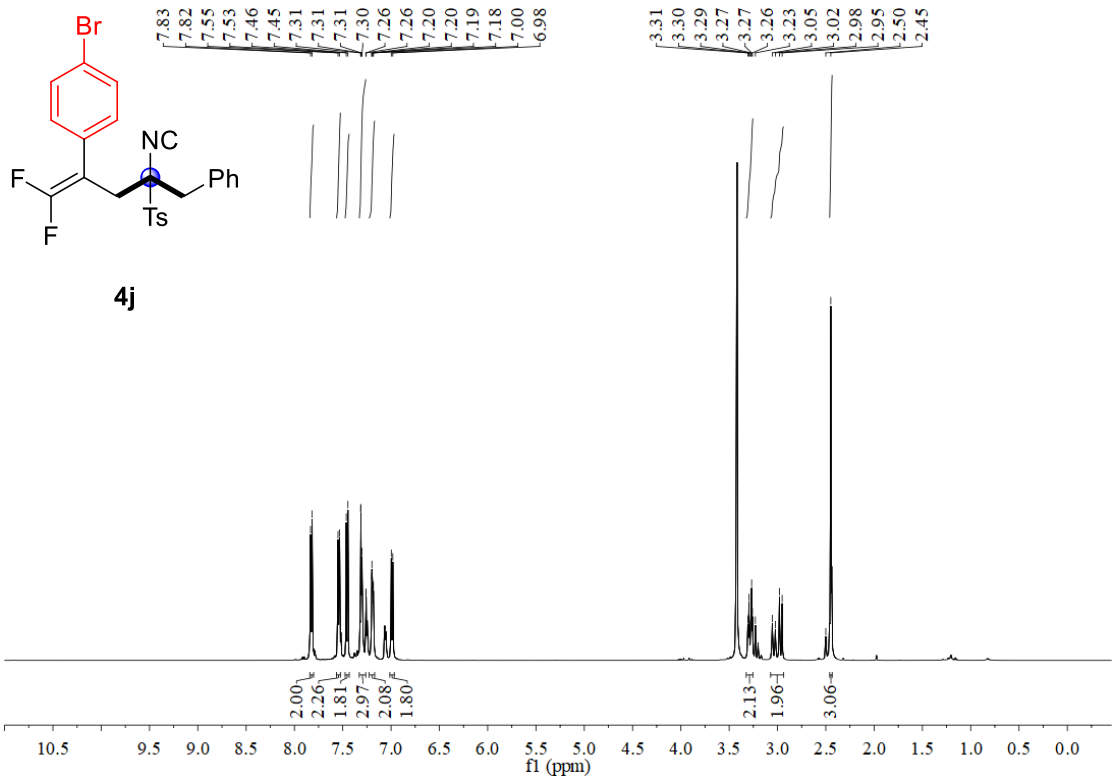
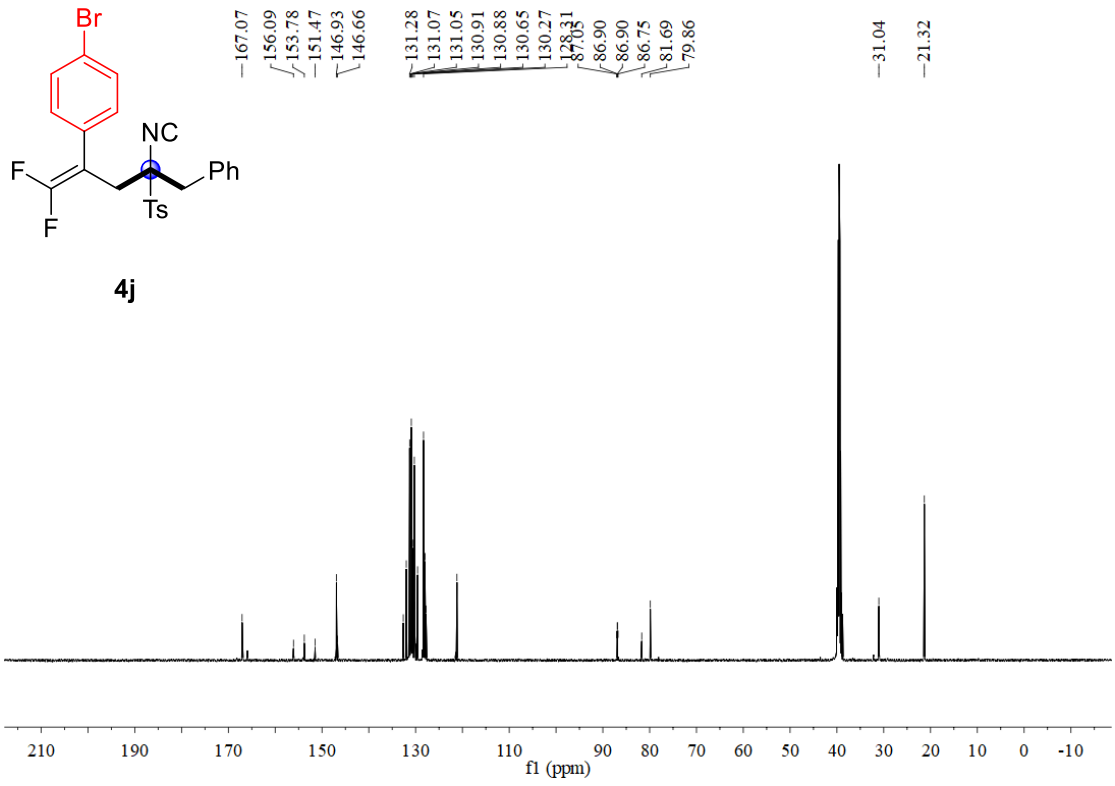
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

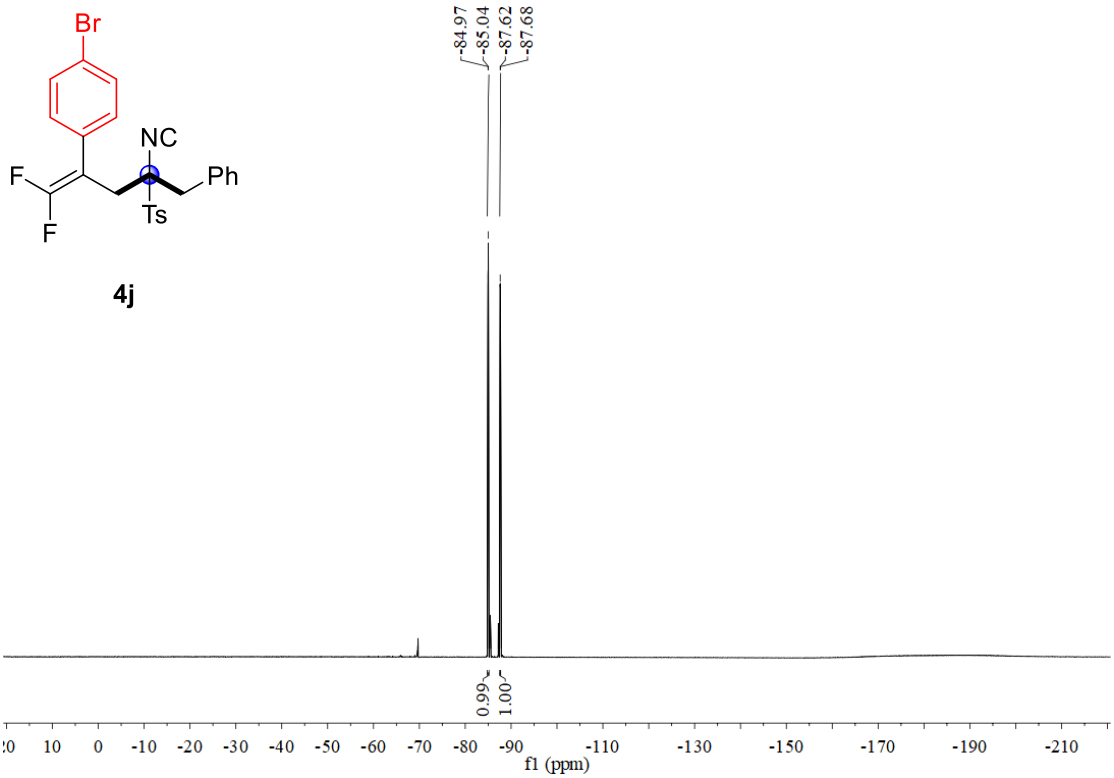
4i


Br
NC
F
Ph
F
Ts
7.83
7.82
7.55
7.53
7.46
7.45
7.31
7.31
7.31
7.30
7.26
7.26
7.20
7.20
7.19
7.18
7.00
6.98
3.31
3.30
3.29
3.27
3.27
3.26
3.23
3.05
3.02
2.98
2.95
2.50
2.45
2.00
2.26
1.81
2.97
2.08
1.80
2.13
1.96
3.06
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

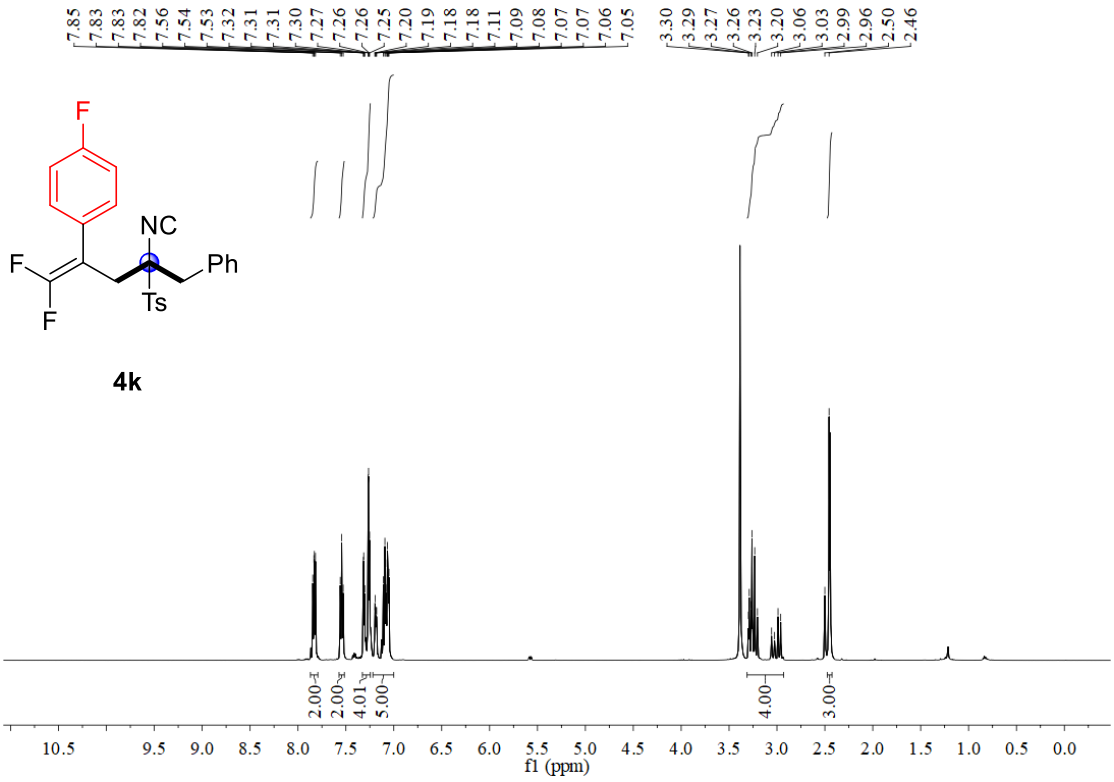
4j


Br
NC
F
Ph
F
Ts
167.07
156.09
153.78
151.47
146.93
146.66
131.28
131.07
131.05
130.91
130.88
130.65
130.27
128.31
87.05
86.90
86.90
86.75
81.69
79.86
31.04
21.32
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

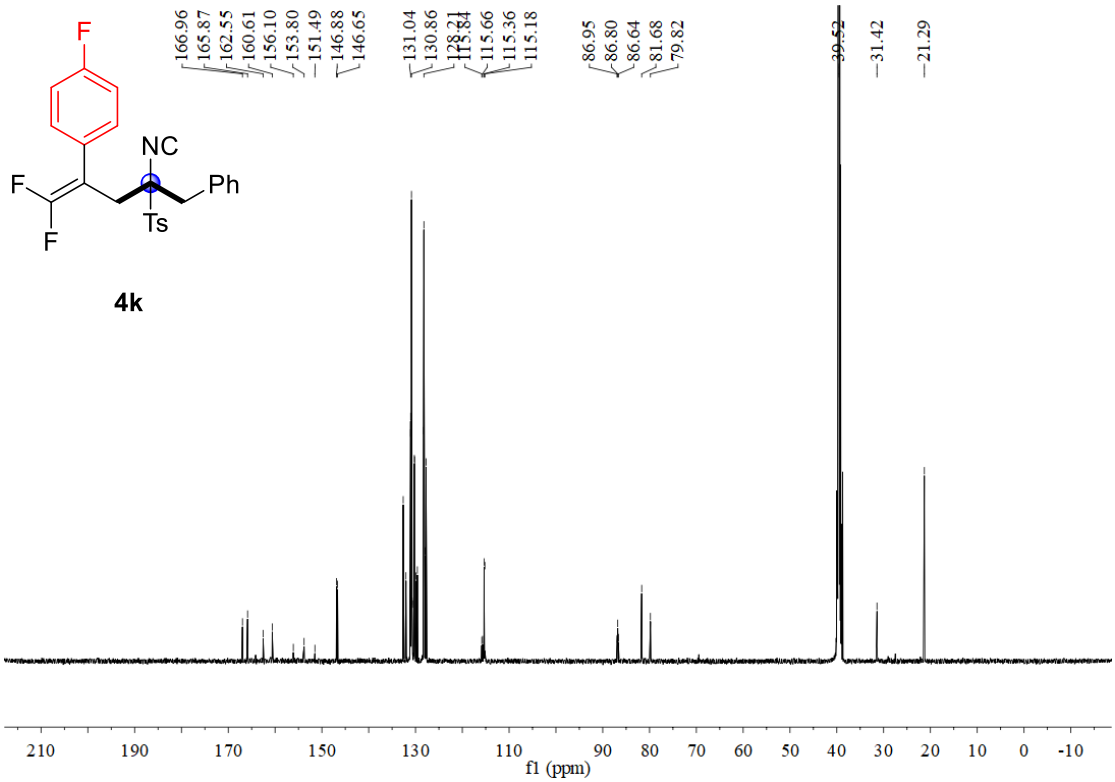
4j

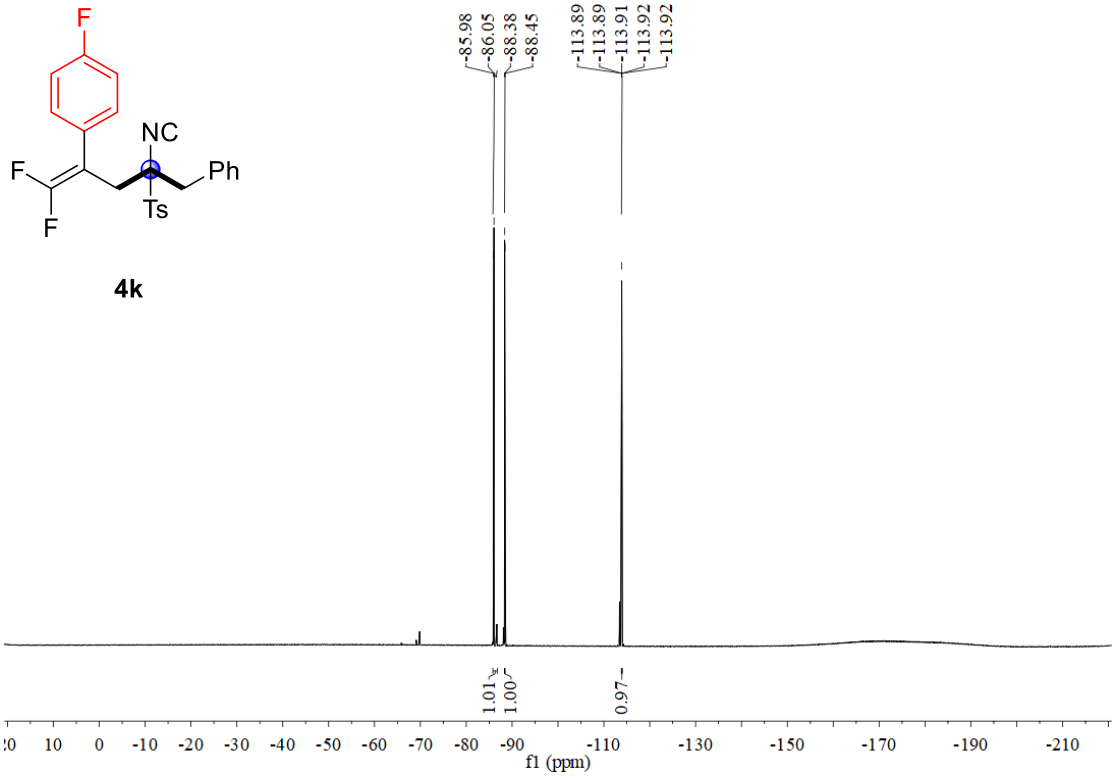

Br
NC
F
Ph
F
Ts
-84.97
-85.04
-87.62
-87.68
0.99
1.00
f1 (ppm)

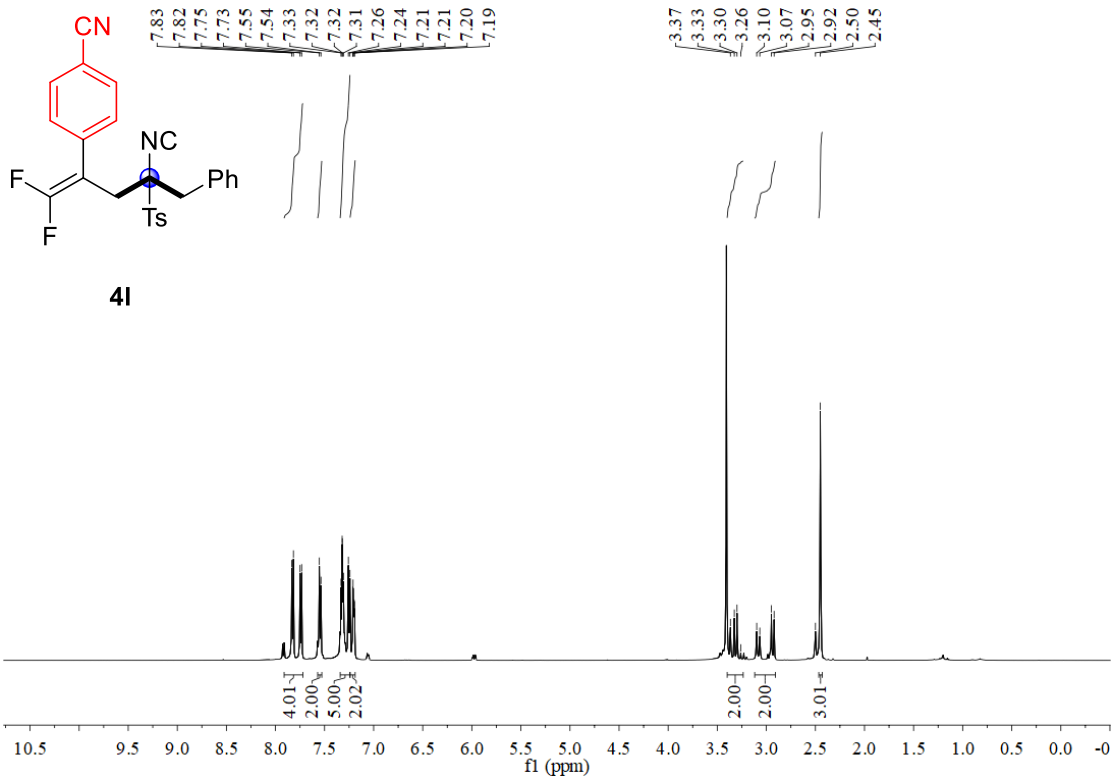
4j


7.85
7.83
7.83
7.82
7.56
7.54
7.53
7.32
7.31
7.31
7.30
7.27
7.26
7.26
7.25
7.20
7.19
7.18
7.11
7.09
7.08
7.07
7.07
7.06
7.05
3.30
3.29
3.27
3.26
3.23
3.20
3.06
3.03
2.99
2.96
2.50
2.46
F
NC
F
Ph
F
Ts
2.00
2.00
4.01
5.00
4.00
3.00
f1 (ppm)

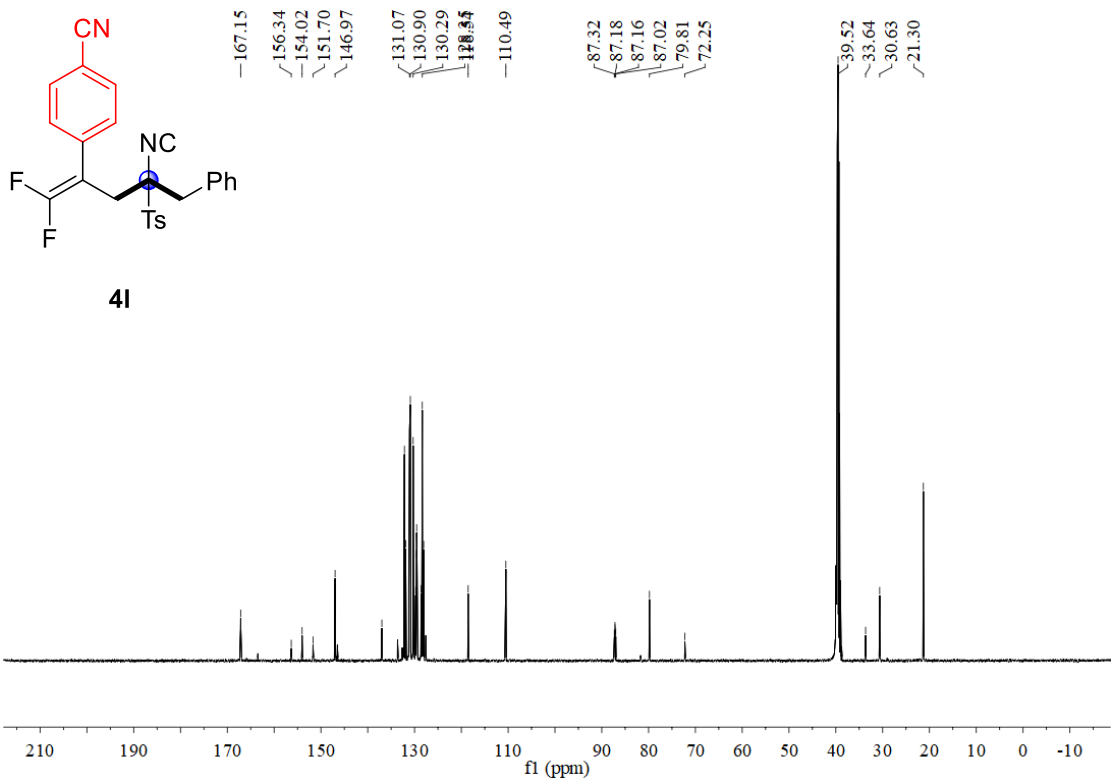
4k


F
NC
F
Ph
F
Ts
4k
166.96
165.87
162.55
160.61
156.10
153.80
151.49
146.88
146.65
131.04
130.86
115.66
115.36
115.18
86.95
86.80
86.64
81.68
79.82
39.52
31.42
21.29
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

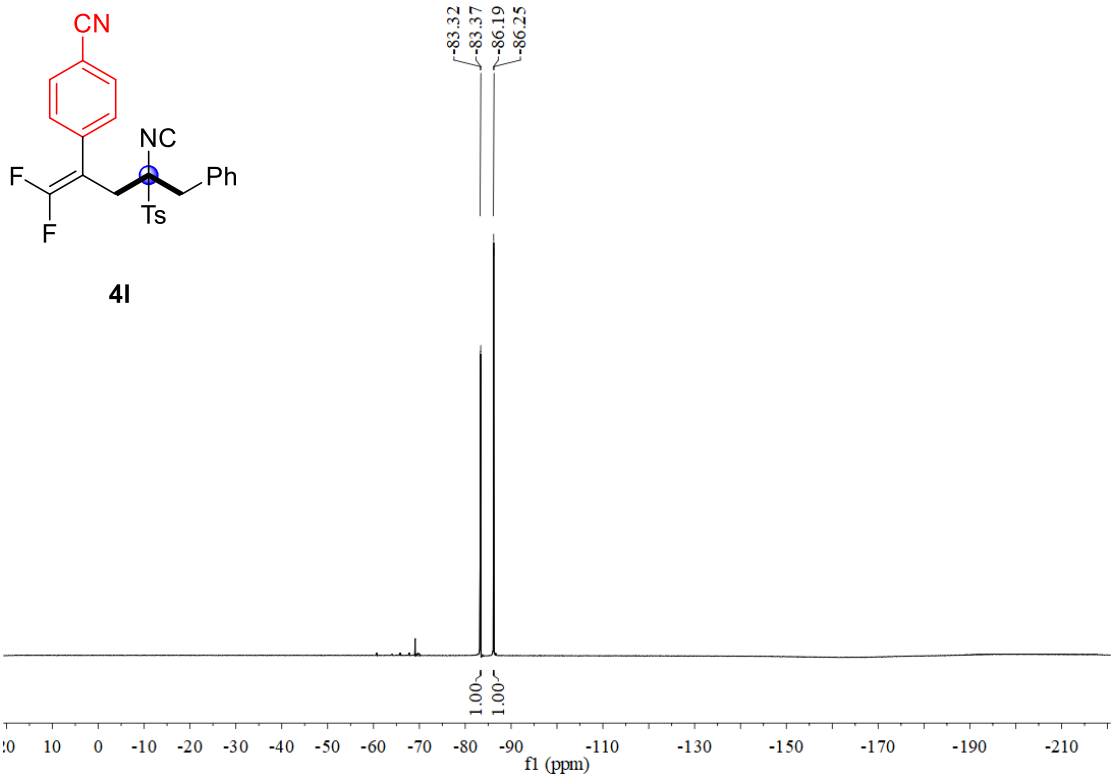

F
NC
F
Ph
F
Ts
4k
-85.98
-86.05
-88.38
-88.45
-113.89
-113.89
-113.91
-113.92
-113.92
1.01
1.00
0.97
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


CN
NC
F
F
Ph
Ts
7.83
7.82
7.75
7.73
7.55
7.54
7.33
7.32
7.32
7.31
7.26
7.24
7.21
7.21
7.20
7.19
3.37
3.33
3.30
3.26
3.10
3.07
2.95
2.92
2.50
2.45
4.01
2.00
5.00
2.02
2.00
2.00
3.01
f1 (ppm)

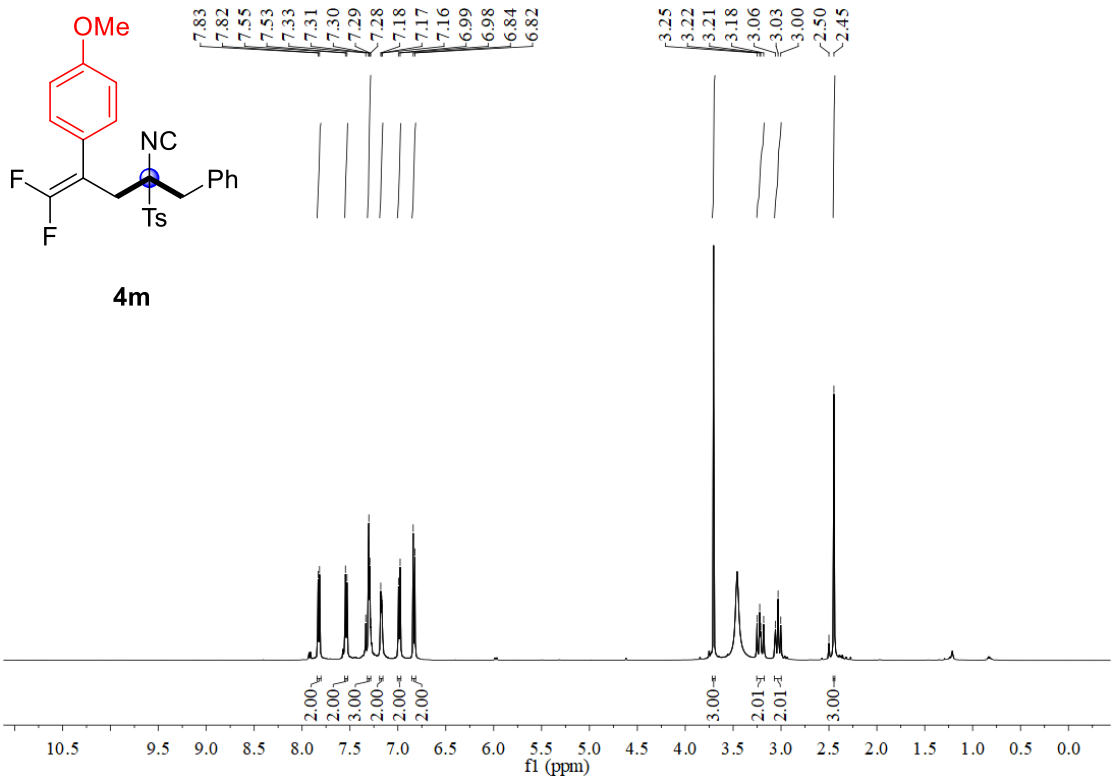
4l


CN
NC
F
F
Ph
Ts
167.15
156.34
154.02
151.70
146.97
131.07
130.90
130.29
110.49
87.32
87.18
87.16
87.02
79.81
72.25
39.52
33.64
30.63
21.30
f1 (ppm)

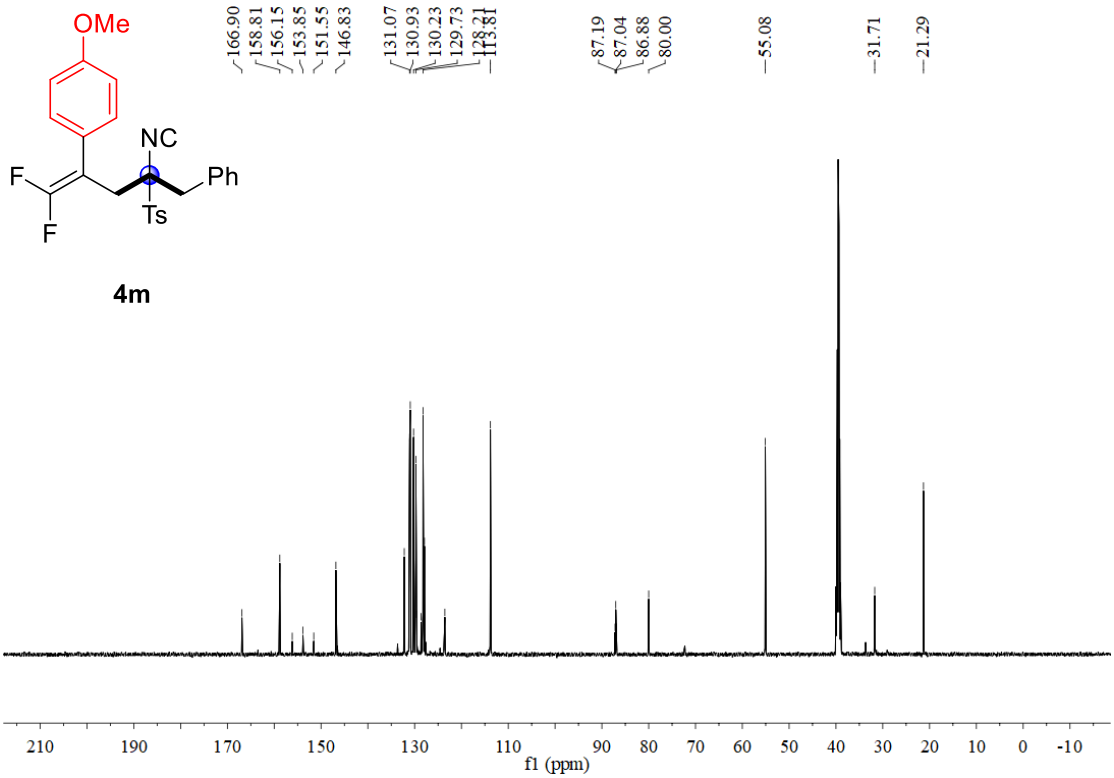
4l

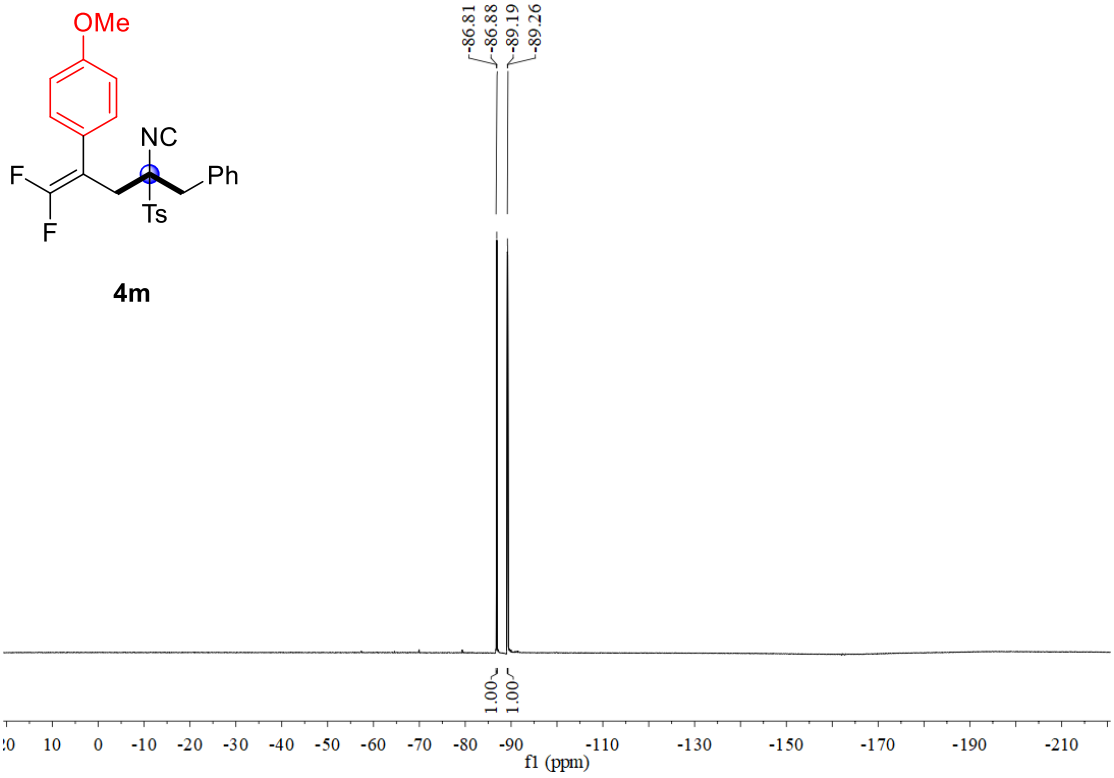

CN
NC
Ph
Ts
F
F
-83.32
-83.37
-86.19
-86.25
1.00
1.00
f1 (ppm)

