Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Palladium-Catalyzed Interannular *meta*-C–H Arylation

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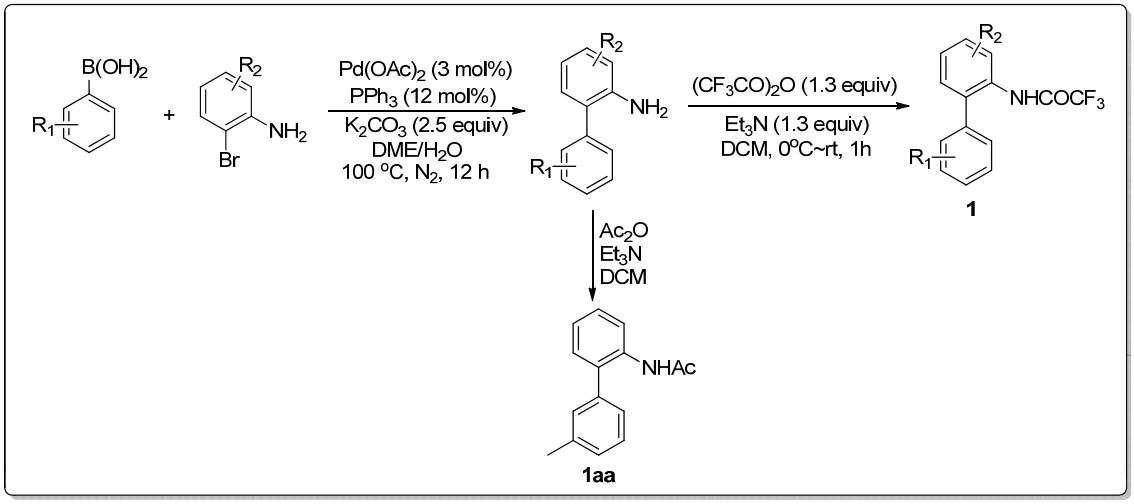
1. General Information

$Pd(OAc)_2$ was obtained from Stream®. 1,2-Dichloroethane were dried by CaH_2 and freshly distilled; Toluene were dried by Na and freshly distilled. The other materials and solvents were purchased from Adamas-beta® and other commercial suppliers and used without additional purification. Nuclear magnetic resonance (NMR) spectra were recorded with Bruker AVANCE 400 MHz.^{1}H, ^{19}F and^{13}C chemical shifts are reported in ppm downfield of tetramethylsilane and referenced to residual solvent peak as following: $CHCl_3$ = 7.26 (^{1}H NMR), $CDCl_3$ = 77.16 (^{13}C NMR). Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad resonance. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or a low-resolution MS instrument using ESI ionization.

2. Experimental Section

2.1 Preparation of Substrates

Procedure A :



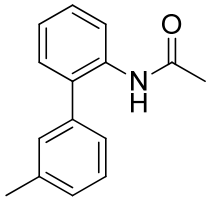
A vessel with a magnetic stir bar was charged with $Pd(OAc)_2$ (3mol%), PPh_3 (12 mol%), K_2CO_3 (2.5 equiv), 2-bromoaniline (5mmol, 1.0 equiv), arylboronic acid (6mmol, 1.2equiv), distilled water (10 mL) and 1,2-dimethoxyethane (10 mL). Then

the mixture was refluxed for 12 h at 100°C under N_2 atmosphere. After being cooled, the mixture was diluted with water (10 mL), extracted with ethyl acetate (2 × 30 mL). The combined organic phase was washed with brine (40 mL), dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent to afford the corresponding biaryl-2-amines.

Ac_2O (4 equiv) was added to 3'-methyl-[1,1'-biphenyl]-2-amine (3mmol, 1 equiv) and triethylamine (2 equiv) in dry dichloromethane (6 mL) at room temperature. Stirring was continued for an additional 12 h at room temperature. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (3 mL), extracted with dichloromethane (10 mL×2). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent to afford the corresponding substrate **1aa**.

$(CF_3CO)_2O$ (1.3 equiv) was added to biaryl-2-amines (3mmol, 1 equiv) and triethylamine (1.3 equiv) in dry dichloromethane (6 mL) at 0 °C under nitrogen atmosphere. Stirring was continued for an additional 1 h at room temperature. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (3 mL), extracted with dichloromethane (10 mL×2). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent to afford the corresponding substrate **1**.

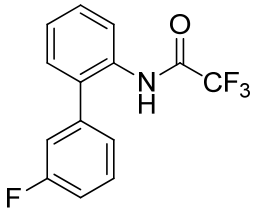
***N*-(3'-methyl-[1,1'-biphenyl]-2-yl)acetamide (1aa)**



1aa is a known compound.[1] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.2 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.21 – 7.13 (m, 4H), 2.42 (s, 3H), 2.02

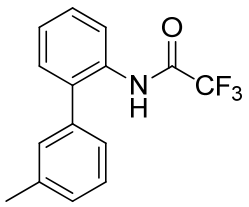
(s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.36, 139.07, 138.21, 134.84, 132.32, 130.14, 129.04, 128.83, 128.44, 126.27, 124.38, 121.59, 24.75, 21.60.

2,2,2-Trifluoro-*N*-(3'-fluoro-[1,1'-biphenyl]-2-yl)acetamide (1a)



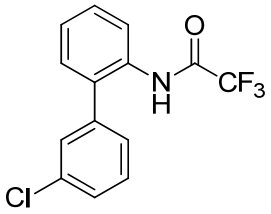
The title compound **1a** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 15 : 1 gave **1a** as a white solid (92% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 1H), 7.93 (brs, 1H), 7.52 – 7.43 (m, 2H), 7.35 – 7.31 (m, 2H), 7.20 – 7.13 (m, 2H), 7.08 (ddd, *J* = 9.6 Hz,*J* = 2.0 Hz,1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.05, -110.94; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.34 (d, *J* = 249.8 Hz), 154.78 (q, *J* = 37.4 Hz), 139.13 (d, *J* = 7.6 Hz), 132.27 (d, *J* = 1.9 Hz), 132.10, 131.13 (d, *J* = 8.6 Hz), 130.39, 129.33, 126.62, 124.72 (d, *J* = 3.1 Hz), 121.95,116.46 (d, *J* = 22.0 Hz), 115.77 (d, *J* = 21.1 Hz), 115.76 (q, *J* = 289.9 Hz); **HRMS**(EI-TOF) *m/z*: 283.0623(M^+); calc. for $C_{14}H_9F_4NO$:283.0620.

2,2,2-Trifluoro-*N*-(3'-methyl-[1,1'-biphenyl]-2-yl)acetamide (1b)



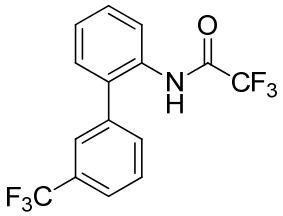
The title compound **1b** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 15 : 1 gave **1b** as a white solid (88% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.07 (brs, 1H), 7.46 – 7.38 (m, 2H), 7.36 – 7.26 (m, 3H), 7.20 – 7.14 (m, 2H), 2.43 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.10; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.62 (q, *J* = 37.3 Hz), 139.48, 136.77, 133.31, 132.31, 130.38, 129.88, 129.46, 129.42, 128.73, 126.28, 126.09, 121.31, 115.82 (q, *J* = 290.1 Hz), 21.49; **HRMS** (EI-TOF) *m/z*: 279.0872(M^+); calc. for $C_{15}H_{12}F_3NO$: 279.0871.

***N*-(3'-Chloro-[1,1'-biphenyl]-2-yl)-2,2,2-trifluoroacetamide (1c)**



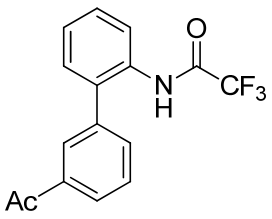
The title compound **1c** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 20 : 1 gave **1c** as a white solid (82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.2 Hz, 1H), 7.91 (brs, 1H), 7.50 – 7.43 (m, 3H), 7.40 – 7.37 (m, 1H), 7.36 – 7.31 (m, 2H), 7.28 – 7.24 (m, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.01; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.82 (q, *J* = 37.5 Hz), 138.76, 135.56, 132.26, 132.04, 130.63, 130.41, 129.47, 129.36, 128.88, 127.12, 126.70, 122.16,115.76 (q, *J* = 290.1 Hz); **HRMS** (EI-TOF) *m/z*: 299.0328(M^+); calc. for $C_{14}H_9ClF_3NO$: 299.0325.

2,2,2-Trifluoro-*N*-(3'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (1d)



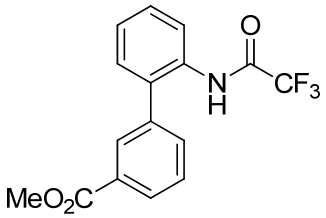
The title compound **1d** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 20 : 1 gave **1d** as a white solid (91% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 7.80 (brs, 1H), 7.75 – 7.70 (m, 1H), 7.68 – 7.62 (m, 2H), 7.59 – 7.55 (m, 1H), 7.51 – 7.45 (m, 1H), 7.39 – 7.34 (m, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.91, -76.09; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.96 (q, *J* = 37.6 Hz), 137.94, 132.51, 132.50, 132.00 (q, *J* = 32.8 Hz), 131.96, 130.58, 130.02, 129.58, 127.03,126.09 (q, *J* = 3.8 Hz), 125.46 (q, *J* = 3.8 Hz), 123.87 (q, *J* = 273.6 Hz), 122.75,115.75 (q, *J* = 289.9 Hz);**HRMS** (EI-TOF) *m/z*: 333.0588(M^+); calc. for $C_{15}H_9F_6NO$: 333.0588.

***N*-(3'-Acetyl-[1,1'-biphenyl]-2-yl)-2,2,2-trifluoroacetamide (1e)**



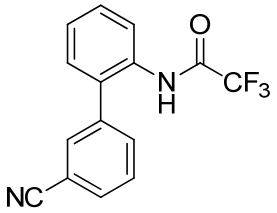
The title compound **1e** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 4 : 1 gave **1e** as a white solid (84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.2 Hz, 1H), 8.02 (dt, *J* = 7.6, 1.5 Hz, 1H), 7.98 – 7.87 (m, 2H), 7.64 – 7.55 (m, 2H), 7.50 – 7.44 (m, 1H), 7.37 – 7.33 (m, 2H), 2.61 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.95; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 197.59, 154.91 (q, *J* = 37.4 Hz), 138.10, 137.65, 133.59, 133.06, 132.01, 130.59, 129.74, 129.34, 129.00, 128.48, 126.92, 122.62, 115.76 (q, *J* = 289.9 Hz), 26.72; **HRMS** (EI-TOF) *m/z*: 307.0816(M^+); calc. for $C_{16}H_{12}F_3NO_2$: 307.0820.

Methyl 2'-(2,2,2-trifluoroacetamido)-[1,1'-biphenyl]-3-carboxylate (1f)



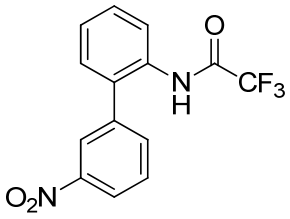
The title compound **1f** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 7 : 1 gave **1f** as a white solid (85% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 1H), 8.10 (dt, *J* = 7.1, 1.8 Hz, 1H), 8.04 (s, 1H), 7.92 (brs, 1H), 7.60 – 7.54 (m, 2H), 7.48 – 7.43 (m, 1H), 7.36 – 7.32 (m, 2H), 3.91 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.02; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.49, 154.90 (q, *J* = 37.4 Hz), 137.36, 133.42, 132.91, 132.04, 131.41, 130.54, 130.27, 129.72, 129.52, 129.25, 126.83, 122.51, 115.75 (q, *J* = 289.9 Hz), 52.45; **HRMS** (EI-TOF) *m/z*: 323.0769(M^+); calc. for $C_{16}H_{12}F_3NO_3$: 323.0772.

***N*-(3'-Cyano-[1,1'-biphenyl]-2-yl)-2,2,2-trifluoroacetamide (1g)**



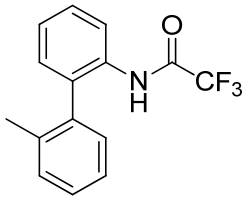
The title compound **1g** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 4 : 1 gave **1g** as a white solid (87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.79 (brs, 1H), 7.75 – 7.71 (m, 1H), 7.68 – 7.65 (m, 1H), 7.63 – 7.59 (m, 2H), 7.49 (td, *J* = 7.6, 1.6 Hz, 1H), 7.38 (td, *J* = 7.6, 0.8 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.6 Hz, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.89; **^{13}C NMR** (101 MHz, $CDCl_3$) δ155.09 (q, *J* = 37.6 Hz), 138.72, 133.40, 132.74, 132.45, 132.13, 131.76, 130.54, 130.12, 129.85, 127.38, 123.52,118.13, 115.72 (q, *J* = 289.9 Hz), 113.74; **HRMS** (EI-TOF) *m/z*: 290.0667(M^+); calc. for $C_{15}H_9F_3N_2O$: 290.0667.

2,2,2-Trifluoro-*N*-(3'-nitro-[1,1'-biphenyl]-2-yl)acetamide (1h)



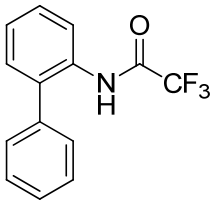
The title compound **1h** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 5 : 1 gave **1h** as an orange solid (90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28 (dt, *J* = 7.6, 2.0 Hz, 1H), 8.26 – 8.22 (m,1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.84 (brs, 1H), 7.73 – 7.66 (m, 2H), 7.53 – 7.48 (m, 1H), 7.43 – 7.36 (m, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.93; **^{13}C NMR** (101 MHz, $CDCl_3$) δ155.16 (q, *J* = 37.6 Hz), 148.81, 139.07, 135.02, 132.52, 131.71, 130.65, 130.31, 129.93, 127.53, 124.16, 123.77, 123.41, 115.71 (q, *J* = 289.9 Hz); **HRMS** (EI-TOF) *m/z*: 310.0567 (M^+); calc. for $C_{14}H_9F_3N_2O_3$: 310.0565.

2,2,2-Trifluoro-*N*-(2'-methyl-[1,1'-biphenyl]-2-yl)acetamide (1i)



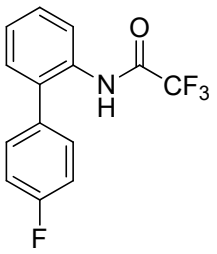
The title compound **1i** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 20 : 1 gave **1i** as a pale yellow oil (90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.0 Hz, 1H), 7.63 (brs, 1H), 7.48 – 7.43 (m, 1H), 7.40 – 7.36 (m, 2H), 7.35 – 7.28 (m, 2H), 7.25 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 1H), 2.10 (s, 3H);**^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.30;**^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.50 (q, *J* = 37.2 Hz), 136.71, 135.58, 132.90, 132.45, 131.04, 130.16, 129.91, 129.26, 128.83, 126.85, 126.05, 120.68, 115.66 (q, *J* = 290.0 Hz), 19.63; **HRMS**(EI-TOF) *m/z*: 279.0874 (M^+); calc. for $C_{15}H_{12}F_3NO$: 279.0871.

***N*-([1,1'-Biphenyl]-2-yl)-2,2,2-trifluoroacetamide (1j)**



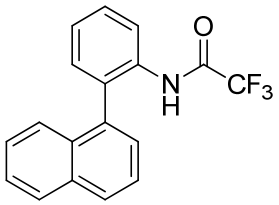
The title compound **1j** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 10 : 1 gave **1j** as a white solid (90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.01 (brs, 1H), 7.56 – 7.50 (m, 2H), 7.49 – 7.41 (m, 2H), 7.39 – 7.29 (m, 4H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.08; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.67 (q, *J* = 37.4 Hz), 136.86, 133.30, 132.29, 130.47, 129.55, 129.15, 128.86, 128.76, 126.37, 121.46, 115.78 (q, *J* = 289.9 Hz); **HRMS** (EI-TOF) *m/z*: 265.0714 (M^+); calc. for $C_{14}H_{10}F_3NO$: 265.0714.

2,2,2-Trifluoro-*N*-(4'-fluoro-[1,1'-biphenyl]-2-yl)acetamide (1k)



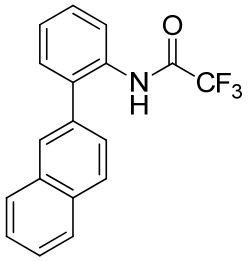
The title compound **1k** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 20 : 1 gave **1k** as a white solid (88% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.87 (brs, 1H), 7.47 – 7.41 (m, 1H), 7.37 – 7.29 (m, 4H), 7.24 – 7.18 (m, 2H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.04, -112.68; **^{13}C NMR** (101 MHz, $CDCl_3$) δ162.95 (d, *J* = 249.9 Hz), 154.75 (q, *J* = 37.4 Hz), 132.86 (d, *J* = 3.5 Hz), 132.54, 132.25, 130.99 (d, *J* = 8.2 Hz), 130.59, 129.06, 126.57, 121.89,116.59 (d, *J* = 21.7 Hz), 115.77 (q, *J* = 290.1 Hz); **HRMS** (EI-TOF) *m/z*: 283.0624 (M^+); calc. for $C_{14}H_9F_4NO$: 283.0620.

2,2,2-Trifluoro-*N*-(2-(naphthalen-1-yl)phenyl)acetamide (1l)



The title compound **1l** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 15 : 1 gave **1l** as a pale yellow solid (92% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.4 Hz, 1H), 7.98 (t, *J* = 8.0 Hz, 2H), 7.65 – 7.53 (m, 4H), 7.51 – 7.37 (m, 5H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.45; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.62 (q, *J* = 37.4 Hz), 133.96, 133.79, 133.42, 131.41, 131.38, 131.31, 129.55, 129.18, 128.84, 127.99, 127.32, 126.75, 126.22, 125.72, 125.06, 121.27, 115.48 (q, *J* = 289.9 Hz); **HRMS** (EI-TOF) *m/z*: 315.0872(M^+); calc. for $C_{18}H_{12}F_3NO$: 315.0871.

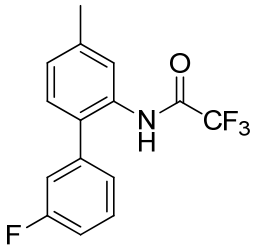
2,2,2-Trifluoro-*N*-(2-(naphthalen-2-yl)phenyl)acetamide (1m)



The title compound **1m** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 20 : 1 gave **1m** as a white solid (90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.0 Hz, 1H), 8.09 (brs, 1H),

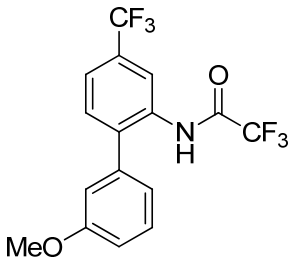
8.01 (d, *J* = 8.4 Hz, 1H), 7.96 – 7.88 (m, 2H), 7.86 (s, 1H), 7.62 – 7.56 (m, 2H), 7.51 – 7.43 (m, 3H), 7.36 (td, *J* = 7.6, 0.8 Hz, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.98; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.78 (q, *J* = 37.3 Hz), 134.21, 133.64, 133.27, 133.02, 132.42, 130.78, 129.45, 128.94, 128.52, 128.18, 128.02, 127.17, 127.07, 126.56, 126.50, 121.69, 115.77 (q, *J* = 290.1 Hz); **HRMS** (EI-TOF) *m/z*: 315.0874(M^+); calc. for $C_{18}H_{12}F_3NO$: 315.0871.

2,2,2-Trifluoro-*N*-(3'-fluoro-4-methyl-[1,1'-biphenyl]-2-yl)acetamide (1n)



The title compound **1n** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 15 : 1 gave **1n** as a white solid (90% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.90 (brs, 1H), 7.51 – 7.43 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.17 – 7.10 (m, 3H), 7.09 – 7.03 (m, 1H), 2.44 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.04, -111.11; **^{13}C NMR** (101 MHz, $CDCl_3$) δ163.33 (d, *J* = 249.7 Hz), 154.76 (q, *J* = 37.5 Hz), 139.63, 139.24 (d, *J* = 7.6 Hz), 131.83, 131.04 (d, *J* = 8.6 Hz), 130.18, 129.51 (d, *J* = 1.9 Hz), 127.43, 124.77 (d, *J* = 3.0 Hz), 122.48,116.48 (d, *J* = 21.8 Hz), 115.79 (q, *J* = 289.9 Hz), 115.54 (d, *J* = 21.0 Hz), 21.54; **HRMS** (EI-TOF) *m/z*: 297.0780(M^+); calc. for $C_{15}H_{11}F_4NO$: 297.0777.

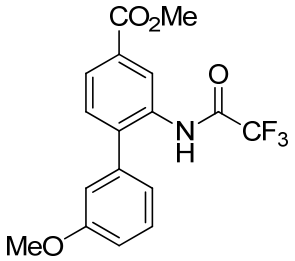
2,2,2-Trifluoro-*N*-(3'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (1o)



The title compound **1o** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 12 : 1 gave **1o** as a white solid

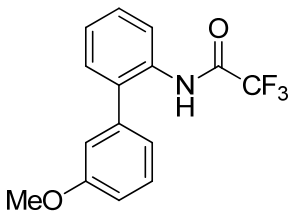
(92% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.19 (brs, 1H), 7.56 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.05 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.93 (d, *J* = 7.2 Hz, 1H), 6.89 – 6.86 (m, 1H), 3.86 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.79, -76.09; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.72, 154.82 (q, *J* = 37.9 Hz), 136.82, 136.12, 132.98, 131.23 (q, *J* = 33.1 Hz), 131.02, 130.85, 123.73 (q, *J* = 273.5 Hz), 122.86 (q, *J* = 3.7 Hz), 120.84, 118.14 (q, *J* = 4.0 Hz), 115.59 (q, *J* = 289.9 Hz), 115.11, 114.52, 55.53; **HRMS** (EI-TOF) *m/z*: 363.0694(M^+); calc. for $C_{16}H_{11}F_6NO_2$: 363.0694.

Methyl 3'-methoxy-2-(2,2,2-trifluoroacetamido)-[1,1'-biphenyl]-4-carboxylate (1p)



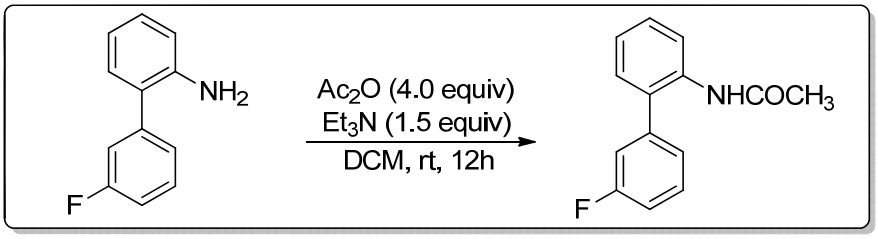
The title compound **1p** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 6 : 1 gave **1p** as a white solid (93% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 1.6 Hz, 1H), 8.15 (brs, 1H), 7.96 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.01 (ddd, *J* = 8.4, 2.4, 0.8 Hz, 1H), 6.94 – 6.91 (m, 1H), 6.88 – 6.86 (m, 1H), 3.94 (s, 3H), 3.84 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.00; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.25, 160.55, 154.80 (q, *J* = 37.7 Hz), 137.55, 137.33, 132.37, 130.79, 130.75, 130.48, 127.49, 122.67, 120.84, 115.68 (q, *J* = 289.9 Hz), 114.95, 114.38, 55.49, 52.52; **HRMS** (EI-TOF) *m/z*: 353.0878(M^+); calc. for $C_{17}H_{14}F_3NO_4$: 353.0875.

2,2,2-Trifluoro-*N*-(3'-methoxy-[1,1'-biphenyl]-2-yl)acetamide (1q)



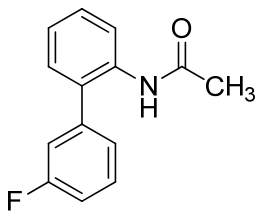
The title compound **1q** was prepared according to **Procedure A** and purified by chromatography in petroleum ether : ethyl acetate = 10 : 1 gave **1q** as a white solid (87% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.0 Hz, 1H), 8.10 (brs, 1H), 7.46 – 7.41 (m, 2H), 7.36 – 7.28 (m, 2H), 7.02 – 6.97 (m, 1H), 6.95 – 6.92 (m, 1H), 6.90 – 6.87 (m, 1H), 3.85 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.01; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.50, 154.65 (q, *J* = 37.2 Hz), 138.20, 133.03, 132.31, 130.65, 130.34, 128.92, 126.29, 121.28, 121.19, 115.80 (q, *J* = 290.0 Hz), 114.63, 114.53, 55.48; **HRMS** (EI-TOF) *m/z*: 295.0818(M^+); calc. for $C_{15}H_{12}F_3NO_2$: 295.0820.

Procedure B :



Ac_2O (4 equiv) was added to 3'-fluoro-[1,1'-biphenyl]-2-amine (3mmol, 1 equiv) and triethylamine (1.5 equiv) in dry dichloromethane (6 mL) at room atmosphere under N_2 atmosphere. Stirring was continued for an additional 12 h at room temperature. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (3 mL), extracted with dichloromethane (15 mL). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated.The residue was purified by flash column chromatography with petroleum ether and ethyl acetate (2 : 1) as eluent to afford the corresponding substrate **1ab** in 90% yield.

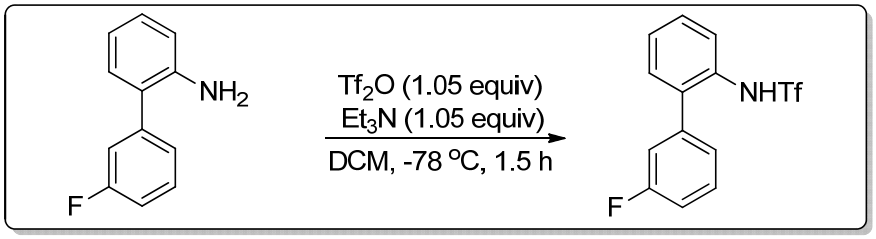
***N*-(3'-Fluoro-[1,1'-biphenyl]-2-yl)acetamide (1ab)**



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.40 – 7.35 (m, 1H), 7.25 – 7.06 (m, 6H), 2.02 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -111.69; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.44, 163.14 (d, *J* = 248.8 Hz), 140.58 (d,

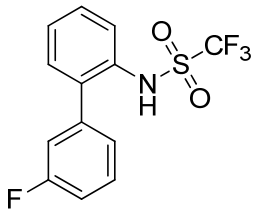
J = 7.7 Hz), 134.65, 131.44, 130.71 (d, *J* = 8.5 Hz), 130.05, 128.95, 124.99 (d, *J* = 3.0 Hz), 124.75, 122.42, 116.43 (d, *J* = 21.7 Hz), 115.02 (d, *J* = 21.0 Hz), 24.59; **HRMS** (EI-TOF) *m/z*: 229.0901(M^+); calc. for $C_{14}H_{12}FNO$: 229.0903.

Procedure C :



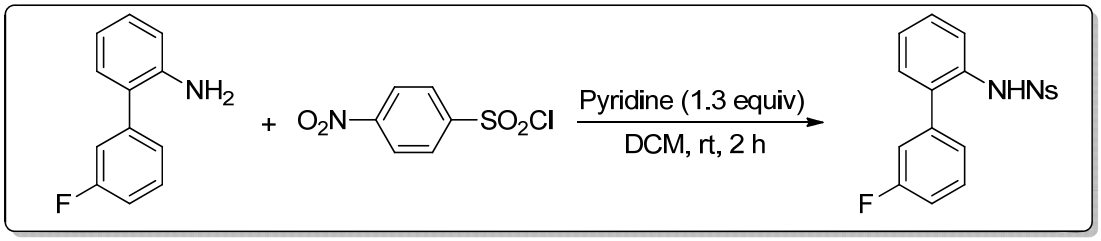
Tf_2O (1.05 equiv, 0.5 M in DCM) was added dropwise to 3'-fluoro-[1,1'-biphenyl]-2-amine (3mmol, 1 equiv) and triethylamine (1.05 equiv) in dry dichloromethane (6 mL) at -78°C under N_2 atmosphere. Stirring was continued for an additional 1.5 h at -78°C. The reaction mixture was quenched with H_2O (3 mL), extracted with dichloromethane (15 mL). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by flash column chromatography with petroleum ether and ethyl acetate (3 : 1) as eluent to afford the corresponding substrate **1ac** in 85% yield.

1,1,1-Trifluoro-*N*-(3'-fluoro-[1,1'-biphenyl]-2-yl)methanesulfonamide (1ac)



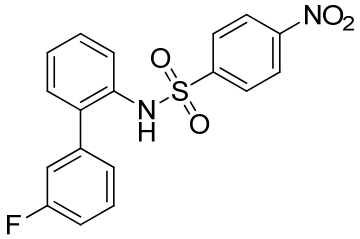
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 8.4, 0.8 Hz, 1H), 7.52 – 7.40 (m, 2H), 7.37 – 7.28 (m, 2H), 7.20 – 7.10 (m, 2H), 7.08 – 7.02 (m, 1H), 6.73 (brs, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.96, -110.98; **^{13}C NMR** (101 MHz, $CDCl_3$) δ163.21 (d, *J* = 249.9 Hz), 139.15 (d, *J* = 7.7 Hz), 134.20 (d, *J* = 1.8 Hz), 131.54, 131.13 (d, *J* = 8.6 Hz), 130.80, 129.53, 127.08, 124.91 (d, *J* = 3.1 Hz), 122.56,119.64 (q, *J* = 323.8 Hz), 116.54 (d, *J* = 21.9 Hz), 115.82 (d, *J* = 21.0 Hz); **HRMS** (EI-TOF) *m/z*: 319.0294(M^+); calc. for $C_{13}H_9F_4NO_2S$: 319.0290.

Procedure D :



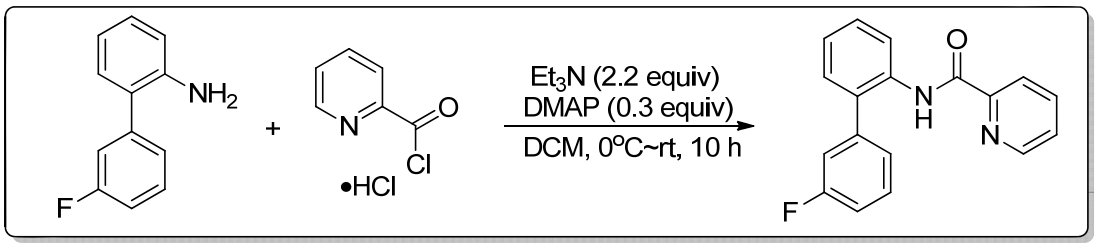
4-Nitrobenzene-1-sulfonyl chloride (1.3 equiv) was added to 3'-fluoro-[1,1'-biphenyl]-2-amine (3mmol, 1 equiv) and pyridine (1.3 equiv) in dry dichloromethane (6 mL) at room temperature under N_2 atmosphere. Stirring was continued for an additional 2 h at room temperature. The reaction mixture was quenched with H_2O (3 mL), extracted with dichloromethane (15 mL). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated.The residue was purified by flash column chromatography with petroleum ether and ethyl acetate (3 : 1) as eluent to afford the corresponding substrate **1ad** in 88% yield.

***N*-(3'-Fluoro-[1,1'-biphenyl]-2-yl)-4-nitrobenzenesulfonamide (1ad)**



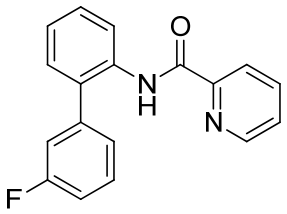
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 – 8.19 (m, 2H), 7.71 – 7.66 (m, 3H), 7.41 (td, *J* = 8.0, 1.6 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.27 – 7.23 (m, 1H), 7.13 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.09 – 7.03 (m, 1H), 6.73 (s, 1H), 6.71 – 6.67 (m, *J* = 7.6 Hz, 1H), 6.44 – 6.38 (m, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -110.89; **^{13}C NMR** (101 MHz, $CDCl_3$) δ162.92 (d, *J* = 250.1 Hz), 150.34, 144.70, 139.30 (d, *J* = 7.6 Hz), 134.17 (d, *J* = 2.0 Hz), 132.38, 130.95 (d, *J* = 8.6 Hz), 130.49, 129.52, 128.43, 126.65, 124.41 (d, *J* = 3.0 Hz), 124.31, 123.77, 116.01 (d, *J* = 21.7 Hz), 115.39 (d, *J* = 20.9 Hz); **HRMS** (EI-TOF) *m/z*: 372.0577(M^+); calc. for $C_{18}H_{13}FN_2O_4S$: 372.0580.

Procedure E :



3'-Fluoro-[1,1'-biphenyl]-2-amine (3mmol, 1 equiv) and triethylamine (2.2 equiv) was added dropwise to pyridine-2-carbonyl chloride hydrochloride (1.1 equiv) and 4-dimethylaminopyridine (0.3 equiv) in dry dichloromethane (6 mL) at 0 ºC under N_2 atmosphere. Stirring was continued for an additional 10 h at room temperature. The reaction mixture was quenched with H_2O (6 mL), extracted with dichloromethane (15 mL). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated.The residue was purified by flash column chromatography with petroleum ether and ethyl acetate (10 : 1) as eluent to afford the corresponding substrate **1ae** in 82% yield..

***N*-(3'-Fluoro-[1,1'-biphenyl]-2-yl)picolinamide (1ae)**



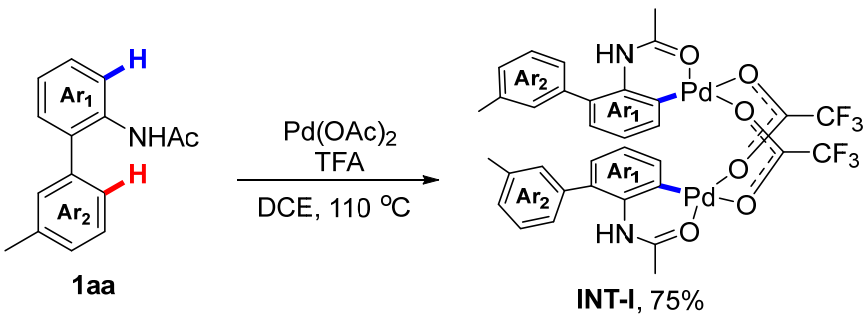
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (brs, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 8.42 – 8.36 (m, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 7.85 (td, *J* = 7.6, 1.6 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.38 (ddd, *J* = 7.6, 4.8, 1.2 Hz, 1H), 7.31 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.27 – 7.11 (m, 4H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -112.36; **^{13}C NMR** (101 MHz, $CDCl_3$) δ163.15 (d, *J* = 248.2 Hz), 162.10, 149.96, 148.11, 140.46 (d, *J* = 7.7 Hz), 137.64, 134.89, 131.39 (d, *J* = 1.9 Hz), 130.56 (d, *J* = 8.5 Hz), 130.17, 129.03, 126.37, 125.40 (d, *J* = 2.9 Hz), 124.44, 122.37, 120.99, 116.71 (d, *J* = 21.8 Hz), 114.86 (d, *J* = 21.1 Hz); **HRMS** (EI-TOF) *m/z*: 292.1009(M^+); calc. for $C_{18}H_{13}FN_2O$: 292.1012.

2.2 Acetamide-Promoted Intraannular C–H Activation and Preparation of Palladacycle INT-I.

***N*-(4''-Acetyl-3-methyl-[1,1':3',1''-terphenyl]-2'-yl)acetamide (2aa)**

To a solution of **1aa** (0.15 mmol) in TFA (0.5 M) were added 4-Ac-C_6H_4I (3 equiv), $Pd(OAc)_2$ (10 mol%) and AgOAc (2 equiv). The resulting mixture was stirred at 120 °C for 15 h. After the reaction was completed, the reaction mixture was poured into water and basified with sat. $NaHCO_3$, and then the product was extracted with CH_2Cl_2 (three times), dried over $MgSO_4$, and concentrated in vacuo. A purification by preparative TLC in hexane : ethyl acetate = 2 : 1 gave **2aa** as a pale yellow solid (76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.46 – 7.27 (m, 4H), 7.21 – 7.13 (m, 3H), 6.76 (s, 1H), 2.61 (s, 3H), 2.38 (s, 3H), 1.69 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.06, 169.30, 145.36, 140.67, 139.93, 139.24, 138.17, 135.84, 131.27, 130.54, 129.78, 129.68, 128.99, 128.43, 128.36, 127.85, 125.93, 26.75, 22.98, 21.58; **HRMS** (EI-TOF) *m/z*: 343.1570 (M^+); calc. for $C_{23}H_{21}NO_2$: 343.1572.

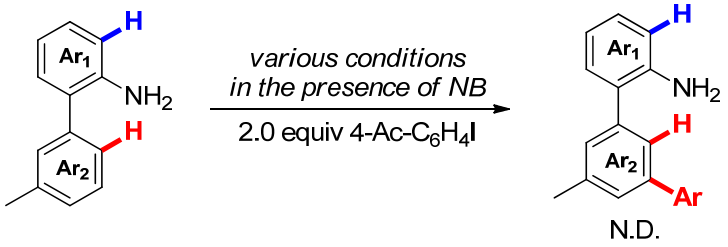
Preparation of palladacycle INT-I.



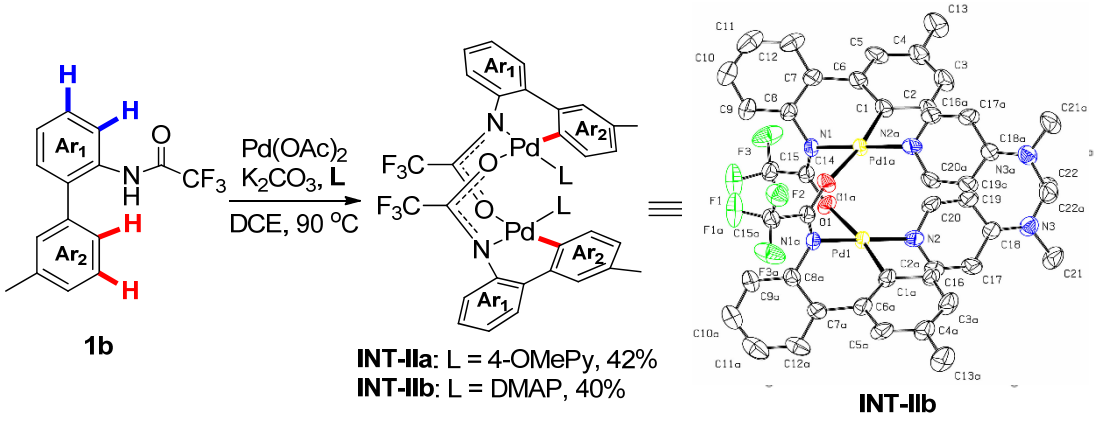
To a solution of **1aa** (1 mmol) in DCE (0.5 M) were added $Pd(OAc)_2$ (1 equiv) and TFA (1.5 equiv). The resulting mixture was stirred at 110 °C for 4 h. After the reaction

was completed, the reaction mixture was concentrated in vacuo. To the crude product, diethyl ether (4 mL) was addedand then the purified product was collected by vacuum filtration, washed with diethyl ether, and dried under vacuum to afford **INT-I** as a yellow solid (75% yield).**^{1}H NMR** (400 MHz, CD_2Cl_2) δ 8.05 (s, 1H), 7.34 – 7.20 (m, 2H), 7.05 – 7.00 (m, 1H), 6.99 – 6.65 (m, 4H), 2.35 (s, 3H), 1.42 (s, 3H); **^{13}C NMR** (101 MHz, CD_2Cl_2) δ 166.87, 165.84 (q, J = 38.2 Hz), 140.24, 137.22, 132.94, 129.72, 129.61, 129.49, 128.44, 127.35, 126.37, 124.98, 123.53, 116.08, 115.30 (q, J = 288.6 Hz), 21.38, 20.98.

Study on interannular *meta*-C–H activation of biaryl-2-amine substrate.



2.3 Preparation of Interannular*ortho*-Palladacycle Complex INT-II



To a 50 mL Schlenk tube, **1b** (1 mmol), $Pd(OAc)_2$ (1 mmol), K_2CO_3 (1.2 mmol), **L** (0.5 mmol) and DCE (8 mL) were added. The tube was charged with N_2 and heated at 90 °C for 10 hours. After cooling to room temperature, the reaction mixture was filtered through a pad of Celite and washed by dichloromethane. The solvent was removed in vacuum. To the crude product, diethyl ether (4 mL) was added and then the purified product was collected by vacuum filtration, washed with diethyl ether:

hexane = 3:1, and dried under vacuum to afford **INT-II**.

When **L** = 4-methoxypyridine, palladacycle complex **INT-IIa** was obtained as a pale yellow solid (42% yield).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 6.8 Hz, 2H), 7.61 – 7.54 (m, 1H), 7.36 (s, 1H), 7.25 – 7.19 (m, 2H), 7.18 – 7.12 (m, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.61 (d, *J* = 7.6 Hz, 1H), 6.40 (d, *J* = 6.8 Hz, 2H), 3.75 (s, 3H), 2.38 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -64.11; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.33, 158.36 (q, *J* = 32.1 Hz), 154.49, 143.70, 140.96, 140.55, 140.12, 136.96, 134.32, 127.37, 127.13, 125.39, 125.33, 123.26 (q, *J* = 2.8 Hz), 116.93 (q, *J* = 290.9 Hz), 110.23, 55.65, 21.00; **HRMS** (ESI)*m/z*: 985.0666 ($M+H^+$); calc. for $C_{42}H_{35}F_6N_4O_4Pd_2$: 985.0627.

When **L** = DMAP, palladacycle complex **INT-IIb** was obtained as a yellow solid (40% yield). A single crystal of **INT-IIb**suitable for X-ray diffraction analysis was obtained by recrystallization from $CHCl_3$/hexane.

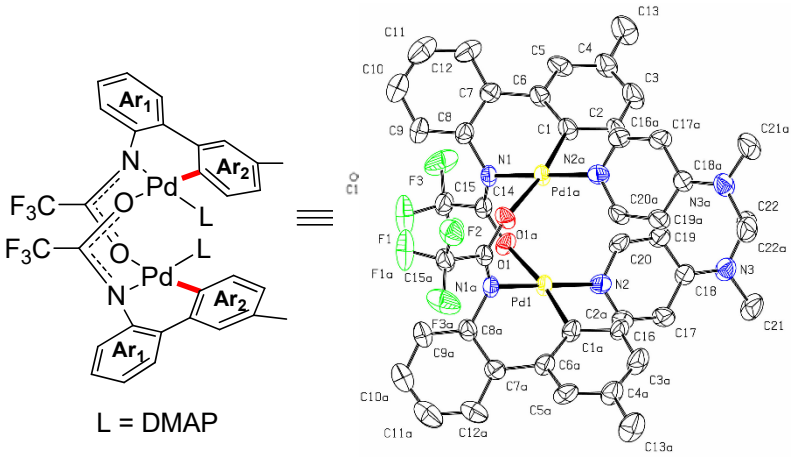


Figure S1. X-ray Crystal Structure for Palladacycle IntermediateINT-IIb

Bond precision: C-C = 0.0131 A Wavelength=0.71073

Cell: a = 14.6512(11) b = 20.1004(15) c = 17.7586(13)

α = 90 β = 92.884(7) γ = 90

Temperature: 293 K

	Calculated	Reported
Volume	5223.2(7)	5223.2(7)
Space group	C 2/c	C 1 2/c 1

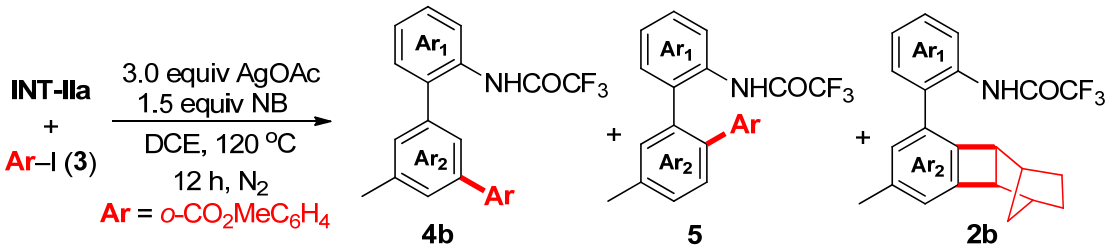
Hall group	-C 2yc	-C 2yc
Moiety formula	C_{44} H_{40} F_6 N_6 O_2 Pd_2	C_{44} H_{40} F_6 N_6 O_2 Pd_2
Sum formula	C_{44} H_{40} F_6 N_6 O_2 Pd_2	C_{44} H_{40} F_6 N_6 O_2 Pd_2
Mr	1011.62	1011.62
Dx,g cm^{-3}	1.286	1.286
Z	4	4
Mu (mm^{-1})	0.746	0.746
F000	2032.0	2032.0
F000’	2024.96	
h,k,lmax	17, 24, 21	17, 24, 21
Nref	4786	4755
Tmin,Tmax	0.745,0.805	0.582, 1.000
Tmin’	0.708	

Correction method= # Reported T Limits: Tmin=0.582 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.994	Theta(max)= 25.350
R(reflections)= 0.0954(3301)	wR2(reflections)= 0.2782(4755)
S = 1.036	Npar= 274

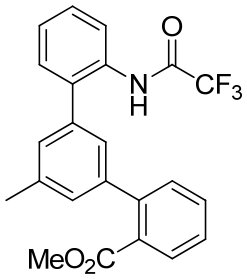
2.4 Stoichiometric Reaction of Palladacycle INT-Iia (GP1)



Entry	Variation from Standard Conditions	Yield (%)[a]		
		4b	**5**	**2b**
1	None	84	0	trace
2	no NB	0	17	0
3	0.2 equiv NB	65	trace	trace
4	0.5 equiv NB	76	trace	trace
5	no Methyl 2-Iodobenzoate	0	0	38

GP1: To a 50 mL Schlenk tube, **INT-IIa**(0.1 mmol), aryl iodide **3a** (3.0 equiv), $Pd(OAc)_2$ (0.1 equiv), AgOAc (3.0 equiv), Norbornene (1.5 equiv) and DCE (1.0 mL) were added. The tube was charged with N_2 and heated at 120 °C for 12 hours. After cooling to room temperature, the reaction mixture was diluted with dichloromethane and filtered through a pad of Celite and washed by dichloromethane. After concentration, the resulting residue was purified by preparative TLC to give the desired product.

Methyl5'-methyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxyl ate (4b)

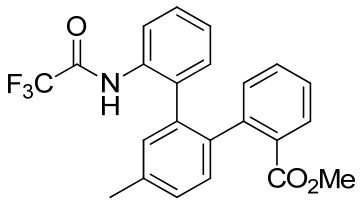


The title compound **4b** was prepared according to **GP1**. A purification by preparative TLC in hexane : ethyl acetate = 9 : 1 gave **4b** as a white solid (84% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.0 Hz, 1H), 8.21 (brs, 1H), 7.89 (dd, J = 7.6, 1.2 Hz, 1H), 7.55 (td, J = 7.6, 1.6 Hz, 1H), 7.46 – 7.40 (m, 2H), 7.39 – 7.36 (m, 2H), 7.29 (td, J = 7.6, 1.2 Hz, 1H), 7.22 – 7.19 (m, 1H), 7.17 (s, 1H), 7.12 (s, 1H), 3.68 (s, 3H), 2.46

(s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.91; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.60, 154.74 (q, *J* = 37.3 Hz), 142.73, 142.14, 138.99, 136.51, 133.29, 132.48, 131.63, 130.75, 130.47, 130.33, 130.25, 129.42, 128.77, 128.58, 127.67, 126.41, 126.23, 121.48, 115.82 (q, *J* = 290.1 Hz), 52.02, 21.47; **HRMS** (EI-TOF) *m/z*: 413.1243 (M^+); calc. for $C_{23}H_{18}F_3NO_3$: 413.1239.

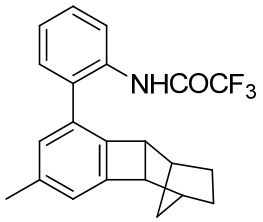
Methyl

4'-methyl-2''-(2,2,2-trifluoroacetamido)-[1,1':2',1''-terphenyl]-2-carboxylate (5)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (brs, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 7.2 Hz, 2H), 7.24 – 7.17 (m, 2H), 7.06 (s, 1H), 6.97 (t, *J* = 7.2 Hz, 1H), 6.94 – 6.88 (m, 1H), 3.65 (s, 3H), 2.42 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.92; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.70, 155.57 (q, *J* = 37.3 Hz), 142.80, 138.59, 137.58, 135.61, 133.74, 132.95, 132.53, 131.83, 131.69, 130.62, 130.44, 129.61, 129.25, 128.71, 128.00, 127.42, 125.51, 123.37, 116.09 (q, *J* = 289.8 Hz), 52.02, 21.09; **HRMS** (EI-TOF) *m/z*: 413.1242 (M^+); calc. for $C_{23}H_{18}F_3NO_3$: 413.1239.

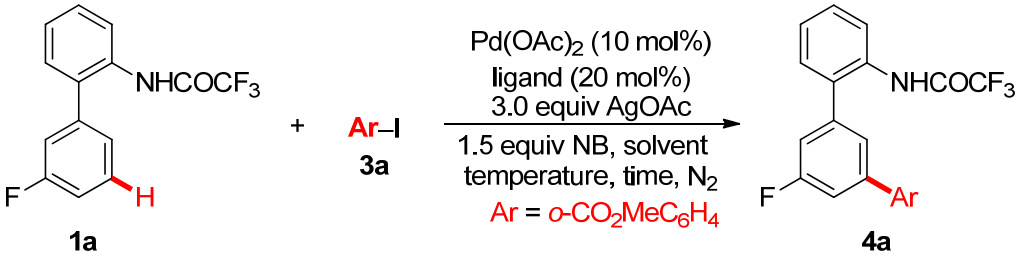
2,2,2-Trifluoro-*N*-(2-(7-methyl-1,2,3,4,4a,8b-hexahydro-1,4-methanobiphenylen-5-yl)phenyl)acetamide (2b)



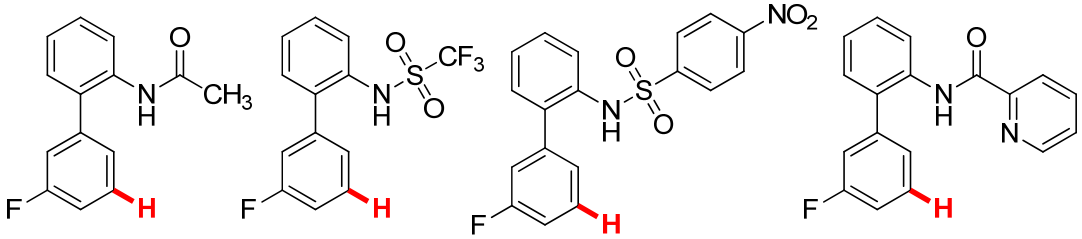
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.12 (brs, 1H), 7.44 – 7.38 (m, 1H), 7.31 – 7.24 (m, 2H), 6.96 (s, 1H), 6.92 (s, 1H), 3.21 (d, *J* = 3.6 Hz, 1H), 3.05 (d, *J* = 3.6 Hz, 1H), 2.38 (s, 3H), 2.30 (d, *J* = 2.8 Hz, 1H), 2.01 (d, *J* = 2.8 Hz, 1H), 1.60 – 1.49 (m, 2H), 1.21 – 1.13 (m, 1H), 1.12 – 1.02 (m, 1H), 0.97 (d, *J* = 10.4 Hz,

1H), 0.83 (d, J = 10.4 Hz, 1H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.97; **^{13}C NMR** (101 MHz, $CDCl_3$) δ154.53 (q, J = 37.3 Hz), 147.99, 142.00, 138.78, 132.57, 130.73, 130.21, 130.15, 128.68, 128.33, 125.93, 123.25, 120.75, 115.81 (q, J = 290.0 Hz), 50.05, 49.94, 36.70, 36.52, 31.98, 27.80, 22.09; **HRMS** (EI-TOF) *m/z*: 371.1495 (M^+); calc. for $C_{22}H_{20}F_3NO$: 371.1497.

2.5 Optimization of the Reaction Conditions for Interannular *meta*-Arylation.

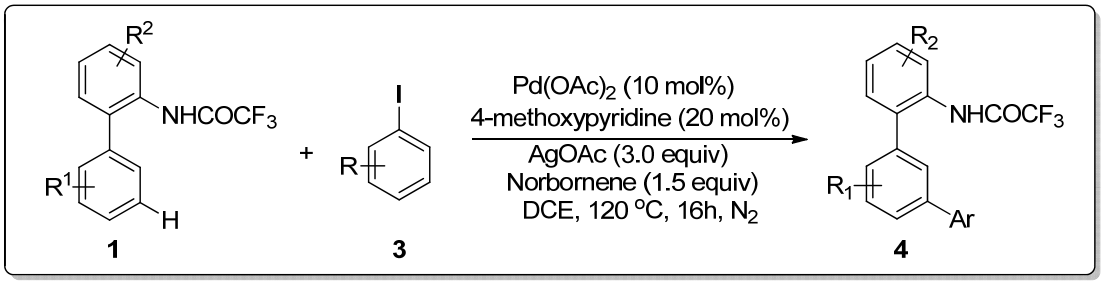


Entry	Ligand	Solvent	Temperature (°C)	Time (h)	Yield (%)[b]
1	pyridine	toluene	100	24	42
2	quinoline	toluene	100	24	30
3	2-picoline	toluene	100	24	38
4	pyridine	toluene	120	16	66
5	pyridine	dioxane	120	16	57
6	pyridine	THF	120	16	49
7	pyridine	DCE	120	16	75
8	2-methoxypyridine	DCE	120	16	25
9	DMAP	DCE	120	16	72
10	4-methoxypyridine	DCE	120	16	81[c]
11[d]	4-methoxypyridine	DCE	120	16	0
12	–	DCE	120	16	0
13[e]	4-methoxypyridine	DCE	120	16	0



[a] Reaction conditions: **1a** (0.1 mmol, 1.0 equiv), **3a** (3.0 equiv), $Pd(OAc)_2$ (10 mol%), ligand (20 mol%), AgOAc (3.0 equiv), NB (1.5 equiv), solvent (1.5 mL), N_2. [b] Isolated yield. [c] 13% **1a** was recovered. [d] No NB. [e] No AgOAc. DMAP = 4-dimethylaminopyridine. N.D. = no detected.

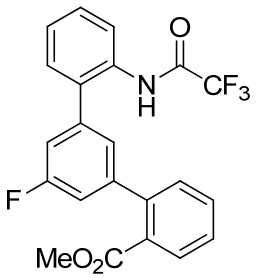
2.6 General Procedure for Palladium/Norbornene-Catalyzed Interannular *meta*-C–H Arylation (GP2).



To a 50 mL Schlenk tube, **1** (0.15 mmol), aryl iodide **3** (0.45 mmol), $Pd(OAc)_2$ (3.4 mg, 0.015 mmol), 4-methoxypyridine (3.3 mg, 0.03 mmol), AgOAc (75.0 mg, 0.45 mmol), NB (22.0 mg, 0.225 mmol) and DCE (1.5 mL) were added. The tube was charged with N_2 and heated at 120 °C for 16 hours. After cooling to room temperature, the reaction mixture was filtered through a pad of Celite with dichloromethane as the eluent. The resulting residue was concentrated and purified by preparative TLC to give the desired product **4**.

Methyl

5'-fluoro-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4a)

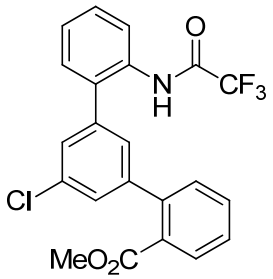


The title compound **4a** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4a** as a pale yellow solid (81% yield).**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1H), 8.11 (brs, 1H), 7.94 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.57 (td, *J* = 7.6, 1.6 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.39 – 7.29 (m, 3H), 7.12 – 7.04 (m, 3H), 3.71 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.83, -111.93; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.90, 162.75 (d, *J* = 249.8 Hz), 154.93 (q, *J* = 37.5 Hz), 144.97 (d, *J* = 8.7 Hz), 141.09 (d, *J* = 2.1 Hz), 138.52 (d, *J* = 8.3 Hz), 132.36 (d, *J* = 2.0 Hz), 132.32, 131.91, 130.68, 130.58, 130.34, 130.07, 129.31, 128.27, 126.51,

125.18 (d, J = 2.8 Hz), 122.12, 115.84 (d, J = 22.0 Hz), 115.77 (q, J = 289.9 Hz), 114.95 (d, J = 22.1 Hz); 52.18; **HRMS** (EI-TOF) *m/z*: 417.0987(M^+); calc. for $C_{22}H_{15}F_4NO_3$: 417.0988.

Methyl

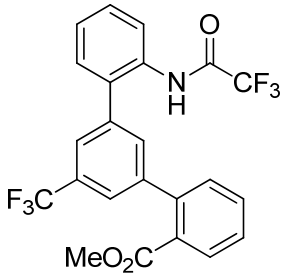
5'-chloro-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate(4c)



The title compound **4c** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4c** as a white solid (70% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.0 Hz, 1H), 8.12 (brs, 1H), 7.95 (dd, J = 7.6, 1.2 Hz, 1H), 7.57 (td, J = 7.6, 1.6 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.39 – 7.29 (m, 5H), 7.20 – 7.18 (m, 1H), 3.72 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.77; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.83, 155.00 (q, J = 37.5 Hz), 144.32, 140.99, 138.18, 134.84, 132.31, 131.97, 130.74, 130.65, 130.36, 129.94, 129.33, 128.68, 128.29, 127.91, 127.65, 126.58, 122.34, 115.78 (q, J = 289.9 Hz), 52.19; **HRMS** (EI-TOF) *m/z*: 433.0694(M^+); calc. for $C_{22}H_{15}ClF_3NO_3$: 433.0693.

Methyl

2''-(2,2,2-trifluoroacetamido)-5'-(trifluoromethyl)-[1,1':3',1''-terphenyl]-2-carbo xylate (4d)

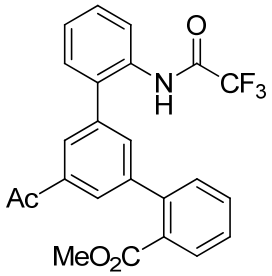


The title compound **4d** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4d** as a white solid (76% yield). **^{1}H NMR**

(400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.0 Hz, 1H), 8.04 (brs, 1H), 7.99 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.63 – 7.57 (m, 3H), 7.53 – 7.45 (m, 3H), 7.41 – 7.33 (m, 3H), 3.70 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.64, -75.87; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.77, 155.12 (q, *J* = 37.7 Hz), 143.61, 140.94, 137.54, 132.81, 132.59, 132.25, 132.11, 131.50 (q, *J* = 32.8 Hz), 130.85, 130.83, 130.50, 129.95, 129.52, 128.49, 126.88, 125.47 (q, *J* = 3.7 Hz), 124.61 (q, *J* = 3.7 Hz), 123.87 (q, *J* = 273.8 Hz), 122.89, 115.77 (q, *J* = 289.9 Hz),52.17; **HRMS** (EI-TOF) *m/z*: 467.0956(M^+); calc. for $C_{23}H_{15}F_6NO_3$: 467.0956.

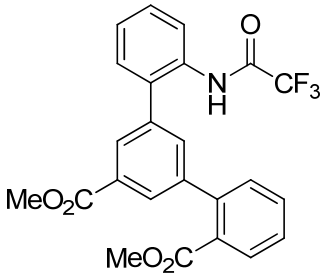
Methyl

5'-acetyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4e)



The title compound **4e** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 4 : 1 gave **4e** as a white solid (77% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.0 Hz, 1H), 8.13 (brs, 1H), 7.98 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.95 – 7.92 (m, 2H), 7.58 (td, *J* = 7.6, 1.2 Hz, 1H), 7.52 (t, *J* = 1.6 Hz, 1H), 7.49 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.45 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.40 – 7.31 (m, 3H), 3.70 (s, 3H), 2.63 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.73; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 197.39, 167.77, 155.06 (q, *J* = 37.6 Hz), 143.20, 141.52, 137.71, 137.14, 133.88, 133.03, 132.30, 132.05, 130.93, 130.71, 130.53, 129.80, 129.28, 128.42, 128.26, 127.69, 126.76, 122.69, 115.77 (q, *J* = 289.9 Hz), 52.17, 26.81; **HRMS** (EI-TOF) *m/z*: 441.1192(M^+); calc. for $C_{24}H_{18}F_3NO_4$: 441.1188.

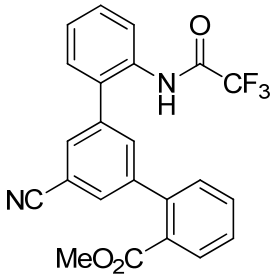
Dimethyl 2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2,5'-dicarboxylate (4f)



The title compound **4f** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 6 : 1 gave **4f** as a white solid (79% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.0 Hz, 1H), 8.10 (brs, 1H), 8.05 – 8.02 (m, 2H), 7.97 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.57 (td, *J* = 7.6, 1.2 Hz, 1H), 7.51 (t, *J* = 1.6 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.40 – 7.30 (m, 3H), 3.92 (s, 3H), 3.69 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.79; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.78, 166.43, 155.03 (q, *J* = 37.6 Hz), 143.06, 141.47, 136.91, 133.73, 132.82, 132.33, 132.00, 131.03, 130.92, 130.69, 130.51, 129.83, 129.67, 129.23, 128.91, 128.20, 126.65, 122.52, 115.77 (q, *J* = 289.9 Hz), 52.49, 52.14; **HRMS** (EI-TOF) *m/z*: 457.1138(M^+); calc. for $C_{24}H_{18}F_3NO_5$: 457.1137.

Methyl

5'-cyano-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4g)

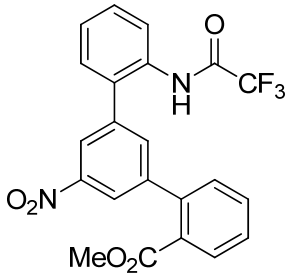


The title compound **4g** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 4 : 1 gave **4g** as a white solid (28% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.0 Hz, 1H), 8.03 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.97 (brs, 1H), 7.65 – 7.62 (m, 2H), 7.59 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.55 – 7.46 (m, 3H), 7.38 – 7.35 (m, 2H), 7.31 (dd, *J* = 7.6, 0.8 Hz, 1H), 3.73 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.67; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.23, 155.23 (q, *J* = 37.7 Hz), 143.94, 140.54, 138.02, 133.95, 132.34, 132.19, 132.16, 131.90, 131.22, 131.05, 130.86, 130.47, 129.79, 129.39, 128.78, 127.05, 123.31, 118.19, 115.75 (q, *J* = 289.9

Hz), 113.30, 52.32; **HRMS** (EI-TOF) *m/z*: 424.1032(M^+); calc. for $C_{23}H_{15}F_3N_2O_3$: 424.1035.

Methyl

5'-nitro-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4h)



The title compound **4h** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 4 : 1 gave **4h** as a pale yellow solid (68% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ8.26 – 8.19 (m, 2H), 8.12 (brs, 1H), 8.09 – 8.02 (m, 2H), 7.66 – 7.59 (m, 2H), 7.55 – 7.46 (m, 2H), 7.44 – 7.34 (m, 3H), 3.74 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.64; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.22, 155.34 (q, *J* = 37.7 Hz), 148.42, 144.21, 140.52, 138.27, 135.47, 132.41, 132.34, 132.14, 131.07, 130.92, 130.57, 129.83, 129.32, 128.86, 127.21, 123.69, 123.33, 122.72, 115.75 (q, *J* = 289.9 Hz), 52.34; **HRMS** (EI-TOF) *m/z*: 444.0935 (M^+); calc. for $C_{22}H_{15}F_3N_2O_5$: 444.0933.

The structure of complex **4h** was determined by X-ray diffraction analysis. A single crystal of this complexsuitable for X-ray diffraction analysis was obtained by recrystallization from ethyl acetate/hexane.

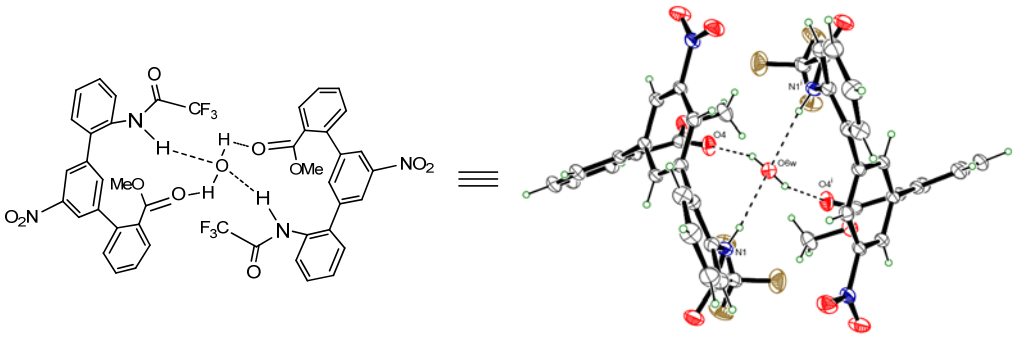


Figure S2. X-ray Crystal Structure for 2(4h)·H_2O

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell:	a=26.3419(12)	b=10.5684(5)	c=19.9298(9)
α=90		β=131.599(1)	γ=90
Temperature:	296 K		
	Calculated		Reported
Volume	4149.1(3)		4149.1(3)
Space group	C 2/c		C 1 2/c 1
Hall group	-C 2yc		-C 2yc
Moiety formula	$2(C_{22}H_{15}F_3N_2O_5)\cdot H_2O$		$2(C_{22}H_{15}F_3N_2O_5)\cdot H_2O$
Sum formula	$C_{44}H_{32}F_6N_4O_{11}$		$C_{44}H_{32}F_6N_4O_{11}$
Mr	906.74		906.74
Dx,g cm^{-3}	1.452		1.452
Z	4		4
Mu (mm^{-1})	0.123		0.123
F000	1864.0		1864.0
F000’	1865.28		
h,k,lmax	34,13,25		34,13,25
Nref	4757		4741
Tmin,Tmax	0.946,0.954		0.947,0.955
Tmin’	0.946		

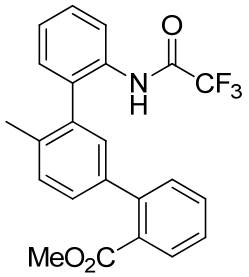
Correction method= # Reported T Limits: Tmin=0.947 Tmax=0.955

AbsCorr = MULTI-SCAN

Data completeness= 0.997	Theta(max)= 27.460
R(reflections)= 0.0500(2649)	wR2(reflections)= 0.1755(4741)
S = 1.001	Npar= 296

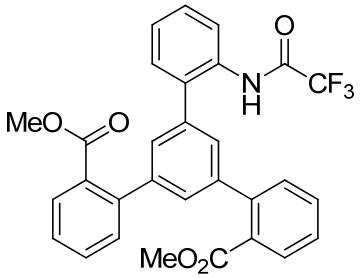
Methyl

4'-methyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4i)



The title compound **4i** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4i** as a white solid (35% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 1H), 7.87 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.79 (brs, 1H), 7.54 (td, *J* = 7.6, 1.2 Hz, 1H), 7.48 – 7.37 (m, 4H), 7.34 – 7.27 (m, 3H), 7.16 (d, *J* = 1.6 Hz, 1H), 3.68 (s, 3H), 2.13 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.07; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.61, 154.75 (q, *J* = 37.4 Hz), 141.97, 139.86, 135.67, 135.34, 133.08, 132.51, 131.69, 130.83, 130.64, 130.41, 130.34, 130.14, 130.04, 129.13, 128.88, 127.58, 126.08, 121.05, 115.73 (q, *J* = 290.1 Hz), 52.04, 19.41; **HRMS** (EI-TOF) *m/z*: 413.1236 (M^+); calc. for $C_{23}H_{18}F_3NO_3$: 413.1239.

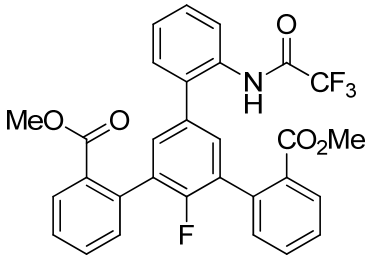
Dimethyl 5'-(2-(2,2,2-trifluoroacetamido)phenyl)-[1,1':3',1''-terphenyl]-2,2''-dicarboxylate (4j)



The title compound **4j** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 7 : 1 gave **4j** as a white solid (76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.39 (brs, 1H), 8.27 (d, *J* = 8.0 Hz, 1H), 7.91 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.56 (td, *J* = 7.6, 1.6 Hz, 2H), 7.47 – 7.39 (m, 6H), 7.33 – 7.28 (m, 4H), 3.70 (s, 6H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.66; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.42, 155.02.75 (q, *J* = 37.4 Hz), 142.43, 141.89, 136.31, 133.31, 132.74, 131.71, 130.90, 130.45, 130.39, 130.37, 128.89, 128.70, 128.09, 127.82, 126.23, 121.89,115.82 (q, *J* = 289.9 Hz), 52.11; **HRMS** (EI-TOF) *m/z*: 533.1446 (M^+); calc. for $C_{30}H_{22}F_3NO_5$:

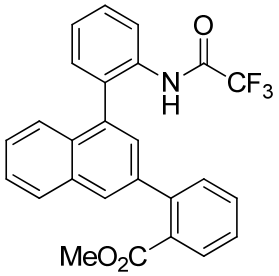
533.1450.

Dimethyl 2'-fluoro-5'-(2-(2,2,2-trifluoroacetamido)phenyl)-[1,1':3',1''-terphenyl]-2,2''-dicarboxylate (4k)



The title compound **4k** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 6 : 1 gave **4k** as a white solid (83% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.42 (brs, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.02 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.59 (td, *J* = 7.6, 1.2 Hz, 2H), 7.50 – 7.39 (m, 6H), 7.33 – 7.27 (m, *J* = 12.9, 3.7 Hz, 3H), 3.74 (s, 6H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.63, -119.60; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.47, 156.12 (d, *J* = 248.6 Hz), 154.98 (q, *J* = 37.5Hz), 136.03, 132.60, 132.27 (d, *J* = 4.3 Hz), 132.06, 131.50, 130.59, 130.55, 130.21 (d, *J* = 18.0 Hz), 128.94, 128.41, 126.40, 122.15, 115.85 (q, *J* = 290.1 Hz), 52.15; **HRMS** (EI-TOF) *m/z*: 551.1352 (M^+); calc. for $C_{30}H_{21}F_4NO_5$: 551.1356.

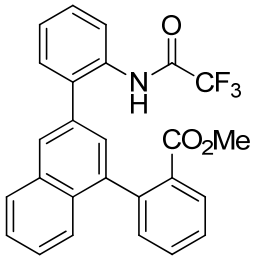
Methyl 2-(4-(2-(2,2,2-trifluoroacetamido)phenyl)naphthalen-2-yl)benzoate (4l)



The title compound **4l** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 9 : 1 gave **4l** as a white solid (49% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.99 – 7.95 (m, 2H), 7.91 (d, *J* = 1.6 Hz, 1H), 7.82 (brs, 1H), 7.63 – 7.41 (m, 9H), 7.37 (td, *J* = 7.2, 1.2 Hz, 1H), 3.65 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -76.21; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.34,

154.92 (q, *J* = 37.5 Hz), 142.26, 138.87, 133.81, 133.73, 133.15, 131.92, 131.46, 131.21, 131.13, 130.63, 130.58, 130.28, 129.57, 129.19, 128.94, 128.16, 127.85, 127.34, 127.03, 126.16, 125.03, 121.61, 115.54 (q, *J* = 289.9 Hz), 52.10; **HRMS** (EI-TOF) *m/z*: 449.1241(M^+); calc. for $C_{26}H_{18}F_3NO_3$: 449.1239.

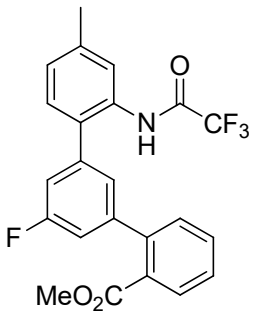
Methyl 2-(3-(2-(2,2,2-trifluoroacetamido)phenyl)naphthalen-1-yl)benzoate (4m)



The title compound **4m** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 8 : 1 gave **4m** as a white solid (63% yield). **^{1}H NMR**(400 MHz, $CDCl_3$) δ 8.38 – 8.26 (m, 2H), 8.11 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 0.8 Hz, 1H), 7.65 (td, *J* = 7.6, 1.2 Hz, 1H), 7.58 – 7.32 (m, 9H), 3.44 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.80; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.28, 154.86 (q, *J* = 37.3 Hz), 141.56, 140.89, 133.59, 133.49, 133.23, 132.55, 132.13, 131.85, 131.77, 130.99, 130.83, 130.56, 128.91, 128.52, 128.17, 128.00, 127.11, 126.84, 126.45, 126.42, 125.72, 121.83, 115.80 (q, *J* = 290.0 Hz), 51.88; **HRMS** (EI-TOF) *m/z*: 449.1241(M^+); calc. for $C_{26}H_{18}F_3NO_3$: 449.1239.

Methyl

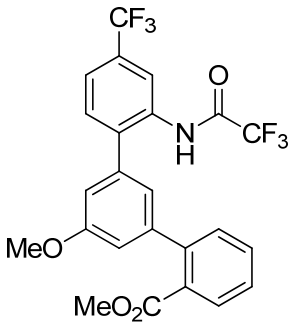
5'-fluoro-4''-methyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carbo xylate (4n)



The title compound **4n** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 13 : 1 gave **4n** as a white solid (80% yield). **^{1}H NMR**

(400 MHz, $CDCl_3$) δ 8.10 (brs, 1H), 8.04 (s, 1H), 7.93 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.56 (td, *J* = 7.6, 1.2 Hz, 1H), 7.46 (td, *J* = 7.6, 1.2 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.15 – 7.11 (m, 1H), 7.09 – 7.03 (m, 3H), 3.71 (s, 3H), 2.43 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.83, -112.12; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.96, 162.72 (d, *J* = 249.6 Hz), 154.92 (q, *J* = 37.4 Hz), 144.85 (d, *J* = 8.7Hz), 141.13 (d, *J* = 2.1 Hz), 139.57, 138.68 (d, *J* = 8.3 Hz), 132.02, 131.88, 130.66, 130.53, 130.13, 130.10, 129.64 (d, *J* = 1.9 Hz), 128.21, 127.36, 125.19 (d, *J* = 2.7 Hz), 122.71, 115.8 (d, *J* = 290.0 Hz), 115.59 (d, *J* = 22.0 Hz), 114.99 (d, *J* = 21.9 Hz), 52.16, 21.52; **HRMS** (EI-TOF) *m/z*: 431.1146(M^+); calc. for $C_{23}H_{17}F_4NO_3$: 431.1145.

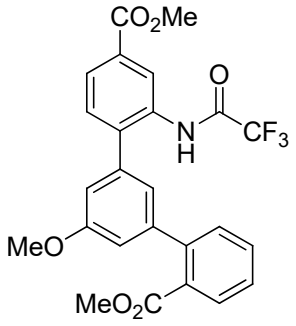
Methyl 5'-methoxy-2''-(2,2,2-trifluoroacetamido)-4''-(trifluoromethyl)-[1,1':3',1''-terphenyl]-2-carboxylate (4o)



The title compound **4o** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 9 : 1 gave **4o** as a white solid (80% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.36 (brs, 1H), 7.92 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.52 – 7.43 (m, 2H), 7.37 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.98 – 6.95 (m, 1H), 6.89 – 6.85 (m, 2H), 3.86 (s, 3H), 3.71 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.75, -75.86; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.20, 160.25, 155.00 (q, *J* = 37.9 Hz), 144.58, 141.78, 136.34, 136.24, 133.20, 131.79, 131.22 (q, *J* = 33.1 Hz), 130.82, 130.67, 130.40, 130.27, 128.03, 123.92 (q, *J* = 273.5 Hz), 122.79 (q, *J* = 3.7 Hz), 121.41, 118.38 (q, *J* = 3.9 Hz), 115.61 (q, *J* = 289.9 Hz), 115.18, 113.11, 55.63, 52.14; **HRMS** (EI-TOF) *m/z*: 497.1065(M^+); calc. for $C_{24}H_{17}F_6NO_4$: 497.1062.

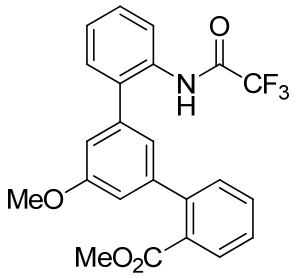
Dimethyl 5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2,4''-dicarboxyla

te (4p)



The title compound **4p** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 5 : 1 gave **4p** as a white solid (69% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.89 (d, *J* = 1.6 Hz, 1H), 8.30 (brs, 1H), 7.97 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.89 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.55 (td, *J* = 7.6, 1.2 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.36 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.95 – 6.93 (m, 1H), 6.88 – 6.85 (m, 2H), 3.94 (s, 3H), 3.85 (s, 3H), 3.69 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.80; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.27, 166.24, 160.12, 154.95 (q, *J* = 37.8 Hz), 144.37, 141.77, 137.59, 136.88, 132.59, 131.72, 130.79, 130.64, 130.46, 130.33, 130.31, 127.95, 127.42, 122.82, 121.35, 115.70 (q, *J* = 290.1 Hz), 115.04, 113.02, 55.61, 52.52, 52.12; **HRMS** (EI-TOF) *m/z*: 487.1241(M^+); calc. for $C_{25}H_{20}F_3NO_6$: 487.1243.

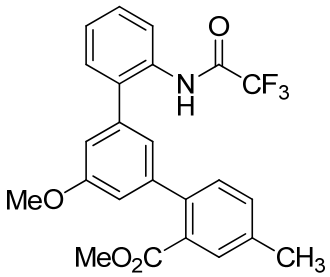
Methyl 5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4q)



The title compound **4q** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 7 : 1 gave **4q** as a white solid (80% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.32 – 8.28 (m, 1H), 8.25 (brs, 1H), 7.89 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.55 (td, *J* = 7.6, 1.6 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.38 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.29 (td, *J* = 7.6, 1.2 Hz, 1H), 6.93 (dd, *J* = 2.4, 1.6 Hz, 1H), 6.90 – 6.88 (m, 1H), 6.87

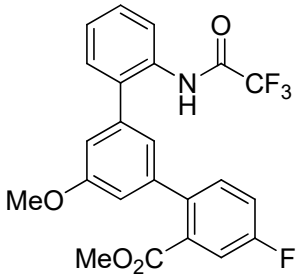
(dd, *J* = 2.4, 1.6 Hz, 1H), 3.85 (s, 3H), 3.69 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.83; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.47, 160.04, 154.75 (q, *J* = 37.4 Hz), 144.18, 141.88, 137.77, 133.07, 132.45, 131.63, 130.63, 130.51, 130.29, 130.22, 128.91, 127.84, 126.22, 121.66, 121.44, 115.80 (q, *J* = 290.1 Hz), 114.57, 113.30, 55.56, 52.10; **HRMS** (EI-TOF) *m/z*: 429.1187(M^+); calc. for $C_{23}H_{18}F_3NO_4$: 429.1188.

Methyl 5'-methoxy-4-methyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4r)



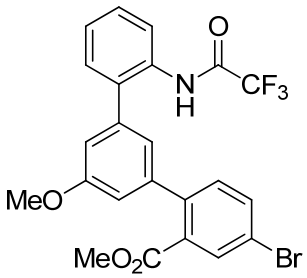
The title compound **4r** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4r** as a white solid (76% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.4 Hz, 1H), 8.23 (brs, 1H), 7.68 (s, 1H), 7.44 – 7.39 (m, 1H), 7.38 – 7.32 (m, 2H), 7.30 – 7.23 (m, 2H), 6.91 – 6.88 (m, 1H), 6.87 – 6.82 (m, 2H), 3.83 (s, 3H), 3.66 (s, 3H), 2.41 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.84; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.70, 160.02, 154.73 (q, *J* = 37.3 Hz), 144.18, 139.01, 137.81, 137.71, 133.10, 132.46, 132.35, 130.71, 130.54, 130.32, 130.29, 128.88, 126.20, 121.70, 121.38, 115.80.75 (q, *J* = 290.1 Hz), 114.63, 114.36, 55.54, 52.05, 21.06; **HRMS** (EI-TOF) *m/z*: 443.1340(M^+); calc. for $C_{24}H_{20}F_3NO_4$: 443.1344.

