Supporting Information *for*

A Class of Economic and Effective of Decarboxylative Perfluoroalkylating Reagents: $[(phen)_2Cu](O_2CR_F)$

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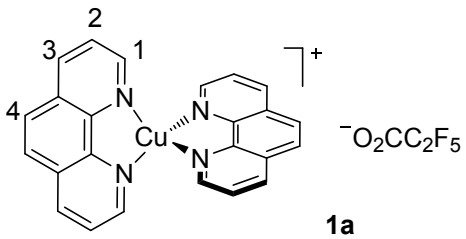
General Information

^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded using Bruker AVIII 400 spectrometer. ^{1}H NMR and ^{13}C NMR chemical shifts were reported in parts per million (ppm) downfield from tetramethylsilane and ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ as the external standard and low field is positive. Coupling constants (*J*) are reported in Hertz (Hz). The residual solvent peak was used as an internal reference: ^{1}H NMR (chloroform δ 7.26) and ^{13}C NMR (chloroform δ 77.0). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. HRMS were obtained on Waters GCT-TOF at the Shanghai Institute of Organic Chemistry. 2-Iodo-3,17-dimethoxy-β-estra-1,3,5(10)-triene was prepared according to the published procedures.[1] Other reagents were received from commercial sources. Solvents were freshly dried and degassed according to the published procedures prior to use. Column chromatography purifications were performed by flash chromatography using Merck silica gel 60.

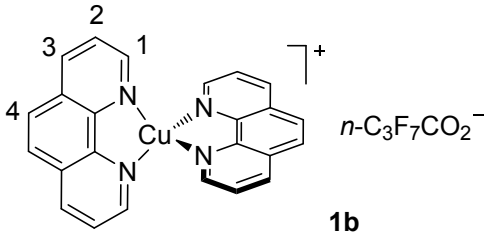
Synthesis of [(phen)$_2$Cu][$O_2CC_2F_5$] (1a).



1a

A solution of NaO*t*-Bu (345 mg, 3.6 mmol) in 10.0 mL of THF was added to a suspension of CuCl (297 mg, 3.0 mmol) in 60 mL of THF, and the resulting mixture was stirred at room temperature for 120 min. The resulting light yellow mixture was filtered through a layer of Celite. To this filtrate was added a solution of 1,10-phenanthroline (1080 mg, 6.0 mmol) in 10 mL of THF. The resulting solution turned reddish brown immediately and was stirred at room temperature for an additional 5 min. A THF solution (1 mL) of $C_2F_5CO_2H$ (810 mg, 3.0 mmol) was added dropwise and the mixture was further stirred at room temperature for 20 min. The solution was filtered, and the filtrate was dried under vacuum to yield a reddish brown solid. The resulting solid were washed with 2 × 2 mL of diethyl ether and dried under vacuum to obtain 1.38 g (79%) of **1a**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.02 (d, J = 3.7 Hz, 4H, H_1), 8.82 (dd, J = 8.1, 1.1 Hz, 4H, H_3), 8.27 (s, 4H, H_4), 7.99 (dd, J = 8.1, 4.7 Hz, 4H, H_2). ^{19}F NMR (376 MHz, DMSO-d_6) δ -81.5 (t, J = 1.4 Hz, 3F, CF_3), -118.1 (d, J = 1.4 Hz, 2F, CF_2). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.3 (t, J = 21.9 Hz), 149.8 (s), 143.5 (s), 137.7 (s), 129.4 (s), 127.5 (s), 126.2 (s), 120.0 (qt, J_{CF} = 286.4, 36.4 Hz, CF_3), 107.6 (tq, J_{CF} = 266.6, 35.4 Hz, CF_2). Elemental Analysis(%) calculated for $C_{27}H_{16}CuF_5N_4O_2$: C 55.25, H 2.75, N 9.54. Found: C 55.47, H 2.89, N 9.77.

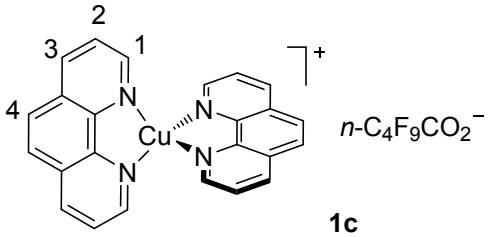
Synthesis of [(phen)$_2$Cu][*n*-$C_3F_7CO_2$] (1b).