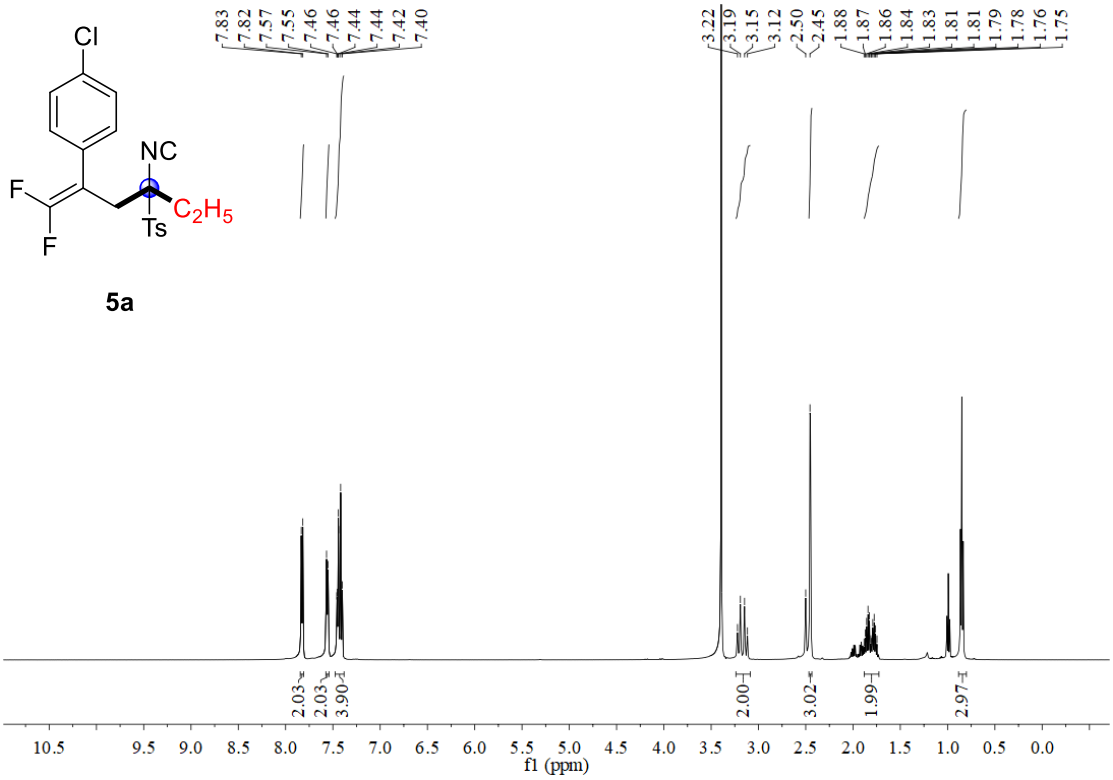
4l


OMe
NC
Ph
Ts
F
F
7.83
7.82
7.55
7.53
7.33
7.31
7.30
7.29
7.28
7.18
7.17
7.16
6.99
6.98
6.84
6.82
3.25
3.22
3.21
3.18
3.06
3.03
3.00
2.50
2.45
2.00
2.00
3.00
2.00
2.00
2.00
3.00
2.01
2.01
3.00
f1 (ppm)

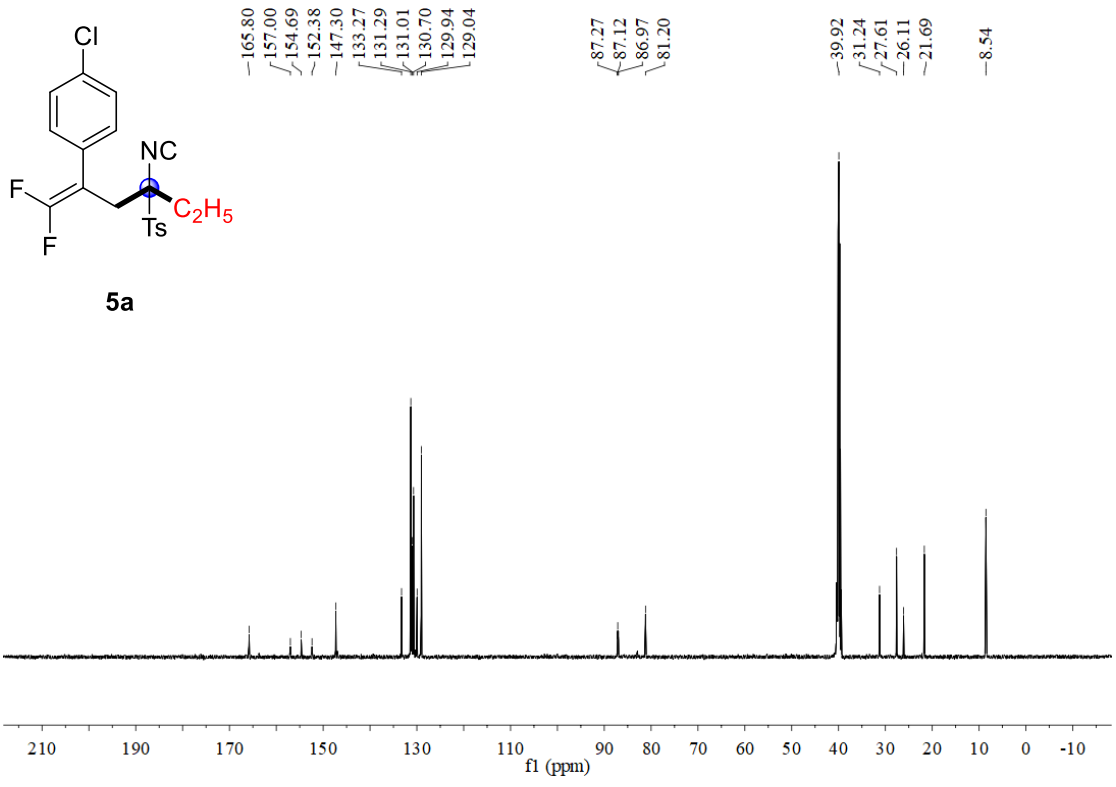
4m


OMe
NC
F
Ph
Ts
F
4m
166.90
158.81
156.15
153.85
151.55
146.83
131.07
130.93
130.23
129.73
128.21
115.81
87.19
87.04
86.88
80.00
55.08
31.71
21.29
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

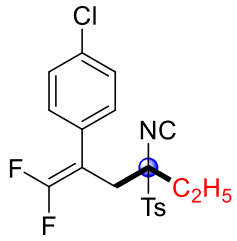

OMe
NC
F
Ph
Ts
F
4m
-86.81
-86.88
-89.19
-89.26
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


Cl
NC
F
C_2H_5
F
Ts
7.83
7.82
7.57
7.55
7.46
7.46
7.44
7.44
7.42
7.40
3.22
3.19
3.15
3.12
2.50
2.45
1.88
1.87
1.86
1.84
1.83
1.81
1.81
1.79
1.78
1.76
1.75
2.03
2.03
3.90
2.00
3.02
1.99
2.97
f1 (ppm)

5a

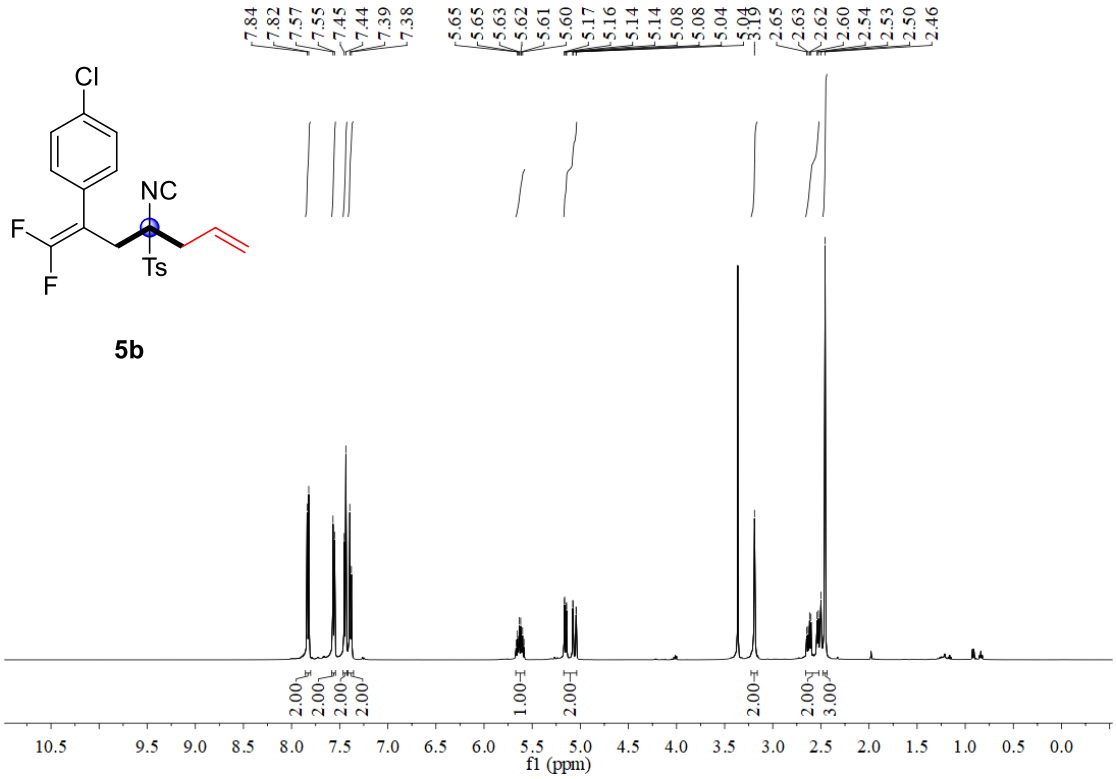

Cl
NC
F
C_2H_5
F
Ts
165.80
157.00
154.69
152.38
147.30
133.27
131.29
131.01
130.70
129.94
129.04
87.27
87.12
86.97
81.20
39.92
31.24
27.61
26.11
21.69
8.54
f1 (ppm)

5a


Cl
NC
F
C_2H_5
Ts
F

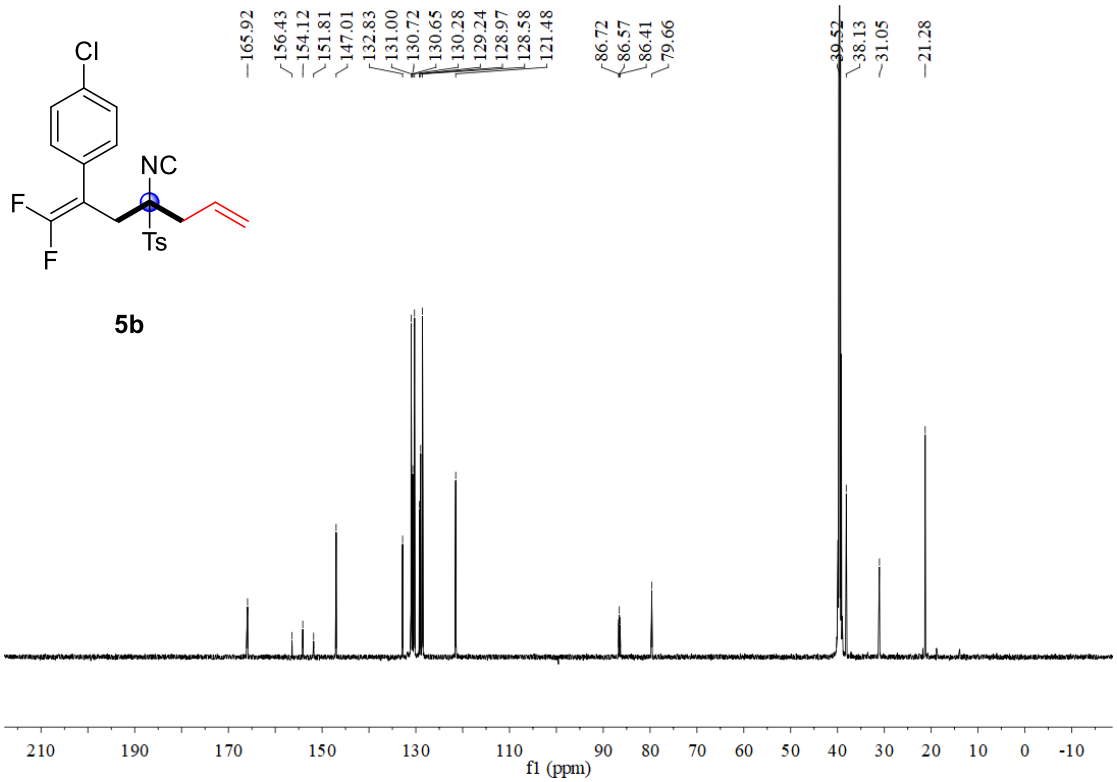
5a

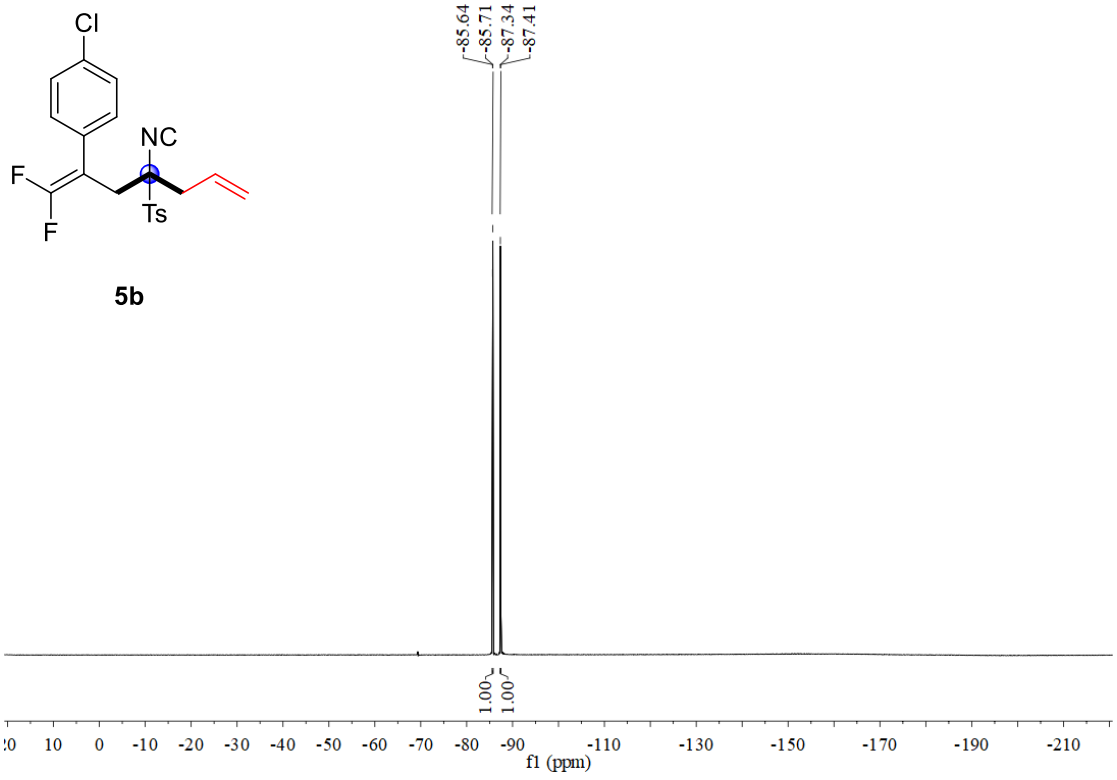
-85.97
-86.04
-87.42
-87.49
1.00
1.01
f1 (ppm)

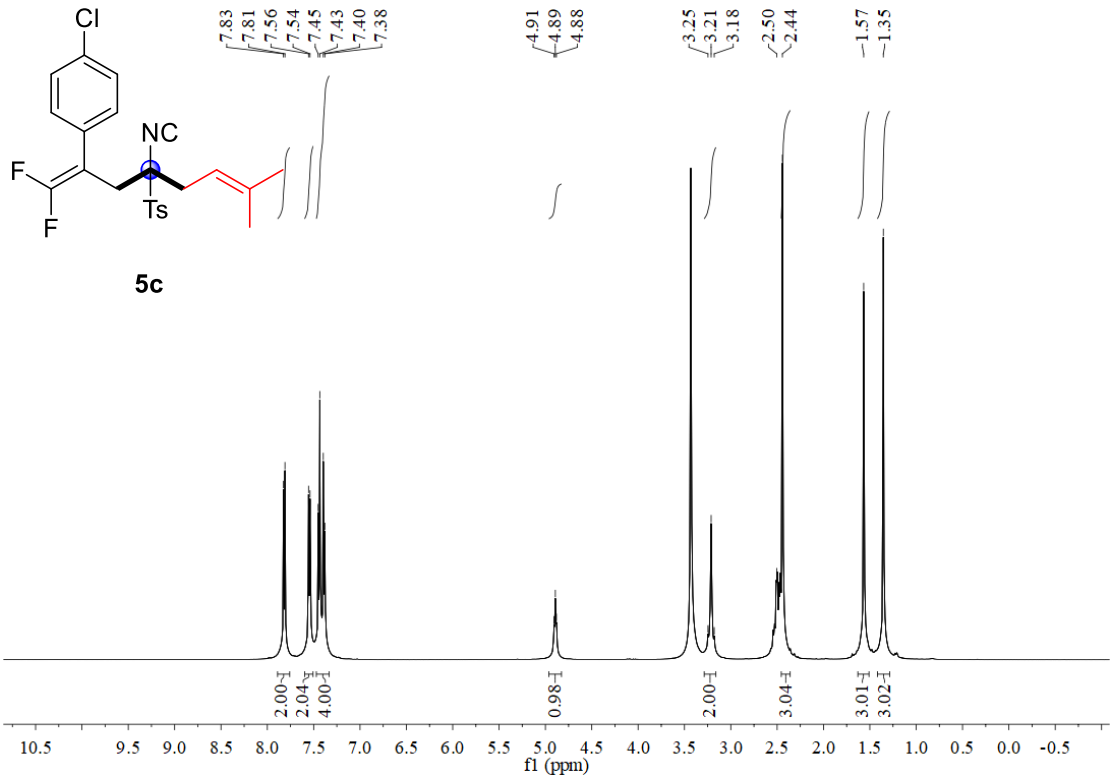

7.84
7.82
7.57
7.55
7.45
7.44
7.39
7.38
5.65
5.65
5.63
5.62
5.61
5.60
5.17
5.16
5.14
5.14
5.08
5.08
5.04
5.04
3.19
2.65
2.63
2.62
2.60
2.54
2.53
2.50
2.46
2.00
2.00
2.00
2.00
1.00
2.00
2.00
3.00
f1 (ppm)

Cl
NC
F
Ts
F

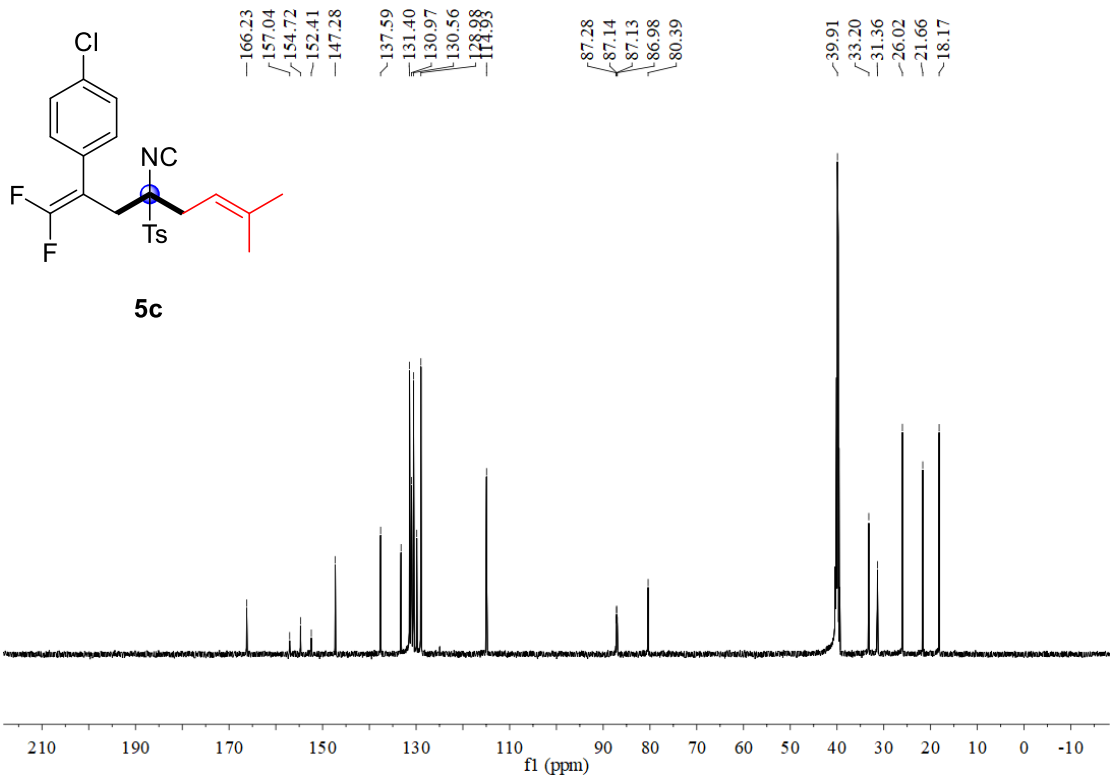
5b


Cl
NC
F
F
Ts
5b
165.92
156.43
154.12
151.81
147.01
132.83
131.00
130.72
130.65
130.28
129.24
128.97
128.58
121.48
86.72
86.57
86.41
79.66
39.52
38.13
31.05
21.28
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

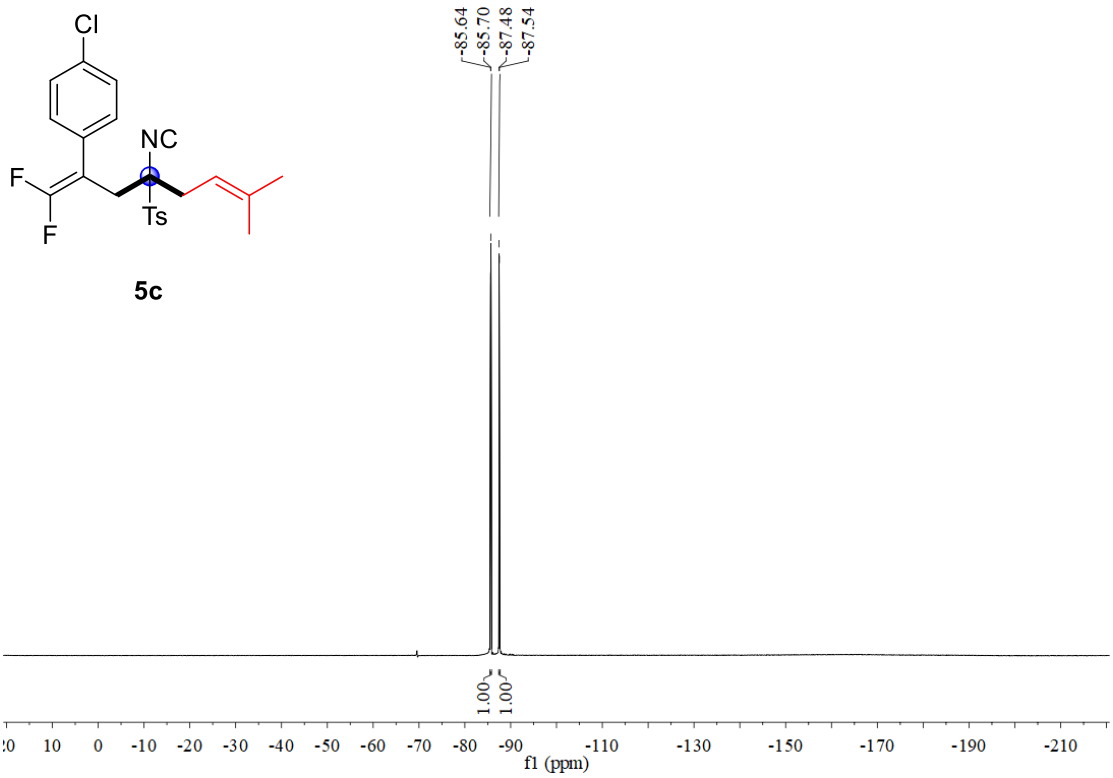

Cl
NC
F
F
Ts
5b
-85.64
-85.71
-87.34
-87.41
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


Cl
NC
F
F
Ts
7.83
7.81
7.56
7.54
7.45
7.43
7.40
7.38
4.91
4.89
4.88
3.25
3.21
3.18
2.50
2.44
1.57
1.35
2.00
2.04
4.00
0.98
2.00
3.04
3.01
3.02
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

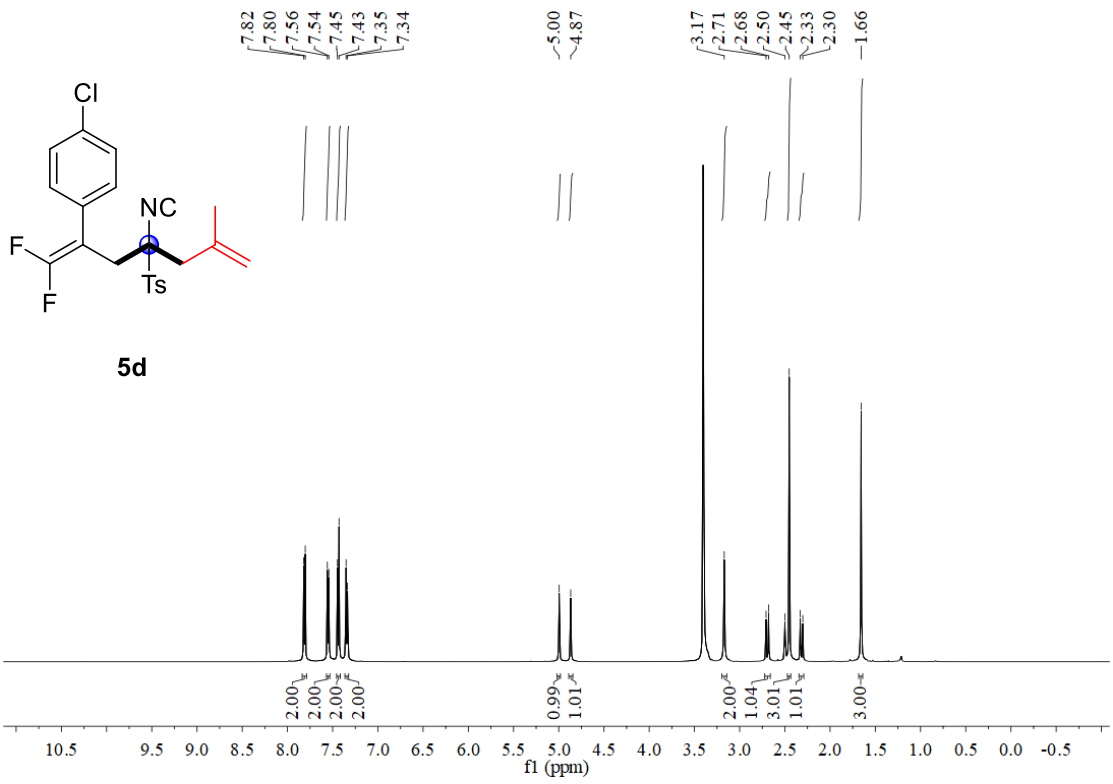
5c


Cl
NC
F
F
Ts
166.23
157.04
154.72
152.41
147.28
137.59
131.40
130.97
130.56
128.98
114.93
87.28
87.14
87.13
86.98
80.39
39.91
33.20
31.36
26.02
21.66
18.17
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

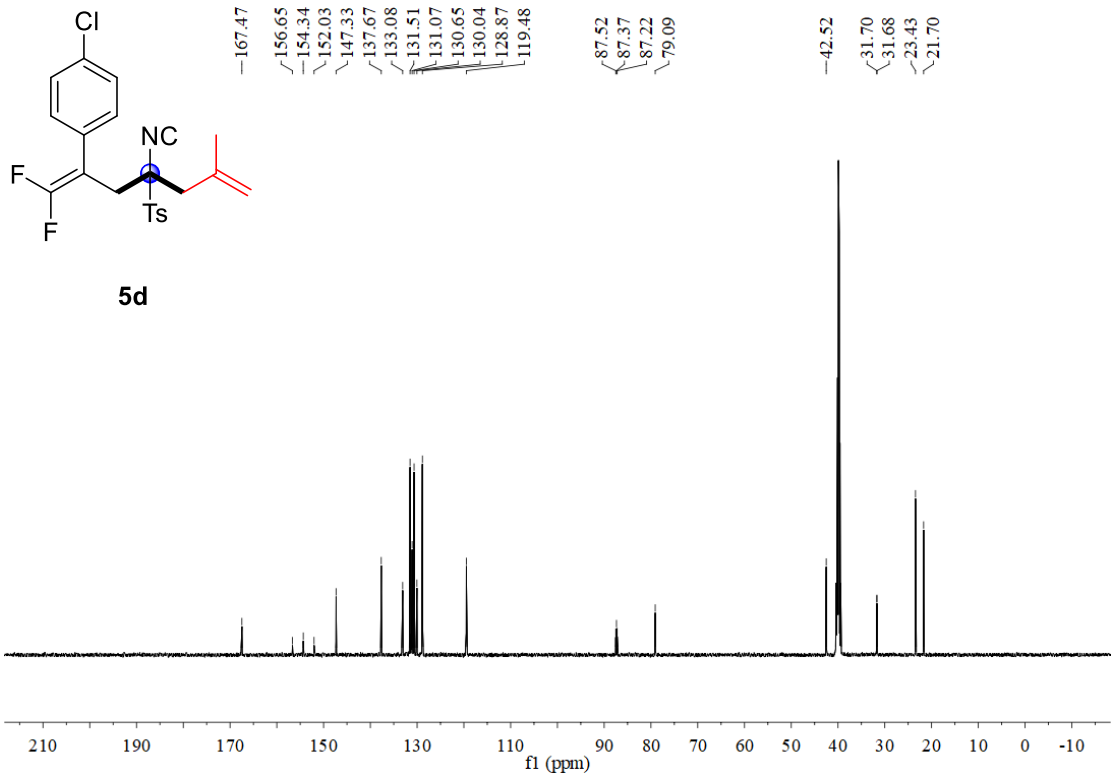
5c


Cl
NC
F
F
Ts
-85.64
-85.70
-87.48
-87.54
1.00
1.00
f1 (ppm)