Methyl 4-fluoro-5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4s)



The title compound **4s** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4s** as a white solid (65% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.4 Hz, 1H), 8.20 (brs, 1H), 7.59 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.38 – 7.33 (m, 2H), 7.32 – 7.22 (m, 2H), 6.90 – 6.86 (m, 2H), 6.86 – 6.84 (m, 1H), 3.85 (s, 3H), 3.70 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.84, -113.64; **^{13}C NMR** (101 MHz, $CDCl_3$) δ167.10 (d, *J* = 2.6 Hz), 161.92 (d, *J* = 249.5 Hz), 160.07, 154.75 (q, *J* = 37.4 Hz), 143.13, 138.08 (d, *J* = 3.5 Hz), 137.87, 133.01, 132.48, 132.42 (d, *J* = 3.1 Hz), 132.05 (d, *J* = 7.5 Hz), 130.28, 128.98, 126.26, 121.75, 121.52, 118.7 (d, *J* = 21.3 Hz), 117.19 (d, *J* = 23.6 Hz), 115.80 (q, *J* = 290.1 Hz), 114.74, 113.37, 55.58, 52.36; **HRMS** (EI-TOF) *m/z*: 447.1093(M^+); calc. for $C_{23}H_{17}F_4NO_4$: 447.1094.

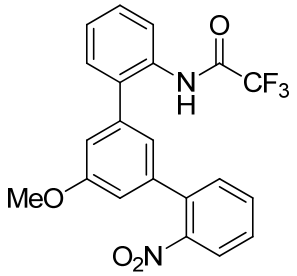
Methyl 4-bromo-5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxylate (4t)



The title compound **4t** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4t** as a white solid (62% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.4 Hz, 1H), 8.18 (brs, 1H), 8.02 (d, *J* = 2.0 Hz, 1H), 7.67 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.38 – 7.34 (m, 1H), 7.30 (td, *J* = 7.6, 1.2 Hz, 1H), 7.26 – 7.23 (m, 1H), 6.89 – 6.87 (m, 2H), 6.86 – 6.83 (m, 1H), 3.85 (s, 3H), 3.70 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.82; **^{13}C NMR** (101 MHz,

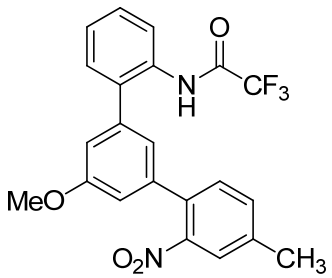
$CDCl_3$) δ 166.98, 160.11, 154.75 (q, *J* = 37.4 Hz), 142.92, 140.80, 137.98, 134.61, 133.12, 132.95, 132.41, 132.20, 132.04, 130.28, 129.02, 126.29, 121.81, 121.56, 121.50, 115.79 (q, *J* = 290.1 Hz), 114.55, 113.53, 55.60, 52.40; **HRMS** (EI-TOF) *m/z*: 507.0297(M^+); calc. for $C_{23}H_{17}BrF_3NO_4$: 507.0293.

2,2,2-Trifluoro-*N*-(5'-methoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)acetamide (4u)



The title compound **4u** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 8 : 1 gave **4u** as a yellow solid (75% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.0 Hz, 1H), 8.08 (brs, 1H), 7.91 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.64 (td, *J* = 7.6, 1.6 Hz, 1H), 7.53 (td, *J* = 8.0, 1.6 Hz, 1H), 7.48 – 7.41 (m, 2H), 7.39 – 7.28 (m, 2H), 6.95 – 6.90 (m, 2H), 6.89 – 6.87 (m, 1H), 3.85 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.88; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.47, 154.83 (q, *J* = 37.4 Hz), 149.14, 140.29, 138.59, 135.65, 132.73, 132.66, 132.30, 131.79, 130.41, 129.13, 128.89, 126.39, 124.41, 121.65, 120.95, 115.77 (q, *J* = 289.9 Hz), 114.26, 114.19, 55.64; **HRMS** (EI-TOF) *m/z*: 416.0986(M^+); calc. for $C_{21}H_{15}F_3N_2O_4$: 416.0984.

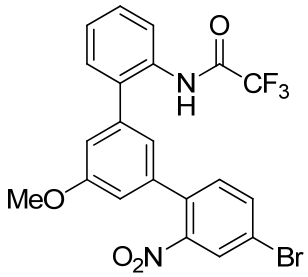
2,2,2-Trifluoro-*N*-(5'-methoxy-4''-methyl-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)acetamide (4v)



The title compound **4v** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4v** as a white solid (72% yield). **^{1}H NMR**

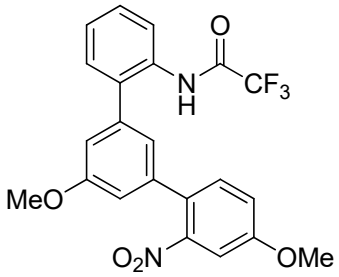
(400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.0 Hz, 1H), 8.11 (brs, 1H), 7.72 (s, 1H), 7.46 – 7.41 (m, 2H), 7.37 – 7.27 (m, 3H), 6.91 – 6.88 (m, 2H), 6.87 – 6.84 (m, 1H), 3.84 (s, 3H), 2.48 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.87; **^{13}C NMR** (101 MHz, $CDCl_3$) δ160.42, 154.82 (q, *J* = 37.4 Hz), 148.94, 140.35, 139.51, 138.49, 133.39, 132.79, 132.78, 132.30, 131.54, 130.40, 129.07, 126.37, 124.72, 121.62, 121.01, 115.76 (q, *J* = 290.1 Hz), 114.25, 114.04, 55.61, 21.01; **HRMS** (EI-TOF) *m/z*: 430.1139(M^+); calc. for $C_{22}H_{17}F_3N_2O_4$: 430.1140.

***N*-(4''-Bromo-5'-methoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)-2,2,2-trifluoroacetamide (4w)**



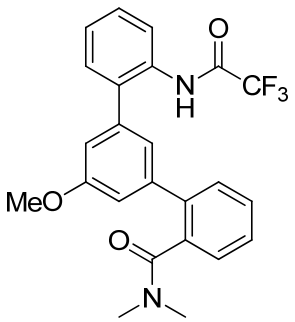
The title compound **4w** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **4w** as a yellow solid (65% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 2.0 Hz, 1H), 8.03 (brs, 1H), 7.77 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.37 – 7.28 (m, 3H), 6.92 (dd, *J* = 2.4, 1.2 Hz, 1H), 6.90 – 6.86 (m, 1H), 6.84 (t, *J* = 1.2 Hz, 1H), 3.85 (s, 3H); **^{19}F NMR**(376 MHz, $CDCl_3$) δ -75.86; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.53, 154.82 (q, *J* = 37.4 Hz), 149.41, 139.15, 138.84, 135.71, 134.50, 133.04, 132.62, 132.24, 130.40, 129.23, 127.38, 126.47, 122.14, 121.79, 120.77, 115.76 (q, *J* = 289.9 Hz), 114.53, 114.12, 55.68; **HRMS** (EI-TOF) *m/z*: 494.0087(M^+); calc. for $C_{21}H_{14}BrF_3N_2O_4$: 494.0089.

***N*-(4'',5'-Dimethoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)-2,2,2-trifluoroacetamide (4x)**



The title compound **4x** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 7 : 1 gave **4x** as a white solid (70% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.4 Hz, 1H), 8.11 (brs, 1H), 7.46 – 7.40 (m, 2H), 7.38 – 7.27 (m, 3H), 7.16 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.88 (d, *J* = 1.6 Hz, 2H), 6.84 (t, *J* = 1.6 Hz, 1H), 3.90 (s, 3H), 3.84 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.87; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.43, 159.64, 154.81 (q, *J* = 37.4 Hz), 149.56, 140.22, 138.47, 132.81, 132.61, 132.30, 130.40, 129.06, 127.85, 126.36, 121.60, 121.14, 118.93, 115.77 (q, *J* = 289.9Hz), 114.37, 113.89, 109.40, 56.08, 55.60; **HRMS** (EI-TOF) *m/z*: 446.1091(M^+); calc. for $C_{22}H_{17}F_3N_2O_5$: 446.1090.

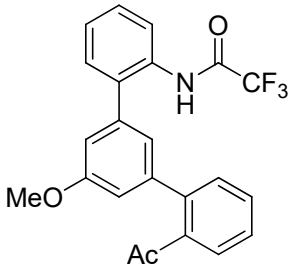
5'-Methoxy-*N*,*N*-dimethyl-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-2-carboxamide (4y)



The title compound **4y** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 1.5 : 1 gave **4y** as a white solid (37% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 – 8.18 (m, 2H), 7.47 – 7.37 (m, 5H), 7.35 – 7.27 (m, 2H), 7.13 – 7.11 (m, 1H), 7.01 (t, *J* = 1.2 Hz, 1H), 6.88 – 6.86 (m, 1H), 3.83 (s, 3H), 2.90 (s, 3H), 2.52 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.80; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.23, 160.24, 154.64 (q, *J* = 37.2 Hz), 142.82, 138.47, 137.81, 135.91, 133.23, 132.18, 130.39, 129.57, 129.37, 129.01, 128.38, 127.55, 126.51, 121.83, 121.47, 115.81 (q, *J* = 290.1 Hz), 114.16, 114.07, 55.67, 38.24, 34.72; **HRMS**

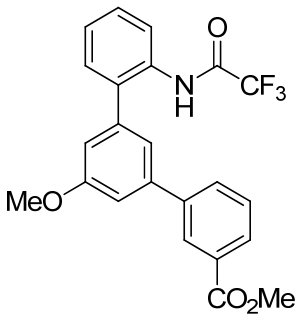
(EI-TOF) *m/z*: 442.1502 (M^+); calc. for $C_{24}H_{21}F_3N_2O_3$: 442.1504.

_N_-(2''-Acetyl-5'-methoxy-[1,1':3',1''-terphenyl]-2-yl)-2,2,2-trifluoroacetamide (4z)



The title compound **4z** was prepared according to **GP2**. A purification by preparative TLC in hexane : ethyl acetate = 8 : 1 gave **4z** as a white solid (51% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.0 Hz, 1H), 8.15 (brs, 1H), 7.59 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.53 (td, *J* = 7.6, 1.6 Hz, 1H), 7.47 – 7.42 (m, *J* = 10.1, 3.6, 1.7 Hz, 2H), 7.40 – 7.28 (m, 3H), 6.96 – 6.89 (m, 3H), 3.85 (s, 3H), 2.17 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.83; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.87, 160.41, 154.69 (q, *J* = 37.5 Hz), 143.73, 140.51, 139.73, 138.62, 132.90, 132.26, 131.07, 130.38, 130.31, 129.12, 128.24, 128.14, 126.44, 121.81, 121.68, 115.79 (q, *J* = 290.2 Hz), 115.06, 113.85, 55.64, 30.32; **HRMS** (EI-TOF) *m/z*: 413.1243(M^+); calc. for $C_{23}H_{18}F_3NO_3$: 413.1239.

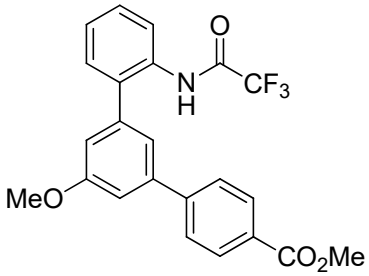
Methyl 5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-3-carboxylate (4aa)



The title compound **4aa** was prepared according to **GP2,** 2-CO_2Me-NB was used instead of NB. A purification by preparative TLC in hexane : ethyl acetate = 8 : 1 gave **4aa** as a white solid (32% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.4 Hz, 1H), 8.27 (s, 1H), 8.18 (brs, 1H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H),

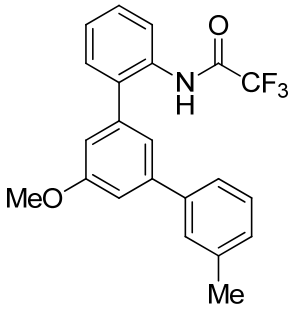
7.53 (t, *J* = 8.0 Hz, 1H), 7.49 – 7.44 (m, 1H), 7.42 – 7.38 (m, 1H), 7.36 – 7.30 (m, 1H), 7.24 – 7.21 (m, 1H), 7.18 (s, 1H), 6.90 (s, 1H), 3.94 (s, 3H), 3.91 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.86; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.98, 160.92, 154.69 (q, *J* = 37.3 Hz), 143.09, 140.59, 138.82, 132.91, 132.28, 131.63, 131.02, 130.43, 129.19, 129.12, 128.40, 126.43, 121.52, 120.32, 115.83 (q, *J* = 289.9 Hz), 113.65, 113.51, 55.71, 52.38; **HRMS** (EI-TOF) *m/z*: 429.1188(M^+); calc. for $C_{23}H_{18}F_3NO_4$: 429.1188.

Methyl 5'-methoxy-2''-(2,2,2-trifluoroacetamido)-[1,1':3',1''-terphenyl]-4-carboxylate (4ab)



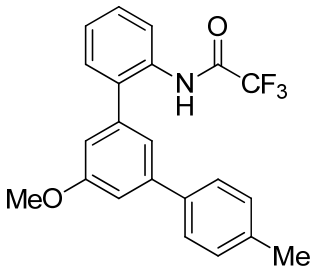
The title compound **4ab** was prepared according to **GP2,** 2-CO_2Me-NB was used instead of NB. A purification by preparative TLC in hexane : ethyl acetate = 8 : 1 gave **4ab** as a white solid (36% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.0 Hz, 1H), 8.15 (br, 1H), 8.11 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.49 – 7.43 (m, 1H), 7.39 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.33 (td, *J* = 7.6, 1.2 Hz, 1H), 7.22 (dd, *J* = 2.0, 1.6 Hz, 1H), 7.18 (t, *J* = 1.6 Hz, 1H), 6.91 (dd, *J* = 2.4, 1.6 Hz, 1H), 3.94 (s, 3H), 3.90 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.85; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 166.94, 160.88, 154.70 (q, *J* = 37.3 Hz), 144.66, 142.94, 138.87, 132.91, 132.25, 130.41, 130.35, 129.73, 129.16, 127.23, 126.48, 121.64, 120.43, 115.82 (q, *J* = 290.2 Hz), 113.92, 113.63, 55.71, 52.33; **HRMS** (EI-TOF) *m/z*: 429.1192(M^+); calc. for $C_{23}H_{18}F_3NO_4$: 429.1188.

2,2,2-Trifluoro-*N*-(5'-methoxy-3''-methyl-[1,1':3',1''-terphenyl]-2-yl)acetamide (4ac)



The title compound **4ac** was prepared according to **GP2,** 2-CO_2Me-NB was used instead of NB. A purification by preparative TLC in hexane : ethyl acetate = 20 : 1 gave **4ac** as a white solid (36% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.21 (brs, 1H), 7.48 – 7.43 (m, 1H), 7.41 – 7.38 (m, 3H), 7.37 – 7.29 (m, 2H), 7.22 – 7.19 (m, 2H), 7.16 (t, *J* = 1.5 Hz, 1H), 6.86 (dd, *J* = 2.4, 1.6 Hz, 1H), 3.90 (s, 3H), 2.42 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.85; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.80, 154.67 (q, *J* = 37.3 Hz), 144.37, 140.30, 138.71, 138.48, 133.03, 132.35, 130.42, 129.00, 128.96, 128.87, 128.09, 126.34, 124.37, 121.34, 120.36, 115.84 (q, *J* = 290.1 Hz), 113.45, 113.14, 55.66, 21.63; **HRMS** (EI-TOF) *m/z*: 385.1287 (M^+); calc. for $C_{22}H_{18}F_3NO_2$: 385.1290.

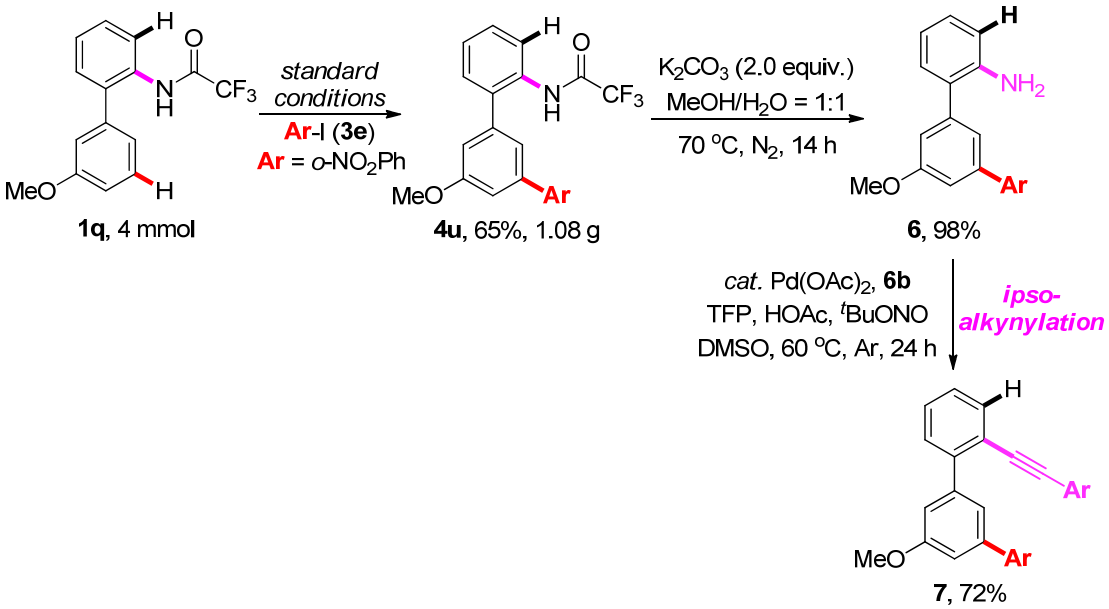
2,2,2-Trifluoro-*N*-(5'-methoxy-4''-methyl-[1,1':3',1''-terphenyl]-2-yl)acetamide(4ad)



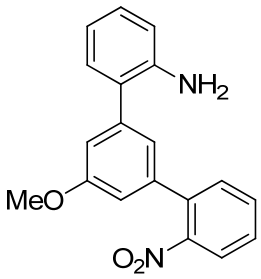
The title compound **4ad** was prepared according to **GP2,** 2-CO_2Me-NB was used instead of NB. A purification by preparative TLC in hexane : ethyl acetate = 20 : 1 gave **4ad** as a white solid (43% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.6 Hz, 1H), 8.21 (brs, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.43 (m, 1H), 7.39 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.31 (td, *J* = 7.6, 1.2 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.19 (dd, *J* = 2.4, 1.6 Hz, 1H), 7.15 (t, *J* = 1.6 Hz, 1H), 6.84 (dd, *J* = 2.4, 1.6 Hz, 1H), 3.89 (s, 3H), 2.41 (s, 3H); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.87; **^{13}C NMR** (101 MHz, $CDCl_3$) δ

160.82, 154.67 (q, J = 37.4 Hz), 144.14, 138.48, 138.05, 137.39, 133.06, 132.35, 130.41, 129.78, 128.99, 127.10, 126.32, 121.31, 120.14, 115.83 (q, J = 290.1 Hz), 113.27, 112.88, 55.63, 21.27; **HRMS** (EI-TOF) *m/z*: 385.1288 (M^+); calc. for $C_{22}H_{18}F_3NO_2$: 385.1290.

2.7 Gram-Scale Synthesis, Removal of PGand *ipso*-Alkynylation



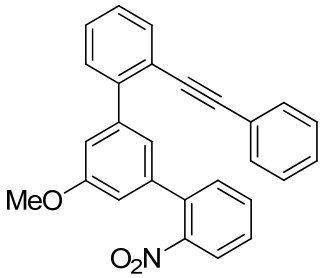
5'-Methoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-amine (6)



To a 100 mL Schlenk tube, **4u** (1 mmol), K_2CO_3 (2.0 equiv), methanol (10 mL) and H_2O (10 mL) was added. The tube was charged with N_2 and heated at 70 °C for 14 hours. After cooling to room temperature, the reaction was diluted with dichloromethane (10 mL), washed by H_2O (10 mL), brine (10 mL), and dried over anhydrous Na_2SO_4. After concentration, The residue was purified by flash column chromatography with ethyl acetate and petroleum ether (4 : 1) as eluent to afford the desired product **6** (98% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, J = 8.4, 1.2 Hz, 1H), 7.62 (td, J = 7.6, 1.2 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.20 – 7.12 (m, 2H), 7.06

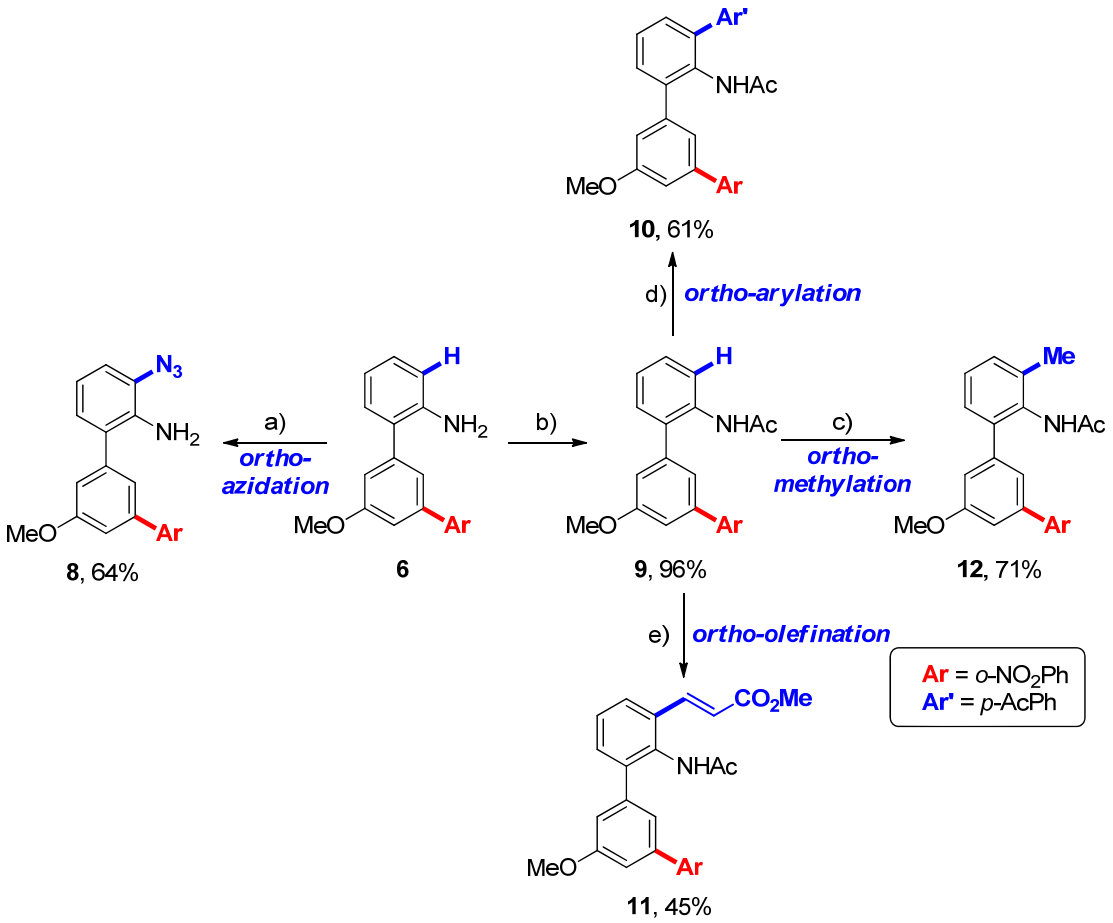
– 6.98 (m, 2H), 6.87 (dd, *J* = 2.4, 1.6 Hz, 1H), 6.81 (td, *J* = 7.6, 1.2 Hz, 1H), 6.76 (dd, *J* = 8.4, 1.2 Hz, 1H), 4.00 – 3.60 (m, 5H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.31, 149.37, 143.77, 141.33, 139.07, 136.18, 132.50, 131.94, 130.34, 128.92, 128.48, 126.81, 124.29, 121.23, 118.58, 115.79, 114.41, 112.80, 55.57; **HRMS** (EI-TOF) *m/z*: 320.1158 (M^+); calc. for $C_{19}H_{16}N_2O_3$: 320.1161.

5'-Methoxy-2-nitro-2''-(phenylethynyl)-1,1':3',1''-terphenyl (7)



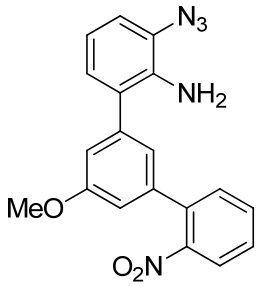
The title compound **7** was prepared according to the literature.[2] A 50 mL Schlenk tube, charged with $Pd(OAc)_2$ (8 mol%), TFP (25 mol%), a stirring bar and septum, was evacuated and backfilled with argon (the cycle was performed three times) and then charged under a positive pressure of argon with DMSO (1 mL), **6** (0.15 mmol), AcOH (1.4equiv), *tert*-BuONO (1.4equiv) and phenyl acetylene **6b** (1.4 equiv) atroom temperature. Then, the Schlenk was transferred to an oil bath and heated at 60 ^oC for 24 hours. The cooled mixture was partitioned between ethyl acetate and saturated NH_4Cl, the organic layer was washed with brine, dried over Na_2SO_4 and concentrated in vacuo. A purification by preparative TLC in hexane : ethyl acetate = 10 : 1 gave **7** as a yellow solid (72% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.64 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.48 – 7.42 (m, 3H), 7.42 – 7.30 (m, 4H), 7.28 – 7.21 (m, 5H), 6.87 (dd, *J* = 2.4, 1.6 Hz, 1H), 3.82 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.41, 149.37, 143.12, 142.36, 138.31, 136.21, 133.13, 132.30, 132.18, 131.56, 129.66, 128.74, 128.36, 128.34, 128.30, 127.54, 124.16, 123.41, 121.67, 121.63, 114.79, 113.10, 92.80, 89.35, 55.56; **HRMS** (EI-TOF) *m/z*: 405.1364 (M^+); calc. for $C_{27}H_{19}NO_3$: 405.1365.

2.8 Further Derivatization via Intraannular *ortho*-C–H Functionlaization.



Reagents and conditions: a) CuBr (10 mol%), $TMSN_3$, TBHP, CH_3CN, 30 °C, Ar; b) Ac_2O, Et_3N, DCM, 30 °C; c) $Pd(OAc)_2$ (20 mol%), MeI, AgOAc, $Cu(OTf)_2$, TFA/DCM (v/v = 4:1), 30 °C, N_2; d) $Pd(OAc)_2$ (10 mol%), 4-AcC_6H_4I, AgOAc, TFA, 130 °C, N_2; e) $Pd(OAc)_2$ (10 mol%), Methyl Acrylate, $K_2S_2O_8$ (1.0 equiv), TFA-DCM, 30 °C, N_2.

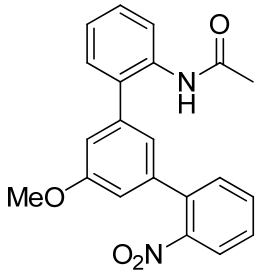
_N_-(3-Azido-5'-methoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)acetamide (8)



The title compound **8** was prepared according to the literature.[3] Substrate **6** (0.15 mmol) and CuBr (0.015 mmol) were added to a 50 mL Schlenk tube under Ar, followed by addition of $TMSN_3$ (0.3 mmol), TBHP (70% in H_2O, 0.3 mmol), CH_3CN (2.0 mL). The formed mixture was stirred at 30 °C under Ar (1 atm) for 3 h as monitored by TLC. The solution was then diluted with ethyl acetate (15 mL), and evaporated under vaccum. A purification by preparative TLC in hexane : ethyl acetate

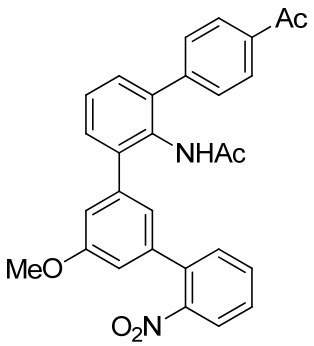
= 8 : 1 gave **8** as a yellow solid (64% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.63 (td, *J* = 7.6, 1.2 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.04 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.00 – 6.98 (m, 1H), 6.98 – 6.94 (m, 2H), 6.88 – 6.86 (m, 1H), 6.82 (t, *J* = 8.0 Hz, 1H), 4.01 (brs, 2H), 3.86 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.37, 149.34, 140.51, 139.27, 136.07, 135.85, 132.56, 131.92, 128.58, 127.63, 126.69, 125.45, 124.35, 121.08, 118.34, 117.74, 114.31, 113.12, 55.61; **HRMS** (ESI-TOF) *m/z*: 362.1178 $(M + H)^+$; calc. for $C_{19}H_{16}N_5O_3$: 362.1175.

***N*-(5'-Methoxy-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)acetamide (9)**



Ac_2O (4 equiv) was added to **6** (2mmol, 1 equiv) and triethylamine (2 equiv) in dry dichloromethane (6 mL) at room temperature. Stirring was continued for an additional 12 h at room temperature. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (3 mL), extracted with dichloromethane (10 mL×2). The organic phase was washed with brine (10 mL), dried over anhydrous Na_2SO_4, filtered and concentrated.The residue was purified by flash column chromatography with ethyl acetate and petroleum ether as eluent to afford the corresponding substrate **9**. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 1H), 7.91 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.64 (td, *J* = 7.6, 1.2 Hz, 1H), 7.52 (td, *J* = 8.0, 1.2 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.39 – 7.33 (m, 1H), 7.26 – 7.21 (m, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 1.6 Hz, 2H), 6.85 (t, *J* = 1.6 Hz, 1H), 3.87 (s, 3H), 2.12 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.03, 160.63, 149.16, 139.91, 139.58, 136.01, 135.21, 132.77, 131.86, 131.40, 129.88, 128.83, 128.79, 124.37, 124.10, 121.54, 121.02, 114.70, 113.55, 55.63, 24.82; **HRMS** (EI-TOF) *m/z*: 362.1269 (M^+); calc. for $C_{21}H_{18}N_2O_4$: 362.1267.

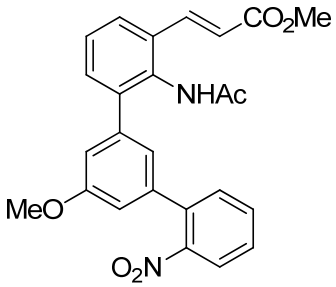
***N*-(4-Acetyl-5''-methoxy-2'''-nitro-[1,1':3',1'':3'',1'''-quaterphenyl]-2'-yl)acetamide (10)**



The title compound **10** was prepared according to the literature.[4] To a solution of **9** (0.15 mmol) in TFA (0.5 M) were added 4-AcC_6H_4I (3 equiv), $Pd(OAc)_2$ (10 mol%) and AgOAc (2 equiv). The resulting mixture was stirred at 130 ºC for 18 h. After the reaction was completed, the reaction mixture was poured into water and basified with sat. $NaHCO_3$, and then the product was extracted with CH_2Cl_2 (three times), dried over $MgSO_4$, and concentrated in vacuo.A purification by preparative TLC in hexane : acetone = 2.5 : 1 gave **10** as a pale yellow solid (61% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.86 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.62 (td, *J* = 7.6, 1.2 Hz, 1H), 7.53 – 7.48 (m, 3H), 7.48 – 7.42 (m, 2H), 7.41 – 7.39 (m, 1H), 7.39 – 7.34 (m, 1H), 6.99 – 6.95 (m, 1H), 6.88 – 6.84 (m, 2H), 6.78 (brs, 1H), 3.83 (s, 3H), 2.62 (s, 3H), 1.75 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 198.03, 169.63, 159.94, 149.32, 145.15, 141.09, 140.20, 140.11, 138.71, 136.04, 135.95, 132.57, 131.92, 131.48, 130.30, 130.19, 128.99, 128.60, 128.42, 127.84, 124.17, 120.87, 114.18, 113.29, 55.60, 26.78, 23.07; **HRMS** (EI-TOF) *m/z*: 480.1689 (M^+); calc. for $C_{29}H_{24}N_2O_5$: 480.1685.

(*E*)-methyl

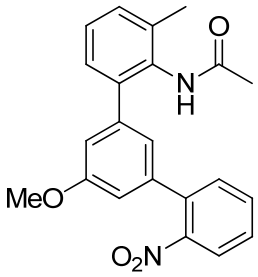
3-(2-acetamido-5'-methoxy-2''-nitro-[1,1':3',1''-terphenyl]-3-yl)acrylate (11)



The title compound **11** was prepared according to the literature.[5] To a solution of **9** (0.15 mmol)in TFA and CH_2Cl_2 (4:1, 0.5 M) were added methyl acrylate (2 equiv),

$Pd(OAc)_2$ (10 mol%), and $K_2S_2O_8$ (1 equiv). The resulting mixture was stirred at 30 °C for 48 h. After the reaction was completed, the reaction mixture was poured into water and basified with sat. $NaHCO_3$, and then the product was extracted with CH_2Cl_2 (three times), dried over $MgSO_4$, and concentrated in vacuo.A purification by preparative TLC in hexane : ethyl acetate = 1.5 : 1 gave **11** as a white solid (45% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.76 (d, *J* = 16.0 Hz, 1H), 7.70 – 7.67 (m, 1H), 7.63 (td, *J* = 7.6, 1.2 Hz, 1H), 7.51 (td, *J* = 7.6, 1.2 Hz, 1H), 7.45 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 – 7.34 (m, 2H), 6.91 – 6.84 (m, 3H), 6.80 (t, *J* = 1.2 Hz, 1H), 6.46 (d, *J* = 16.0 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 2.08 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 170.22, 167.40, 160.08, 141.15, 140.53, 140.22, 139.56, 139.11, 135.96, 133.49, 133.14, 132.68, 131.89, 131.80, 128.73, 127.67, 126.79, 124.27, 120.75, 119.82, 114.18, 113.44, 55.65, 51.90, 23.31; **HRMS** (EI-TOF) *m/z*: 446.1479 (M^+); calc. for $C_{25}H_{22}N_2O_6$: 446.1478.

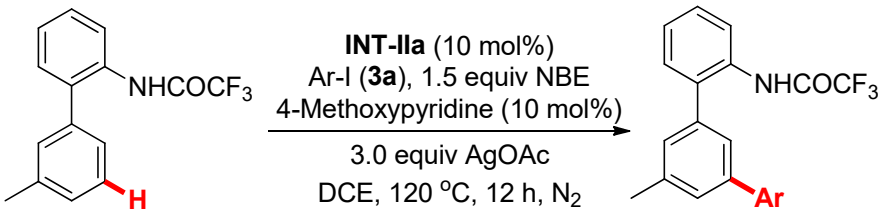
***N*-(5'-Methoxy-3-methyl-2''-nitro-[1,1':3',1''-terphenyl]-2-yl)acetamide (12)**



The title compound **12** was prepared according to the literature.[6]To a solution of **9** (0.15 mmol)in TFA and CH_2Cl_2 (4:1, 0.5 M) were added MeI (3 equiv), $Pd(OAc)_2$ (20 mol%), AgOAc (2 equiv) and $Cu(OTf)_2$ (1 equiv). The resulting mixture was stirred at 30 °C for 15 h. After the reaction was completed, the reaction mixture was poured into water and basified with sat. $NaHCO_3$, and then the product was extracted with CH_2Cl_2 (three times), dried over $MgSO_4$, and concentrated in vacuo. A purification by preparative TLC in hexane : ethyl acetate = 1.5 : 1 gave **12** as a white solid (71% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.61 (td, *J* = 7.6, 1.2 Hz, 1H), 7.49 (td, *J* = 8.0, 1.2 Hz, 1H), 7.44 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.17 (dd, *J* = 7.2, 2.0 Hz, 1H), 6.90 – 6.88 (m, 1H), 6.85 – 6.78 (m, 3H), 3.82 (s, 3H), 2.29 (s, 3H), 2.03 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.62, 159.83,

149.26, 141.53, 139.11, 138.79, 137.09, 136.13, 132.88, 132.58, 131.93, 130.56, 128.56, 127.71, 127.43, 124.17, 120.88, 114.09, 113.10, 55.56, 23.20, 18.77; **HRMS** (EI-TOF) *m/z*: 376.1420 (M^+); calc. for $C_{22}H_{20}N_2O_4$: 376.1423.

2.9 Catalytic Reactivity of Palladacycle INT-IIa.



1b **4b,** 62%

To a 50 mL Schlenk tube, **1b** (0.1 mmol), **3a** (0.3 mmol), **INT-IIa** (0.01 mmol), 4-methoxypyridine (0.01 mmol), AgOAc (0.3 mmol), Norbornene (0.15 mmol) and DCE (1.0 mL) were added. The tube was charged with N_2 and heated at 120 °C for 12 hours. After cooling to room temperature, the reaction mixture was diluted with dichloromethane and filtered through a pad of Celite and washed by dichloromethane. After concentration, the resulting residue was purified by preparative TLC to give the desired product **4b** in 62% yield.

3. References

[1] W. C. P. Tsang, N. Zheng, S. L. Buchwald, *J. Am. Chem. Soc.***2005**, *127*, 14560

[2] X.-F. Wu, H. Neumann, M. Beller,*Chem. Commun.* **2011**, *47*, 7959.

[3] C. Tang, N. Jiao, *J. Am. Chem. Soc.* **2012**, *134*, 18924.

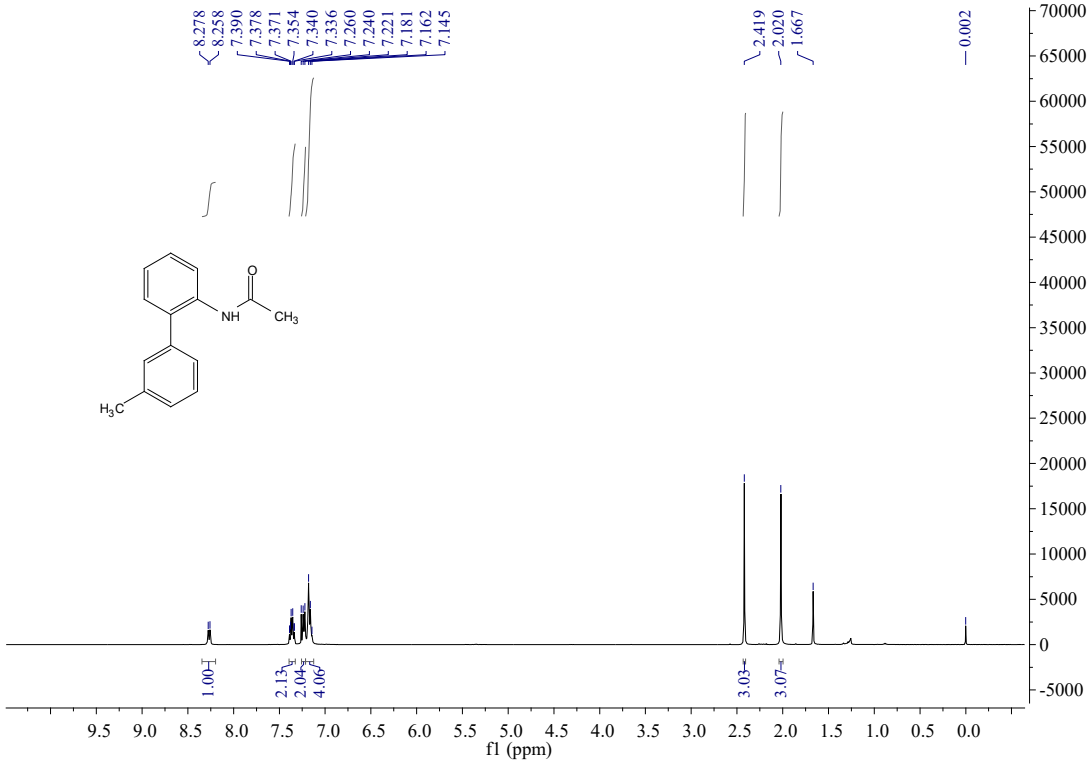
[4] O. Daugulis, V. G. Zaitsev, *Angew. Chem. Int. Ed.* **2005**, *44*, 4046.

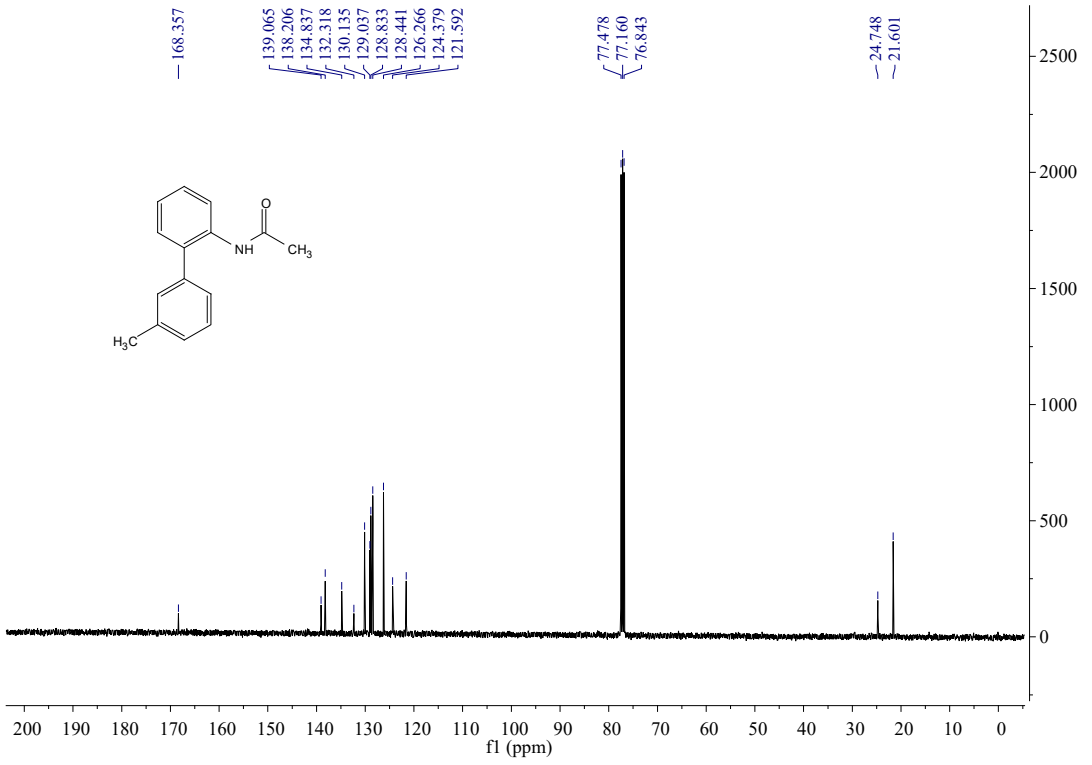
[5] B. S. Kim, C. Jang, D. J. Lee, S. W. Youn, *Chem. Asian J.***2010**, *5*, 2336.

[6] M. Jung, S. W. Youn, *Bull. Korean Chem. Soc.***2011**, *32*, 2865

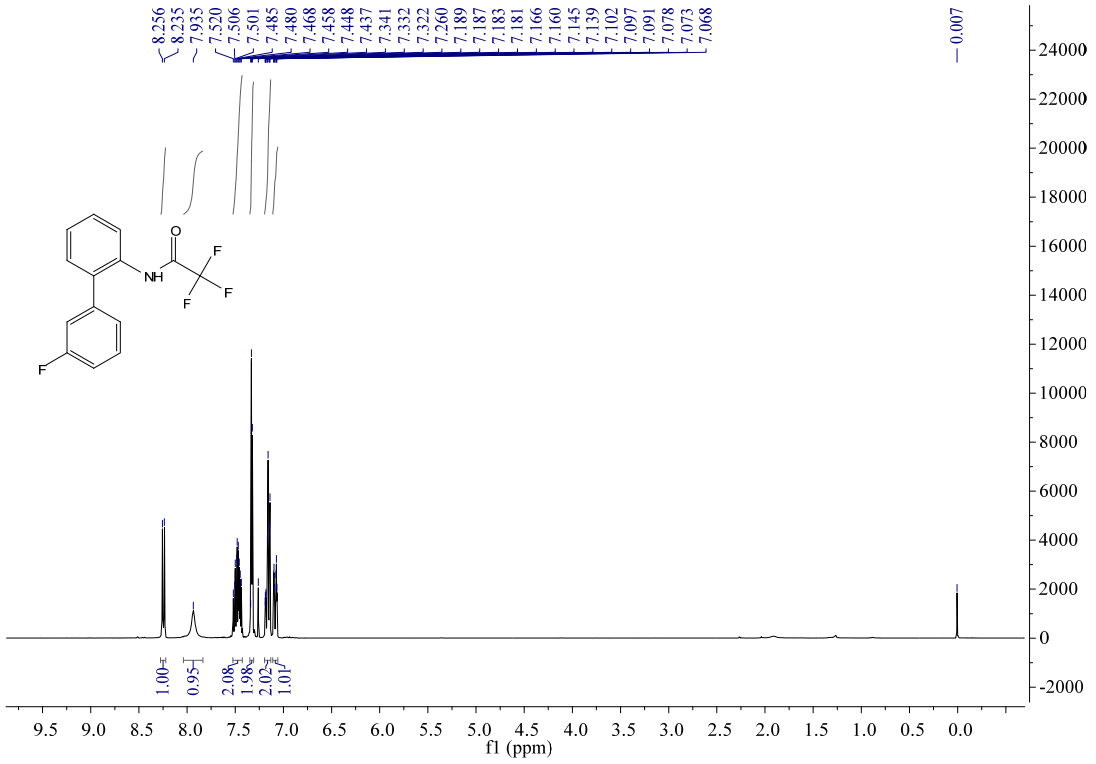
4. NMR Spectra

1aa





1a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7.332
7.322
7.260
7.189
7.187
7.183
7.181
7.166
7.160
7.145
7.139
7.102
7.097
7.091
7.078
7.073
7.068
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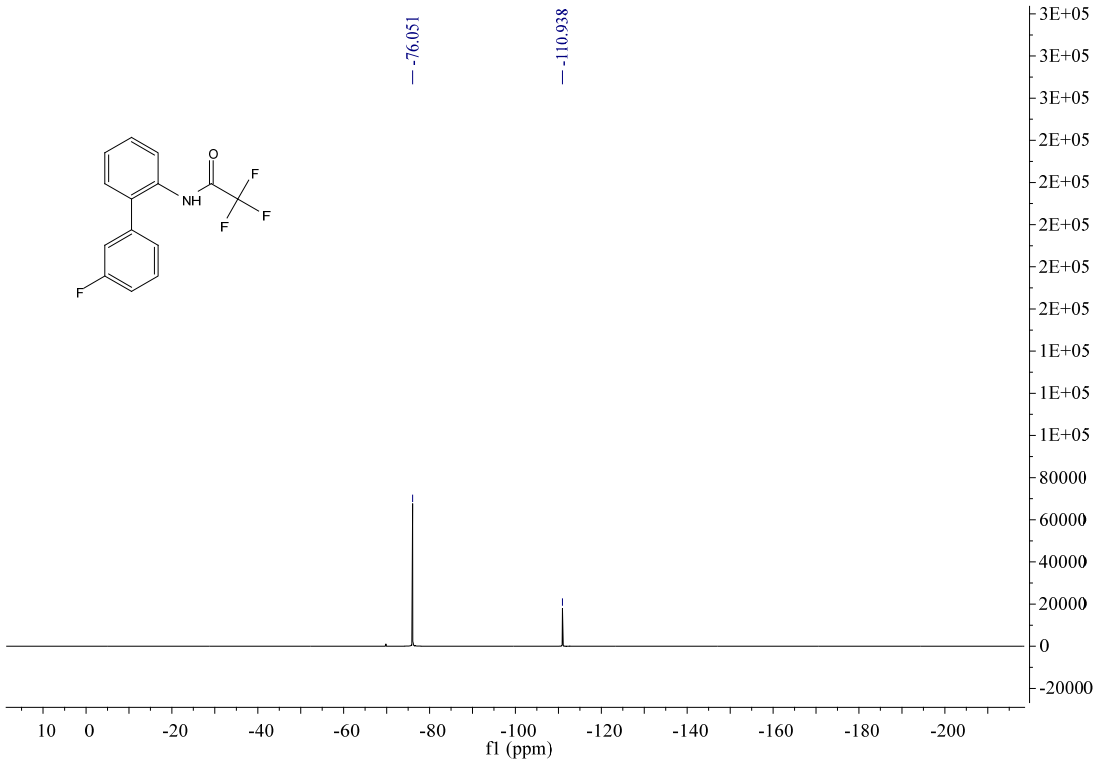
1.00
0.95
2.08
1.98
2.02
1.01
fl (ppm)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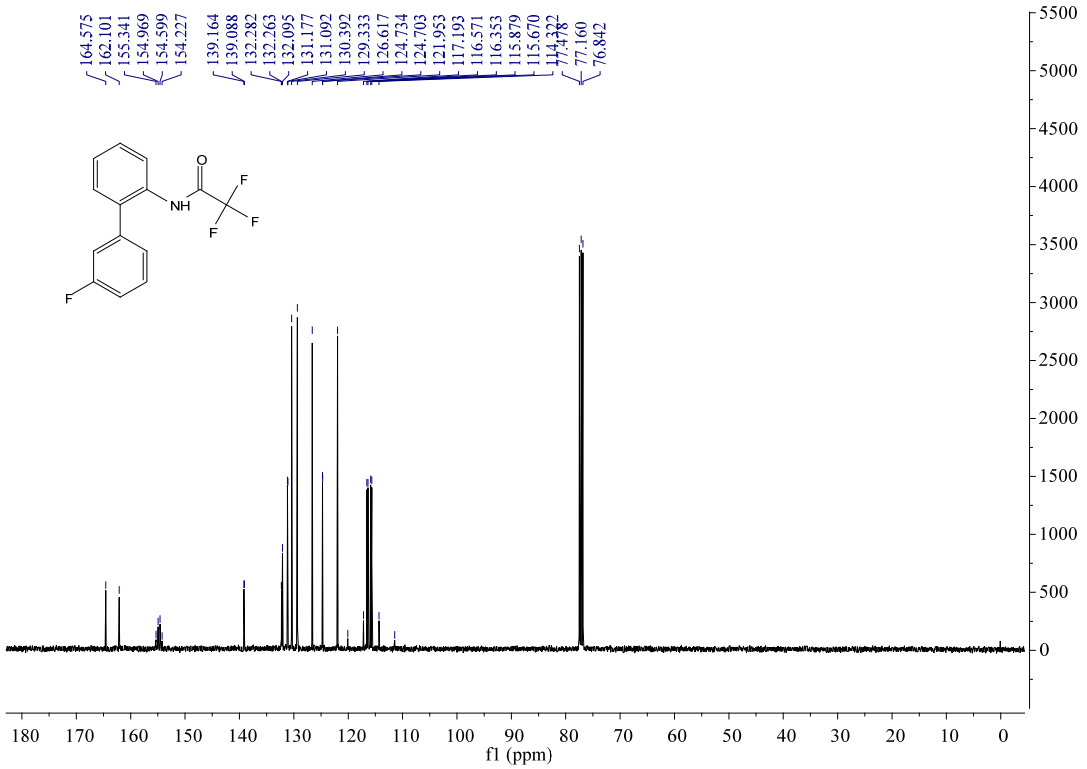
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132.263
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131.092
130.392
129.333
126.617
124.734
124.703
121.953
117.193
116.571
116.353
115.879
115.670
114.322
77.478
77.160
76.842
O
NH
F
F
F
F
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
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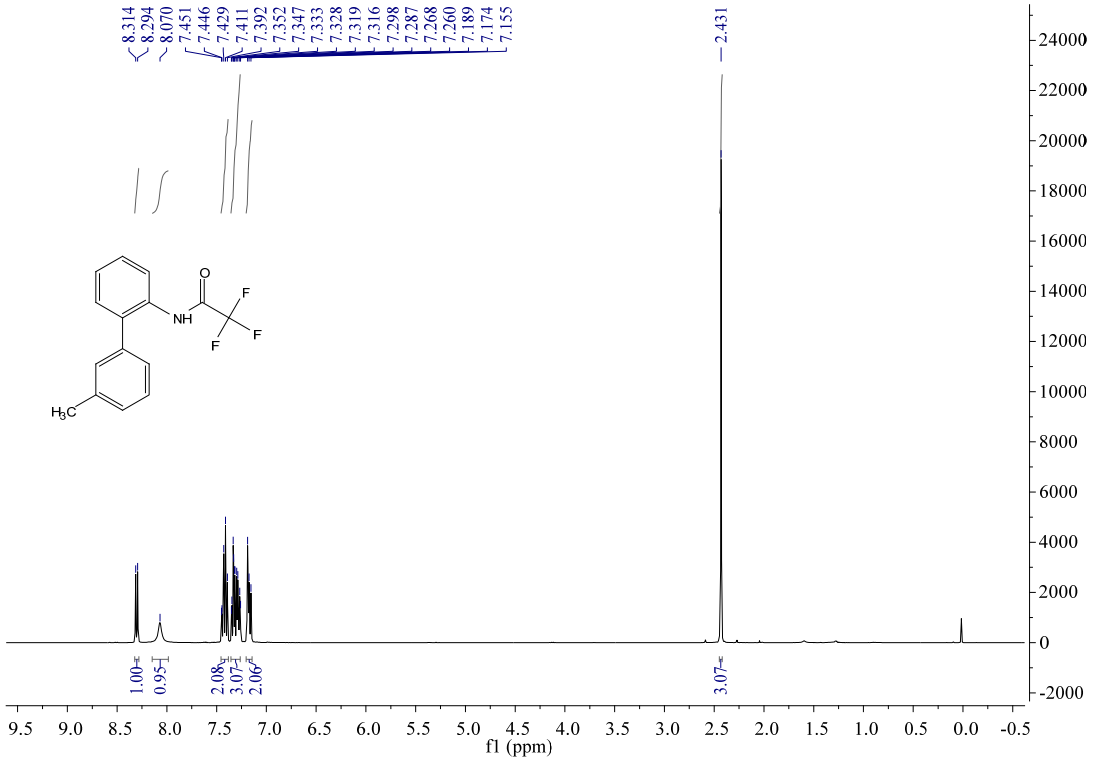
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1b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7.316
7.298
7.287
7.268
7.260
7.189
7.174
7.155
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F
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H3C
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3.07
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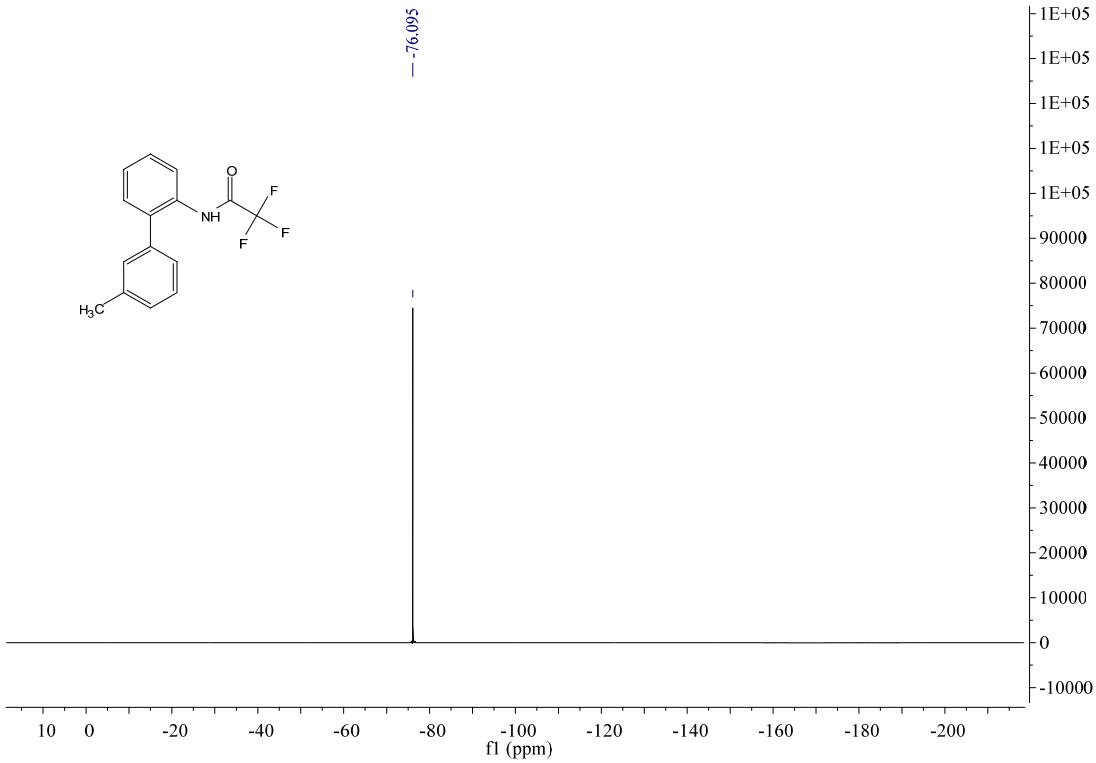
3.07
f1 (ppm)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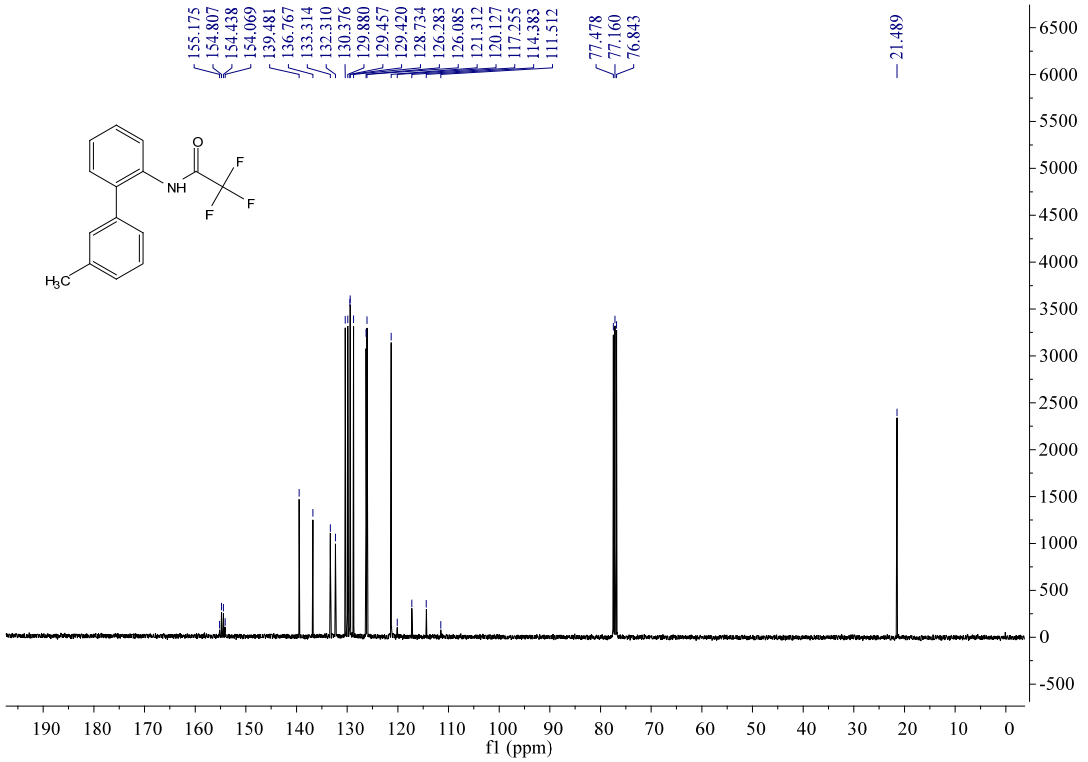
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121.312
120.127
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114.383
111.512
77.478
77.160
76.843
21.489
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NH
F
F
F
H3C
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5500
5000
4500
4000
3500
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1500
1000
500
0
-500
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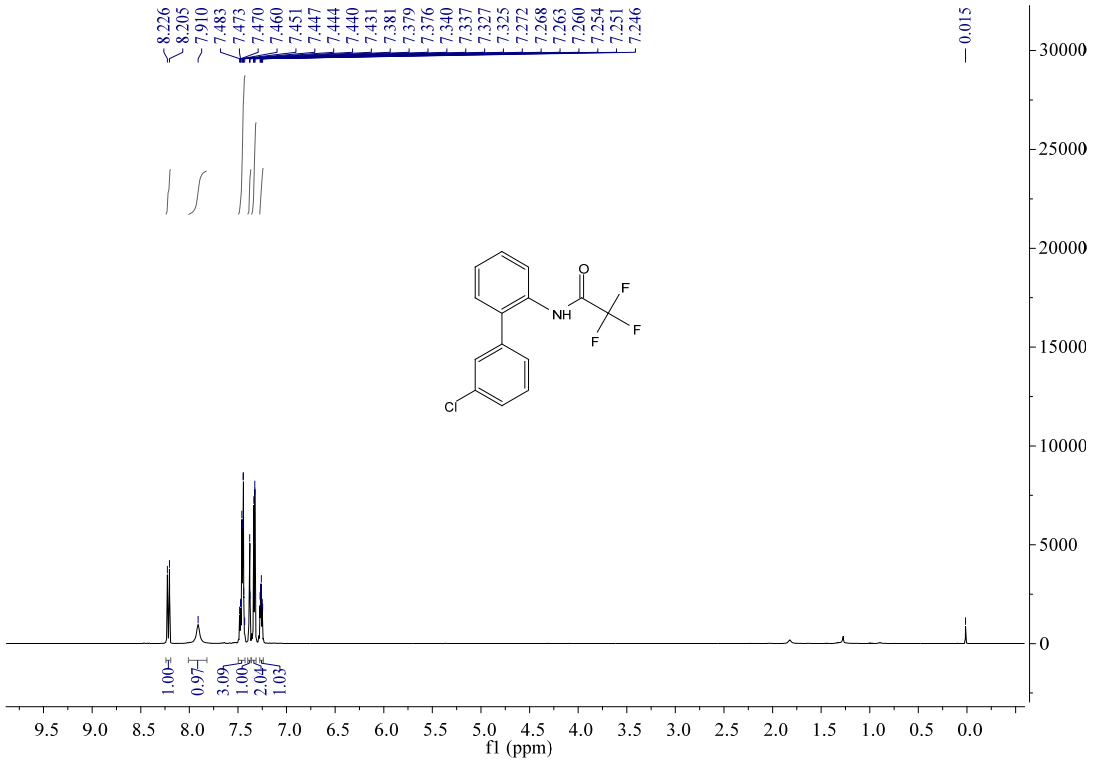
f1 (ppm)

1c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7.379
7.376
7.340
7.337
7.327
7.325
7.272
7.268
7.263
7.260
7.254
7.251
7.246
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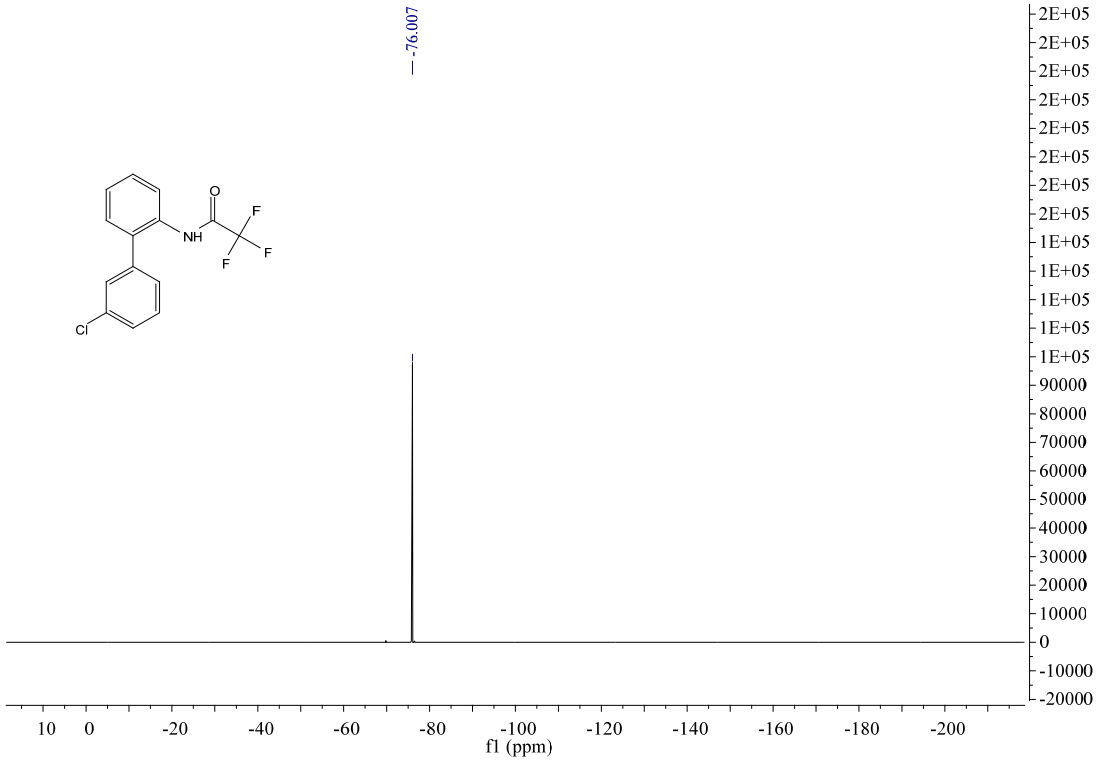
F
F
Cl
f1 (ppm)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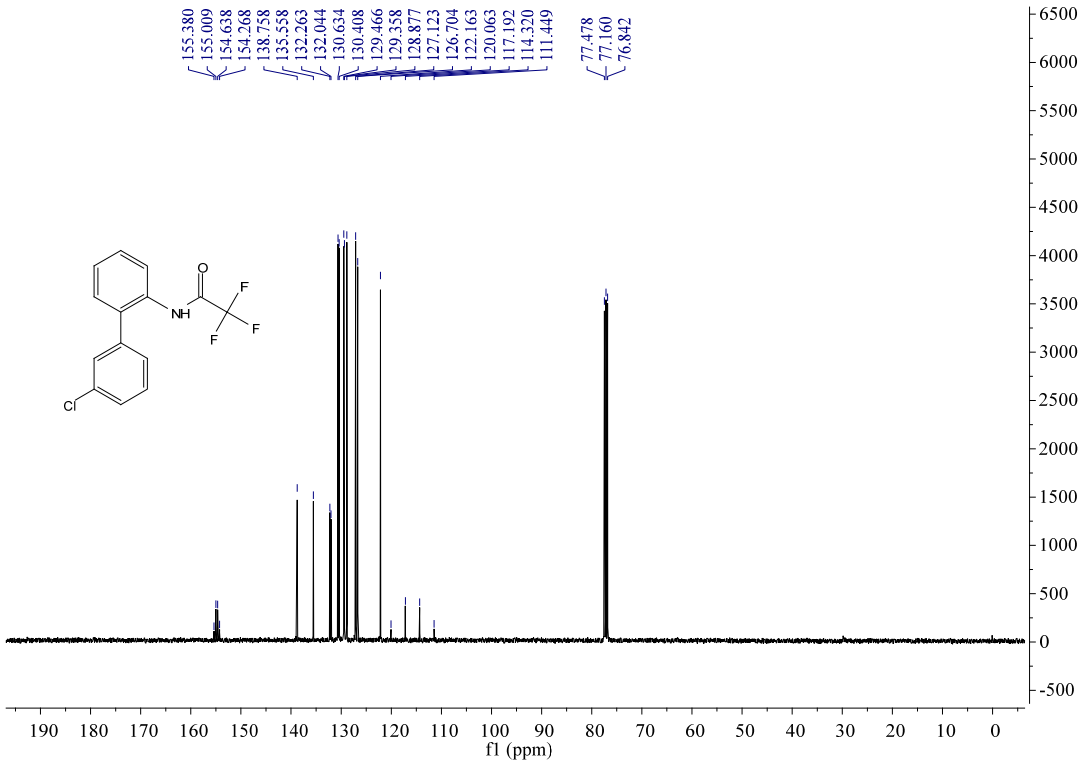
Cl
f1 (ppm)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F
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Cl
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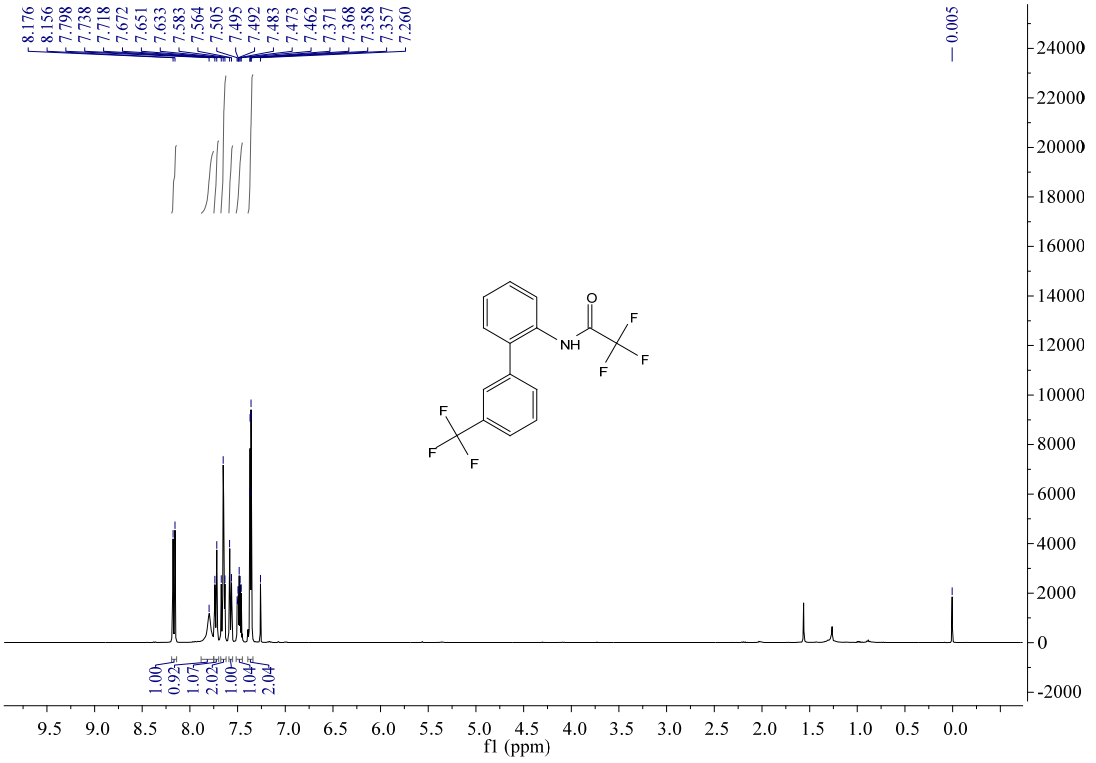
f1 (ppm)

1d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7.495
7.492
7.483
7.473
7.462
7.371
7.368
7.358
7.357
7.260
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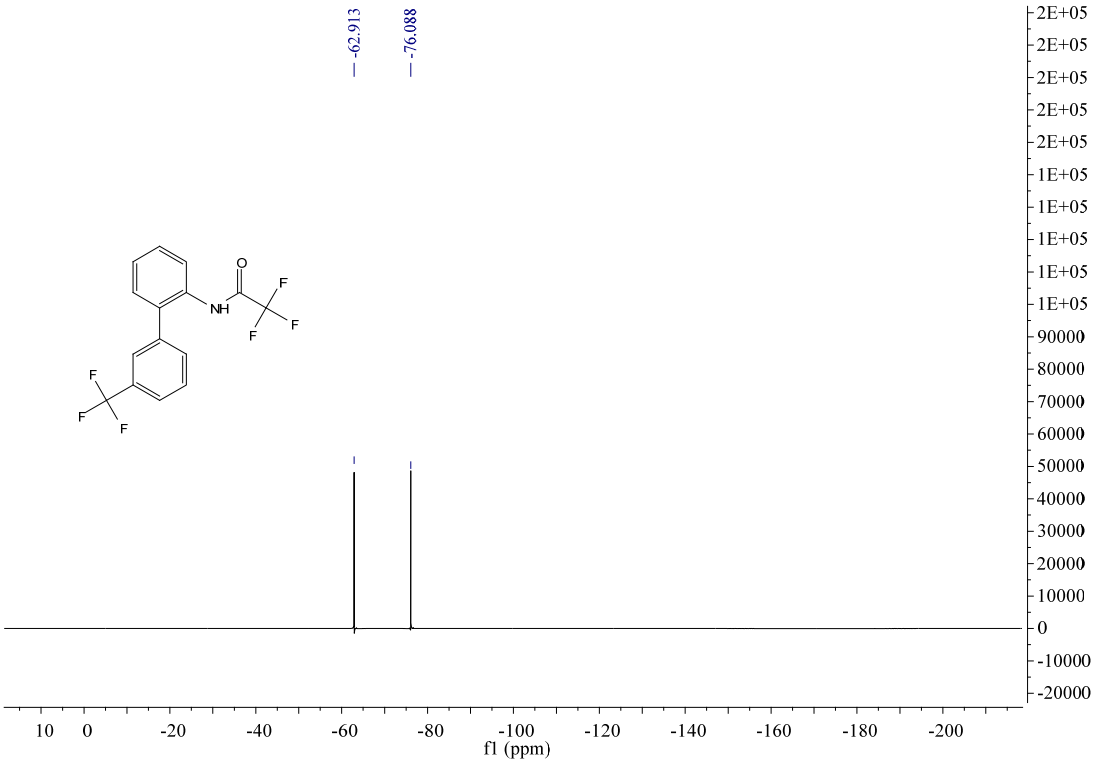
F
F
F
f1 (ppm)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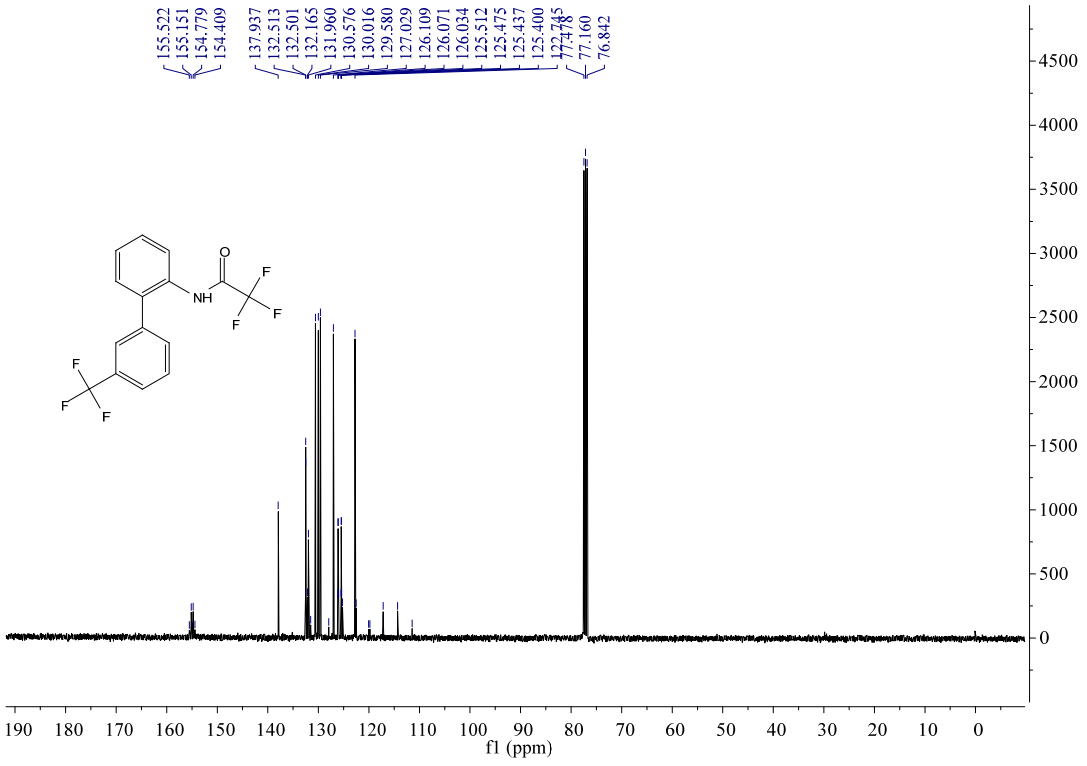
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F
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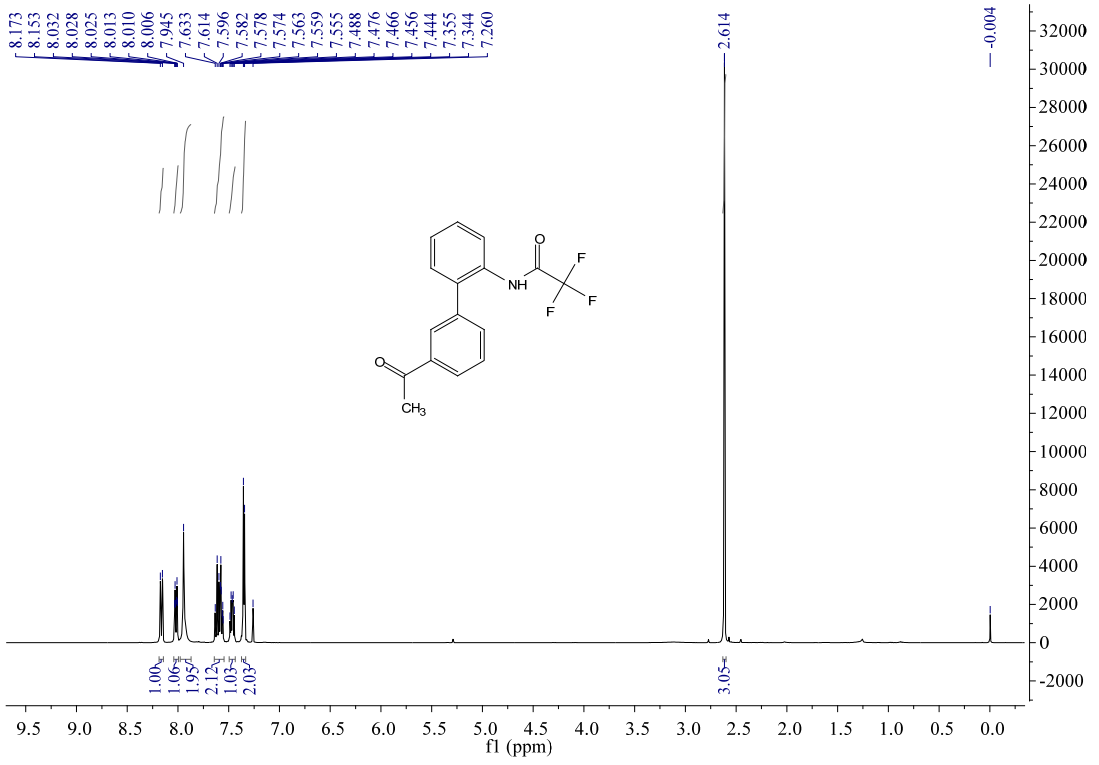
f1 (ppm)