1b

A solution of NaO*t*-Bu (345 mg, 3.6 mmol) in 10 mL of THF was added to a suspension of CuCl (297 mg, 3.0 mmol) in 60 mL of THF, and the resulting mixture was stirred at room temperature for 120 min. The resulting light yellow mixture was filtered through a layer of Celite. To this filtrate was added a solution of 1,10-phenanthroline (1080 mg, 6.0 mmol) in 10 mL of THF. The resulting solution turned reddish brown immediately and was stirred at room temperature for an additional 5 min. A THF solution (1 mL) of *n*-$C_3F_7CO_2H$ (960 mg, 3.0 mmol) was added dropwise and the mixture was further stirred at room temperature for 20 min. The solution was filtered, and the filtrate was dried under vacuum to yield a reddish brown solid. The resulting solid were washed with 2 × 2 mL of diethyl ether and dried under vacuum to obtain 1.14 g (60%) of **1b**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (d, J = 3.7 Hz, 4H, H_1), 8.82 (dd, J = 8.1, 1.0 Hz, 4H, H_3), 8.27 (s, 4H, H_4), 7.99 (dd, J = 8.1, 4.7 Hz, 4H, H_2). ^{19}F NMR (376 MHz, DMSO-d_6) δ -80.2 (t, J = 8.5 Hz, 3F, CF_3), -115.6 (q, J = 8.4 Hz, 2F, CF_2), -126.1 (s, 2F, CF_2). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.0 (t, J = 22.2 Hz), 149.8 (s), 143.5 (s), 137.7 (s), 129.4 (s), 127.5 (s), 126.2 (s), 125.0 – 104.4 (m, $CF_2CF_2CF_3$). Elemental Analysis(%) calculated for $C_{28}H_{16}CuF_7N_4O_2 \cdot C_6H_6$: C 57.11, H 3.10, N 7.83. Found: C 57.32, H 3.19, N 8.06.

Synthesis of [(phen)$_2$Cu][*n*-$C_4F_9CO_2$] (1c).

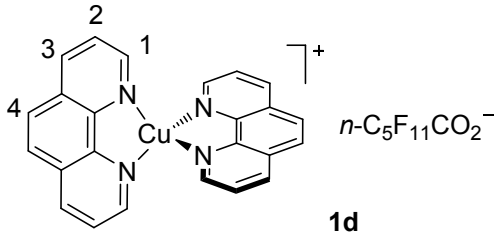


1c

A solution of NaO*t*-Bu (345 mg, 3.6 mmol) in 10 mL of THF was added to a suspension of CuCl (297 mg, 3.0 mmol) in 60 mL of THF, and the resulting mixture was stirred at room temperature for 120 min. The resulting light yellow mixture was filtered through a layer of Celite. To this filtrate was added a solution of 1,10-phenanthroline (1080 mg, 6.0 mmol) in 10 mL of THF. The resulting solution turned reddish brown immediately and was stirred at room temperature for an additional 5 min. A THF solution (1 mL) of *n*-$C_4F_9CO_2H$ (1110 mg, 3.0 mmol) was added dropwise and the mixture was further stirred at room temperature for 20 min. The solution was filtered, and the filtrate was dried under vacuum to yield a reddish brown solid. The resulting solid were washed with 2 × 2 mL of hexanes and dried under

vacuum to obtain 1.02 g (50%) of **1c**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.02 (d, J = 4.2 Hz, 4H, H_1), 8.83 (d, J = 8.1 Hz, 4H, H_3), 8.27 (s, 4H, H_4), 8.00 (dd, J = 8.1, 4.7 Hz, 4H, H_2). ^{19}F NMR (376 MHz, DMSO-d_6) δ -80.7 (tt, J = 9.7, 2.7 Hz, 3F, CF_3), -115.1 (td, J = 11.1, 2.7 Hz, 2F, CF_2), -119.5 – -124.9 (m, 2F, CF_2), -125.4 – -125.6 (m, 2F, CF_2). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.1 (t, J = 22.0 Hz), 149.8 (s), 143.5 (s), 137.7 (s), 129.5 (s), 127.5 (s), 126.2 (s), 124.7 – 106.2 (m, *$CF_2CF_2CF_2CF_3$*). Elemental Analysis(%) calculated for $C_{29}H_{16}CuF_9N_4O_2$: C 50.70, H 2.35, N 8.16. Found: C 50.45, H 2.71, N 8.09.

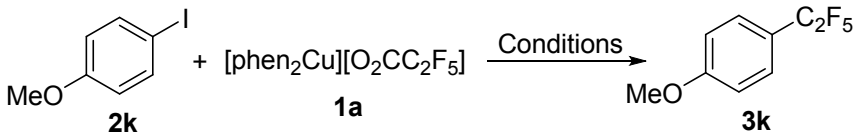
Synthesis of [(phen)$_2$Cu][*n*-$C_5F_{11}CO_2$] (1d).



1d

A solution of NaO*t*-Bu (345 mg, 3.6 mmol) in 10 mL of THF was added to a suspension of CuCl (297 mg, 3.0 mmol) in 60 mL of THF, and the resulting mixture was stirred at room temperature for 120 min. The resulting light yellow mixture was filtered through a layer of Celite. To this filtrate was added a solution of 1,10-phenanthroline (1080 mg, 6.0 mmol) in 10 mL of THF. The resulting solution turned reddish brown immediately and was stirred at room temperature for an additional 5 min. A THF solution (1 mL) of *n*-$C_5F_{11}CO_2H$ (1260 mg, 3.0 mmol) was added dropwise and the mixture was further stirred at room temperature for 20 min. The solution was filtered, and the filtrate was dried under vacuum to yield a reddish brown solid. The resulting solid were washed with 2 × 2 mL of hexanes and dried under vacuum to obtain 1.01 g (51%) of **1d**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.04 (s, 4H, H_1), 8.76 (d, J = 7.6 Hz, 4H, H_3), 8.21 (s, 4H, H_4), 8.07 – 7.71 (m, 4H, H_2). ^{19}F NMR (376 MHz, DMSO-d_6) δ -80.6 (t, J = 2.5 Hz, 3F, CF_3), -114.9 (t, J = 11.7 Hz, 2F, CF_2), -122.0 (s, 2F, CF_2), -122.3 (s, 2F, CF_2), -126.1 (s, 2F, CF_2). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.2 (t, J = 21.8 Hz), 150.1 (s), 143.9 (s), 137.5 (s), 129.3 (s), 127.4 (s), 125.7 (s), 124.2 – 102.1 (m, *$CF_2CF_2CF_2CF_2CF_3$*).