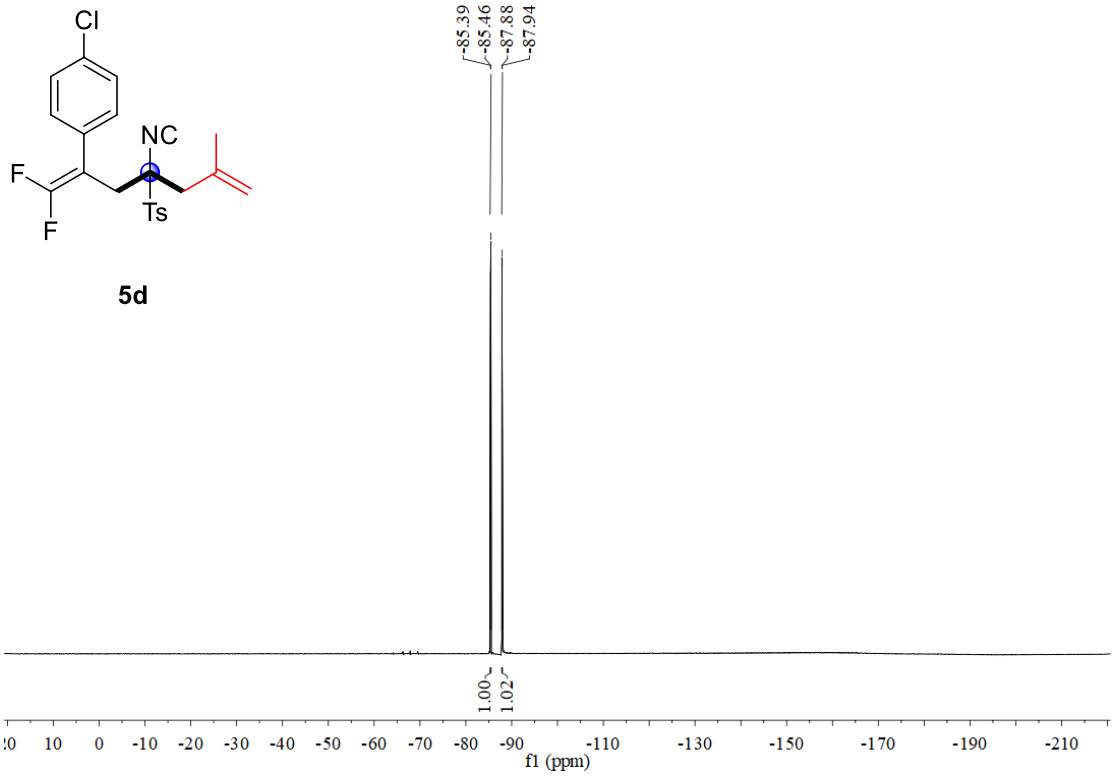
5c


Cl
NC
F
F
Ts
7.82
7.80
7.56
7.54
7.45
7.43
7.35
7.34
5.00
4.87
3.17
2.71
2.68
2.50
2.45
2.33
2.30
1.66
2.00
2.00
2.00
2.00
0.99
1.01
2.00
1.04
3.01
1.01
3.00
f1 (ppm)

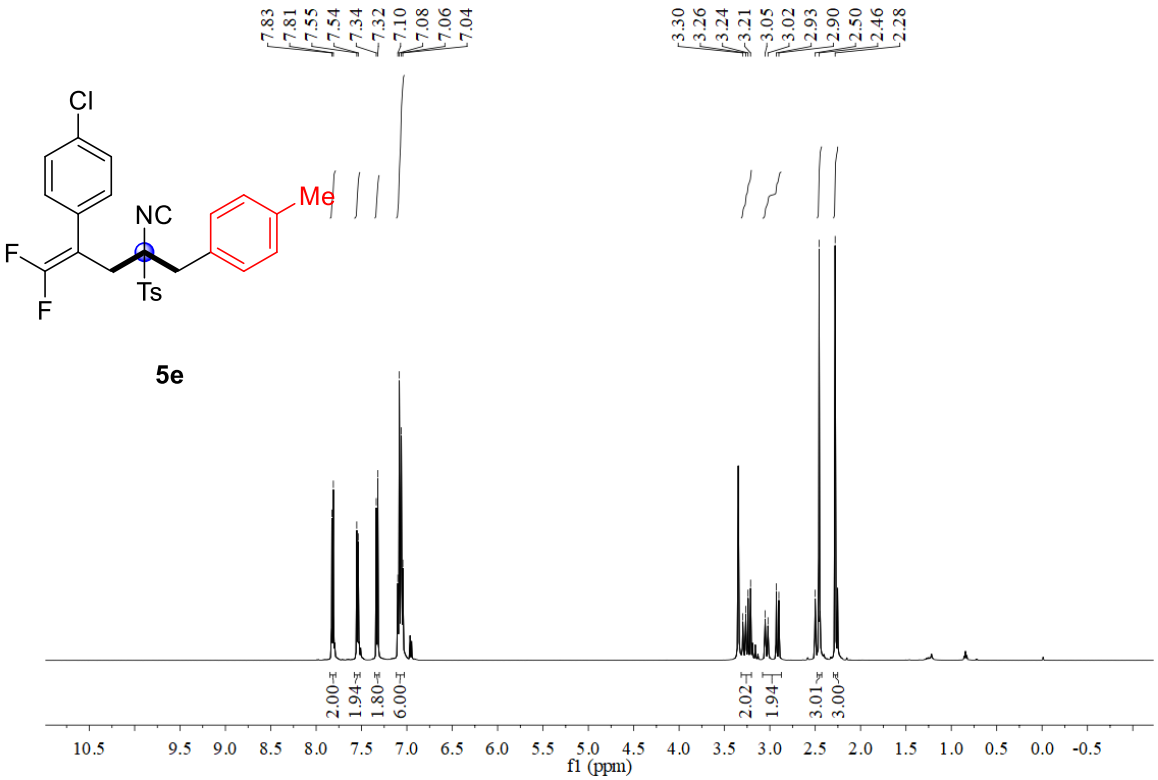
5d


Cl
NC
F
F
Ts
167.47
156.65
154.34
152.03
147.33
137.67
133.08
131.51
131.07
130.65
130.04
128.87
119.48
87.52
87.37
87.22
79.09
42.52
31.70
31.68
23.43
21.70
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

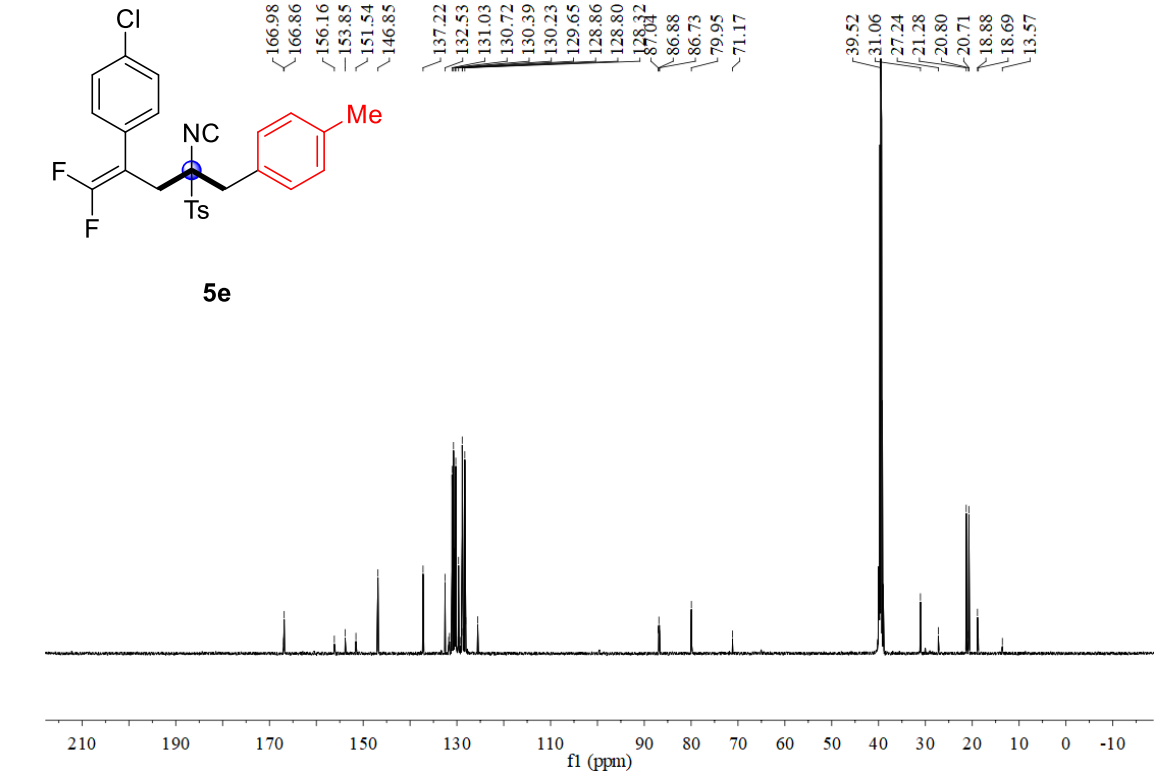
5d


Cl
NC
F
F
Ts
-85.39
-85.46
-87.88
-87.94
1.00
1.02
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

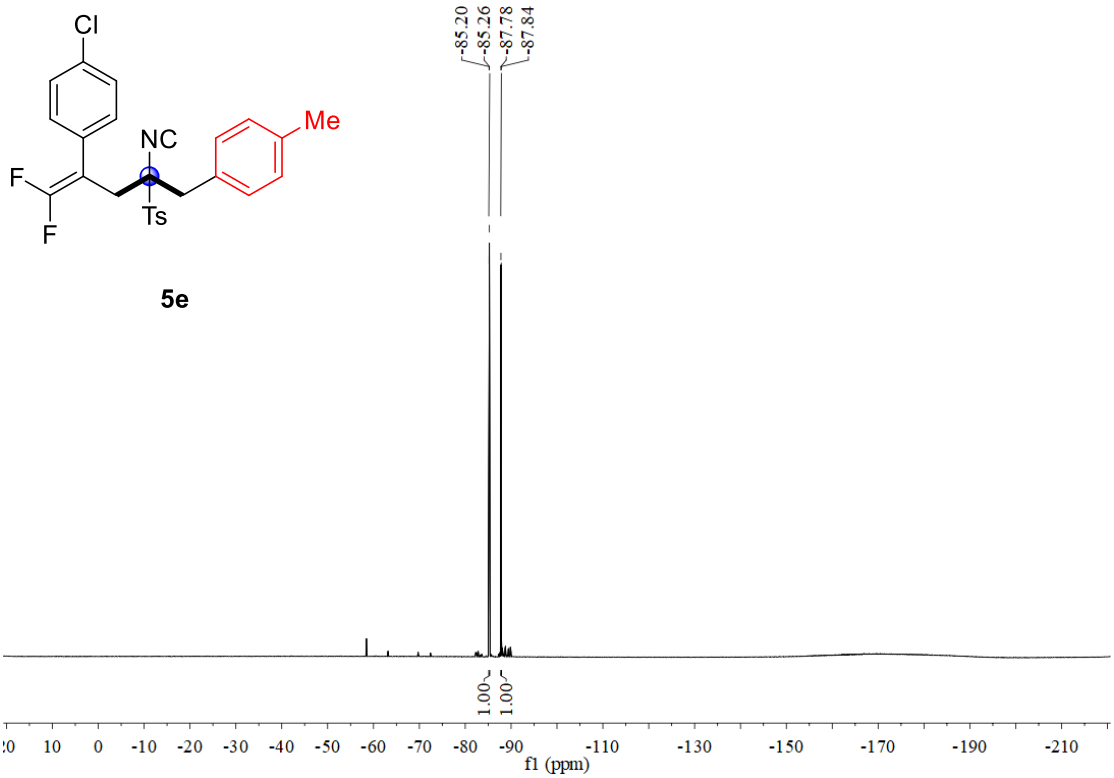
5d


7.83
7.81
7.55
7.54
7.34
7.32
7.10
7.08
7.06
7.04
3.30
3.26
3.24
3.21
3.05
3.02
2.93
2.90
2.50
2.46
2.28
Cl
NC
Me
F
F
Ts
2.00
1.94
1.80
6.00
2.02
1.94
3.01
3.00
f1 (ppm)

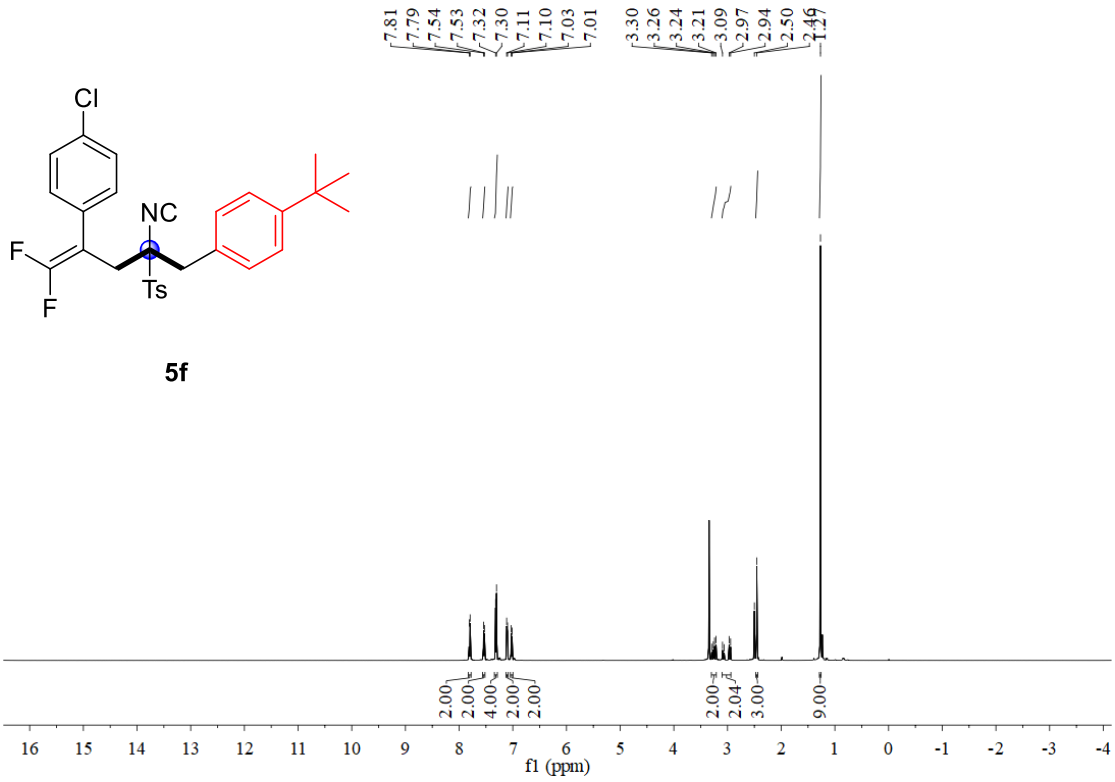
5e


166.98
166.86
156.16
153.85
151.54
146.85
137.22
132.53
131.03
130.72
130.39
130.23
129.65
128.86
128.80
128.32
87.04
86.88
86.73
79.95
71.17
39.52
31.06
27.24
21.28
20.80
20.71
18.88
18.69
13.57
Cl
NC
Me
F
F
Ts
f1 (ppm)

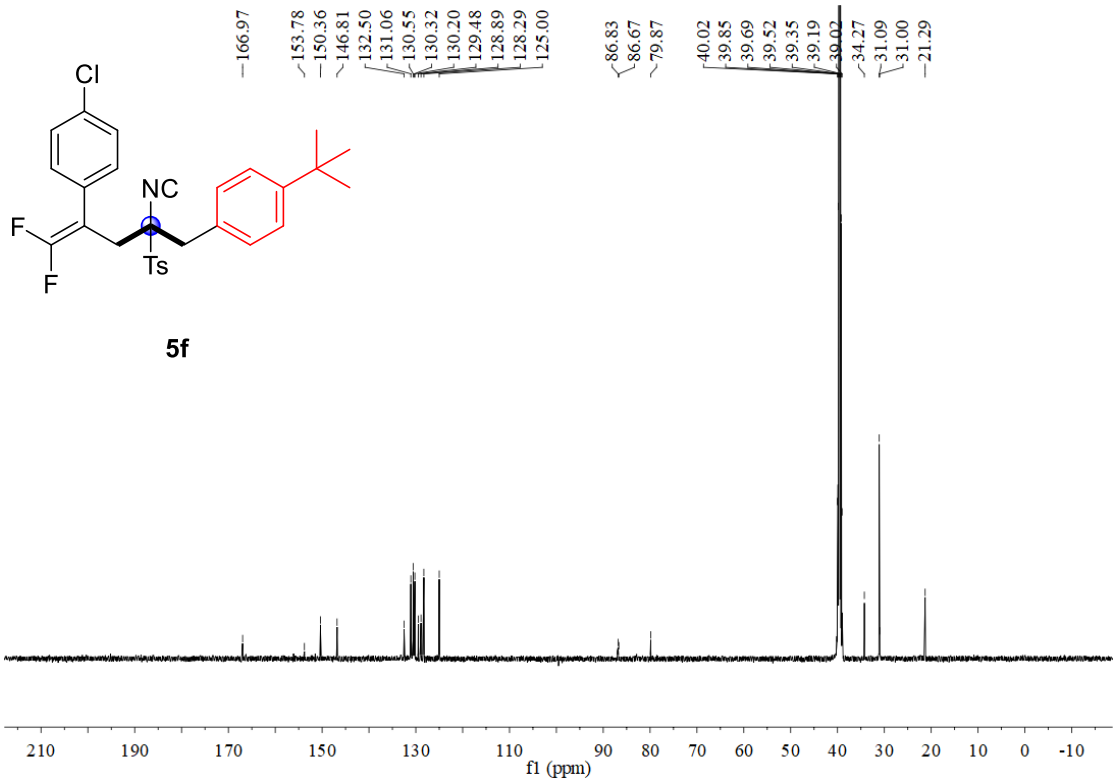
5e


Cl
NC
Me
F
F
Ts
-85.20
-85.26
-87.78
-87.84
1.00
1.00
f1 (ppm)

5e


Cl
NC
F
F
Ts
7.81
7.79
7.54
7.53
7.32
7.30
7.11
7.10
7.03
7.01
3.30
3.26
3.24
3.21
3.09
2.97
2.94
2.50
2.46
1.27
2.00
2.00
4.00
2.00
2.00
2.00
2.04
3.00
9.00
f1 (ppm)

5f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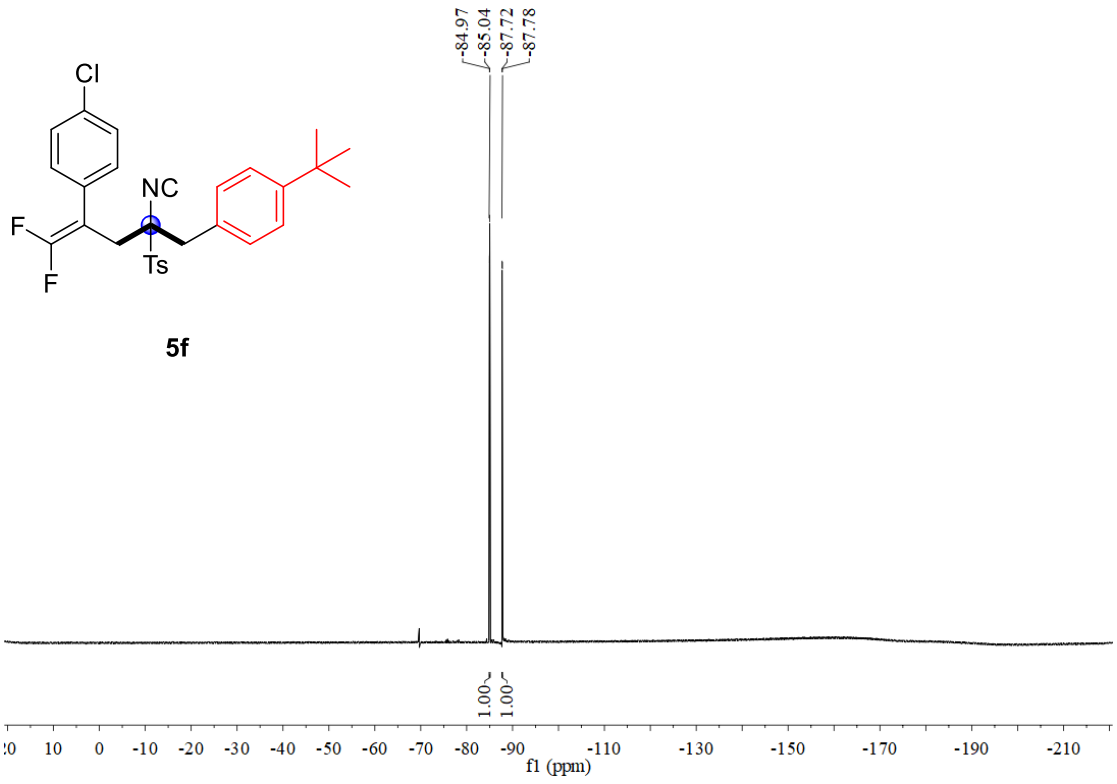
132.50
131.06
130.55
130.32
130.20
129.48
128.89
128.29
125.00
86.83
86.67
79.87
40.02
39.85
39.69
39.52
39.35
39.19
39.02
34.27
31.09
31.00
21.29
Cl
NC
F
F
Ts
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

5f


-84.97
-85.04
-87.72
-87.78
Cl
NC
F
F
Ts
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1.00
10
0
-10
-20
-30
-40
-50
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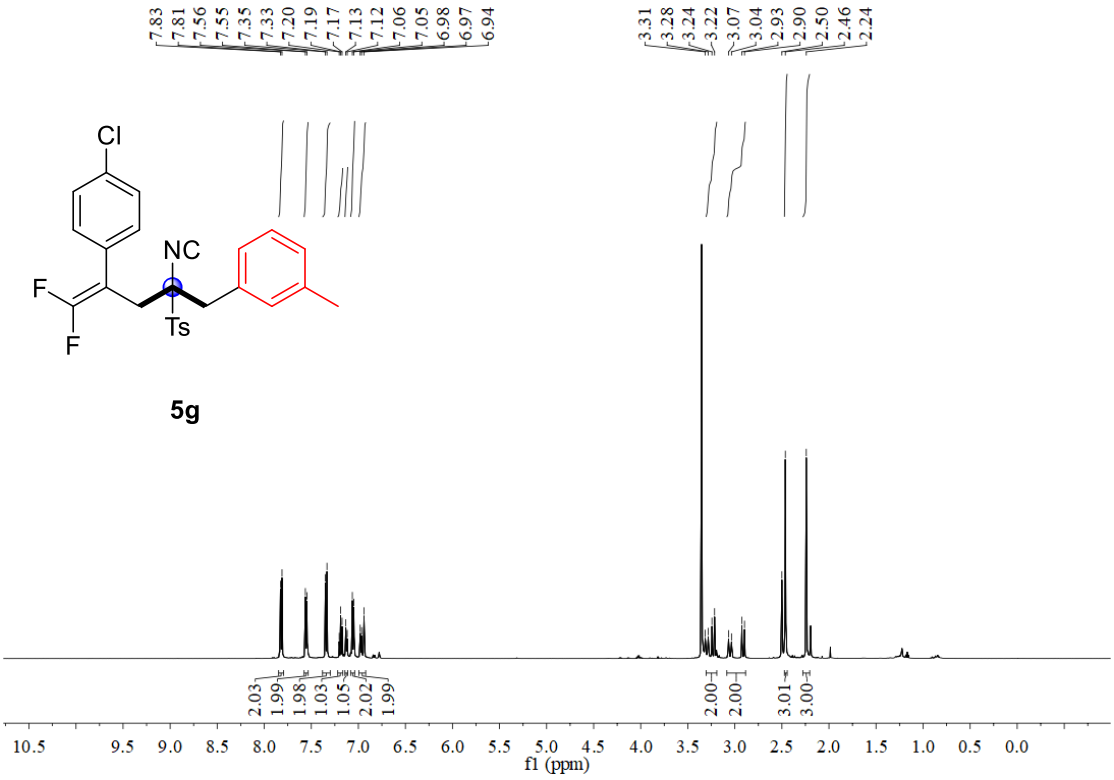
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

5f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7.81
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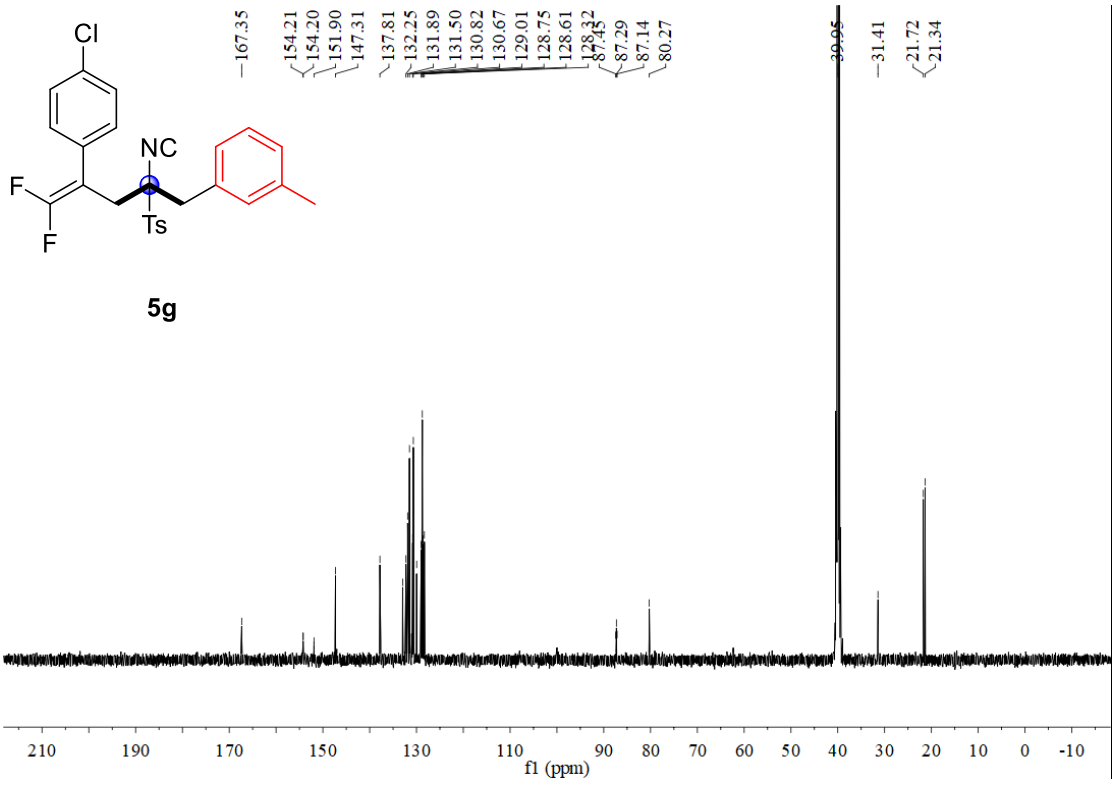
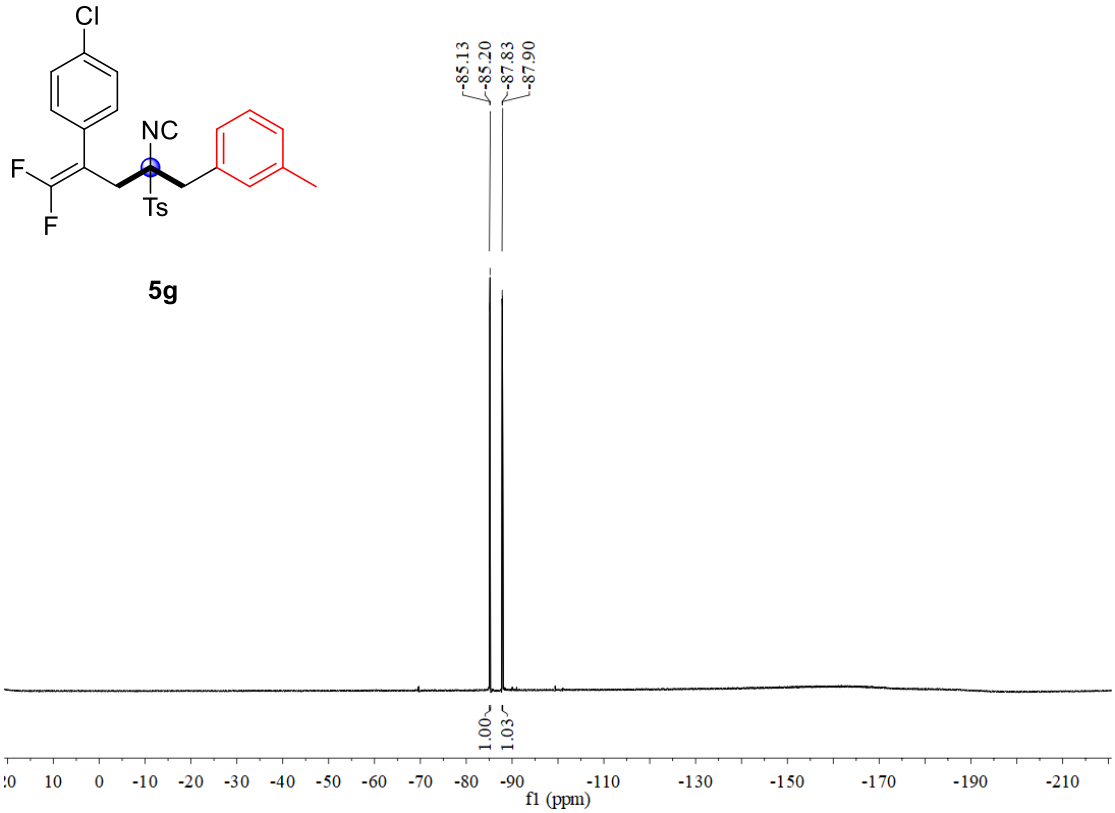
7.55
7.35
7.33
7.20
7.19
7.17
7.13
7.12
7.06
7.05
6.98
6.97
6.94
3.31
3.28
3.24
3.22
3.07
3.04
2.93
2.90
2.50
2.46
2.24
Cl
NC
F
F
Ts
5g
2.03
1.99
1.98
1.03
1.05
2.02
1.99
2.00
2.00
3.01
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.35
154.21
154.20
151.90
147.31
137.81
132.25
131.89
131.50
130.82
130.67
129.01
128.75
128.61
128.32
87.45
87.29
87.14
80.27
39.95
31.41
21.72
21.34
Cl
NC
F
F
Ts
5g
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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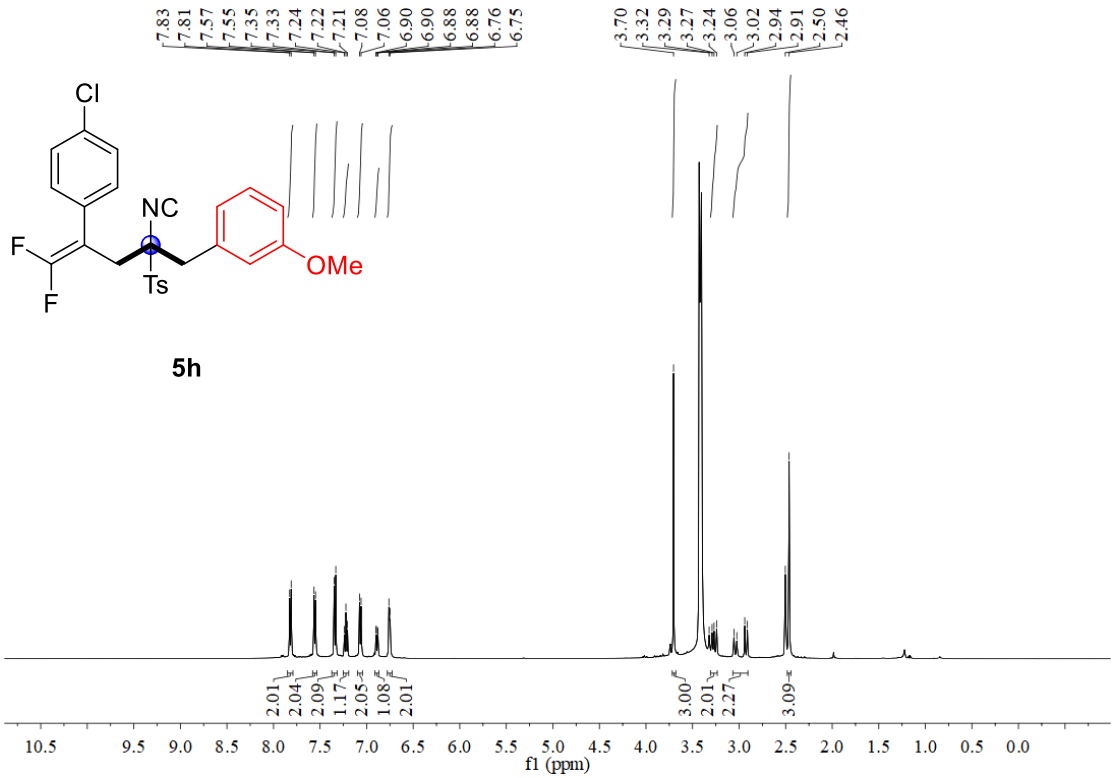
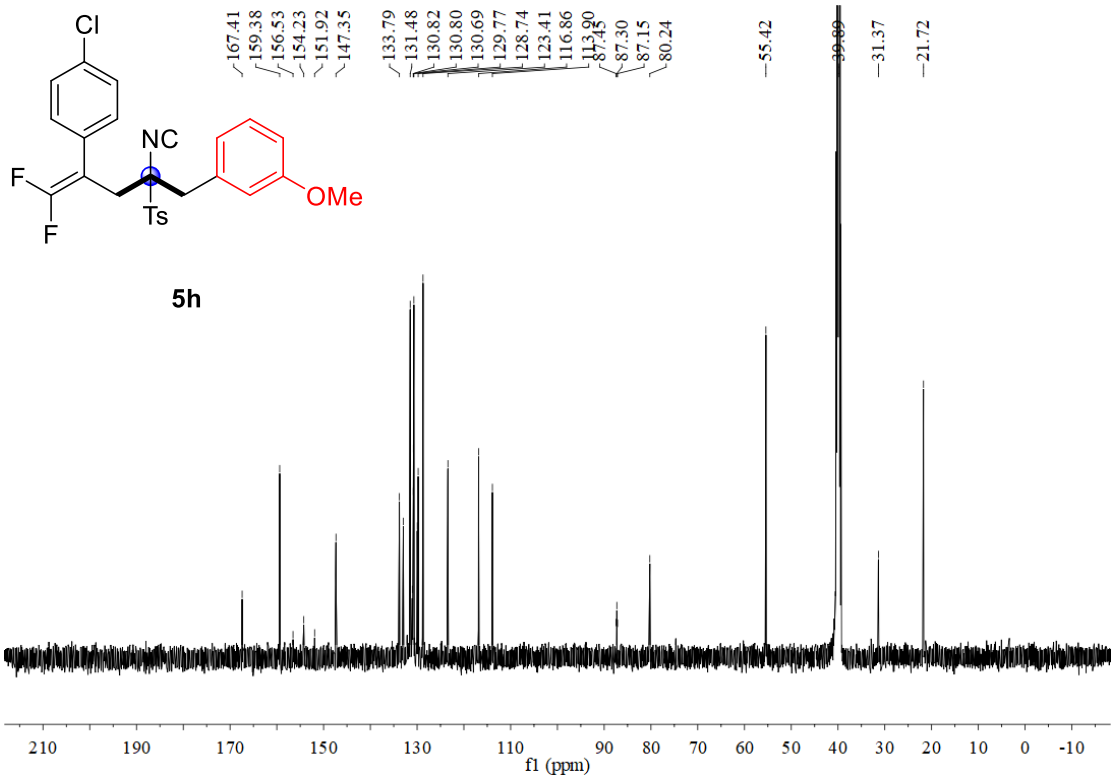
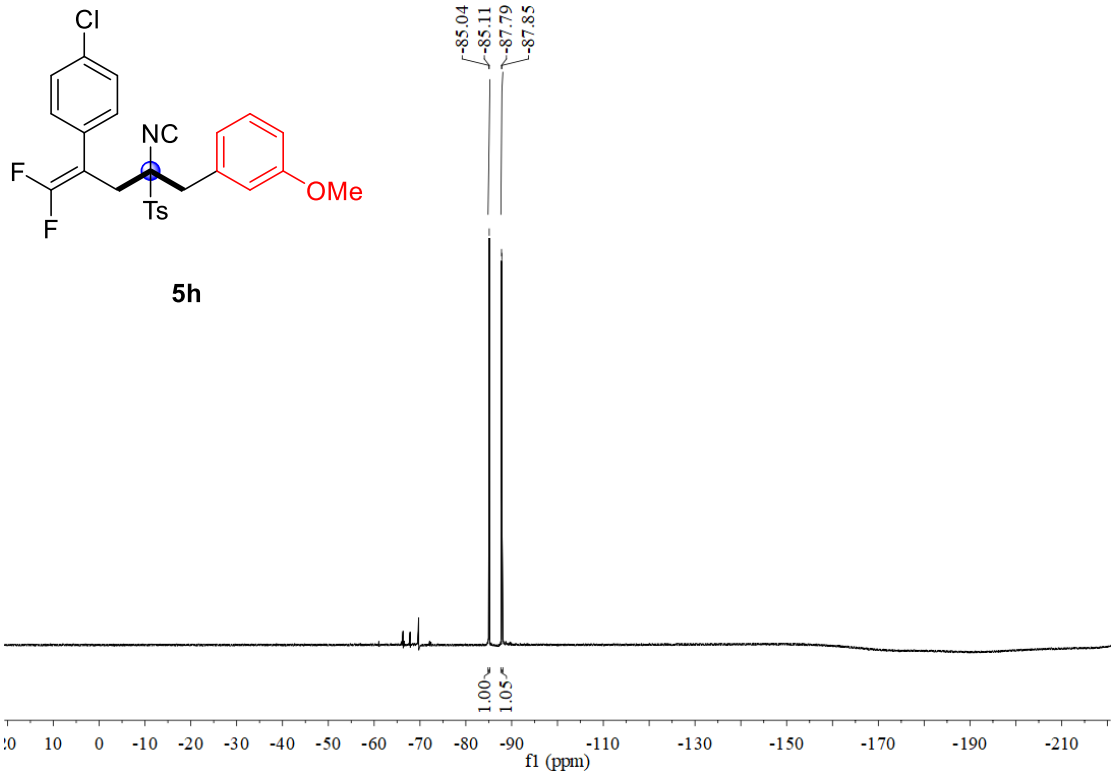
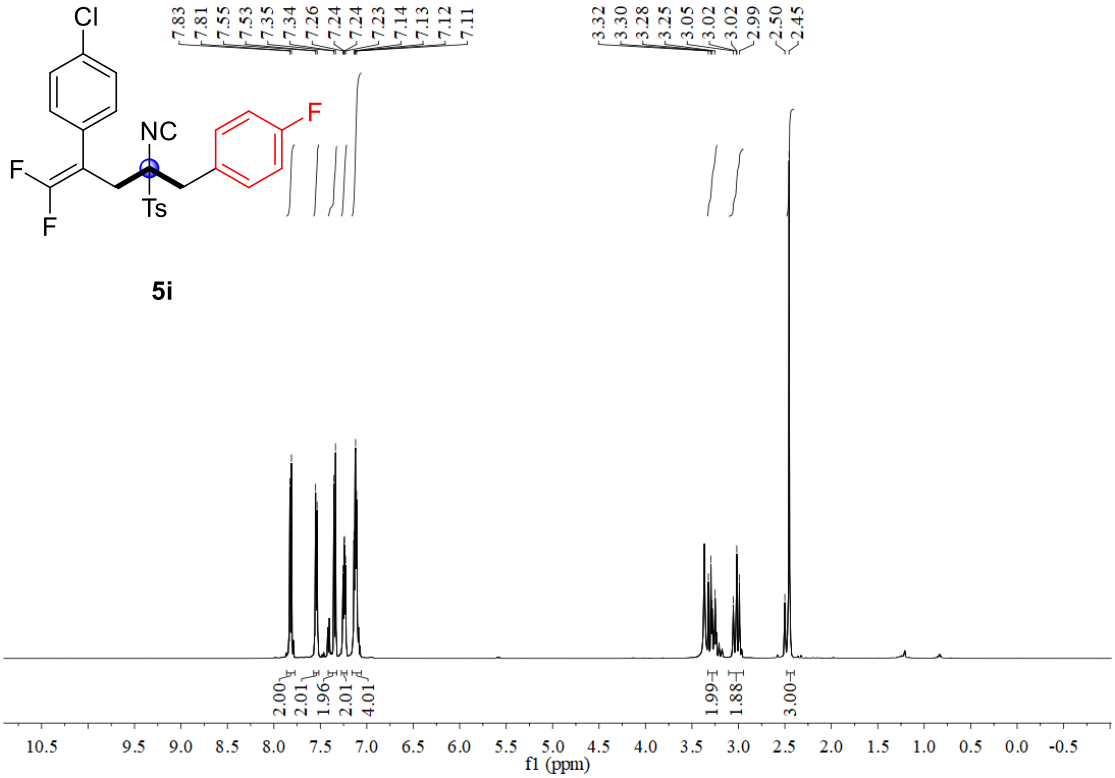
NC
F
F
Ts
5g
-85.13
-85.20
-87.83
-87.90
1.00
1.03
f1 (ppm)