1e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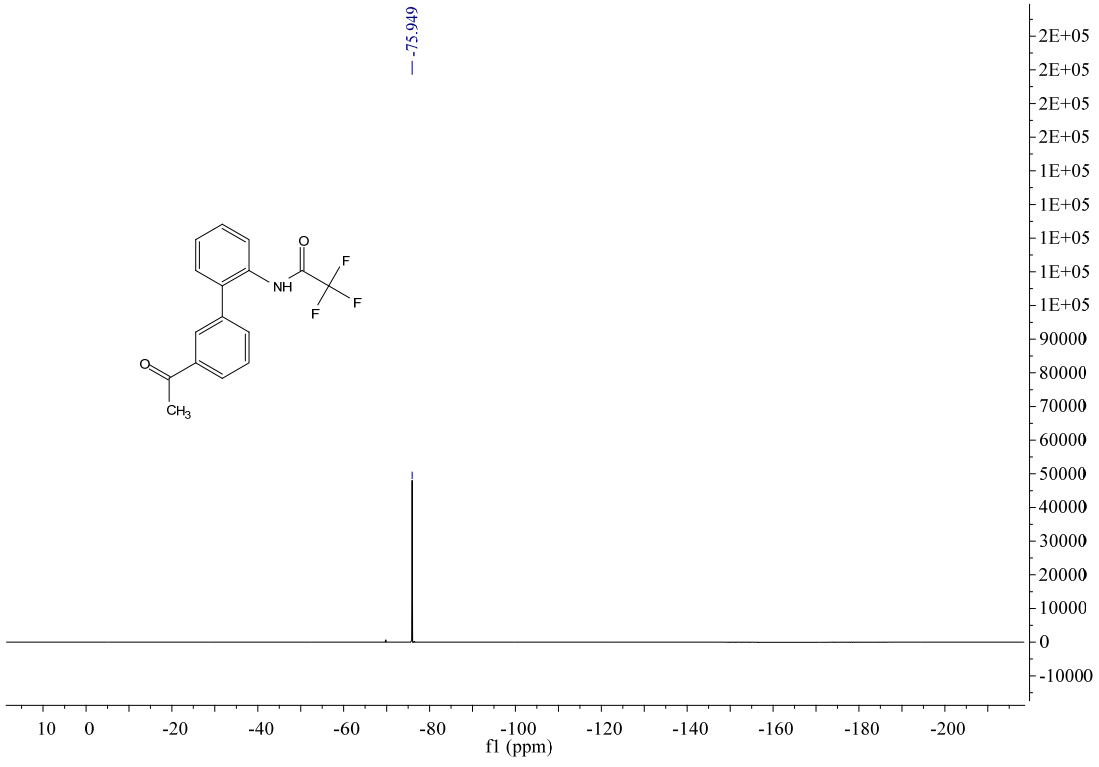
f1 (ppm)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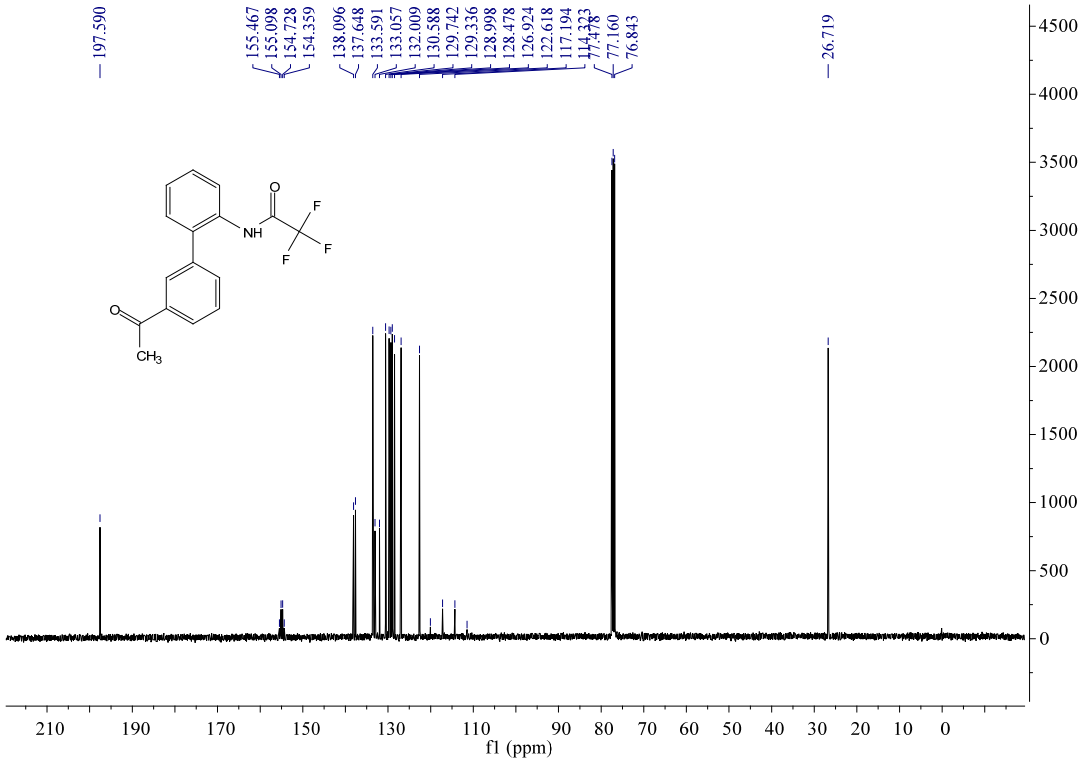
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F
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CH3
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4000
3500
3000
2500
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500
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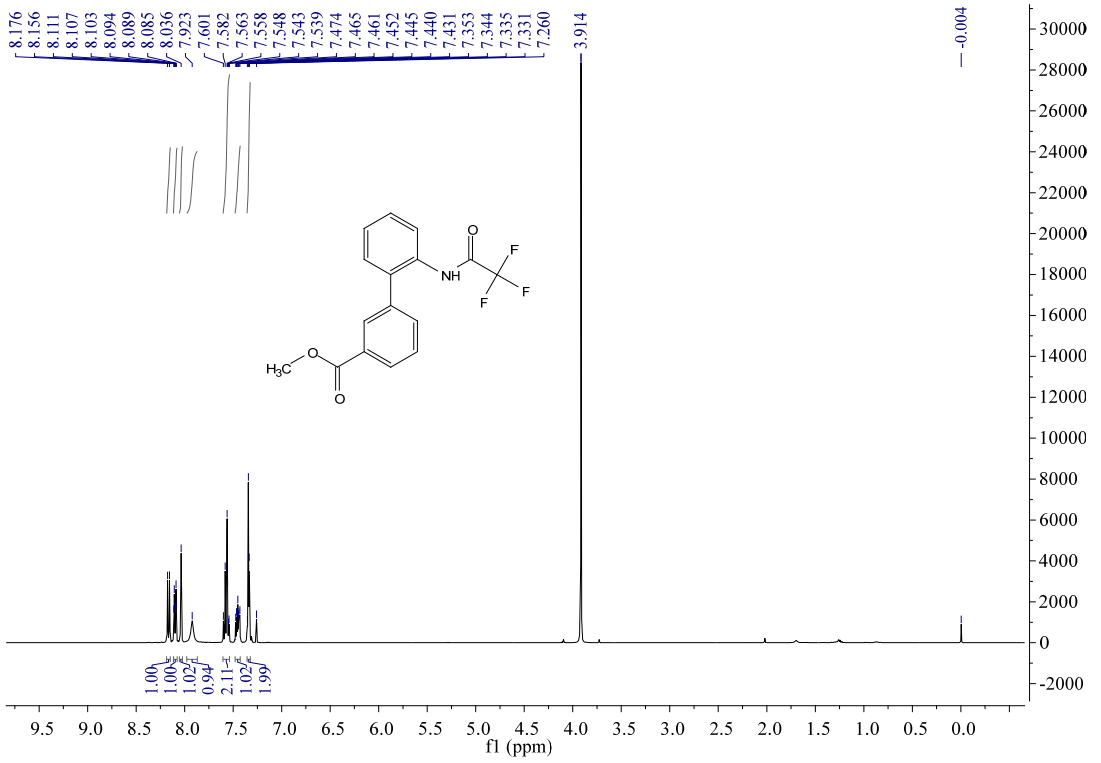
30
20
10
0
f1 (ppm)

1f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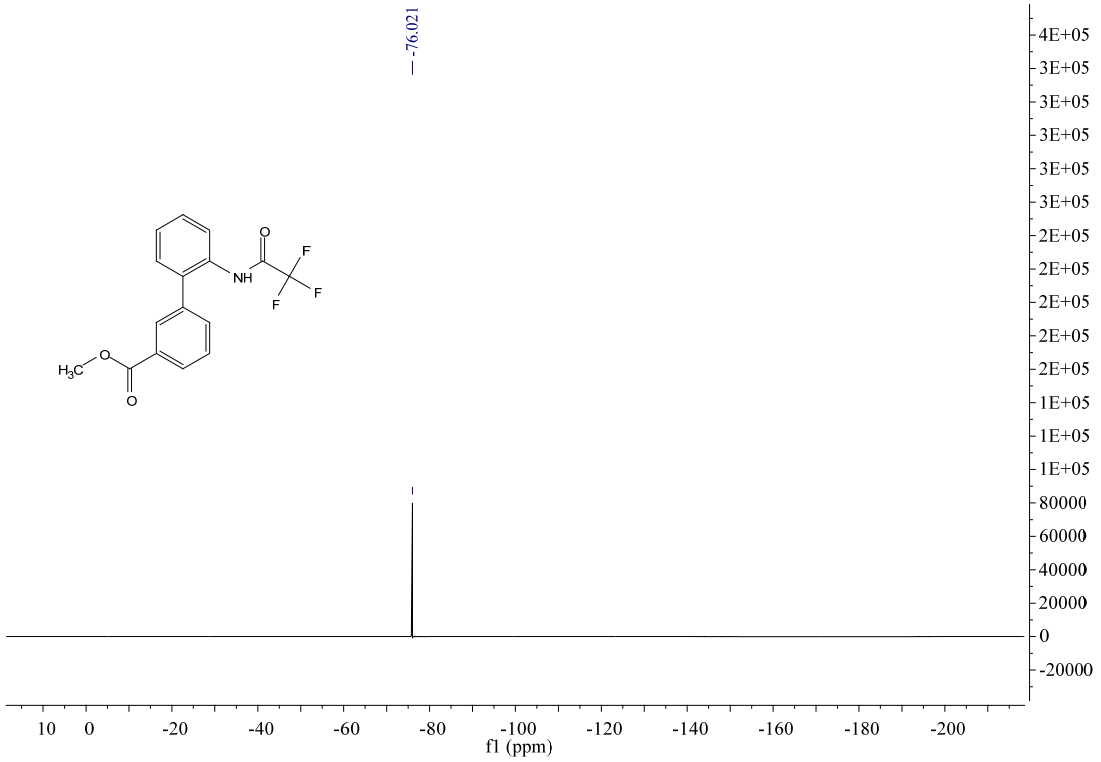
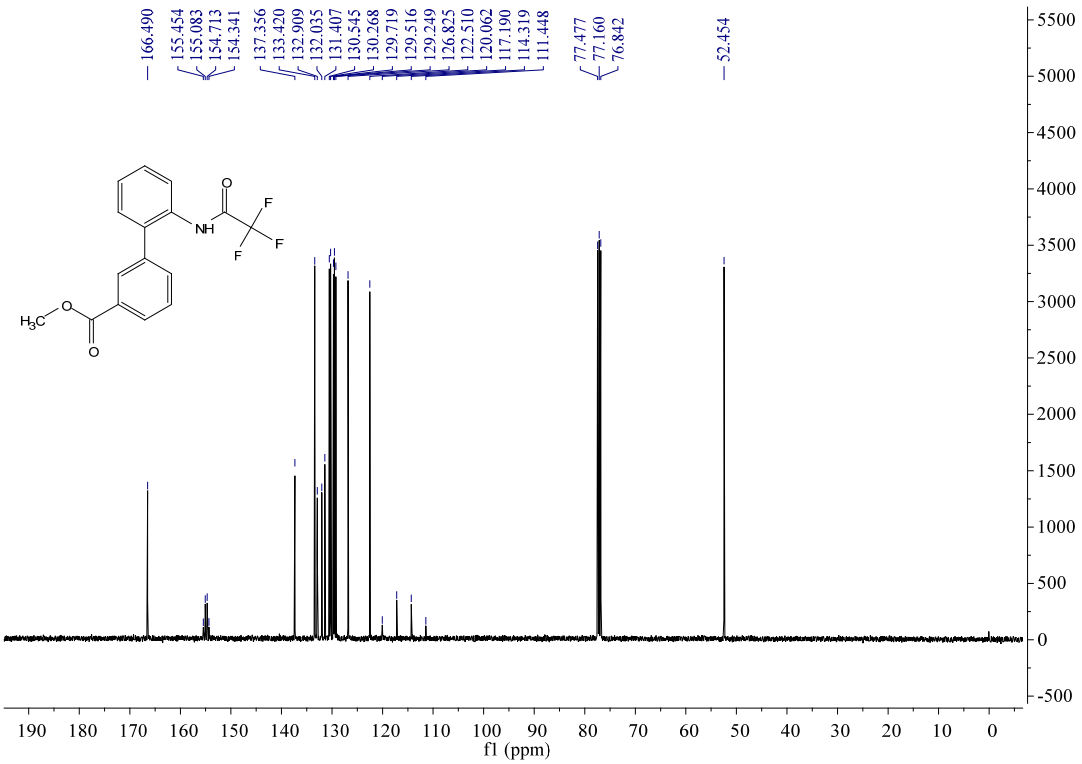
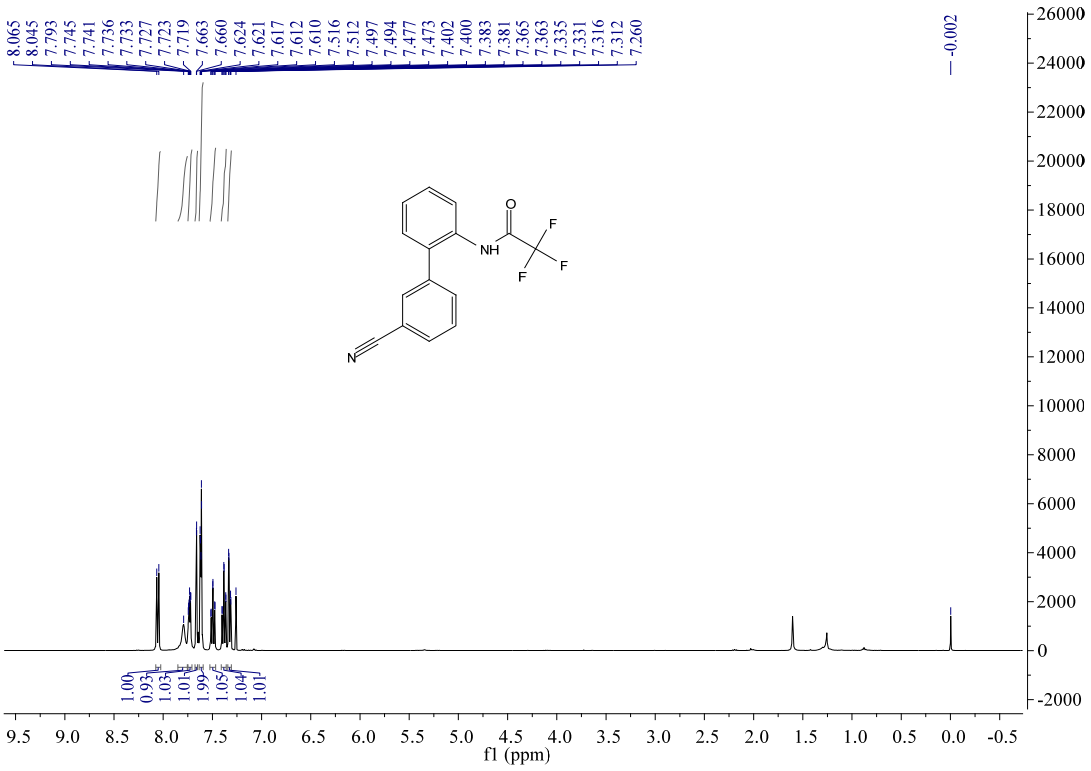
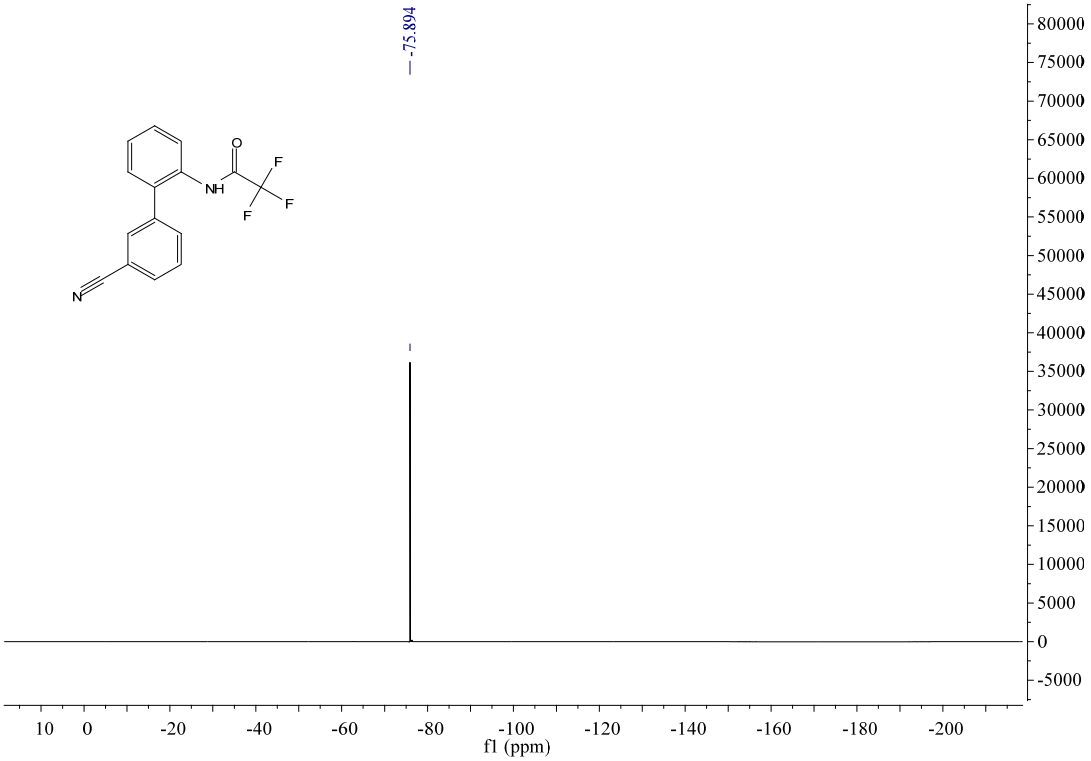
1.99
fl (ppm)

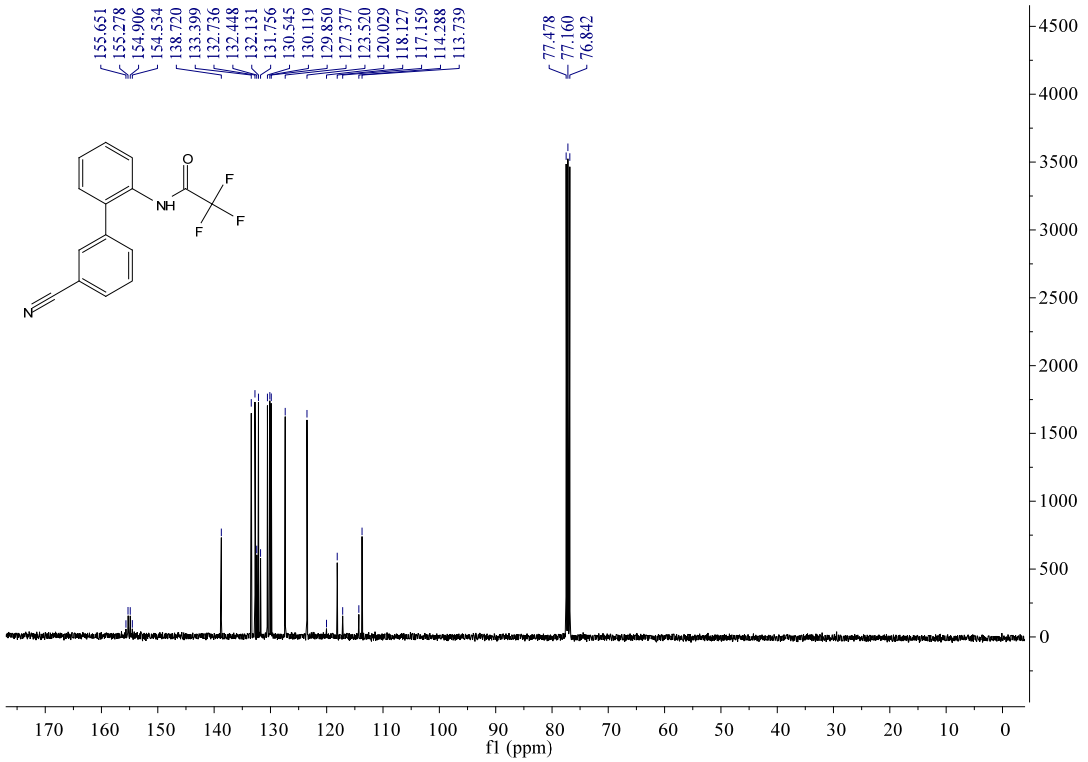

-76.021
NH
O
F
F
F
H3C
O
O
fl (ppm)


166.490
155.454
155.083
154.713
154.341
137.356
133.420
132.909
132.035
131.407
130.545
130.268
129.719
129.516
129.249
126.825
122.510
120.062
117.190
114.319
111.448
77.477
77.160
76.842
52.454
NH
O
F
F
F
H3C
O
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

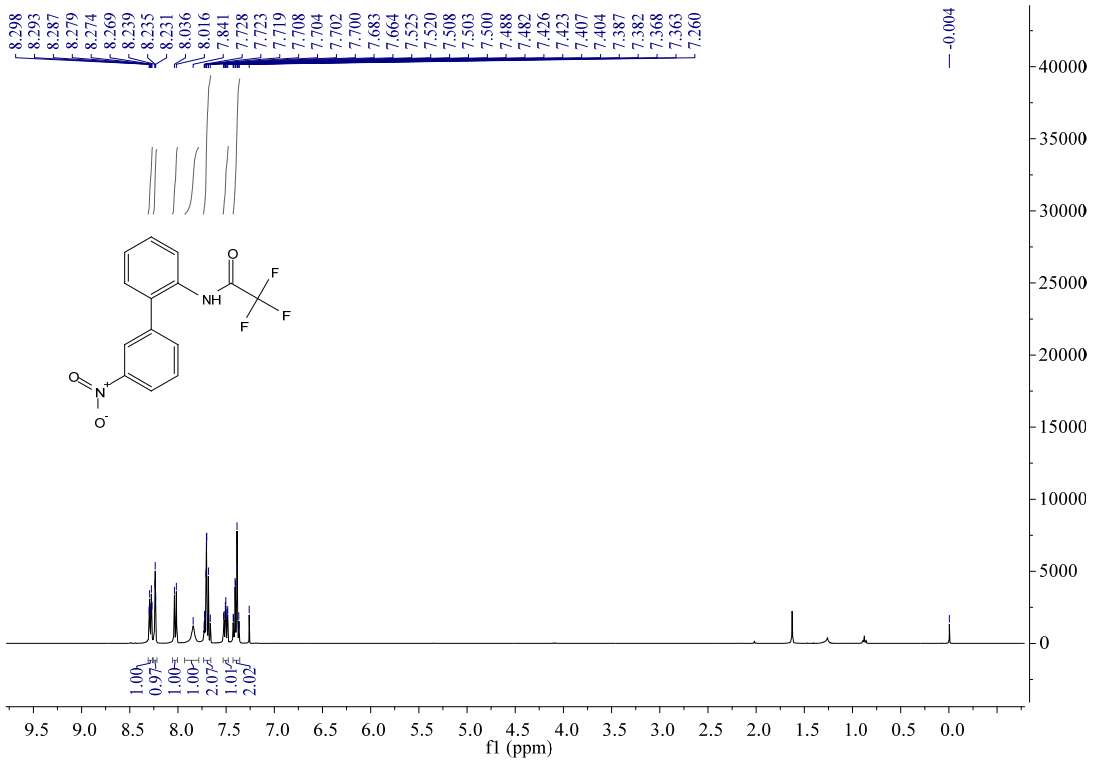
1g

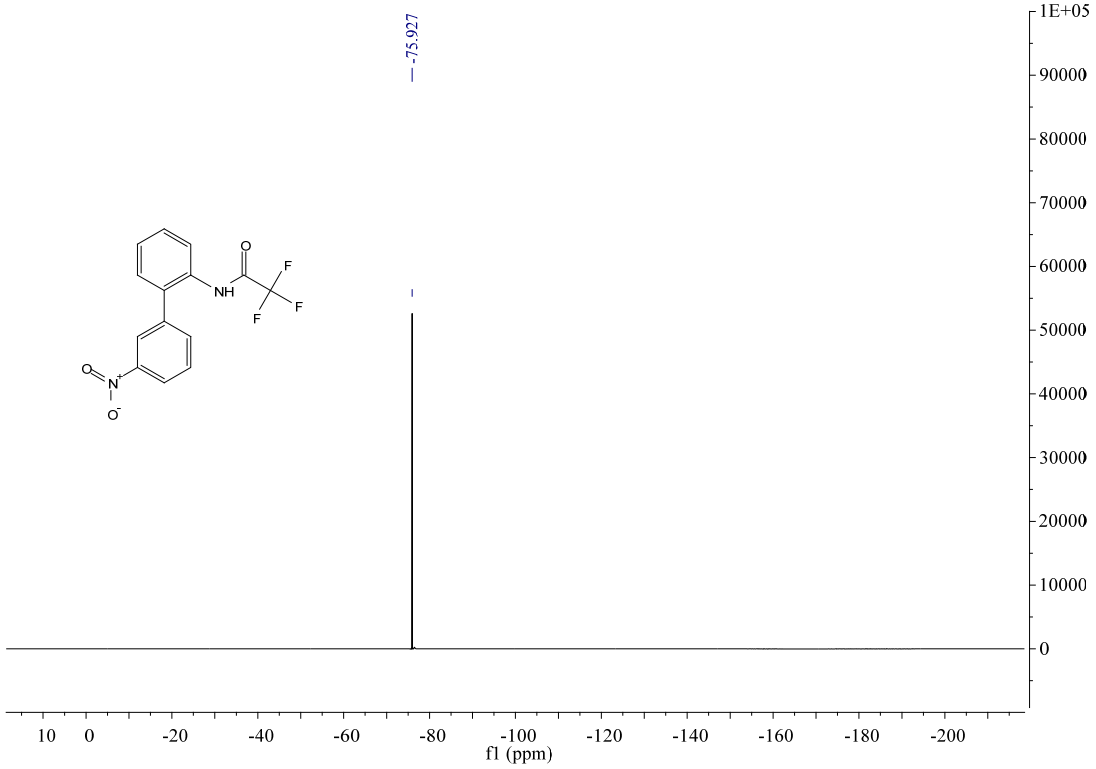

8.065
8.045
7.793
7.745
7.741
7.736
7.733
7.727
7.723
7.719
7.663
7.660
7.624
7.621
7.617
7.612
7.610
7.516
7.512
7.497
7.494
7.477
7.473
7.402
7.400
7.383
7.381
7.365
7.363
7.335
7.331
7.316
7.312
7.260
-0.002
O
NH
F
F
F
N
1.00
0.93
1.03
1.01
1.99
1.05
1.04
1.01
f1 (ppm)

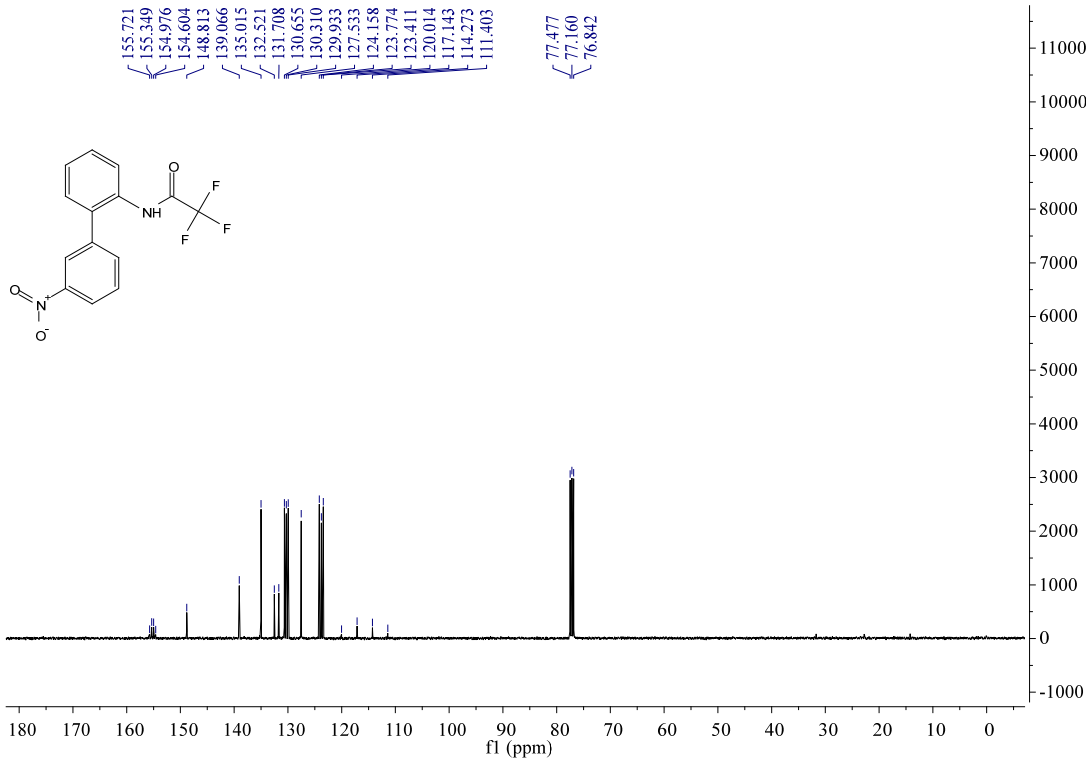

-75.894
O
NH
F
F
F
N
f1 (ppm)


155.651
155.278
154.906
154.534
138.720
133.399
132.736
132.448
132.131
131.756
130.545
130.119
129.850
127.377
123.520
120.029
118.127
117.159
114.288
113.739
77.478
77.160
76.842
O
NH
F
F
F
N
4500
4000
3500
3000
2500
2000
1500
1000
500
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

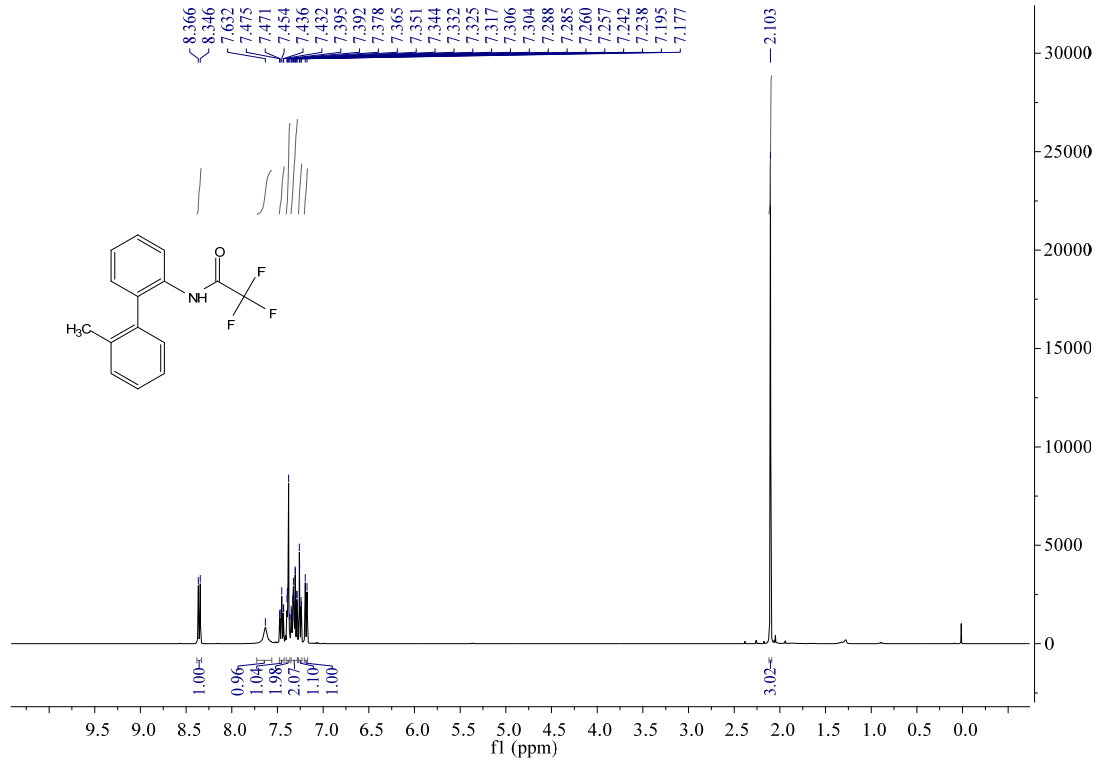
1h

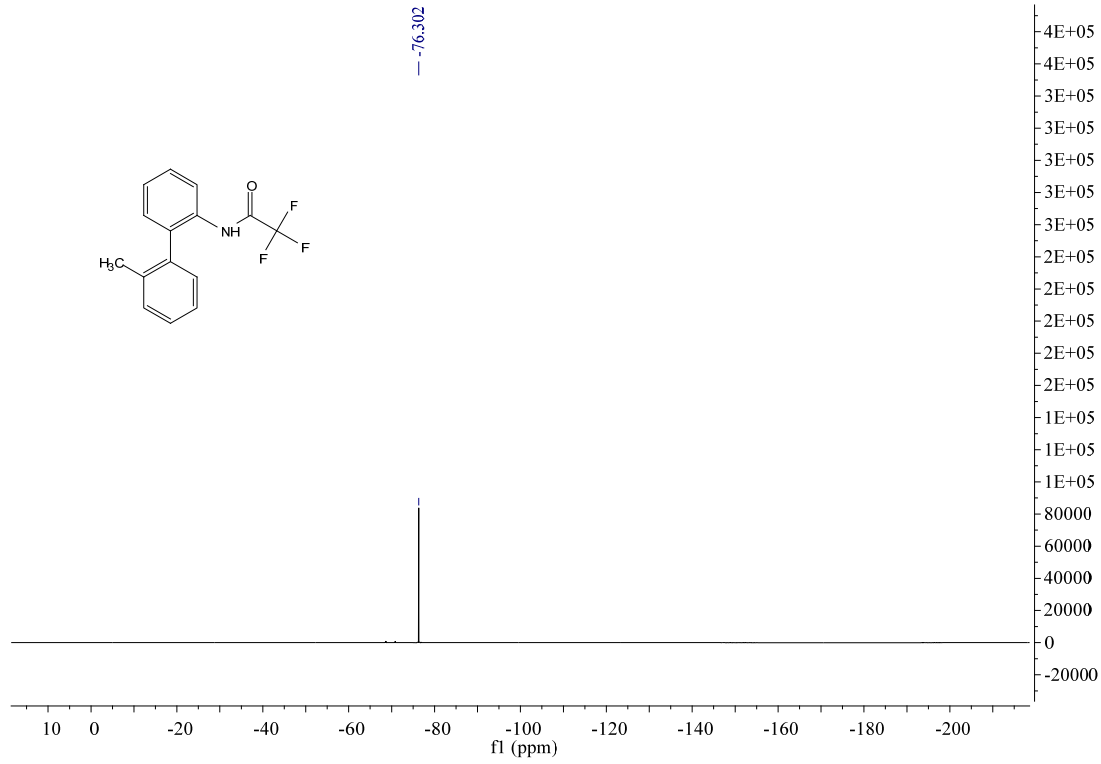

8.298
8.293
8.287
8.279
8.274
8.269
8.239
8.235
8.231
8.036
8.016
7.841
7.728
7.723
7.719
7.708
7.704
7.702
7.700
7.683
7.664
7.525
7.520
7.508
7.503
7.500
7.488
7.482
7.426
7.423
7.407
7.404
7.387
7.382
7.368
7.363
7.260
-0.004
NH
O
F
F
F
N+
O-
1.00
0.97
1.00
1.00
2.07
1.01
2.02
f1 (ppm)

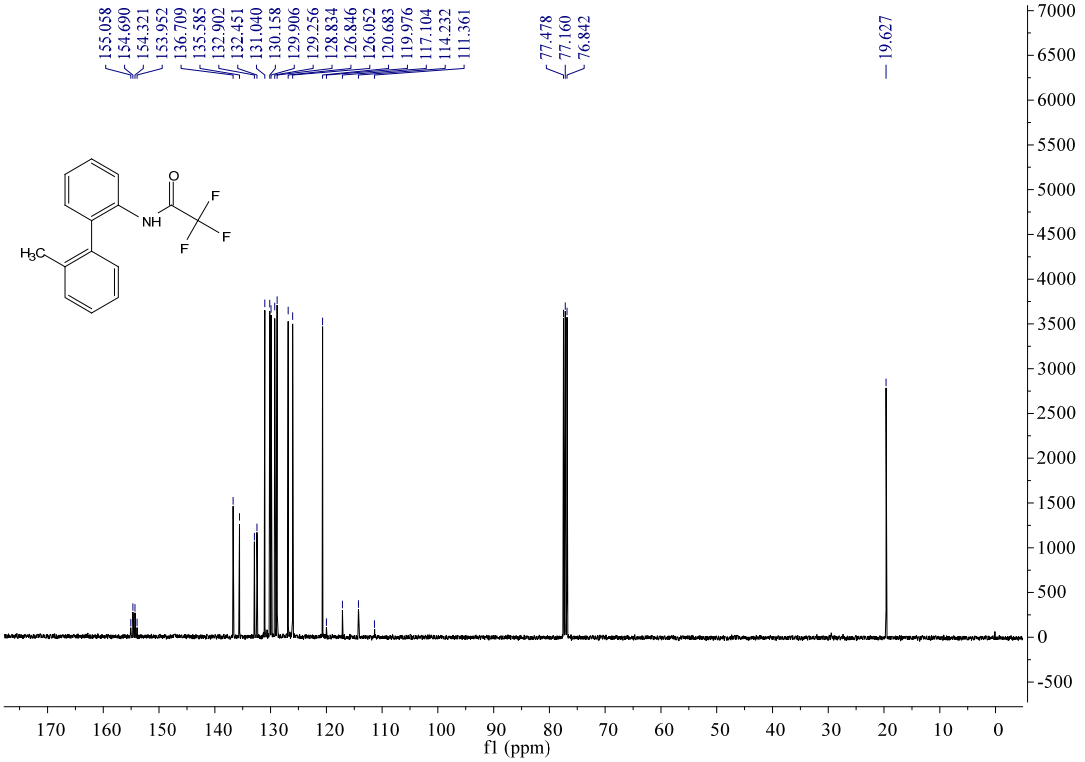

-75.927
NH
O
F
F
F
N+
O-
f1 (ppm)


155.721
155.349
154.976
154.604
148.813
139.066
135.015
132.521
131.708
130.655
130.310
129.933
127.533
124.158
123.774
123.411
120.014
117.143
114.273
111.403
77.477
77.160
76.842
O
NH
F
F
F
O
N+
O-
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

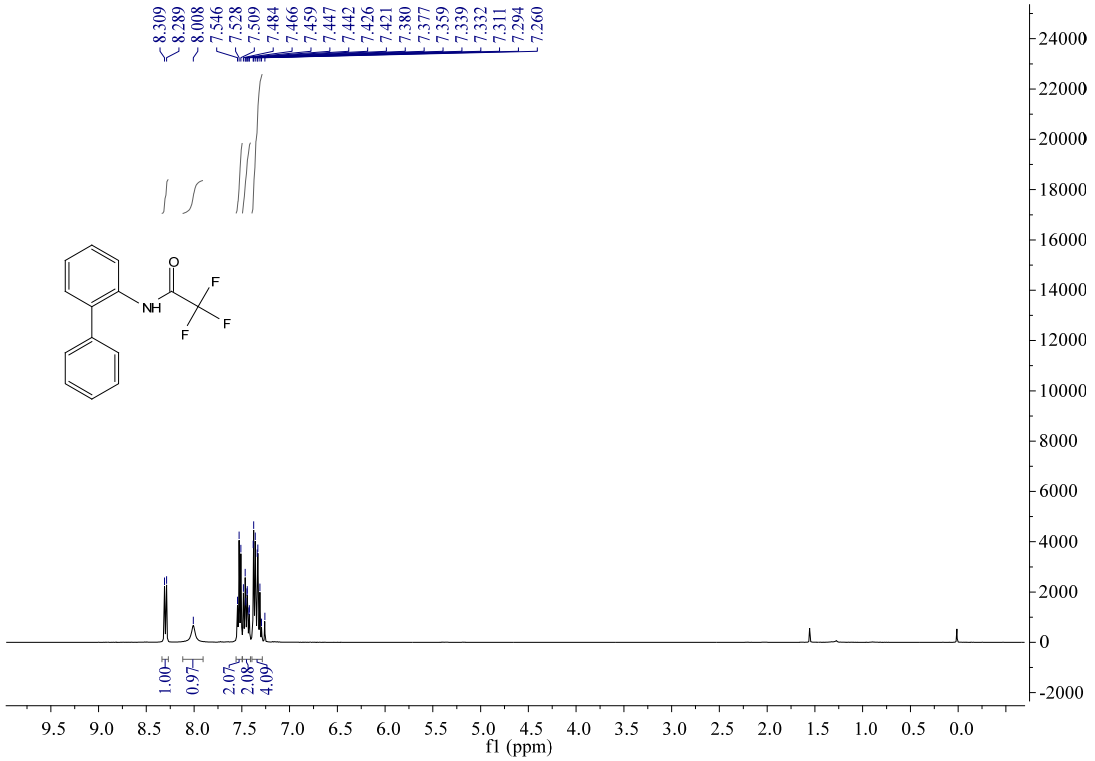
1i

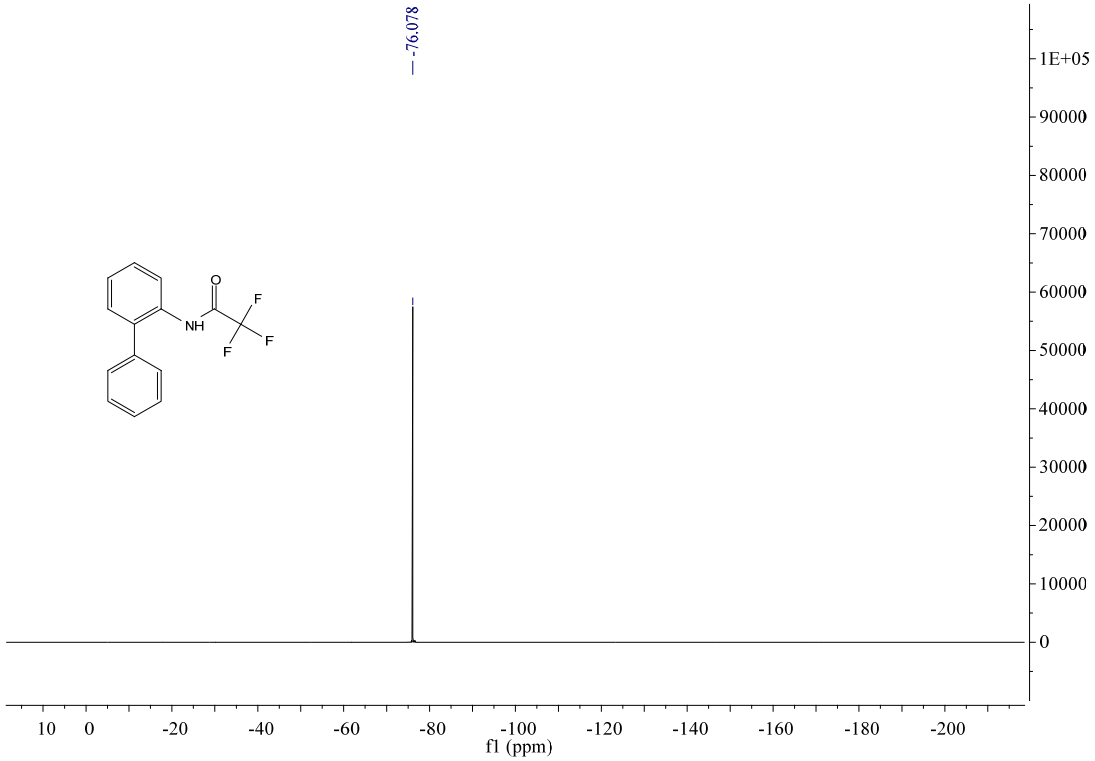

8.366
8.346
7.632
7.475
7.471
7.454
7.436
7.432
7.395
7.392
7.378
7.365
7.351
7.344
7.332
7.325
7.317
7.306
7.304
7.288
7.285
7.260
7.257
7.242
7.238
7.195
7.177
2.103
O
NH
F
F
F
H3C
1.00
0.96
1.04
1.98
2.07
1.10
1.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
30000
25000
20000
15000
10000
5000
0

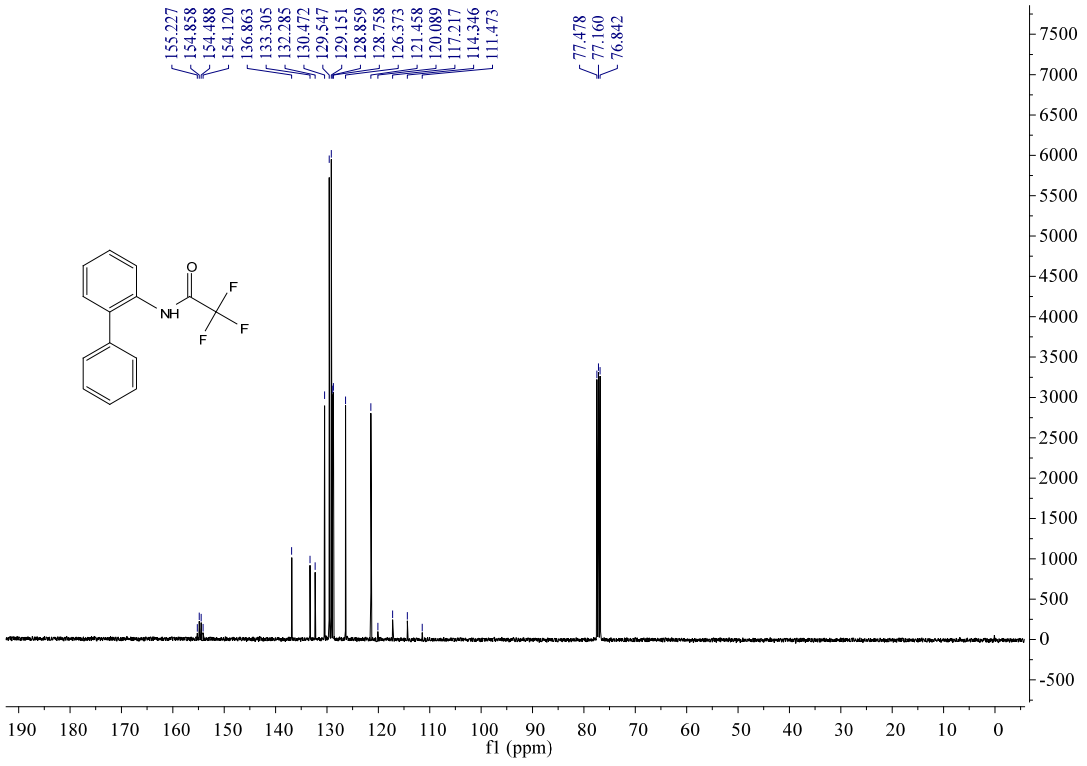

-76.302
O
NH
F
F
F
H3C
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)
4E+05
4E+05
3E+05
3E+05
3E+05
3E+05
3E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
80000
60000
40000
20000
0
-20000


155.058
154.690
154.321
153.952
136.709
135.585
132.902
132.451
131.040
130.158
129.906
129.256
128.834
126.846
126.052
120.683
119.976
117.104
114.232
111.361
77.478
77.160
76.842
19.627
O
NH
F
F
F
H3C
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

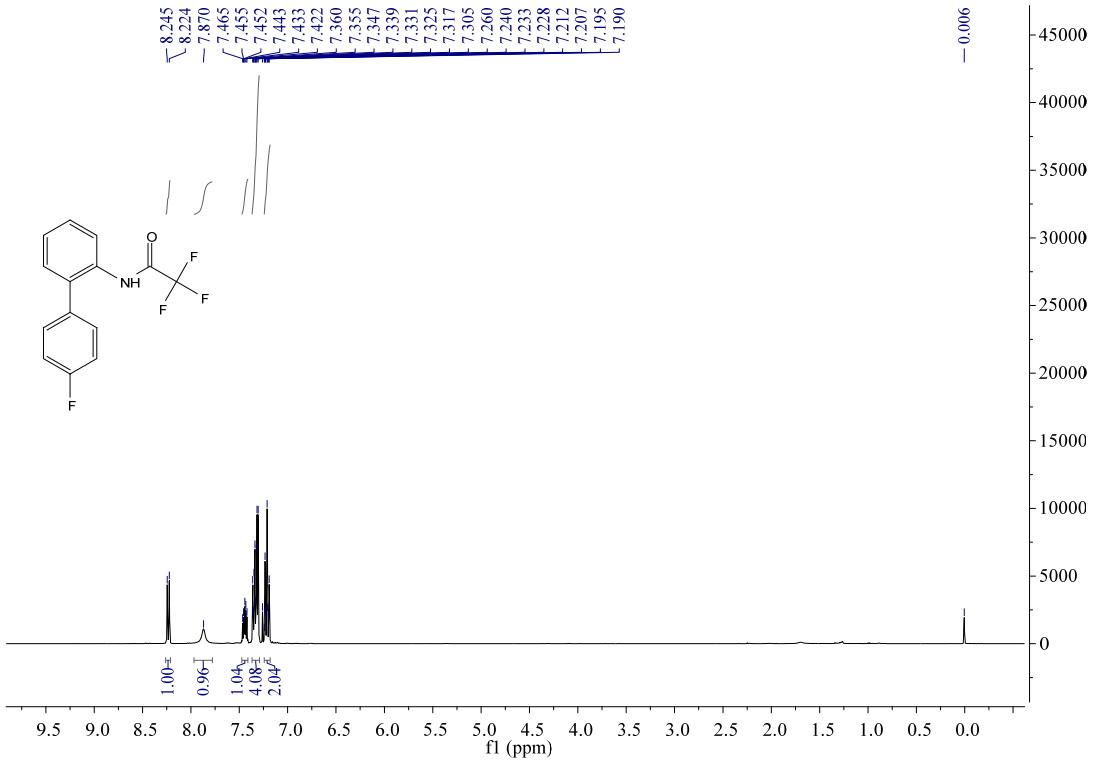
1j

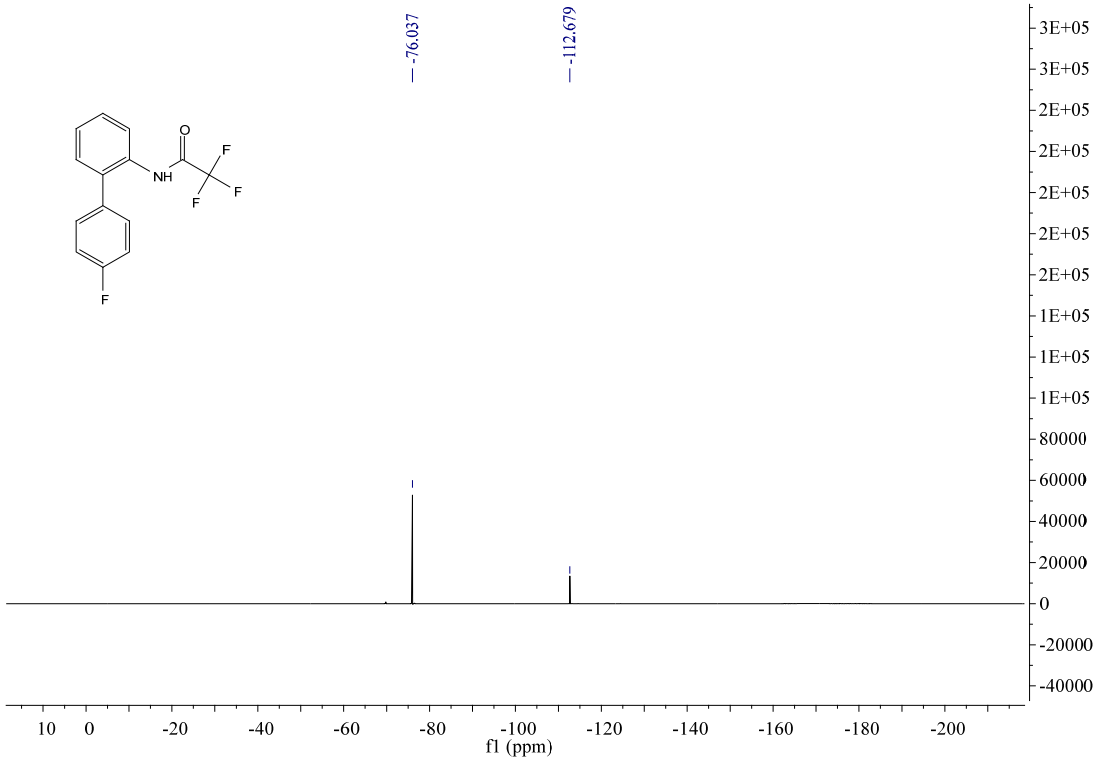

8.309
8.289
8.008
7.546
7.528
7.509
7.484
7.466
7.459
7.447
7.442
7.426
7.421
7.380
7.377
7.359
7.339
7.332
7.311
7.294
7.260
NH
O
F
F
F
1.00
0.97
2.07
2.08
4.09
f1 (ppm)

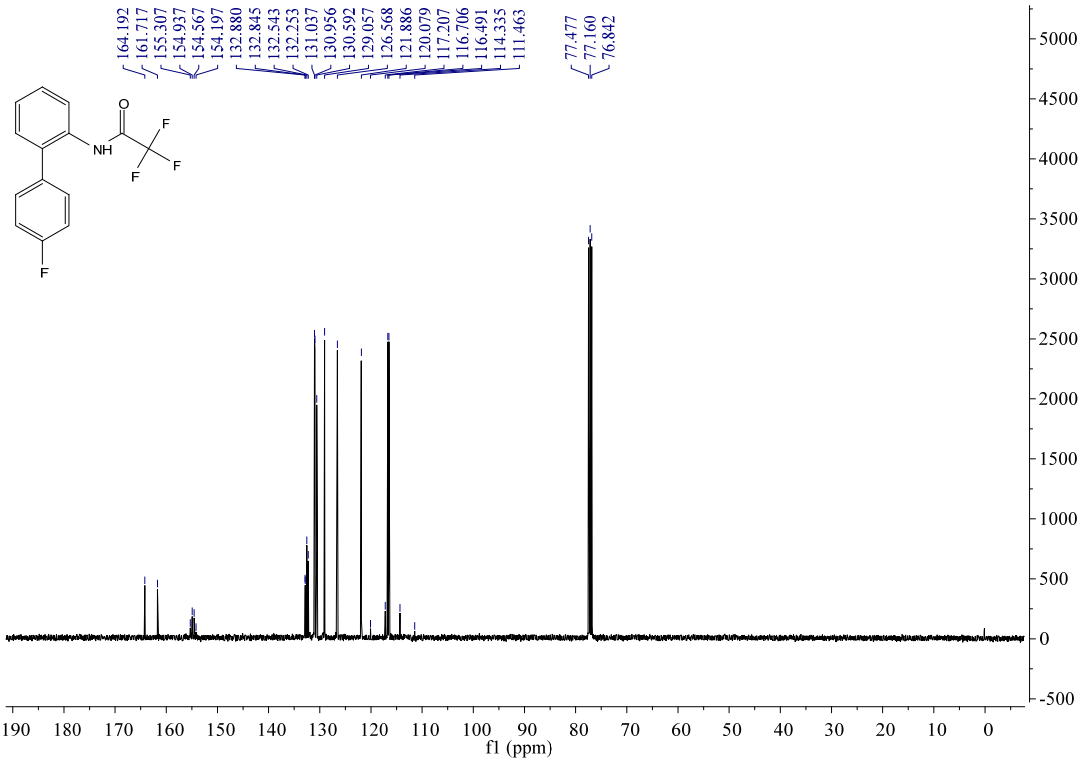

-76.078
NH
O
F
F
F
f1 (ppm)


155.227
154.858
154.488
154.120
136.863
133.305
132.285
130.472
129.547
129.151
128.859
128.758
126.373
121.458
120.089
117.217
114.346
111.473
77.478
77.160
76.842
O
NH
F
F
F
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

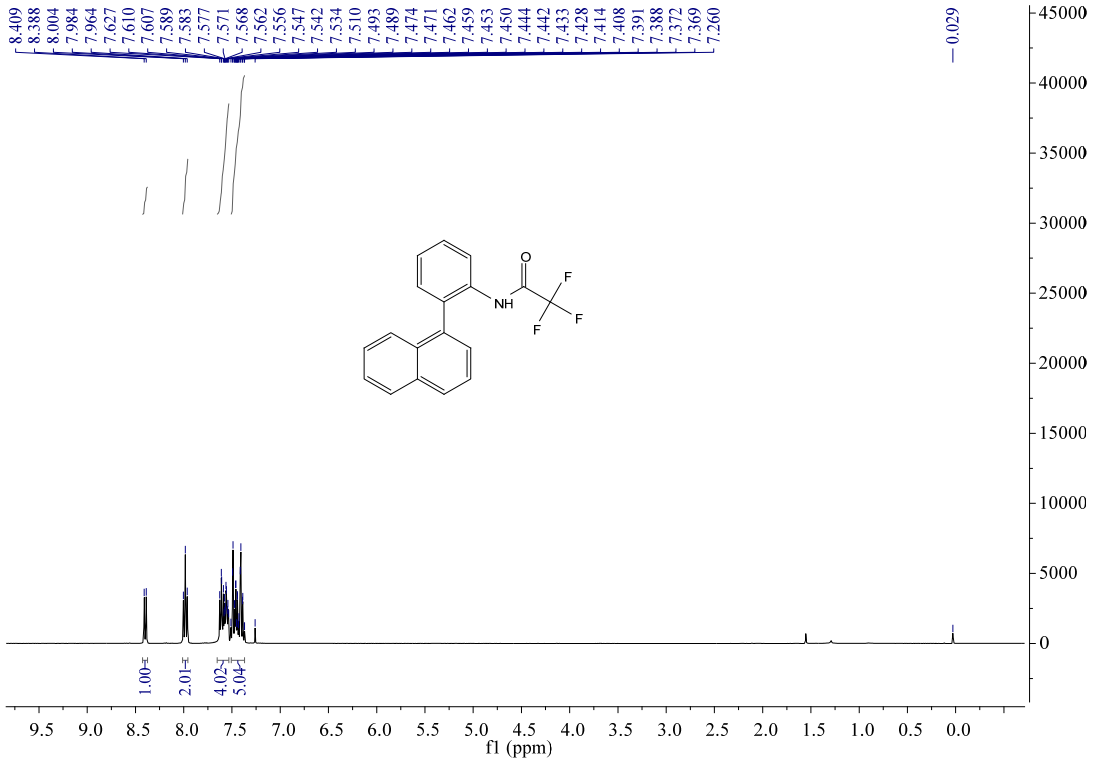
1k

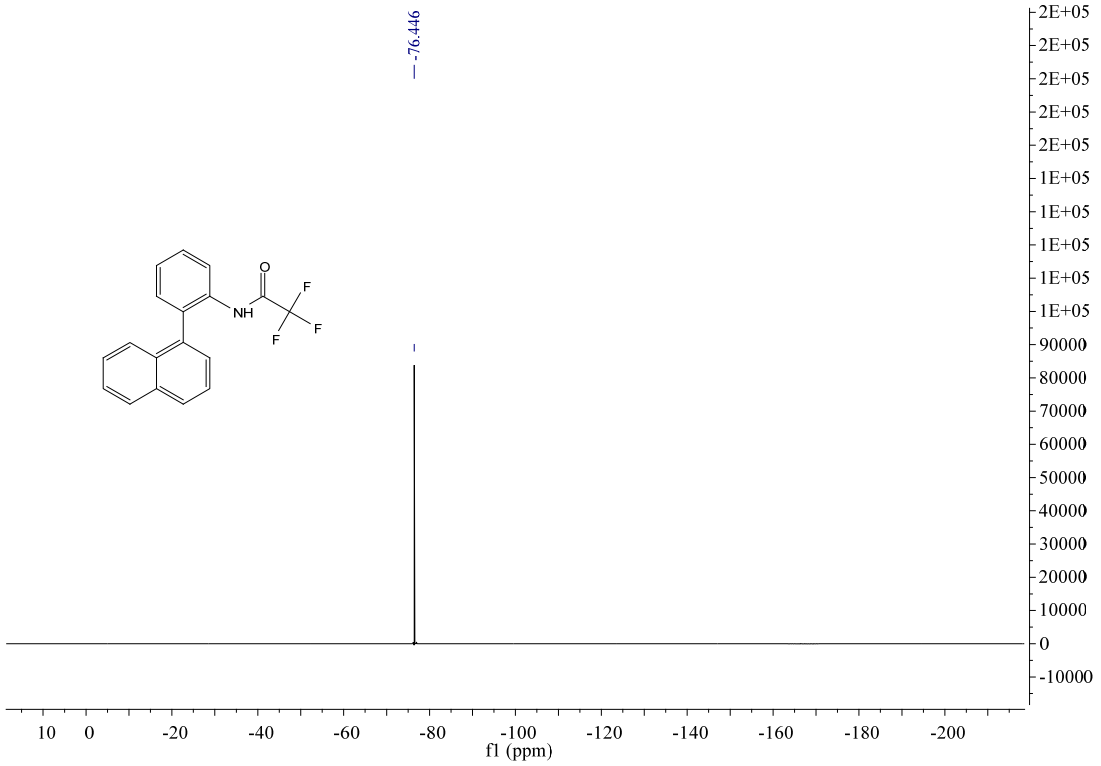

8.245
8.224
7.870
7.465
7.455
7.452
7.443
7.433
7.422
7.360
7.355
7.347
7.339
7.331
7.325
7.317
7.305
7.260
7.240
7.233
7.228
7.212
7.207
7.195
7.190
0.006
NH
O
F
F
F
F
1.00
0.96
1.04
4.08
2.04
fl (ppm)

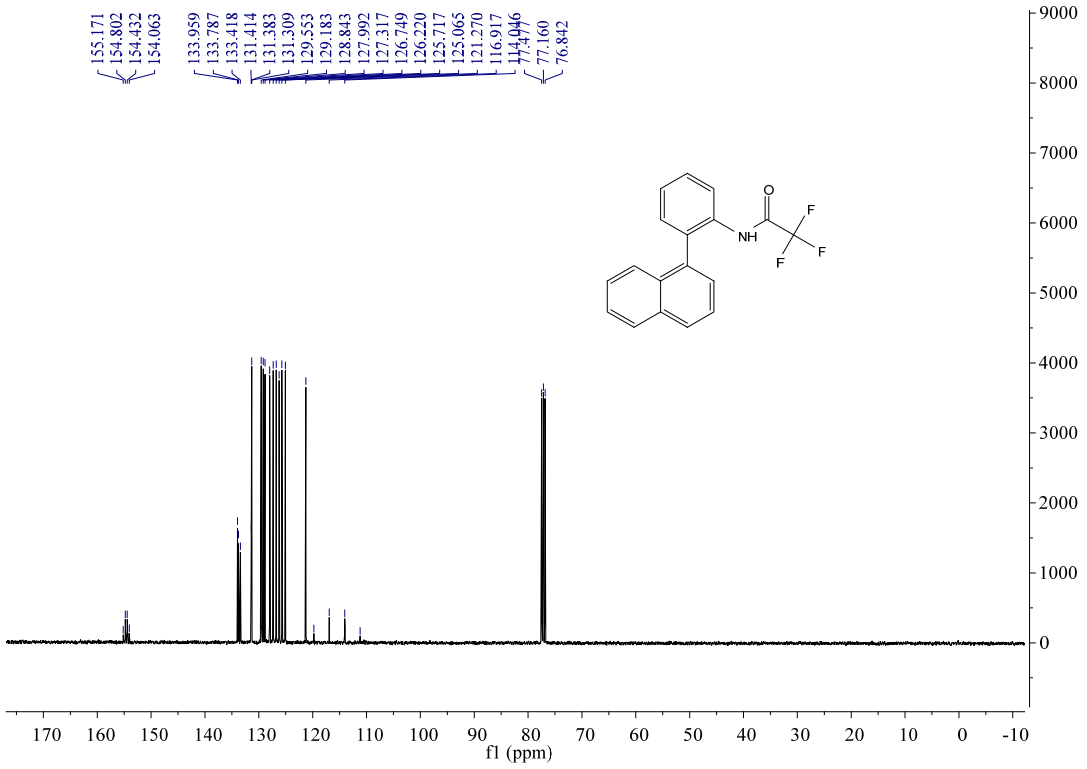

-76.037
-112.679
NH
O
F
F
F
F
fl (ppm)


164.192
161.717
155.307
154.937
154.567
154.197
132.880
132.845
132.543
132.253
131.037
130.956
130.592
129.057
126.568
121.886
120.079
117.207
116.706
116.491
114.335
111.463
77.477
77.160
76.842
O
NH
F
F
F
F
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

1l


8.409
8.388
8.004
7.984
7.964
7.627
7.610
7.607
7.589
7.583
7.577
7.571
7.568
7.562
7.556
7.547
7.542
7.534
7.510
7.493
7.489
7.474
7.471
7.462
7.459
7.453
7.450
7.444
7.442
7.433
7.428
7.414
7.408
7.391
7.388
7.372
7.369
7.260
0.029
O
NH
F
F
F
1.00
2.01
4.02
5.04
f1 (ppm)


-76.446
O
NH
F
F
F
f1 (ppm)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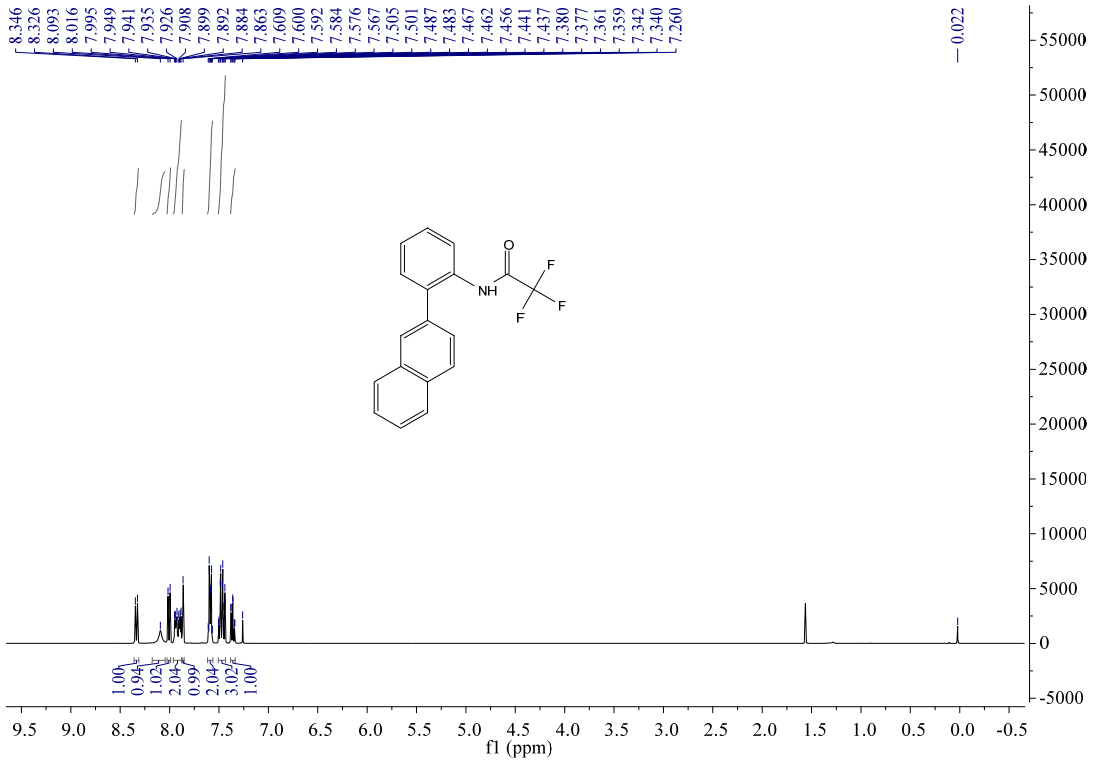
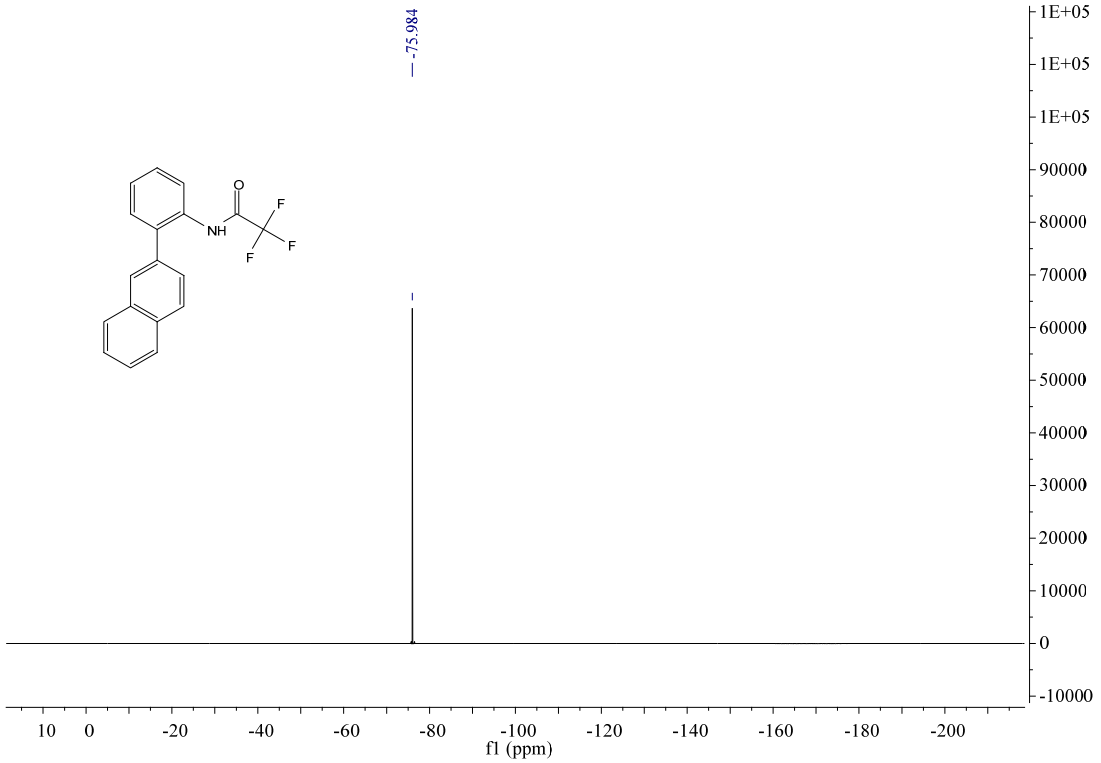
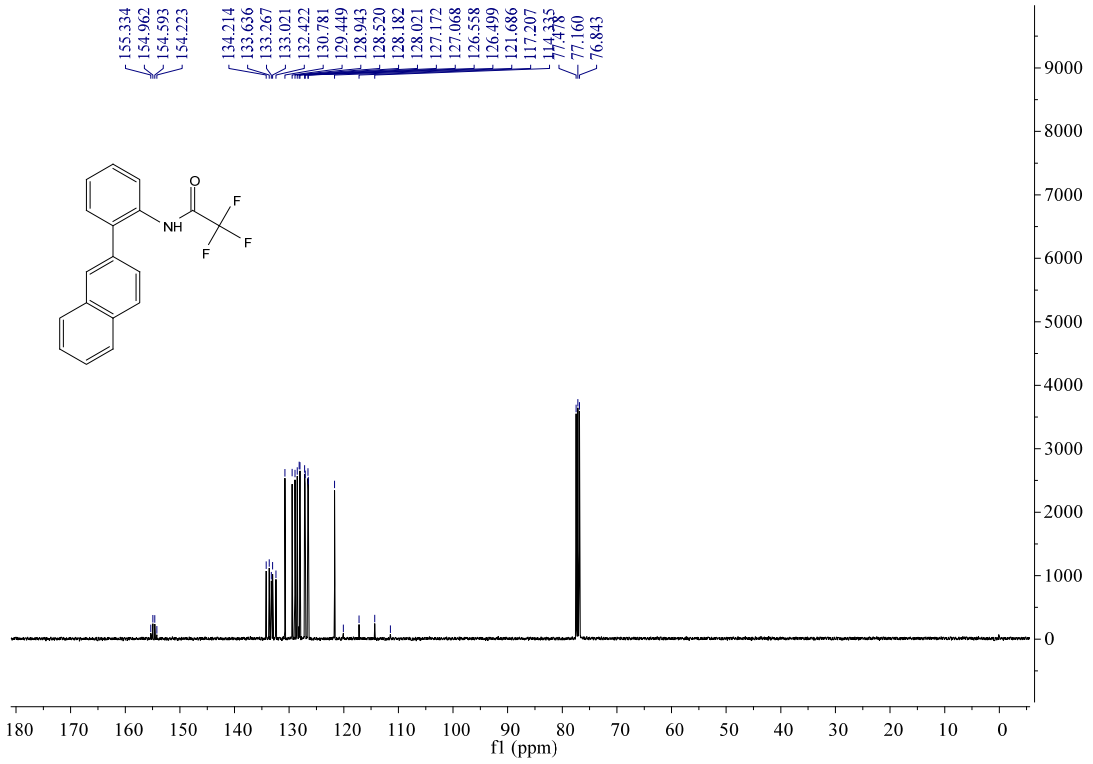
154.802
154.432
154.063
133.959
133.787
133.418
131.414
131.383
131.309
129.553
129.183
128.843
127.992
127.317
126.749
126.220
125.717
125.065
121.270
116.917
114.046
77.477
77.160
76.842
NH
O
F
F
F
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

1m


8.346
8.326
8.093
8.016
7.995
7.949
7.941
7.935
7.926
7.908
7.899
7.892
7.884
7.863
7.609
7.600
7.592
7.584
7.576
7.567
7.505
7.501
7.487
7.483
7.467
7.462
7.456
7.441
7.437
7.380
7.377
7.361
7.359
7.342
7.340
7.260
0.022
O
NH
F
F
F
1.00
0.94
1.02
2.04
0.99
2.04
3.02
1.00
f1 (ppm)


-75.984
O
NH
F
F
F
f1 (ppm)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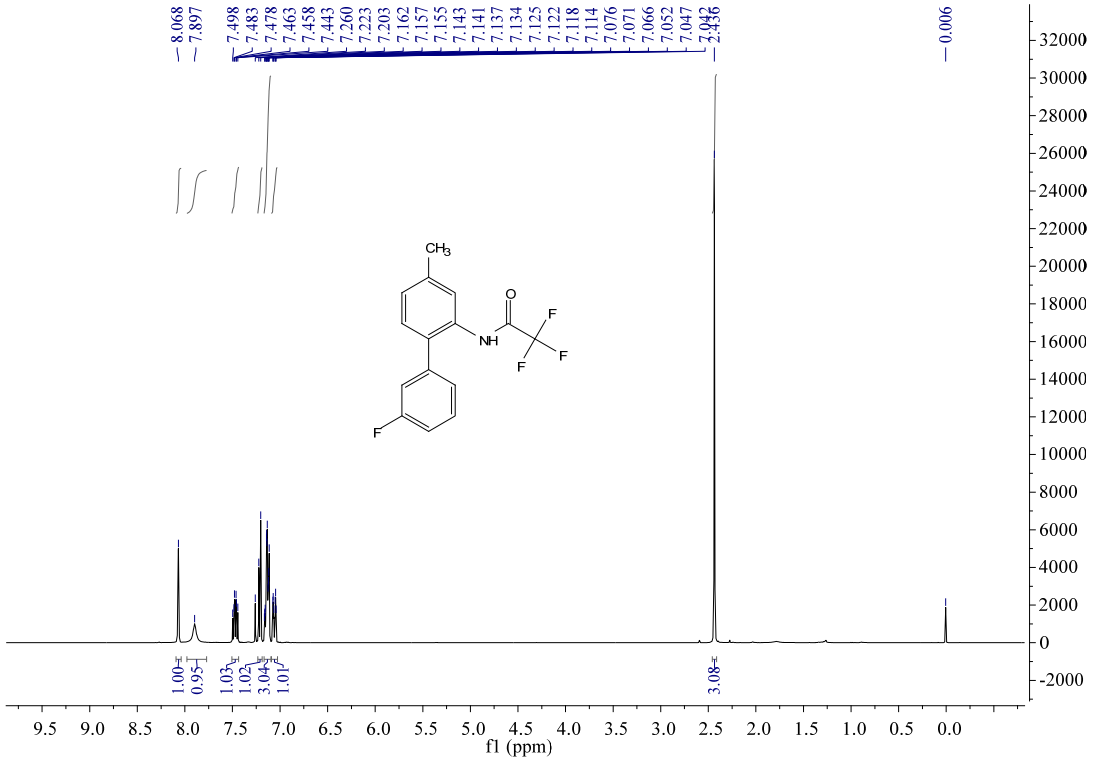
154.593
154.223
134.214
133.636
133.267
133.021
132.422
130.781
129.449
128.943
128.520
128.182
128.021
127.172
127.068
126.558
126.499
121.686
117.207
77.478
77.160
76.843
O
NH
F
F
F
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1n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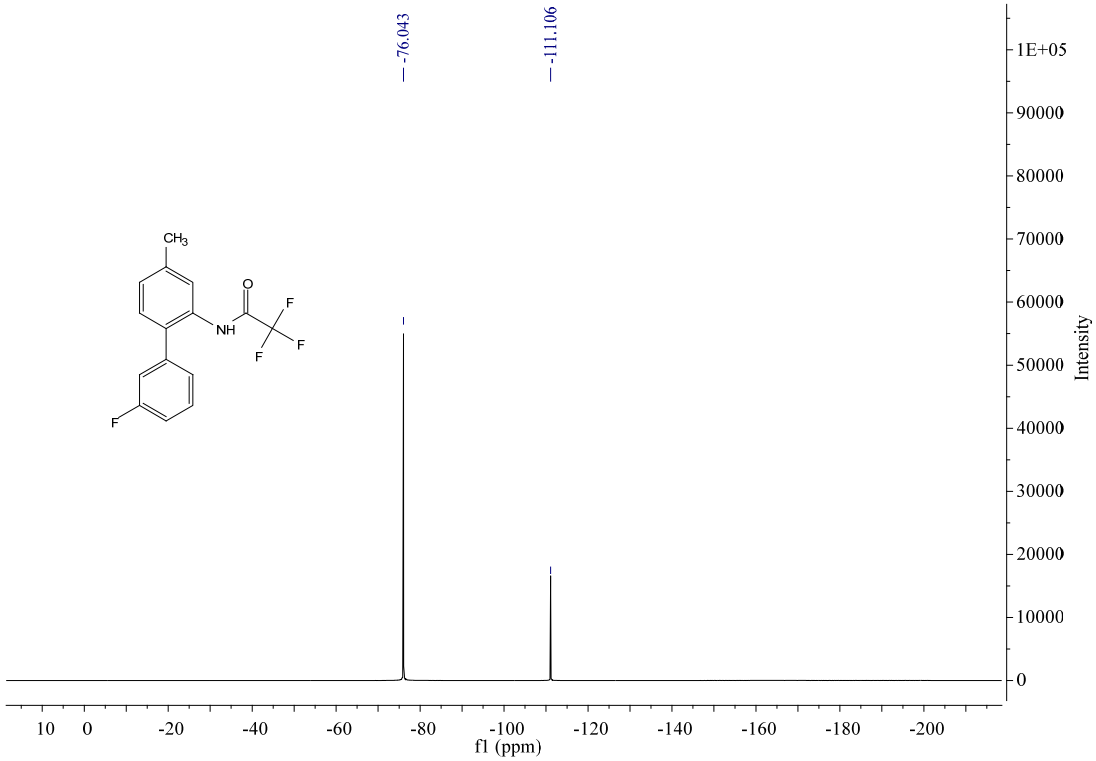
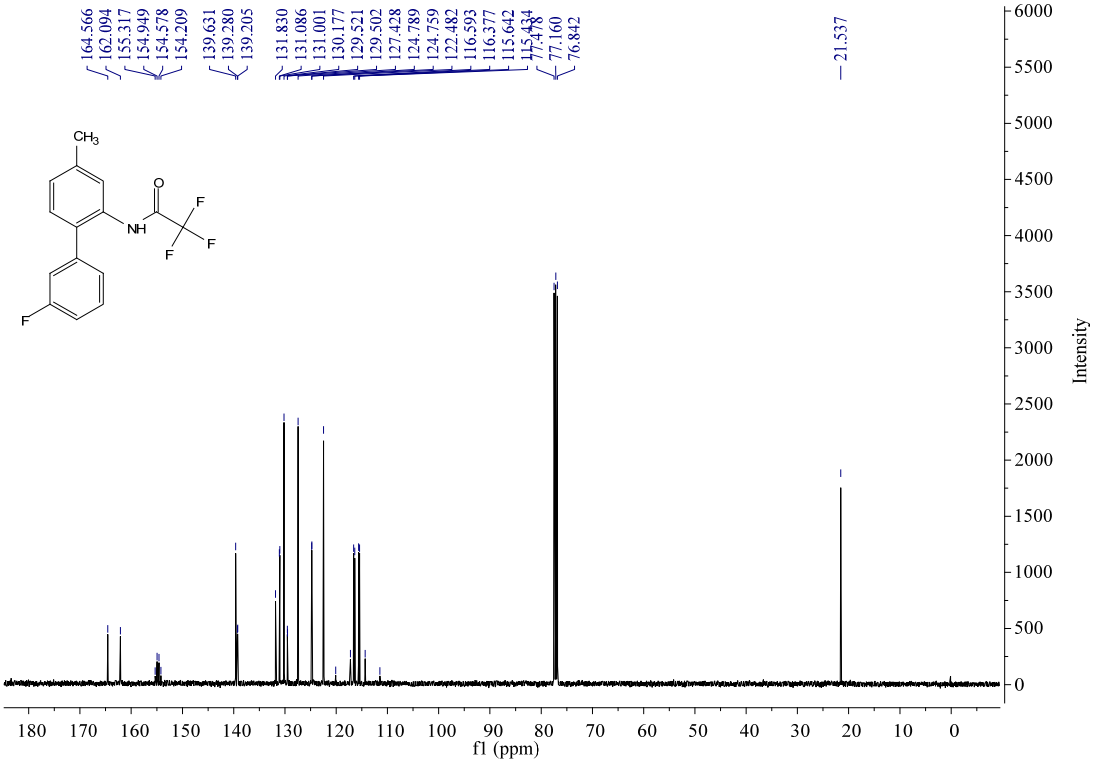
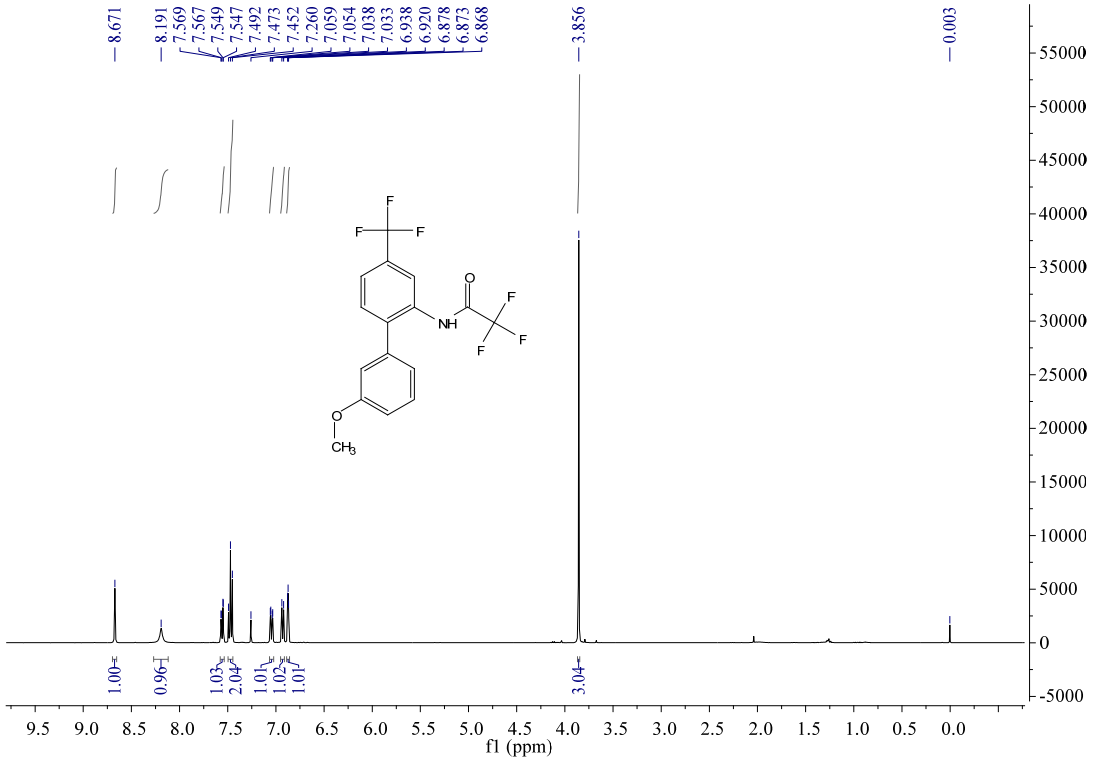
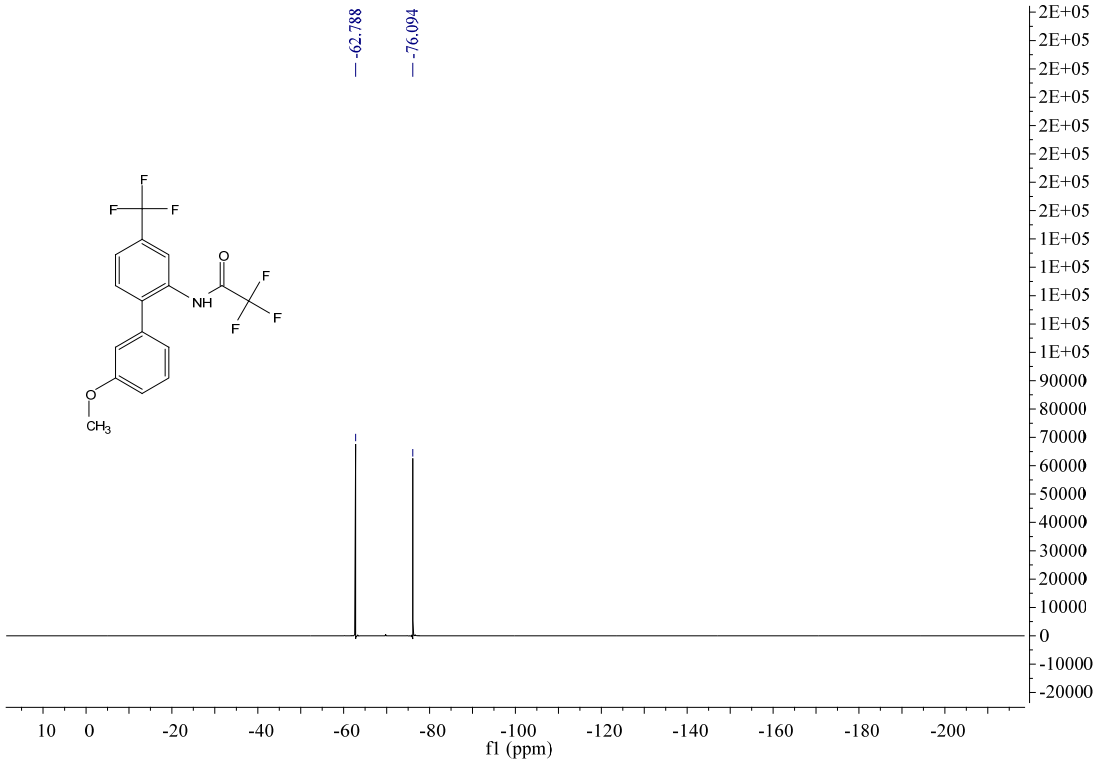
7.897
7.498
7.483
7.478
7.463
7.458
7.443
7.260
7.223
7.203
7.162
7.157
7.155
7.143
7.141
7.137
7.134
7.125
7.122
7.118
7.114
7.076
7.071
7.066
7.052
7.047
7.042
2.436
0.006
CH3
O
NH
F
F
F
F
1.00
0.95
1.03
1.02
3.04
1.01
3.08
fl (ppm)


-76.043
-111.106
CH3
O
NH
F
F
F
F
Intensity
fl (ppm)


164.566
162.094
155.317
154.949
154.578
154.209
139.631
139.280
139.205
131.830
131.086
131.001
130.177
129.521
129.502
127.428
124.789
124.759
122.482
116.593
116.377
115.642
115.434
77.478
77.160
76.842
21.537
CH3
O
NH
F
F
F
F
Intensity
f1 (ppm)

1o


8.671
8.191
7.569
7.567
7.549
7.547
7.492
7.473
7.452
7.260
7.059
7.054
7.038
7.033
6.938
6.920
6.878
6.873
6.868
3.856
0.003
1.00
0.96
1.03
2.04
1.01
1.02
1.01
3.04
f1 (ppm)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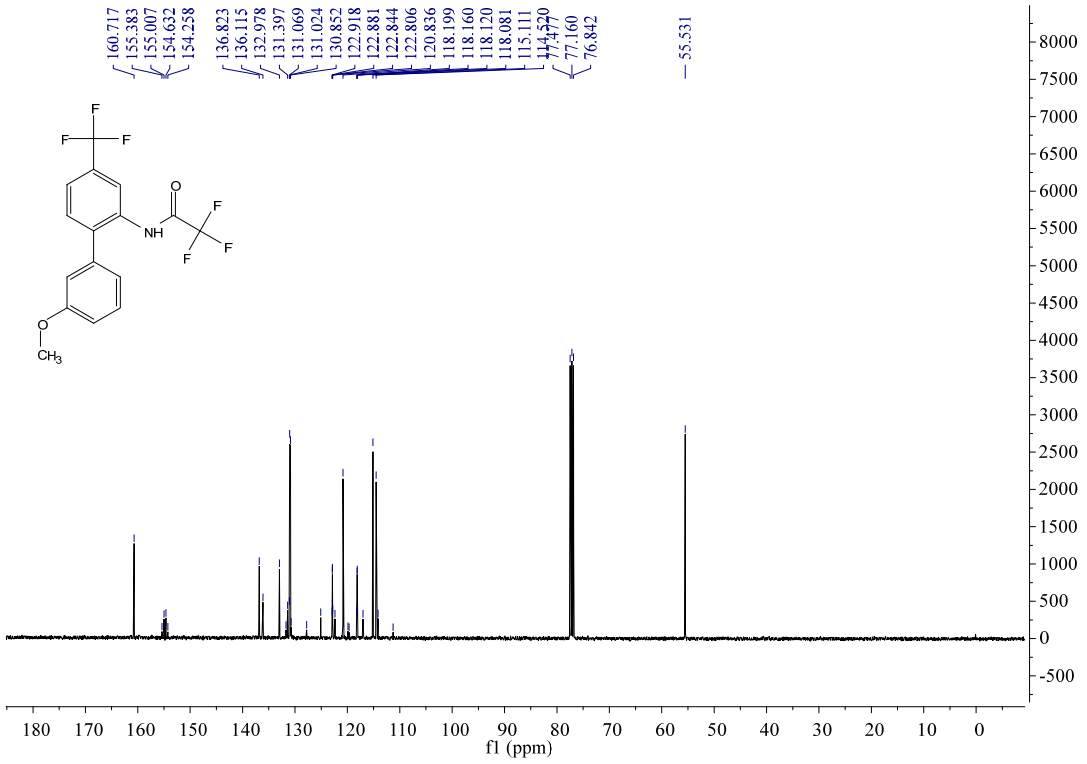
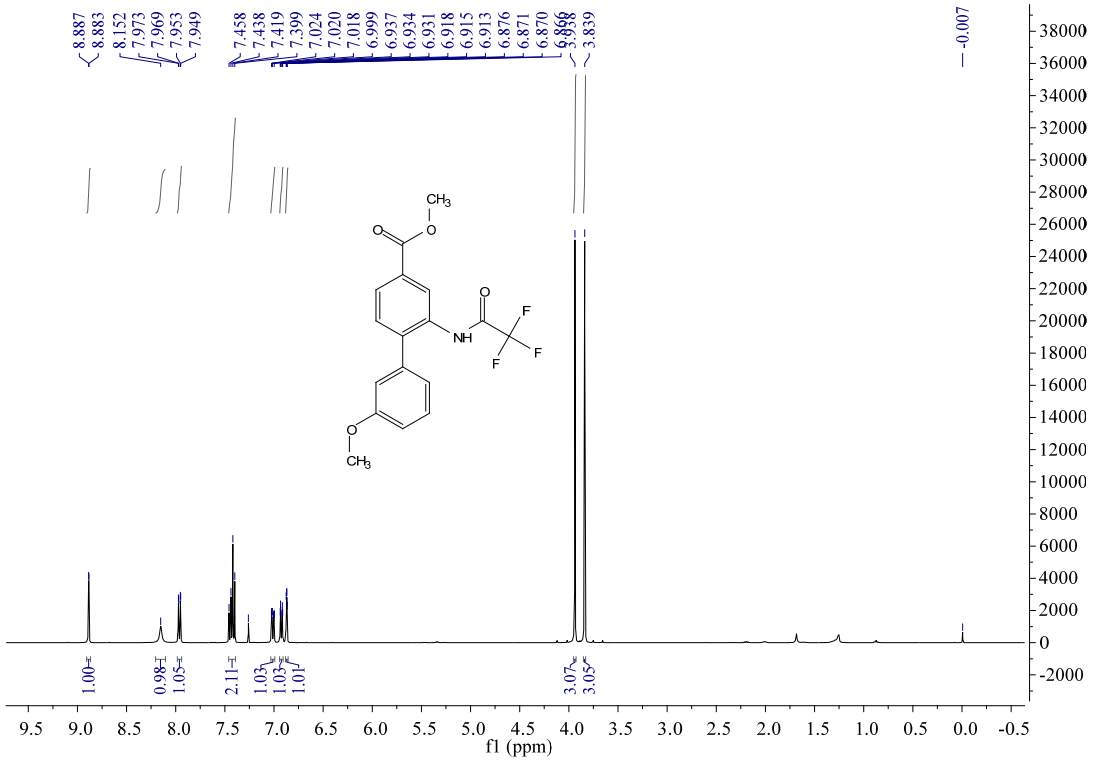
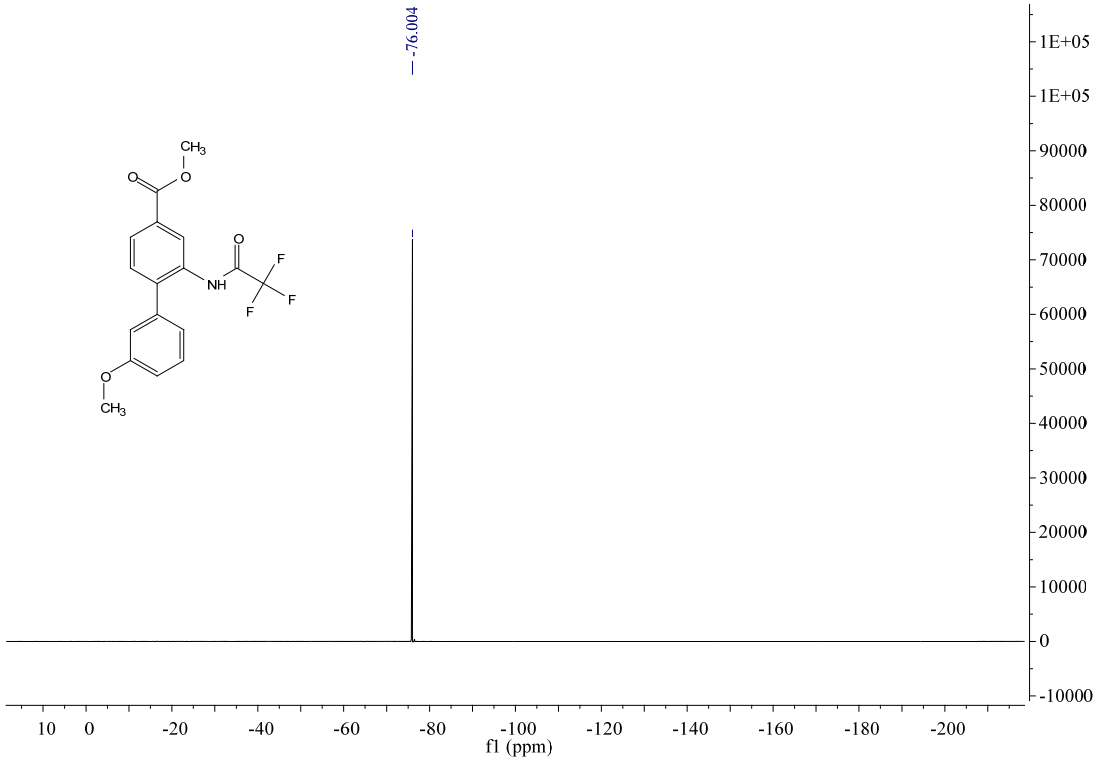
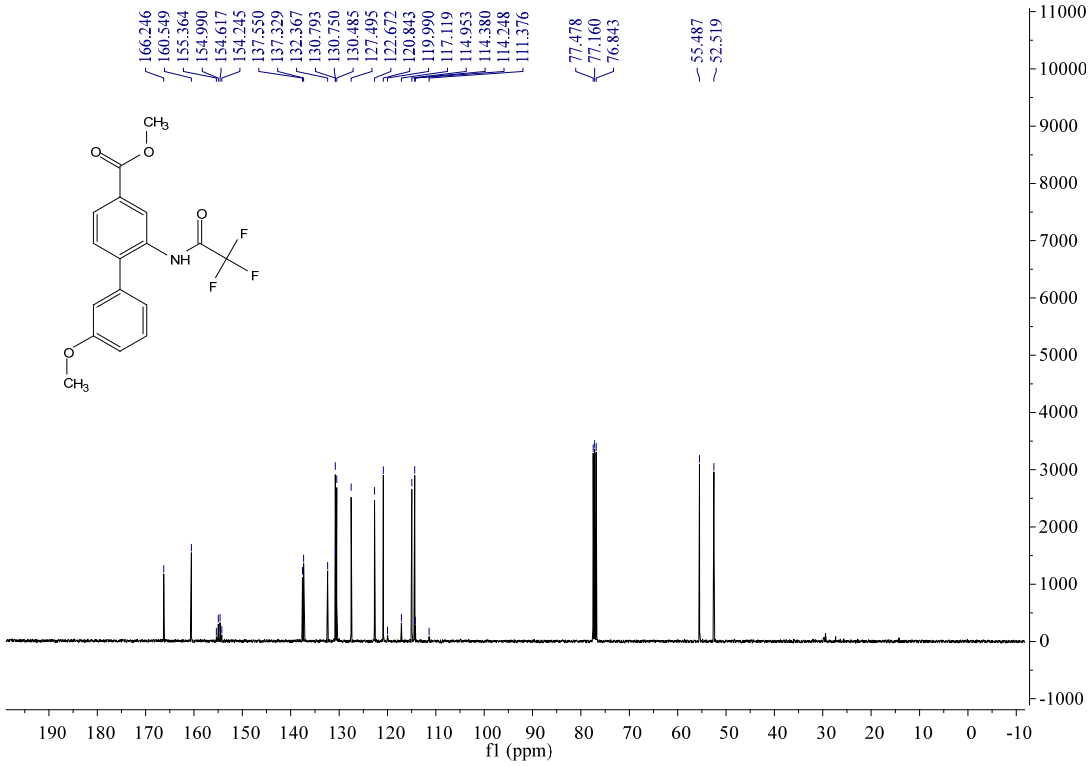
-76.094
f1 (ppm)


160.717
155.383
155.007
154.632
154.258
136.823
136.115
132.978
131.397
131.069
131.024
130.852
122.918
122.881
122.844
122.806
120.836
118.199
118.160
118.120
118.081
115.111
77.477
77.160
76.842
55.531
F
F
F
O
NH
F
F
F
O
CH3
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

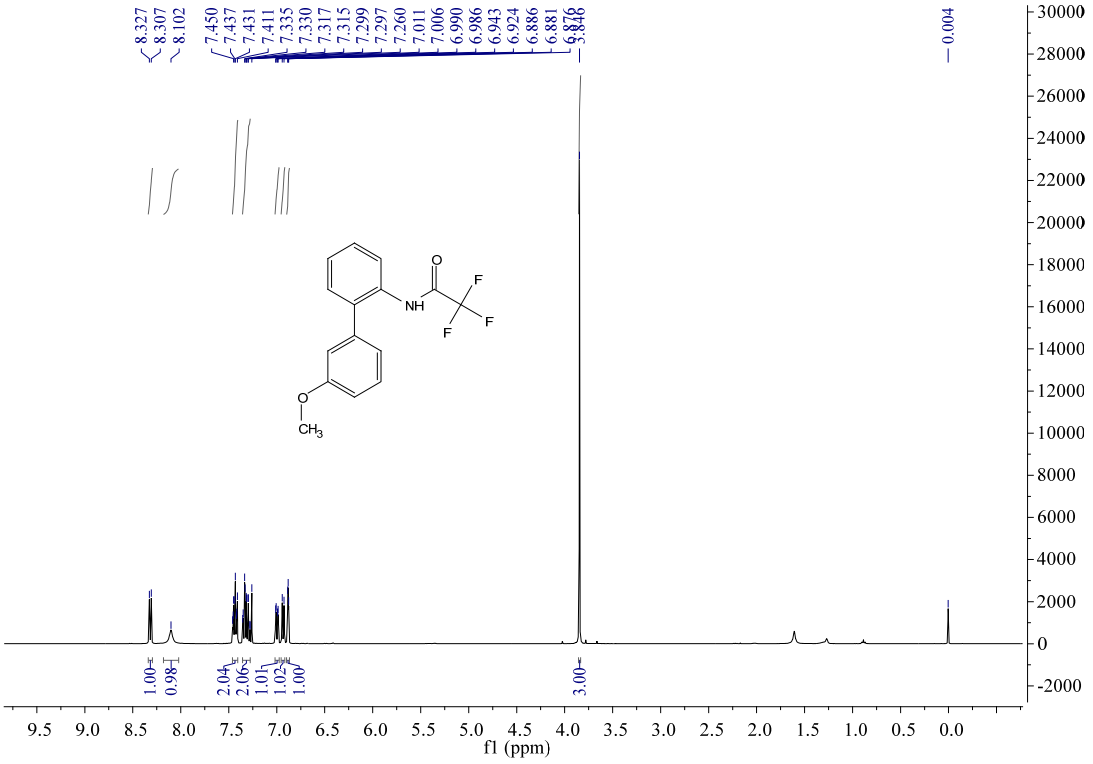
1p

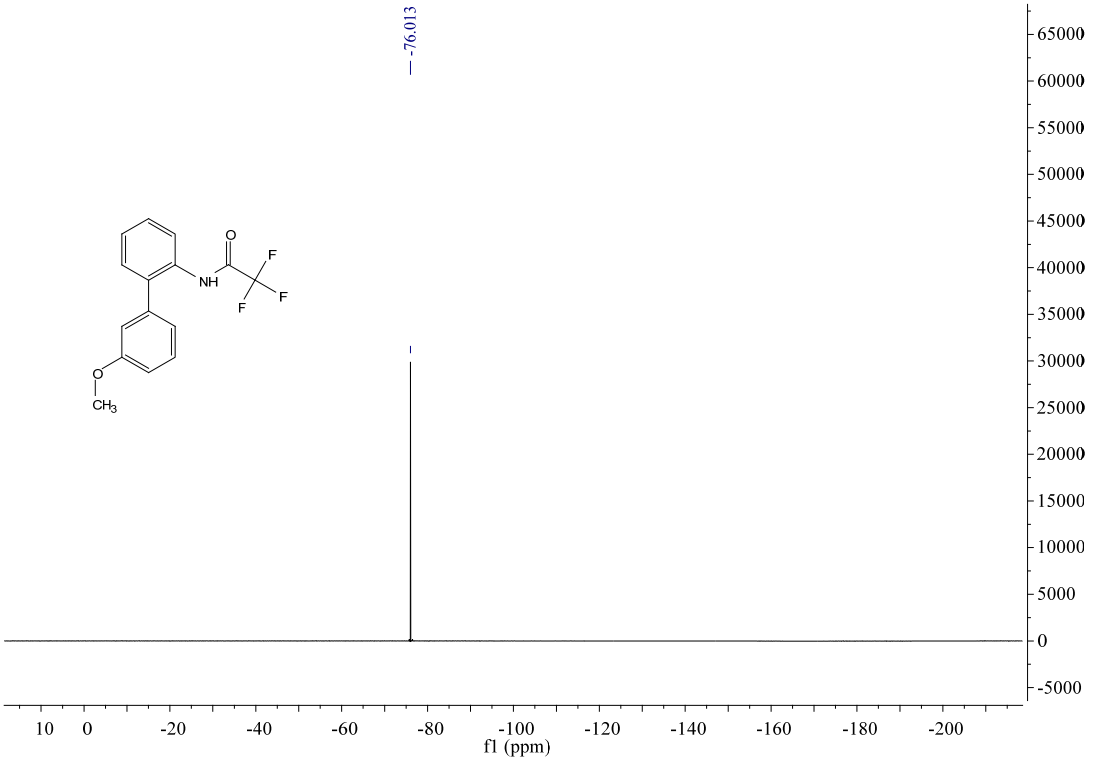

8.887
8.883
8.152
7.973
7.969
7.953
7.949
7.458
7.438
7.419
7.399
7.024
7.020
7.018
6.999
6.937
6.934
6.931
6.918
6.915
6.913
6.876
6.871
6.870
3.958
3.839
-0.007
1.00
0.98
1.05
2.11
1.03
1.03
1.01
3.07
3.05
CH3
O
O
NH
F
F
F
O
CH3
fl (ppm)

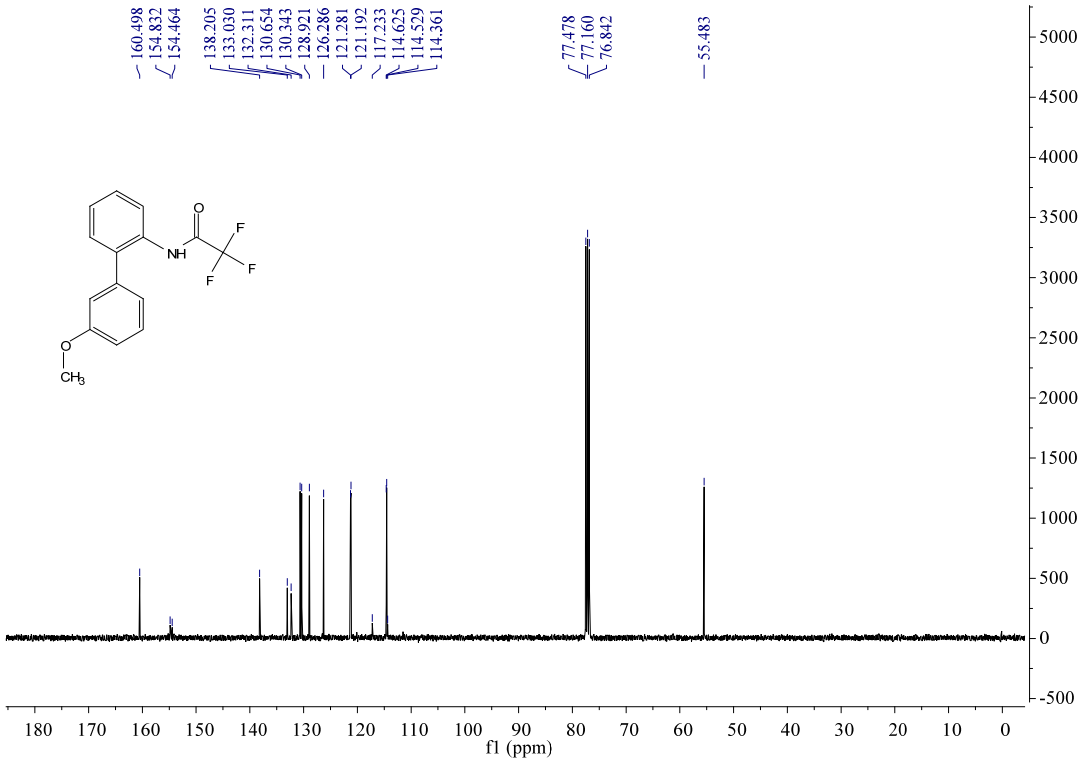

-76.004
CH3
O
O
NH
F
F
F
O
CH3
fl (ppm)


166.246
160.549
155.364
154.990
154.617
154.245
137.550
137.329
132.367
130.793
130.750
130.485
127.495
122.672
120.843
119.990
117.119
114.953
114.380
114.248
111.376
77.478
77.160
76.843
55.487
52.519
CH3
O
O
O
NH
F
F
F
O
CH3
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

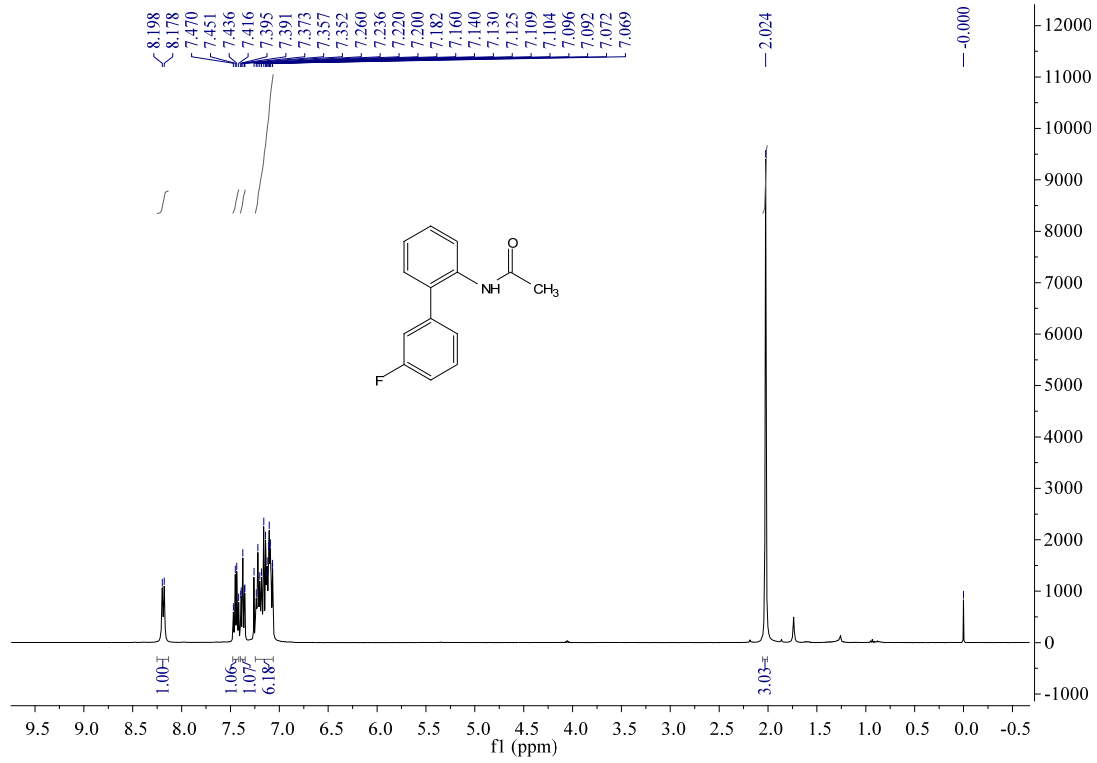
1q

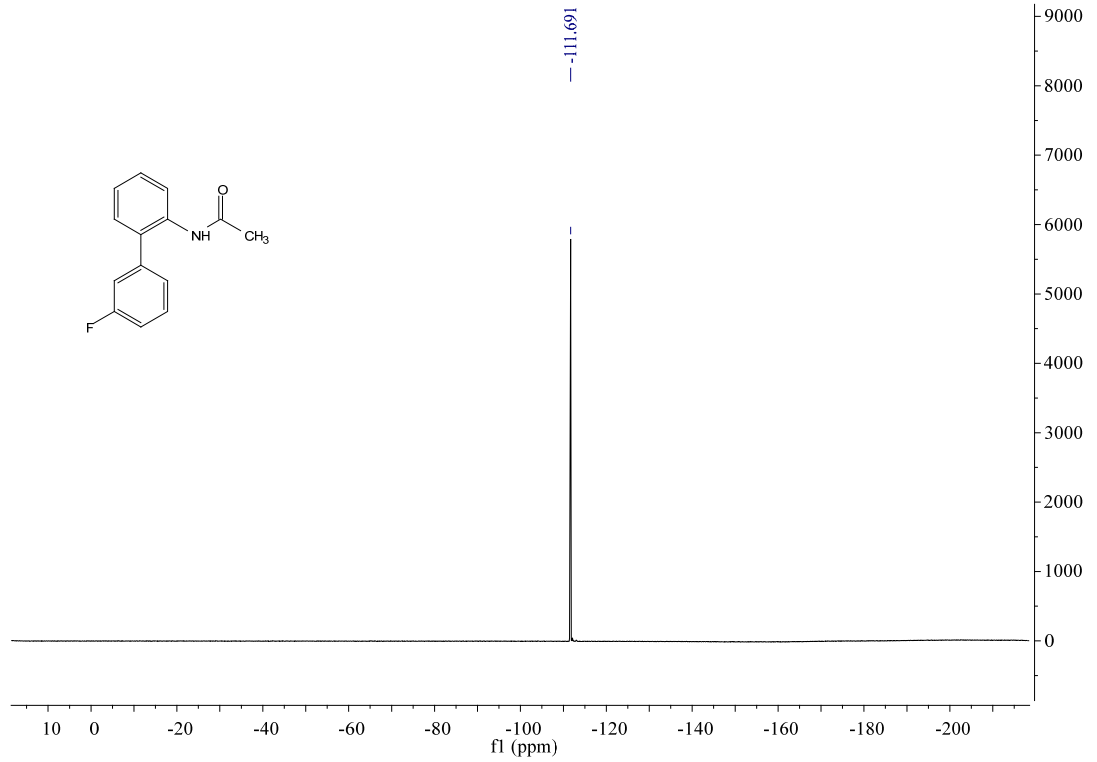

8.327
8.307
8.102
7.450
7.437
7.431
7.411
7.335
7.330
7.317
7.315
7.299
7.297
7.260
7.011
7.006
6.990
6.986
6.943
6.924
6.886
6.881
3.848
0.004
1.00
0.98
2.04
2.06
1.01
1.02
1.00
3.00
NH
O
F
F
F
O
CH3
f1 (ppm)

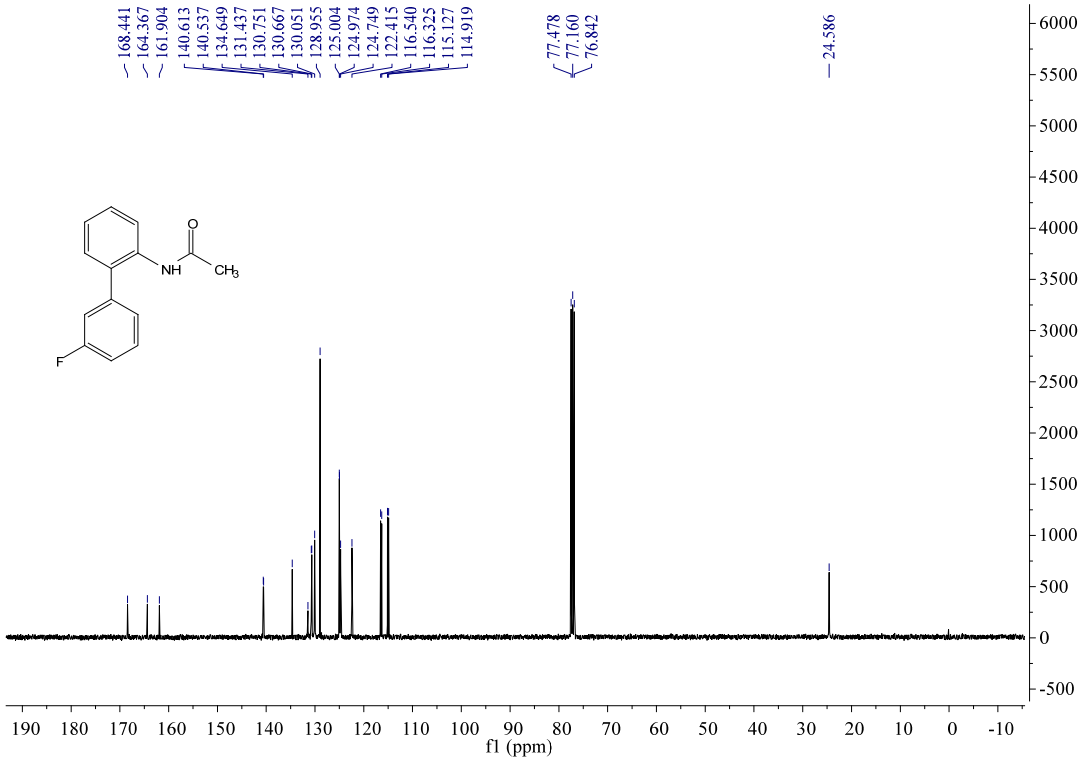

-76.013
NH
O
F
F
F
O
CH3
f1 (ppm)


160.498
154.832
154.464
138.205
133.030
132.311
130.654
130.343
128.921
126.286
121.281
121.192
117.233
114.625
114.529
114.361
77.478
77.160
76.842
55.483
NH
O
F
F
F
O
CH3
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

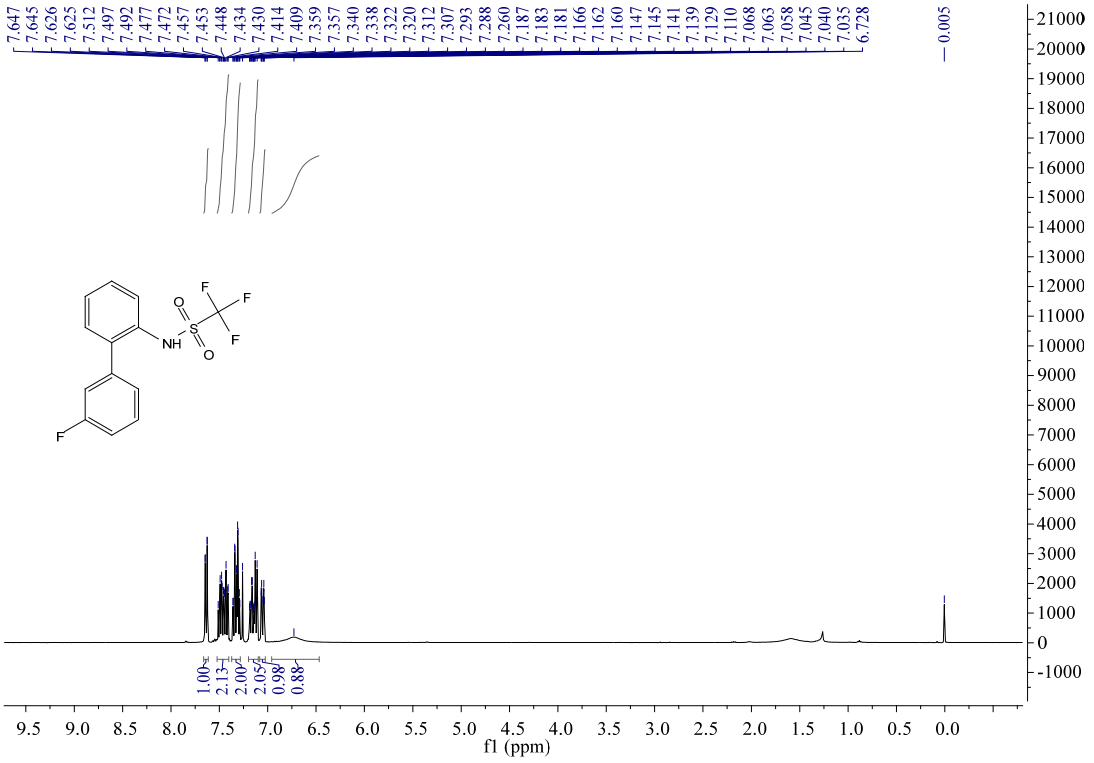
1ab

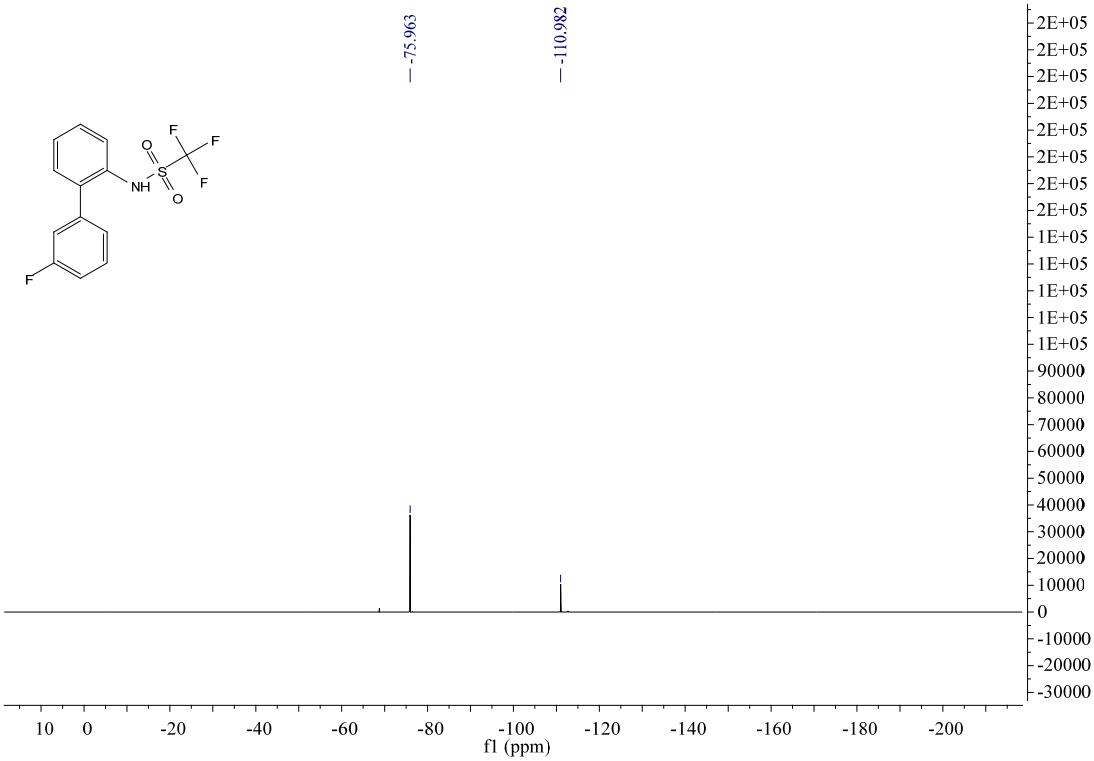

8.198
8.178
7.470
7.451
7.436
7.416
7.395
7.391
7.373
7.357
7.352
7.260
7.236
7.220
7.200
7.182
7.160
7.140
7.130
7.125
7.109
7.104
7.096
7.092
7.072
7.069
2.024
-0.000
NH
CH3
O
F
1.00
1.06
1.07
6.18
3.03
f1 (ppm)

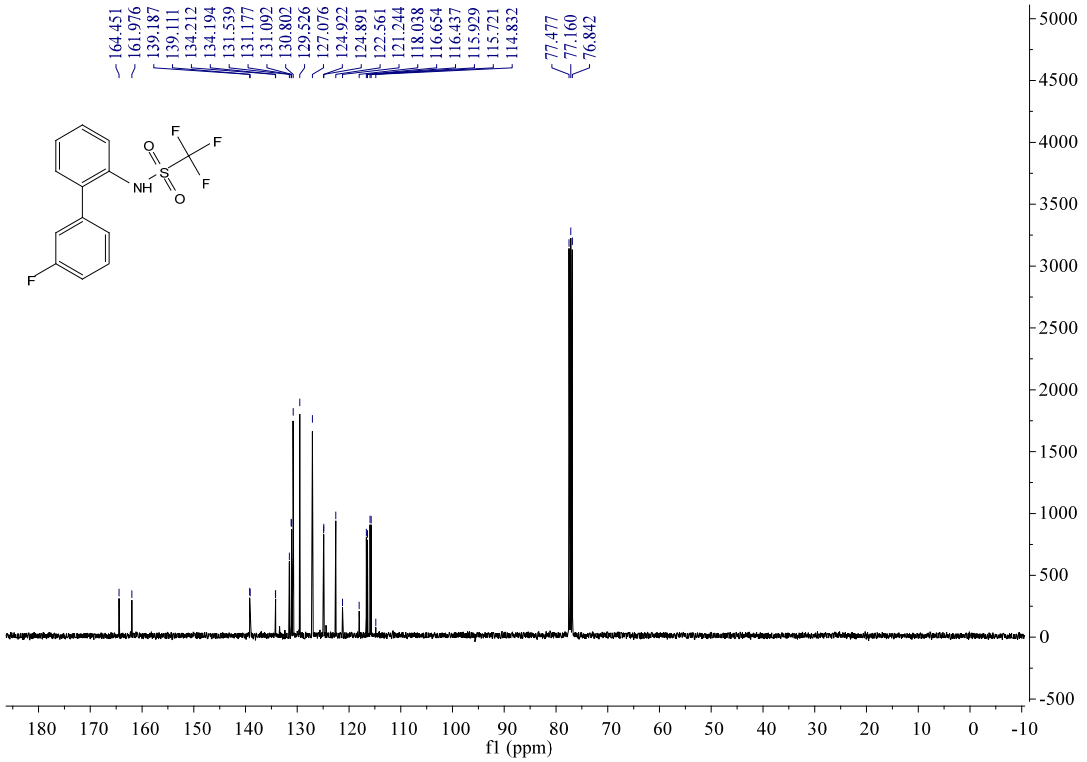

-111.691
NH
CH3
O
F
f1 (ppm)


168.441
164.367
161.904
140.613
140.537
134.649
131.437
130.751
130.667
130.051
128.955
125.004
124.974
124.749
122.415
116.540
116.325
115.127
114.919
77.478
77.160
76.842
24.586
NH
O
CH3
F
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

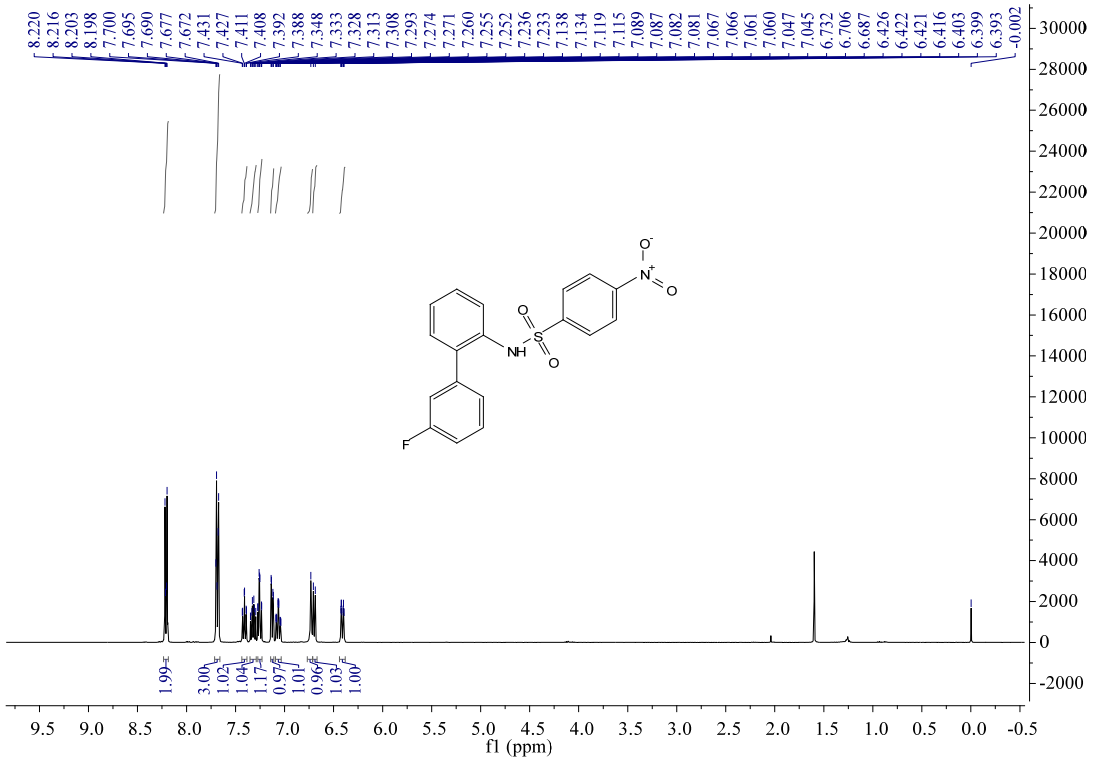
1ac

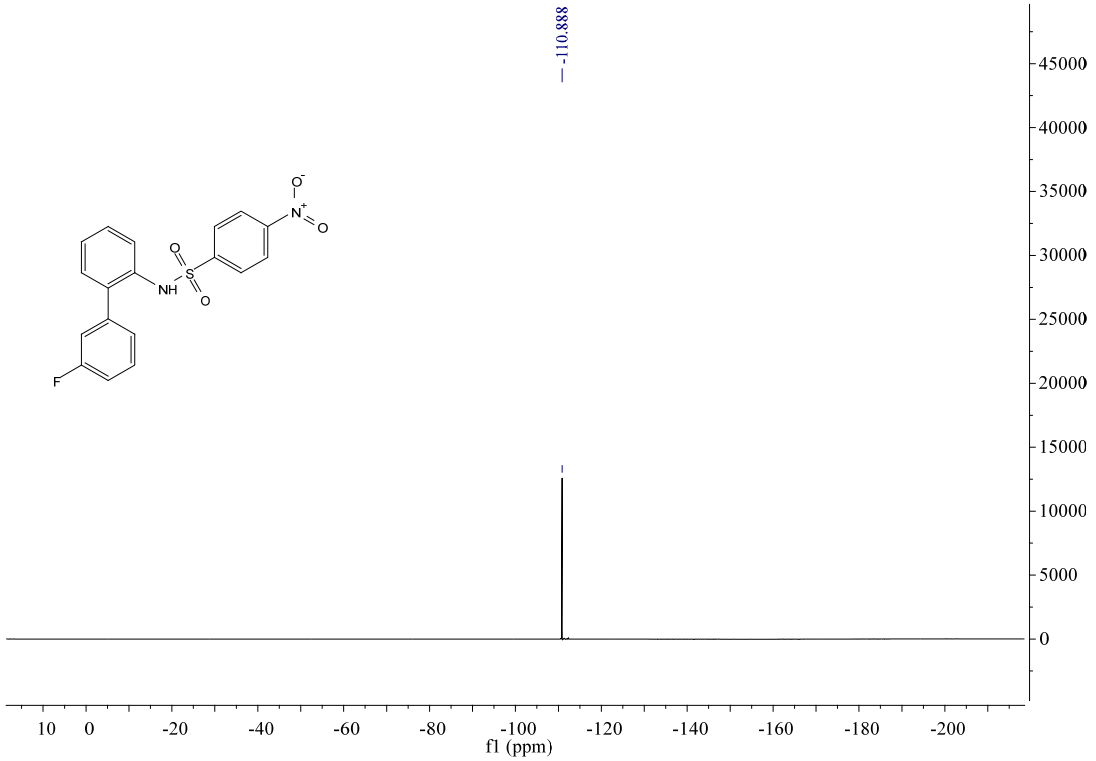

7.647
7.645
7.626
7.625
7.512
7.497
7.492
7.477
7.472
7.457
7.453
7.448
7.434
7.430
7.414
7.409
7.359
7.357
7.340
7.338
7.322
7.320
7.312
7.307
7.293
7.288
7.260
7.187
7.183
7.181
7.166
7.162
7.160
7.147
7.145
7.141
7.139
7.129
7.110
7.068
7.063
7.058
7.045
7.040
7.035
6.728
0.005
1.00
2.13
2.00
2.05
0.98
0.88
f1 (ppm)

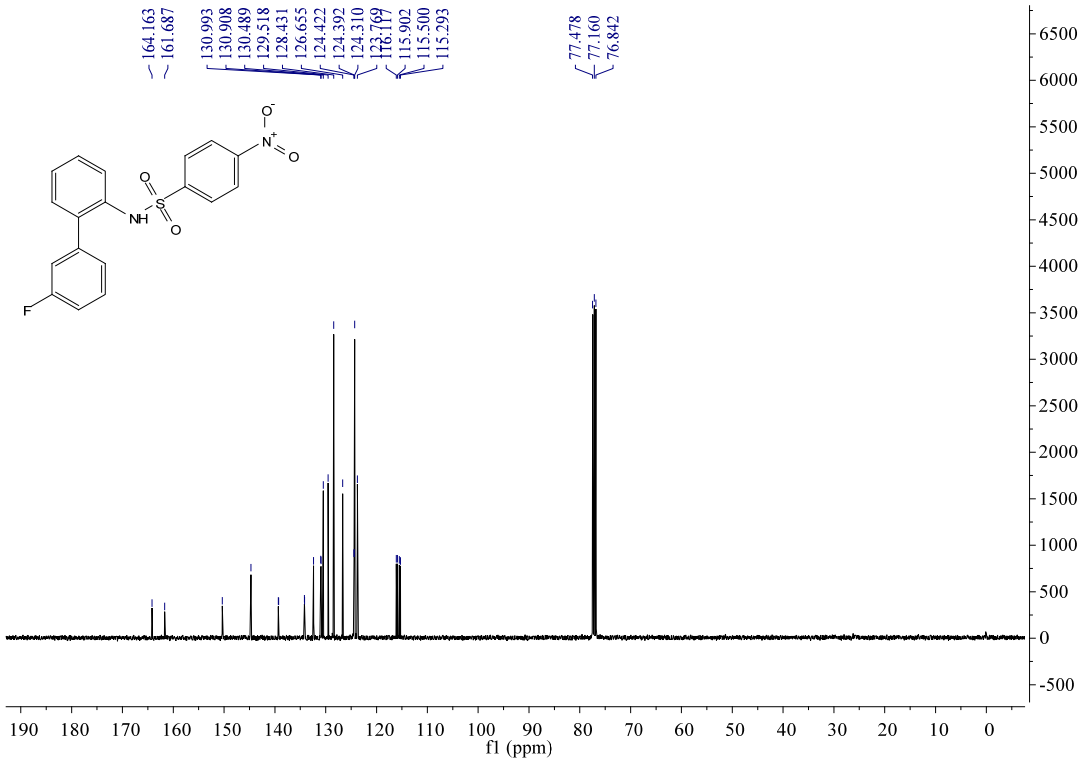

-75.963
-110.982
f1 (ppm)


164.451
161.976
139.187
139.111
134.212
134.194
131.539
131.177
131.092
130.802
129.526
127.076
124.922
124.891
122.561
121.244
118.038
116.654
116.437
115.929
115.721
114.832
77.477
77.160
76.842
F
F
F
O
S
NH
O
F
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

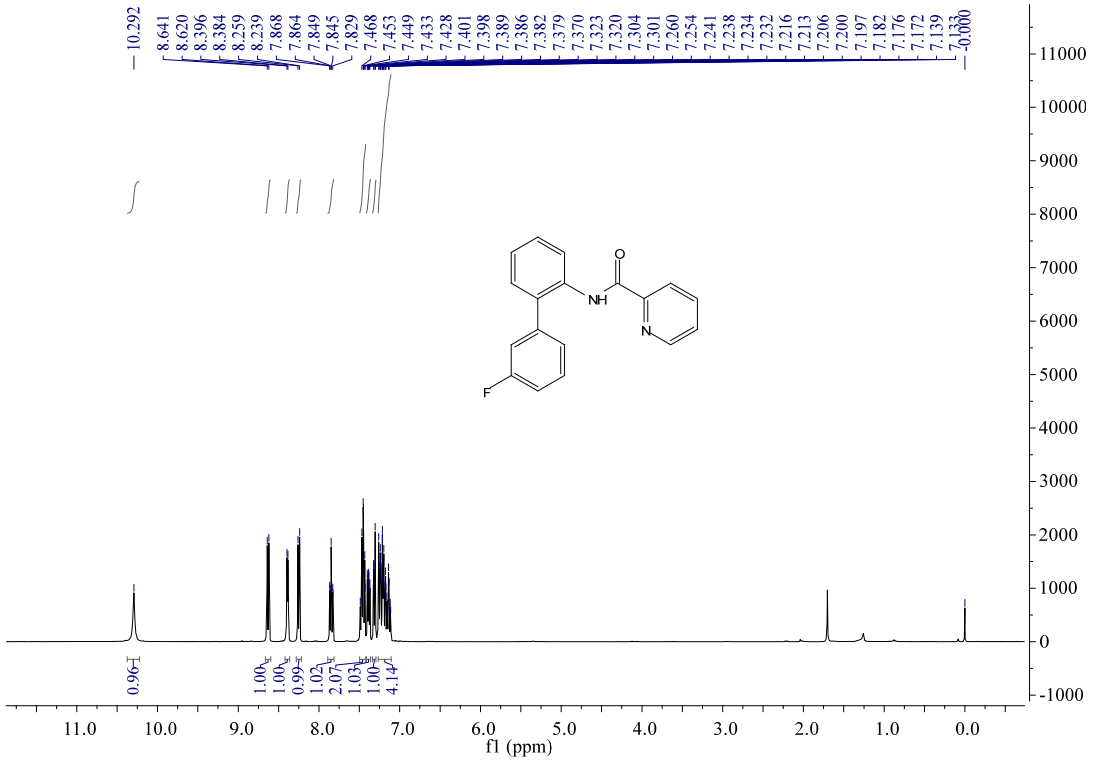
1ad


8.220
8.216
8.203
8.198
7.700
7.695
7.690
7.677
7.672
7.431
7.427
7.411
7.408
7.392
7.388
7.348
7.333
7.328
7.313
7.308
7.293
7.274
7.271
7.260
7.255
7.252
7.236
7.233
7.138
7.134
7.119
7.115
7.089
7.087
7.082
7.081
7.067
7.066
7.061
7.060
7.047
7.045
6.732
6.706
6.687
6.426
6.422
6.421
6.416
6.403
6.399
6.393
-0.002
1.99
3.00
1.02
1.04
1.17
0.97
1.01
0.96
1.03
1.00
f1 (ppm)

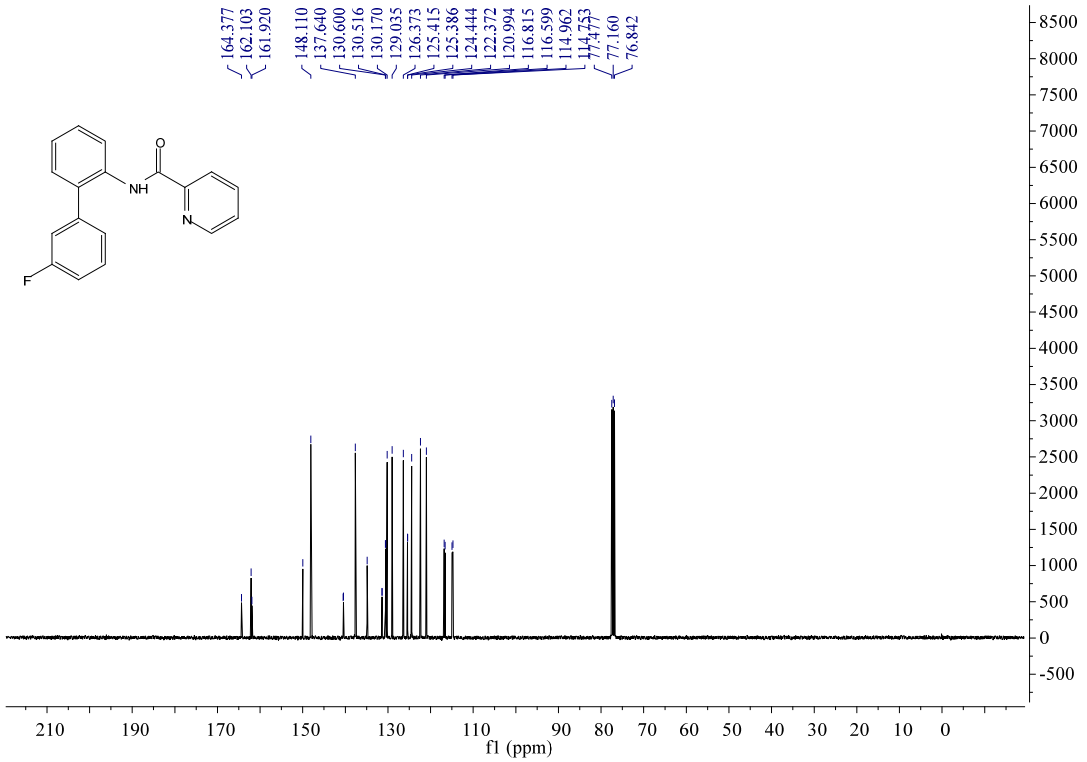

-110.888
f1 (ppm)


164.163
161.687
130.993
130.908
130.489
129.518
128.431
126.655
124.422
124.392
124.310
123.769
123.717
116.117
115.902
115.500
115.293
77.478
77.160
76.842
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

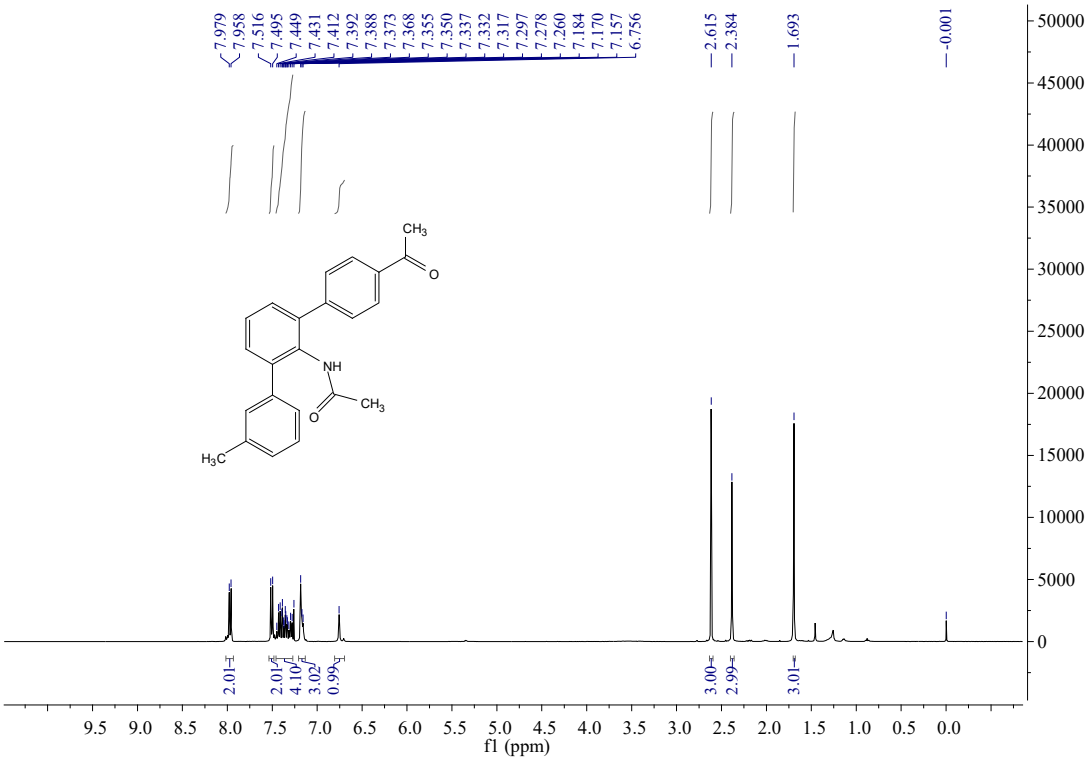
1ae

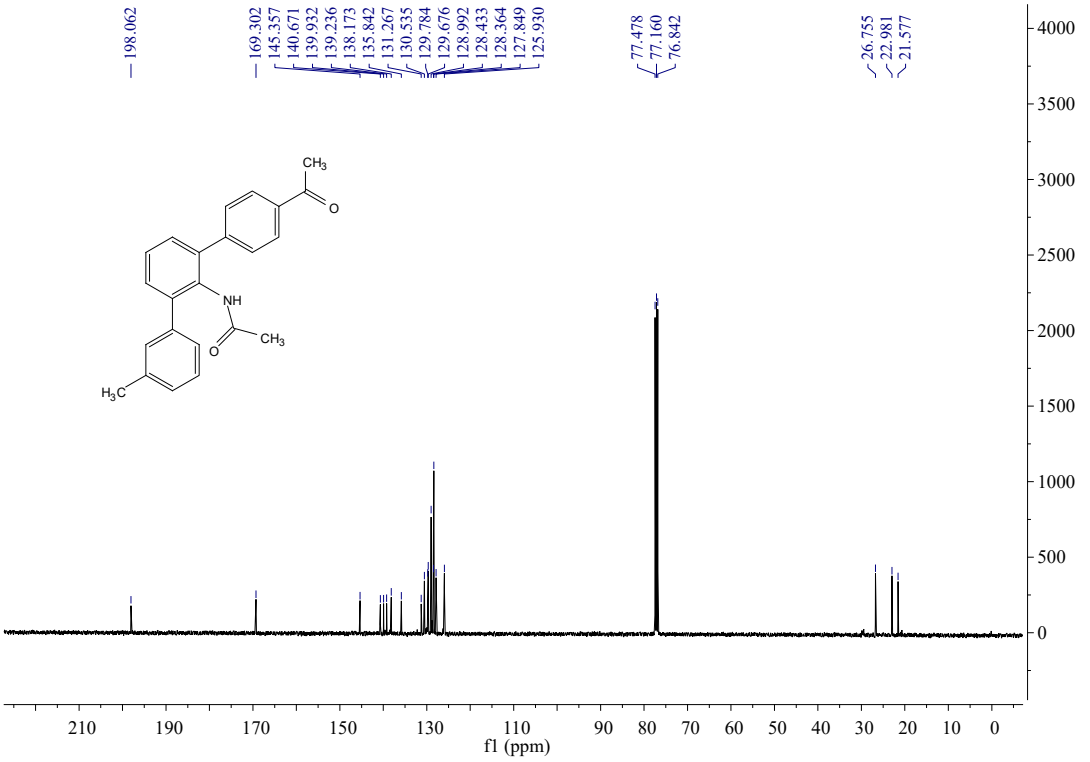

10.292
8.641
8.620
8.396
8.384
8.259
8.239
7.868
7.864
7.849
7.845
7.829
7.468
7.453
7.449
7.433
7.428
7.401
7.398
7.389
7.386
7.382
7.379
7.370
7.323
7.320
7.304
7.301
7.260
7.254
7.241
7.238
7.234
7.232
7.216
7.213
7.206
7.200
7.197
7.182
7.176
7.172
7.139
7.133
0.000
O
NH
N
F
0.96
1.00
1.00
0.99
1.02
2.07
1.03
1.00
4.14
f1 (ppm)


-112.357
O
NH
N
F
f1 (ppm)

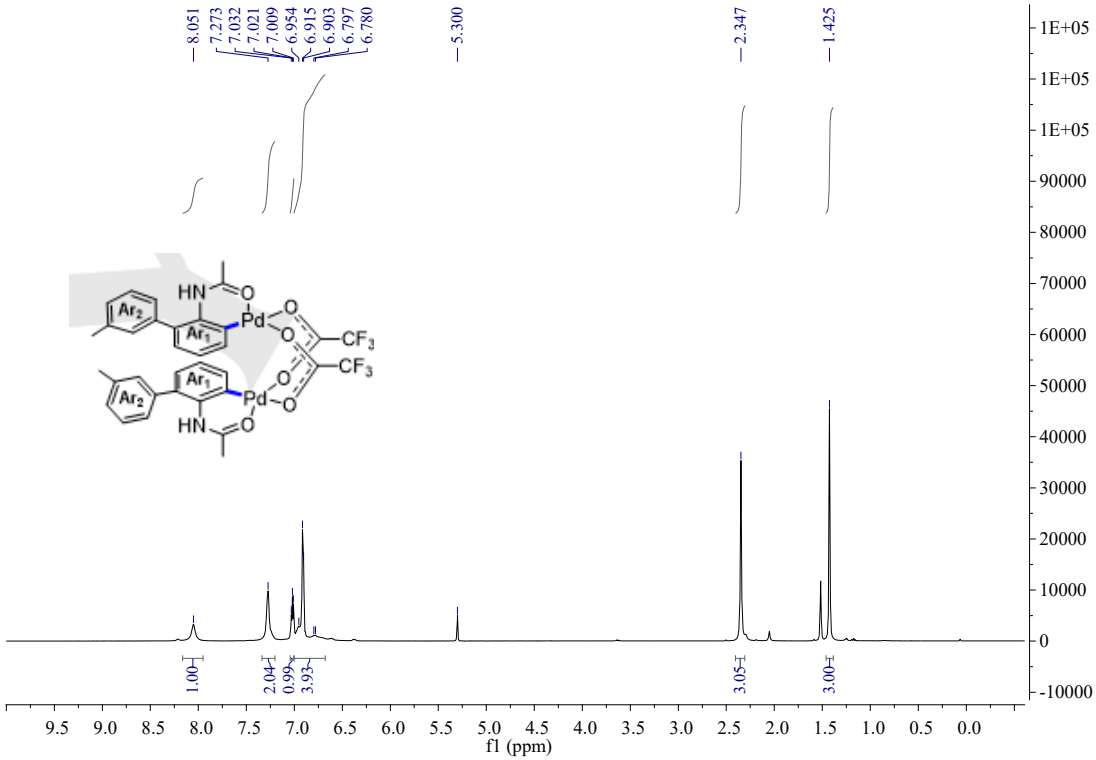

164.377
162.103
161.920
148.110
137.640
130.600
130.516
130.170
129.035
126.373
125.415
125.386
124.444
122.372
120.994
116.815
116.599
114.962
114.753
77.477
77.160
76.842
O
NH
N
F
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

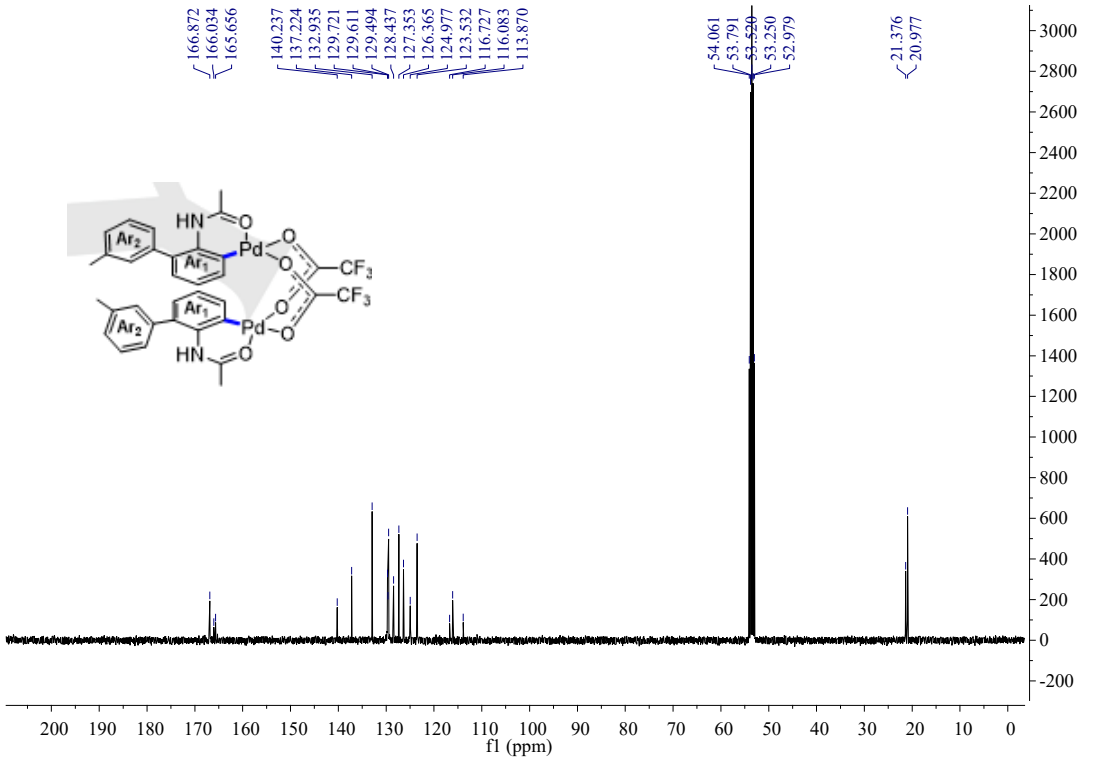
2aa


7.979
7.958
7.516
7.495
7.449
7.431
7.412
7.392
7.388
7.373
7.368
7.355
7.350
7.337
7.332
7.317
7.297
7.278
7.260
7.184
7.170
7.157
6.756
2.615
2.384
1.693
-0.001
CH3
O
NH
CH3
O
H3C
2.01
2.01
4.10
3.02
0.99
3.00
2.99
3.01
fl (ppm)

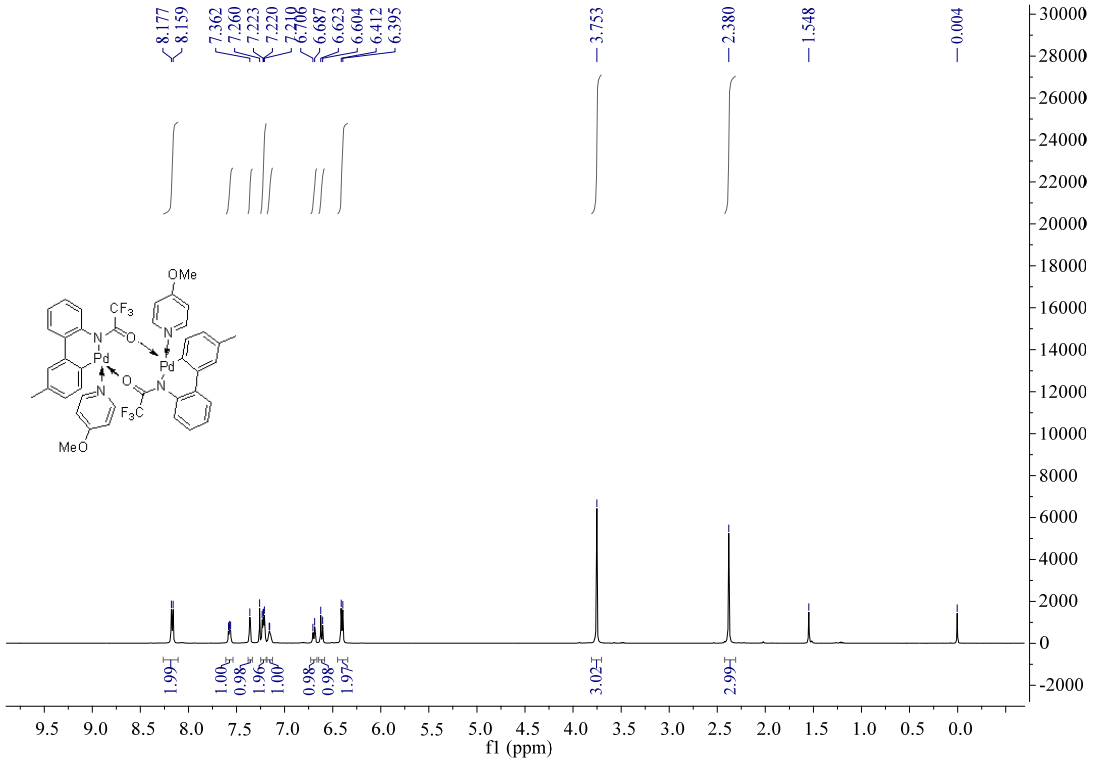

198.062
169.302
145.357
140.671
139.932
139.236
138.173
135.842
131.267
130.535
129.784
129.676
128.992
128.433
128.364
127.849
125.930
77.478
77.160
76.842
26.755
22.981
21.577
CH3
O
NH
CH3
O
H3C
fl (ppm)

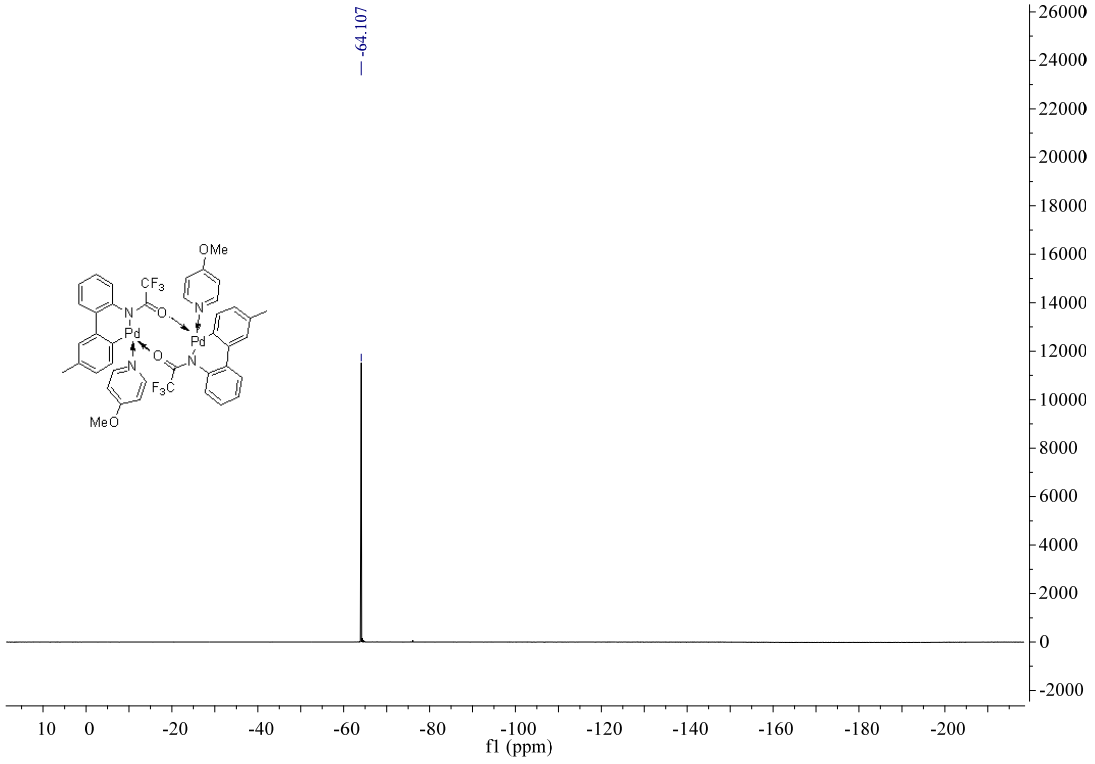
INT-I

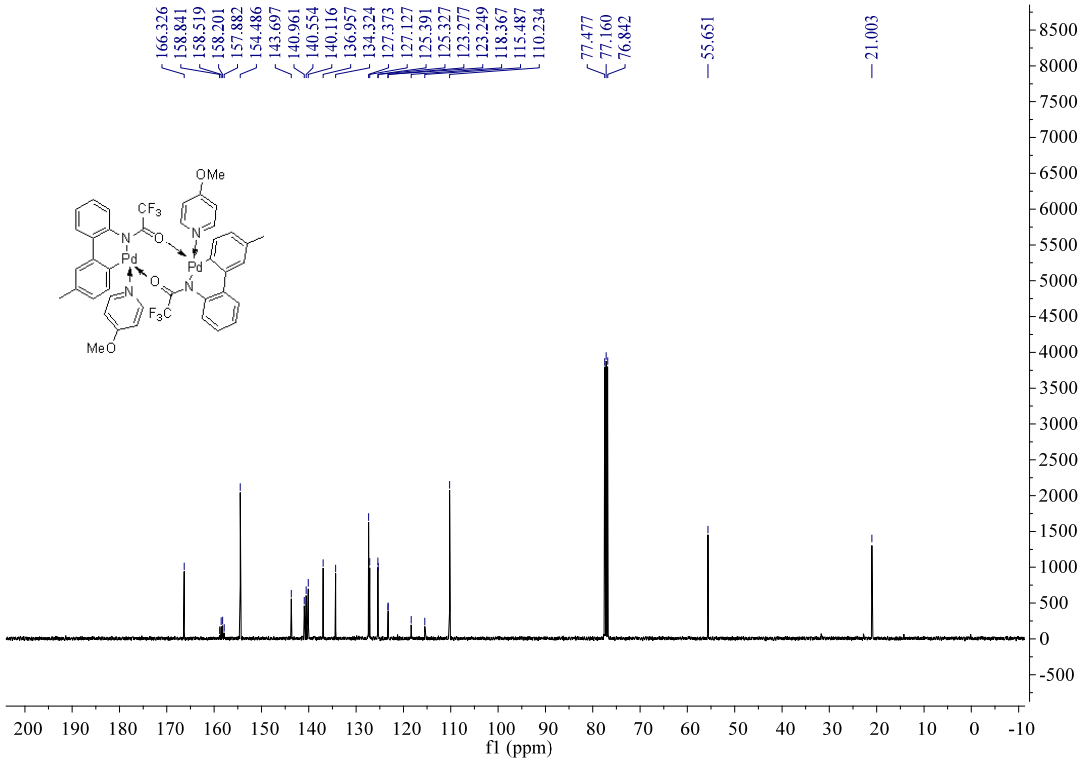

8.051
7.273
7.032
7.021
7.009
6.954
6.915
6.903
6.797
6.780
5.300
2.347
1.425
1.00
2.04
0.99
3.93
3.05
3.00
f1 (ppm)


166.872
166.034
165.656
140.237
137.224
132.935
129.721
129.611
129.494
128.437
127.353
126.365
124.977
123.532
116.727
116.083
113.870
54.061
53.791
53.520
53.250
52.979
21.376
20.977
f1 (ppm)