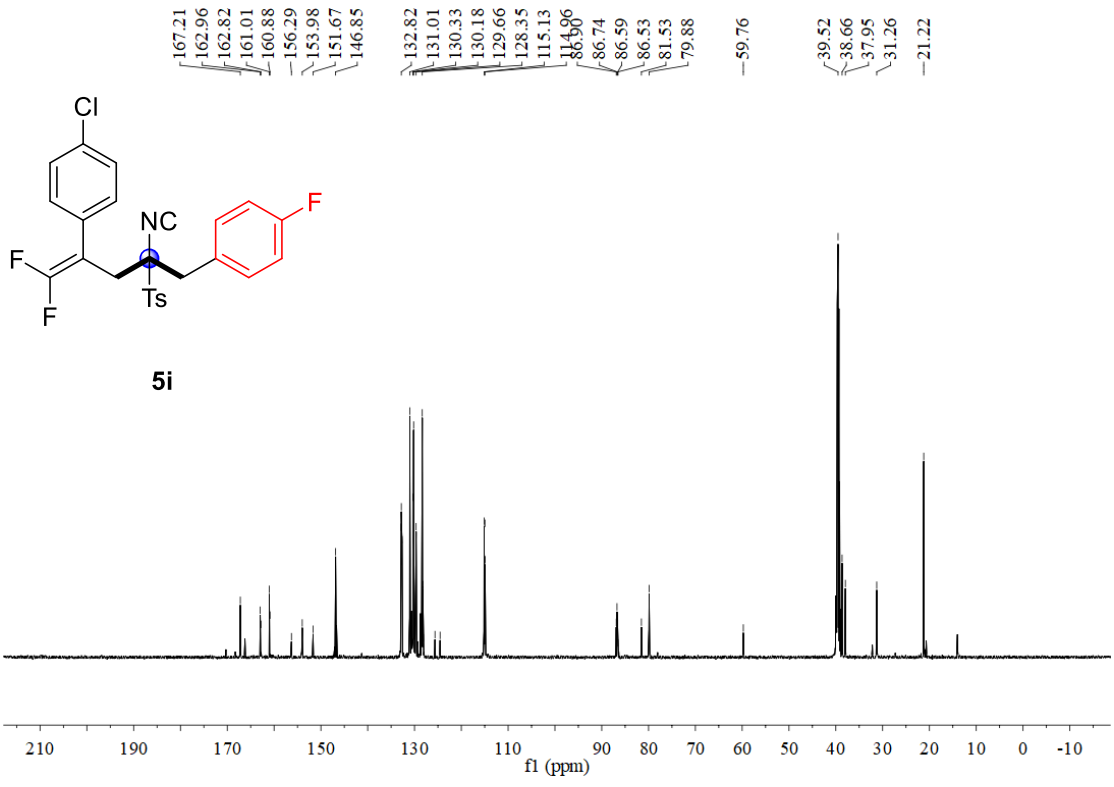

7.83
7.81
7.57
7.55
7.35
7.33
7.24
7.22
7.21
7.08
7.06
6.90
6.90
6.88
6.76
6.75
3.70
3.32
3.29
3.27
3.24
3.06
3.02
2.94
2.91
2.50
2.46
Cl
NC
F
F
Ts
OMe
5h
2.01
2.04
2.09
1.17
2.05
1.08
2.01
3.00
2.01
2.27
3.09
f1 (ppm)


Cl
NC
F
F
Ts
OMe
5h
167.41
159.38
156.53
154.23
151.92
147.35
133.79
131.48
130.82
130.80
130.69
129.77
128.74
123.41
116.86
113.90
87.45
87.30
87.15
80.24
55.42
39.89
31.37
21.72
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

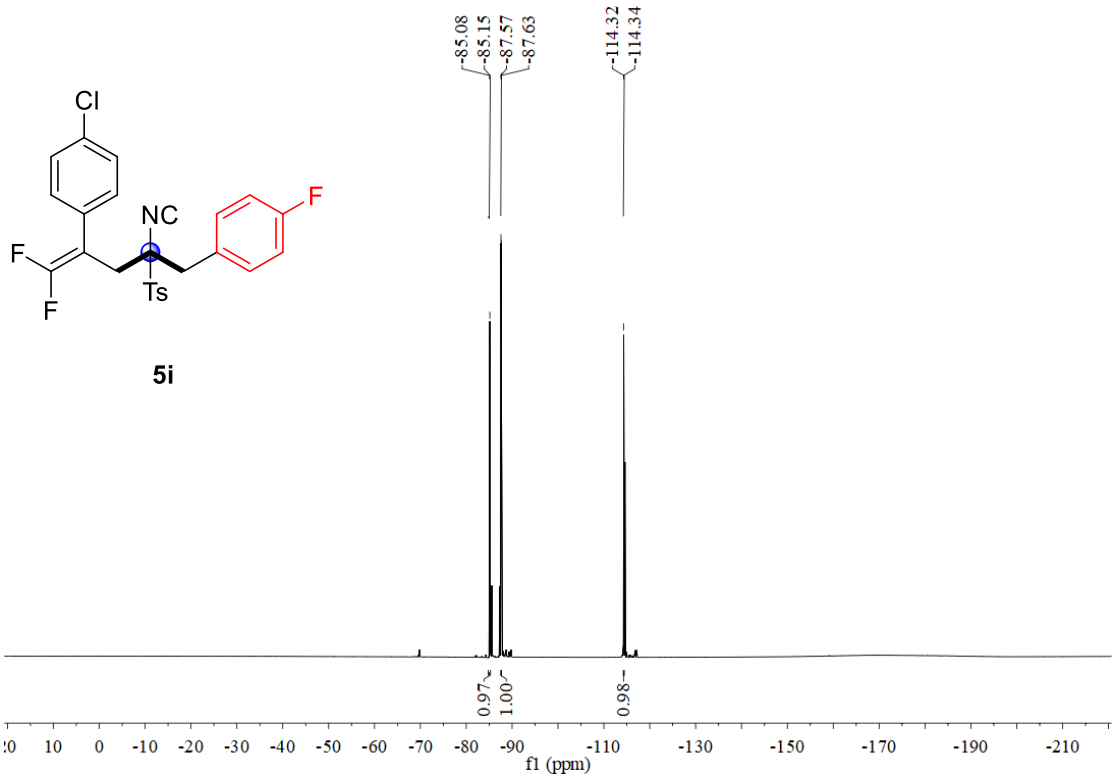

Cl
NC
F
F
Ts
OMe
5h
-85.04
-85.11
-87.79
-87.85
1.00
1.05
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


Cl
NC
F
F
F
Ts
7.83
7.81
7.55
7.53
7.35
7.34
7.26
7.24
7.24
7.23
7.14
7.13
7.12
7.11
3.32
3.30
3.28
3.25
3.05
3.02
3.02
2.99
2.50
2.45
2.00
2.01
1.96
2.01
4.01
1.99
1.88
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

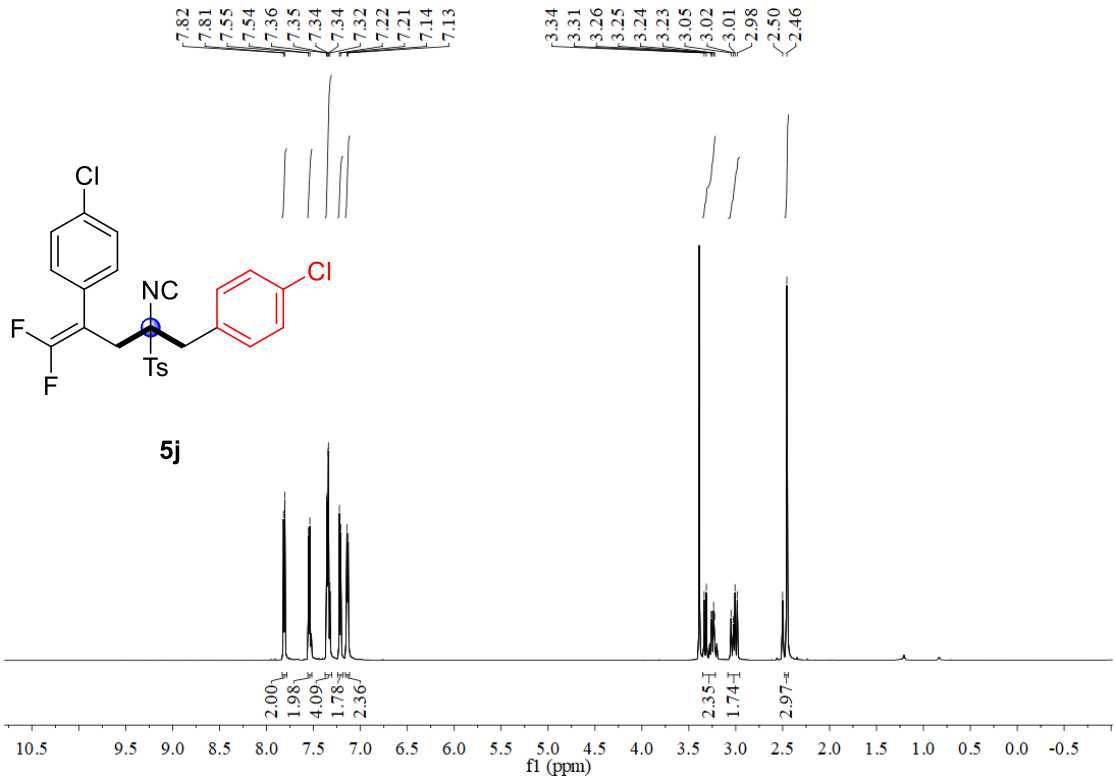
5i


Cl
NC
F
F
F
Ts
167.21
162.96
162.82
161.01
160.88
156.29
153.98
151.67
146.85
132.82
131.01
130.33
130.18
129.66
128.35
115.13
114.96
86.90
86.74
86.59
86.53
81.53
79.88
59.76
39.52
38.66
37.95
31.26
21.22
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

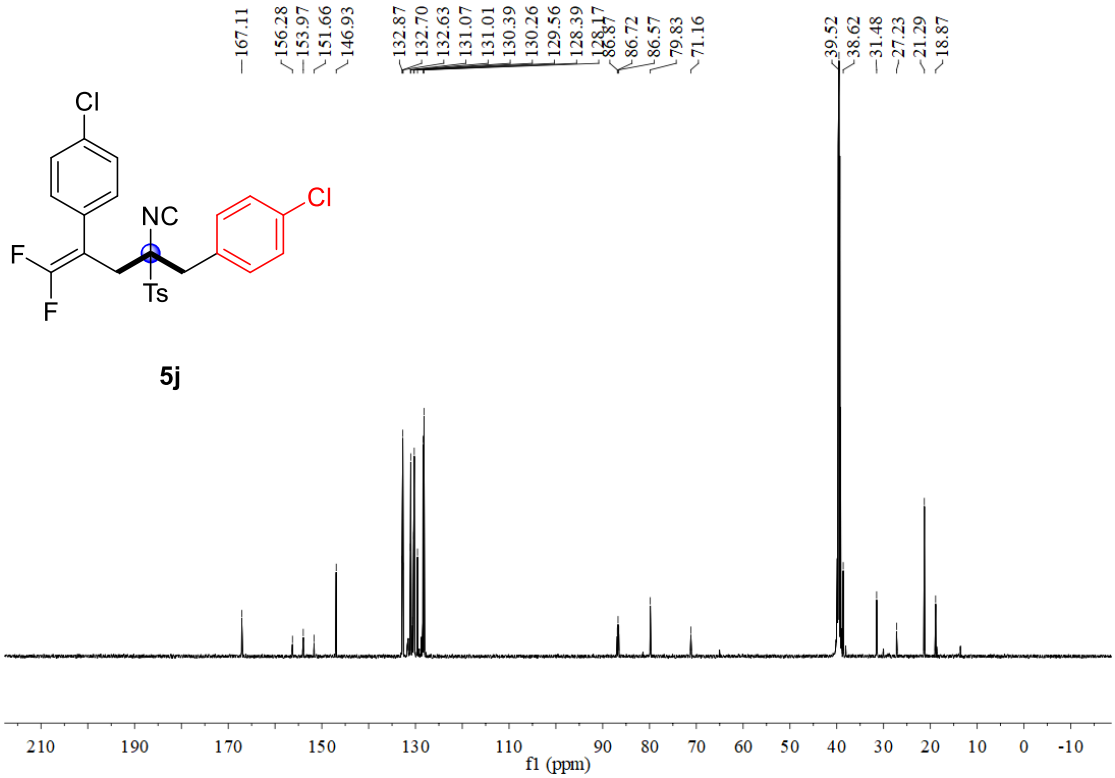
5i


Cl
NC
F
F
F
Ts
-85.08
-85.15
-87.57
-87.63
-114.32
-114.34
0.97
1.00
0.98
f1 (ppm)

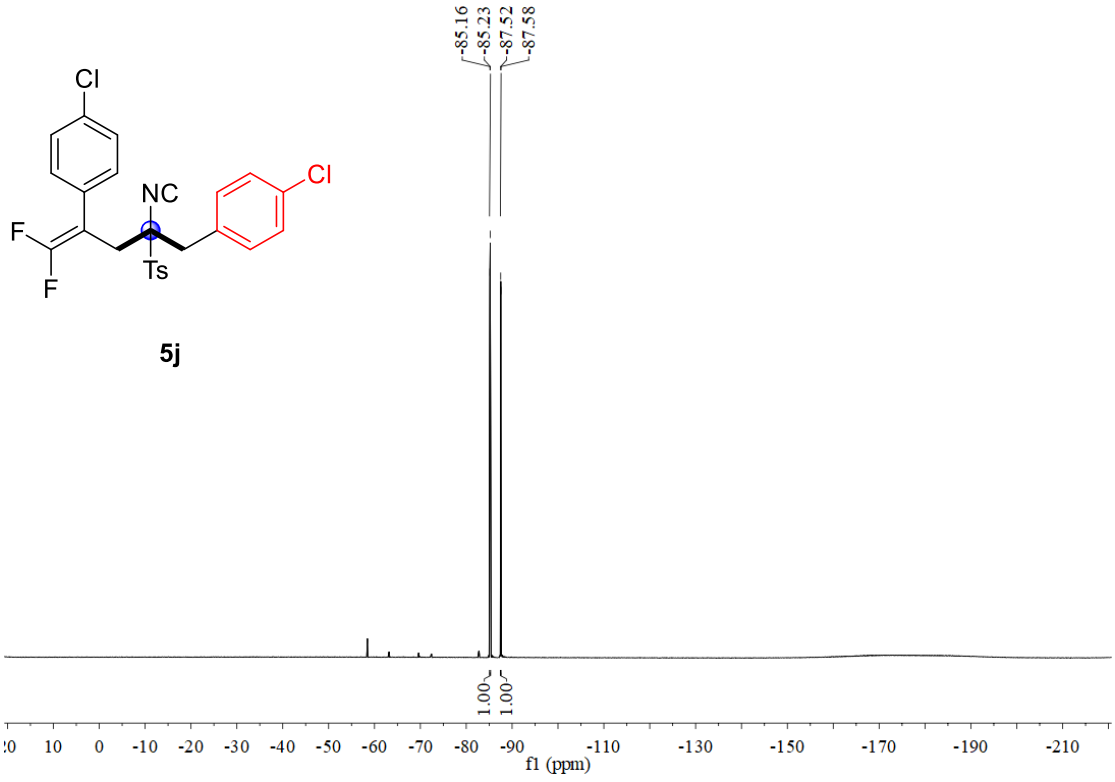
5i


7.82
7.81
7.55
7.54
7.36
7.35
7.34
7.34
7.32
7.22
7.21
7.14
7.13
3.34
3.31
3.26
3.25
3.24
3.23
3.05
3.02
3.01
2.98
2.50
2.46
Cl
NC
F
F
Cl
Ts
2.00
1.98
4.09
1.78
2.36
2.35
1.74
2.97
f1 (ppm)

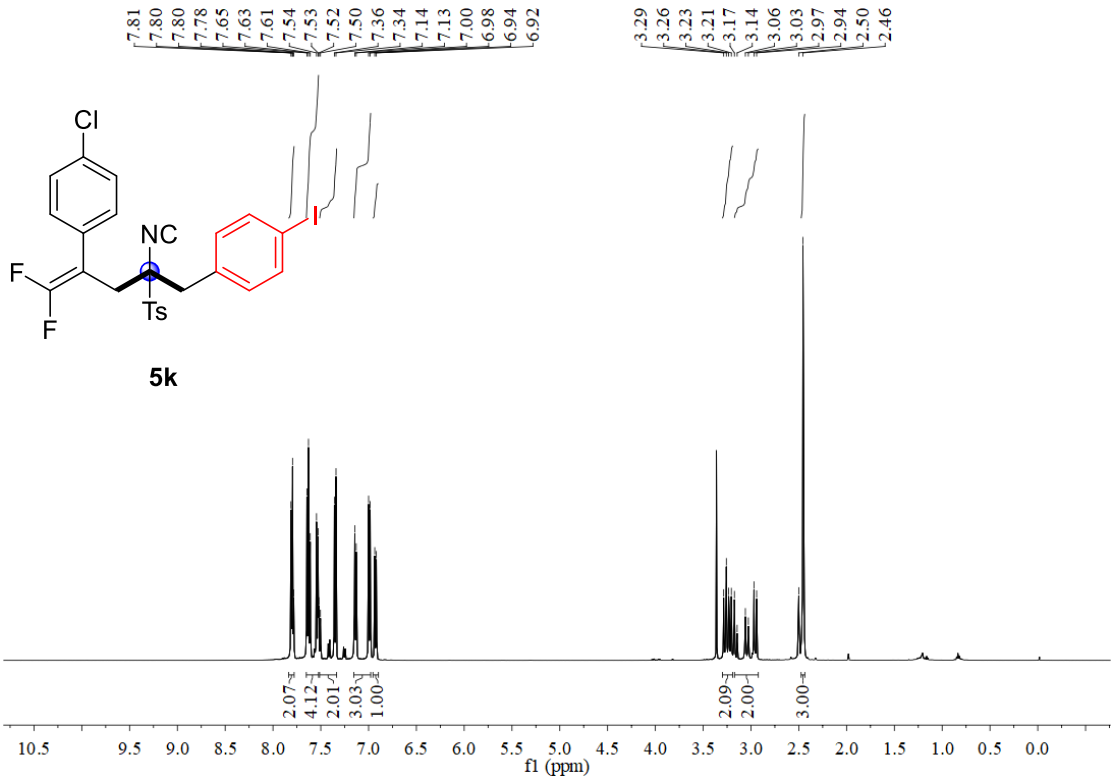
5j


167.11
156.28
153.97
151.66
146.93
132.87
132.70
132.63
131.07
131.01
130.39
130.26
129.56
128.39
128.17
86.87
86.72
86.57
79.83
71.16
39.52
38.62
31.48
27.23
21.29
18.87
Cl
NC
Cl
F
F
Ts
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

5j


-85.16
-85.23
-87.52
-87.58
Cl
NC
Cl
F
F
Ts
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

5j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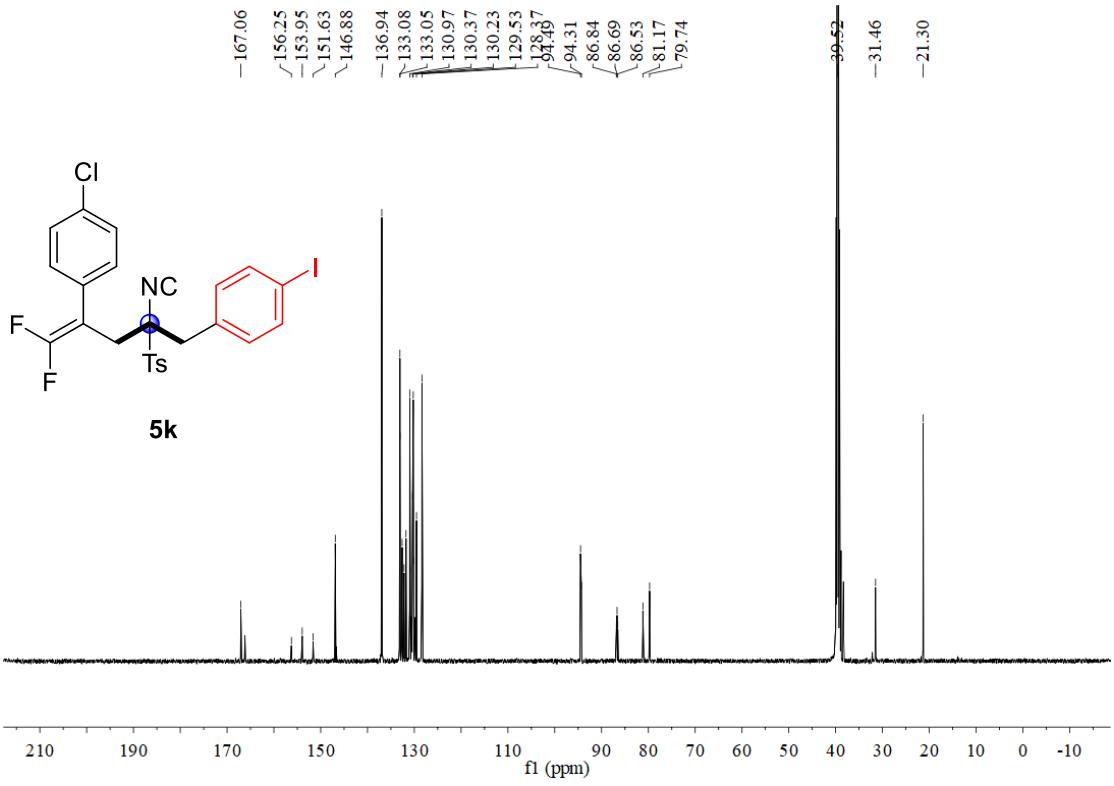
7.80
7.78
7.65
7.63
7.61
7.54
7.53
7.52
7.50
7.36
7.34
7.14
7.13
7.00
6.98
6.94
6.92
3.29
3.26
3.23
3.21
3.17
3.14
3.06
3.03
2.97
2.94
2.50
2.46
Cl
NC
F
F
Ts
I
5k
2.07
4.12
2.01
3.03
1.00
2.09
2.00
3.00
f1 (ppm)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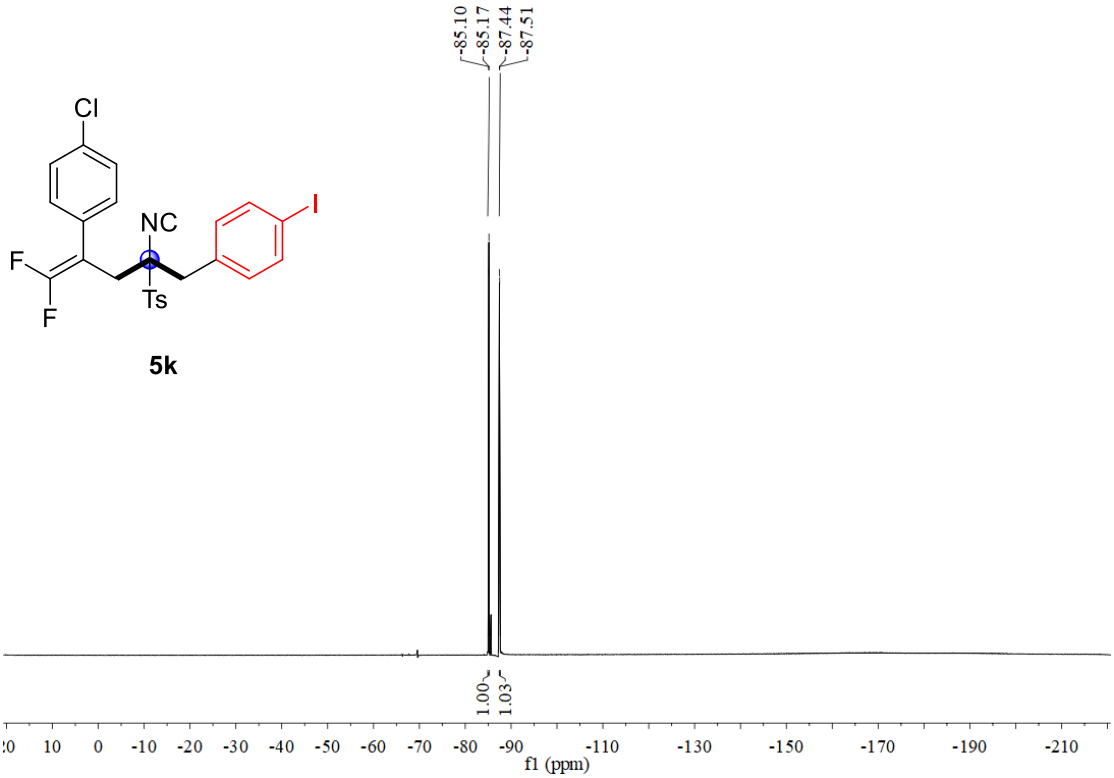
136.94
133.08
133.05
130.97
130.37
130.23
129.53
94.31
86.84
86.69
86.53
81.17
79.74
39.52
31.46
21.30
Cl
NC
F
F
Ts
I
5k
f1 (ppm)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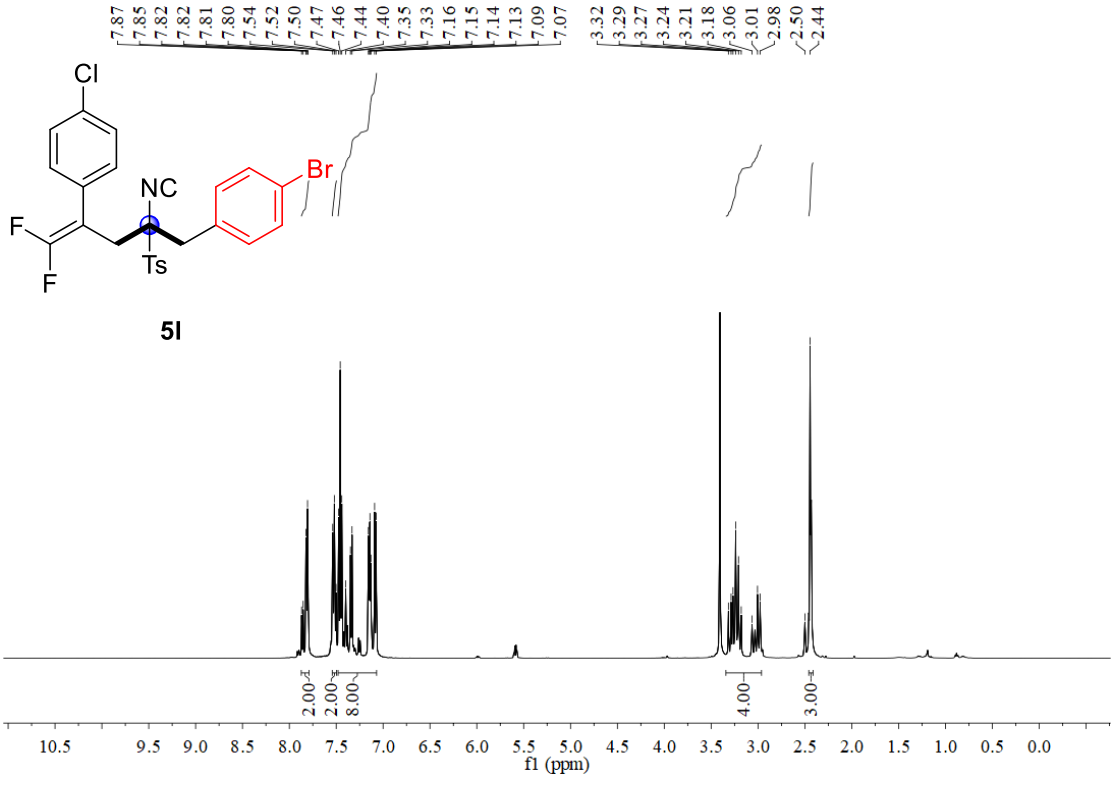
-85.17
-87.44
-87.51
Cl
NC
I
F
F
Ts
1.00
1.03
f1 (ppm)

5k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7.82
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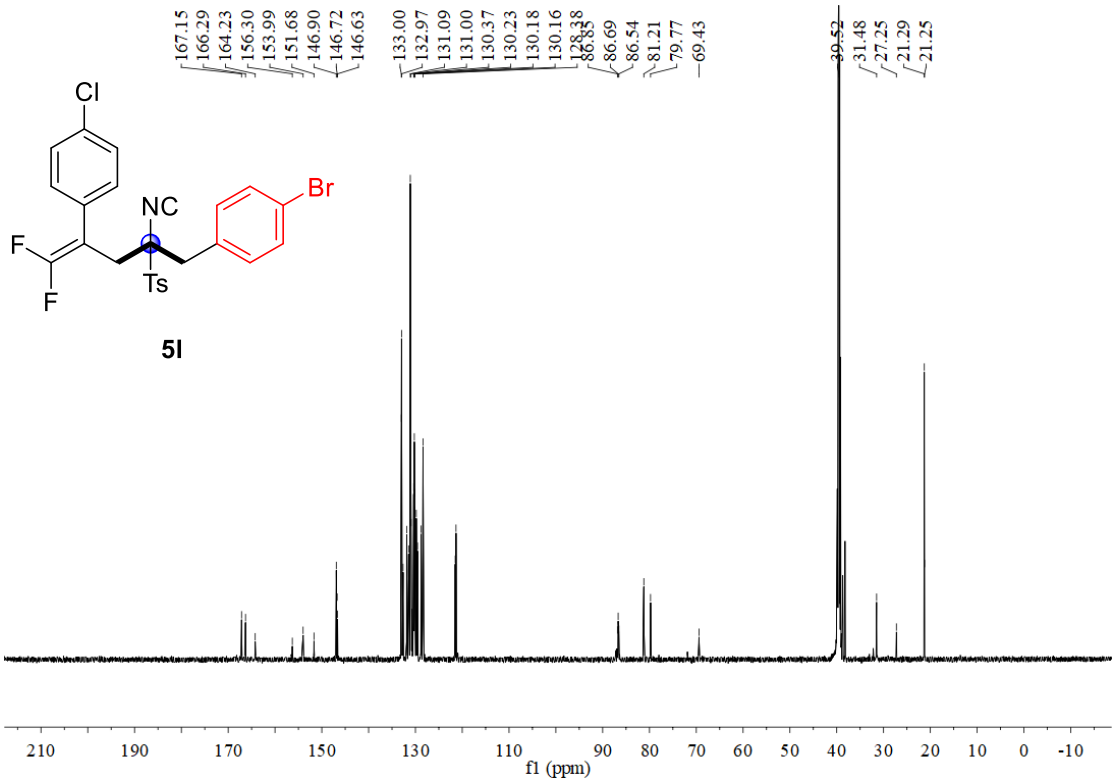
7.80
7.54
7.52
7.50
7.47
7.46
7.44
7.40
7.35
7.33
7.16
7.15
7.14
7.13
7.09
7.07
3.32
3.29
3.27
3.24
3.21
3.18
3.06
3.01
2.98
2.50
2.44
Cl
NC
Br
F
F
Ts
2.00
2.00
8.00
4.00
3.00
f1 (ppm)

5l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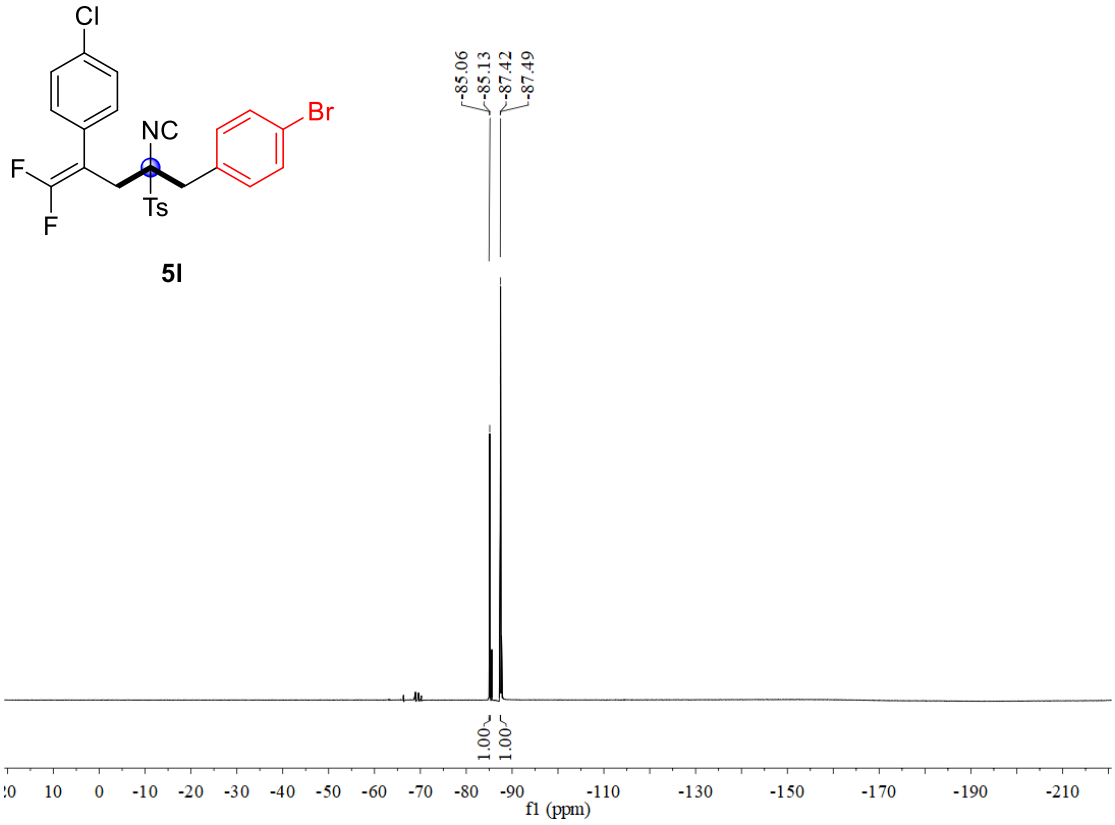
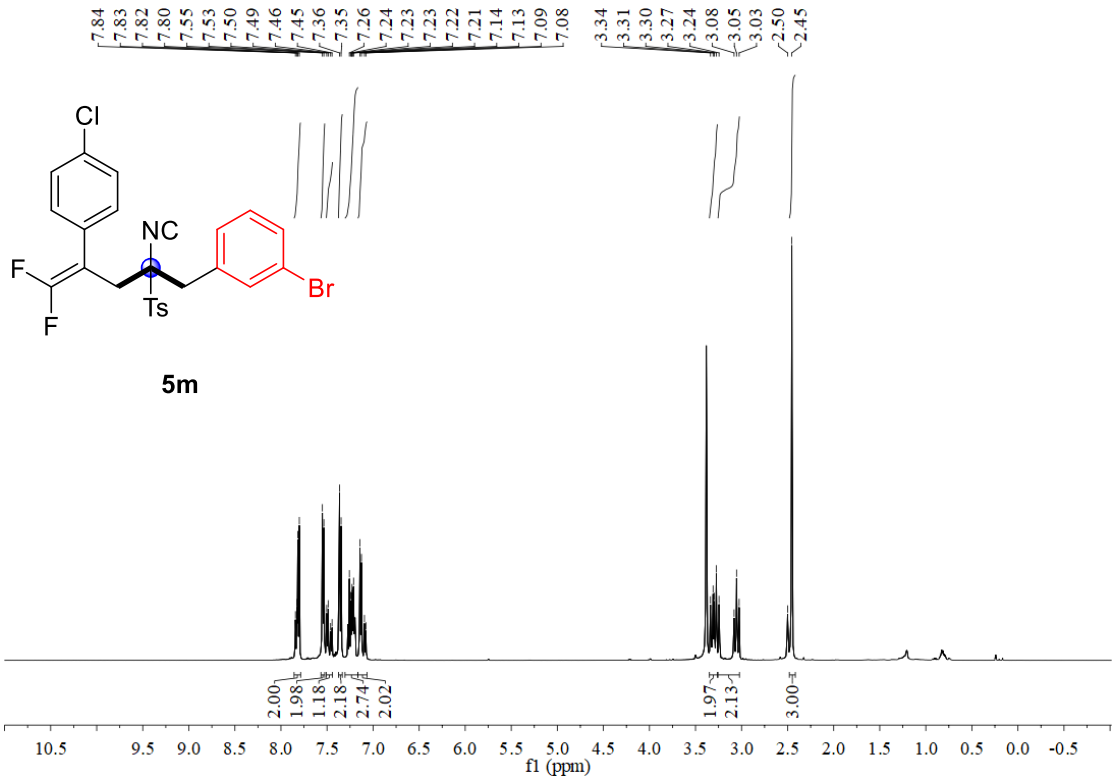
151.68
146.90
146.72
146.63
133.00
132.97
131.09
131.00
130.37
130.23
130.18
130.16
128.38
86.85
86.69
86.54
81.21
79.77
69.43
39.52
31.48
27.25
21.29
21.25
Cl
Br
NC
F
F
Ts
5l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-85.06
-85.13
-87.42
-87.49
Cl
Br
NC
F
F
Ts
5l
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)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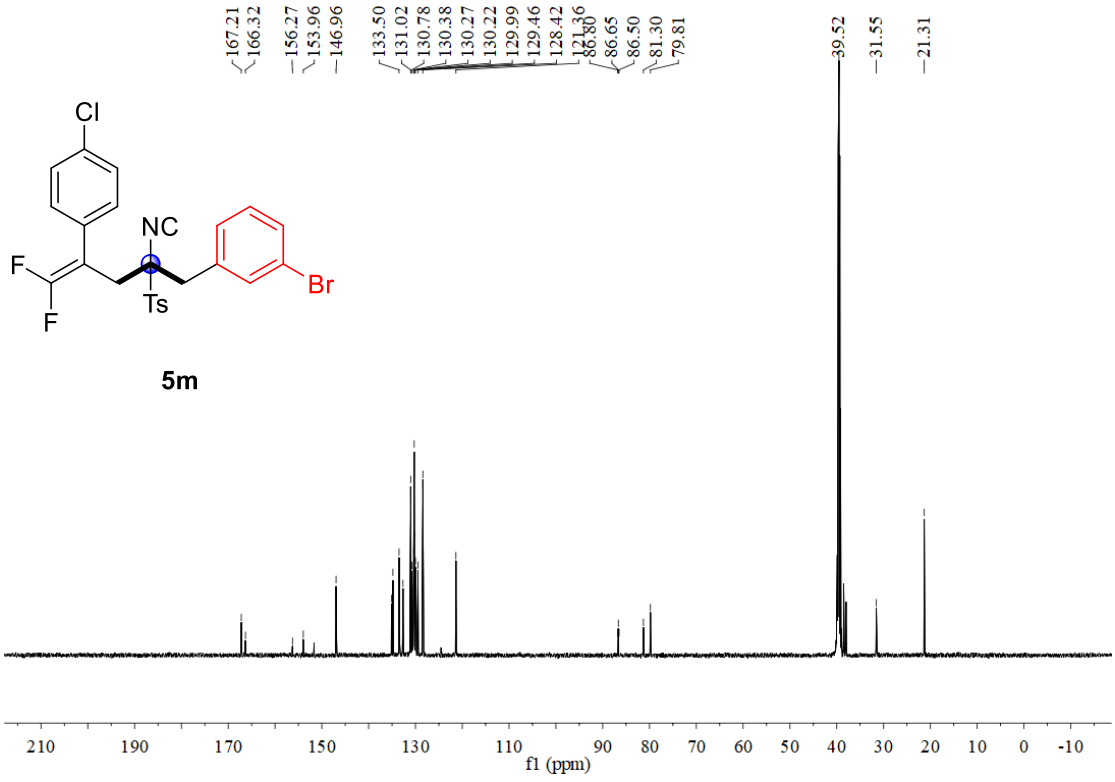
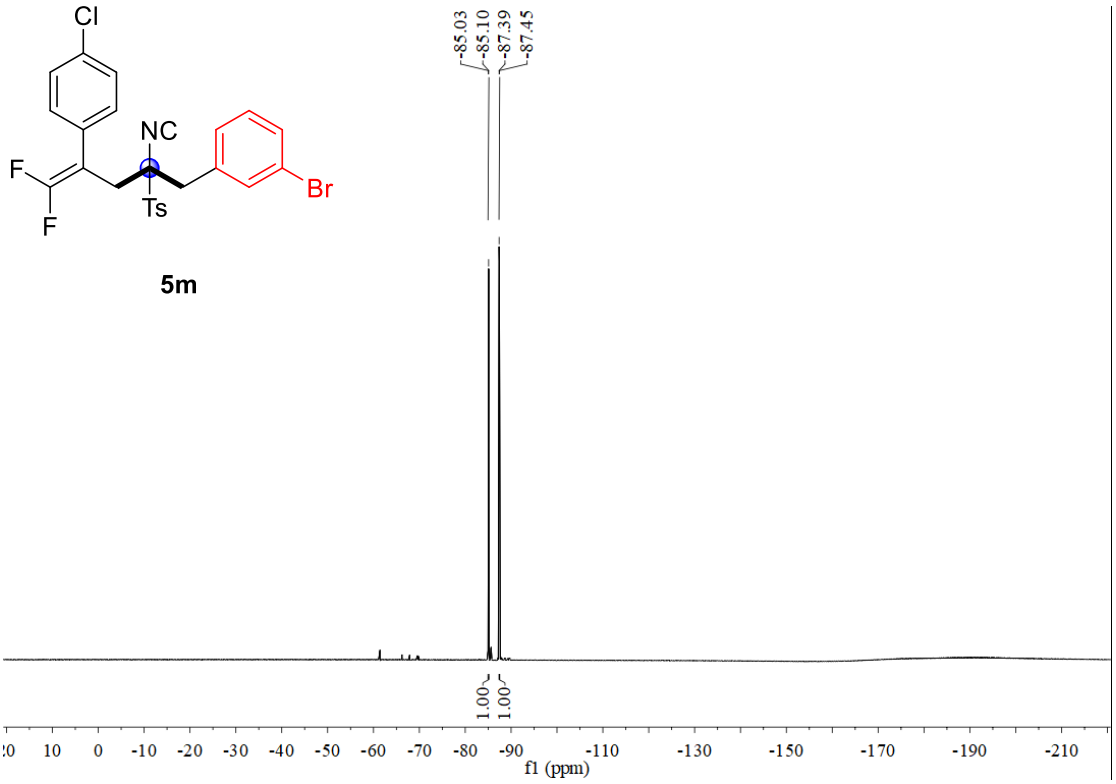
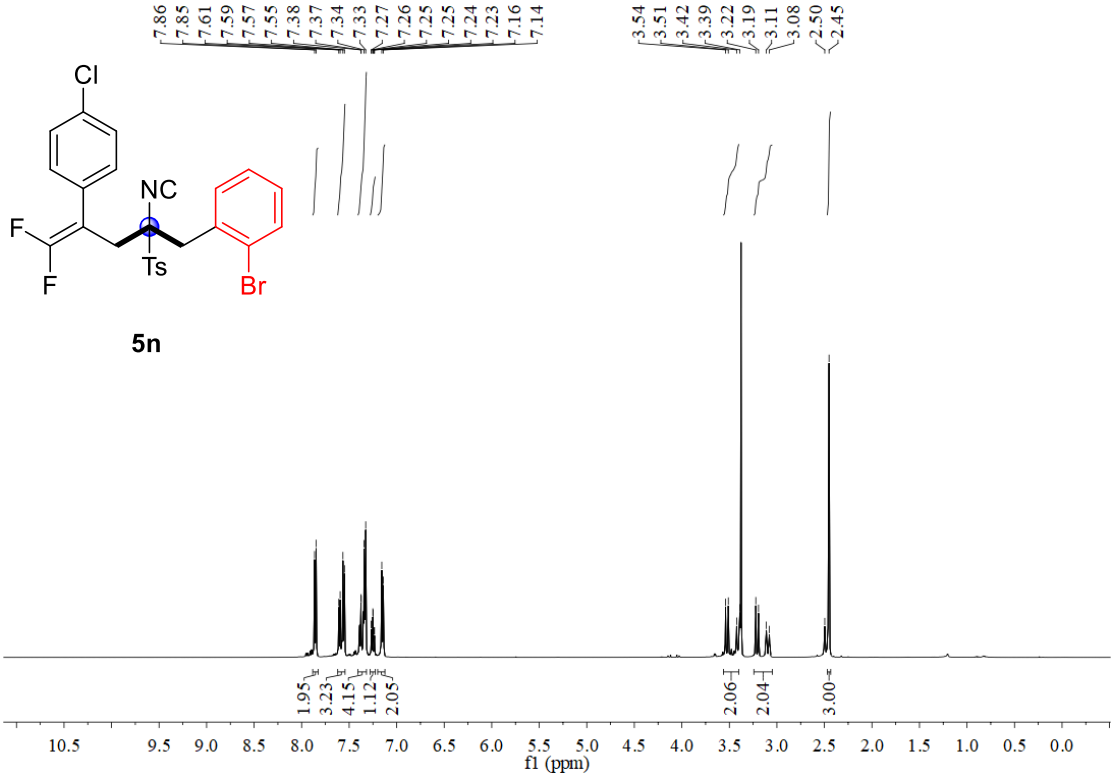
7.45
7.36
7.35
7.26
7.24
7.23
7.23
7.22
7.21
7.14
7.13
7.09
7.08
3.34
3.31
3.30
3.27
3.24
3.08
3.05
3.03
2.50
2.45
Cl
NC
F
F
Ts
Br
5m
2.00
1.98
1.18
2.18
2.74
2.02
1.97
2.13
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


167.21
166.32
156.27
153.96
146.96
133.50
131.02
130.78
130.38
130.27
130.22
129.99
129.46
128.42
121.36
86.80
86.65
86.50
81.30
79.81
39.52
31.55
21.31
Cl
NC
F
F
Ts
Br
5m
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Cl
NC
F
F
Ts
Br
-85.03
-85.10
-87.39
-87.45
1.00
1.00
f1 (ppm)

5m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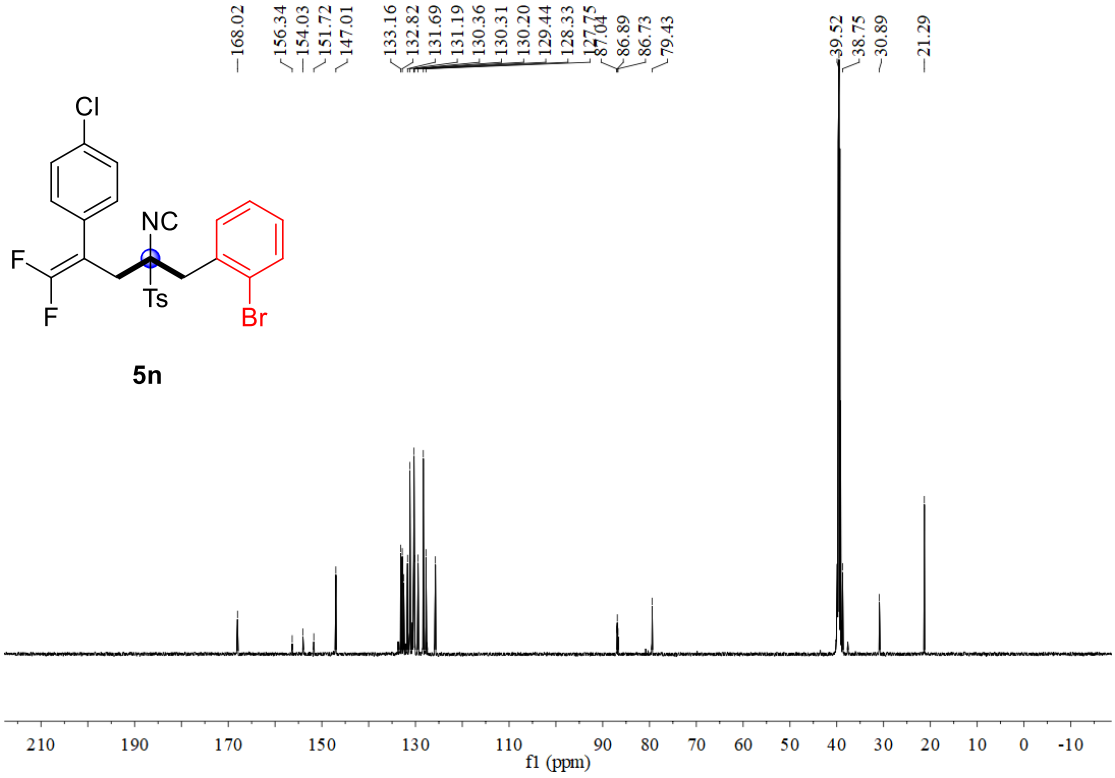
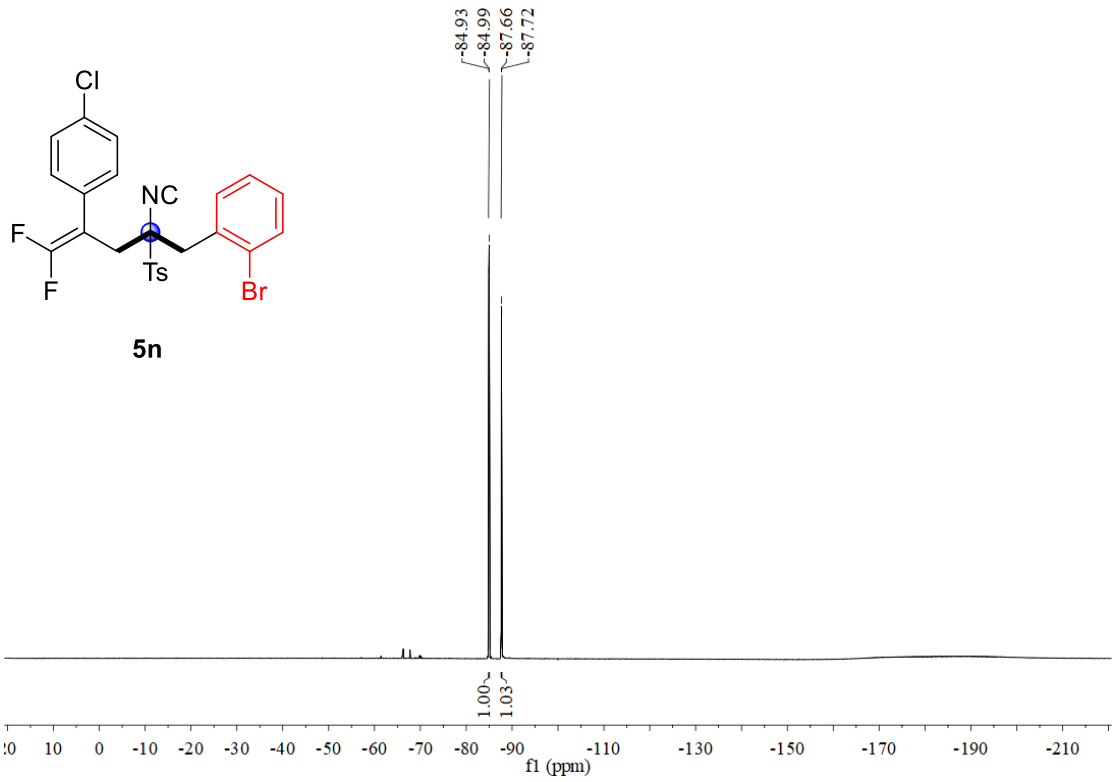
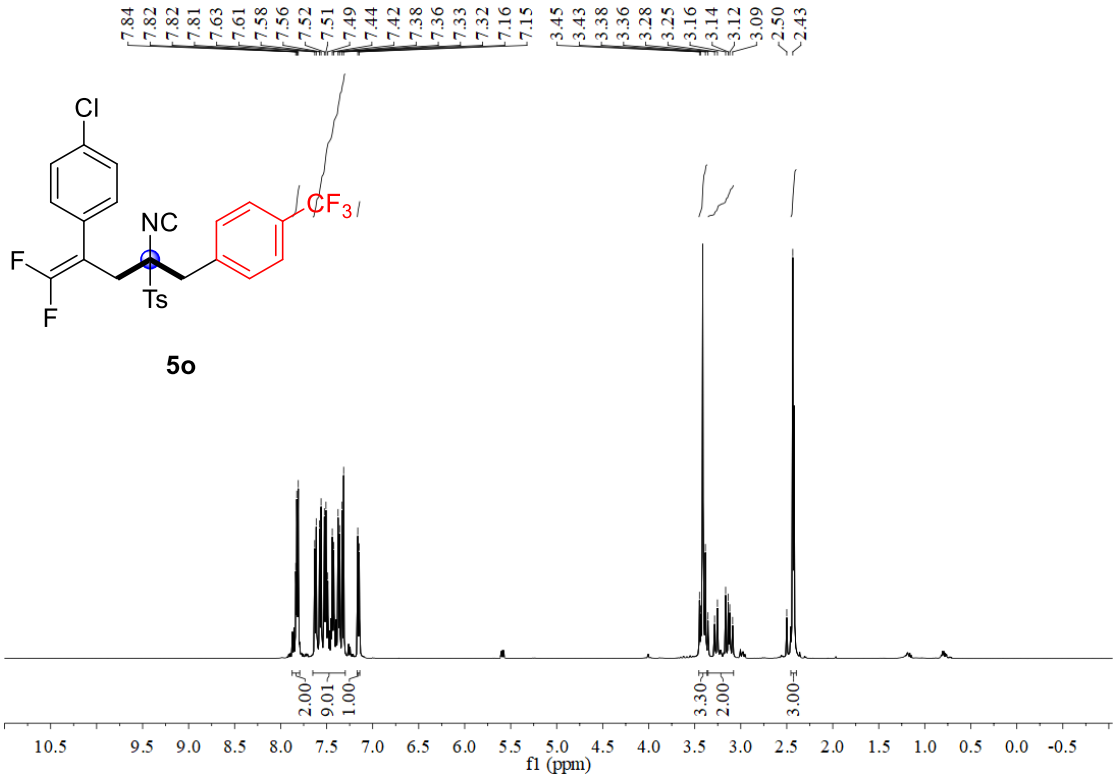
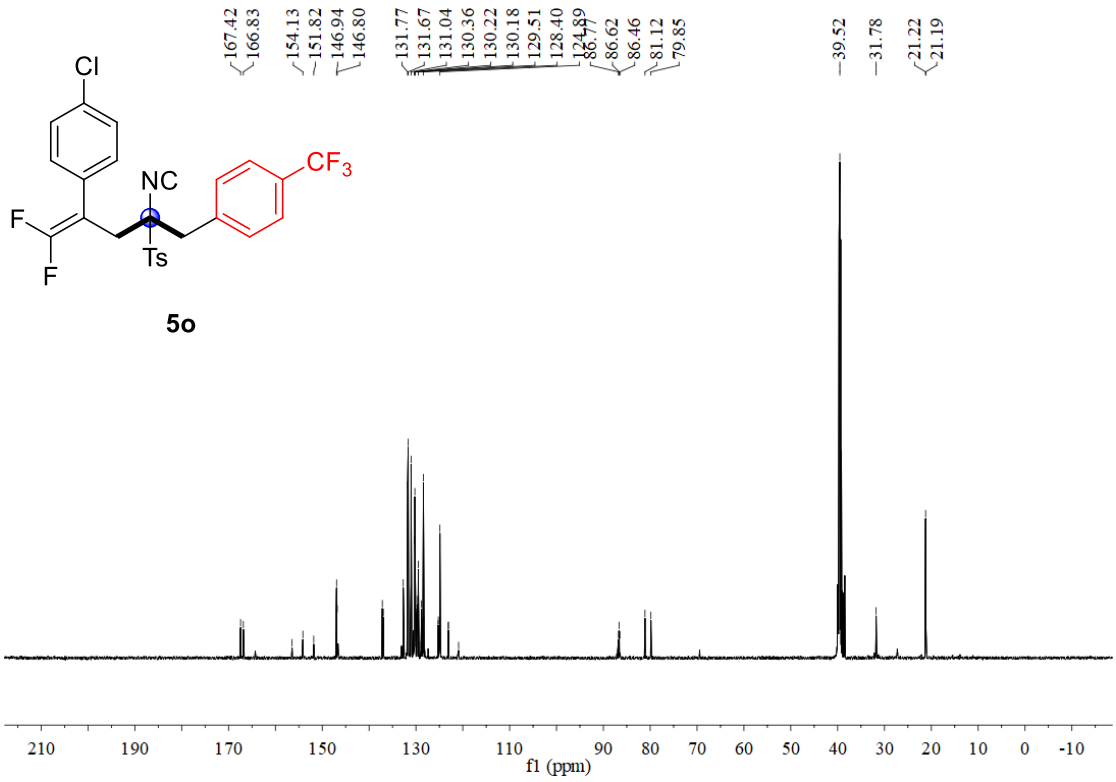
7.59
7.57
7.55
7.38
7.37
7.34
7.33
7.27
7.26
7.25
7.25
7.24
7.23
7.16
7.14
3.54
3.51
3.42
3.39
3.22
3.19
3.11
3.08
2.50
2.45
Cl
NC
F
F
Ts
Br
1.95
3.23
4.15
1.12
2.05
2.06
2.04
3.00
f1 (ppm)

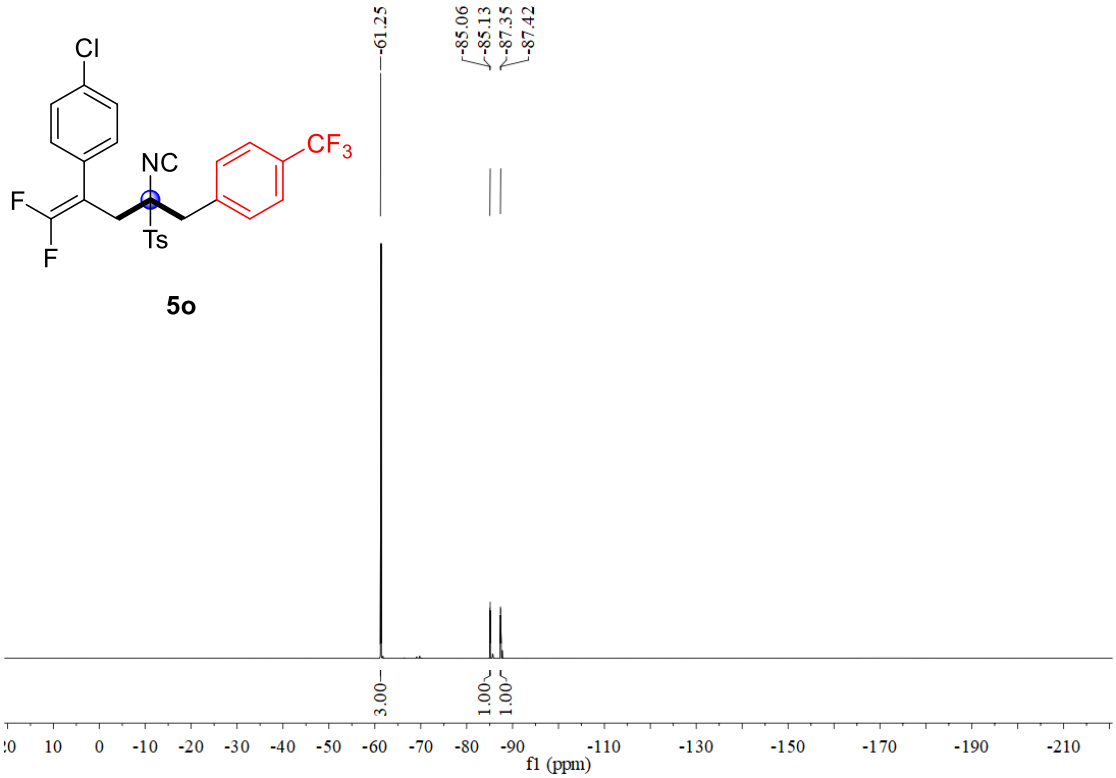
5n


168.02
156.34
154.03
151.72
147.01
133.16
132.82
131.69
131.19
130.36
130.31
130.20
129.44
128.33
127.75
87.04
86.89
86.73
79.43
39.52
38.75
30.89
21.29
Cl
NC
F
F
Ts
Br
5n
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