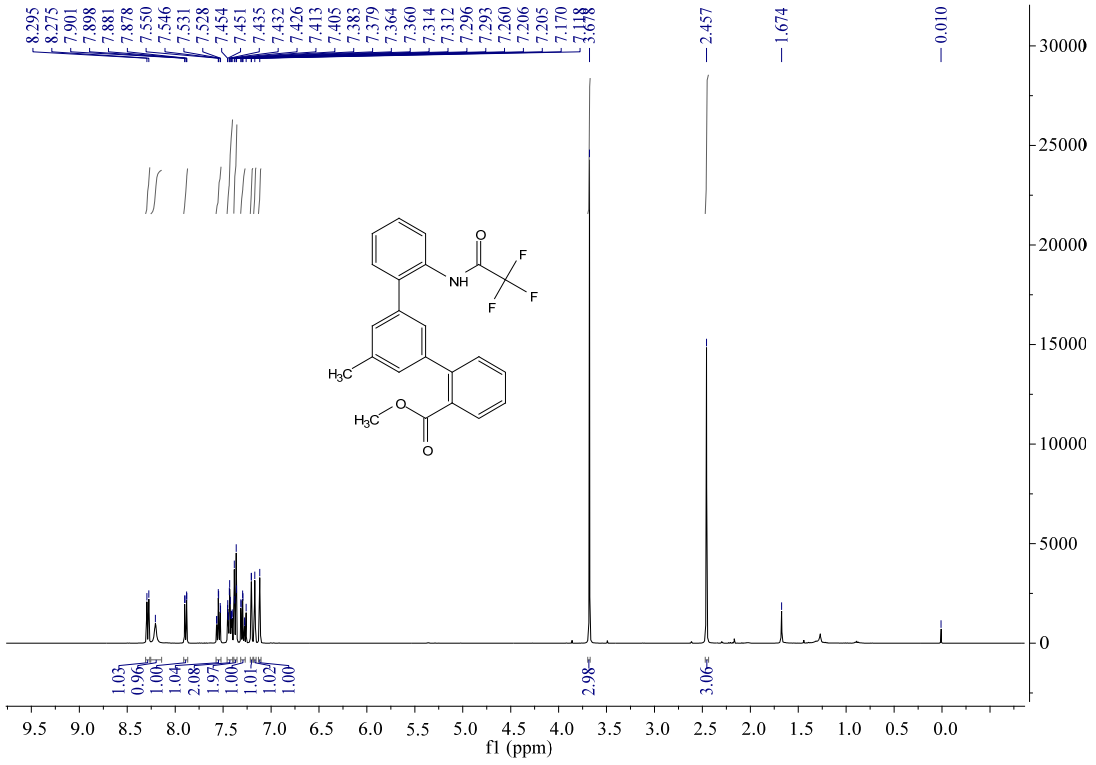
INT-IIa

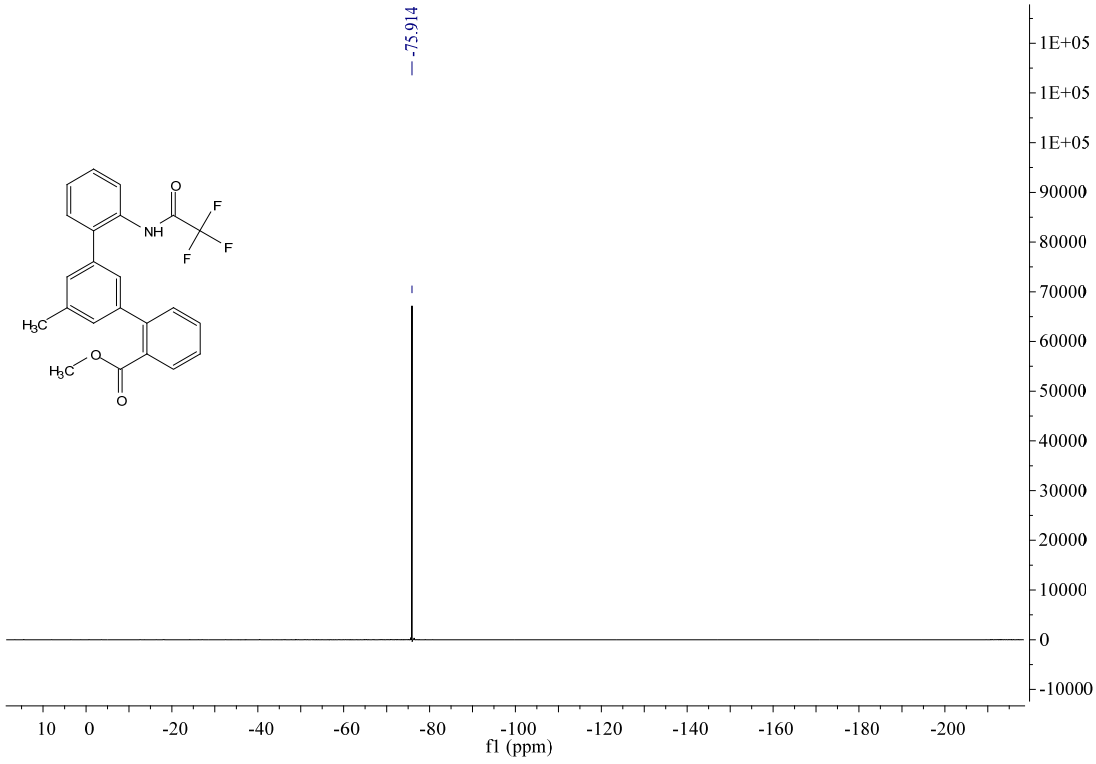

8.177
8.159
7.362
7.260
7.223
7.220
7.210
7.206
6.687
6.623
6.604
6.412
6.395
3.753
2.380
1.548
0.004
OMe
CF3
N
O
Pd
Pd
N
O
N
F3C
MeO
1.99
1.00
0.98
1.96
1.00
0.98
0.98
1.97
3.02
2.99
f1 (ppm)

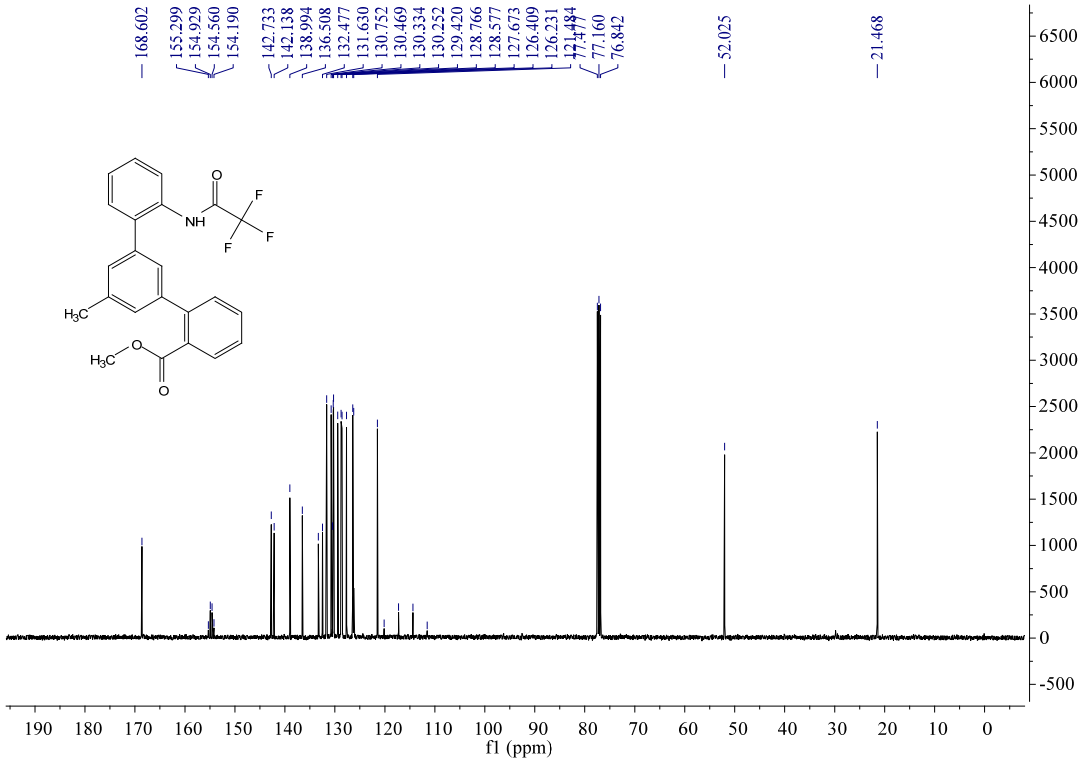

-64.107
OMe
CF3
N
O
Pd
Pd
N
O
N
F3C
MeO
f1 (ppm)


166.326
158.841
158.519
158.201
157.882
154.486
143.697
140.961
140.554
140.116
136.957
134.324
127.373
127.127
125.391
125.327
123.277
123.249
118.367
115.487
110.234
77.477
77.160
76.842
55.651
21.003
OMe
CF3
N
O
Pd
Pd
N
O
N
F3C
MeO
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

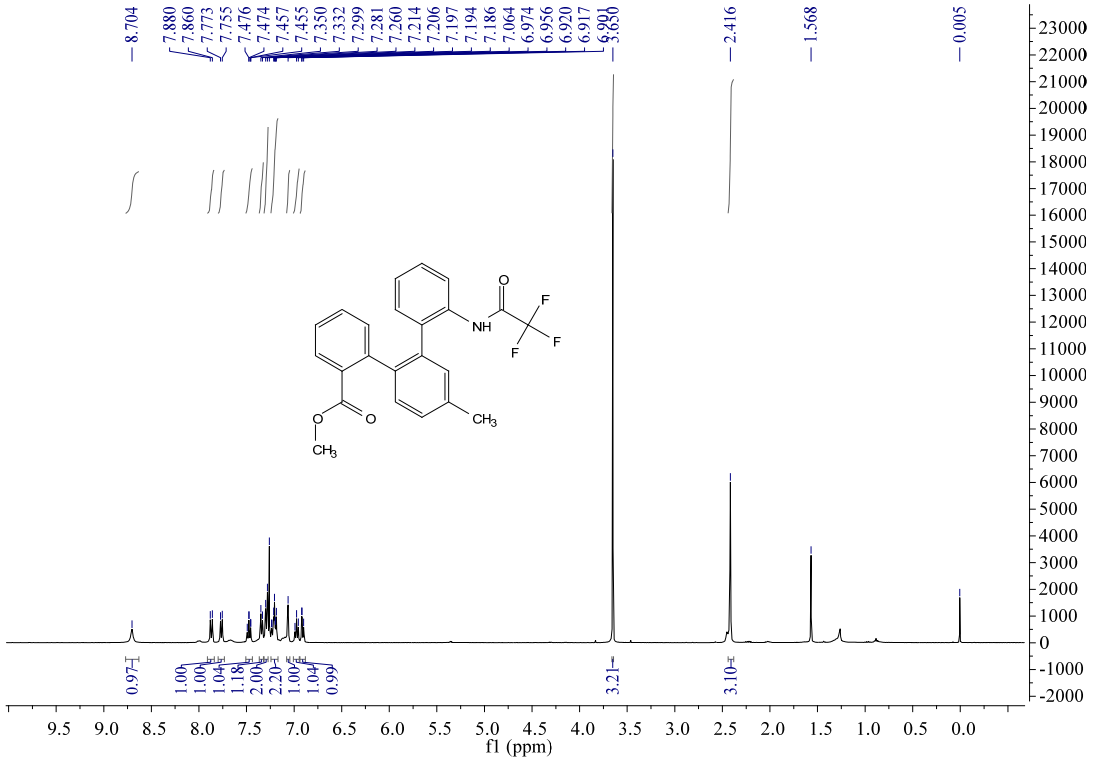
4b


8.295
8.275
7.901
7.898
7.881
7.878
7.550
7.546
7.531
7.528
7.454
7.451
7.435
7.432
7.426
7.413
7.405
7.383
7.379
7.364
7.360
7.314
7.312
7.296
7.293
7.260
7.206
7.205
7.170
7.118
3.678
2.457
1.674
0.010
NH
O
F
F
F
H3C
O
H3C
O
1.03
0.96
1.00
1.04
2.08
1.97
1.00
1.01
1.02
1.00
2.98
3.06
fl (ppm)


-75.914
NH
O
F
F
F
H3C
O
H3C
O
fl (ppm)


168.602
155.299
154.929
154.560
154.190
142.733
142.138
138.994
136.508
132.477
131.630
130.752
130.469
130.334
130.252
129.420
128.766
128.577
127.673
126.409
126.231
121.484
77.160
76.842
52.025
21.468
O
NH
F
F
F
H3C
O
H3C
O
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

5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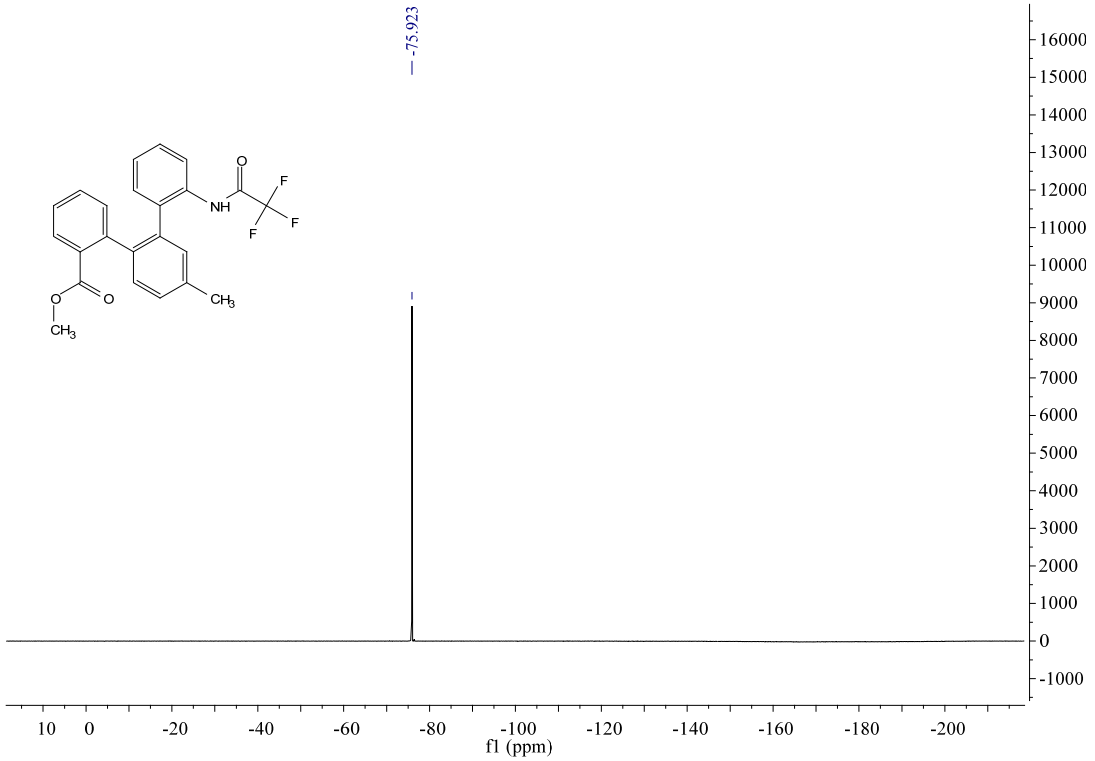
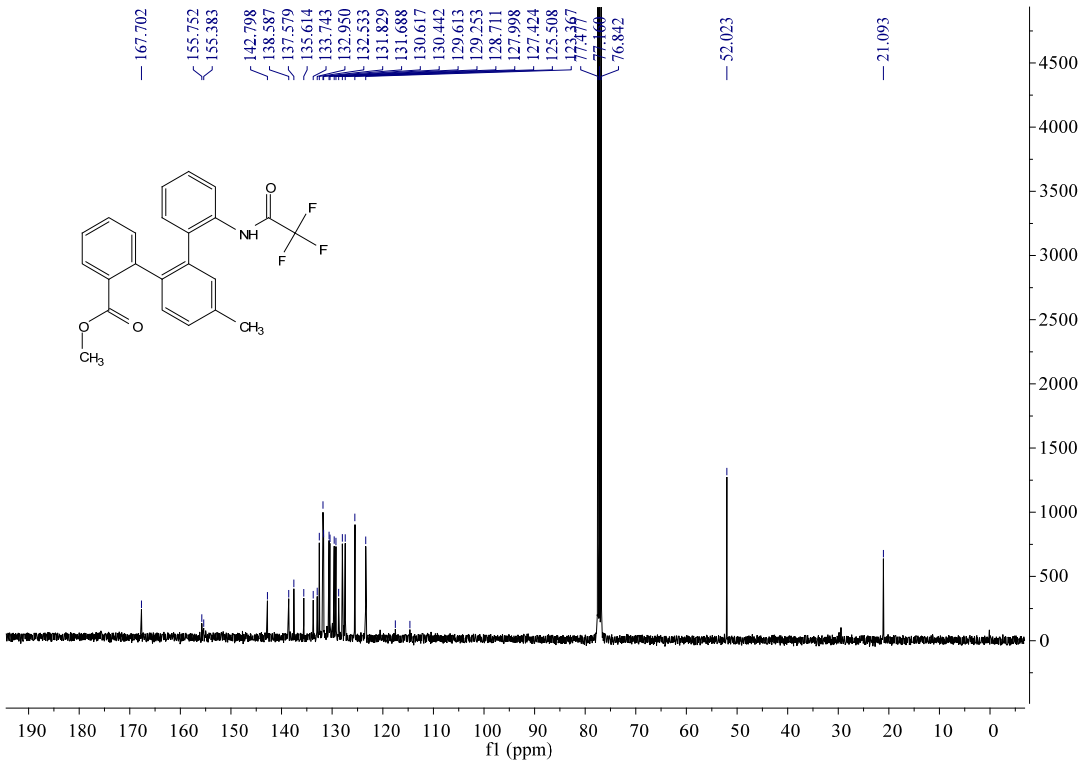
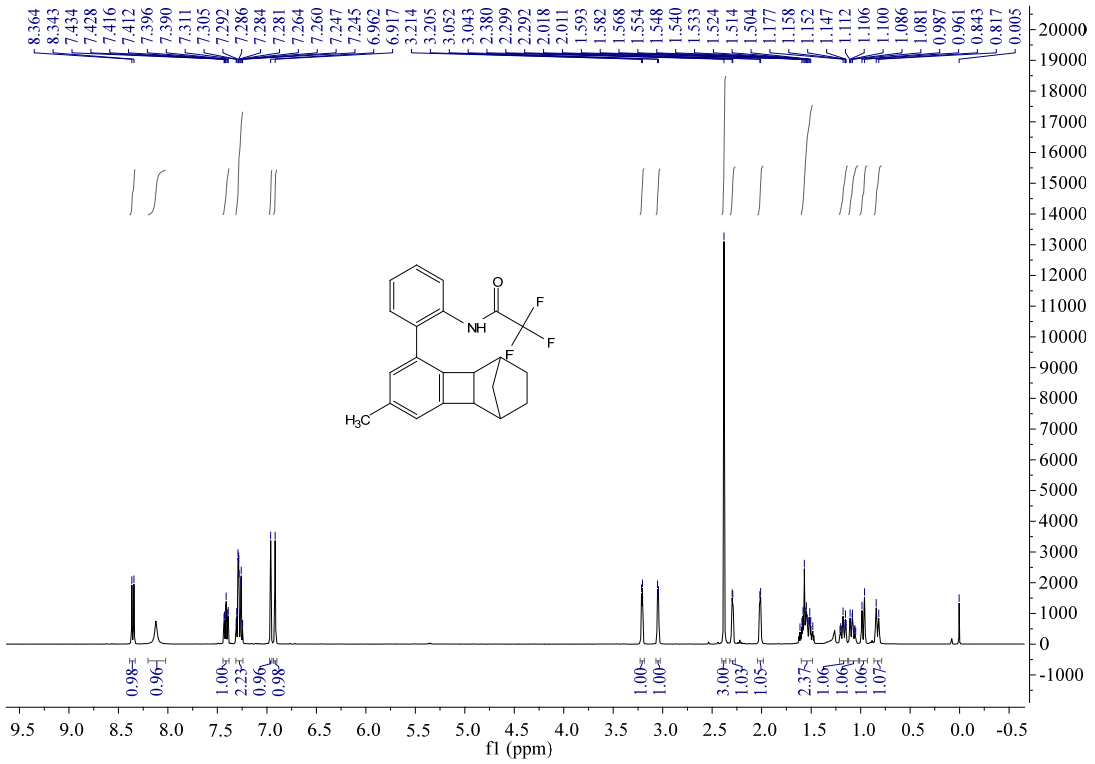
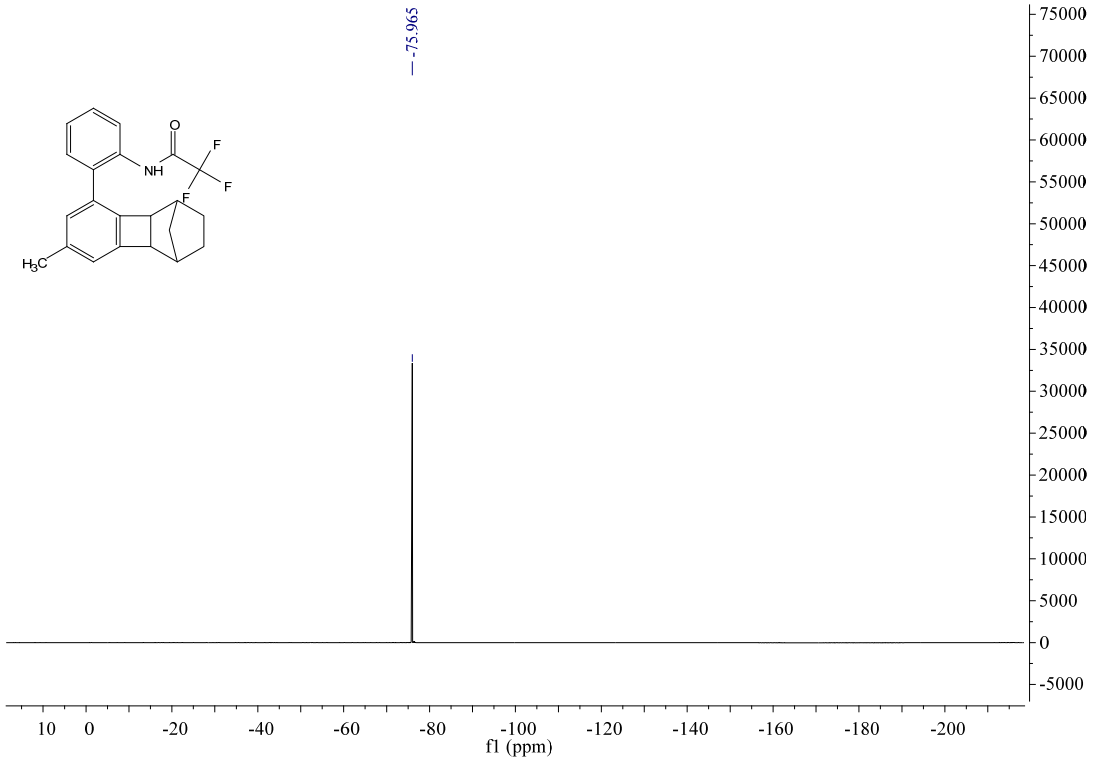
7.880
7.860
7.773
7.755
7.476
7.474
7.457
7.455
7.350
7.332
7.299
7.281
7.260
7.214
7.206
7.197
7.194
7.186
7.064
6.974
6.956
6.920
6.917
6.901
6.850
2.416
1.568
0.005
0.97
1.00
1.00
1.04
1.18
2.00
2.20
1.00
1.04
0.99
3.21
3.10
NH
F
F
F
O
O
O
CH3
CH3
f1 (ppm)

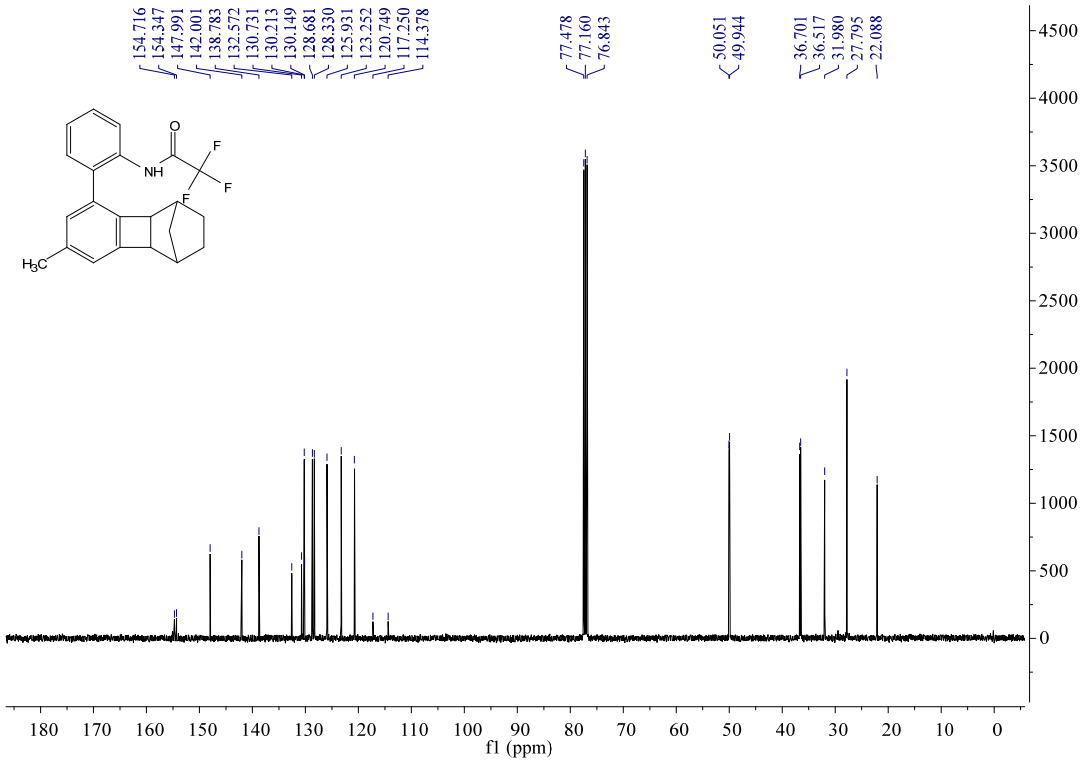

-75.923
NH
F
F
F
O
O
O
CH3
CH3
f1 (ppm)


167.702
155.752
155.383
142.798
138.587
137.579
135.614
133.743
132.950
132.533
131.829
131.688
130.617
130.442
129.613
129.253
128.711
127.998
127.424
125.508
76.842
52.023
21.093
O
NH
F
F
F
O
O
CH3
CH3
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

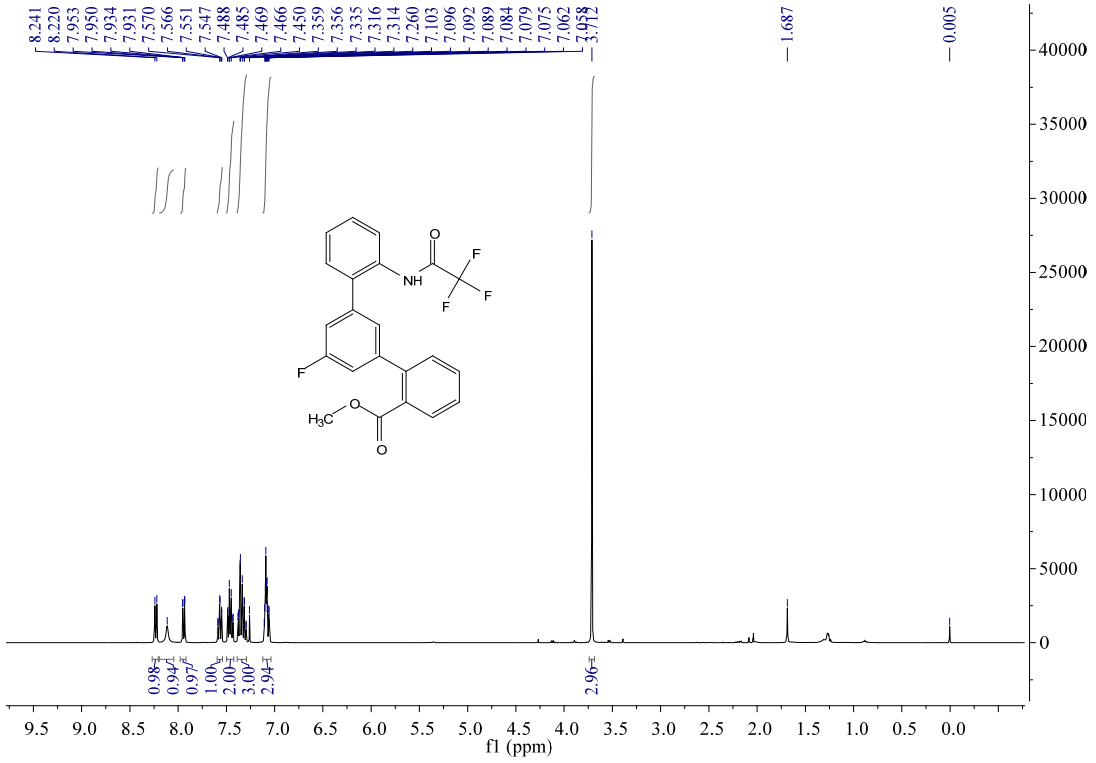
2b

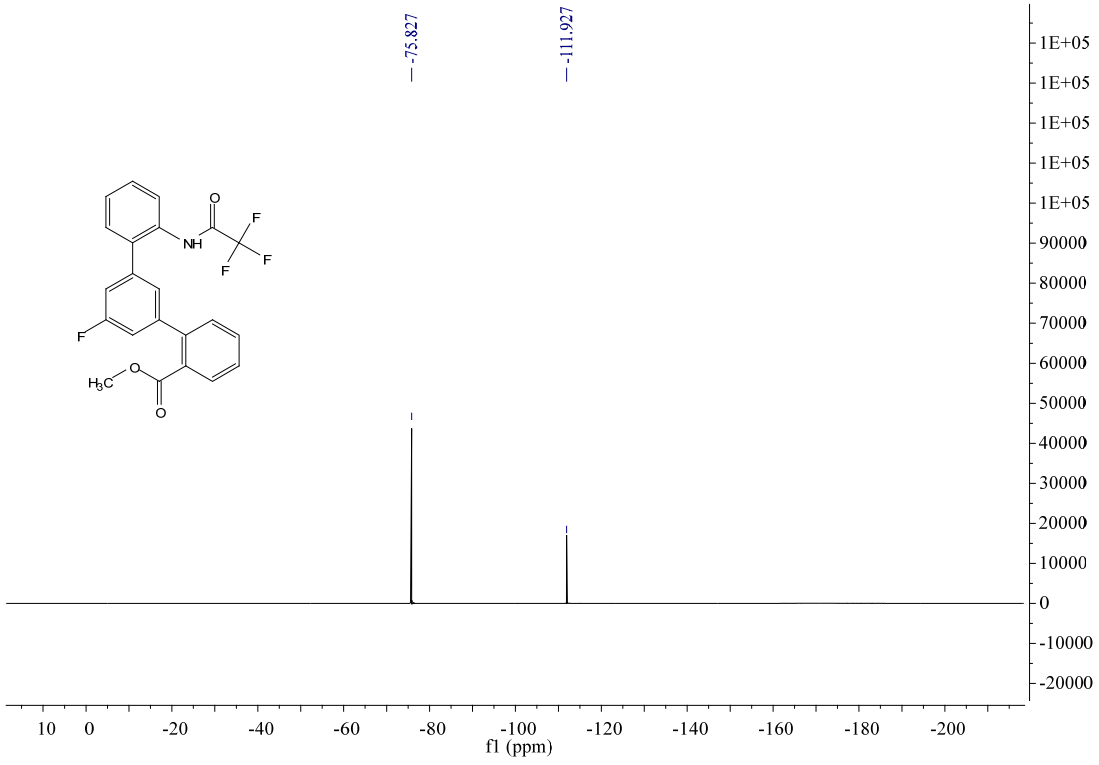

8.364
8.343
7.434
7.428
7.416
7.412
7.396
7.390
7.311
7.305
7.292
7.286
7.284
7.281
7.264
7.260
7.247
7.245
6.962
6.917
3.214
3.205
3.052
3.043
2.380
2.299
2.292
2.018
2.011
1.593
1.582
1.568
1.554
1.548
1.540
1.533
1.524
1.514
1.504
1.177
1.158
1.152
1.147
1.112
1.106
1.100
1.086
1.081
0.987
0.961
0.843
0.817
0.005
O
NH
F
F
F
H3C
0.98
0.96
1.00
2.23
0.96
0.98
1.00
1.00
3.00
1.03
1.05
2.37
1.06
1.06
1.06
1.07
fl (ppm)

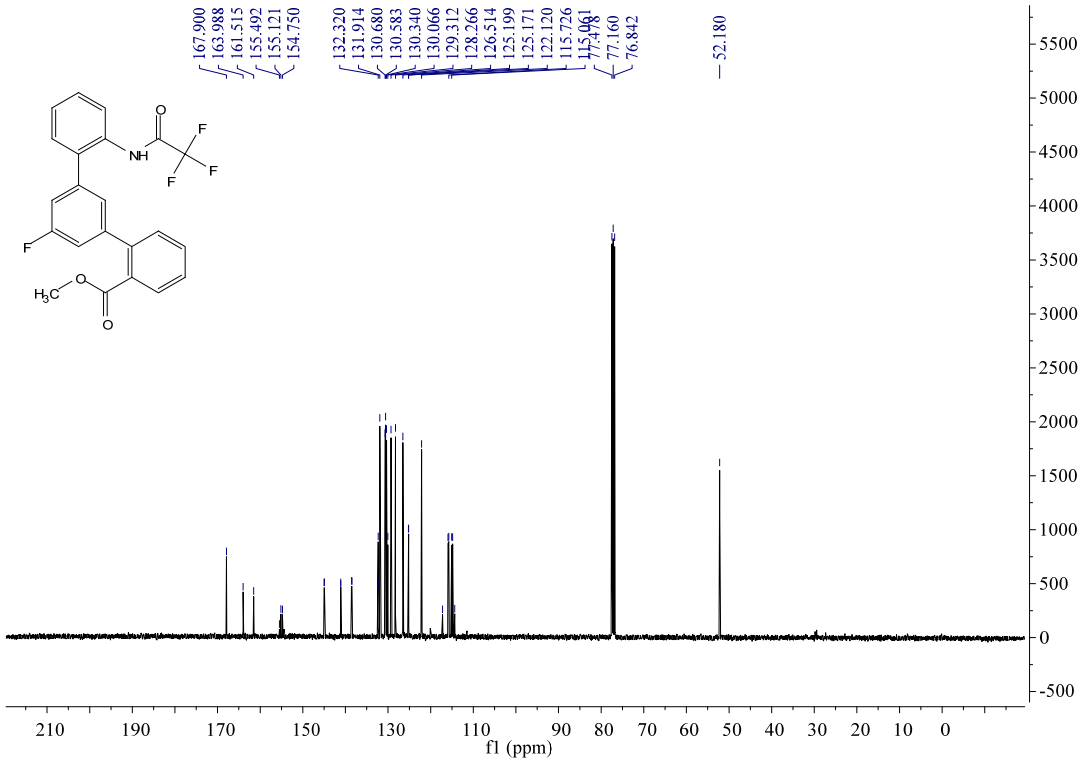

-75.965
O
NH
F
F
F
H3C
fl (ppm)


154.716
154.347
147.991
142.001
138.783
132.572
130.731
130.213
130.149
128.681
128.330
125.931
123.252
120.749
117.250
114.378
77.478
77.160
76.843
50.051
49.944
36.701
36.517
31.980
27.795
22.088
O
NH
F
F
F
H3C
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

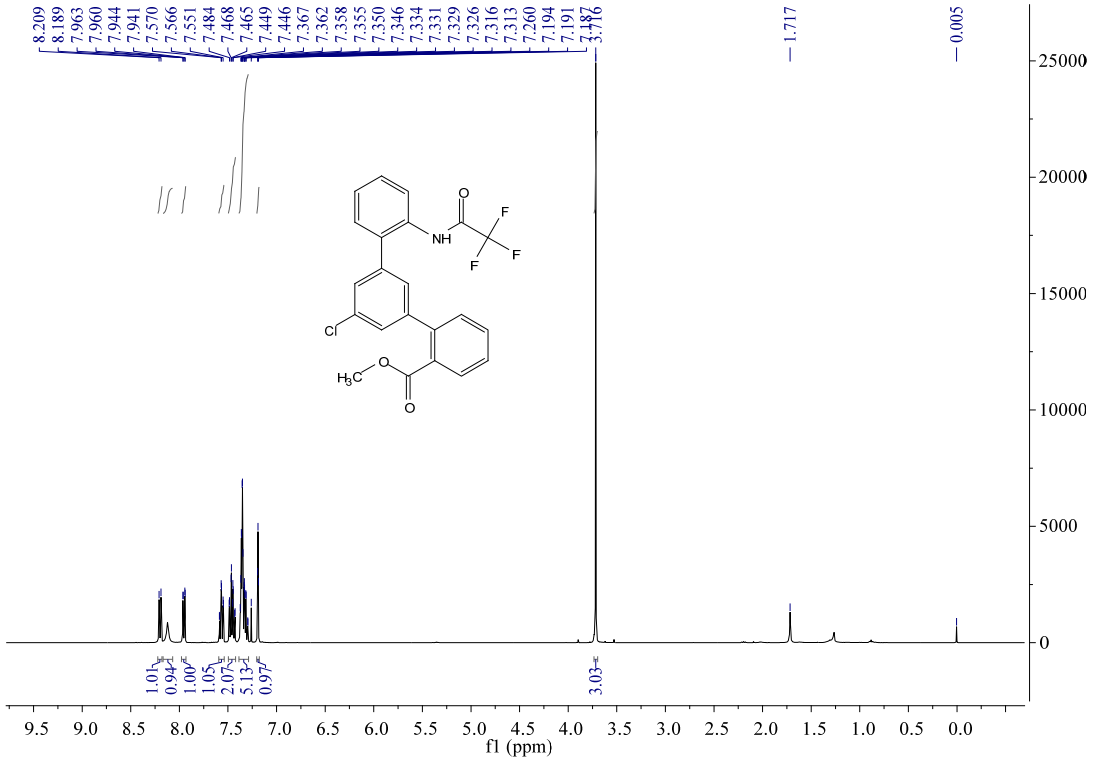
4a

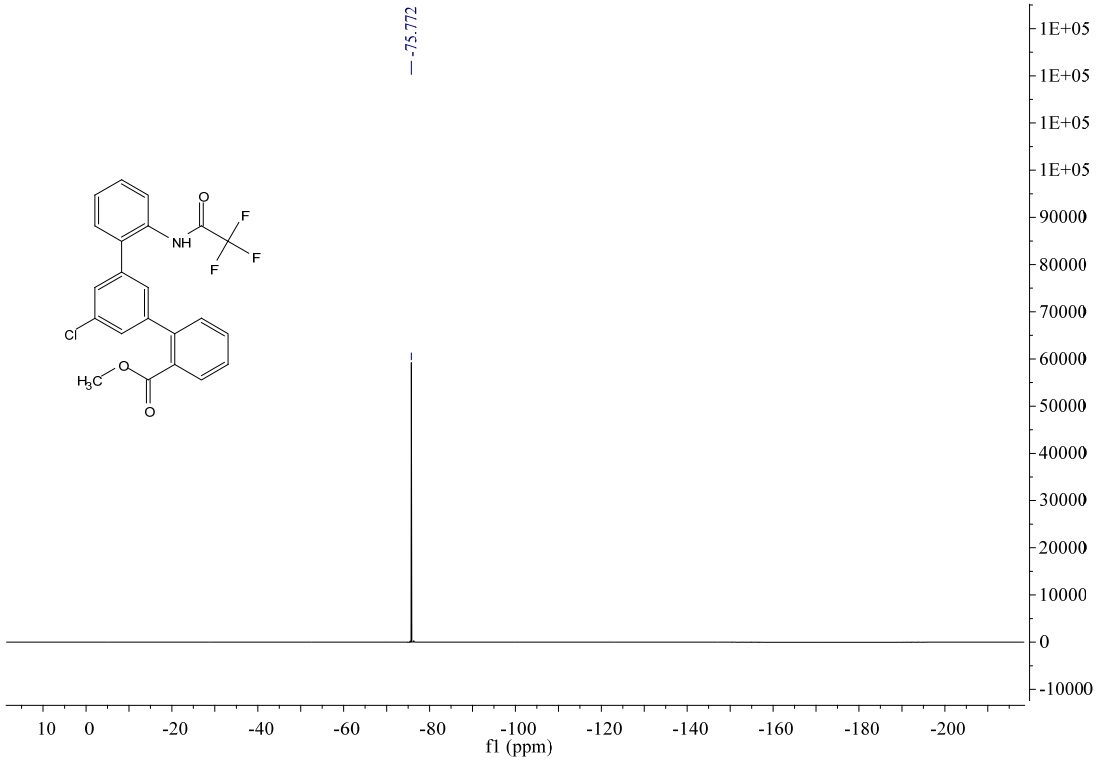

8.241
8.220
7.953
7.950
7.934
7.931
7.570
7.566
7.551
7.547
7.488
7.485
7.469
7.466
7.450
7.359
7.356
7.335
7.316
7.314
7.260
7.103
7.096
7.092
7.089
7.084
7.079
7.075
7.062
3.712
1.687
0.005
0.98
0.94
0.97
1.00
2.00
3.00
2.94
2.96
NH
O
F
F
F
F
H3C
O
O
40000
35000
30000
25000
20000
15000
10000
5000
0
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

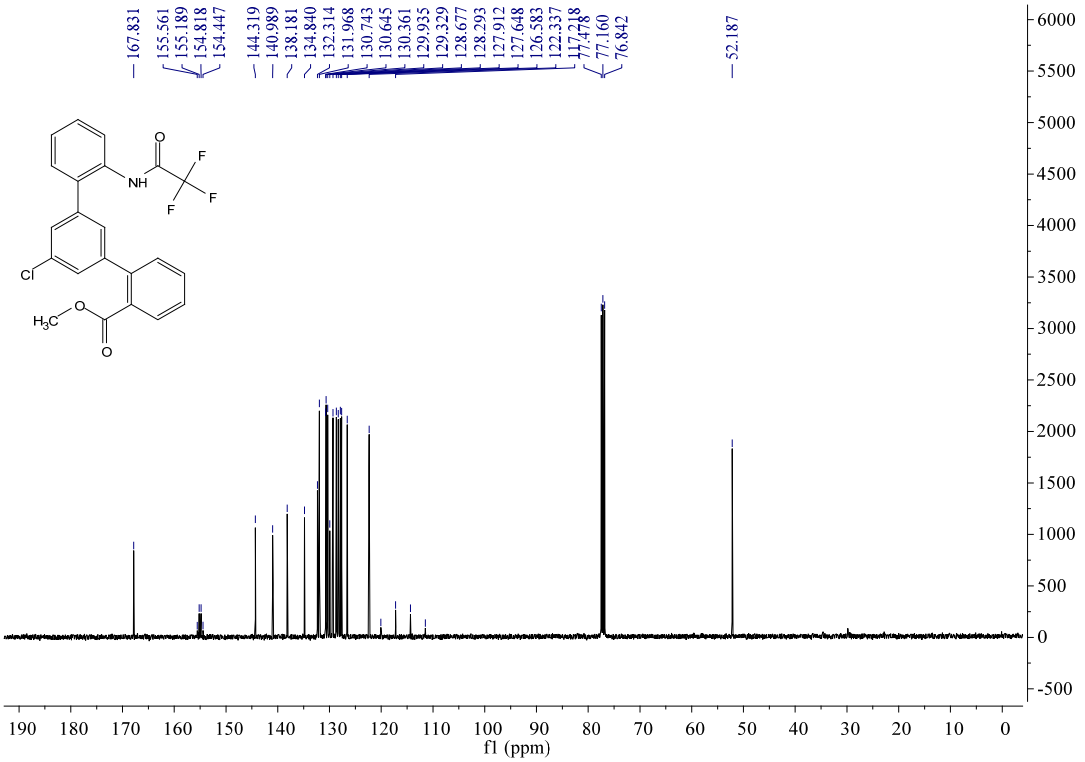

-75.827
-111.927
NH
O
F
F
F
F
H3C
O
O
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


167.900
163.988
161.515
155.492
155.121
154.750
132.320
131.914
130.680
130.583
130.340
130.066
129.312
128.266
126.514
125.199
125.171
122.120
115.726
77.478
77.160
76.842
52.180
NH
O
F
F
F
O
H3C
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

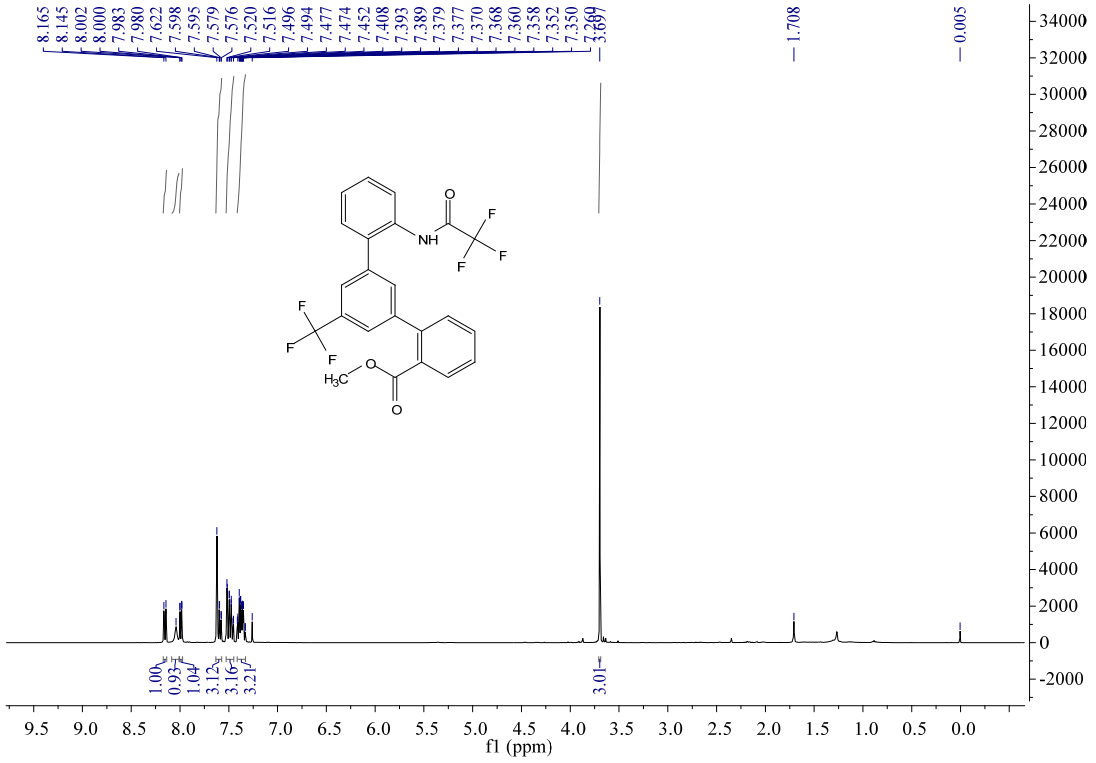
4c

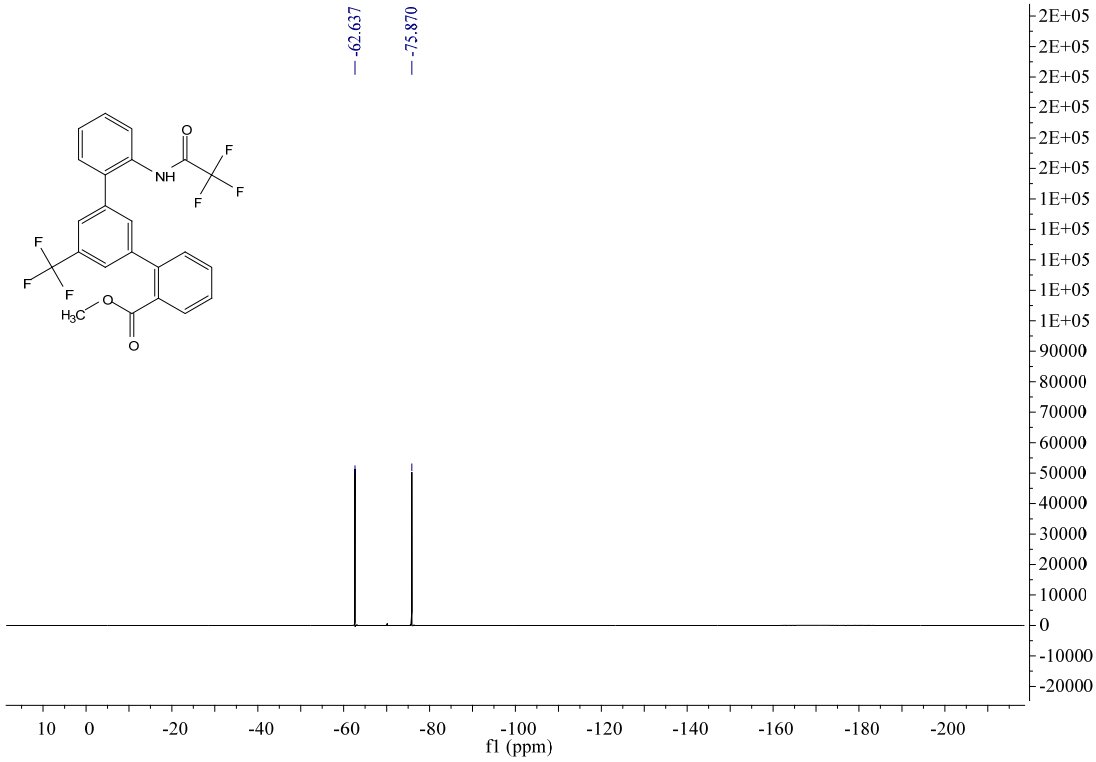

8.209
8.189
7.963
7.960
7.944
7.941
7.570
7.566
7.551
7.484
7.468
7.465
7.449
7.446
7.367
7.362
7.358
7.355
7.350
7.346
7.334
7.331
7.329
7.326
7.316
7.313
7.260
7.194
7.191
3.716
1.717
0.005
1.01
0.94
1.00
1.05
2.07
5.13
0.97
3.03
NH
O
F
F
F
Cl
O
H3C
O
25000
20000
15000
10000
5000
0
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

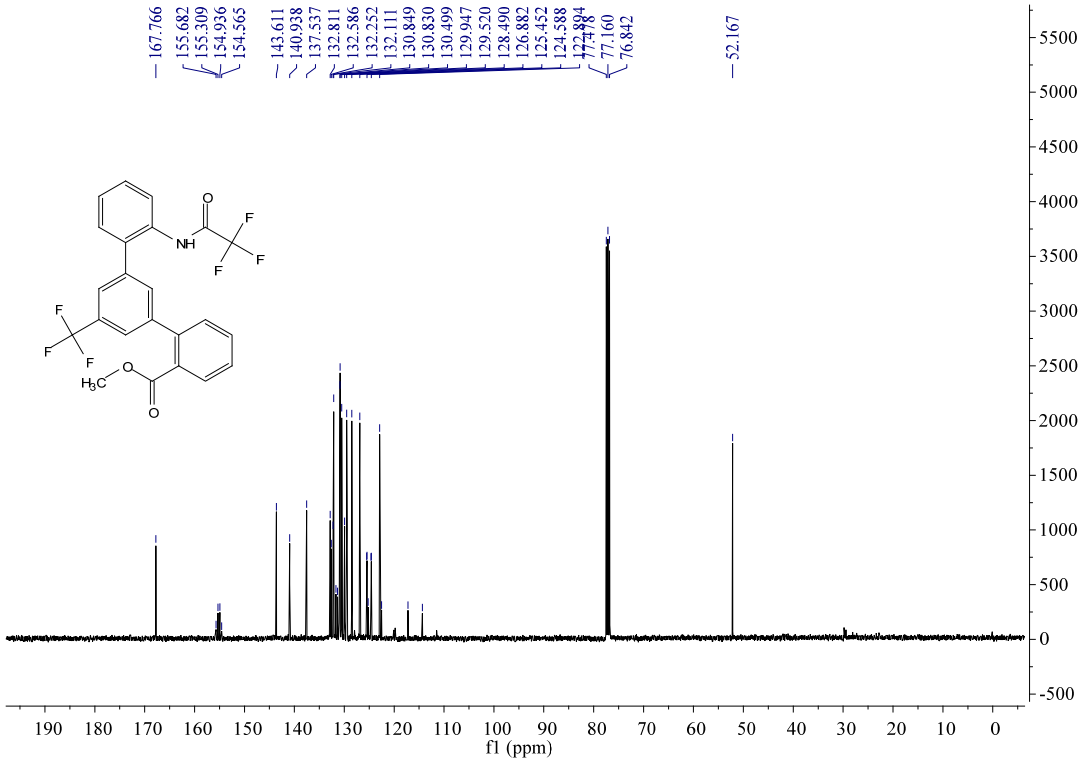

-75.772
NH
O
F
F
F
Cl
O
H3C
O
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


167.831
155.561
155.189
154.818
154.447
144.319
140.989
138.181
134.840
132.314
131.968
130.743
130.645
130.361
129.935
129.329
128.677
128.293
127.912
127.648
126.583
122.337
117.218
77.478
77.160
76.842
52.187
O
NH
F
F
F
Cl
H3C
O
O
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

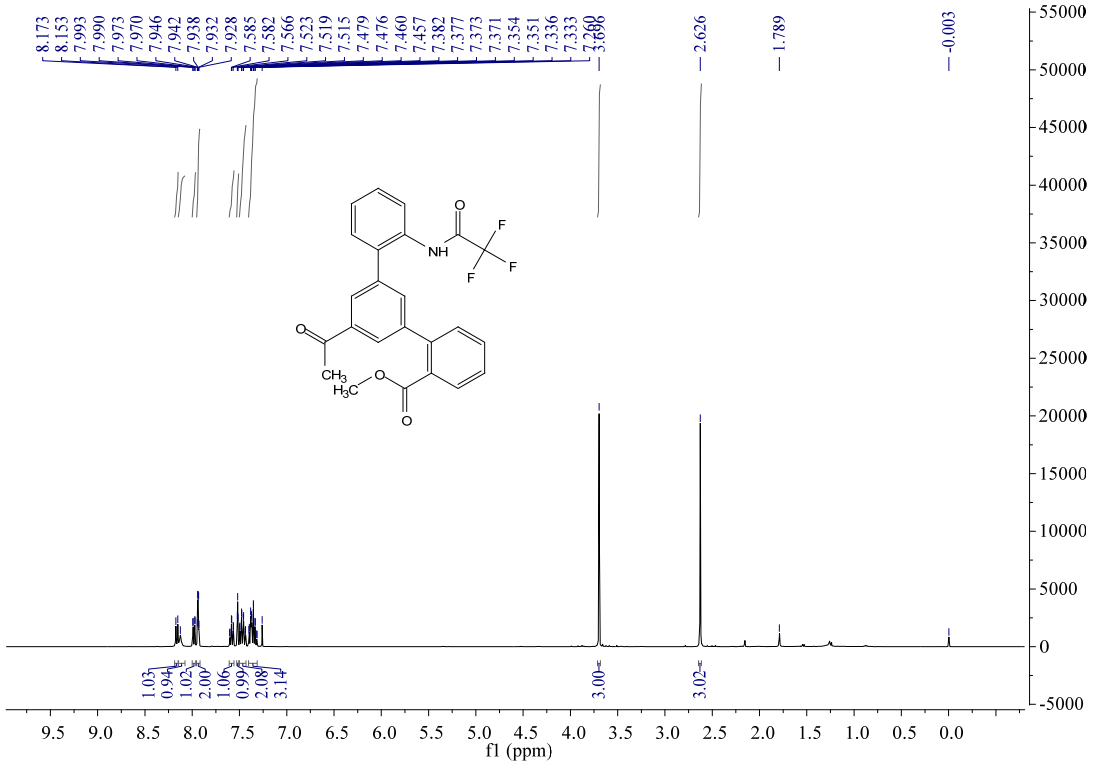
4d

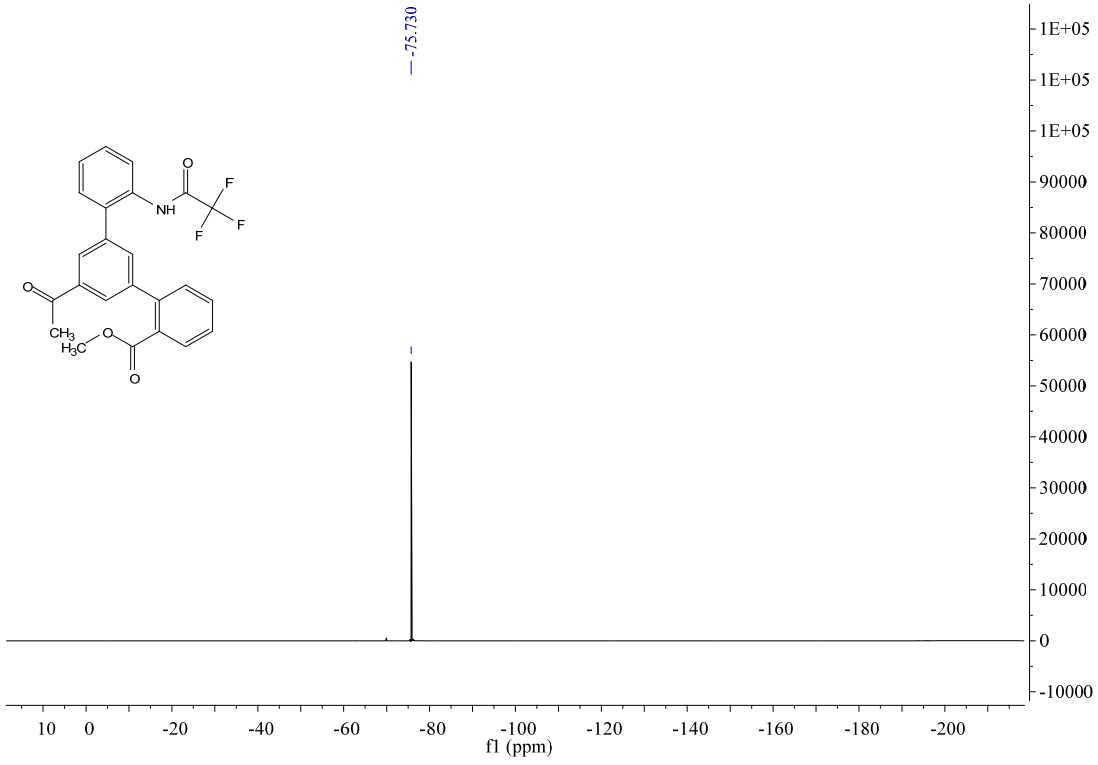

8.165
8.145
8.002
8.000
7.983
7.980
7.622
7.598
7.595
7.579
7.576
7.520
7.516
7.496
7.494
7.477
7.474
7.452
7.408
7.393
7.389
7.379
7.377
7.370
7.368
7.360
7.358
7.352
7.350
7.269
3.697
1.708
0.005
1.00
0.93
1.04
3.12
3.16
3.21
3.01
NH
O
F
F
F
F
F
H3C
O
O
fl (ppm)

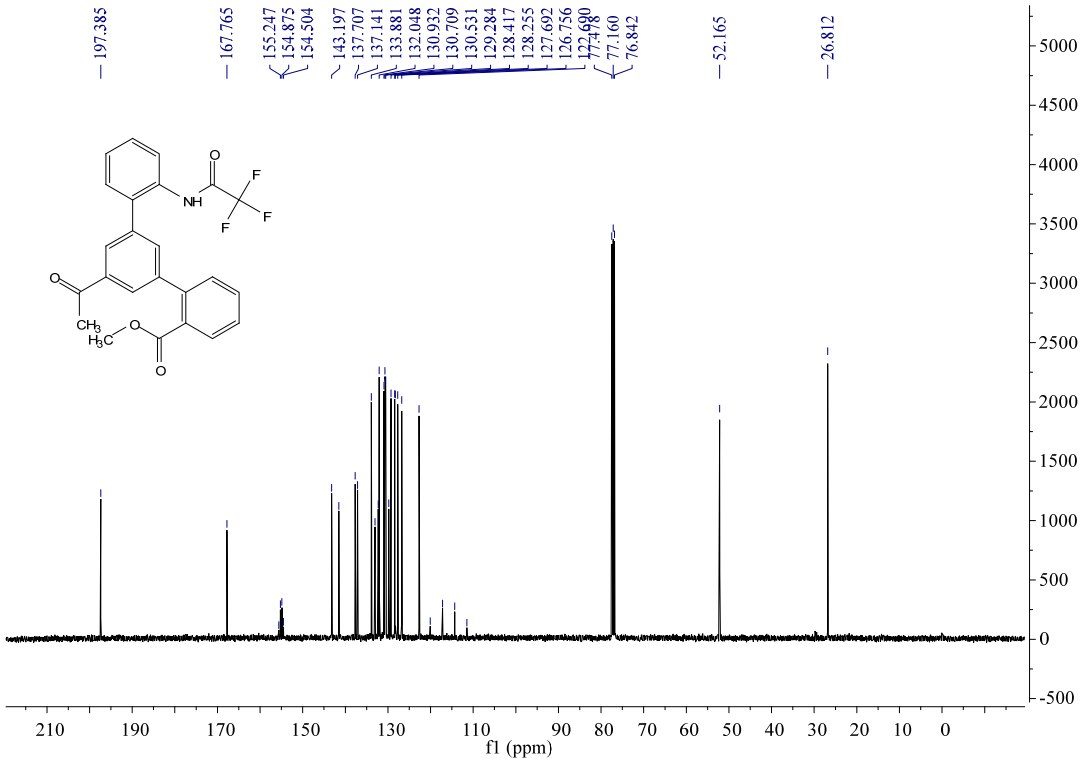

-62.637
-75.870
NH
O
F
F
F
F
F
H3C
O
O
fl (ppm)


167.766
155.682
155.309
154.936
154.565
143.611
140.938
137.537
132.811
132.586
132.252
132.111
130.849
130.830
130.499
129.947
129.520
128.490
126.882
125.452
124.588
122.894
77.478
77.160
76.842
52.167
NH
O
F
F
F
F
F
O
H3C
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

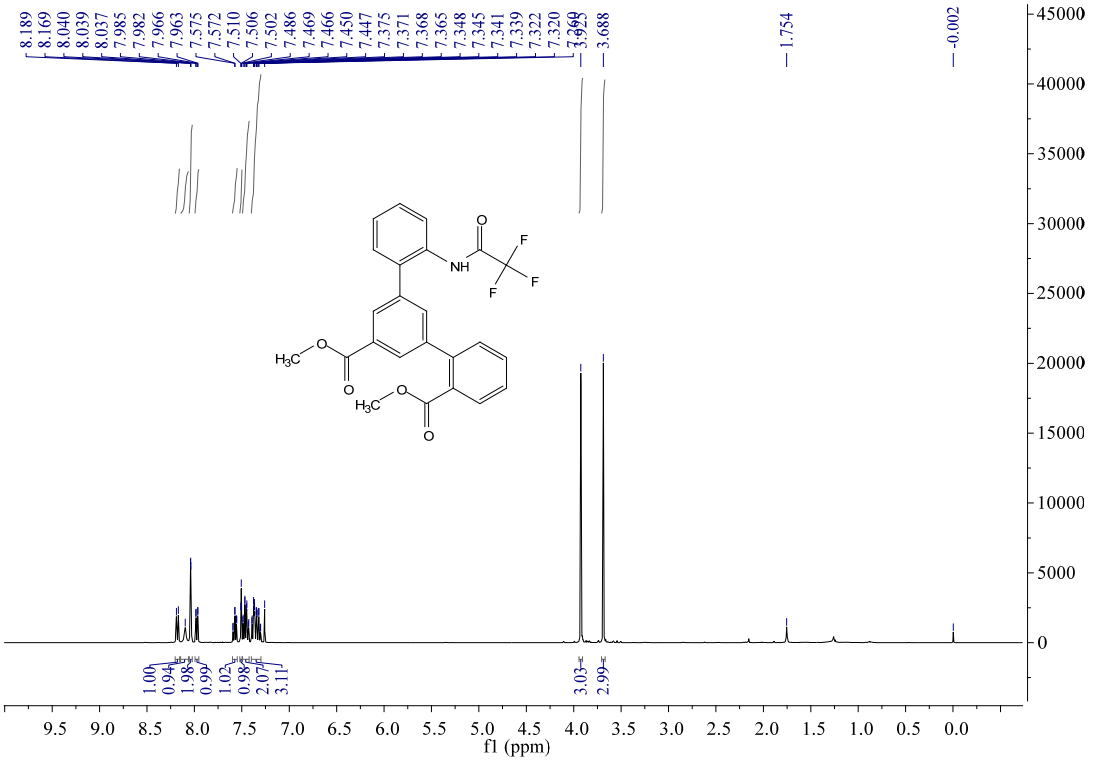
4e

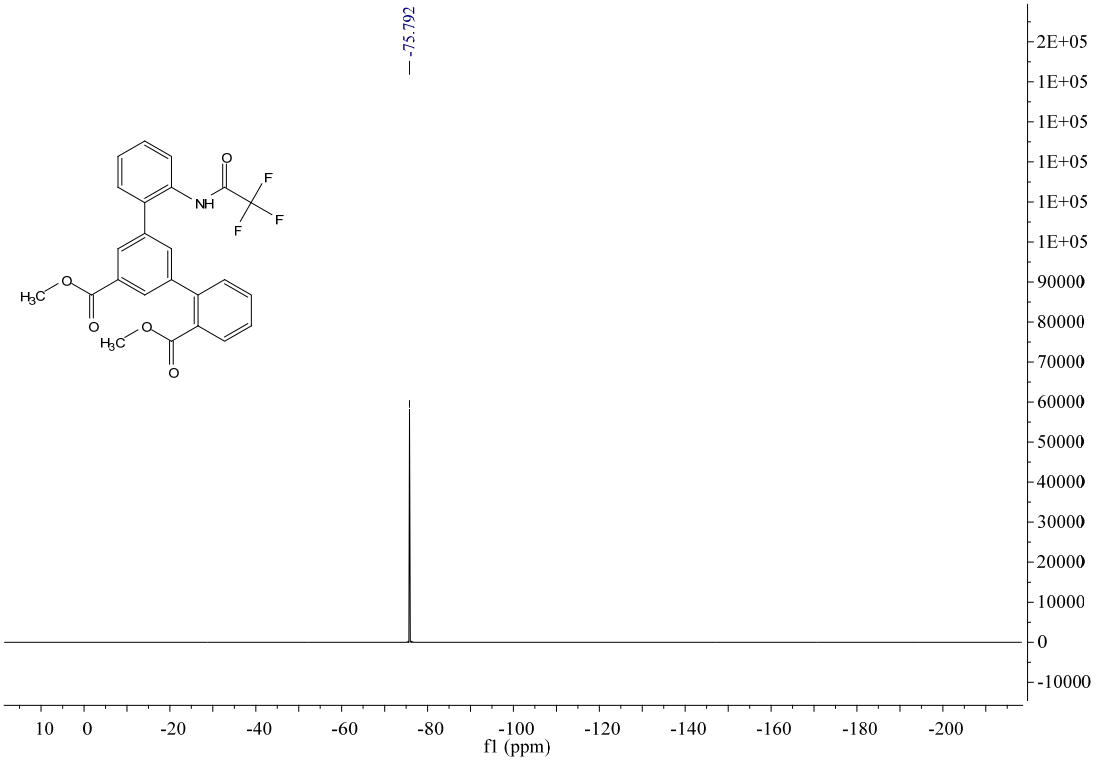

8.173
8.153
7.993
7.990
7.973
7.970
7.946
7.942
7.938
7.932
7.928
7.585
7.582
7.566
7.523
7.519
7.515
7.479
7.476
7.460
7.457
7.382
7.377
7.373
7.371
7.354
7.351
7.336
7.333
3.698
2.626
1.789
-0.003
NH
F
F
F
O
O
CH3
H3C
O
O
1.03
0.94
1.03
2.00
1.06
0.99
2.08
3.14
3.00
3.02
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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)

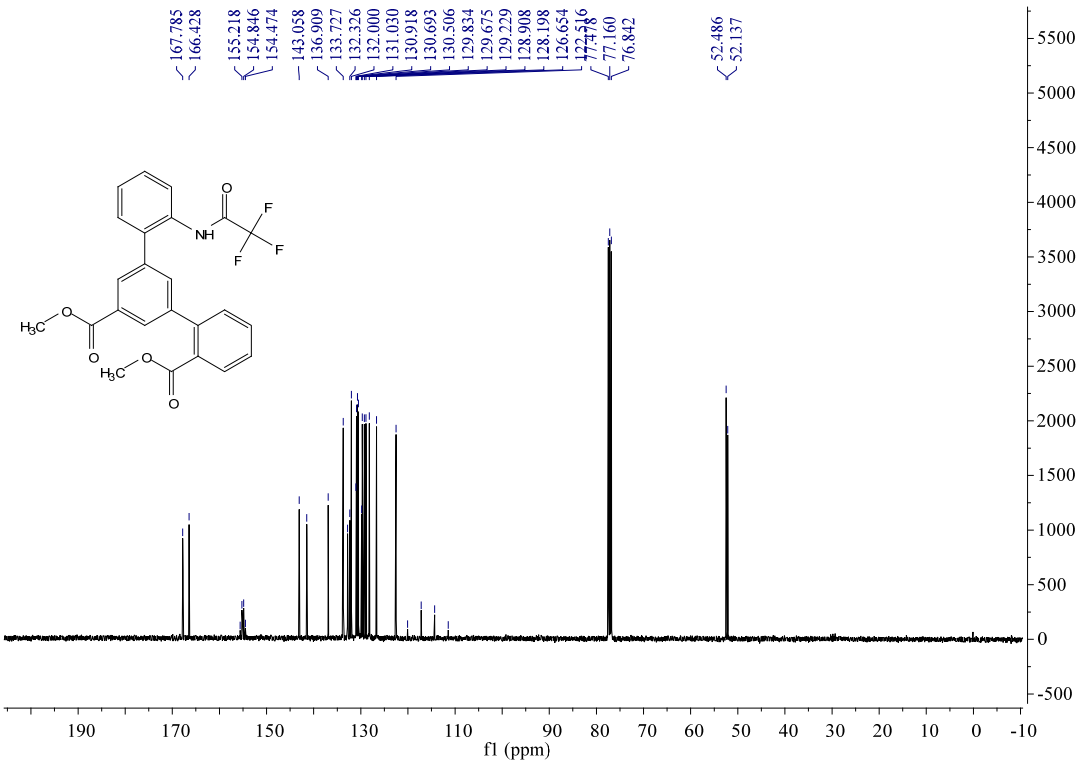

-75.730
NH
F
F
F
O
O
CH3
H3C
O
O
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


197.385
167.765
155.247
154.875
154.504
143.197
137.707
137.141
133.881
132.048
130.932
130.709
130.531
129.284
128.417
128.255
127.692
126.756
77.160
76.842
52.165
26.812
NH
O
F
F
F
O
CH3
H3C
O
O
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

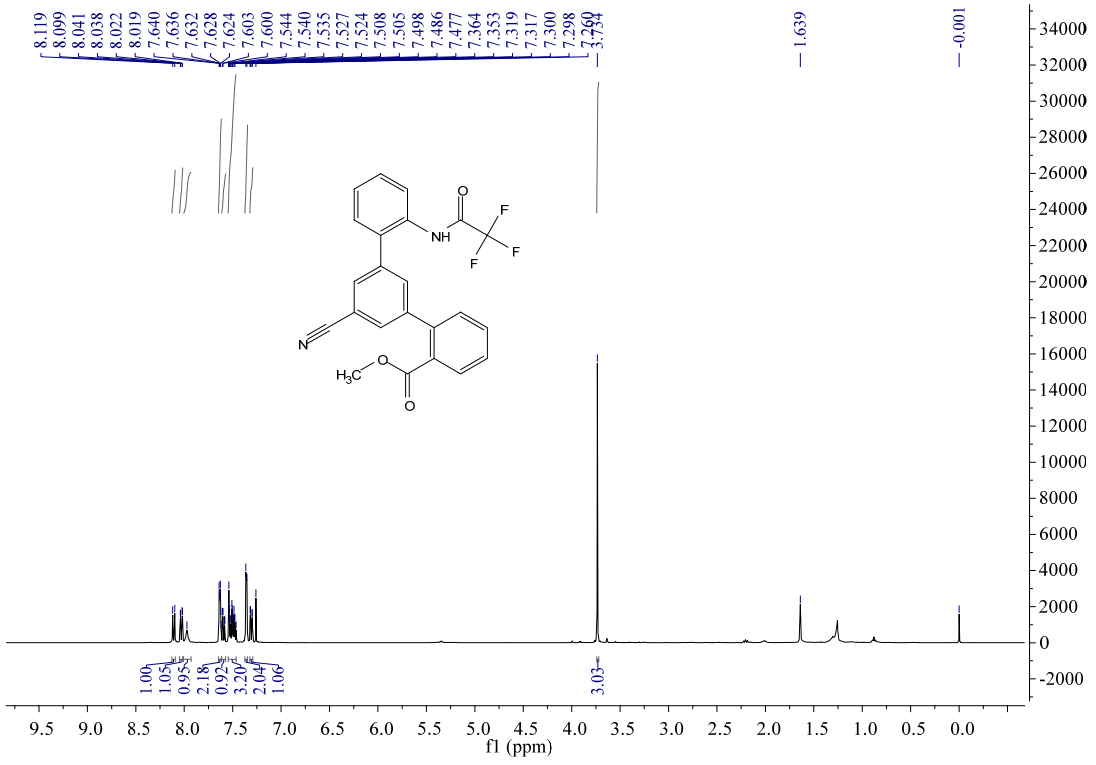
4f

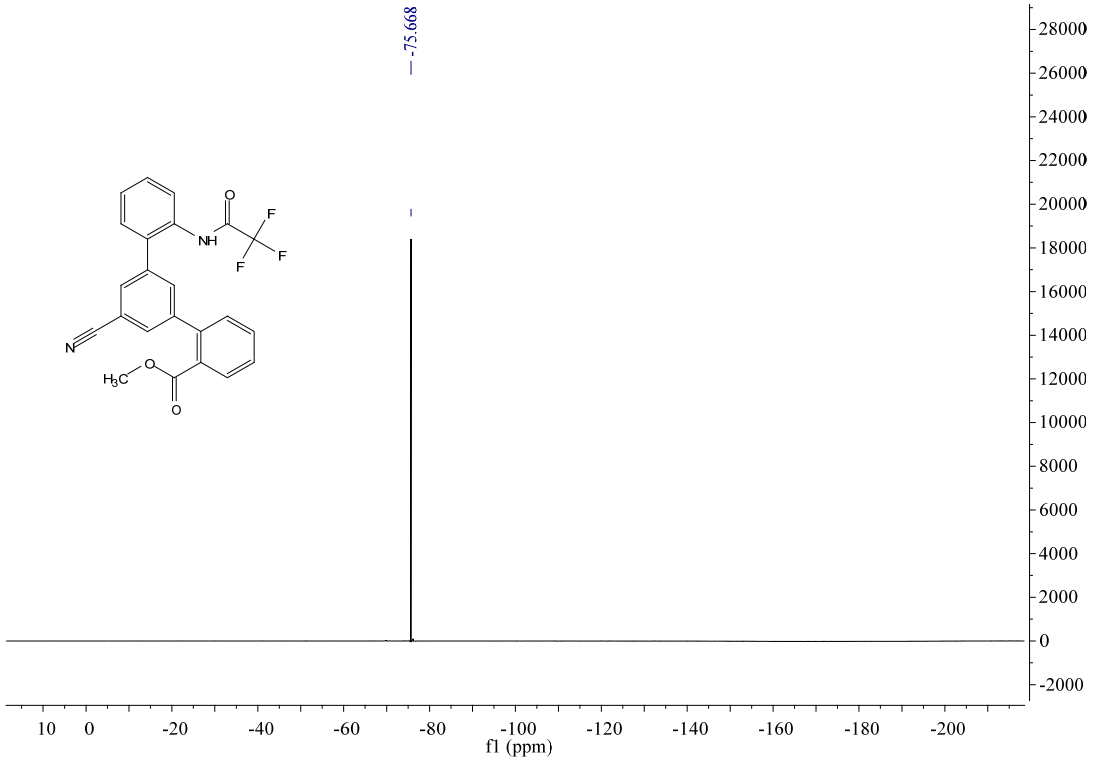

8.189
8.169
8.040
8.039
8.037
7.985
7.982
7.966
7.963
7.575
7.572
7.510
7.506
7.502
7.486
7.469
7.466
7.450
7.447
7.375
7.371
7.368
7.365
7.348
7.345
7.341
7.339
7.322
7.320
3.925
3.688
1.754
-0.002
1.00
0.94
1.98
0.99
1.02
0.98
2.07
3.11
3.03
2.99
O
NH
F
F
F
H3C
O
O
H3C
O
O
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

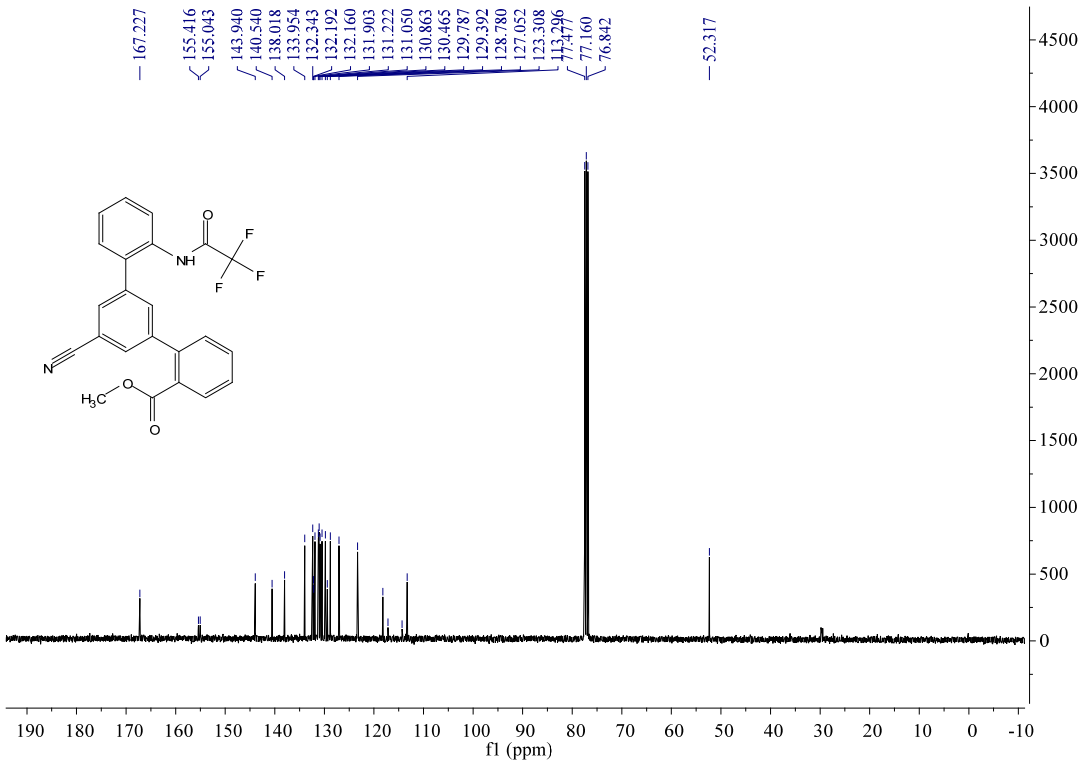

-75.792
O
NH
F
F
F
H3C
O
O
H3C
O
O
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


167.785
166.428
155.218
154.846
154.474
143.058
136.909
133.727
132.326
132.000
131.030
130.918
130.693
130.506
129.834
129.675
129.229
128.908
128.198
126.654
122.516
77.160
76.842
52.486
52.137
NH
O
F
F
F
H3C
O
O
H3C
O
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