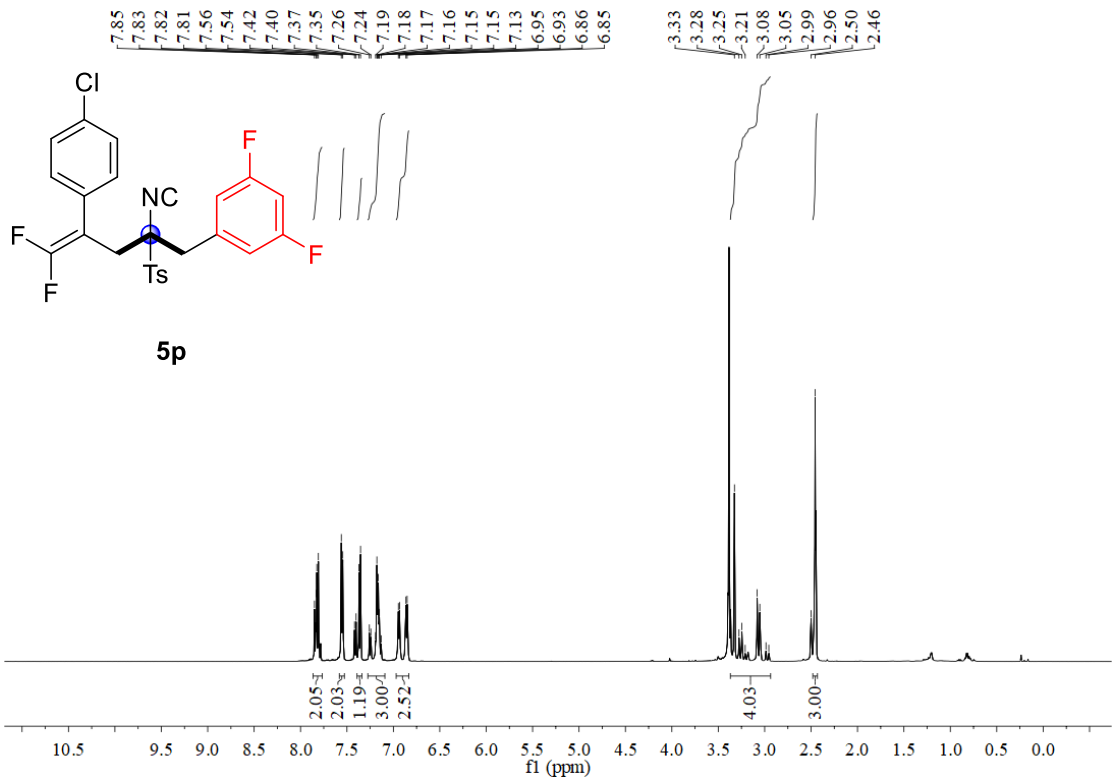

-84.93
-84.99
-87.66
-87.72
Cl
NC
F
F
Ts
Br
5n
1.00
1.03
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


7.84
7.82
7.82
7.81
7.63
7.61
7.58
7.56
7.52
7.51
7.49
7.44
7.42
7.38
7.36
7.33
7.32
7.16
7.15
3.45
3.43
3.38
3.36
3.28
3.25
3.16
3.14
3.12
3.09
2.50
2.43
Cl
NC
CF3
F
F
Ts
5o
2.00
9.01
1.00
3.30
2.00
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

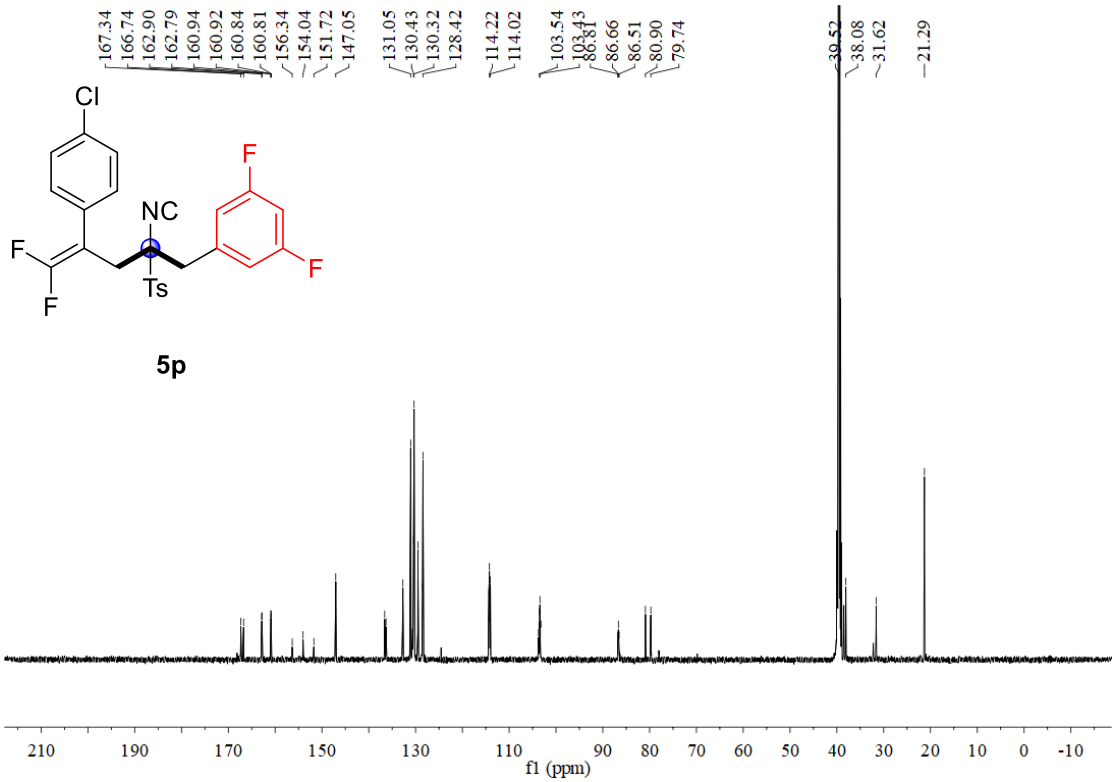

167.42
166.83
154.13
151.82
146.94
146.80
131.77
131.67
131.04
130.36
130.22
130.18
129.51
128.40
124.89
88.77
86.62
86.46
81.12
79.85
39.52
31.78
21.22
21.19
Cl
NC
CF3
F
F
Ts
5o
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

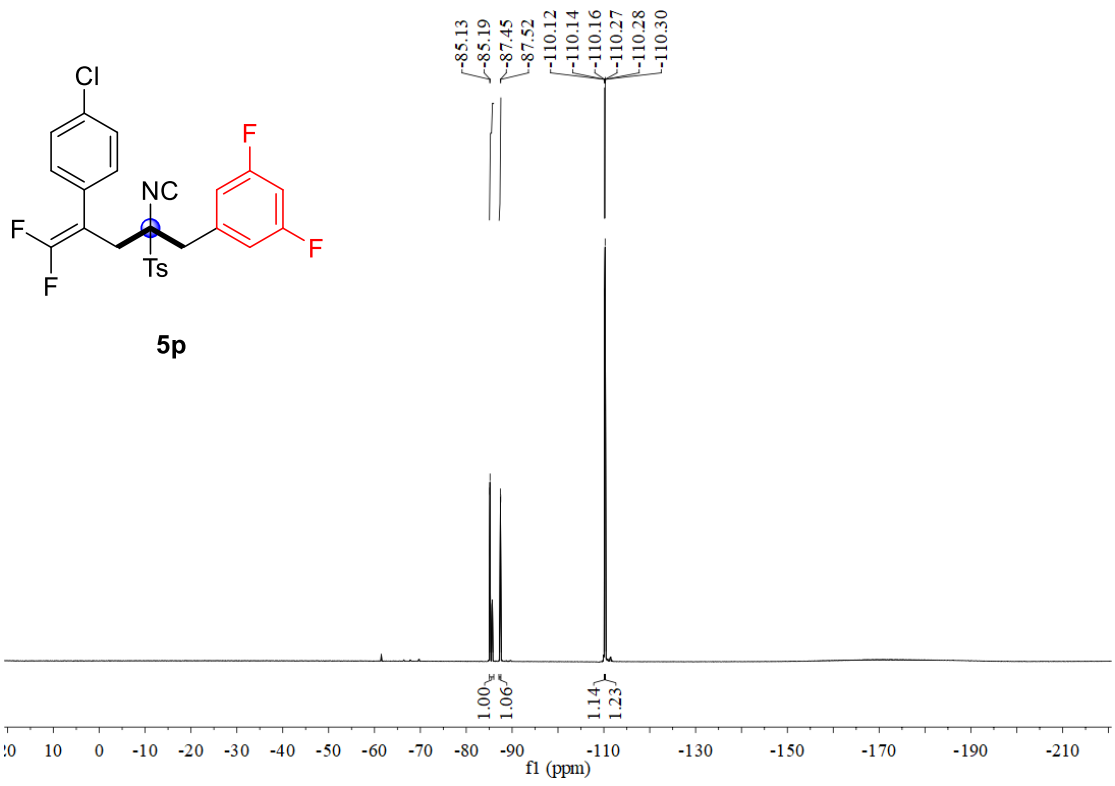

Cl
NC
Ts
F
F
CF3
-61.25
-85.06
-85.13
-87.35
-87.42
3.00
1.00
1.00
f1 (ppm)

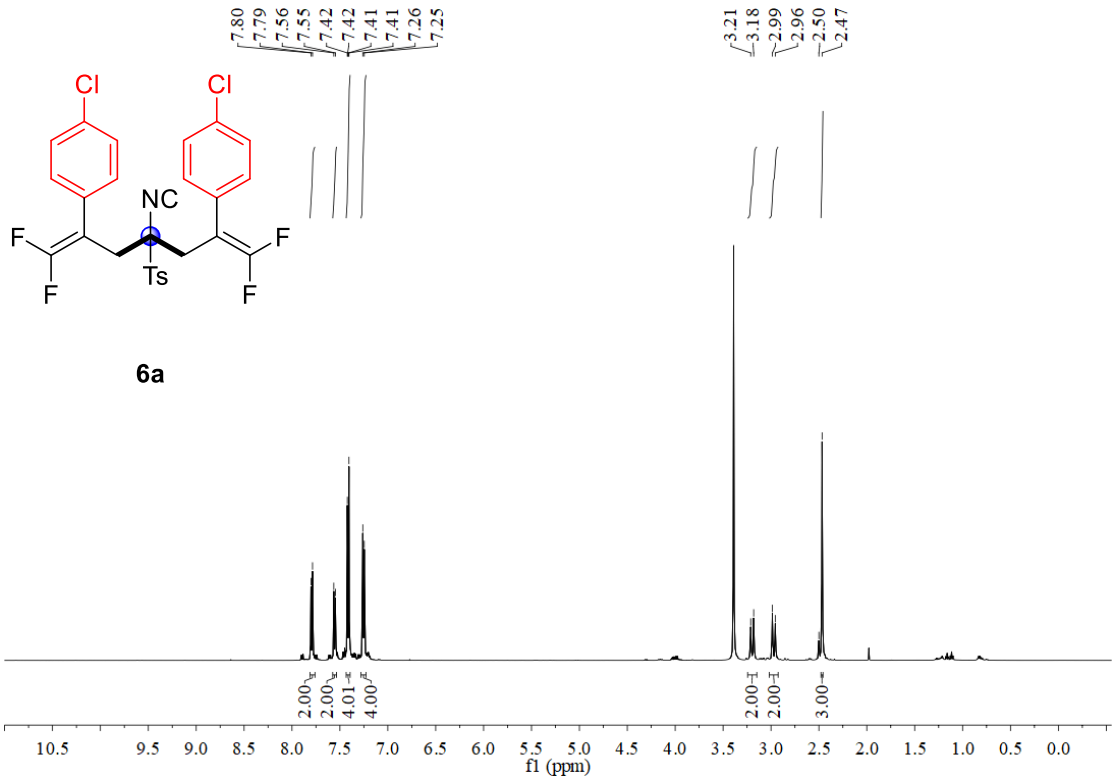
5o

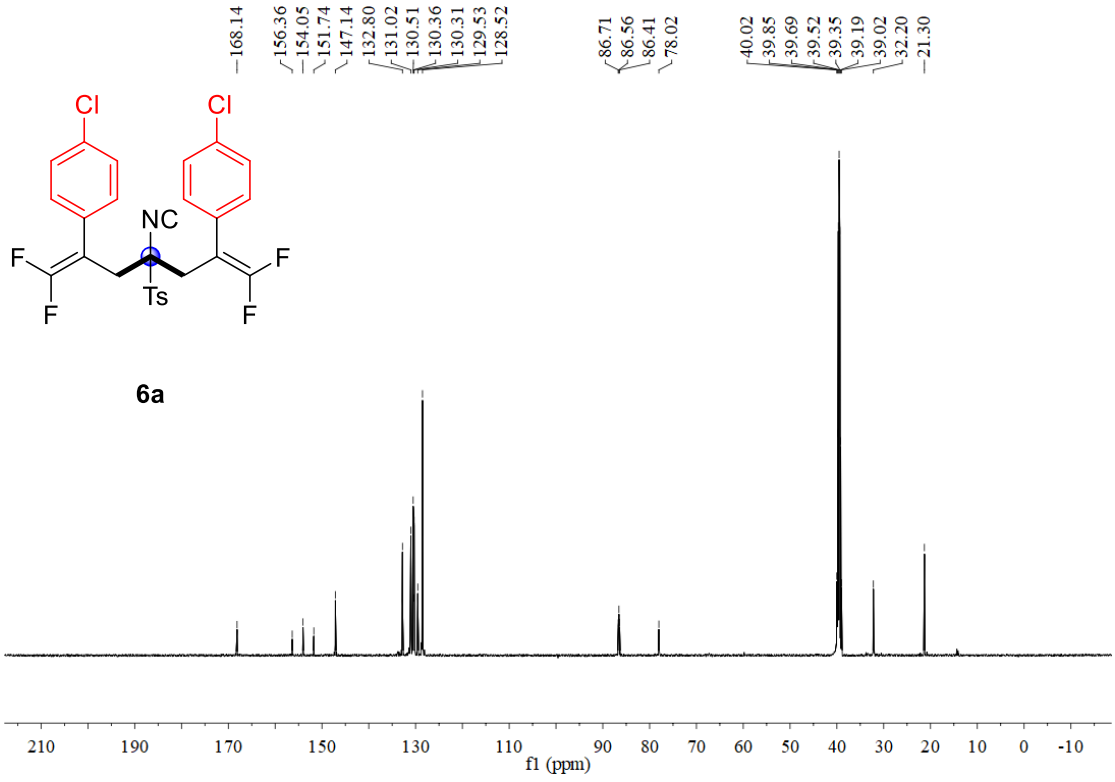

7.85
7.83
7.82
7.81
7.56
7.54
7.42
7.40
7.37
7.35
7.26
7.24
7.19
7.18
7.17
7.16
7.15
7.15
7.13
6.95
6.93
6.86
6.85
3.33
3.28
3.25
3.21
3.08
3.05
2.99
2.96
2.50
2.46
Cl
NC
Ts
F
F
F
2.05
2.03
1.19
3.00
2.52
4.03
3.00
f1 (ppm)

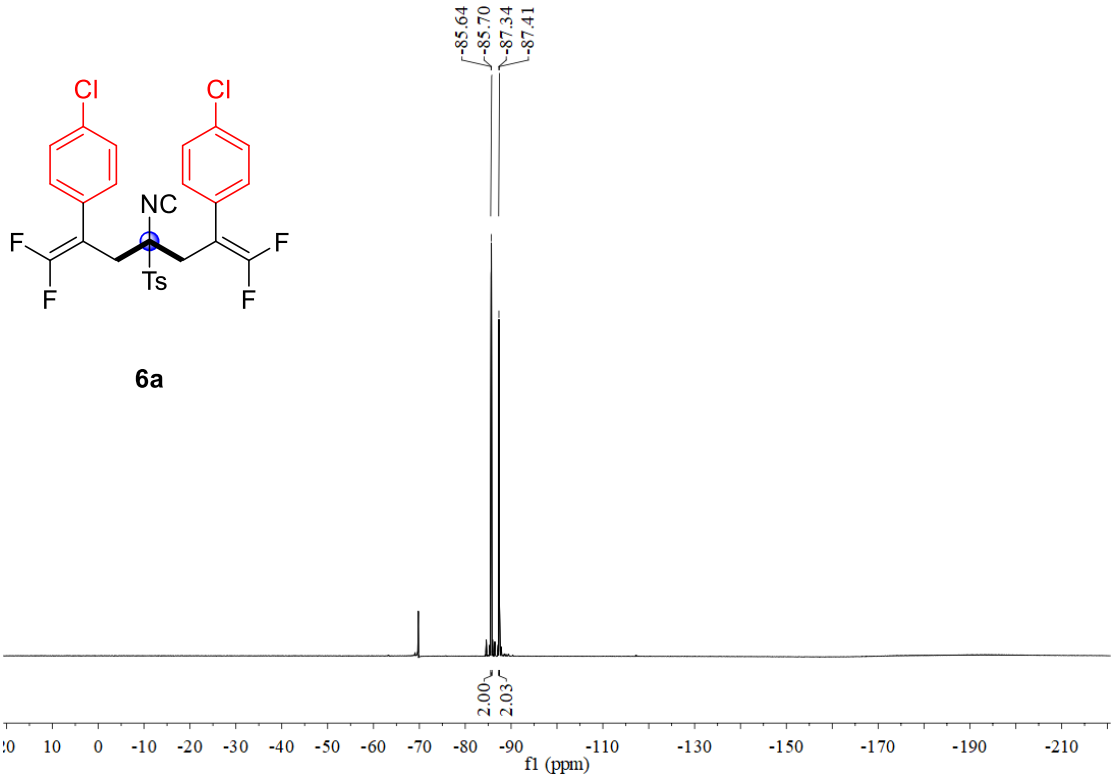
5p


167.34
166.74
162.90
162.79
160.94
160.92
160.84
160.81
156.34
154.04
151.72
147.05
131.05
130.43
130.32
128.42
114.22
114.02
103.54
103.43
88.81
86.66
86.51
80.90
79.74
39.52
38.08
31.62
21.29
Cl
F
NC
F
F
Ts
F
5p
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

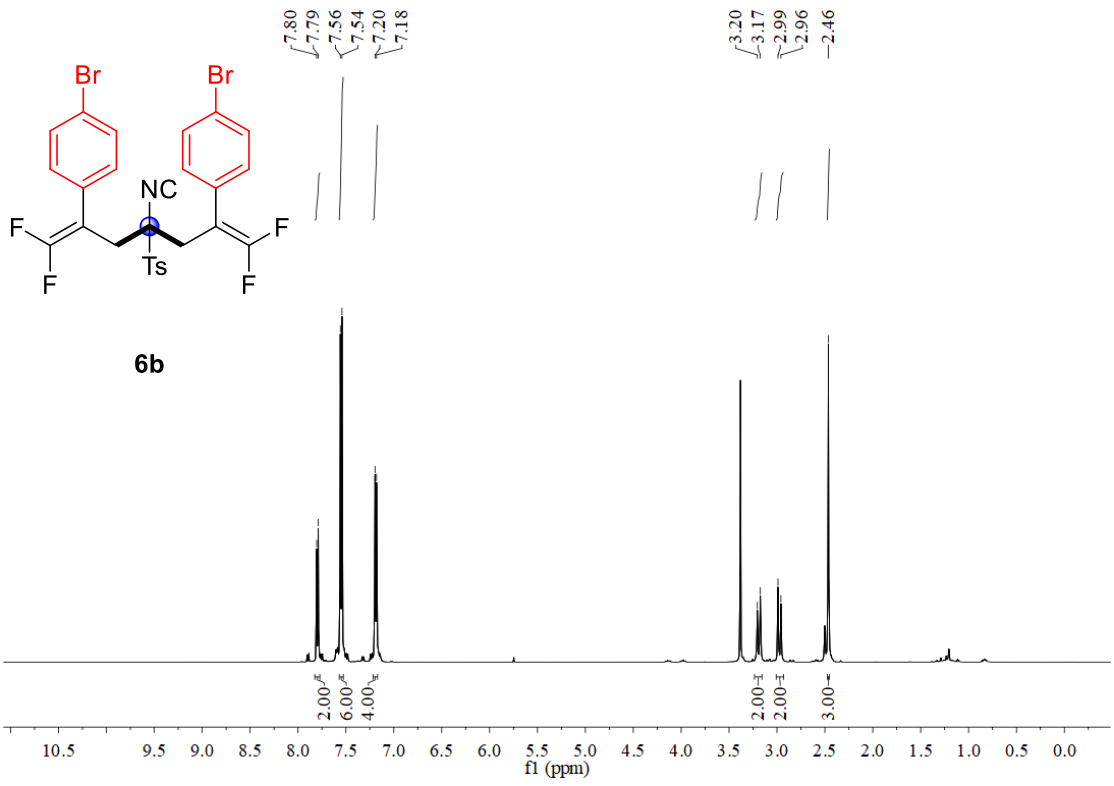

-85.13
-85.19
-87.45
-87.52
-110.12
-110.14
-110.16
-110.27
-110.28
-110.30
Cl
F
NC
F
F
Ts
F
5p
1.00
1.06
1.14
1.23
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


7.80
7.79
7.56
7.55
7.42
7.42
7.41
7.41
7.26
7.25
3.21
3.18
2.99
2.96
2.50
2.47
Cl
Cl
NC
F
F
F
F
Ts
6a
2.00
2.00
4.01
4.00
2.00
2.00
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

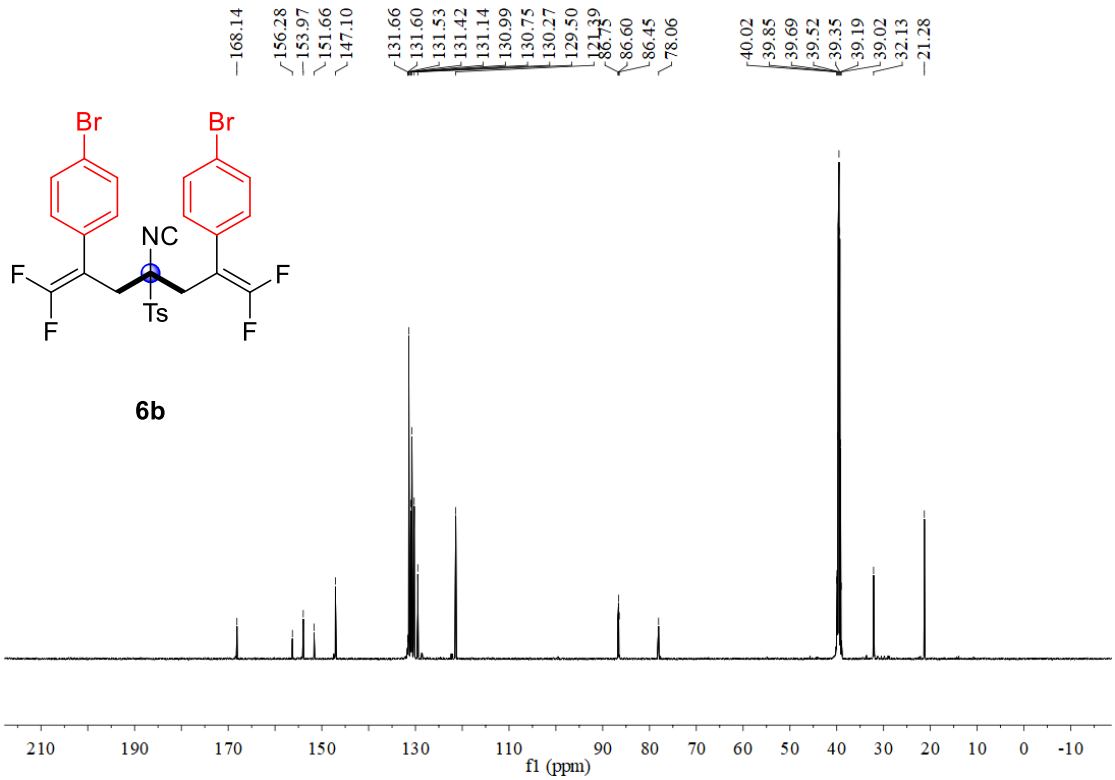

168.14
156.36
154.05
151.74
147.14
132.80
131.02
130.51
130.36
130.31
129.53
128.52
86.71
86.56
86.41
78.02
40.02
39.85
39.69
39.52
39.35
39.19
39.02
32.20
21.30
Cl
Cl
NC
F
F
F
F
Ts
6a
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

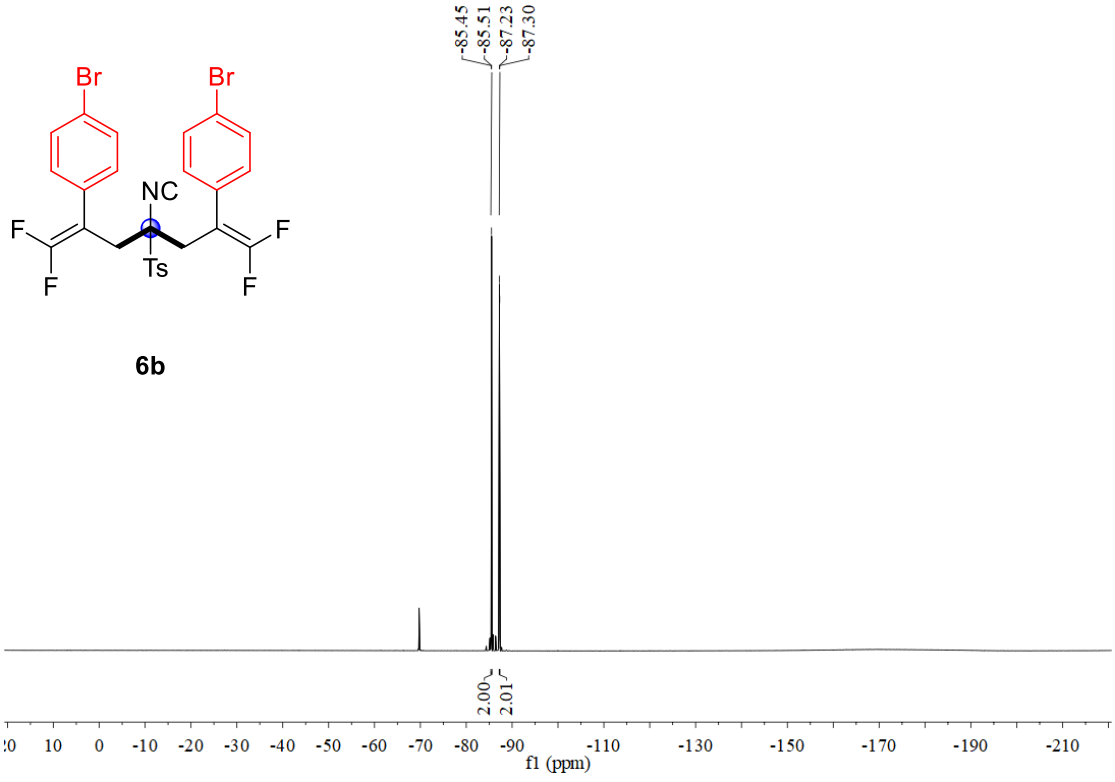

Cl
Cl
NC
F
F
F
F
Ts
-85.64
-85.70
-87.34
-87.41
2.00
2.03
f1 (ppm)

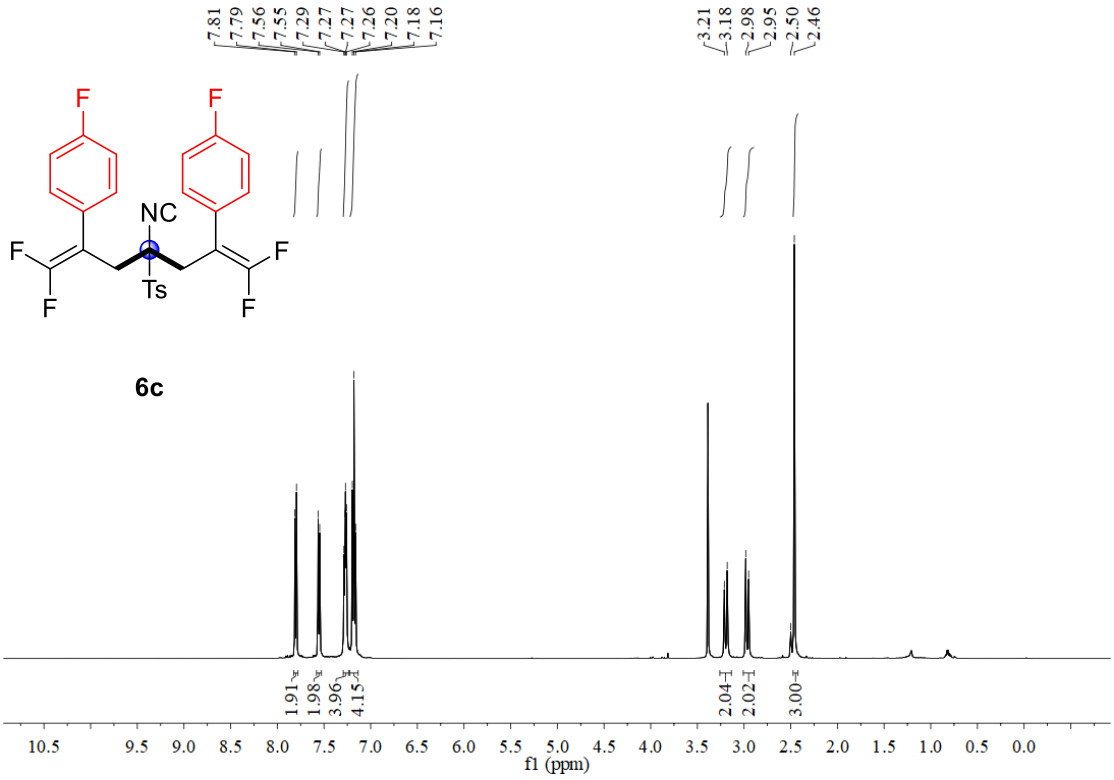
6a

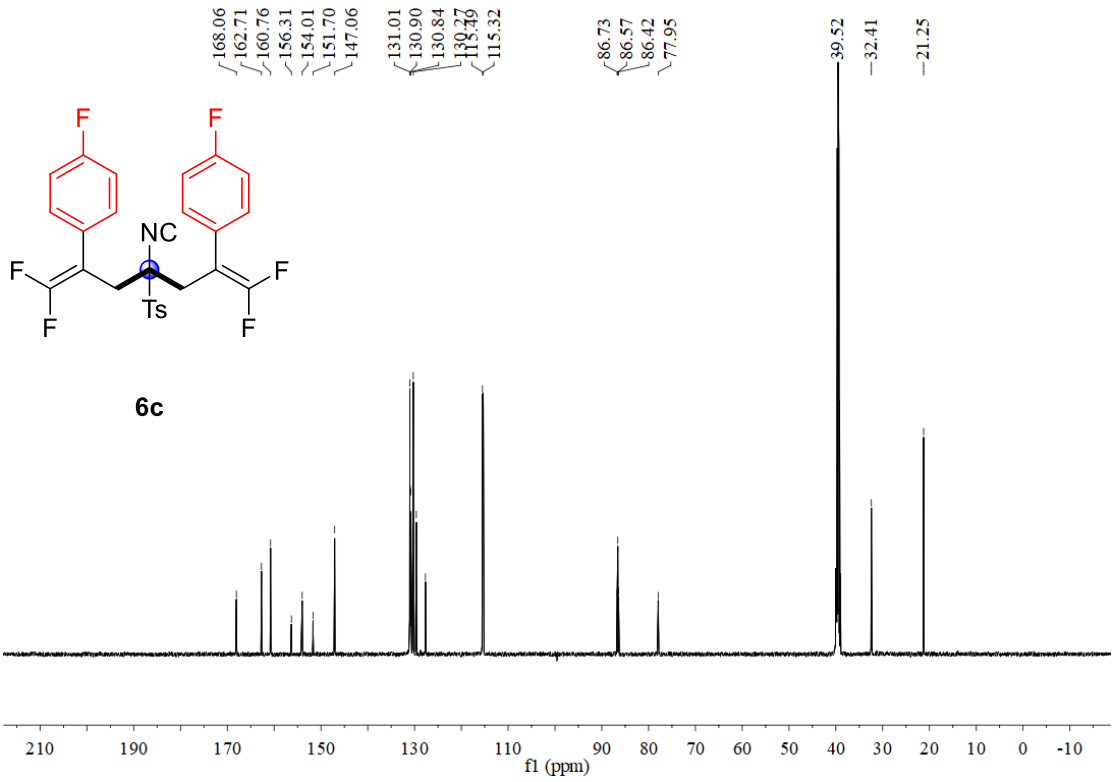

Br
Br
NC
F
F
F
F
Ts
7.80
7.79
7.56
7.54
7.20
7.18
3.20
3.17
2.99
2.96
2.46
2.00
6.00
4.00
2.00
2.00
3.00
f1 (ppm)