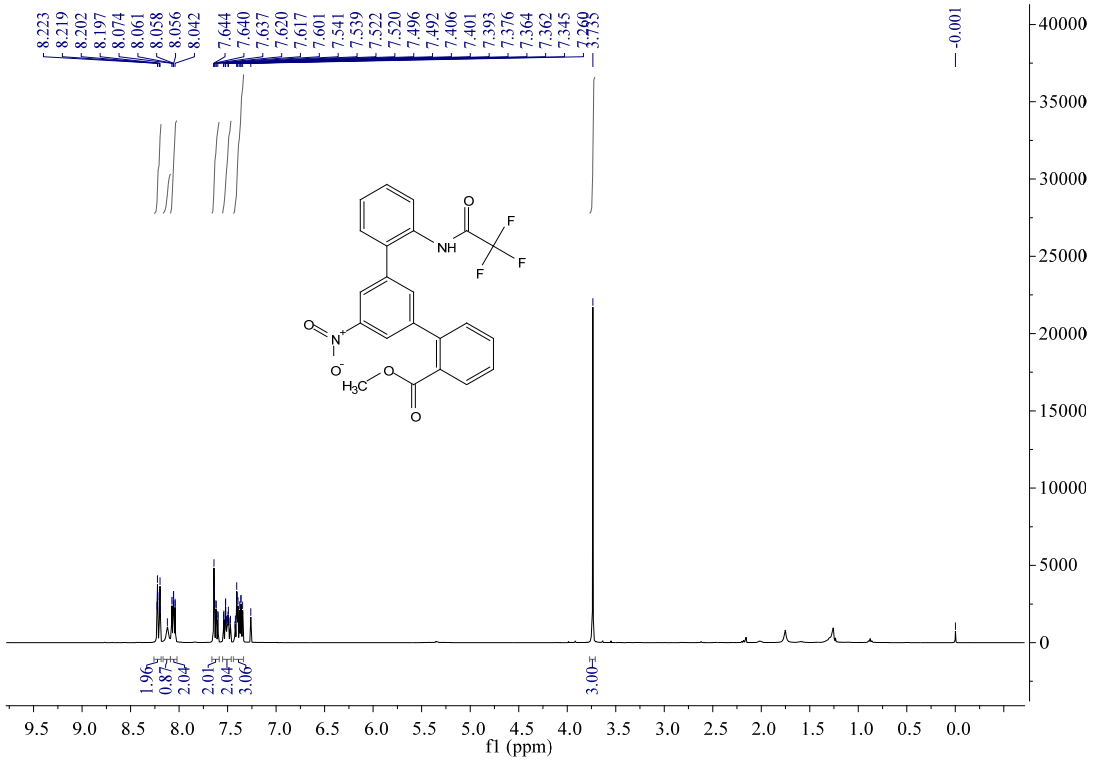
4g

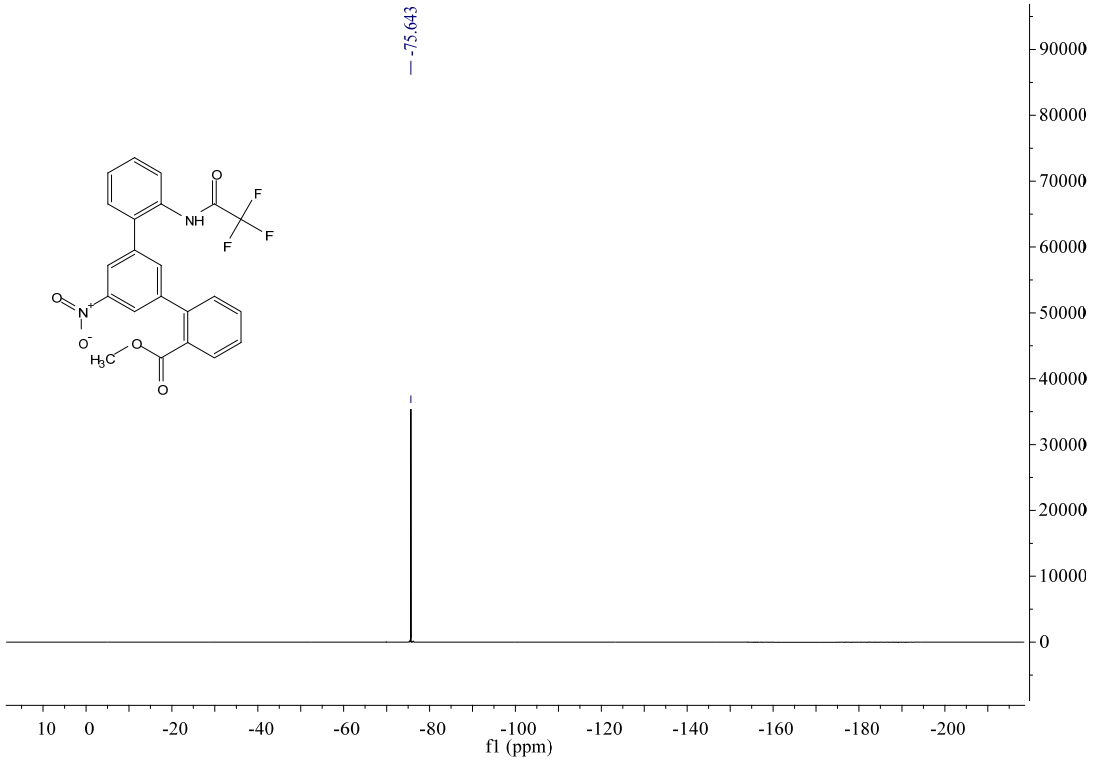

8.119
8.099
8.041
8.038
8.022
8.019
7.640
7.636
7.632
7.628
7.624
7.603
7.600
7.544
7.540
7.535
7.527
7.524
7.508
7.505
7.498
7.486
7.477
7.364
7.353
7.319
7.317
7.300
7.298
7.260
3.734
1.639
-0.001
1.00
1.05
0.95
2.18
0.92
3.20
2.04
1.06
3.03
f1 (ppm)

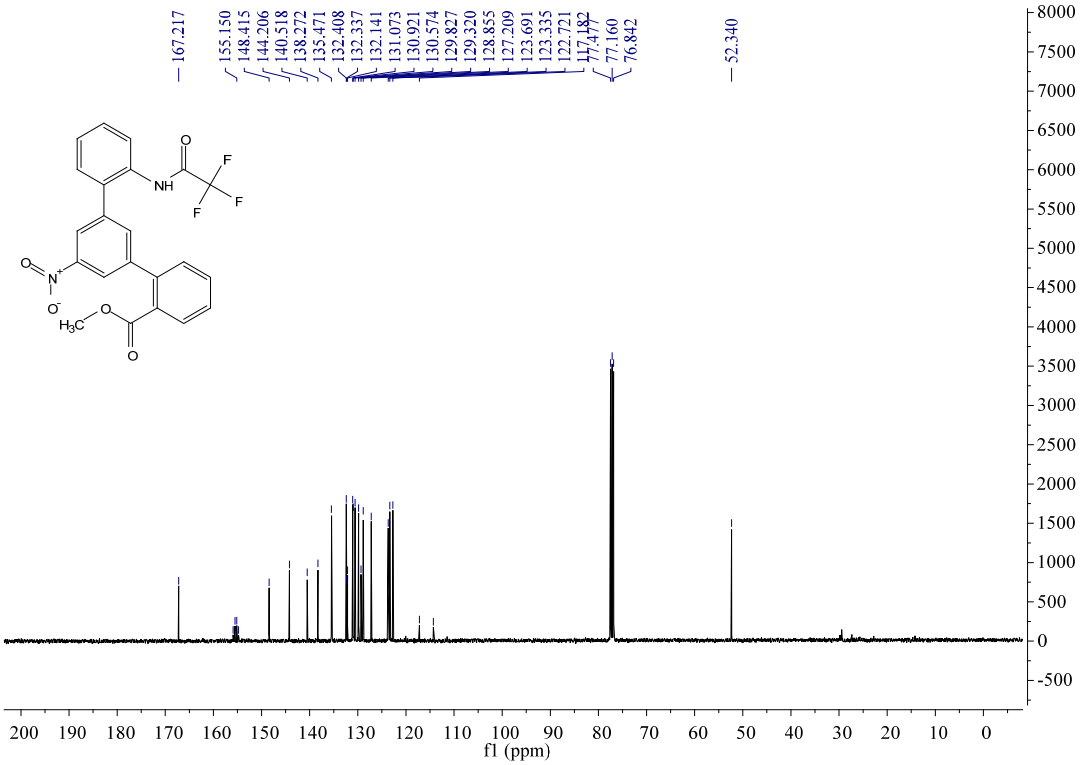

-75.668
f1 (ppm)


167.227
155.416
155.043
143.940
140.540
138.018
133.954
132.343
132.192
132.160
131.903
131.222
131.050
130.863
130.465
129.787
129.392
128.780
127.052
123.308
77.477
77.160
76.842
52.317
NH
O
F
F
F
N
H3C
O
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

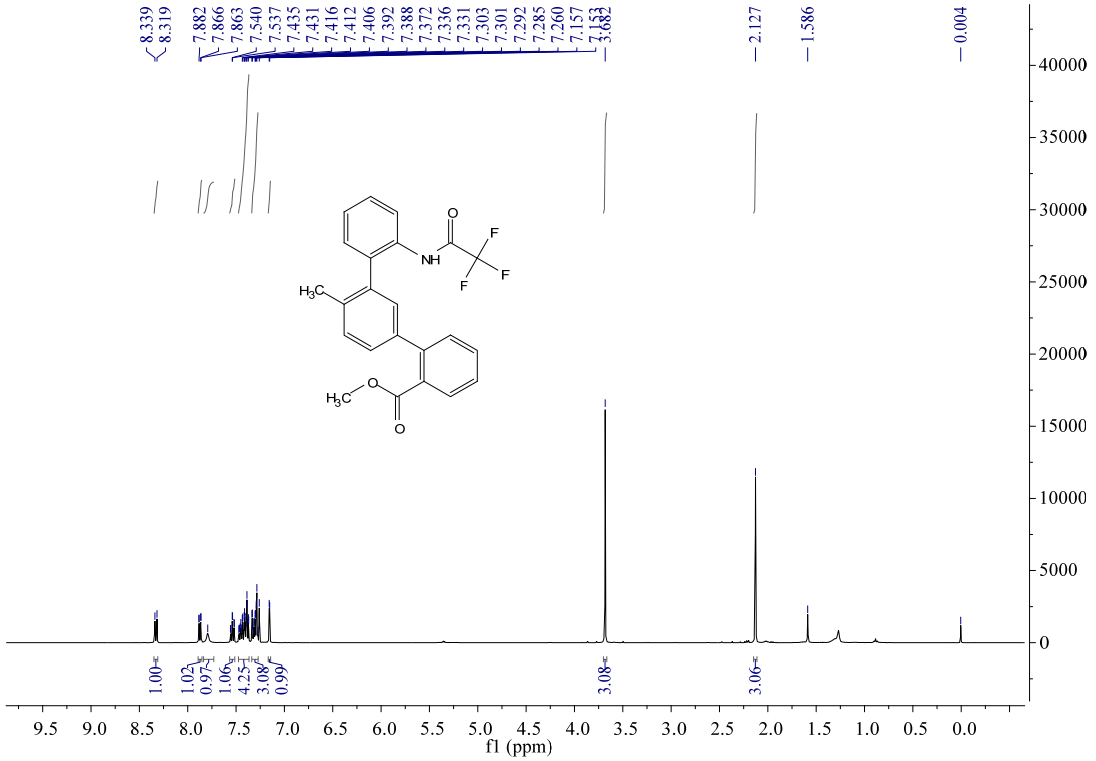
4h

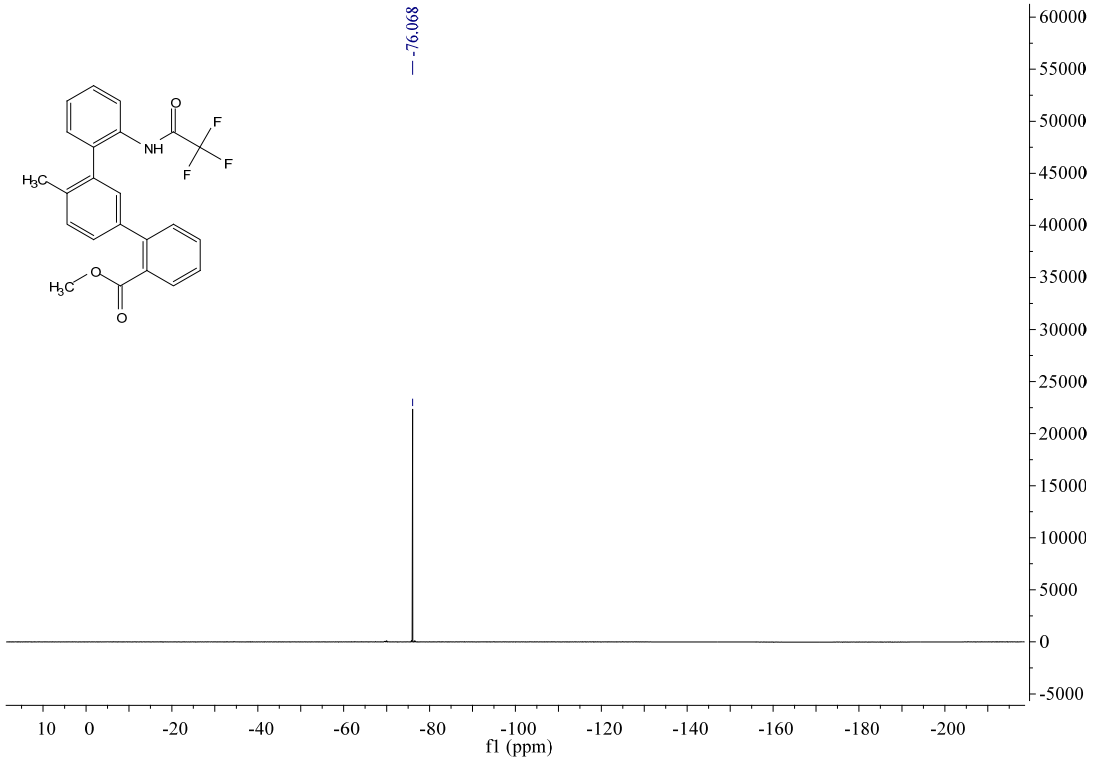

8.223
8.219
8.202
8.197
8.074
8.061
8.058
8.056
8.042
7.644
7.640
7.637
7.620
7.617
7.601
7.541
7.539
7.522
7.520
7.496
7.492
7.406
7.401
7.393
7.376
7.364
7.362
7.345
7.260
3.733
-0.001
1.96
0.87
2.04
2.01
2.04
3.06
3.00
fl (ppm)

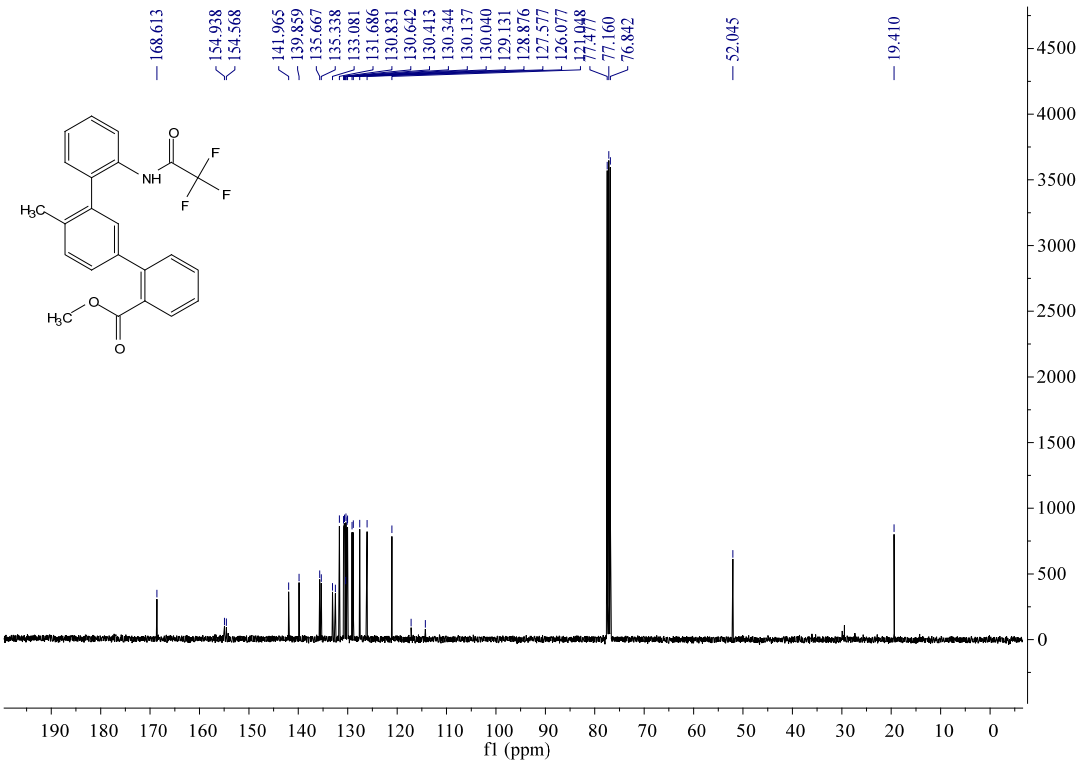

-75.643
fl (ppm)


167.217
155.150
148.415
144.206
140.518
138.272
135.471
132.408
132.337
132.141
131.073
130.921
130.574
129.827
129.320
128.855
127.209
123.691
123.335
122.721
77.160
76.842
52.340
NH
O
F
F
F
O
N
O
H3C
O
O
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

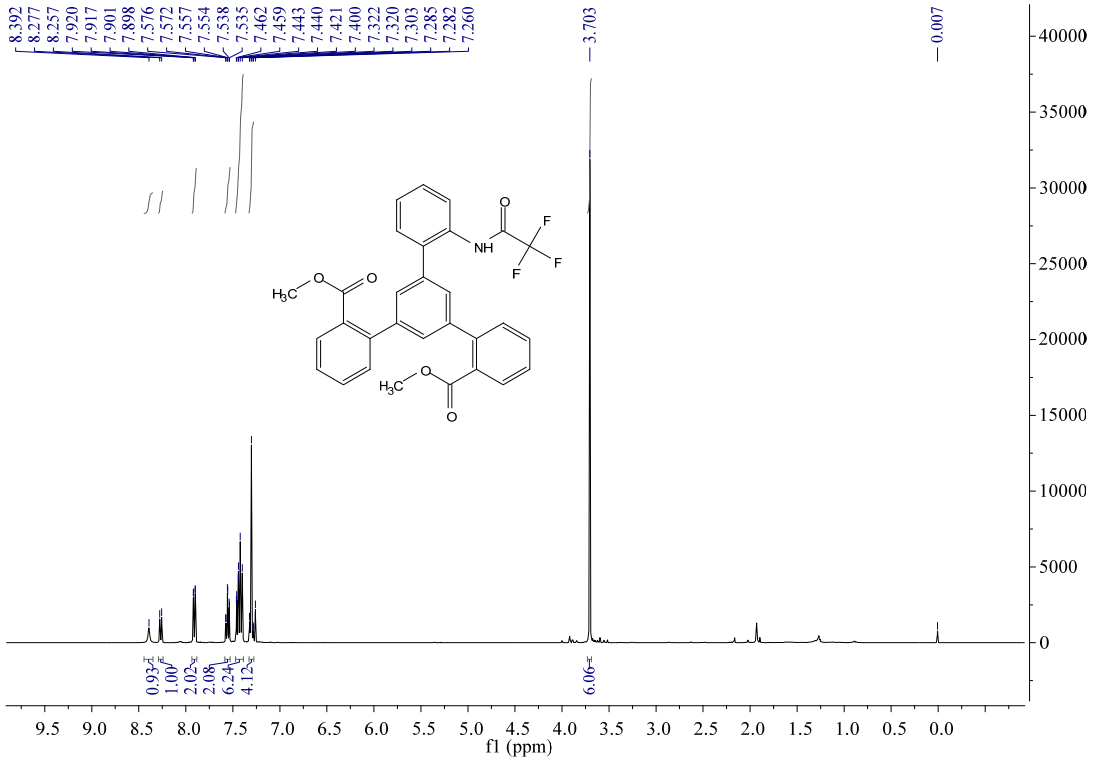
4i

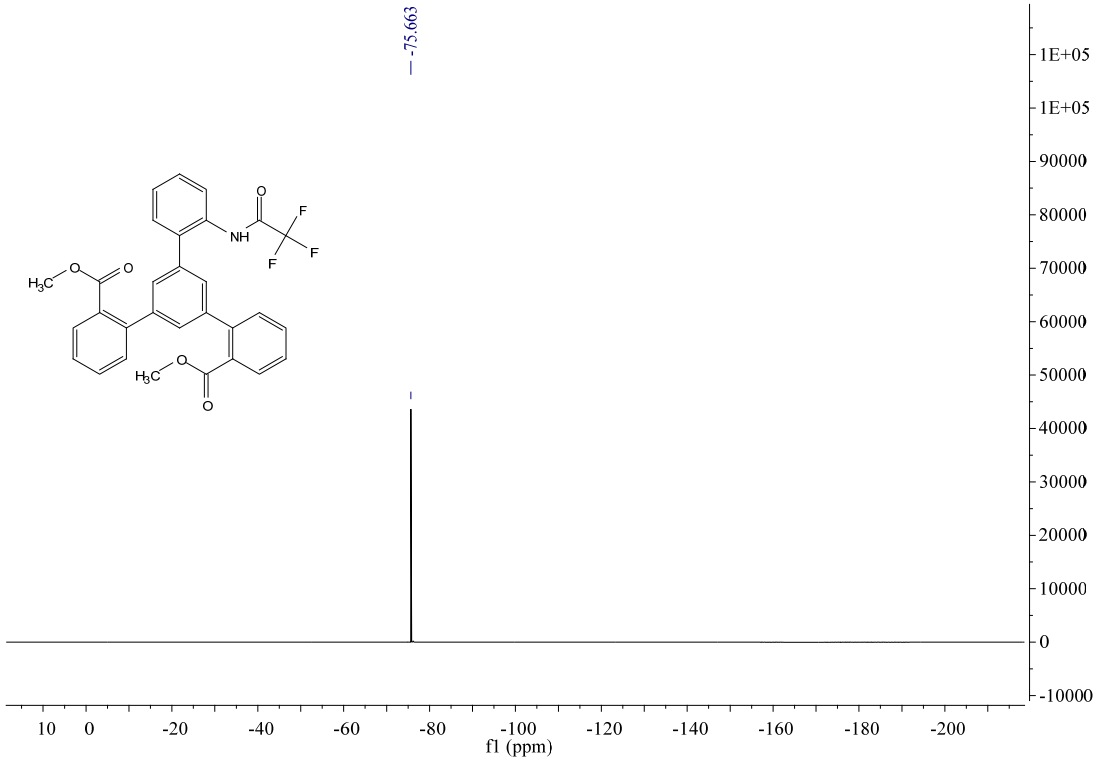

8.339
8.319
7.882
7.866
7.863
7.540
7.537
7.435
7.431
7.416
7.412
7.406
7.392
7.388
7.372
7.336
7.331
7.303
7.301
7.292
7.285
7.260
7.157
7.153
3.682
2.127
1.586
0.004
1.00
1.02
0.97
1.06
4.25
3.08
0.99
3.08
3.06
f1 (ppm)

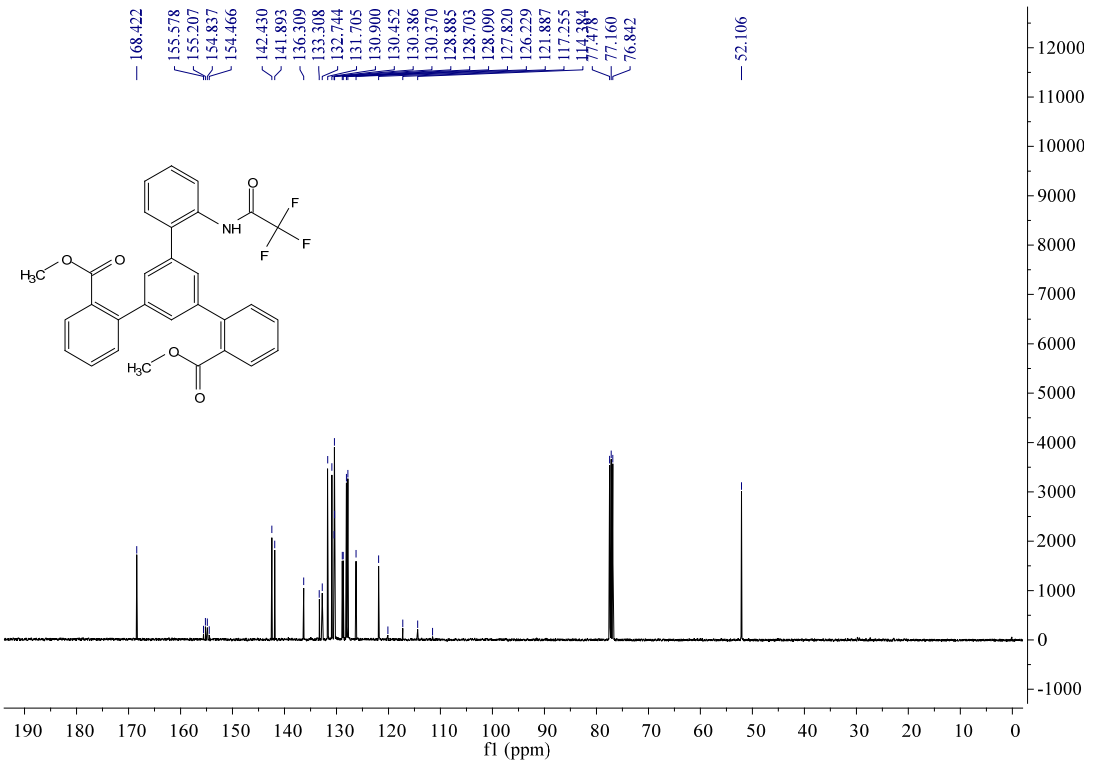

-76.068
f1 (ppm)


168.613
154.938
154.568
141.965
139.859
135.667
135.338
133.081
131.686
130.831
130.642
130.413
130.344
130.137
130.040
129.131
128.876
127.577
126.077
121.048
77.160
76.842
52.045
19.410
NH
O
F
F
F
H3C
O
H3C
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

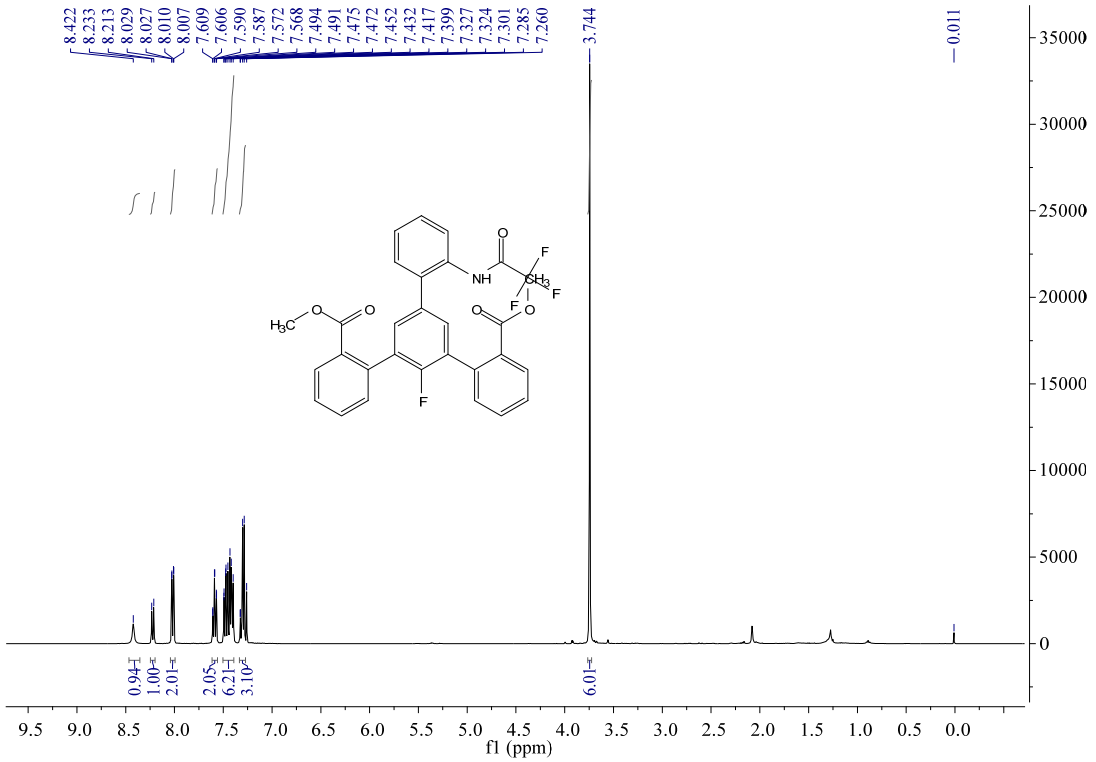
4j

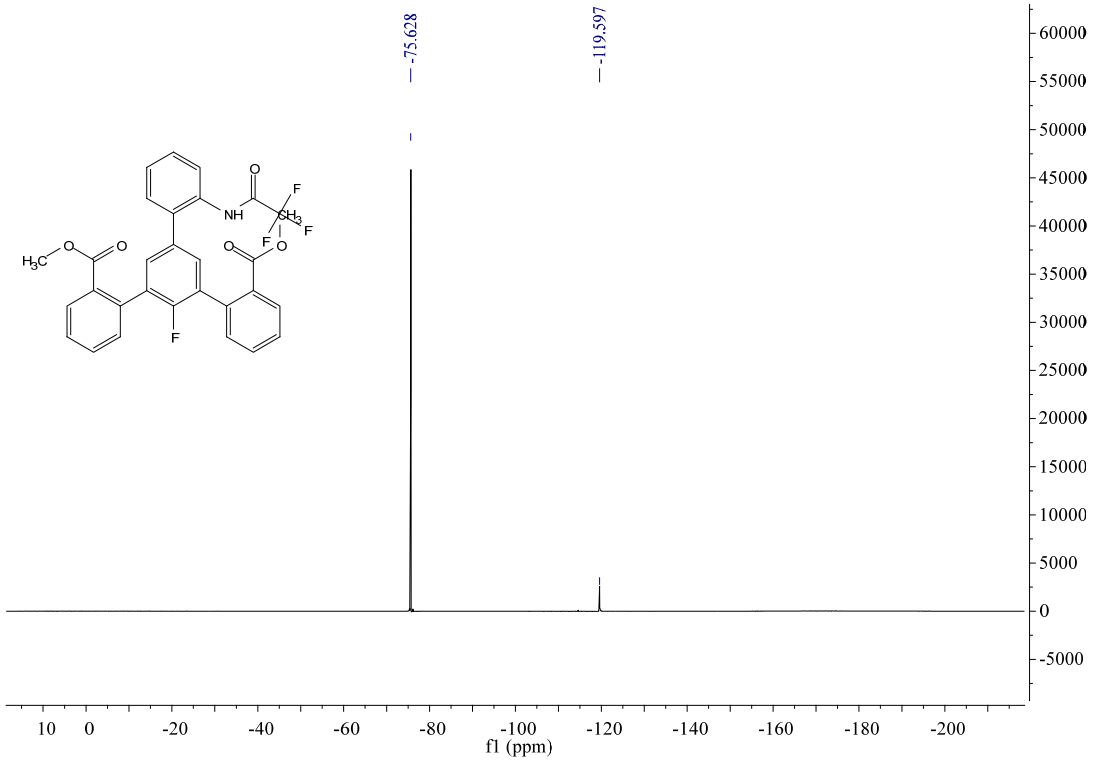

8.392
8.277
8.257
7.920
7.917
7.901
7.898
7.576
7.572
7.557
7.554
7.538
7.535
7.462
7.459
7.443
7.440
7.421
7.400
7.322
7.320
7.303
7.285
7.282
7.260
3.703
0.007
0.93
1.00
2.02
2.08
6.24
4.12
6.06
NH
F
F
F
O
O
H3C
O
O
H3C
O
O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
40000
35000
30000
25000
20000
15000
10000
5000
0

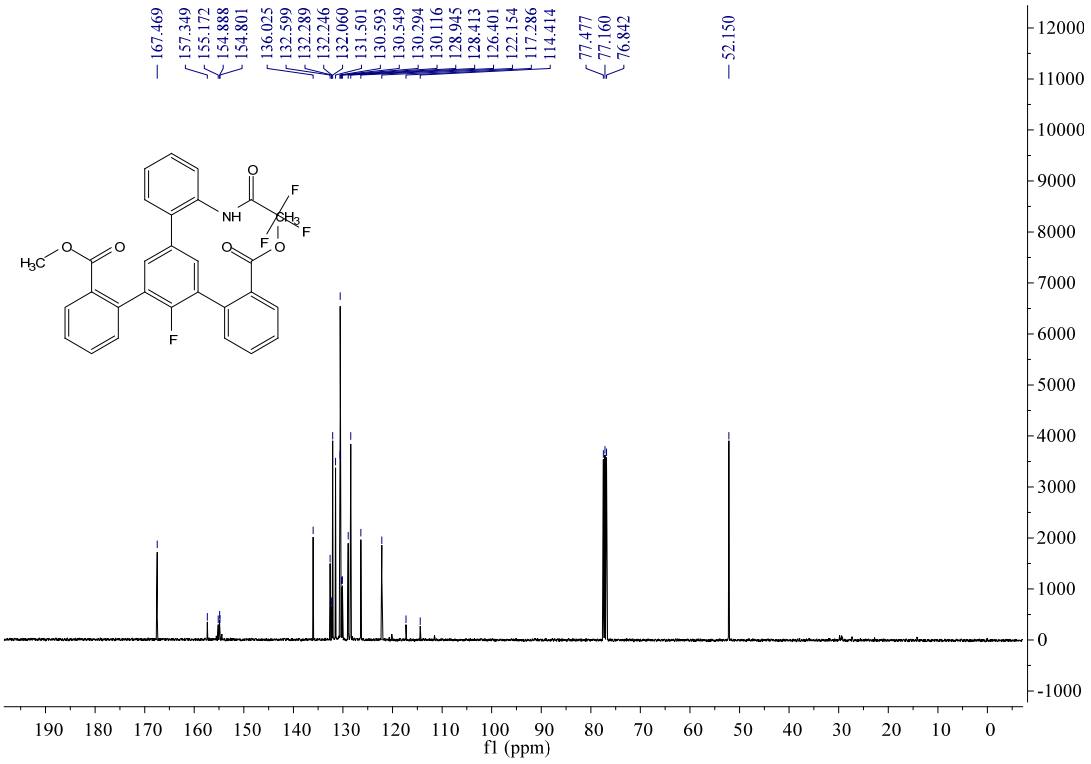

-75.663
NH
F
F
F
O
O
H3C
O
O
H3C
O
O
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000


168.422
155.578
155.207
154.837
154.466
142.430
141.893
136.309
133.308
132.744
131.705
130.900
130.452
130.386
130.370
128.885
128.703
128.090
127.820
126.229
121.887
117.255
77.160
76.842
52.106
O
NH
F
F
F
H3C
O
O
H3C
O
O
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

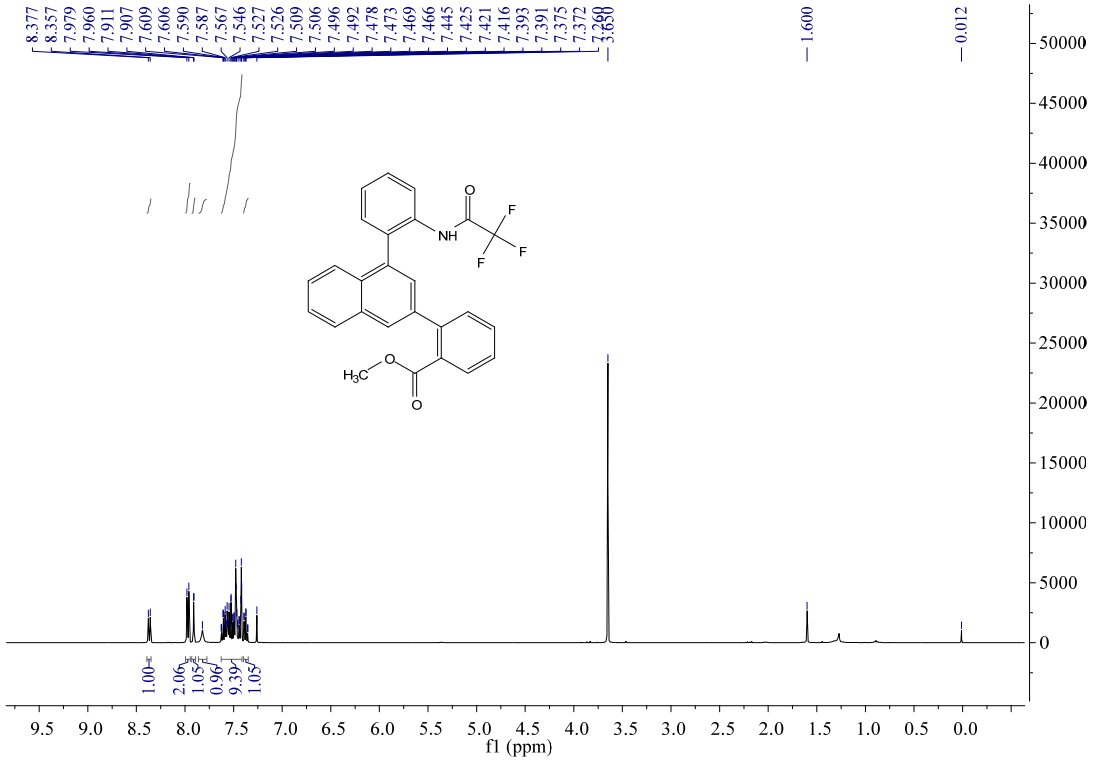
4k

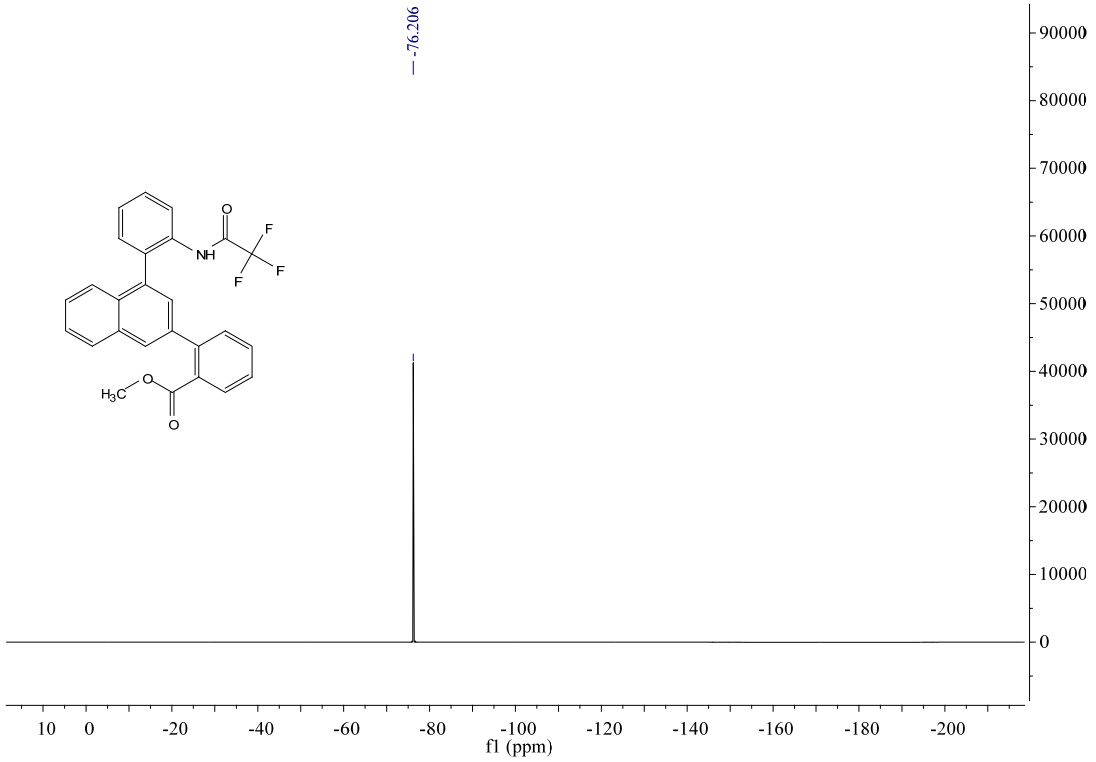

8.422
8.233
8.213
8.029
8.027
8.010
8.007
7.609
7.606
7.590
7.587
7.572
7.568
7.494
7.491
7.475
7.472
7.452
7.432
7.417
7.399
7.327
7.324
7.301
7.285
7.260
3.744
0.011
0.94
1.00
2.01
2.05
6.21
3.10
6.01
f1 (ppm)

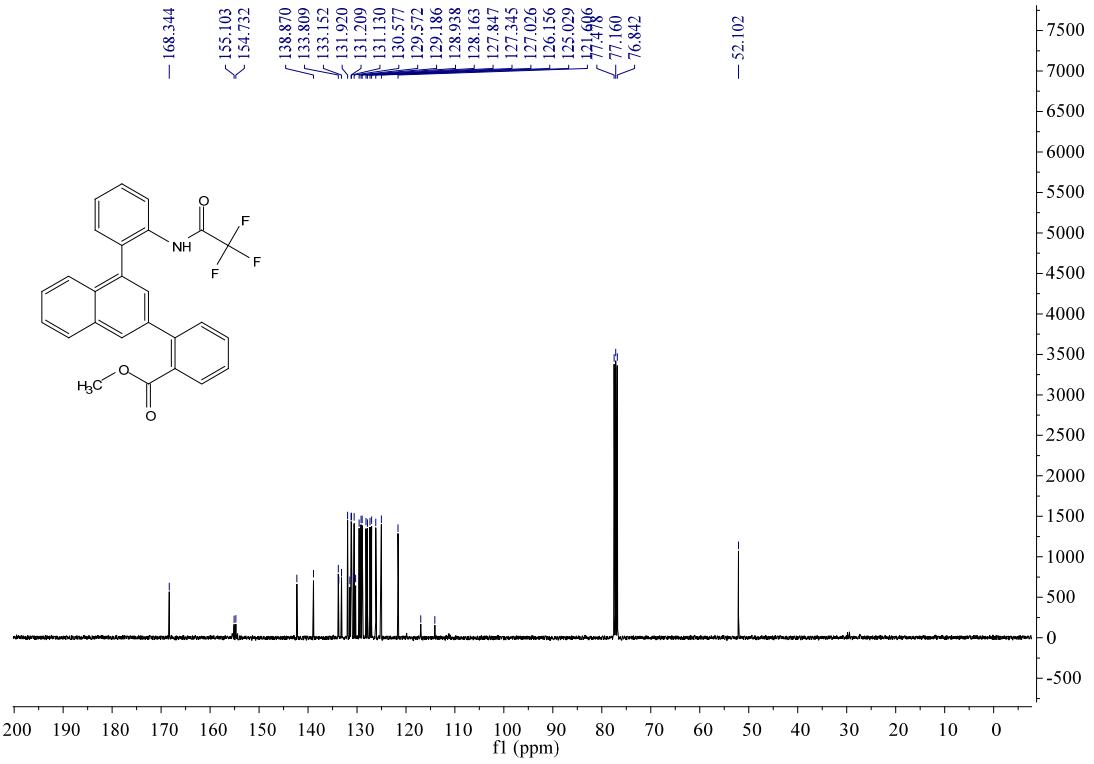

-75.628
-119.597
f1 (ppm)


167.469
157.349
155.172
154.888
154.801
136.025
132.599
132.289
132.246
132.060
131.501
130.593
130.549
130.294
130.116
128.945
128.413
126.401
122.154
117.286
114.414
77.477
77.160
76.842
52.150
NH
O
F
CH3
F
F
O
O
O
H3C
O
F
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

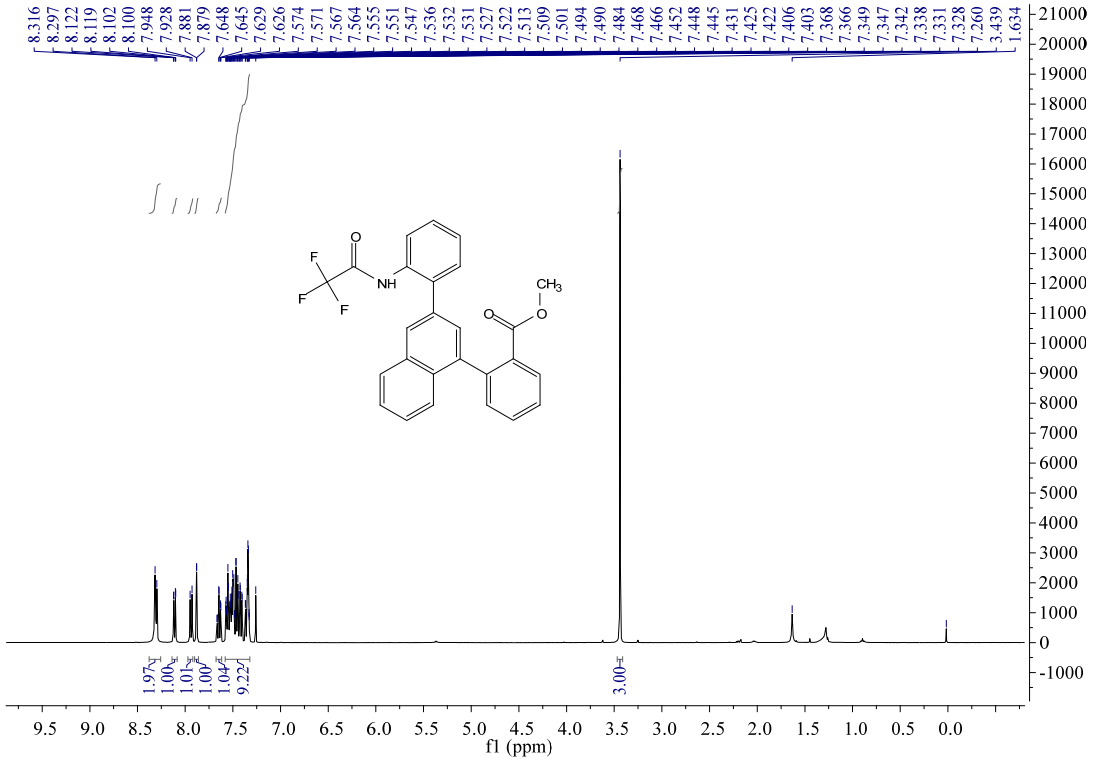
4l

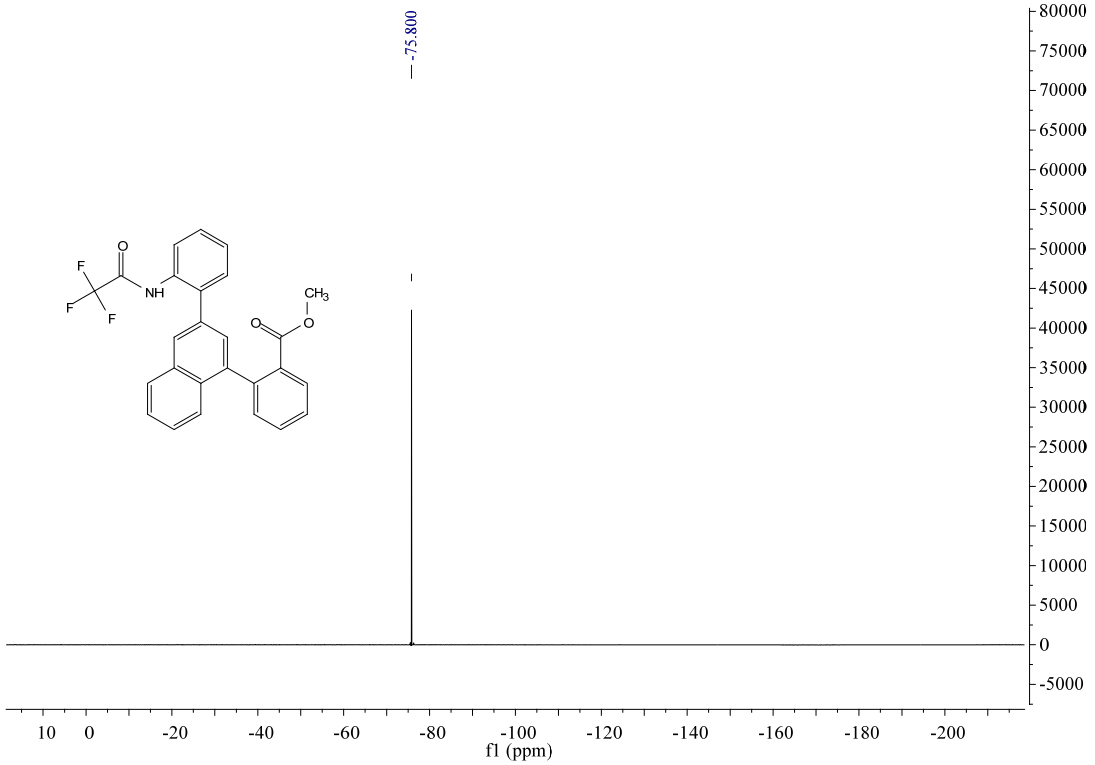

8.377
8.357
7.979
7.960
7.911
7.907
7.609
7.606
7.590
7.587
7.567
7.546
7.527
7.526
7.509
7.506
7.496
7.492
7.478
7.473
7.469
7.466
7.445
7.425
7.421
7.416
7.393
7.391
7.375
7.372
3.650
1.600
0.012
NH
O
F
F
F
H3C
O
O
1.00
2.06
1.05
0.96
9.39
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0

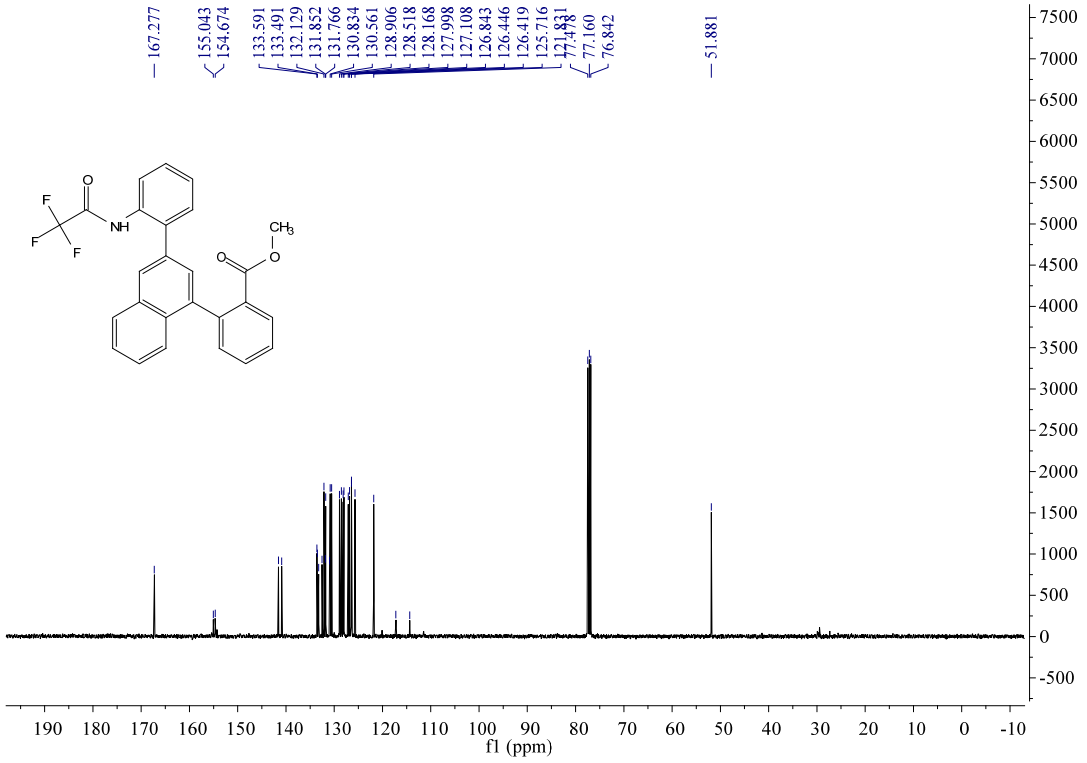

-76.206
NH
O
F
F
F
H3C
O
O
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)
90000
80000
70000
60000
50000
40000
30000
20000
10000
0


168.344
155.103
154.732
138.870
133.809
133.152
131.920
131.209
131.130
130.577
129.572
129.186
128.938
128.163
127.847
127.345
127.026
126.156
125.029
121.606
77.478
77.160
76.842
52.102
NH
O
F
F
F
H3C
O
O
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

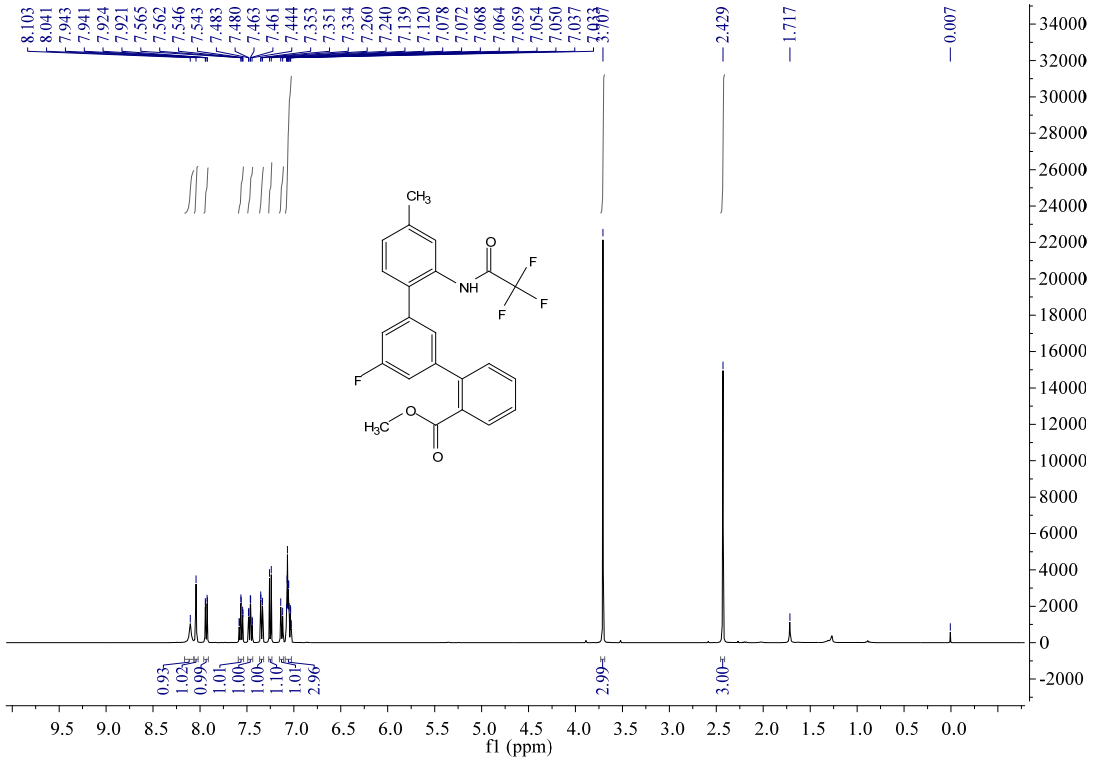
4m

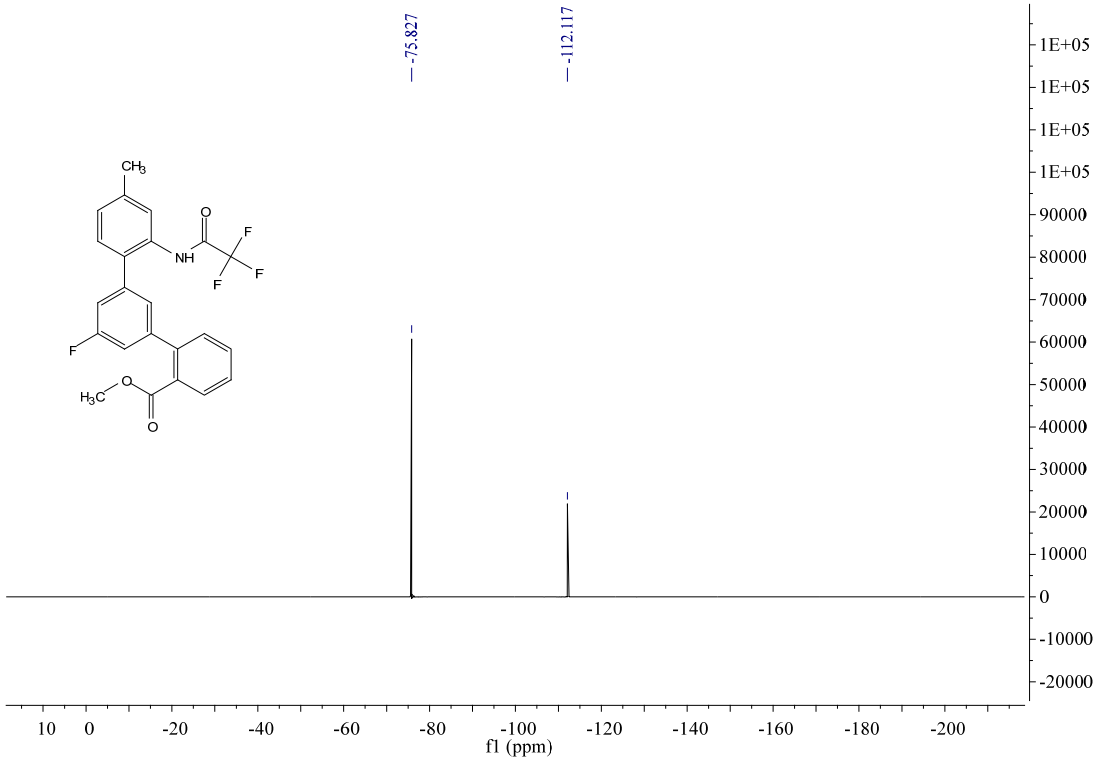

8.316
8.297
8.122
8.119
8.102
8.100
7.948
7.928
7.881
7.879
7.648
7.645
7.629
7.626
7.574
7.571
7.567
7.564
7.555
7.551
7.547
7.536
7.532
7.531
7.527
7.522
7.513
7.509
7.501
7.494
7.490
7.484
7.468
7.466
7.452
7.448
7.445
7.431
7.425
7.422
7.406
7.403
7.368
7.366
7.349
7.347
7.342
7.338
7.331
7.328
7.260
3.439
1.634
F
F
F
O
NH
CH3
O
O
1.97
1.00
1.01
1.00
1.04
9.22
3.00
f1 (ppm)

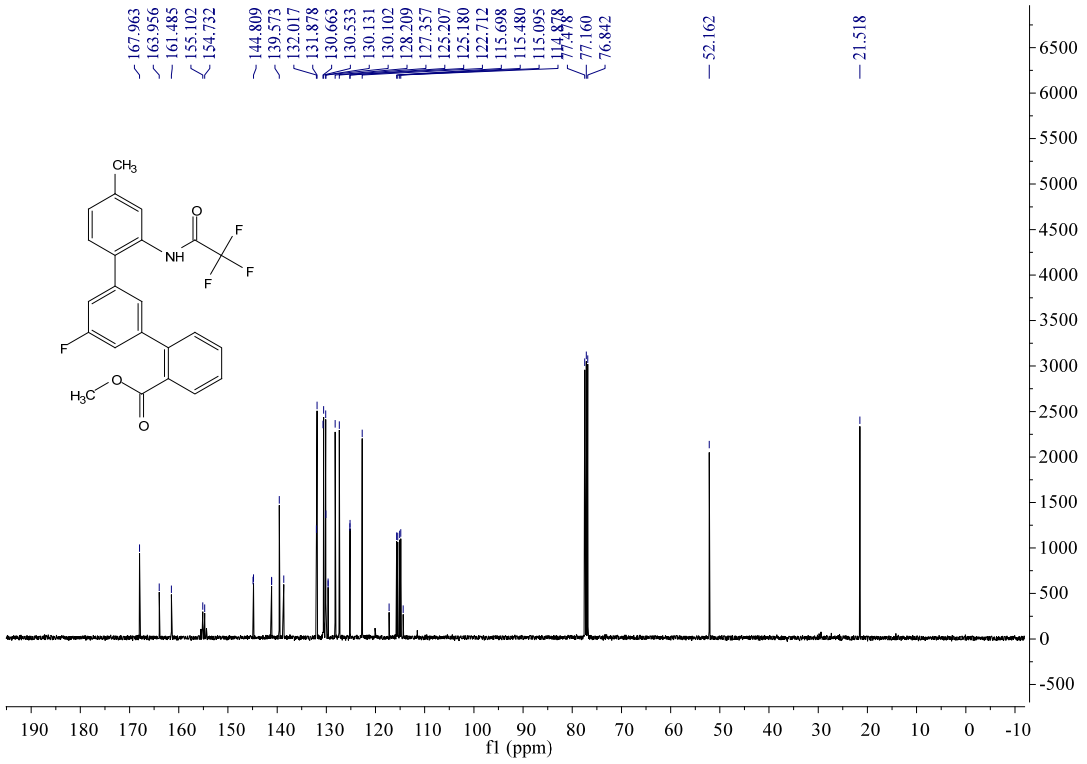

-75.800
F
F
F
O
NH
CH3
O
O
f1 (ppm)


167.277
155.043
154.674
133.591
133.491
132.129
131.852
131.766
130.834
130.561
128.906
128.518
128.168
127.998
127.108
126.843
126.446
126.419
125.716
121.831
77.478
77.160
76.842
51.881
F
F
F
O
NH
O
O
CH3
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

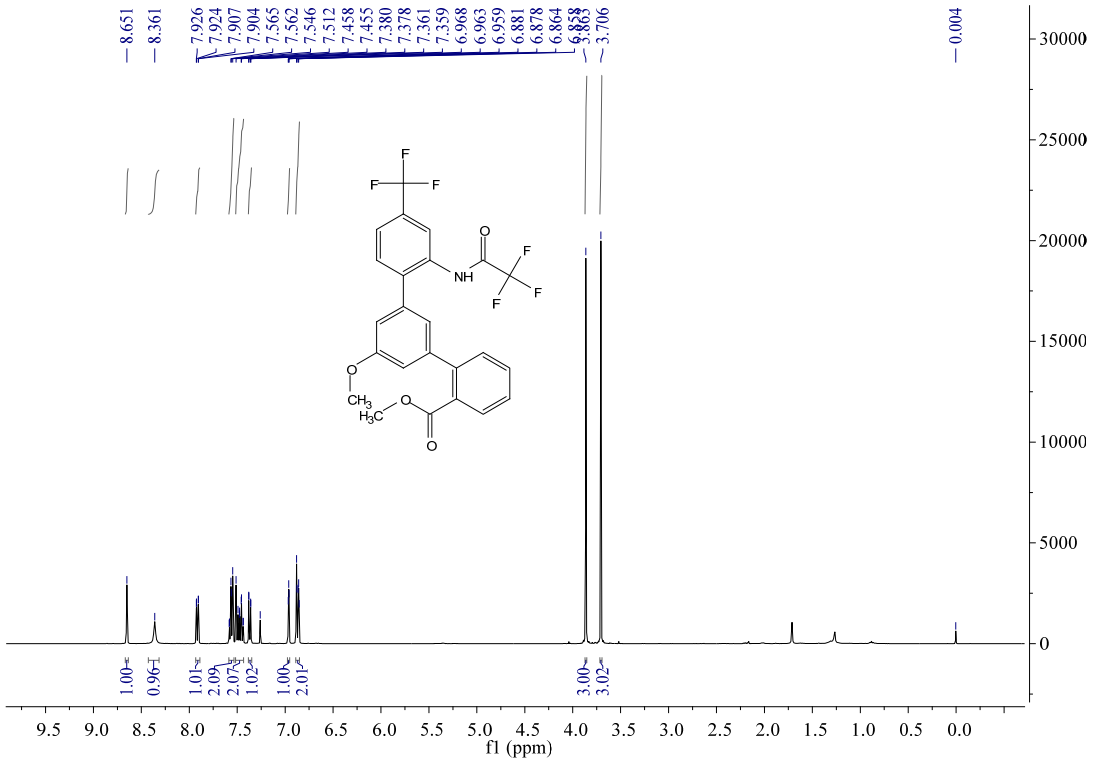
4n

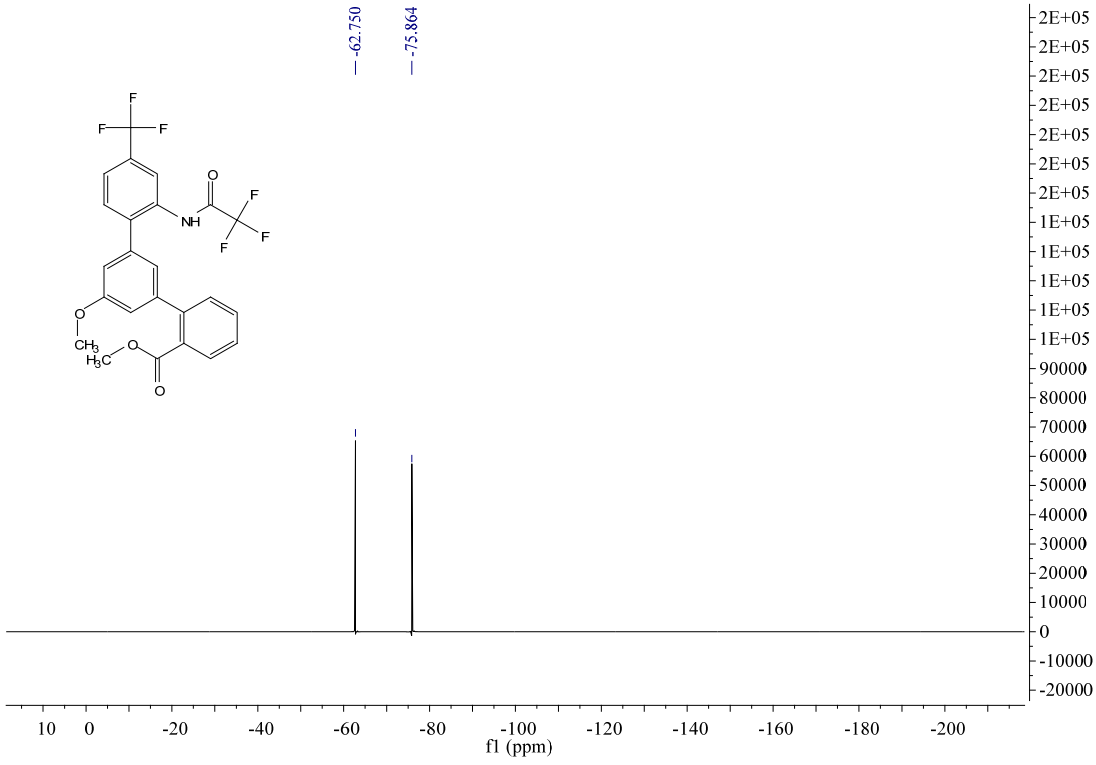

8.103
8.041
7.943
7.941
7.924
7.921
7.565
7.562
7.546
7.543
7.483
7.480
7.463
7.461
7.444
7.353
7.351
7.334
7.260
7.240
7.139
7.120
7.078
7.072
7.068
7.064
7.059
7.054
7.050
7.037
7.033
3.000
2.429
1.717
0.007
CH3
NH
O
F
F
F
F
H3C
O
O
0.93
1.02
0.99
1.01
1.00
1.00
1.10
1.01
2.96
2.99
3.00
fl (ppm)

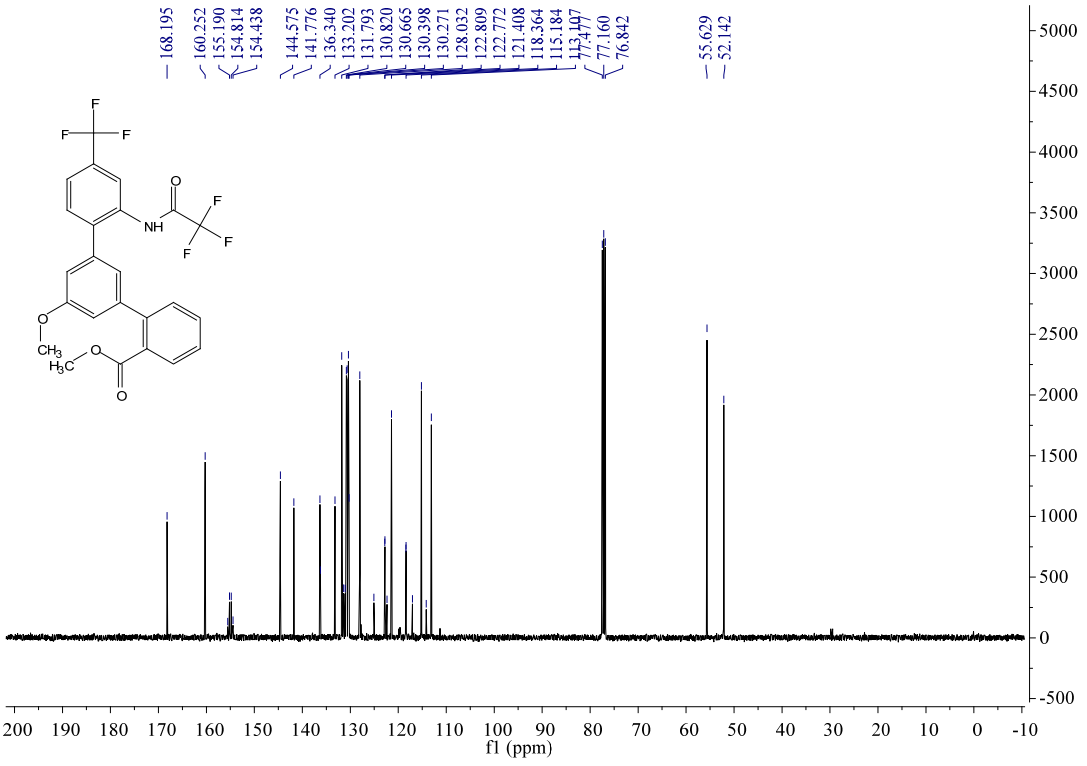

-75.827
-112.117
CH3
NH
O
F
F
F
F
H3C
O
O
fl (ppm)


167.963
163.956
161.485
155.102
154.732
144.809
139.573
132.017
131.878
130.663
130.533
130.131
130.102
128.209
127.357
125.207
125.180
122.712
115.698
115.480
115.095
77.478
77.160
76.842
52.162
21.518
CH3
NH
O
F
F
F
F
H3C
O
O
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

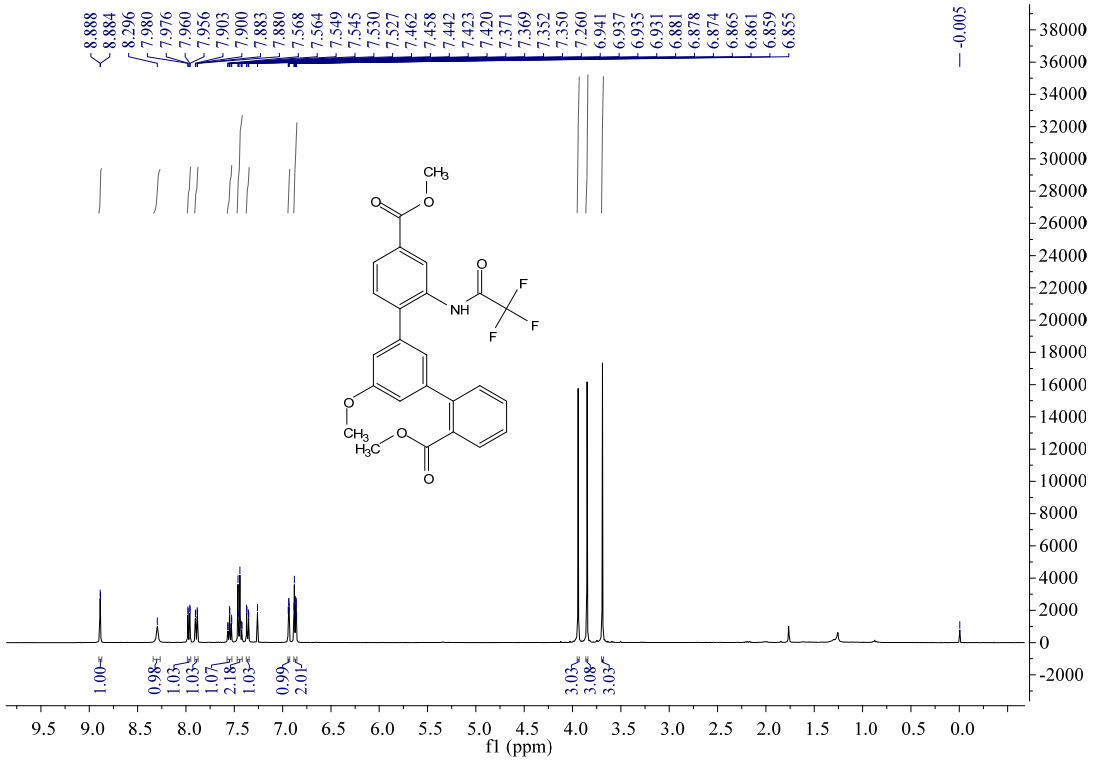
4o

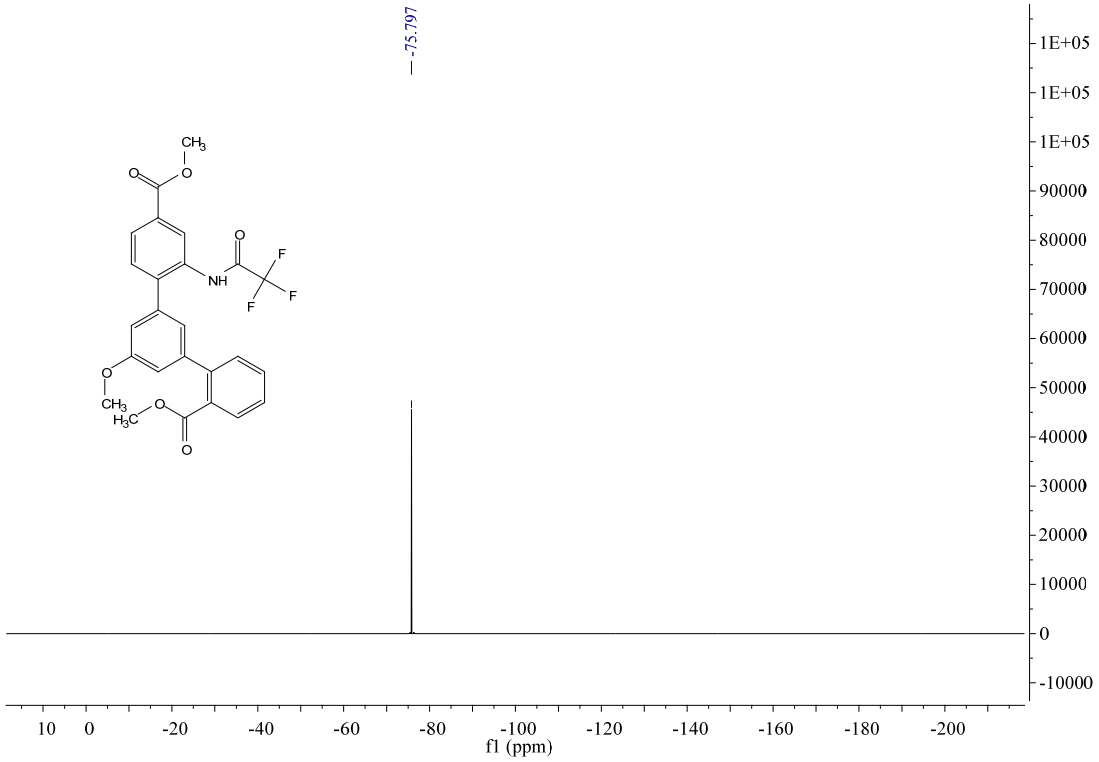

8.651
8.361
7.926
7.924
7.907
7.904
7.565
7.562
7.546
7.512
7.458
7.455
7.380
7.378
7.361
7.359
6.968
6.963
6.959
6.881
6.878
6.864
3.863
3.706
0.004
1.00
0.96
1.01
2.09
2.07
1.02
1.00
2.01
3.00
3.02
f1 (ppm)

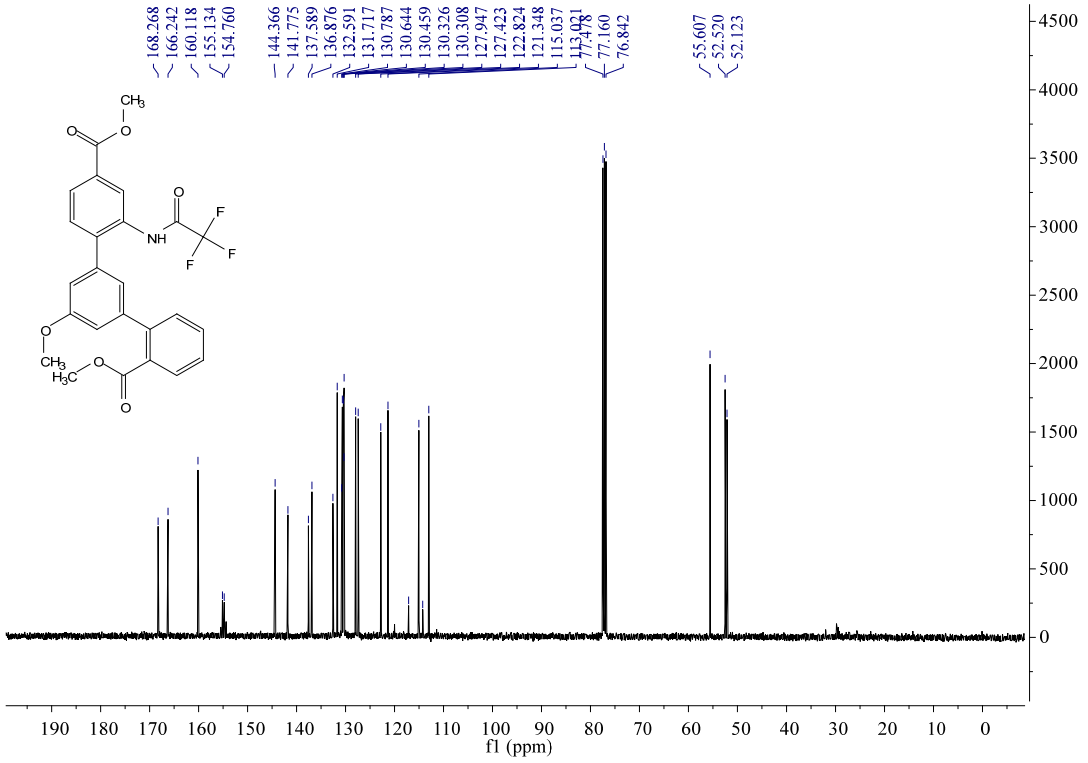

-62.750
-75.864
f1 (ppm)


168.195
160.252
155.190
154.814
154.438
144.575
141.776
136.340
133.202
131.793
130.820
130.665
130.398
130.271
128.032
122.809
122.772
121.408
118.364
115.184
77.160
76.842
55.629
52.142
F
F
F
O
NH
F
F
F
O
CH3
H3C
O
O
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

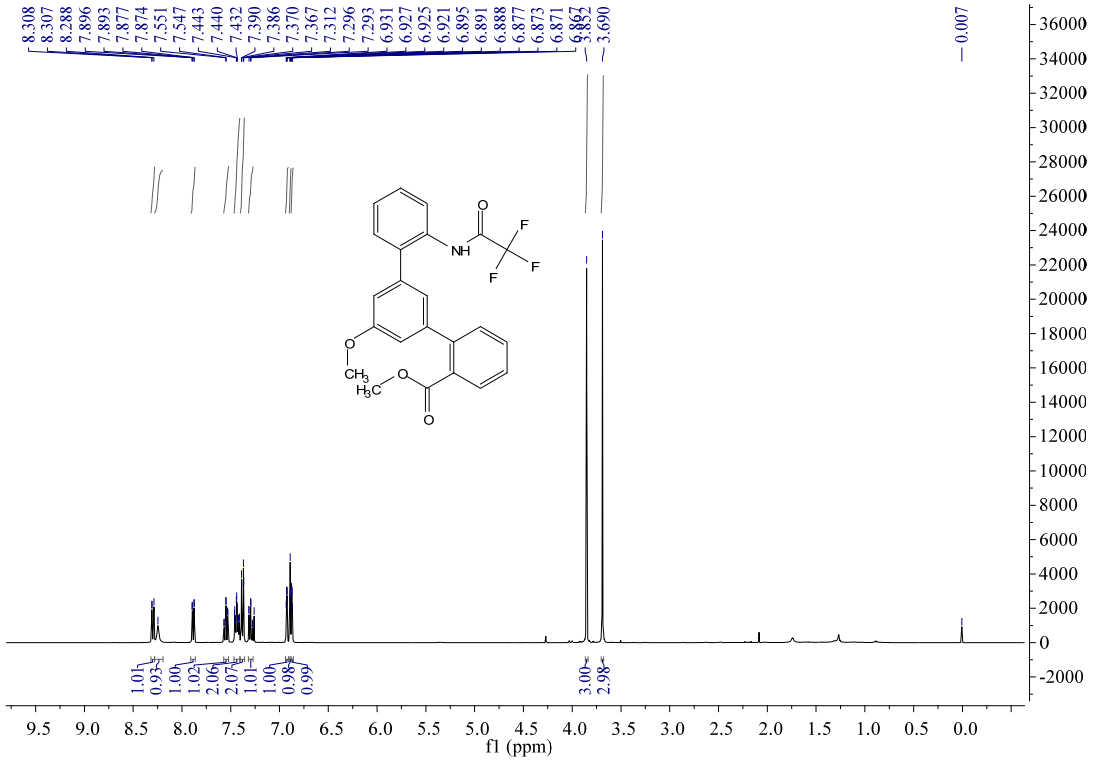
4p


8.888
8.884
8.296
7.980
7.976
7.960
7.956
7.903
7.900
7.883
7.880
7.568
7.564
7.549
7.545
7.530
7.527
7.462
7.458
7.442
7.423
7.420
7.371
7.369
7.352
7.350
7.260
6.941
6.937
6.935
6.931
6.881
6.878
6.874
6.865
6.861
6.859
6.855
-0.005
1.00
0.98
1.03
1.03
1.07
2.18
1.03
0.99
2.01
3.03
3.08
3.03
f1 (ppm)


-75.797
f1 (ppm)


168.268
166.242
160.118
155.134
154.760
144.366
141.775
137.589
136.876
132.591
131.717
130.787
130.644
130.459
130.326
130.308
127.947
127.423
122.824
121.348
115.037
113.021
77.478
77.160
76.842
55.607
52.520
52.123
CH3
O
O
NH
O
F
F
F
O
CH3
H3C
O
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4q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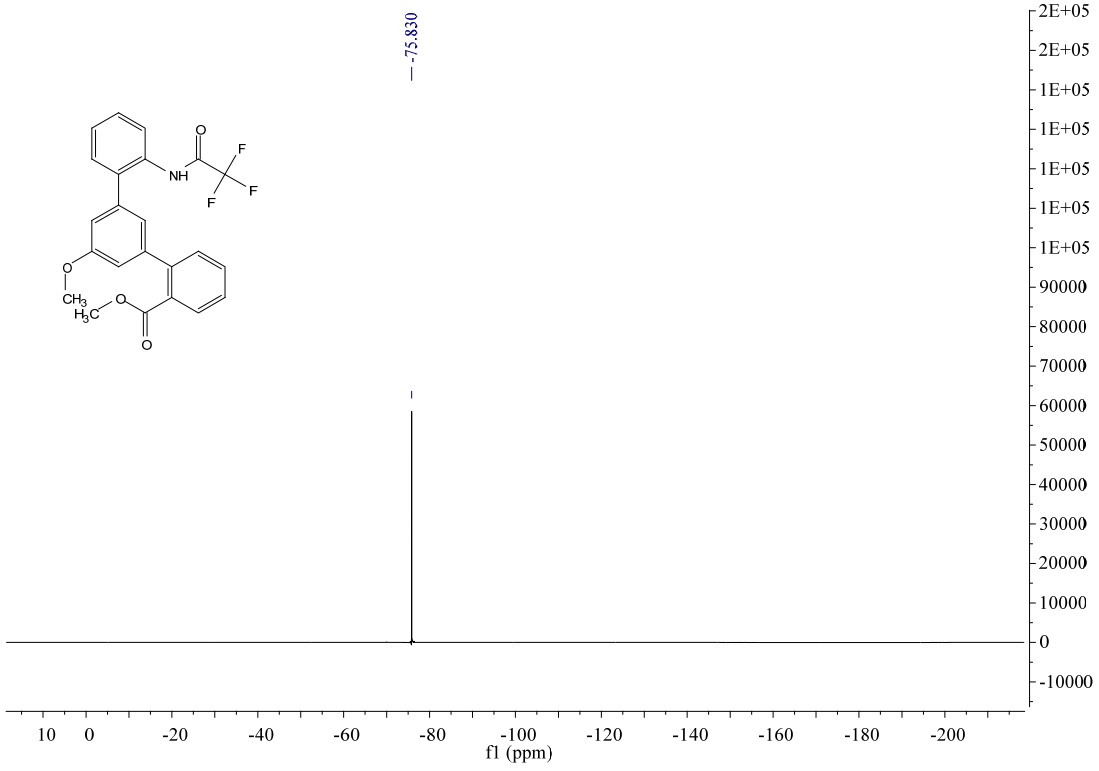
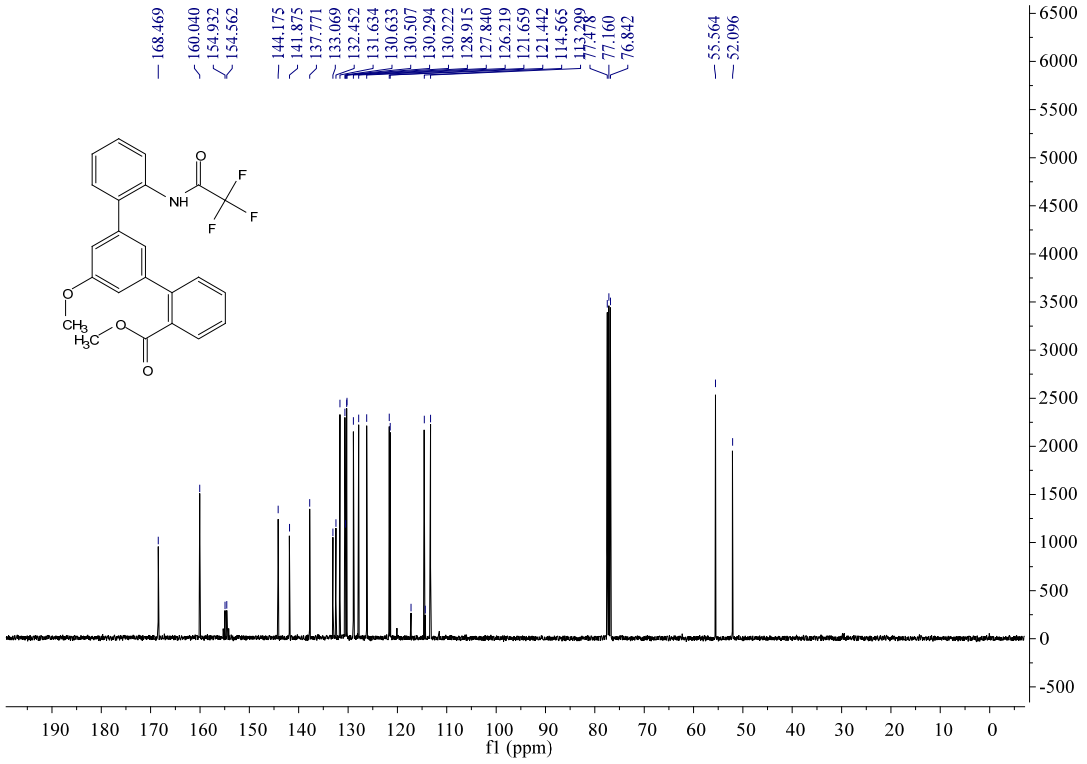
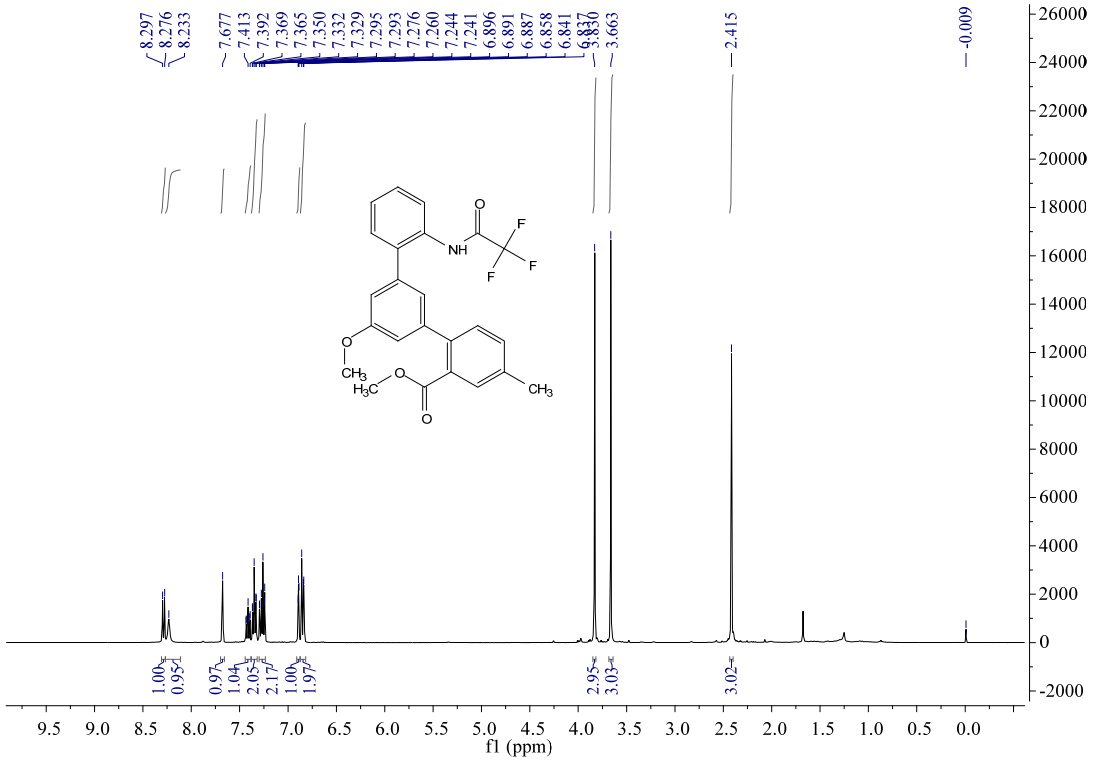
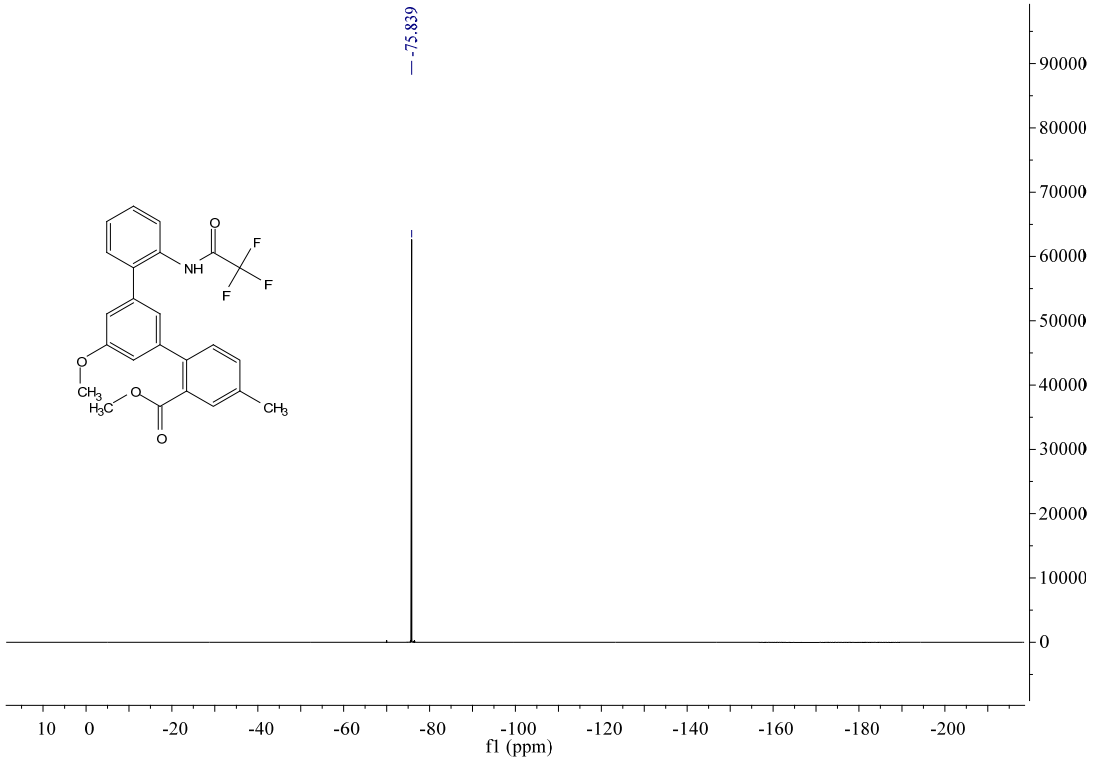
8.307
8.288
7.896
7.893
7.877
7.874
7.551
7.547
7.443
7.440
7.432
7.390
7.386
7.370
7.367
7.312
7.296
7.293
6.931
6.927
6.925
6.921
6.895
6.891
6.888
6.877
6.873
6.871
3.852
3.690
0.007
1.01
0.93
1.00
1.02
2.06
2.07
1.01
1.00
0.98
0.99
3.00
2.98
NH
O
F
F
F
O
CH3
H3C
O
O
fl (ppm)

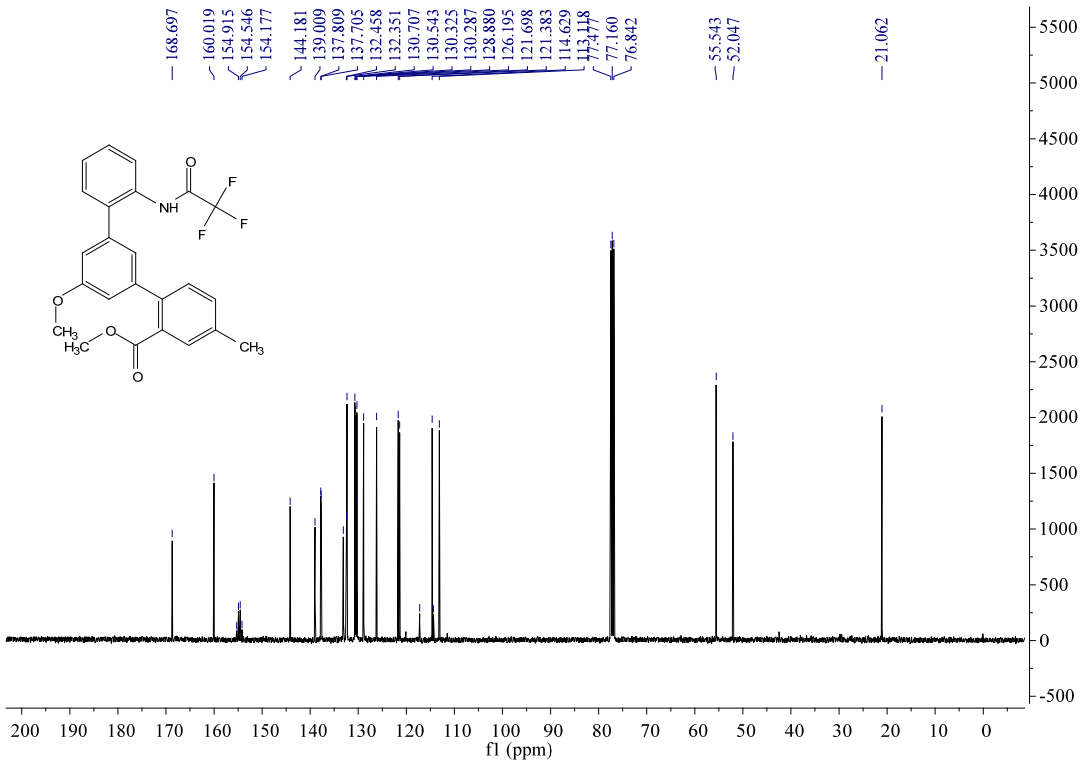

-75.830
NH
O
F
F
F
O
CH3
H3C
O
O
fl (ppm)


168.469
160.040
154.932
154.562
144.175
141.875
137.771
133.069
132.452
131.634
130.633
130.507
130.294
130.222
128.915
127.840
126.219
121.659
121.442
114.565
113.299
77.478
77.160
76.842
55.564
52.096
NH
O
F
F
F
O
CH3
H3C
O
O
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

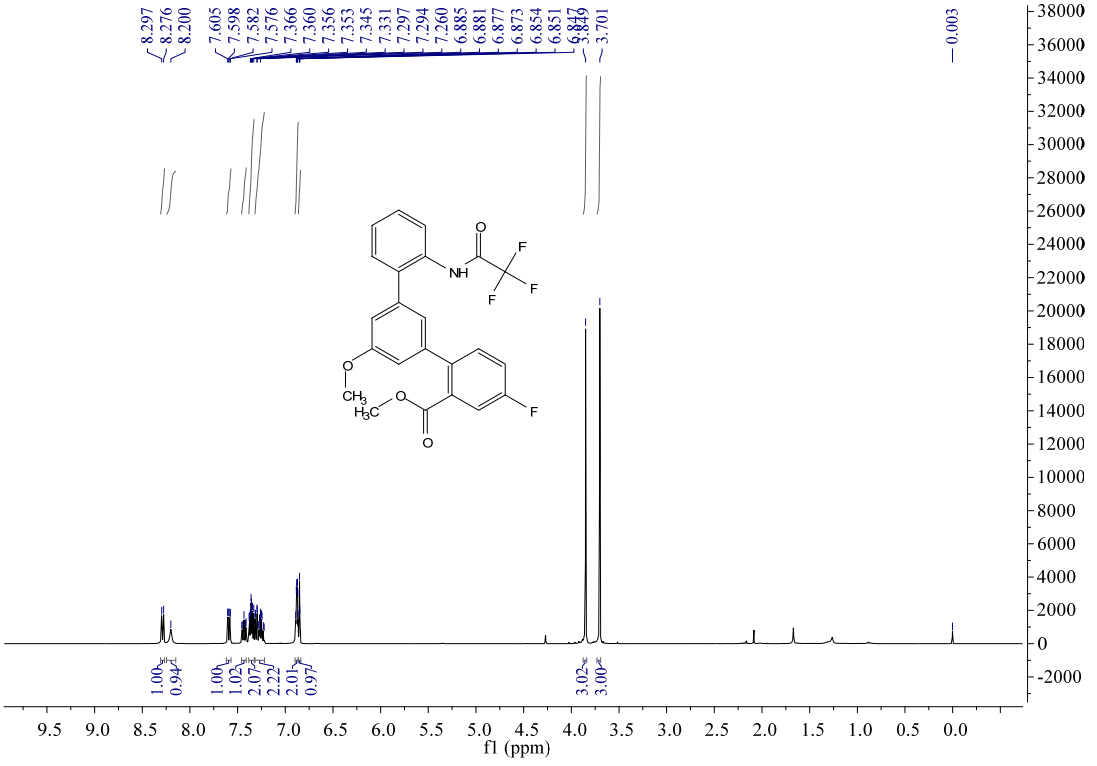
4r

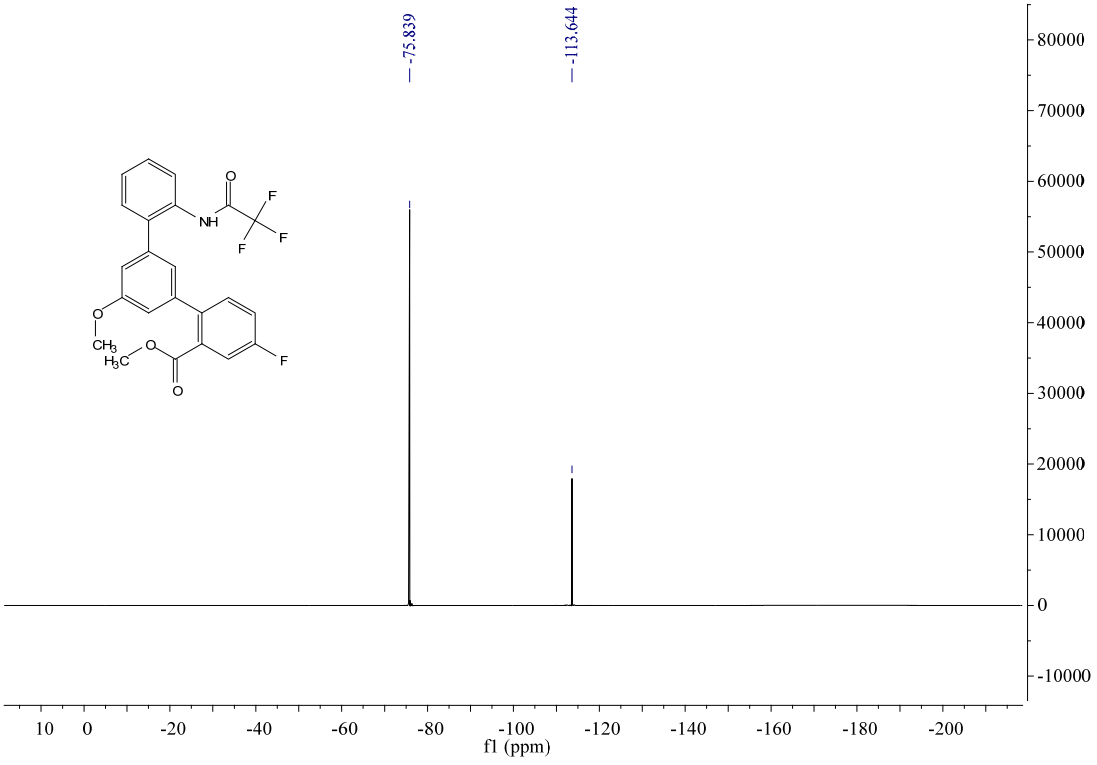

8.297
8.276
8.233
7.677
7.413
7.392
7.369
7.365
7.350
7.332
7.329
7.295
7.293
7.276
7.260
7.244
7.241
6.896
6.891
6.887
6.858
6.841
3.836
3.663
2.415
-0.009
1.00
0.95
0.97
1.04
2.05
2.17
1.00
1.97
2.95
3.03
3.02
O
NH
F
F
F
O
CH3
H3C
O
O
CH3
fl (ppm)

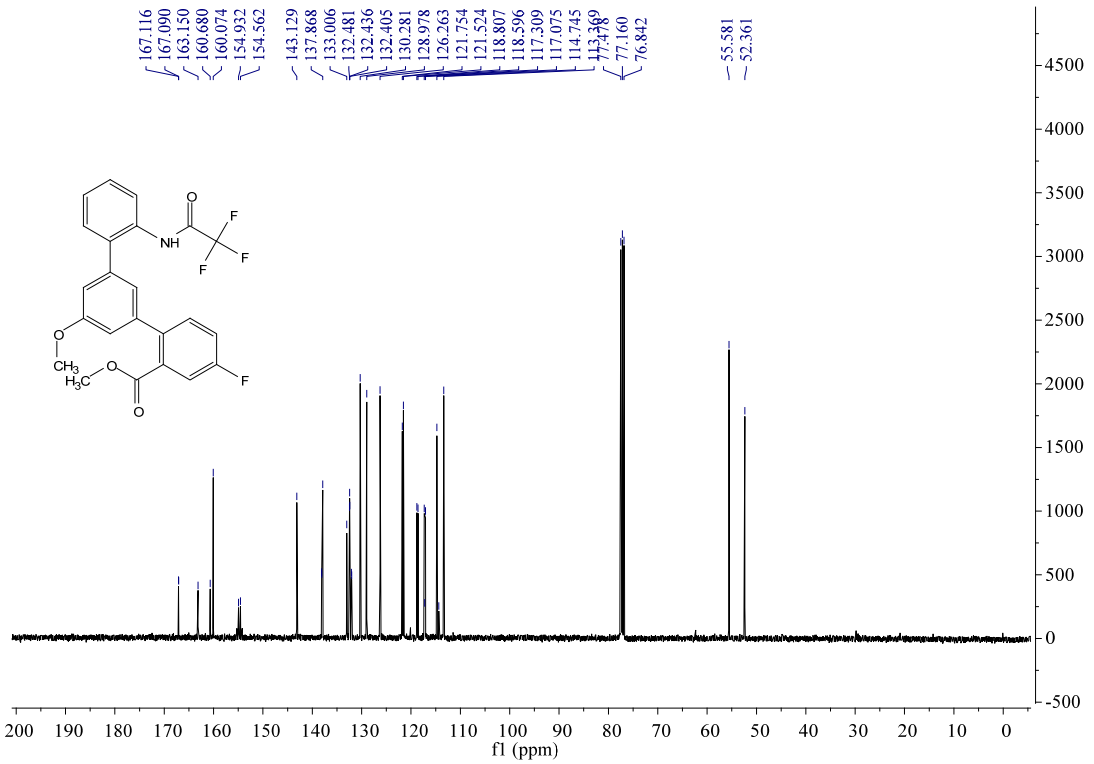

-75.839
O
NH
F
F
F
O
CH3
H3C
O
O
CH3
fl (ppm)


168.697
160.019
154.915
154.546
154.177
144.181
139.009
137.809
137.705
132.458
132.351
130.707
130.543
130.325
130.287
128.880
126.195
121.698
121.383
114.629
113.118
77.477
77.160
76.842
55.543
52.047
21.062
NH
O
F
F
F
O
CH3
H3C
O
O
CH3
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

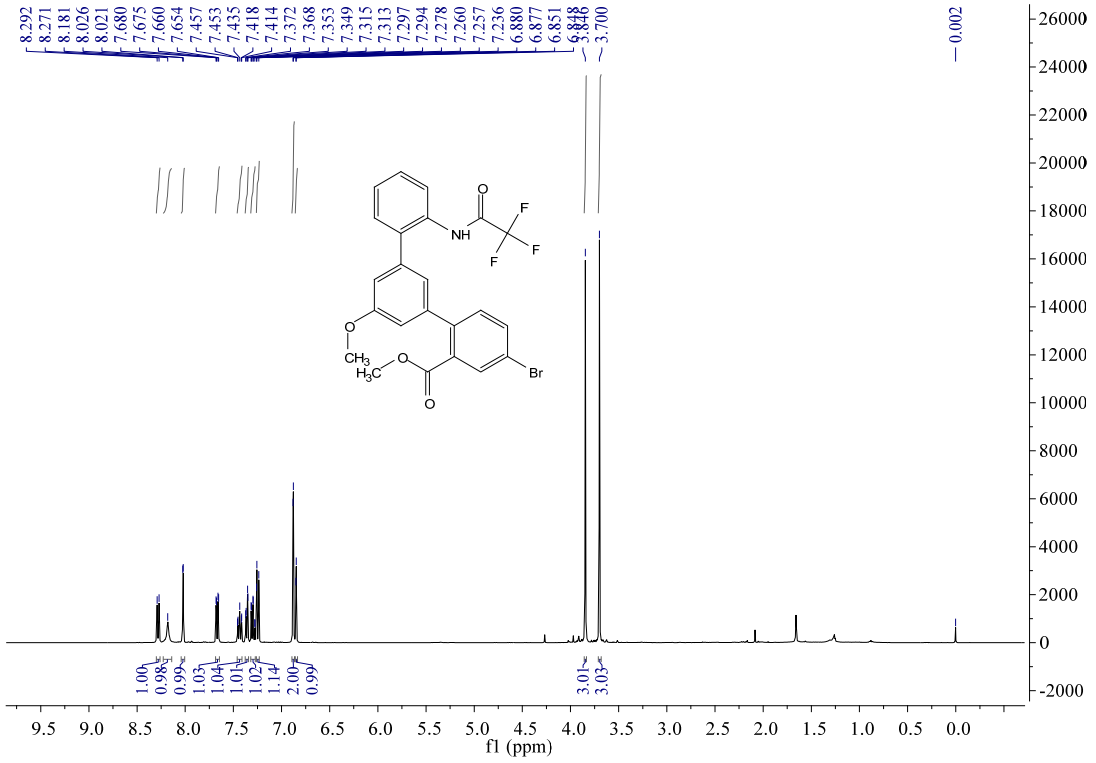
4s

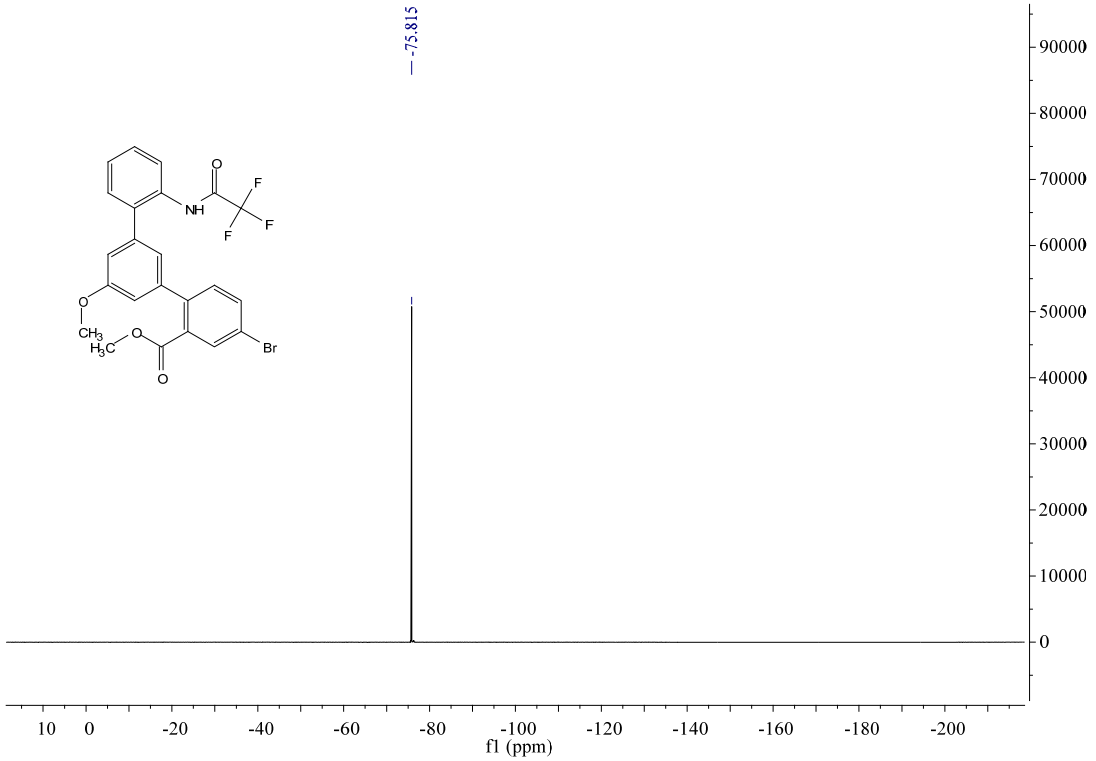

8.297
8.276
8.200
7.605
7.598
7.582
7.576
7.366
7.360
7.356
7.353
7.345
7.331
7.297
7.294
7.260
6.885
6.881
6.877
6.873
6.854
6.851
3.849
3.701
0.003
1.00
0.94
1.00
1.02
2.07
2.22
2.01
0.97
3.02
3.00
NH
O
F
F
F
O
CH3
H3C
O
O
F
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000

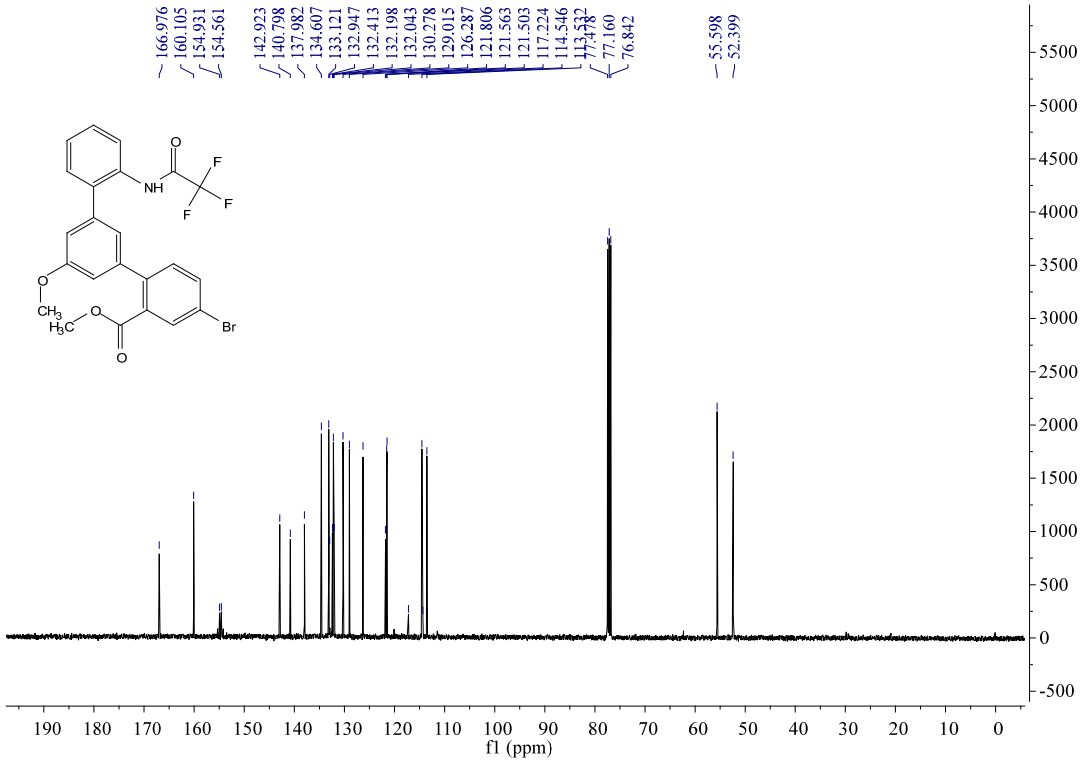

-75.839
-113.644
NH
O
F
F
F
O
CH3
H3C
O
O
F
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000


167.116
167.090
163.150
160.680
160.074
154.932
154.562
143.129
137.868
133.006
132.481
132.436
132.405
130.281
128.978
126.263
121.754
121.524
118.807
118.596
117.309
117.075
114.745
77.160
76.842
55.581
52.361
NH
O
F
F
F
O
CH3
H3C
O
O
F
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

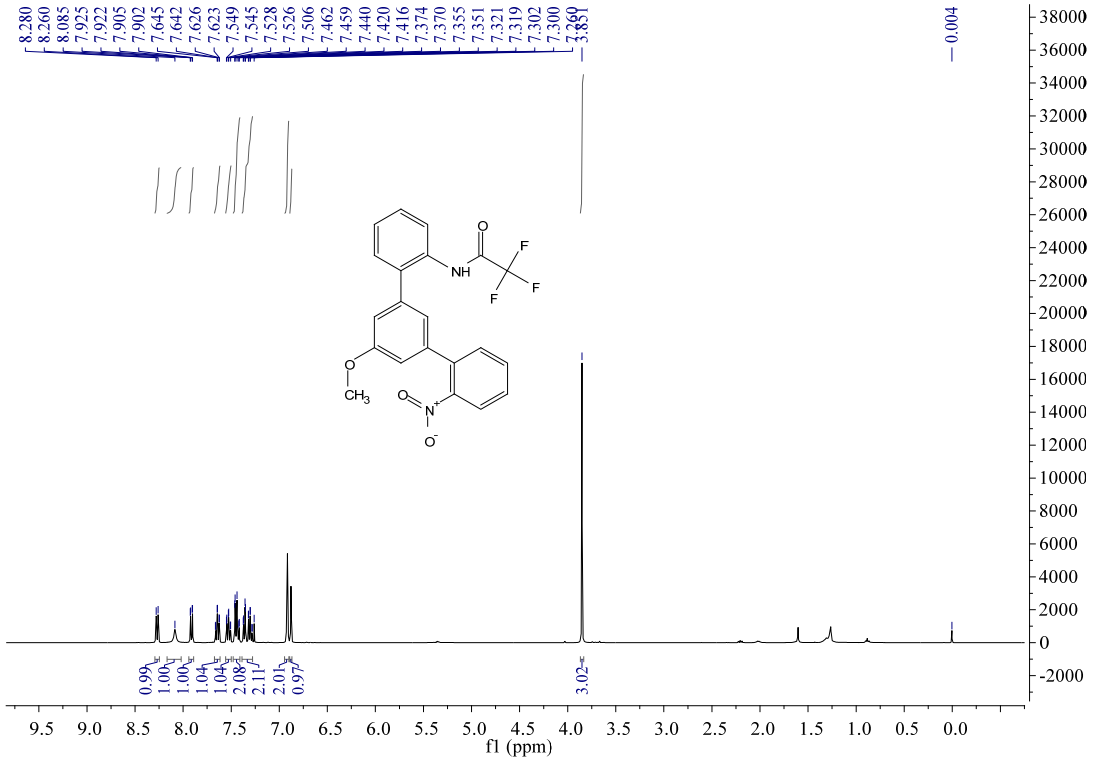
4t

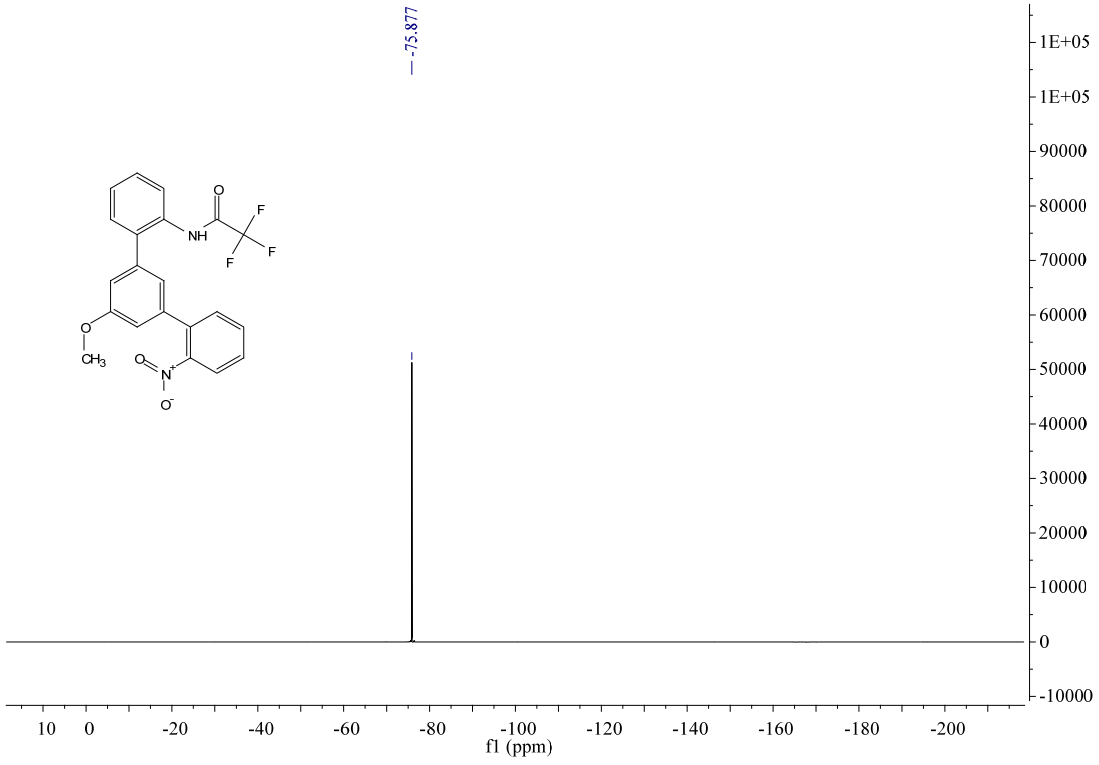

8.292
8.271
8.181
8.026
8.021
7.680
7.675
7.660
7.654
7.457
7.453
7.435
7.418
7.414
7.372
7.368
7.353
7.349
7.315
7.313
7.297
7.294
7.278
7.260
7.257
7.236
6.880
6.877
6.851
3.846
3.700
0.002
1.00
0.98
0.99
1.03
1.04
1.01
1.02
1.14
2.00
0.99
3.01
3.03
NH
O
F
F
F
O
CH3
H3C
O
O
Br
fl (ppm)

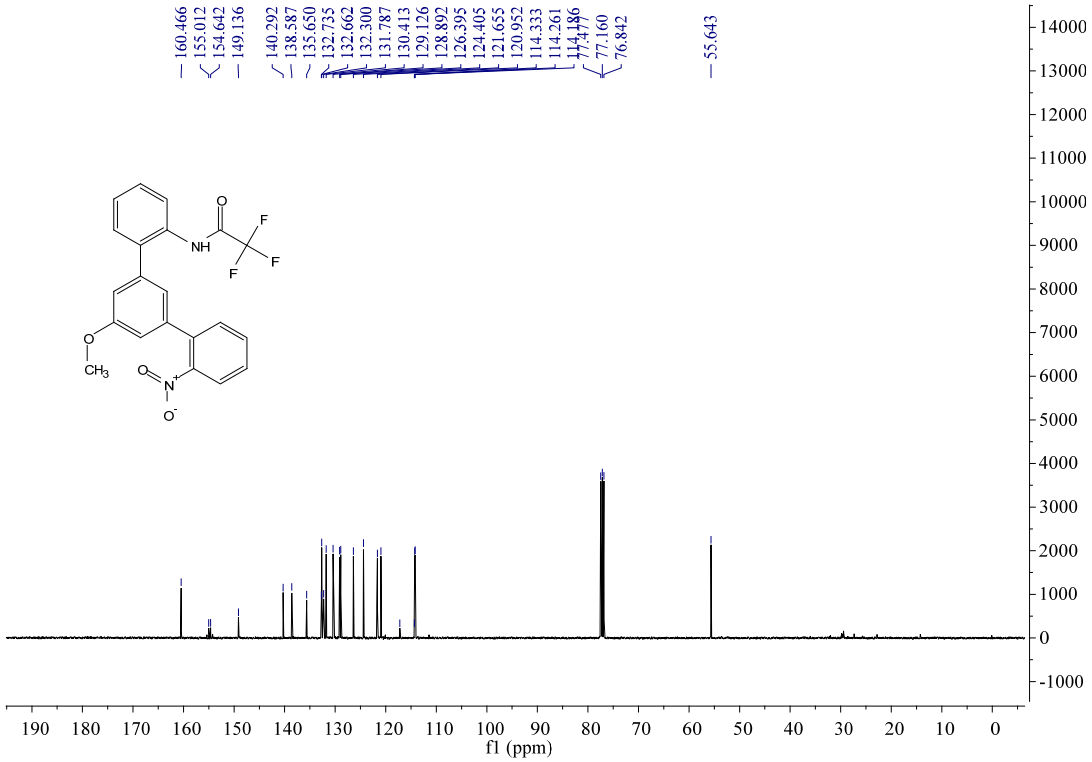

-75.815
NH
O
F
F
F
O
CH3
H3C
O
O
Br
fl (ppm)


166.976
160.105
154.931
154.561
142.923
140.798
137.982
134.607
133.121
132.947
132.413
132.198
132.043
130.278
129.015
126.287
121.806
121.563
121.503
117.224
114.546
113.532
77.478
77.160
76.842
55.598
52.399
NH
O
F
F
F
O
CH3
H3C
O
O
Br
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

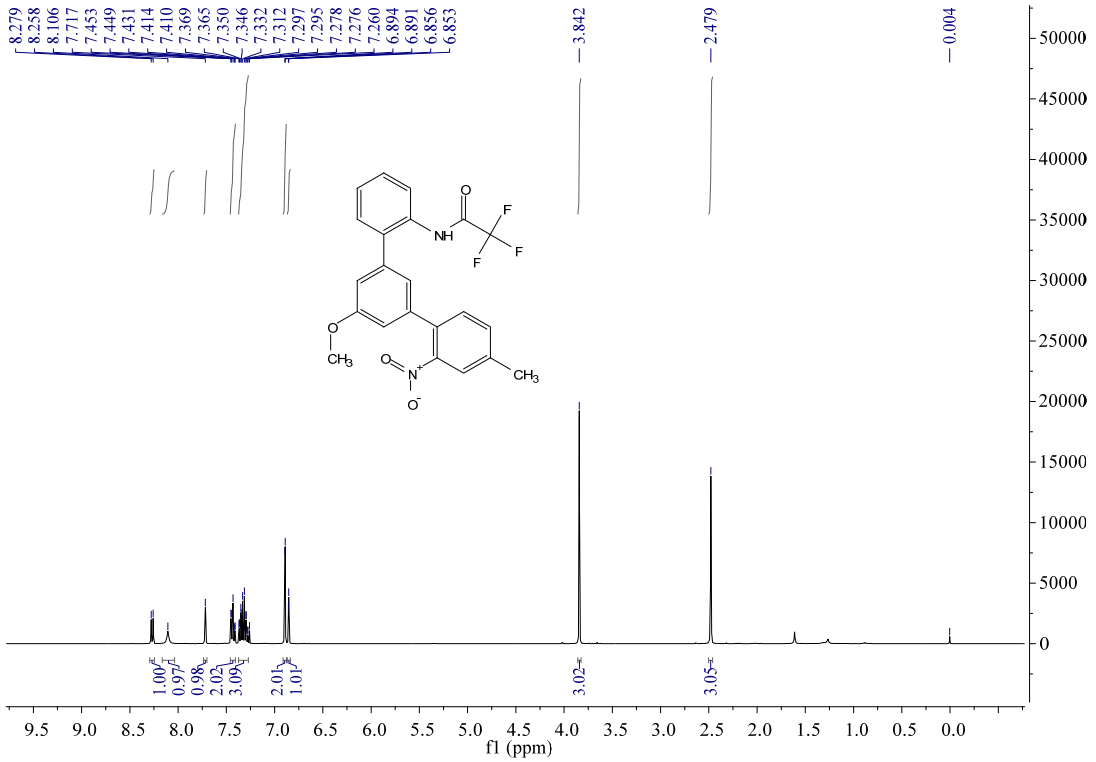
4u

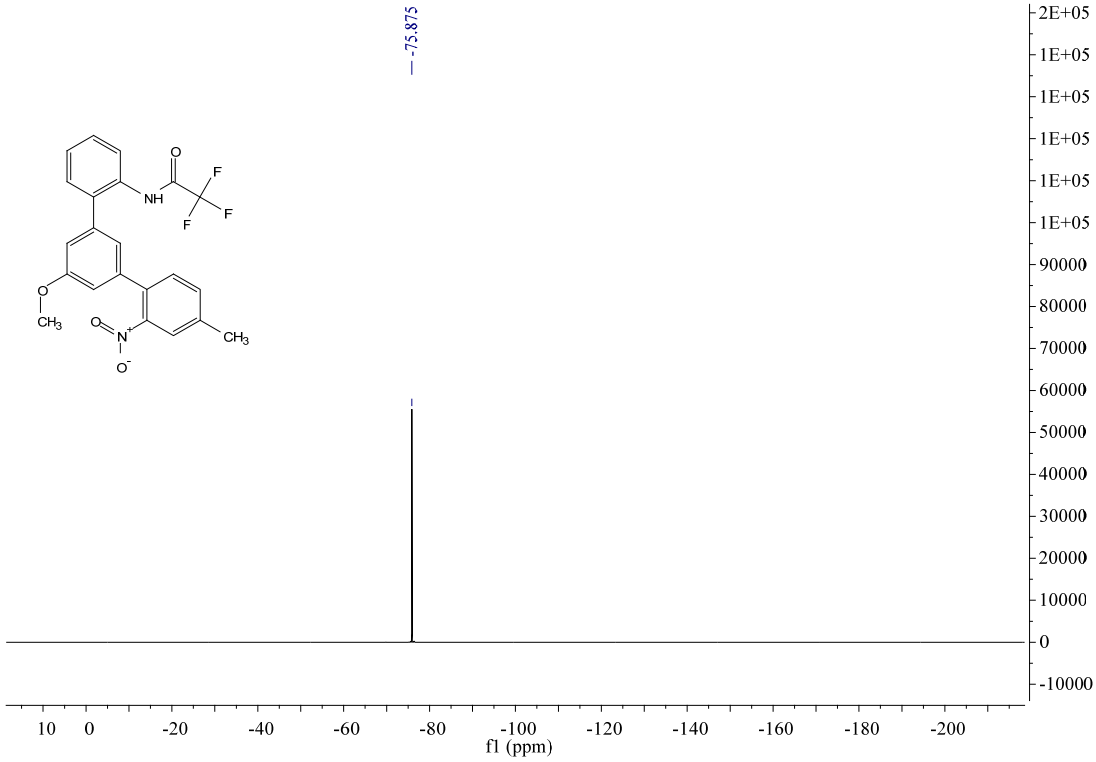

8.280
8.260
8.085
7.925
7.922
7.905
7.902
7.645
7.642
7.626
7.623
7.549
7.545
7.528
7.526
7.506
7.462
7.459
7.440
7.420
7.416
7.374
7.370
7.355
7.351
7.321
7.319
7.302
7.300
3.851
0.004
0.99
1.00
1.00
1.04
1.04
2.08
2.11
2.01
0.97
3.02
NH
O
F
F
F
O
CH3
O
N+
O-
fl (ppm)

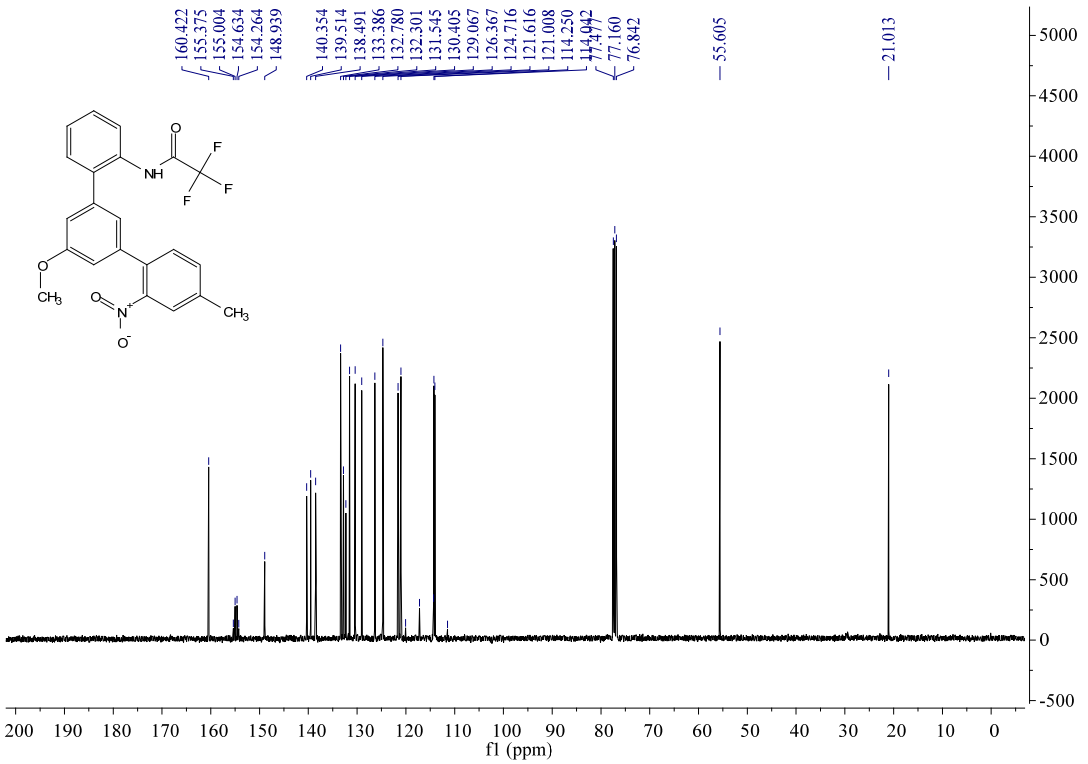

-75.877
NH
O
F
F
F
O
CH3
O
N+
O-
fl (ppm)


160.466
155.012
154.642
149.136
140.292
138.587
135.650
132.735
132.662
132.300
131.787
130.413
129.126
128.892
126.395
124.405
121.655
120.952
114.333
114.261
77.160
76.842
55.643
NH
O
F
F
F
O
CH3
O
N+
O-
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

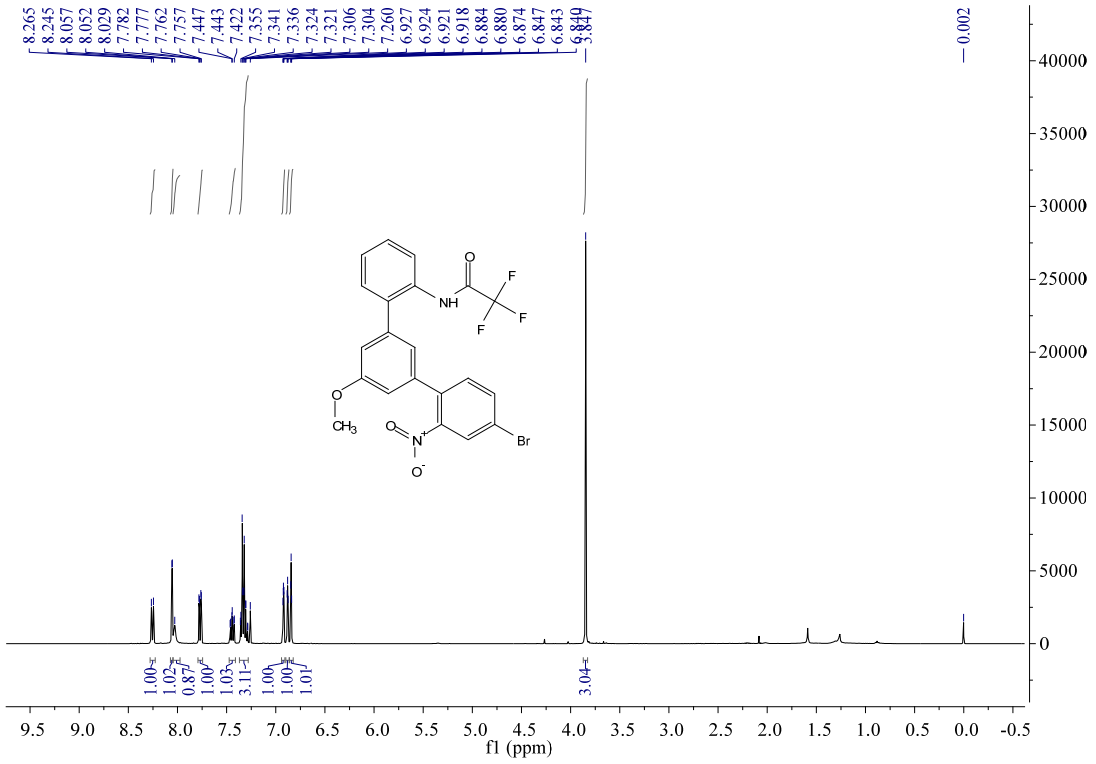
4v

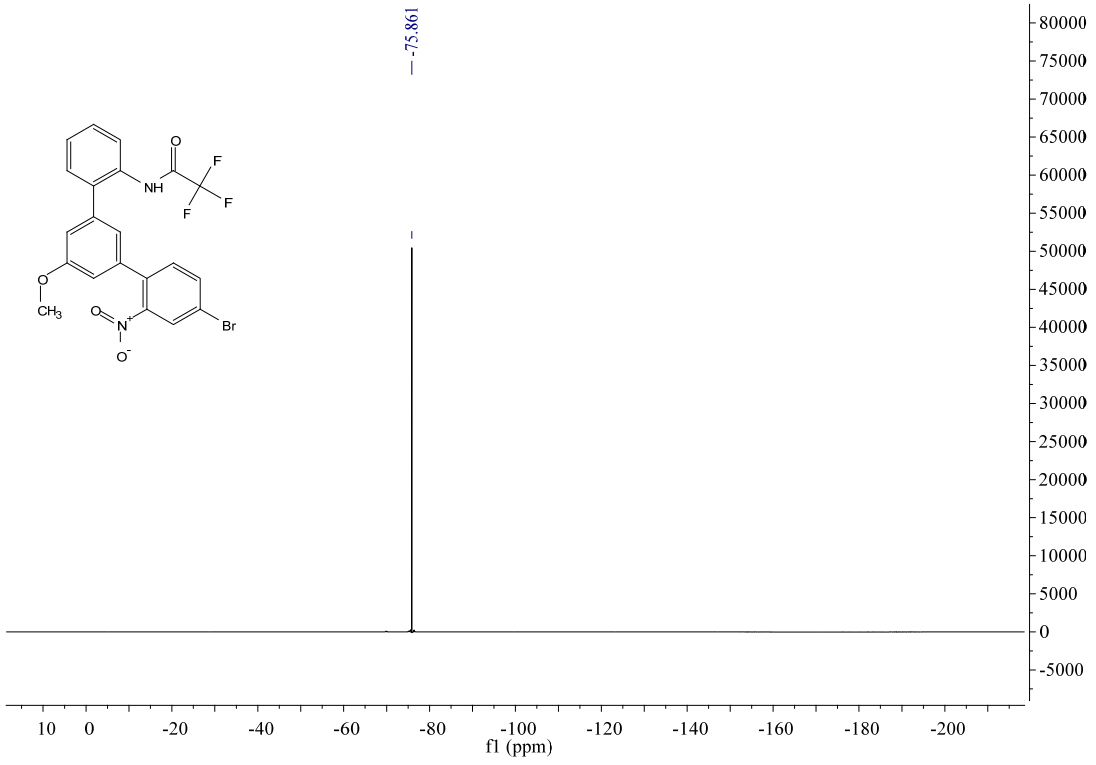

8.279
8.258
8.106
7.717
7.453
7.449
7.431
7.414
7.410
7.369
7.365
7.350
7.346
7.332
7.312
7.297
7.295
7.278
7.276
7.260
6.894
6.891
6.856
6.853
3.842
2.479
0.004
1.00
0.97
0.98
2.02
3.09
2.01
1.01
3.02
3.05
fl (ppm)

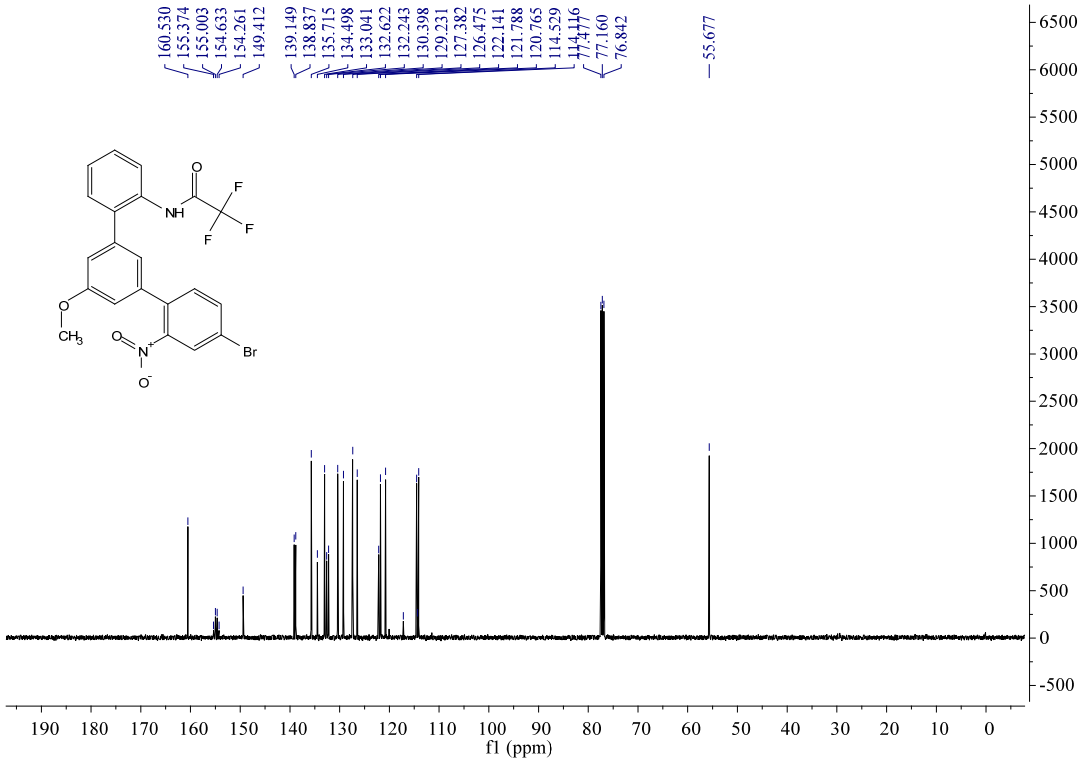

-75.875
fl (ppm)


160.422
155.375
155.004
154.634
154.264
148.939
140.354
139.514
138.491
133.386
132.780
132.301
131.545
130.405
129.067
126.367
124.716
121.616
121.008
114.250
77.477
77.160
76.842
55.605
21.013
O
NH
F
F
F
O
CH3
O
N+
O-
CH3
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

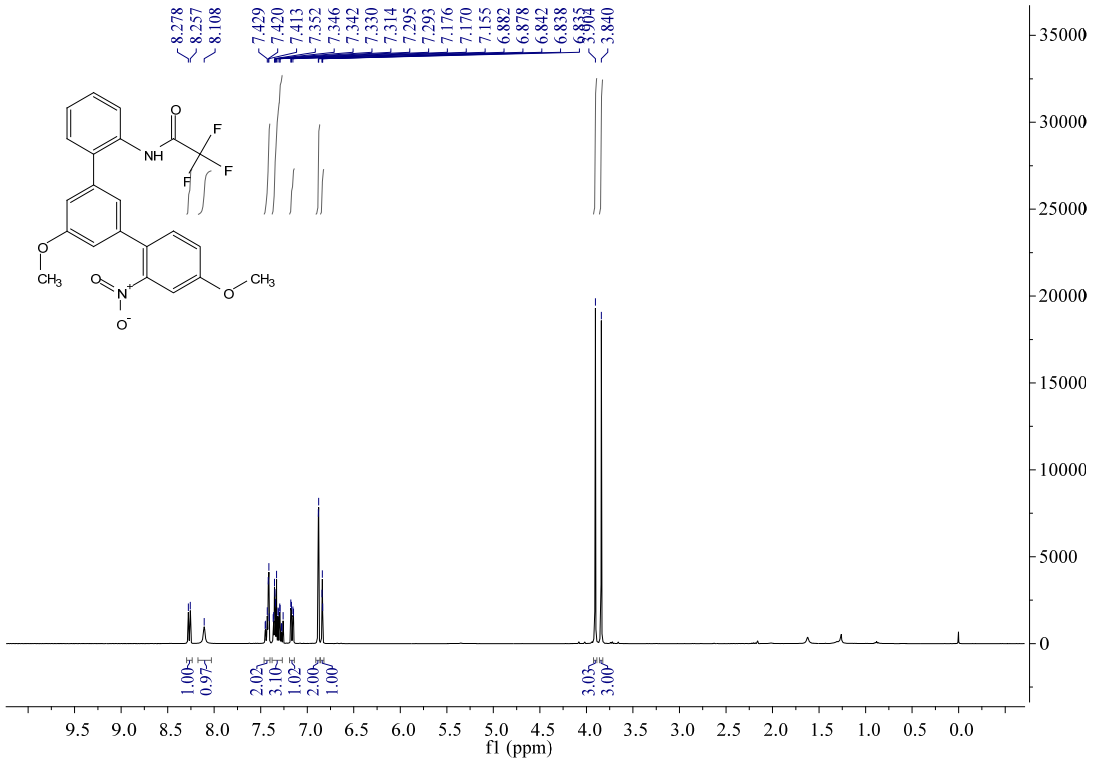
4w

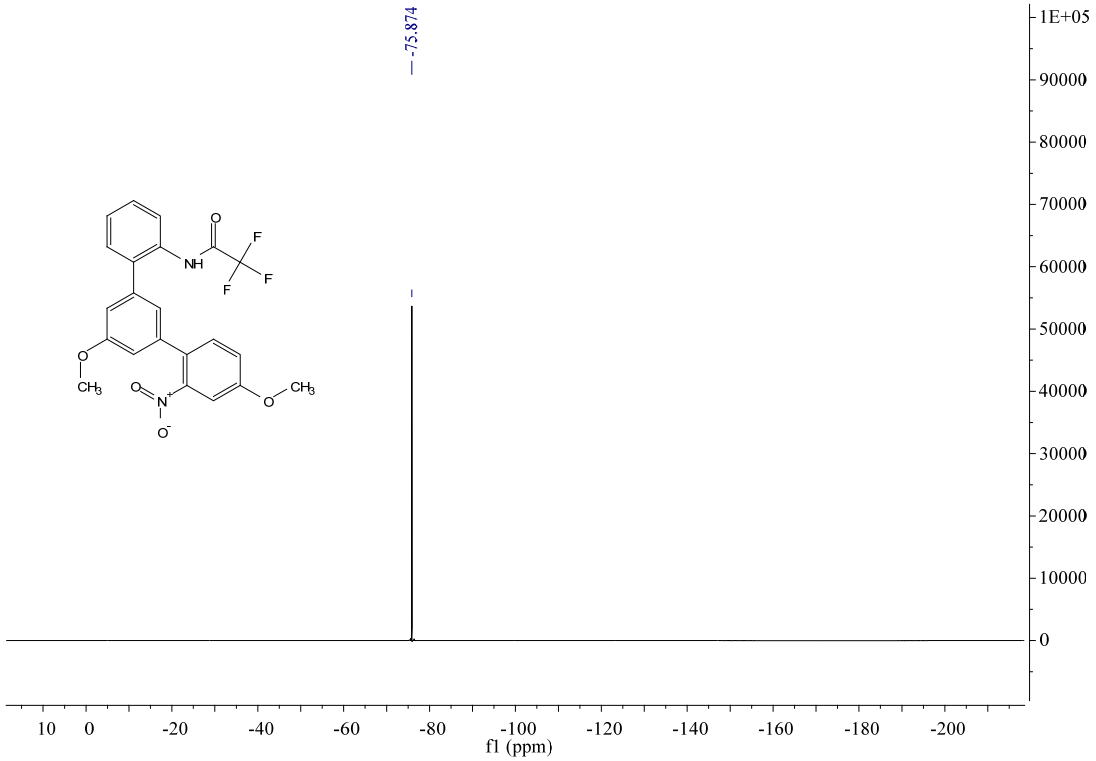

8.265
8.245
8.057
8.052
8.029
7.782
7.777
7.762
7.757
7.447
7.443
7.422
7.355
7.341
7.336
7.324
7.321
7.306
7.304
7.260
6.927
6.924
6.921
6.918
6.884
6.880
6.874
6.847
6.843
6.840
3.847
0.002
1.00
1.02
0.87
1.00
1.03
3.11
1.00
1.00
1.01
3.04
NH
F
F
F
O
O
CH3
N+
O-
Br
fl (ppm)

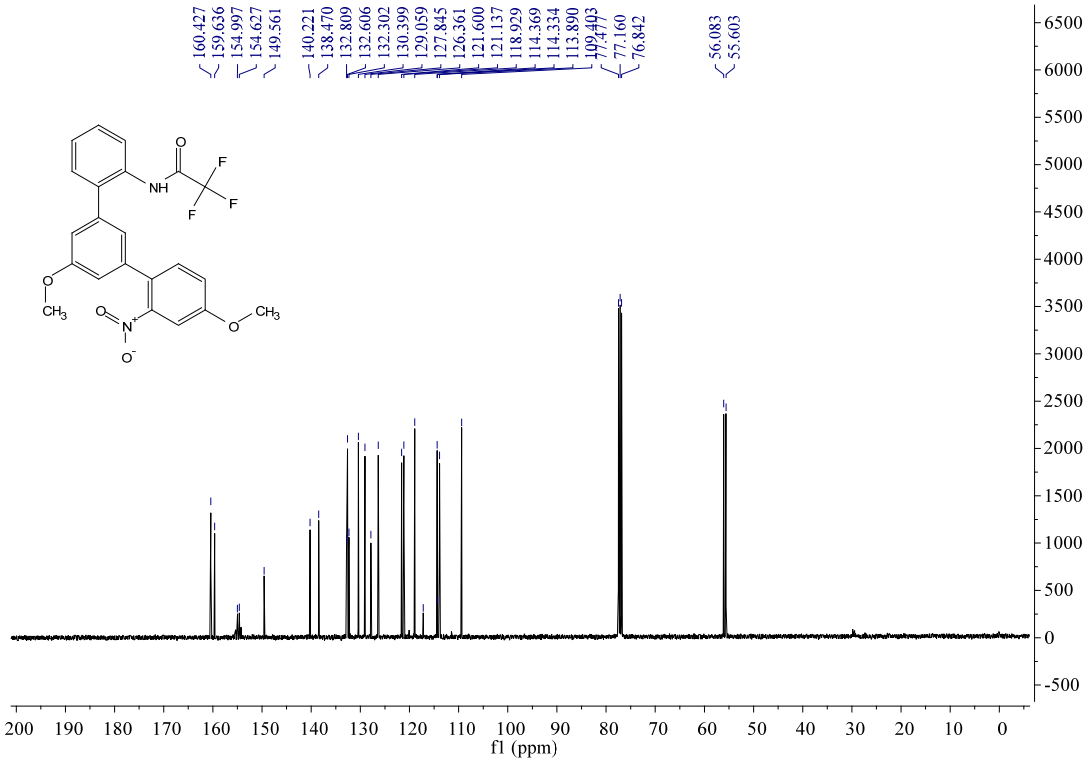

-75.861
NH
F
F
F
O
O
CH3
N+
O-
Br
fl (ppm)


160.530
155.374
155.003
154.633
154.261
149.412
139.149
138.837
135.715
134.498
133.041
132.622
132.243
130.398
129.231
127.382
126.475
122.141
121.788
120.765
114.529
114.116
77.477
77.160
76.842
55.677
NH
O
F
F
F
O
CH3
O
N+
O-
Br
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

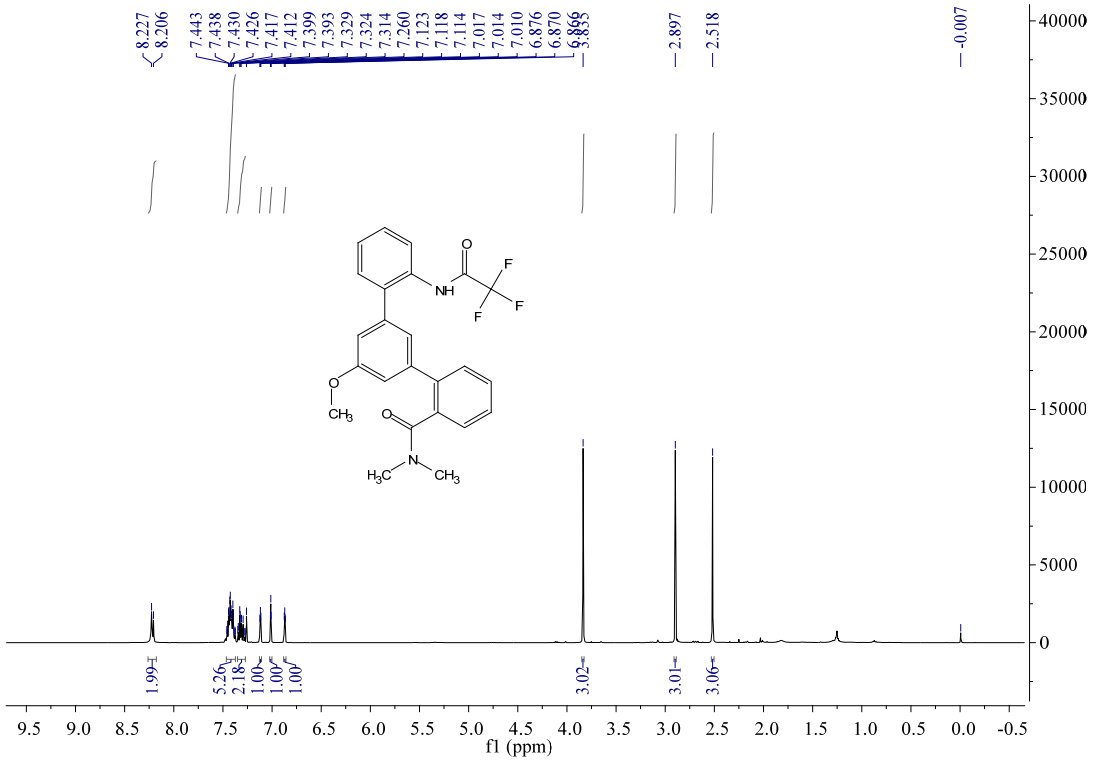
4x

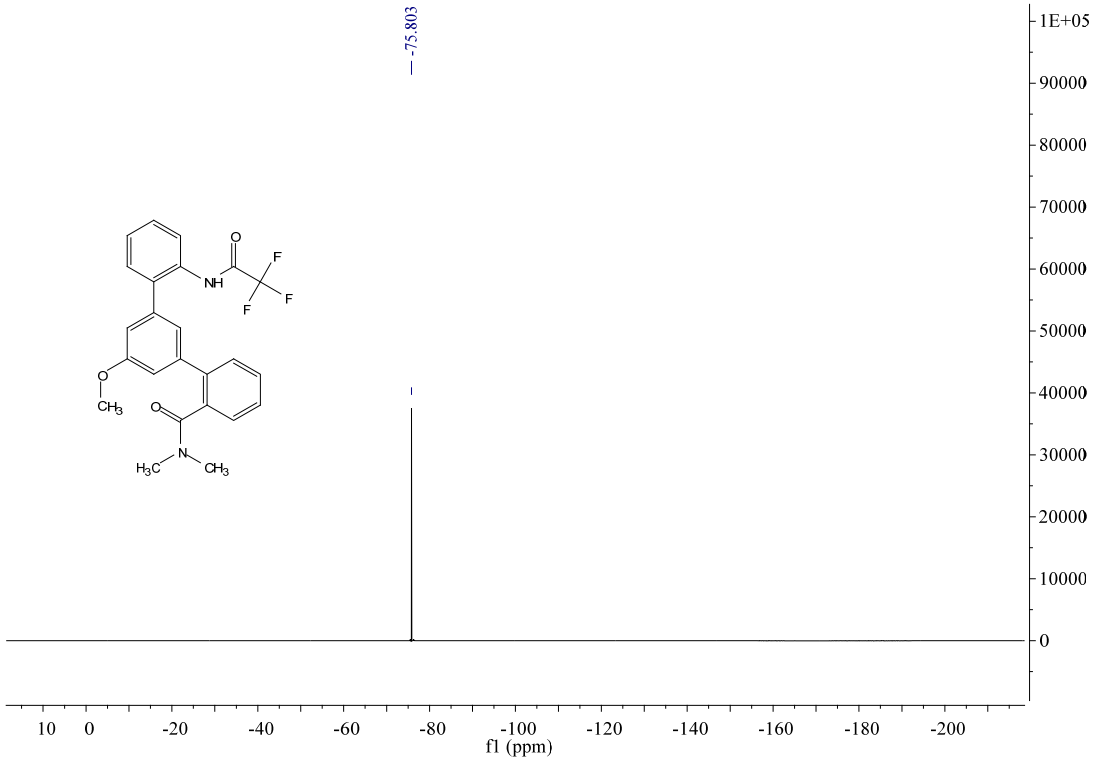

8.278
8.257
8.108
7.429
7.420
7.413
7.352
7.346
7.342
7.330
7.314
7.295
7.293
7.176
7.170
7.155
6.882
6.878
6.842
6.838
6.835
3.904
3.840
1.00
0.97
2.02
3.10
1.02
2.00
1.00
3.03
3.00
f1 (ppm)

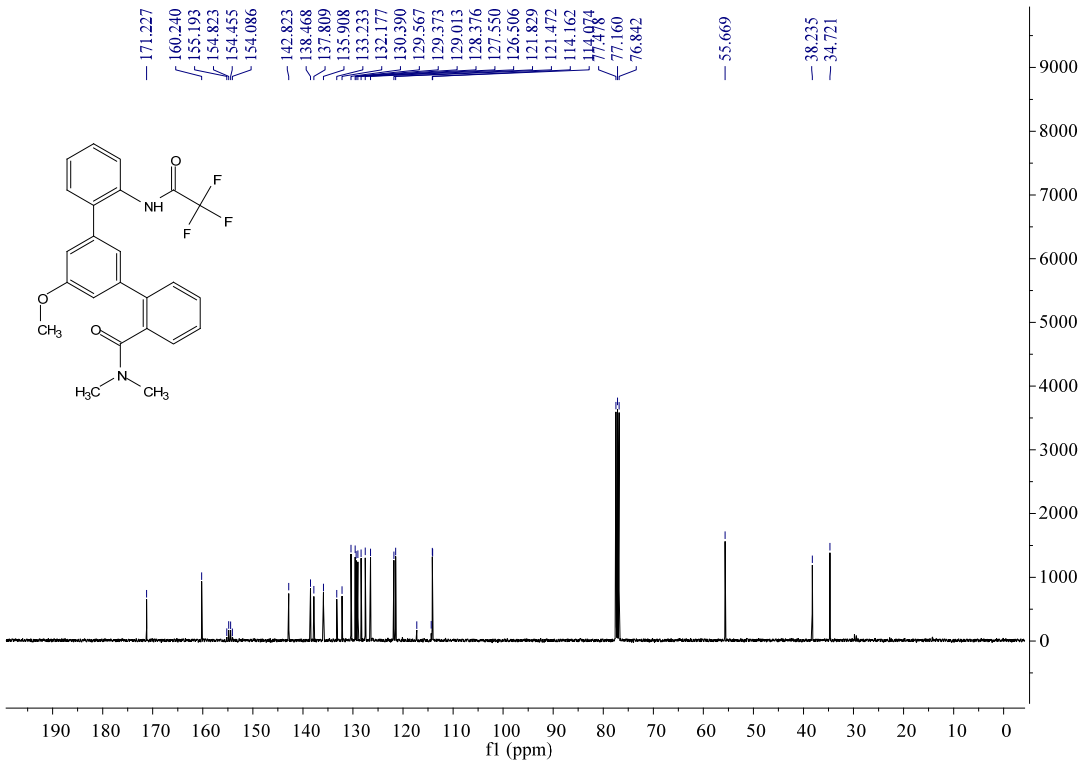

-75.874
f1 (ppm)


160.427
159.636
154.997
154.627
149.561
140.221
138.470
132.809
132.606
132.302
130.399
129.059
127.845
126.361
121.600
121.137
118.929
114.369
114.334
113.890
77.477
77.160
76.842
56.083
55.603
NH
O
F
F
F
O
CH3
O
N+
O-
O
CH3
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

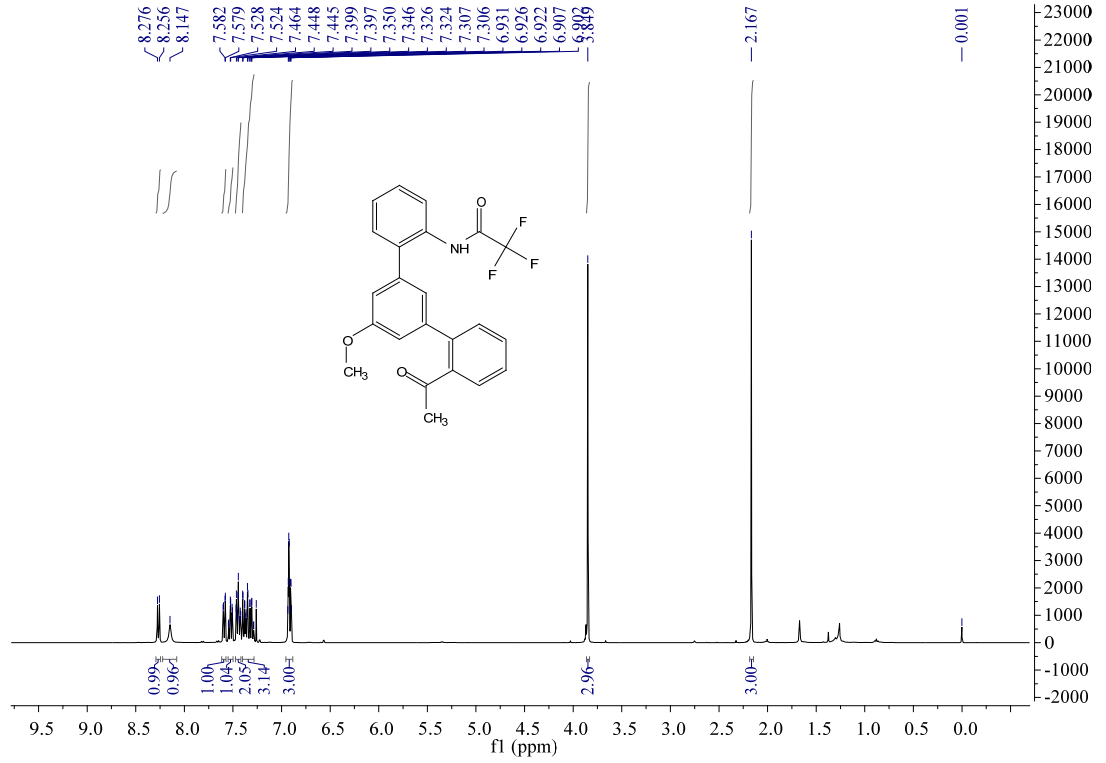
4y


8.227
8.206
7.443
7.438
7.430
7.426
7.417
7.412
7.399
7.393
7.329
7.324
7.314
7.260
7.123
7.118
7.114
7.017
7.014
7.010
6.876
6.870
3.835
2.897
2.518
-0.007
1.99
5.26
2.18
1.00
1.00
1.00
3.02
3.01
3.06
f1 (ppm)


-75.803
f1 (ppm)