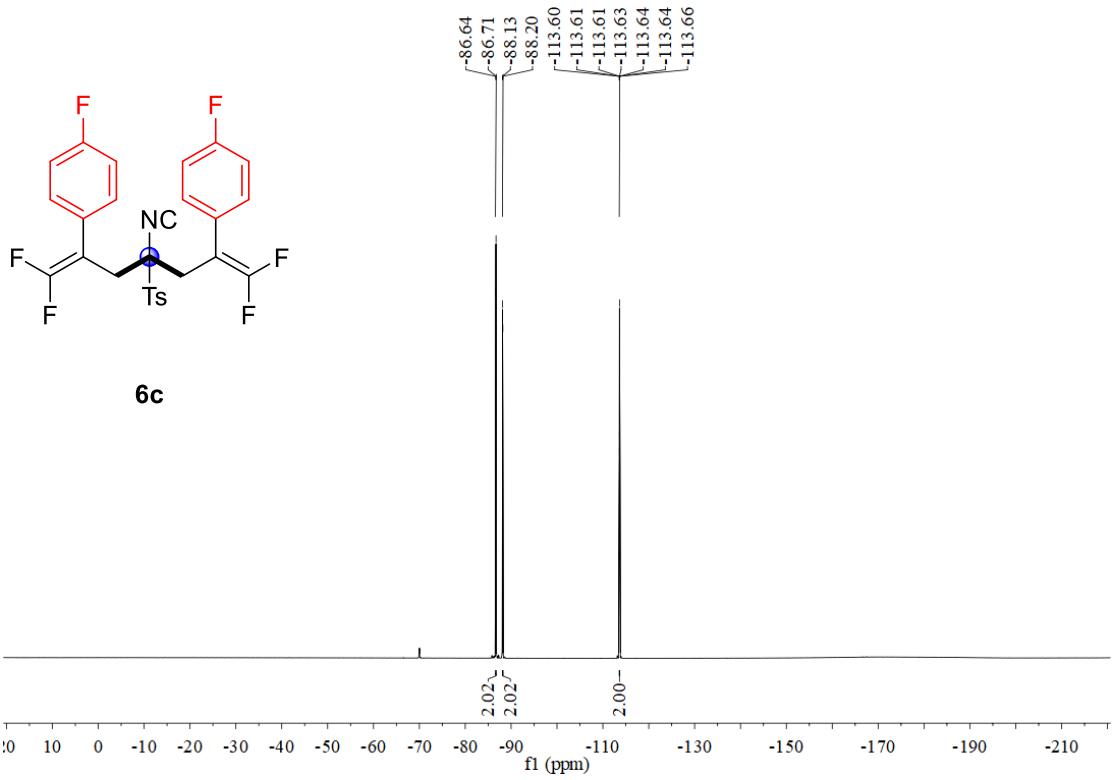
6b


168.14
156.28
153.97
151.66
147.10
131.66
131.60
131.53
131.42
131.14
130.99
130.75
130.27
129.50
127.39
88.75
86.60
86.45
78.06
40.02
39.85
39.69
39.52
39.35
39.19
39.02
32.13
21.28
Br
Br
NC
F
F
F
F
Ts
6b
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

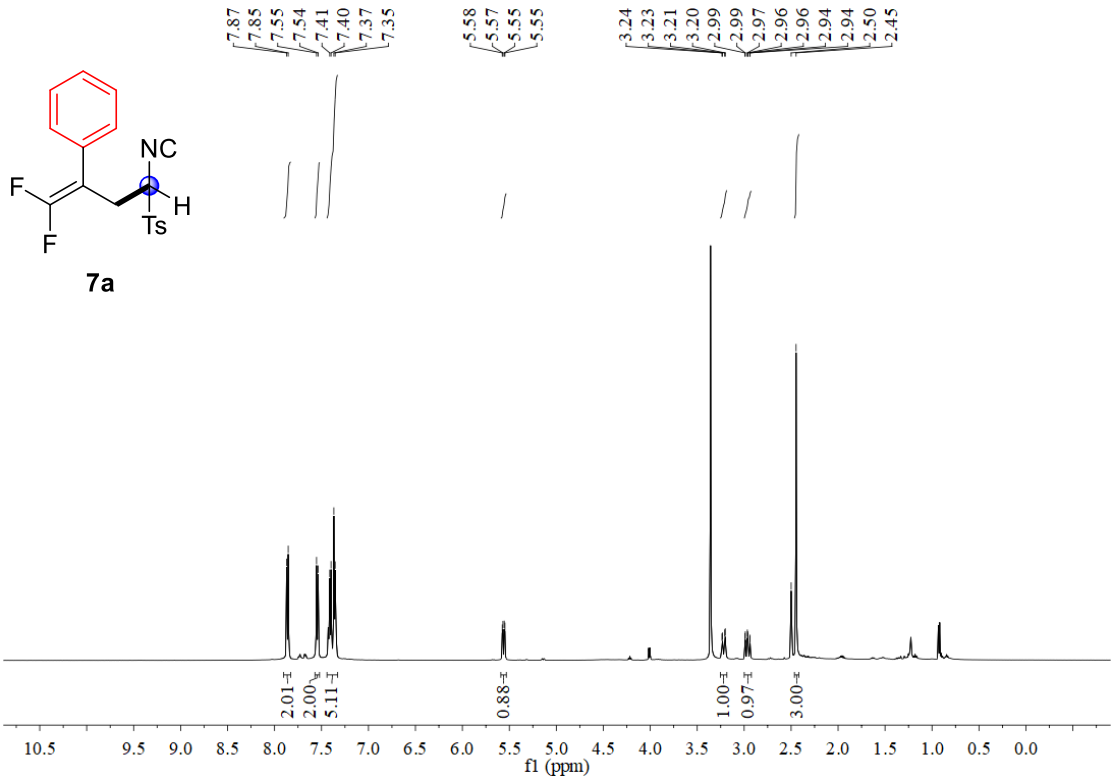

-85.45
-85.51
-87.23
-87.30
Br
Br
NC
F
F
F
F
Ts
6b
2.00
2.01
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


7.81
7.79
7.56
7.55
7.29
7.27
7.27
7.26
7.20
7.18
7.16
3.21
3.18
2.98
2.95
2.50
2.46
F
F
NC
F
F
Ts
F
F
6c
1.91
1.98
3.96
4.15
2.04
2.02
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

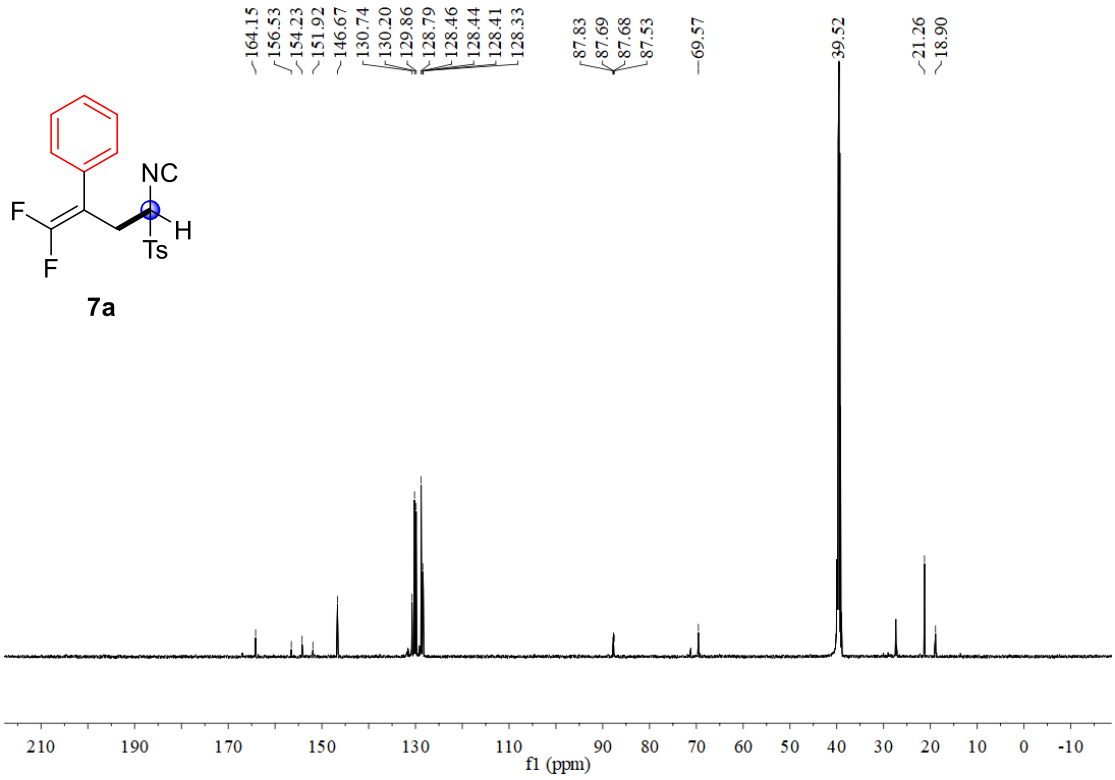

168.06
162.71
160.76
156.31
154.01
151.70
147.06
131.01
130.90
130.84
130.27
115.49
115.32
86.73
86.57
86.42
77.95
39.52
32.41
21.25
F
F
NC
F
F
Ts
F
F
6c
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


F
F
NC
F
F
Ts
F
F
-86.64
-86.71
-88.13
-88.20
-113.60
-113.61
-113.61
-113.63
-113.64
-113.64
-113.66
2.02
2.02
2.00
f1 (ppm)

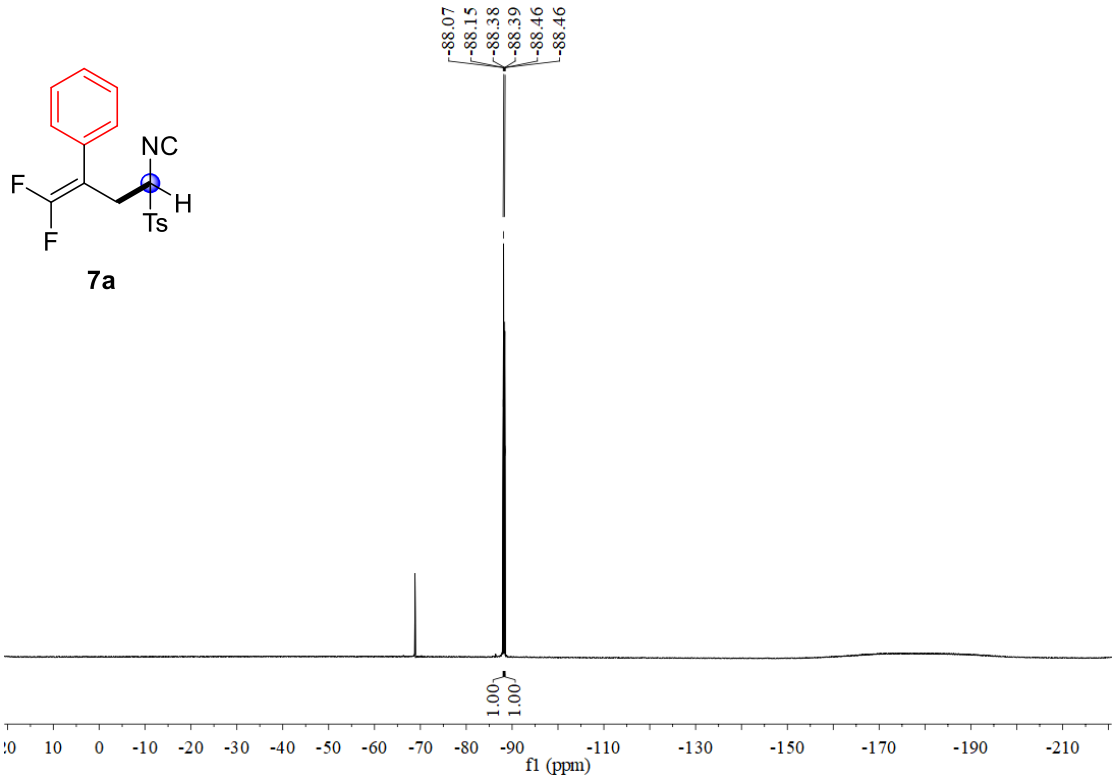
6c


NC
F
F
H
Ts
7.87
7.85
7.55
7.54
7.41
7.40
7.37
7.35
5.58
5.57
5.55
5.55
3.24
3.23
3.21
3.20
2.99
2.99
2.97
2.96
2.96
2.94
2.94
2.50
2.45
2.01
2.00
5.11
0.88
1.00
0.97
3.00
f1 (ppm)

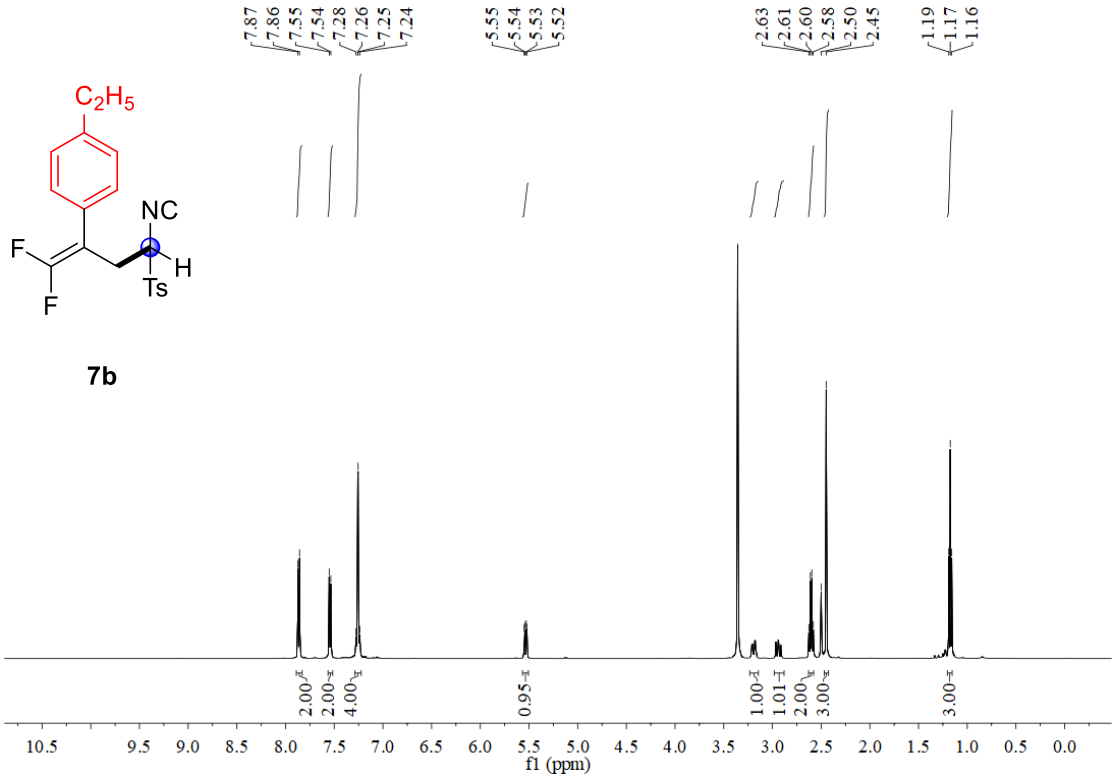
7a


NC
F
F
H
Ts
164.15
156.53
154.23
151.92
146.67
130.74
130.20
129.86
128.79
128.46
128.44
128.41
128.33
87.83
87.69
87.68
87.53
69.57
39.52
21.26
18.90
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

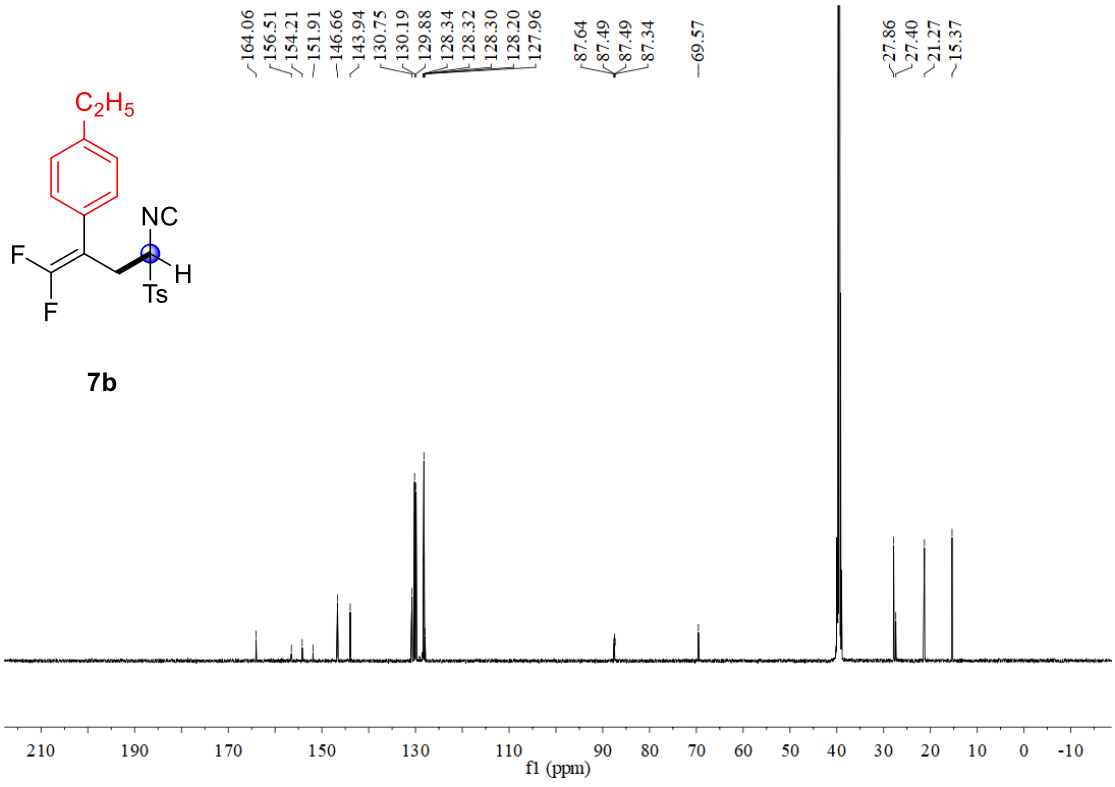
7a


NC
F
F
H
Ts
-88.07
-88.15
-88.38
-88.39
-88.46
-88.46
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

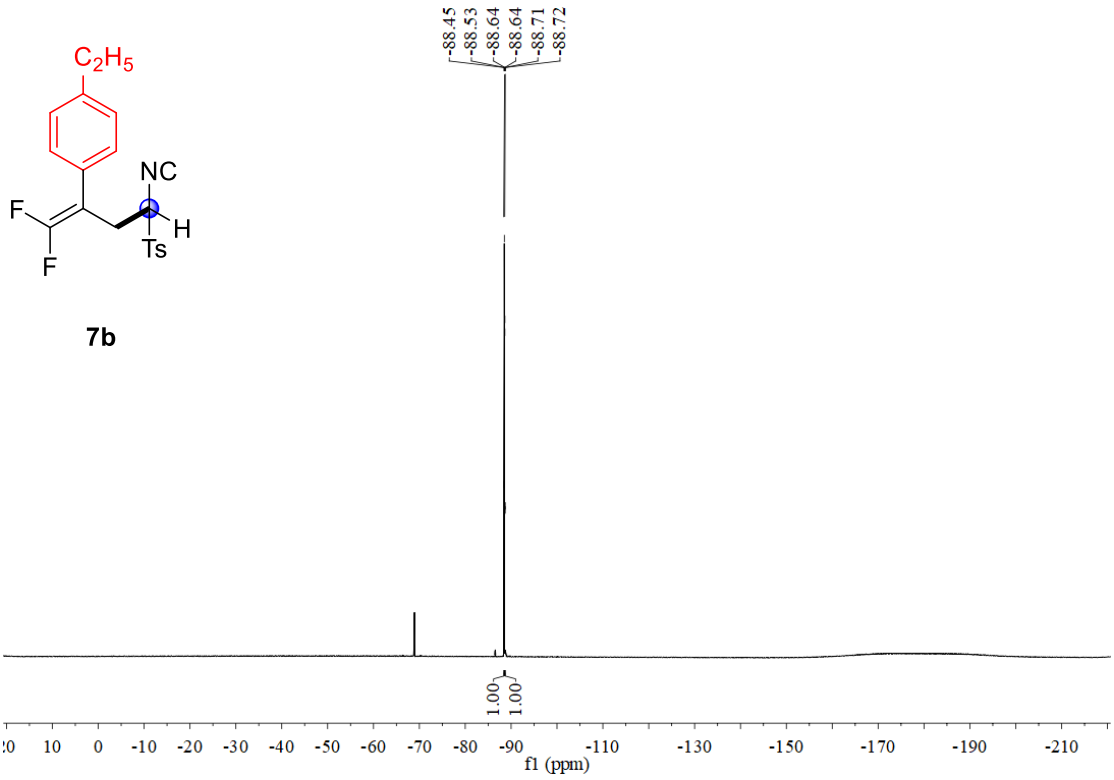
7a


7.87
7.86
7.55
7.54
7.28
7.26
7.25
7.24
5.55
5.54
5.53
5.52
2.63
2.61
2.60
2.58
2.50
2.45
1.19
1.17
1.16
C2H5
NC
F
F
H
Ts
2.00
2.00
4.00
0.95
1.00
1.01
2.00
3.00
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

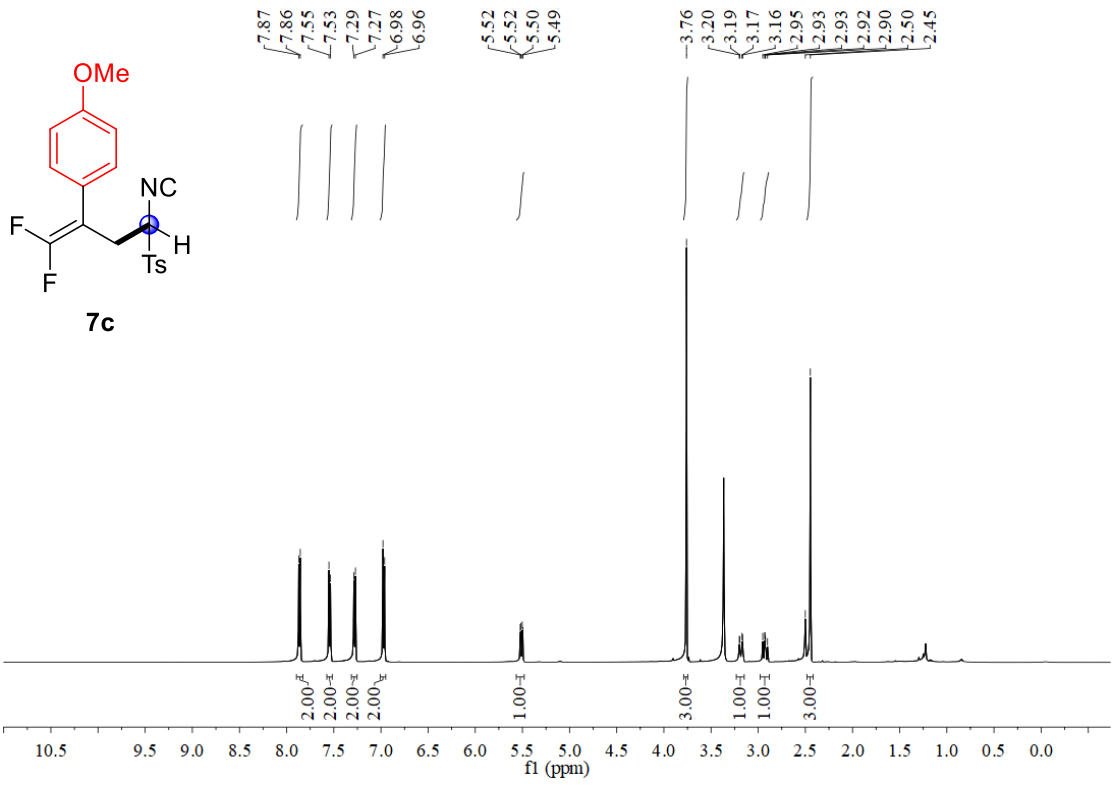
7b


164.06
156.51
154.21
151.91
146.66
143.94
130.75
130.19
129.88
128.34
128.32
128.30
128.20
127.96
87.64
87.49
87.49
87.34
69.57
27.86
27.40
21.27
15.37
C2H5
NC
F
F
H
Ts
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

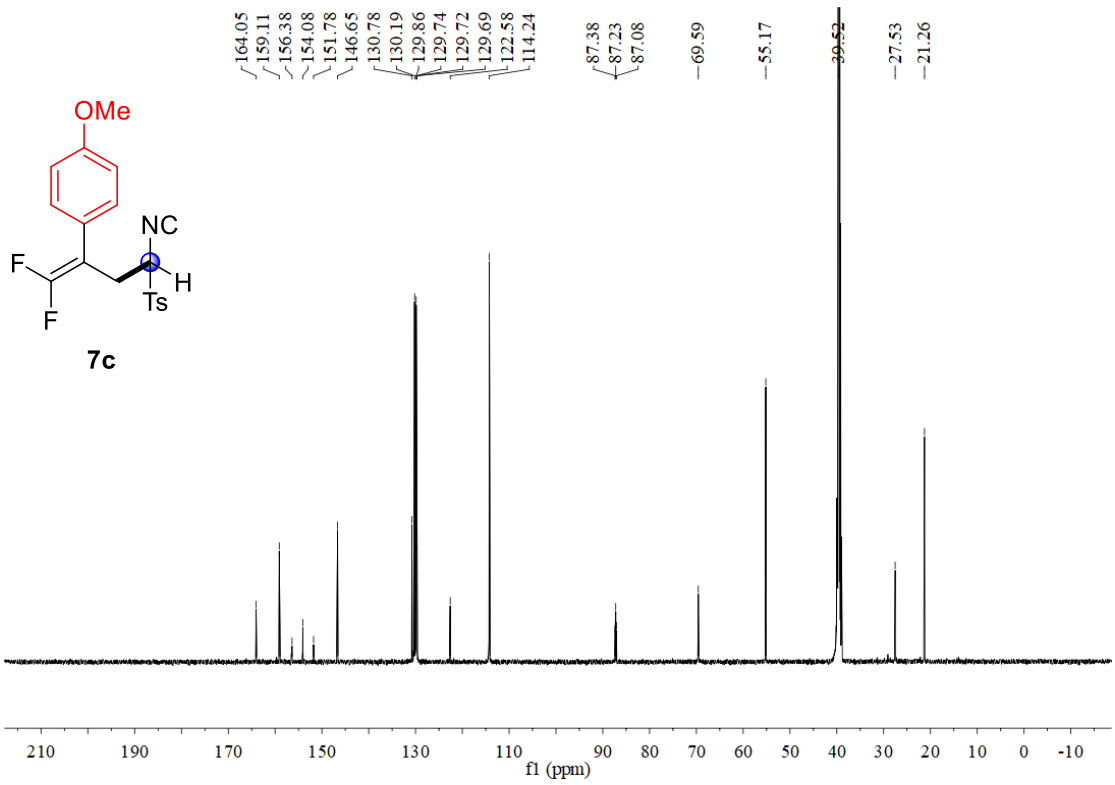
7b

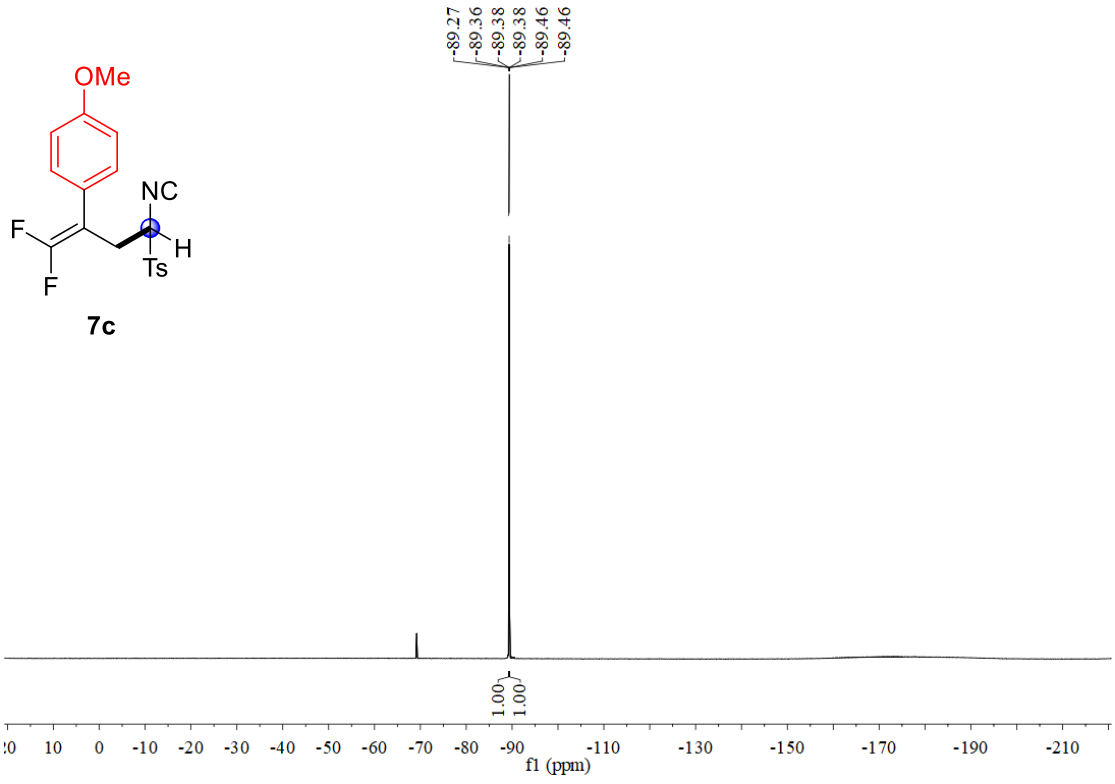

C2H5
NC
F
F
H
Ts
-88.45
-88.53
-88.64
-88.64
-88.71
-88.72
1.00
1.00
f1 (ppm)

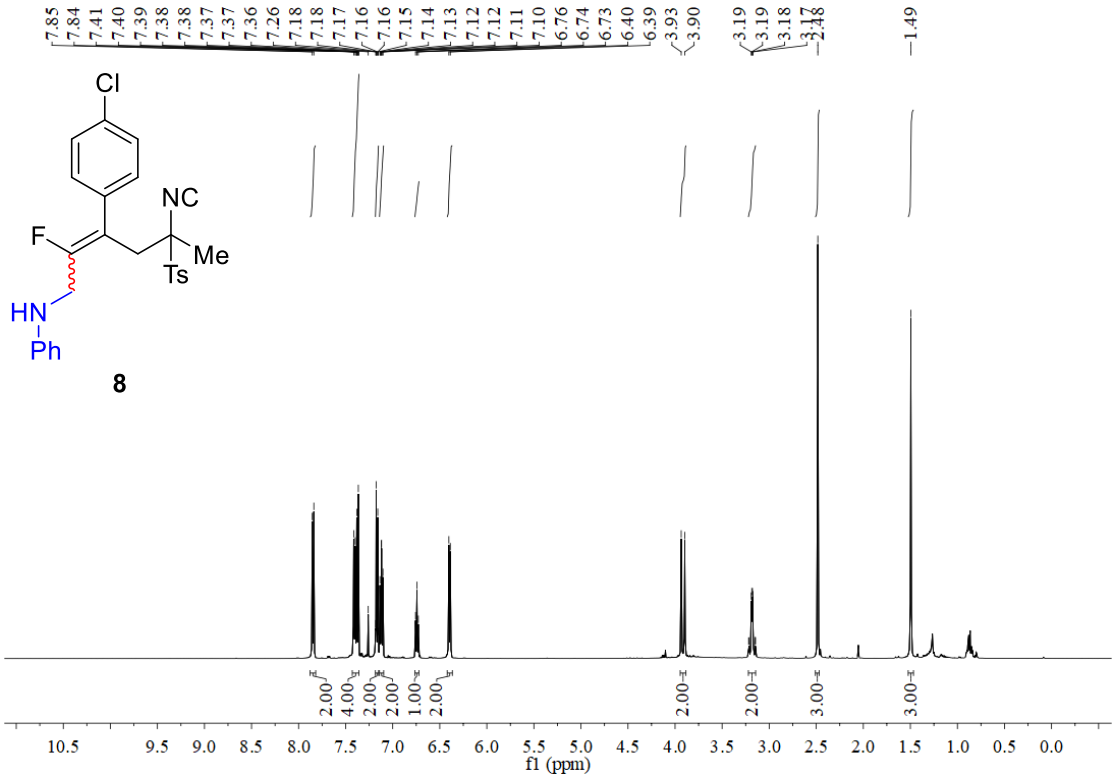
7b

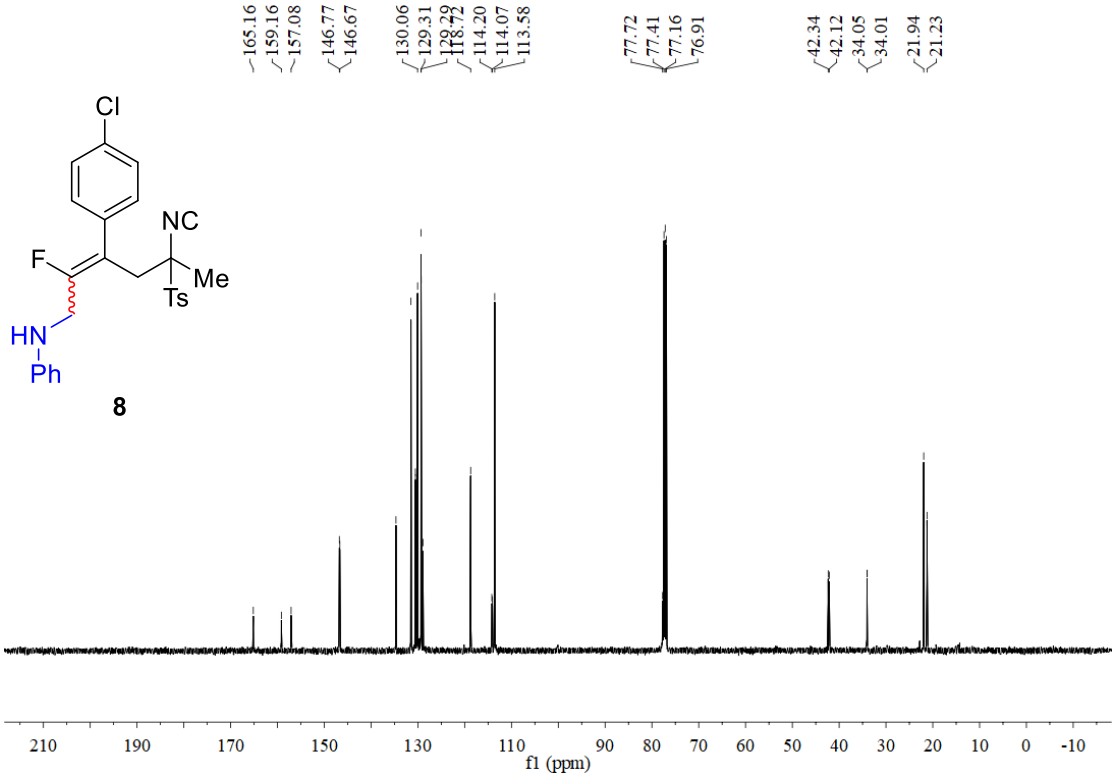

OMe
NC
F
F
H
Ts
7.87
7.86
7.55
7.53
7.29
7.27
6.98
6.96
5.52
5.52
5.50
5.49
3.76
3.20
3.19
3.17
3.16
2.95
2.93
2.93
2.92
2.90
2.50
2.45
2.00
2.00
2.00
2.00
1.00
3.00
1.00
1.00
3.00
f1 (ppm)

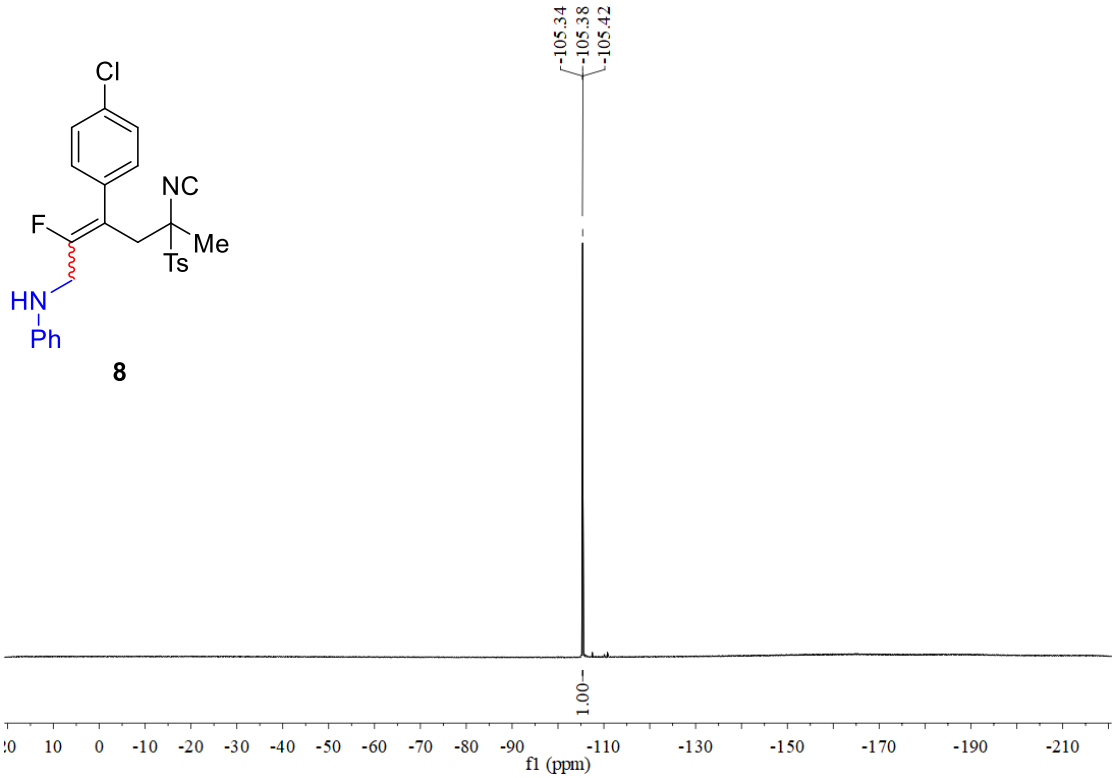
7c


164.05
159.11
156.38
154.08
151.78
146.65
130.78
130.19
129.86
129.74
129.72
129.69
122.58
114.24
87.38
87.23
87.08
69.59
55.17
39.52
27.53
21.26
OMe
NC
F
F
H
Ts
7c
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

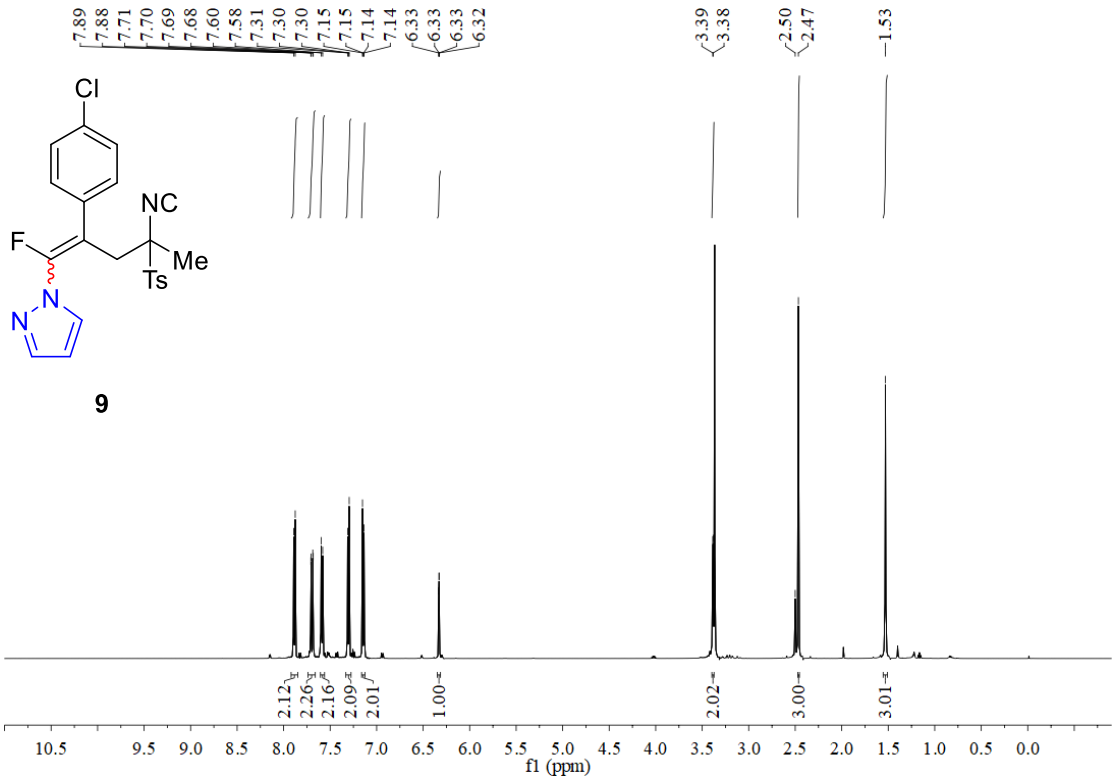

-89.27
-89.36
-89.38
-89.38
-89.46
-89.46
OMe
NC
F
F
H
Ts
7c
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


Cl
NC
F
Me
Ts
HN
Ph
8
f1 (ppm)

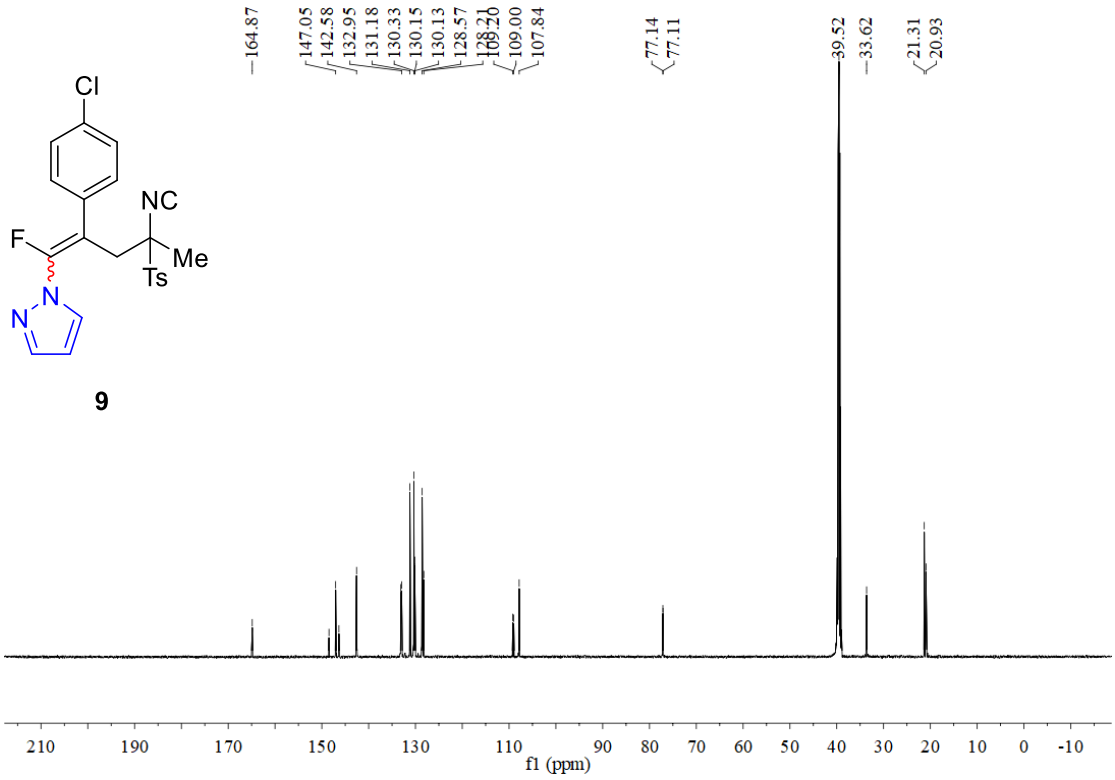

Cl
NC
F
Me
Ts
HN
Ph
8
f1 (ppm)


-105.34
-105.38
-105.42
Cl
NC
F
Me
Ts
HN
Ph
1.00
f1 (ppm)

8


7.89
7.88
7.71
7.70
7.69
7.68
7.60
7.58
7.31
7.30
7.30
7.15
7.15
7.14
7.14
6.33
6.33
6.33
6.32
3.39
3.38
2.50
2.47
1.53
Cl
NC
F
Me
Ts
N
N
2.12
2.26
2.16
2.09
2.01
1.00
2.02
3.00
3.01
f1 (ppm)

9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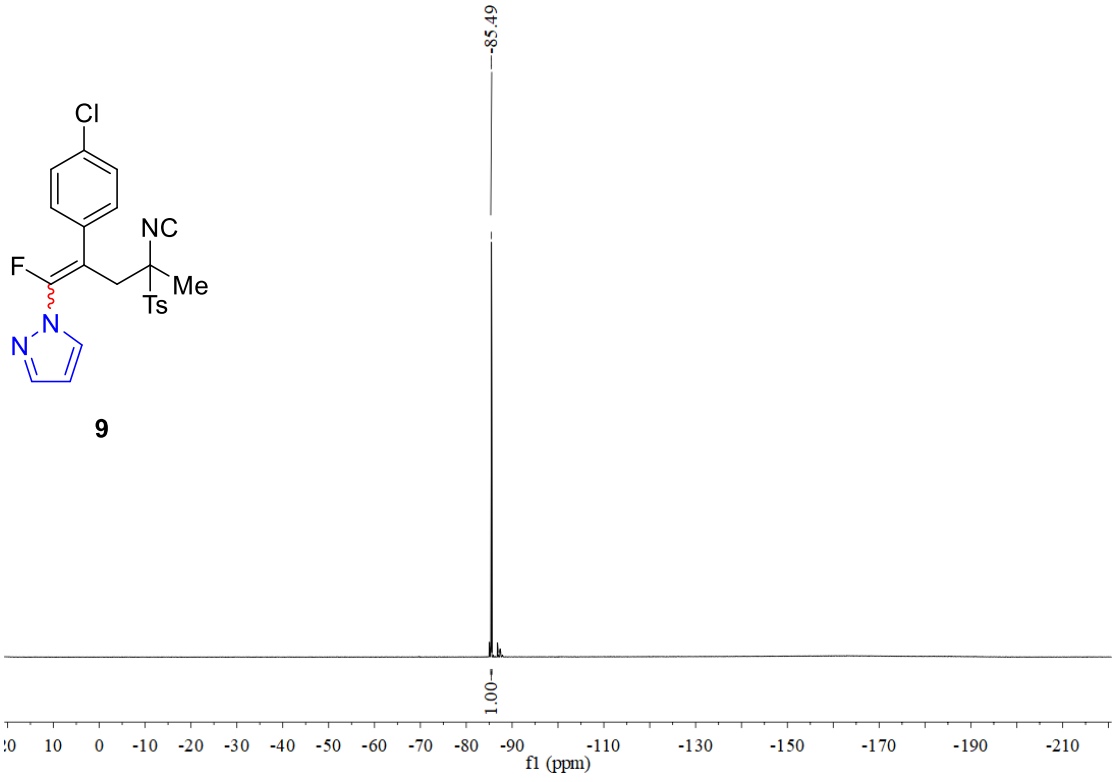
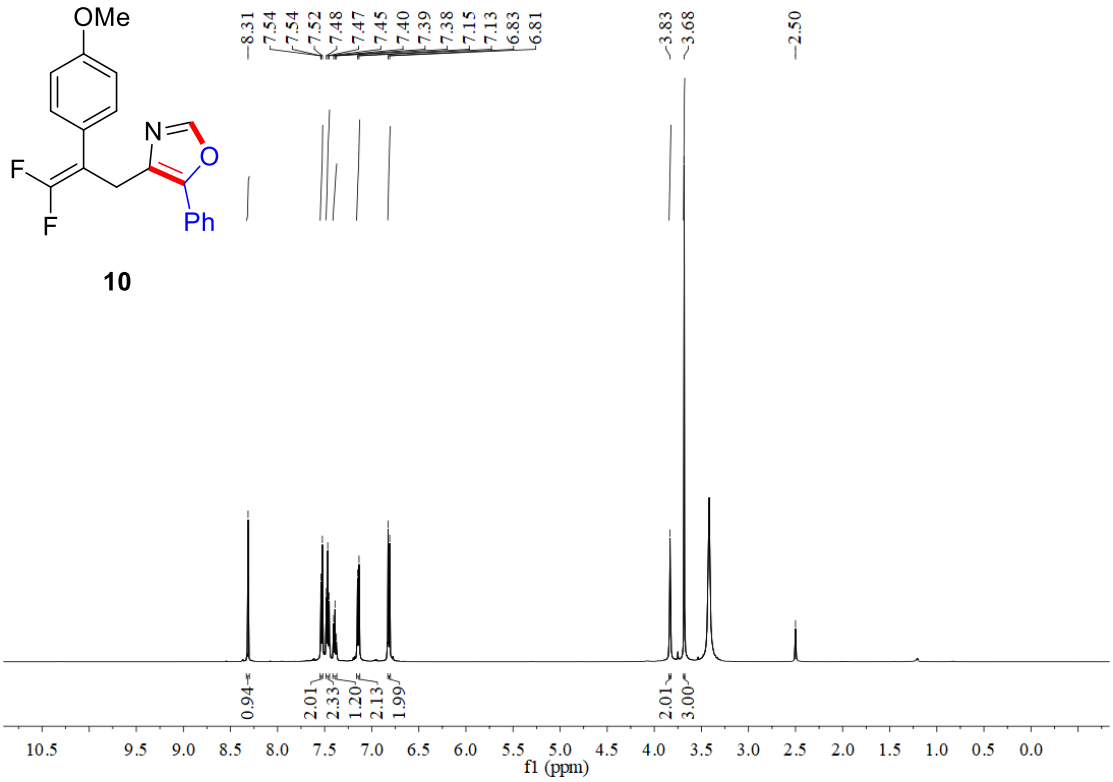
NC
F
Me
Ts
N
N
164.87
147.05
142.58
132.95
131.18
130.33
130.15
130.13
128.57
109.00
107.84
77.14
77.11
39.52
33.62
21.31
20.93
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

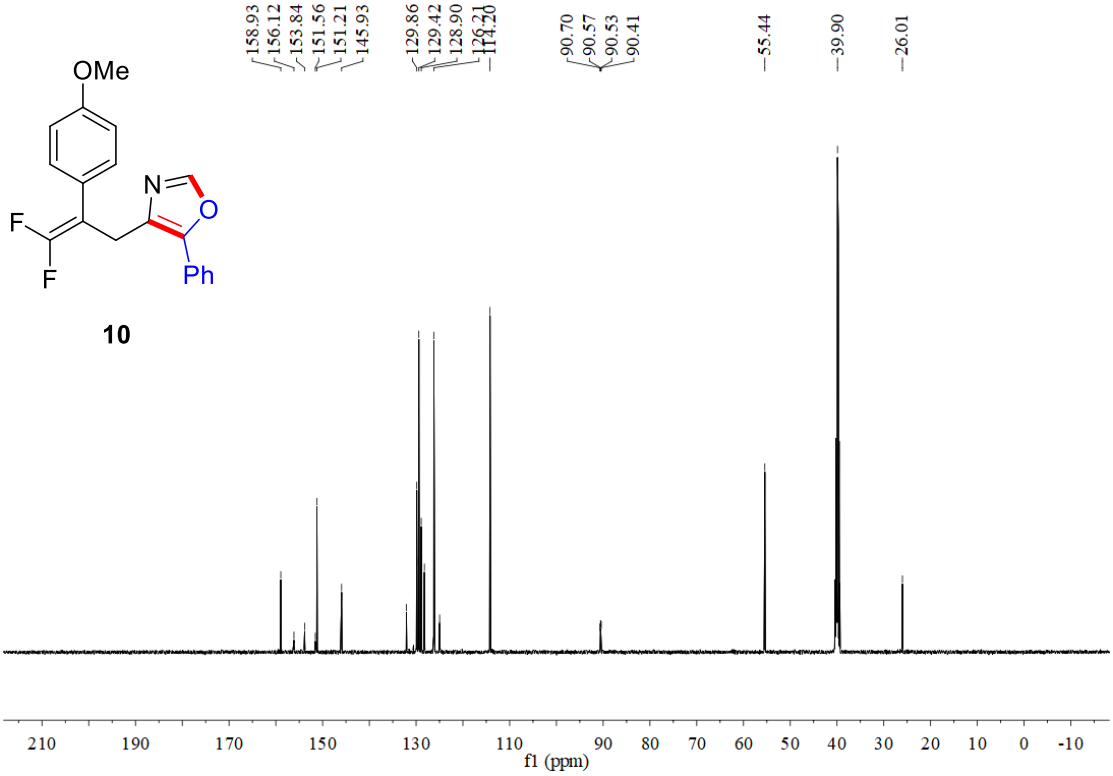
9


Cl
NC
F
Me
Ts
N
N
-85.49
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

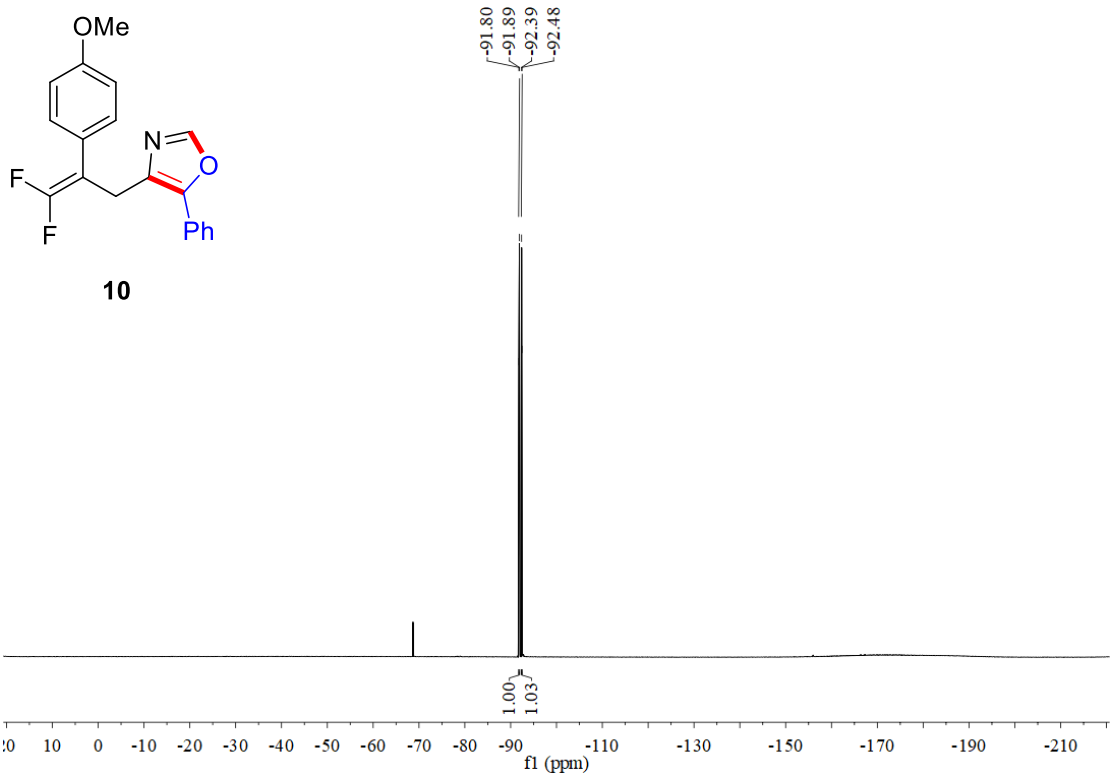
9


OMe
N
O
F
F
Ph
8.31
7.54
7.54
7.52
7.48
7.47
7.45
7.40
7.39
7.38
7.15
7.13
6.83
6.81
3.83
3.68
2.50
0.94
2.01
2.33
1.20
2.13
1.99
2.01
3.00
f1 (ppm)

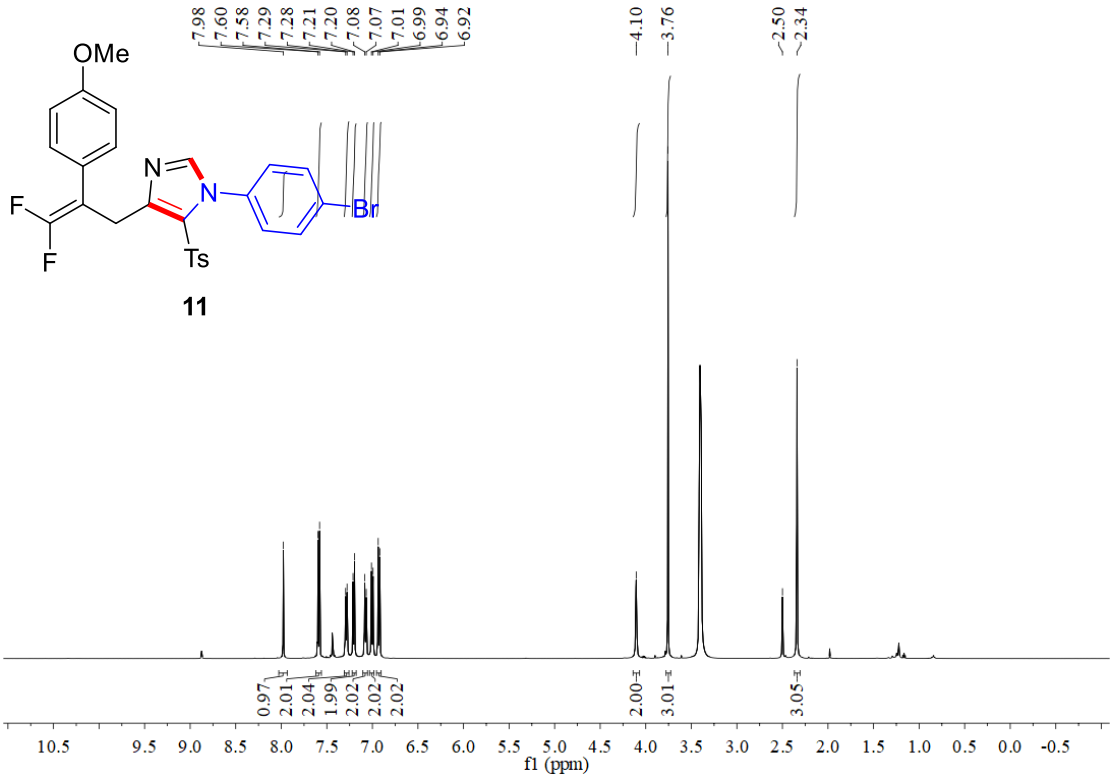
10


OMe
N
O
F
F
Ph
158.93
156.12
153.84
151.56
151.21
145.93
129.86
129.42
128.90
90.70
90.57
90.53
90.41
55.44
39.90
26.01
f1 (ppm)

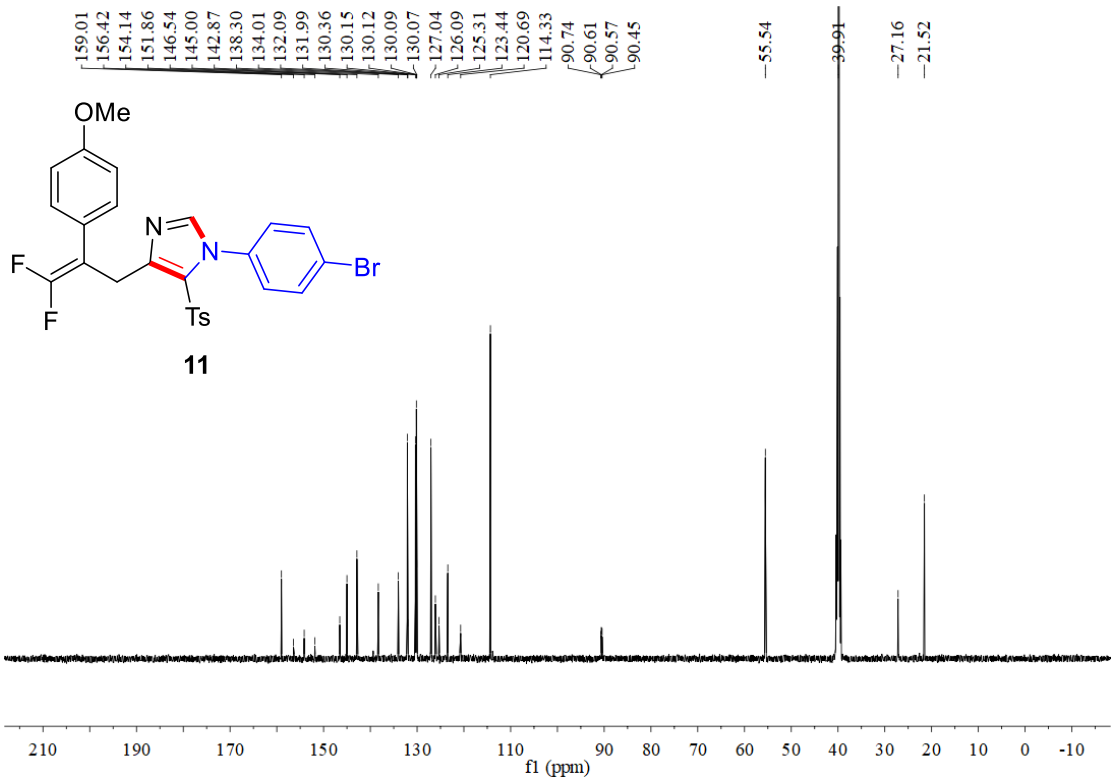
10

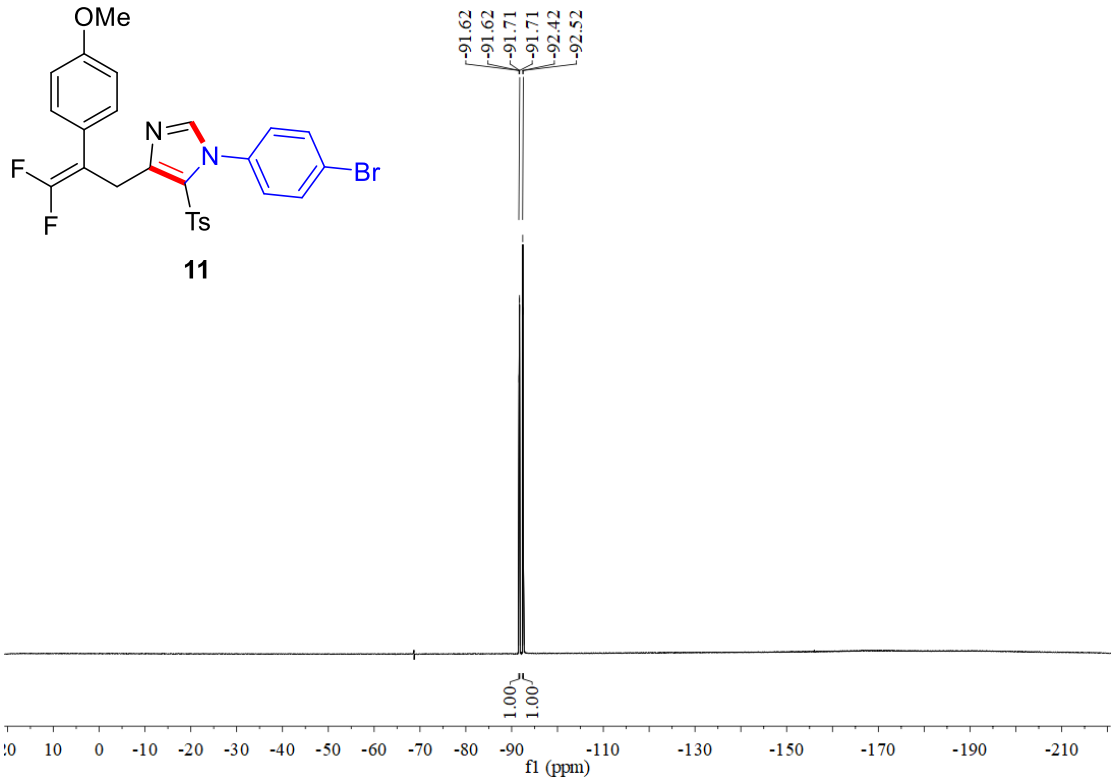

OMe
N
O
F
F
Ph
-91.80
-91.89
-92.39
-92.48
1.00
1.03
f1 (ppm)

10


7.98
7.60
7.58
7.29
7.28
7.21
7.20
7.08
7.07
7.01
6.99
6.94
6.92
4.10
3.76
2.50
2.34
OMe
N
N
Br
F
F
Ts
0.97
2.01
2.04
1.99
2.02
2.02
2.02
2.00
3.01
3.05
f1 (ppm)

11


159.01
156.42
154.14
151.86
146.54
145.00
142.87
138.30
134.01
132.09
131.99
130.36
130.15
130.12
130.09
130.07
127.04
126.09
125.31
123.44
120.69
114.33
90.74
90.61
90.57
90.45
55.54
39.91
27.16
21.52
OMe
N
N
Br
F
F
Ts
11
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-91.62
-91.62
-91.71
-91.71
-92.42
-92.52
OMe
N
N
Br
F
F
Ts
11
1.00
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)