171.227
160.240
155.193
154.823
154.455
154.086
142.823
138.468
137.809
135.908
133.233
132.177
130.390
129.567
129.373
129.013
128.376
127.550
126.506
121.829
121.472
114.162
114.024
77.478
77.160
76.842
55.669
38.235
34.721
NH
O
F
F
F
O
CH3
O
N
H3C
CH3
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4z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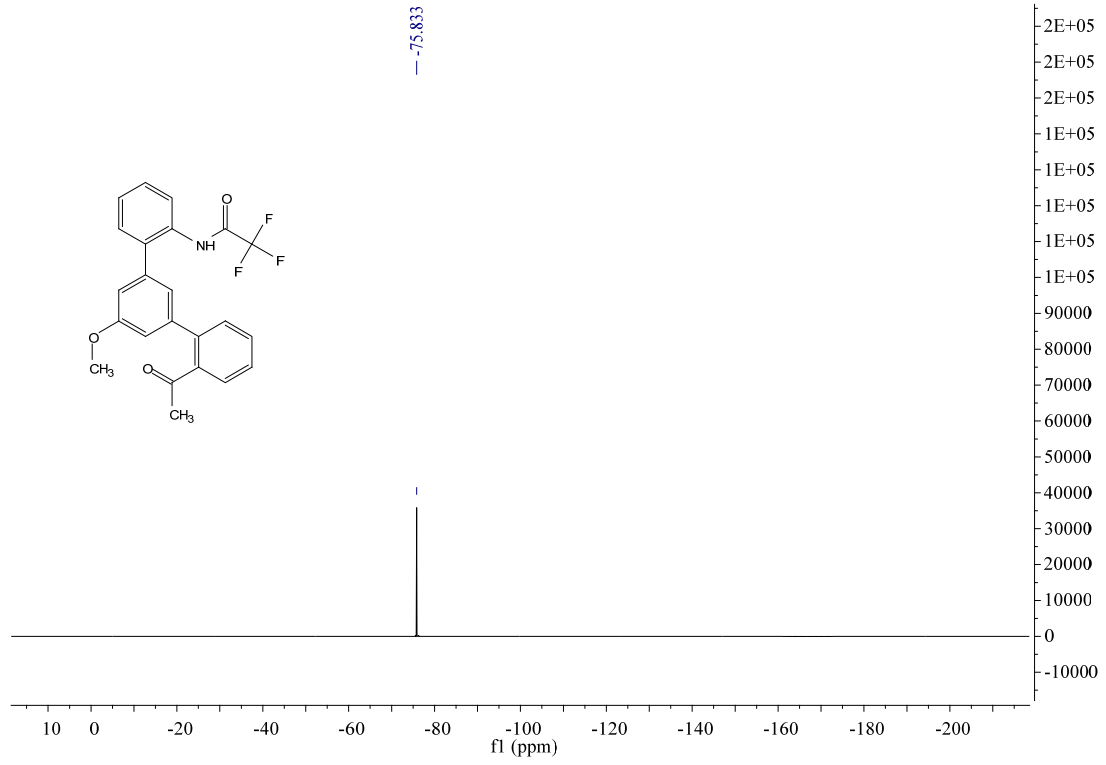
8.256
8.147
7.582
7.579
7.528
7.524
7.464
7.448
7.445
7.399
7.397
7.350
7.346
7.326
7.324
7.307
7.306
6.931
6.926
6.922
6.907
6.902
6.899
3.849
2.167
0.001
0.99
0.96
1.00
1.04
2.05
3.14
3.00
2.96
3.00
NH
O
F
F
F
O
CH3
O
CH3
f1 (ppm)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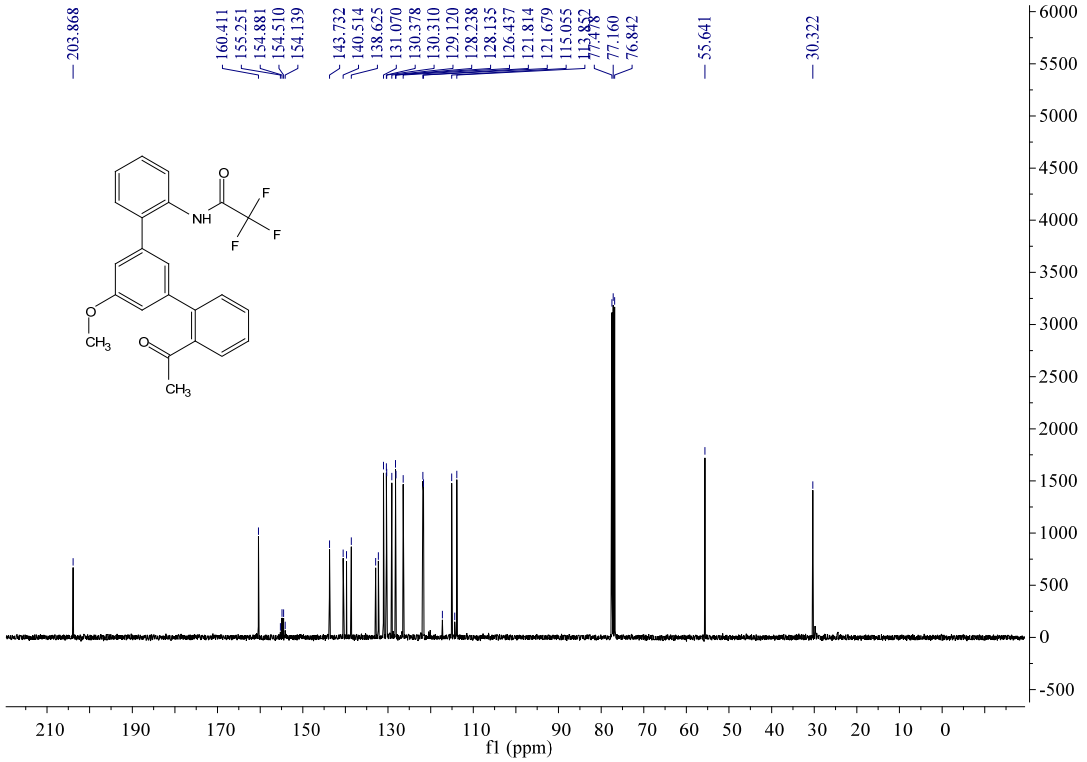
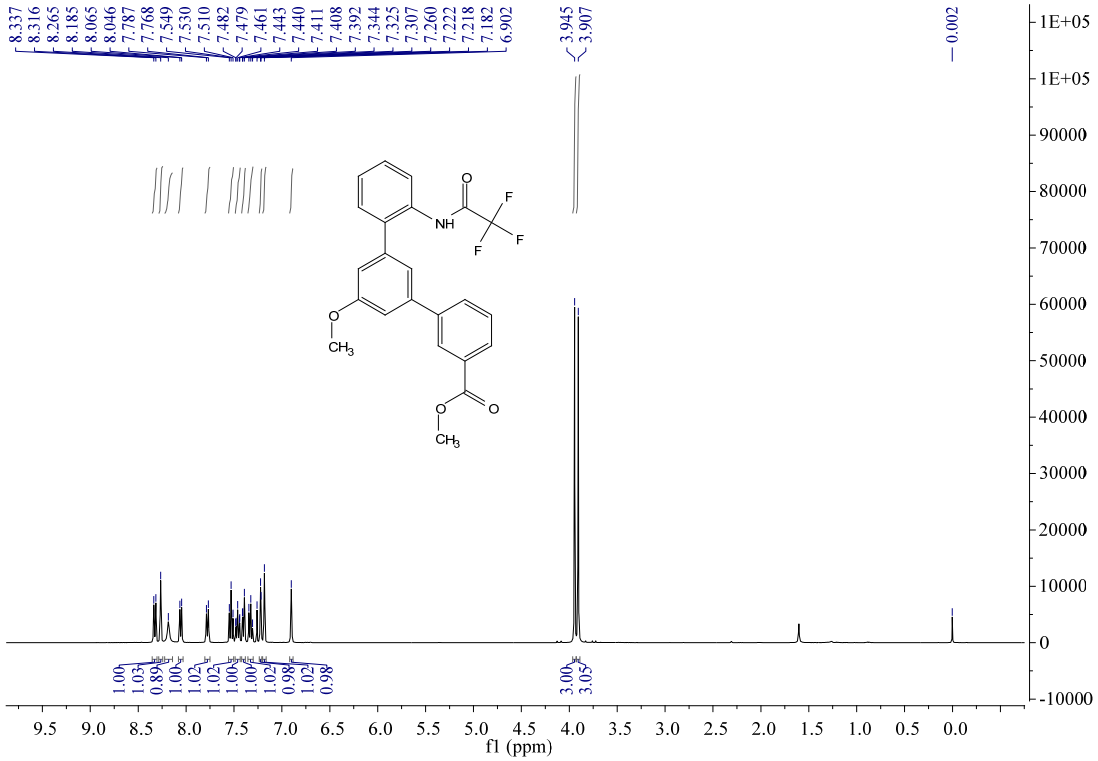
NH
O
F
F
F
O
CH3
O
CH3
f1 (ppm)


203.868
160.411
155.251
154.881
154.510
154.139
143.732
140.514
138.625
131.070
130.378
130.310
129.120
128.238
128.135
126.437
121.814
121.679
115.055
113.852
77.478
77.160
76.842
55.641
30.322
NH
O
F
F
F
O
CH3
O
CH3
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4aa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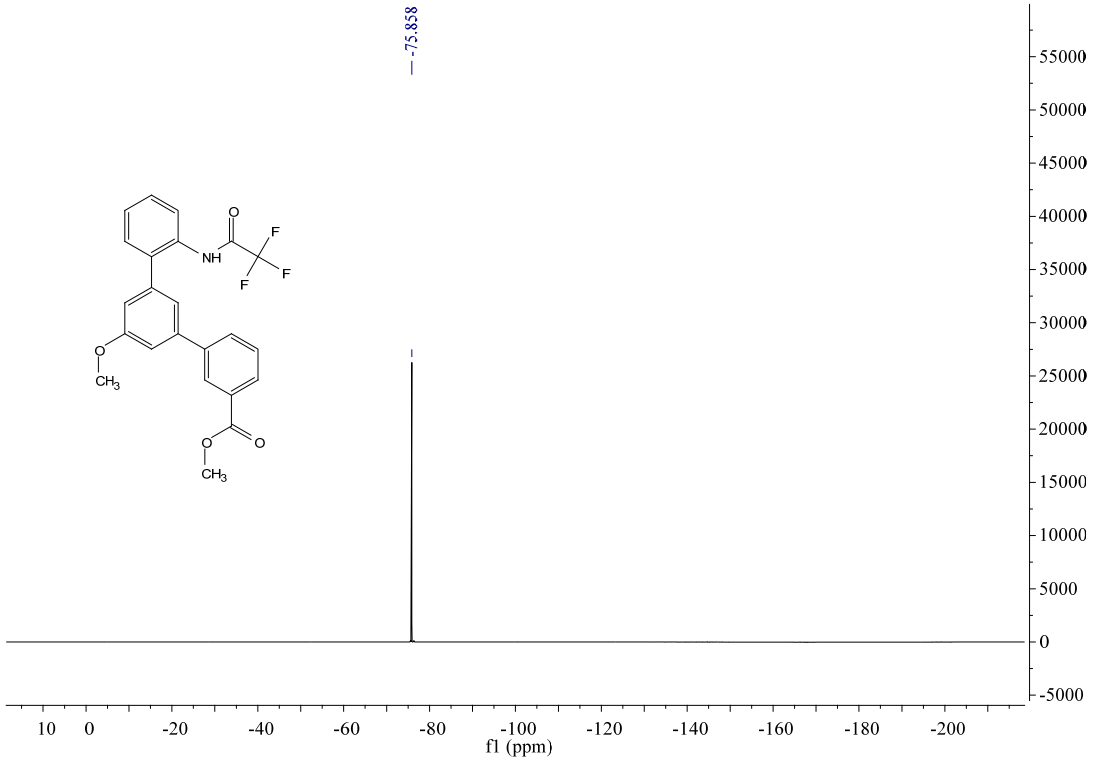
8.316
8.265
8.185
8.065
8.046
7.787
7.768
7.549
7.530
7.510
7.482
7.479
7.461
7.443
7.440
7.411
7.408
7.392
7.344
7.325
7.307
7.260
7.222
7.218
7.182
6.902
3.945
3.907
0.002
1.00
1.03
0.89
1.00
1.02
1.02
1.00
1.00
1.02
0.98
1.02
0.98
3.00
3.05
NH
O
F
F
F
O
CH3
O
O
CH3
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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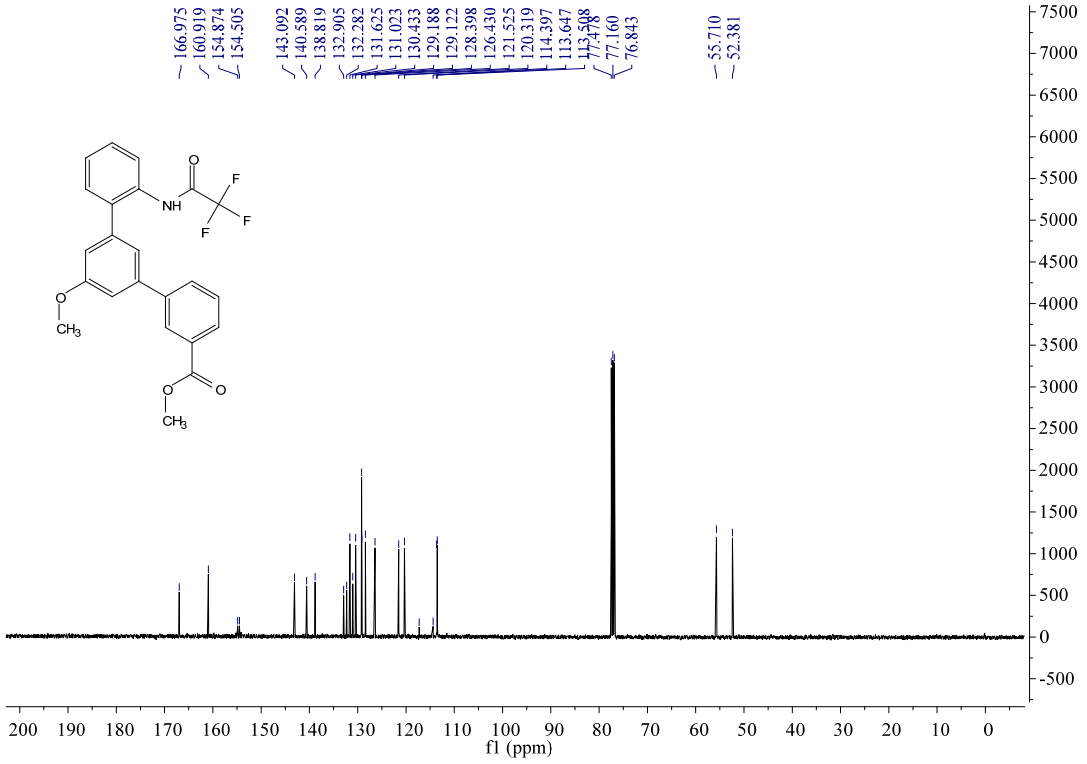
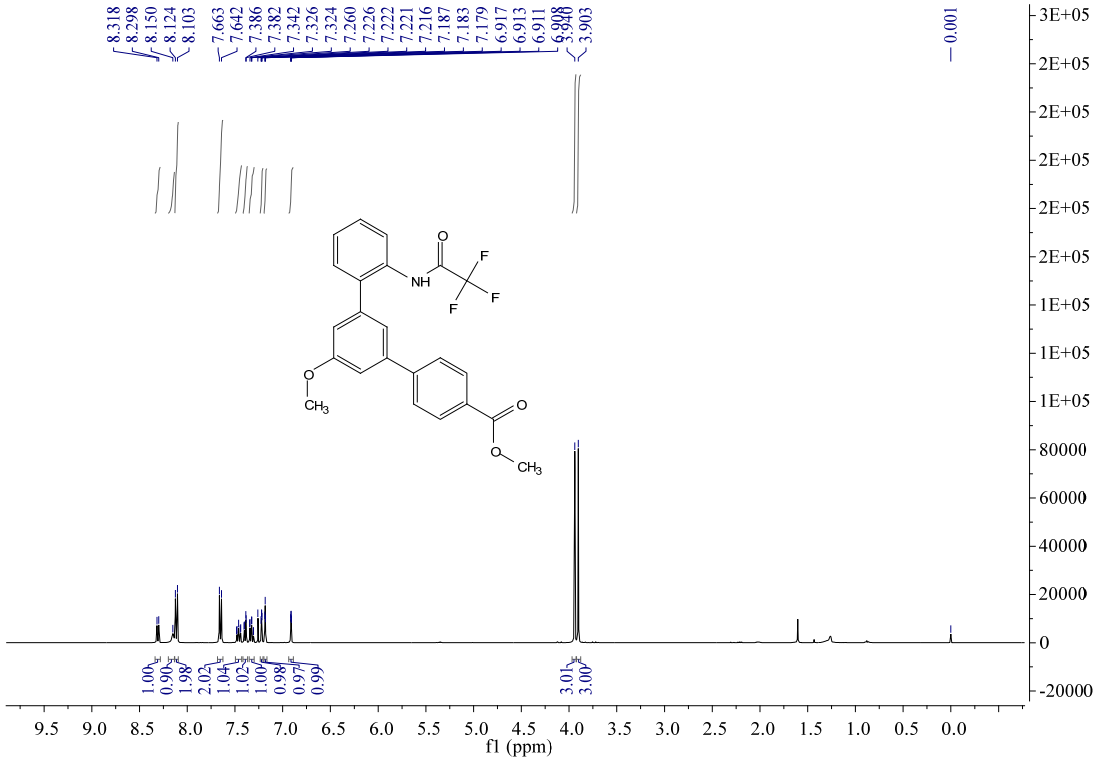
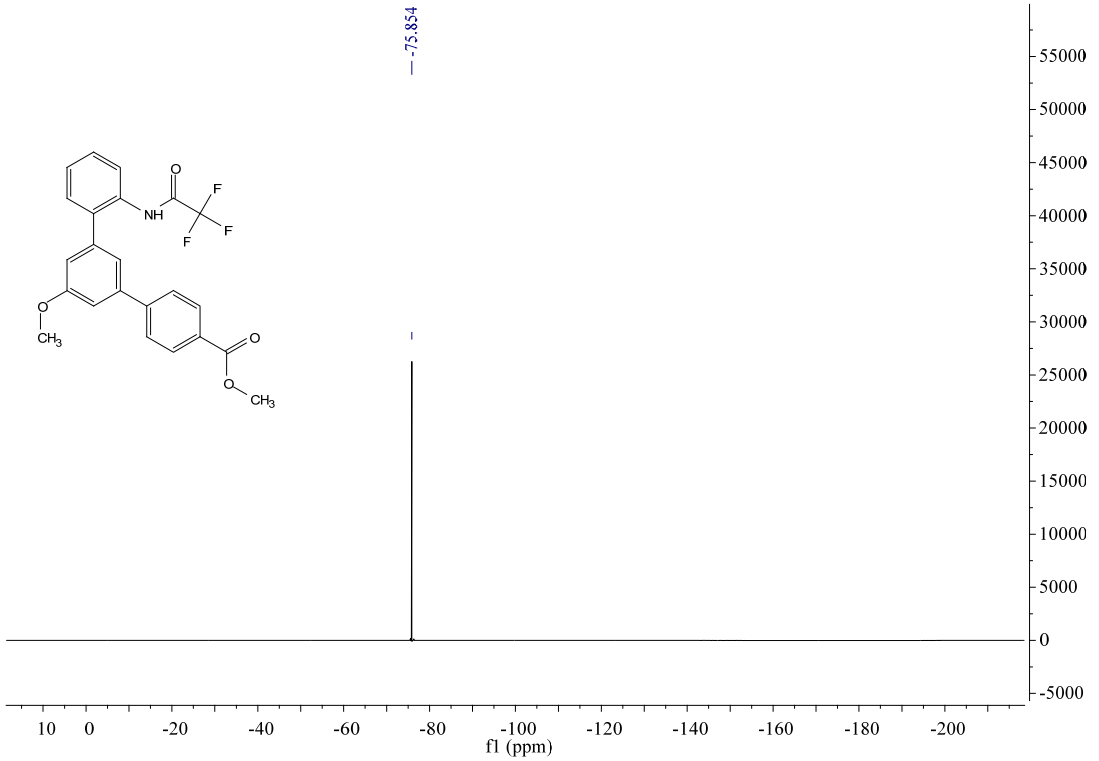
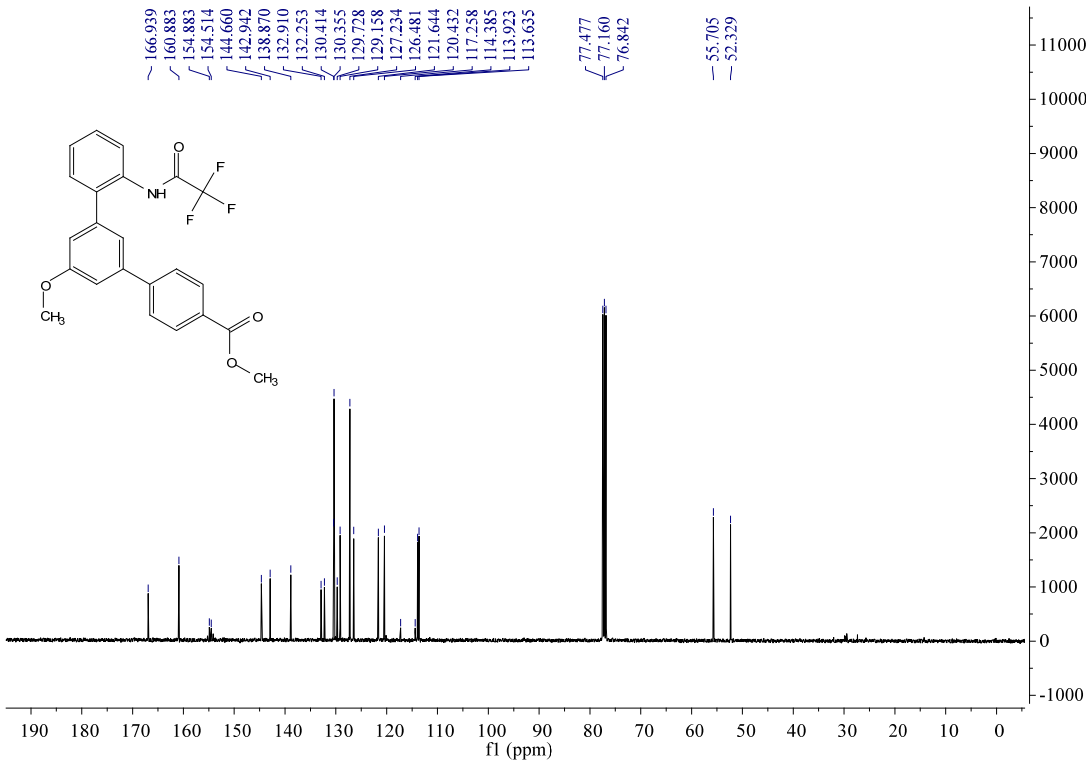
NH
O
F
F
F
O
CH3
O
O
CH3
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200
f1 (ppm)


166.975
160.919
154.874
154.505
143.092
140.589
138.819
132.905
132.282
131.625
131.023
130.433
129.188
129.122
128.398
126.430
121.525
120.319
114.397
113.647
77.160
76.843
55.710
52.381
NH
O
F
F
F
O
CH3
O
O
CH3
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

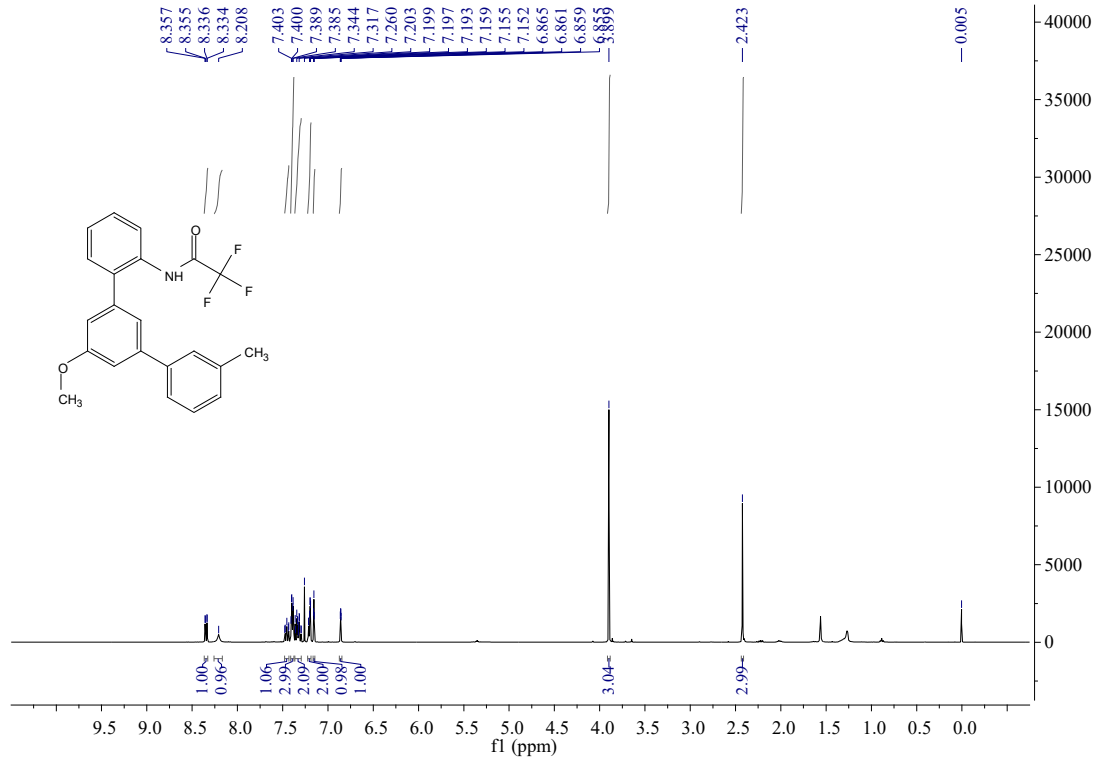
4ab


8.318
8.298
8.150
8.124
8.103
7.663
7.642
7.386
7.382
7.342
7.326
7.324
7.260
7.226
7.222
7.221
7.216
7.187
7.183
7.179
6.917
6.913
6.911
3.940
3.903
0.001
NH
O
F
F
F
O
CH3
O
CH3
1.00
0.90
1.98
2.02
1.04
1.02
1.00
0.98
0.97
0.99
3.01
3.00
fl (ppm)

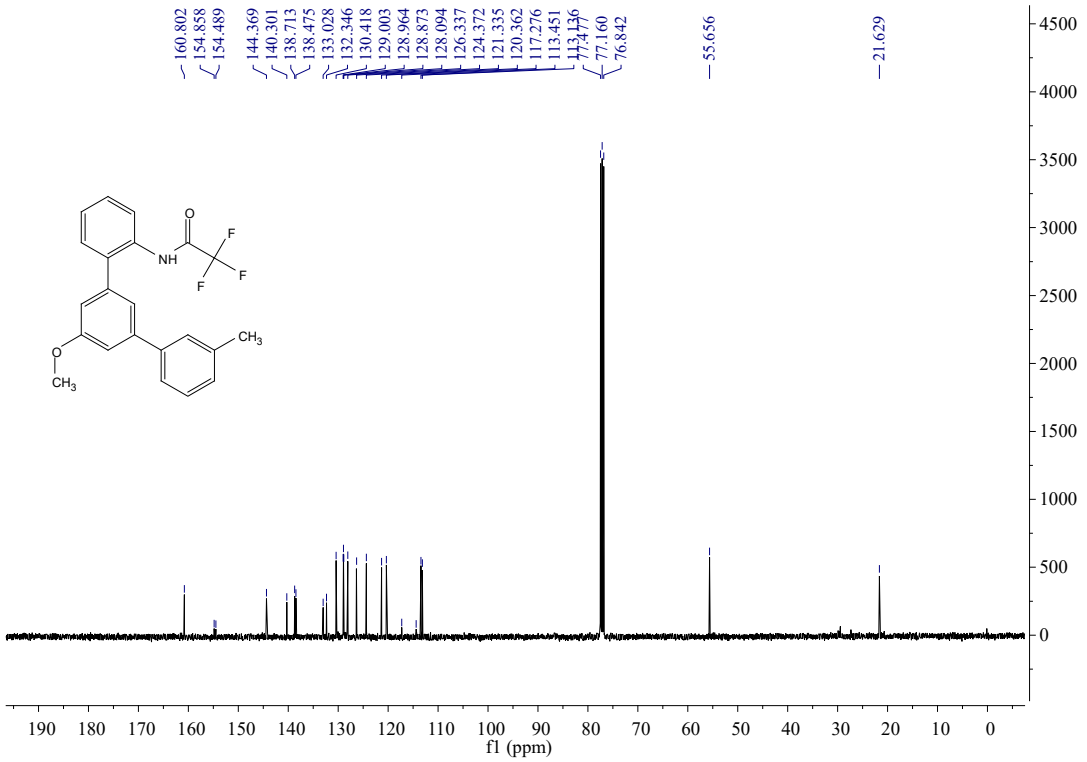

-75.854
NH
O
F
F
F
O
CH3
O
CH3
fl (ppm)


166.939
160.883
154.883
154.514
144.660
142.942
138.870
132.910
132.253
130.414
130.355
129.728
129.158
127.234
126.481
121.644
120.432
117.258
114.385
113.923
113.635
77.477
77.160
76.842
55.705
52.329
NH
O
F
F
F
O
CH3
O
O
CH3
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

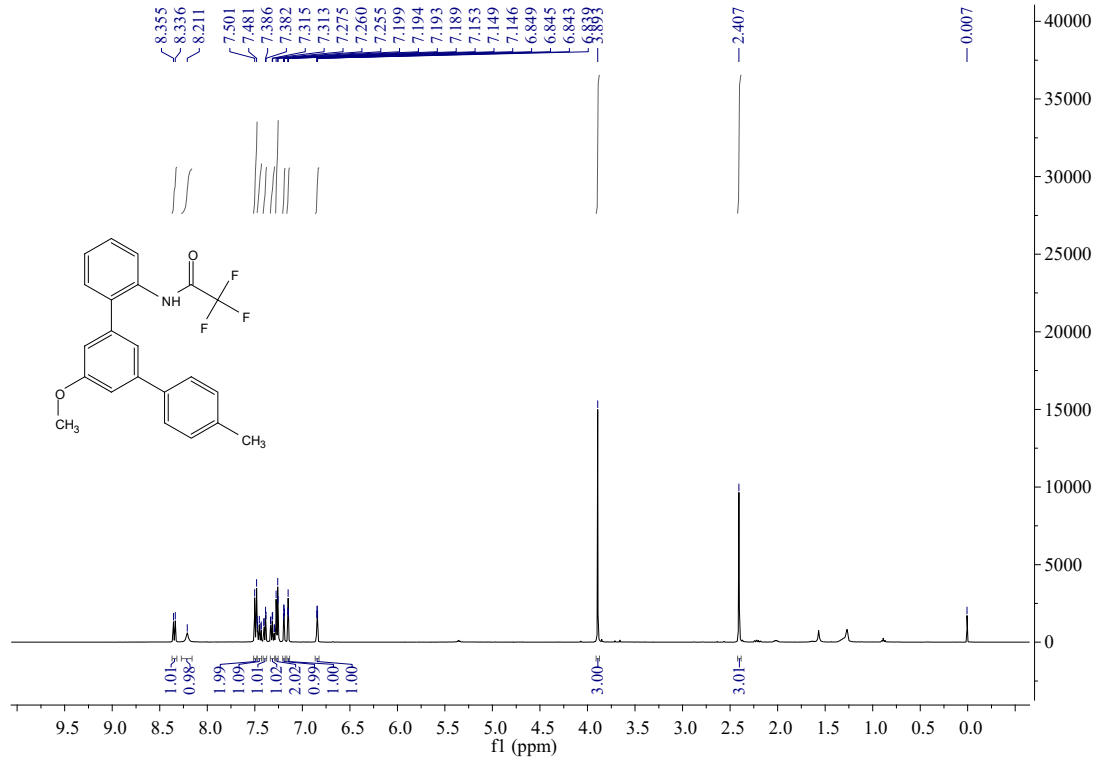
4ac

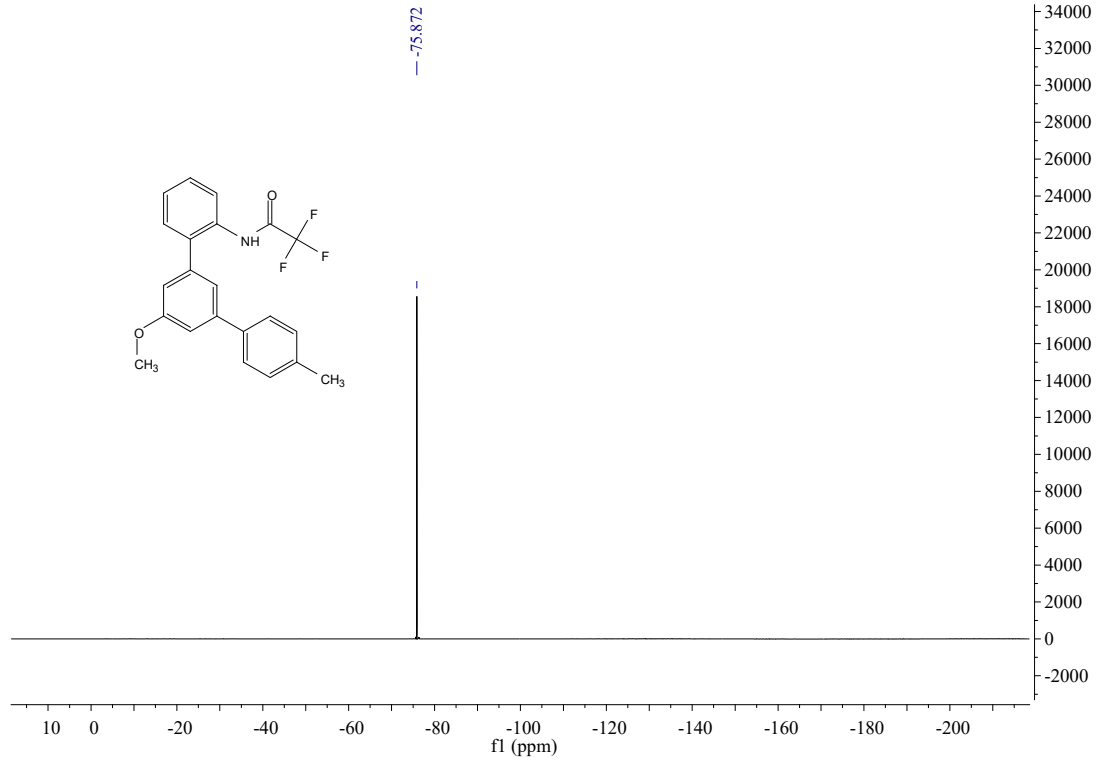

8.357
8.355
8.336
8.334
8.208
7.403
7.400
7.389
7.385
7.344
7.317
7.260
7.203
7.199
7.197
7.193
7.159
7.155
7.152
6.865
6.861
6.859
6.855
3.899
2.423
0.005
NH
O
F
F
F
O
CH3
CH3
1.00
0.96
1.06
2.99
2.09
2.00
0.98
1.00
3.04
2.99
fl (ppm)

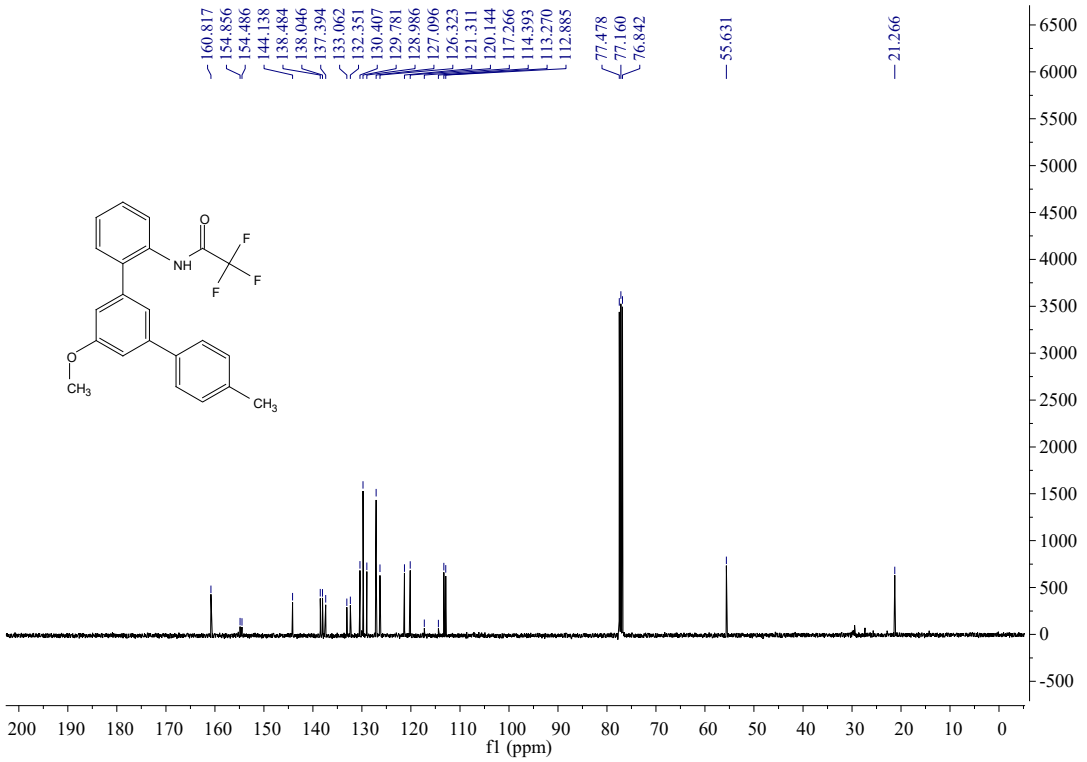

-75.847
NH
O
F
F
F
O
CH3
CH3
fl (ppm)


160.802
154.858
154.489
144.369
140.301
138.713
138.475
133.028
132.346
130.418
129.003
128.964
128.873
128.094
126.337
124.372
121.335
120.362
117.276
113.451
77.477
77.160
76.842
55.656
21.629
NH
O
F
F
F
O
CH3
CH3
4500
4000
3500
3000
2500
2000
1500
1000
500
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

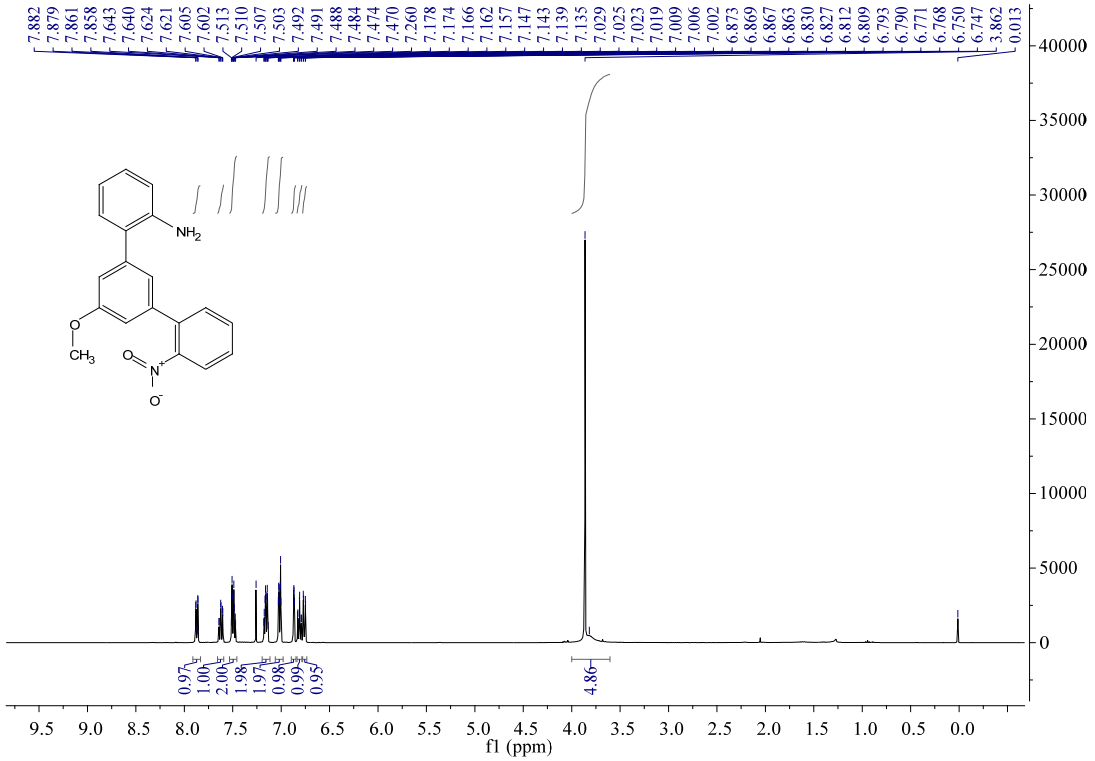
4ad

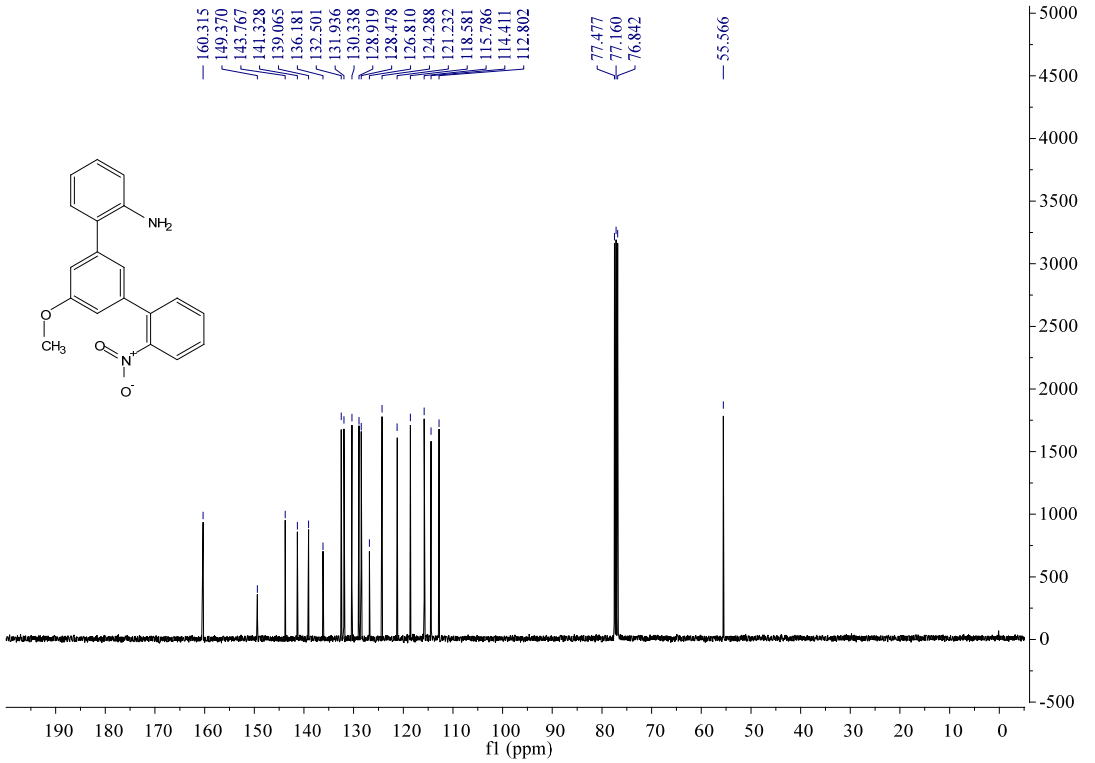

8.355
8.336
8.211
7.501
7.481
7.386
7.382
7.315
7.313
7.275
7.260
7.255
7.199
7.194
7.193
7.189
7.153
7.149
7.146
6.849
6.845
6.843
6.839
6.833
2.407
0.007
NH
O
F
F
F
O
CH3
CH3
1.01
0.98
1.99
1.09
1.01
1.02
2.02
0.99
1.00
1.00
3.00
3.01
fl (ppm)


-75.872
NH
O
F
F
F
O
CH3
CH3
fl (ppm)

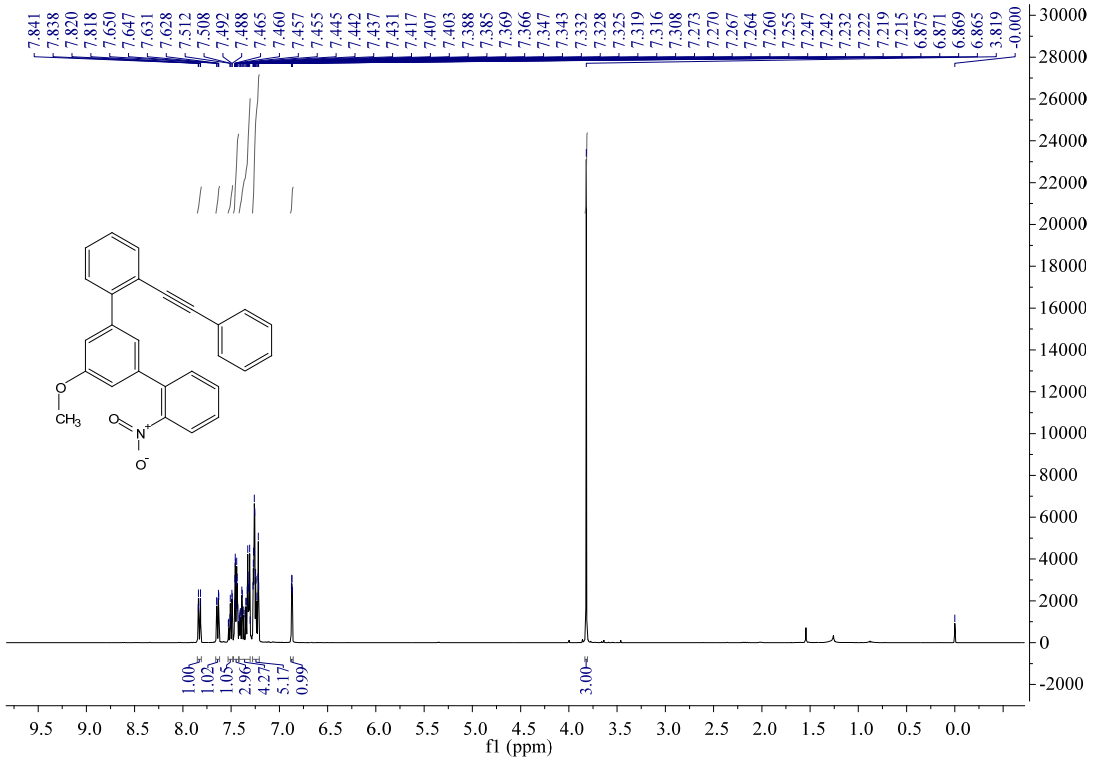

160.817
154.856
154.486
144.138
138.484
138.046
137.394
133.062
132.351
130.407
129.781
128.986
127.096
126.323
121.311
120.144
117.266
114.393
113.270
112.885
77.478
77.160
76.842
55.631
21.266
O
NH
F
F
F
O
CH3
CH3
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

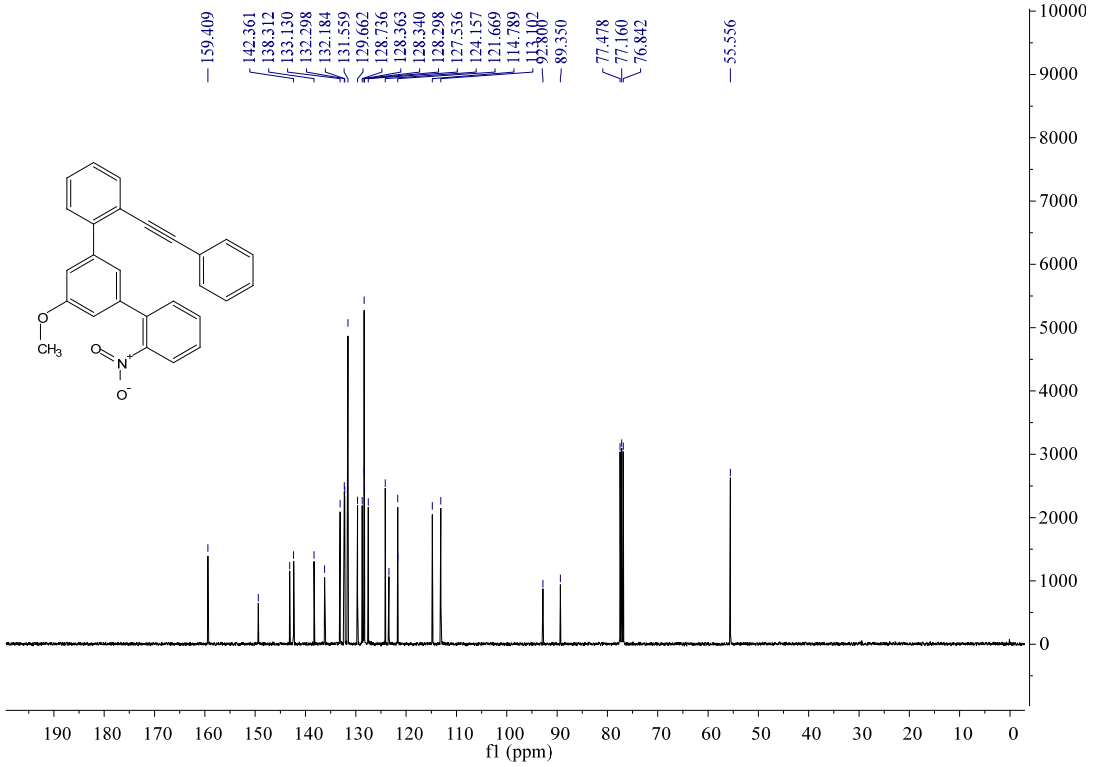
6


7.882
7.879
7.861
7.858
7.643
7.640
7.624
7.621
7.605
7.602
7.513
7.510
7.507
7.503
7.492
7.491
7.488
7.484
7.474
7.470
7.260
7.178
7.174
7.166
7.162
7.157
7.147
7.143
7.139
7.135
7.029
7.025
7.023
7.019
7.009
7.006
7.002
6.873
6.869
6.867
6.863
6.830
6.827
6.812
6.809
6.793
6.790
6.771
6.768
6.750
6.747
3.862
0.013
NH2
O
CH3
O
N+
O-
0.97
1.00
2.00
1.98
1.97
0.98
0.99
0.95
4.86
f1 (ppm)

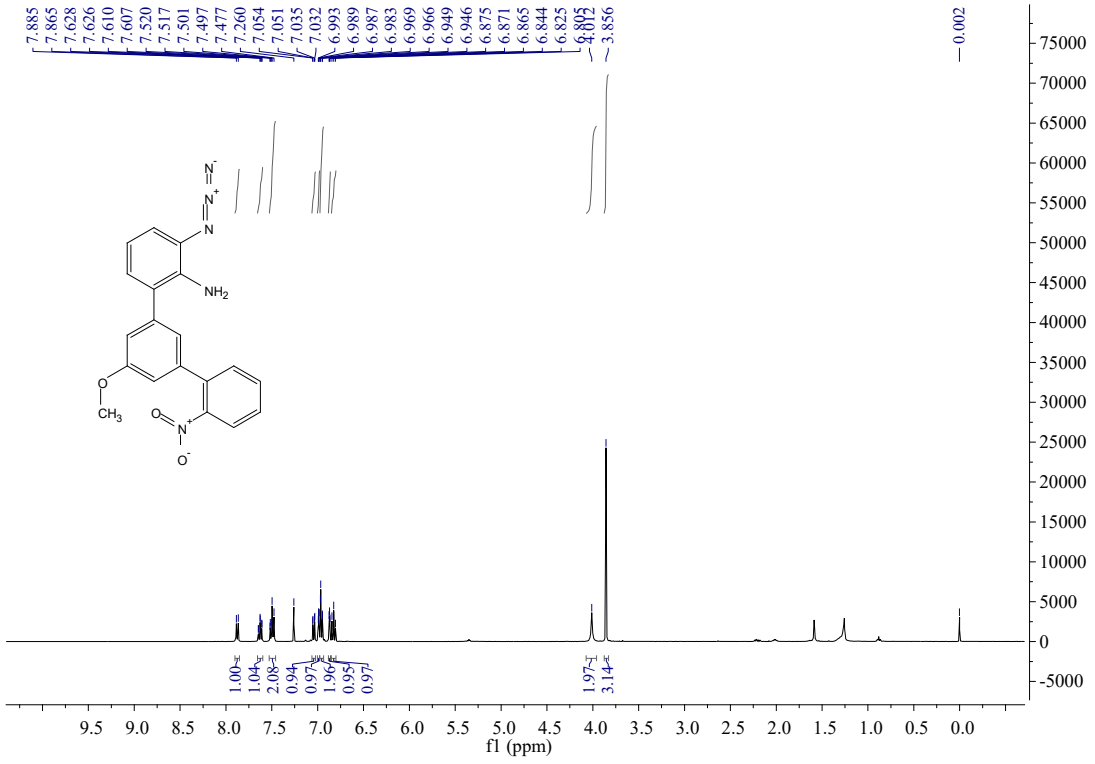

160.315
149.370
143.767
141.328
139.065
136.181
132.501
131.936
130.338
128.919
128.478
126.810
124.288
121.232
118.581
115.786
114.411
112.802
77.477
77.160
76.842
55.566
NH2
O
CH3
O
N+
O-
f1 (ppm)

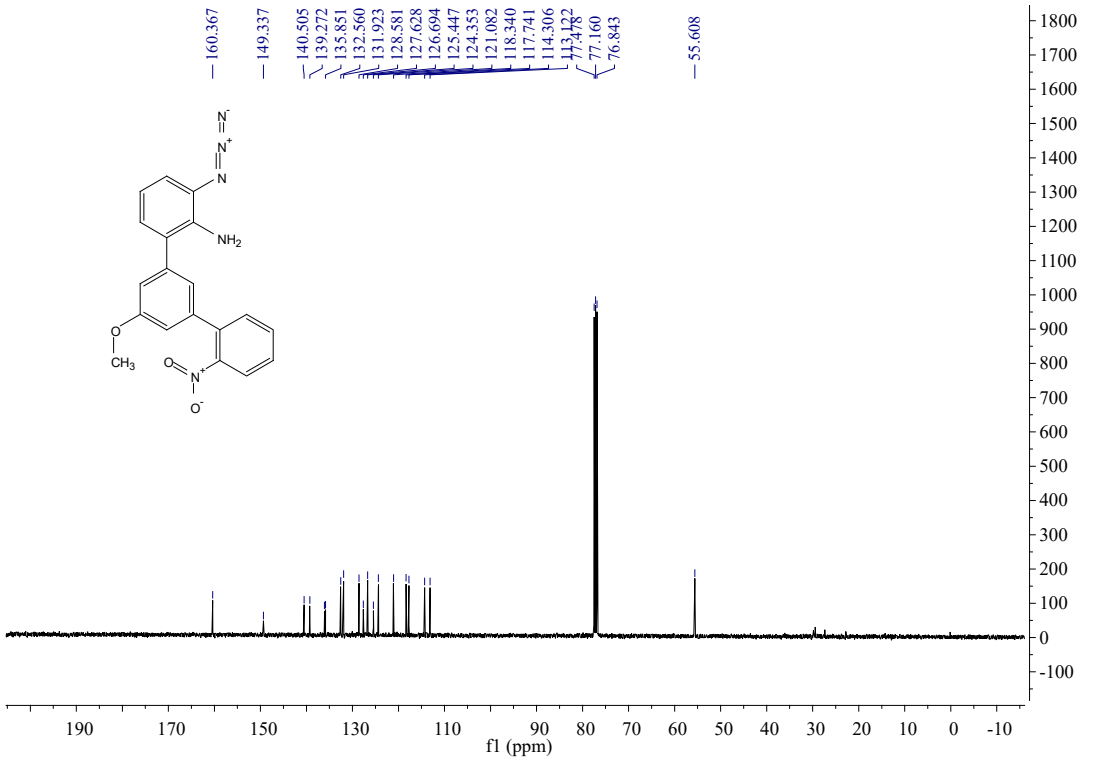
7


7.841
7.838
7.820
7.818
7.650
7.647
7.631
7.628
7.512
7.508
7.492
7.488
7.465
7.460
7.457
7.455
7.445
7.442
7.437
7.431
7.417
7.407
7.403
7.388
7.385
7.369
7.366
7.347
7.343
7.332
7.328
7.325
7.319
7.316
7.308
7.273
7.270
7.267
7.264
7.260
7.255
7.247
7.242
7.232
7.222
7.219
7.215
6.875
6.871
6.869
6.865
3.819
-0.000
1.00
1.02
1.05
2.96
4.27
5.17
0.99
3.00
f1 (ppm)

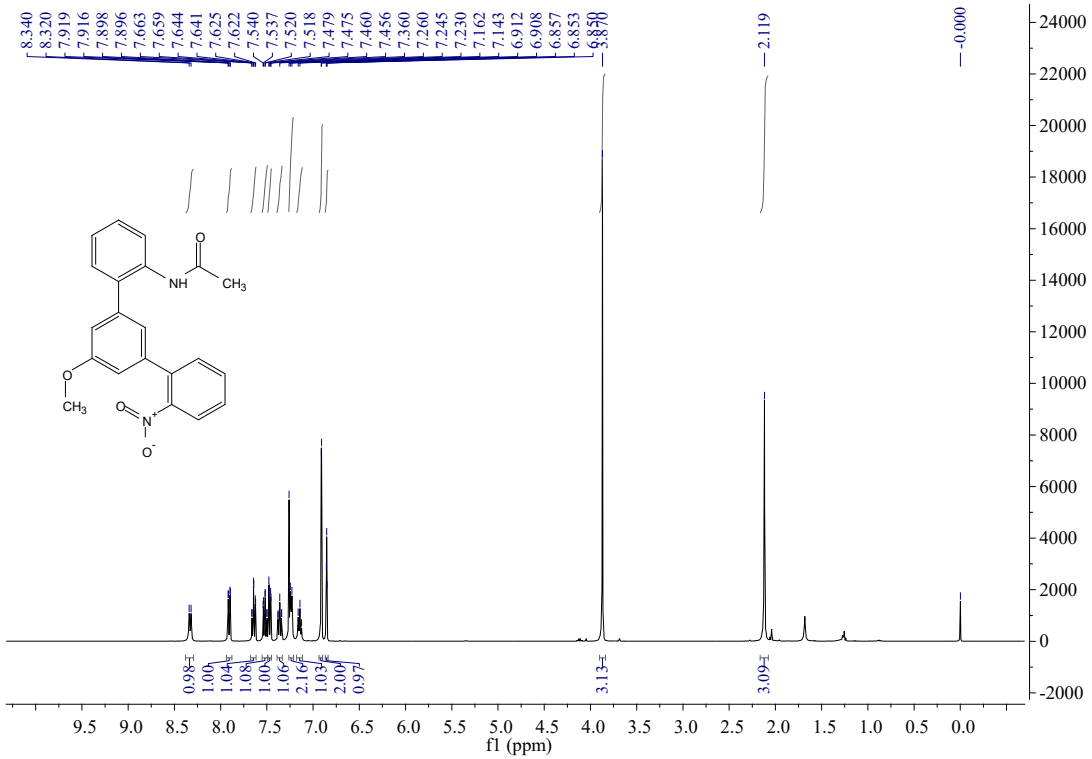

159.409
142.361
138.312
133.130
132.298
132.184
131.559
129.662
128.736
128.363
128.340
128.298
127.536
124.157
121.669
114.789
113.102
92.800
89.350
77.478
77.160
76.842
55.556
f1 (ppm)

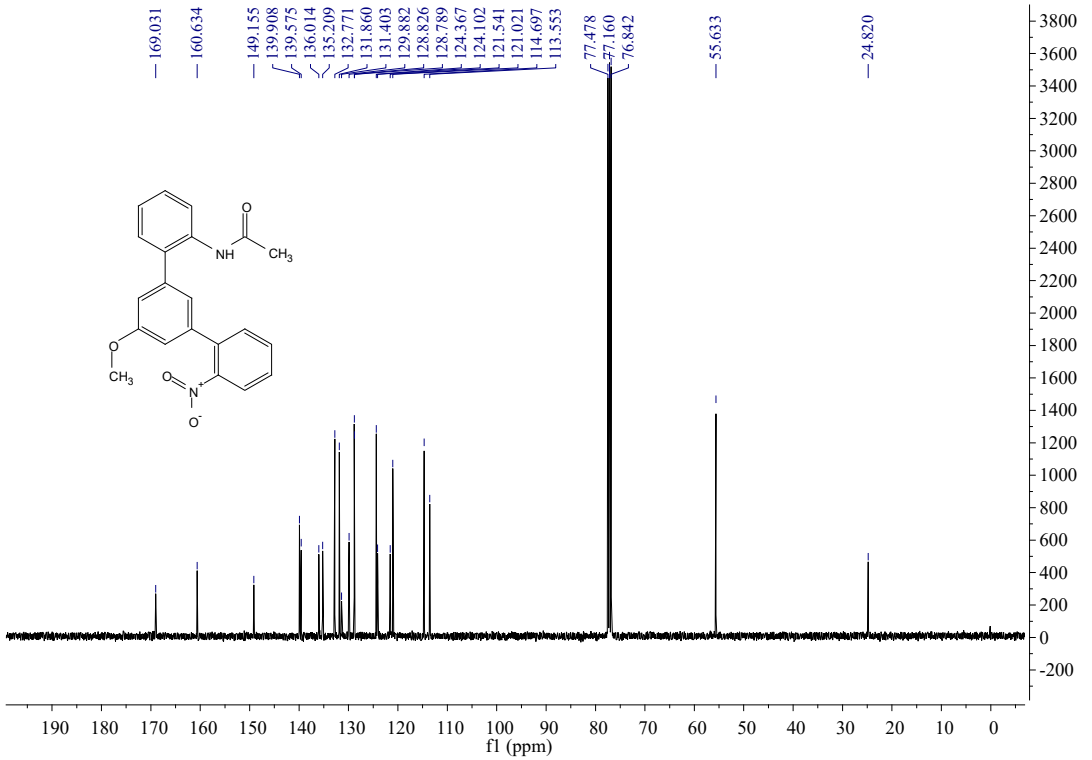
8


7.885
7.865
7.628
7.626
7.610
7.607
7.520
7.517
7.501
7.497
7.477
7.260
7.054
7.051
7.035
7.032
6.993
6.989
6.987
6.983
6.969
6.966
6.949
6.946
6.875
6.871
6.865
6.844
6.825
6.805
4.012
3.856
0.002
1.00
1.04
2.08
0.94
0.97
1.96
0.95
0.97
1.97
3.14
NH2
O
CH3
N+
O-
fl (ppm)

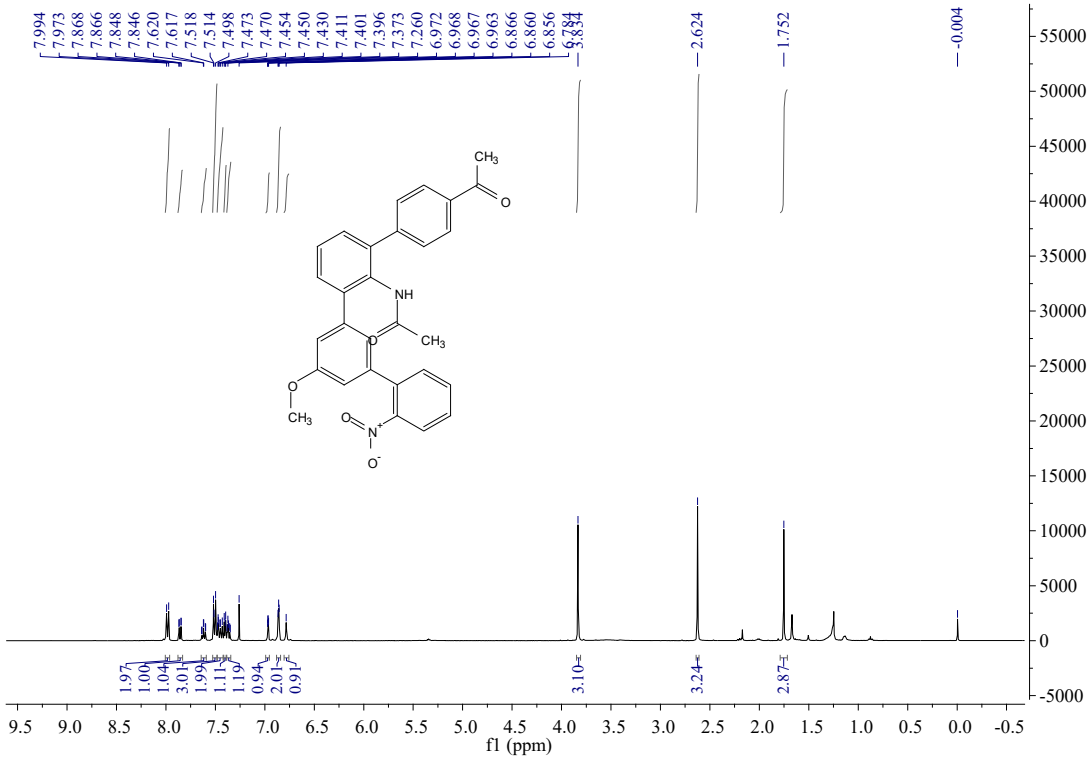

160.367
149.337
140.505
139.272
135.851
132.560
131.923
128.581
127.628
126.694
125.447
124.353
121.082
118.340
117.741
114.306
113.122
77.478
77.160
76.843
55.608
NH2
O
CH3
N+
O-
fl (ppm)

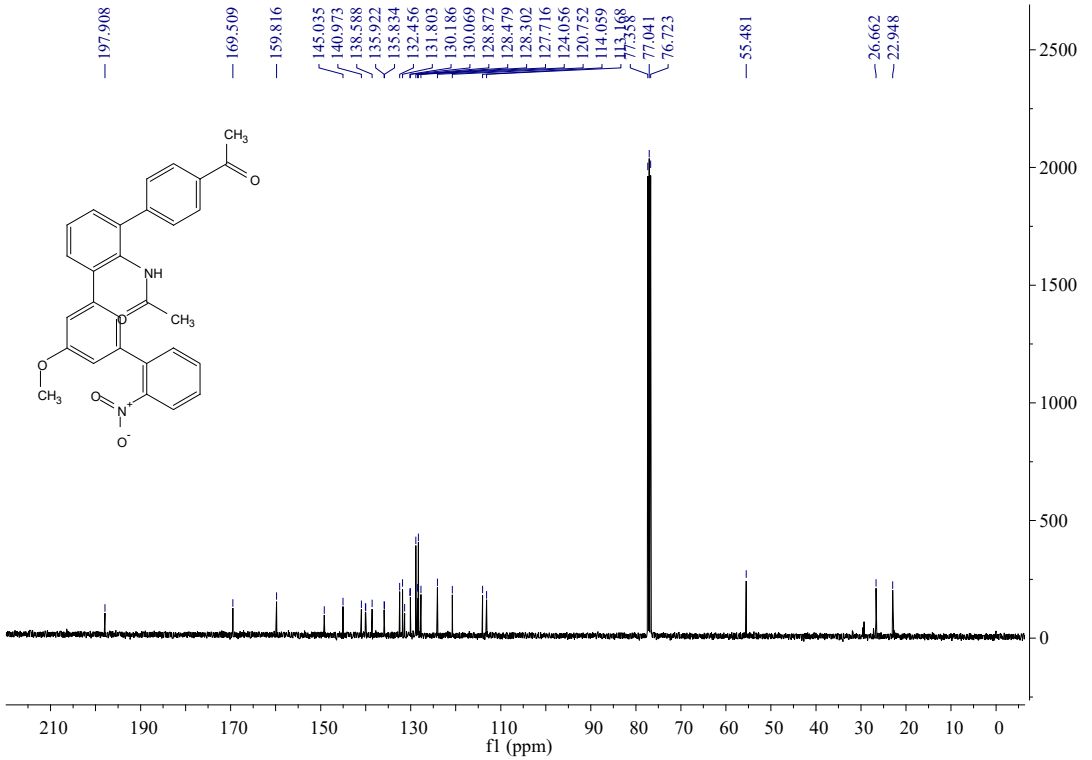
9


8.340
8.320
7.919
7.916
7.898
7.896
7.663
7.659
7.644
7.641
7.625
7.622
7.540
7.537
7.520
7.518
7.479
7.475
7.460
7.456
7.360
7.260
7.245
7.230
7.162
7.143
6.912
6.908
6.857
6.853
6.850
3.870
2.119
-0.000
NH
CH3
O
CH3
N+
O-
0.98
1.00
1.04
1.08
1.00
1.06
2.16
1.03
2.00
0.97
3.13
3.09
f1 (ppm)

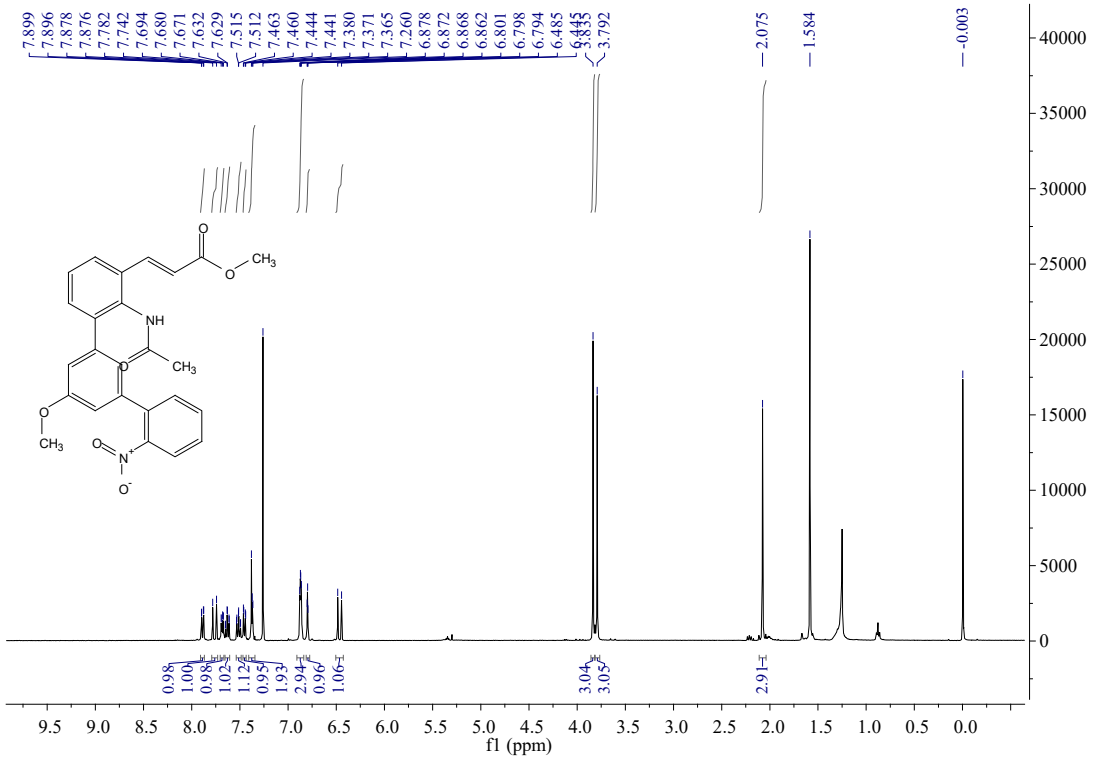

169.031
160.634
149.155
139.908
139.575
136.014
135.209
132.771
131.860
131.403
129.882
128.826
128.789
124.367
124.102
121.541
121.021
114.697
113.553
77.478
77.160
76.842
55.633
24.820
NH
CH3
O
CH3
N+
O-
f1 (ppm)

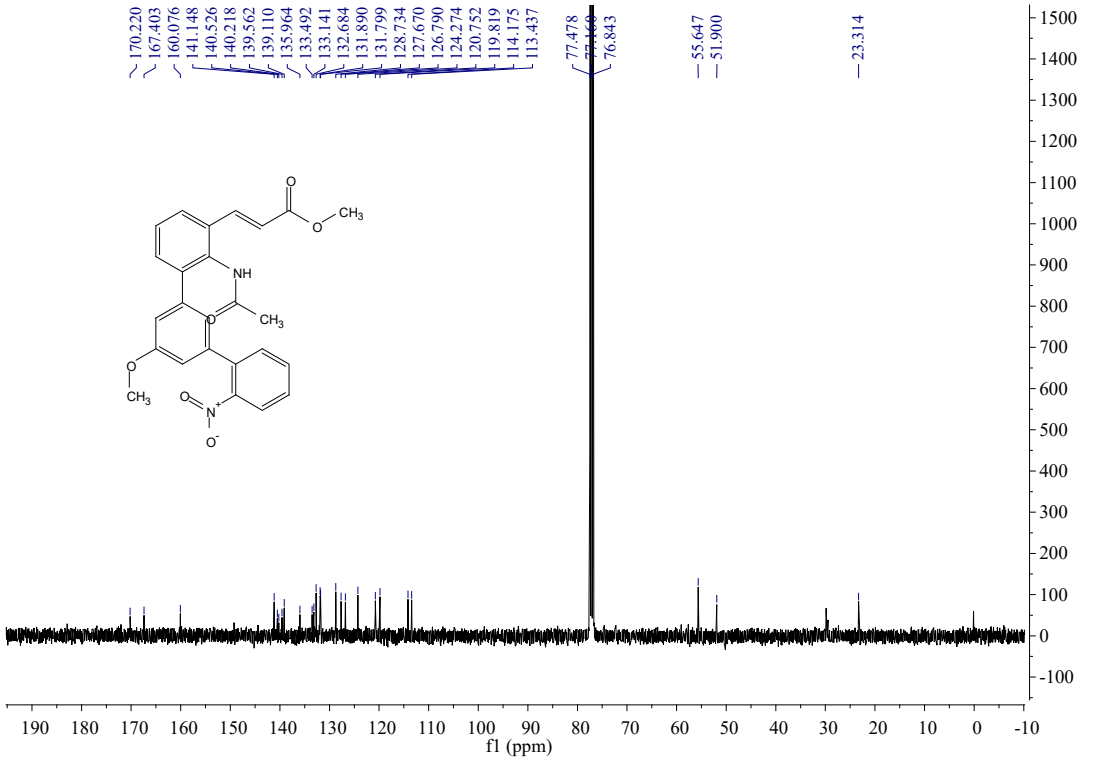
10


7.994
7.973
7.868
7.866
7.848
7.846
7.620
7.617
7.518
7.514
7.498
7.473
7.470
7.454
7.450
7.430
7.411
7.401
7.396
7.373
7.260
6.972
6.968
6.967
6.963
6.866
6.860
6.856
6.784
3.834
2.624
1.752
-0.004
CH3
O
NH
O
CH3
O
CH3
O
N+
O-
1.97
1.00
1.04
3.01
1.99
1.11
1.19
0.94
2.01
0.91
3.10
3.24
2.87
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
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)

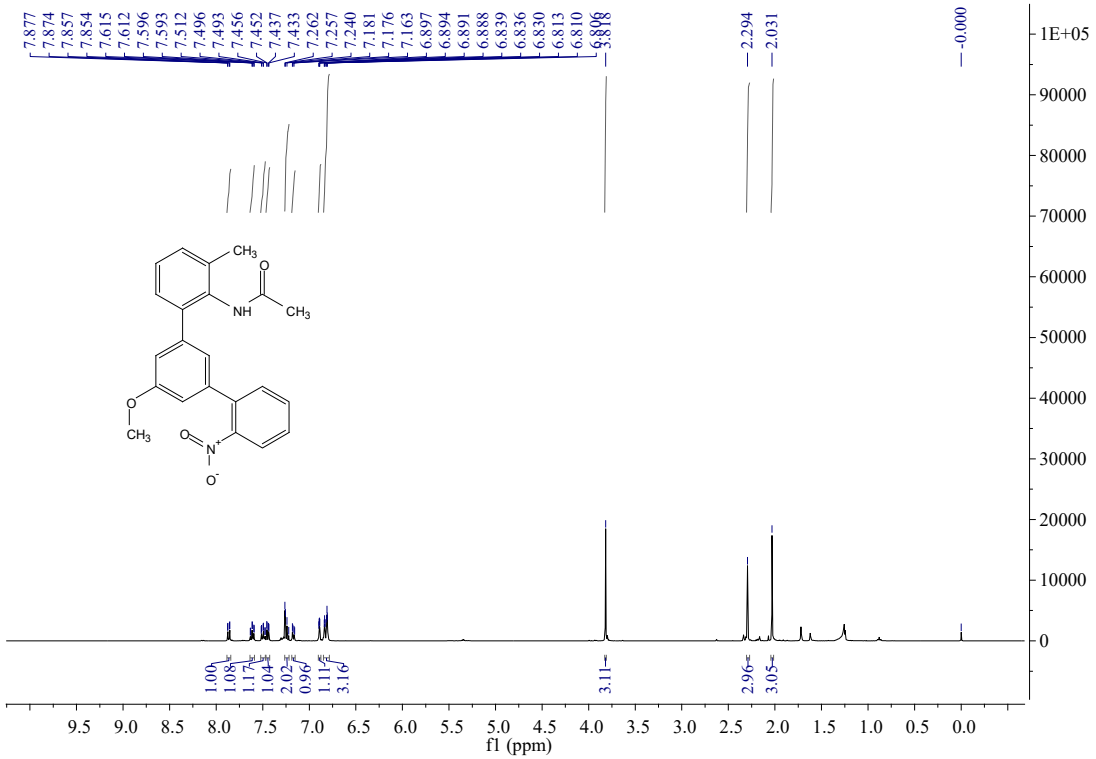

197.908
169.509
159.816
145.035
140.973
138.588
135.922
135.834
132.456
131.803
130.186
130.069
128.872
128.479
128.302
127.716
124.056
120.752
114.059
113.168
77.358
77.041
76.723
55.481
26.662
22.948
CH3
O
NH
O
CH3
O
CH3
O
N+
O-
2500
2000
1500
1000
500
0
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

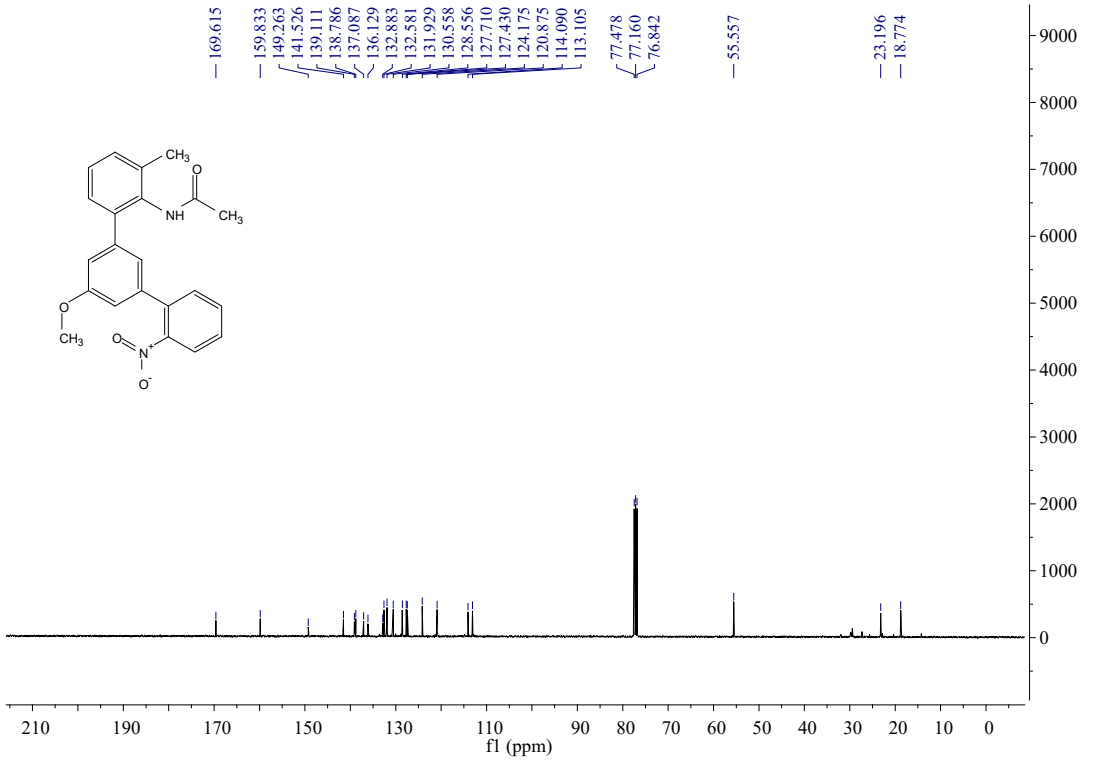
11


7.899
7.896
7.878
7.876
7.782
7.742
7.694
7.680
7.671
7.632
7.629
7.515
7.512
7.463
7.460
7.444
7.441
7.380
7.371
7.365
7.260
6.878
6.872
6.868
6.862
6.801
6.798
6.794
6.485
6.445
3.835
3.792
2.075
1.584
-0.003
0.98
1.00
0.98
1.02
1.12
0.95
1.93
2.94
0.96
1.06
3.04
3.05
2.91
fl (ppm)


170.220
167.403
160.076
141.148
140.526
140.218
139.562
139.110
135.964
133.492
133.141
132.684
131.890
131.799
128.734
127.670
126.790
124.274
120.752
119.819
114.175
113.437
77.478
77.160
76.843
55.647
51.900
23.314
fl (ppm)

12


7.877
7.874
7.857
7.854
7.615
7.612
7.596
7.593
7.512
7.496
7.493
7.456
7.452
7.437
7.433
7.262
7.257
7.240
7.181
7.176
7.163
6.897
6.894
6.891
6.888
6.839
6.836
6.830
6.813
6.810
6.806
3.818
2.294
2.031
-0.000
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
1.00
1.08
1.17
1.04
2.02
0.96
1.11
3.16
3.11
2.96
3.05
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)


169.615
159.833
149.263
141.526
139.111
138.786
137.087
136.129
132.883
132.581
131.929
130.558
128.556
127.710
127.430
124.175
120.875
114.090
113.105
77.478
77.160
76.842
55.557
23.196
18.774
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)