Optimization of pentafluoroethylation of 1-iodo-4-methoxybenzene with 1a. [a]

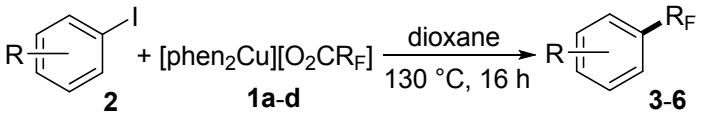


2k **1a** **3k**

Entry	Solvent	Temp (°C)	Time (h)	Yield (%)[b]
1	DMF	130	12	43
2	DMAc	130	12	19
3	NMP	130	12	10
4	DMSO	130	12	3
5	CH_3CN	110	12	5
6	diglyme	130	12	53
7	dioxane	130	12	81
8	dioxane	120	12	25
9	dioxane	130	16	90

[a] Reaction conditions: **1a** (0.15 mmol), **2k** (0.10 mmol), solvent (1.5 mL), under N_2 atmosphere. [b] The yield was determined by ^{19}F NMR spectroscopy with $PhOCF_3$ as internal standard.

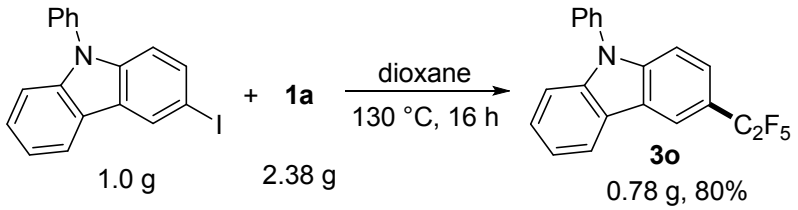
General procedure for Perfluoroalkylation of aryl iodides:



2 **1a-d** **3-6**

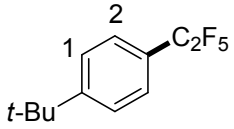
In a dry box, $[phen_2Cu][O_2CR_F]$ (0.75 mmol), aryl or heteroaryl halides (0.50 mmol), and 5.0 mL dioxane were added to a oven dried 25.0 mL test tube with Teflon screw cap. The tube was sealed and the solution was stirred at 130 °C for 16 h. Then the reaction mixture was filtered through a layer of Celite, eluted with diethyl ether. The resulting mixture was extracted by ethyl ether (20 mL × 3), and the combined organic layers was washed with water (60 mL × 3), and then dried over magnesium sulfate. The solvent was removed by rotary evaporation and the resulting product was purified by column chromatography on silica gel with *n*-pentane/Et_2O.

Procedure for gram scale reaction



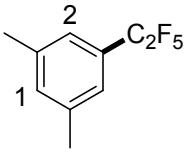
In a dry box, [phen$_2$Cu][$O_2CC_2F_5$] (**1a**) (2.38 g, 4.1 mmol), 3-iodo-*N*-phenylcarbazole (1.0 g, 2.7 mmol), and 20 mL dioxane were added to a oven dried 100 mL test tube with Teflon screw cap. The tube was sealed and the solution was placed into a preheated 130 °C oil bath for 16 h. Then the reaction mixture was filtered through a layer of Celite, eluted with diethyl ether. The resulting mixture was extracted by ethyl ether (50 mL × 3), and the combined organic layers was washed with water (100 mL × 3), and then dried over magnesium sulfate. The solvent was removed by rotary evaporation and the resulting product was purified by column chromatography on silica gel with *n*-pentane/Et_2O. Compound **3o** was obtained in 80% yield (0.78 g).

Data for compounds 3



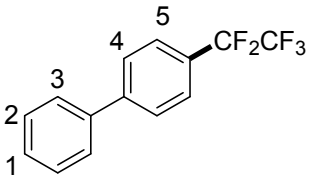
1-*tert*-Butyl-4-(perfluoroethyl)benzene (3a) [2]

Obtained as a colourless oil in 82% yield (103 mg). R_f (*n*-pentane) = 0.88. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.35 (m, 4H, H_1, H_2), 1.35 (s, 9H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3 (t, J = 1.6 Hz), 126.2 (td, J = 6.3, 1.0 Hz), 125.8 (s), 125.7 (s), 119.2 (qt, J_{CF} = 286.8, 39.4 Hz, CF_3), 113.6 (tq, J_{CF} = 253.5, 38.4 Hz, CF_2), 34.9 (s), 31.1 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.8 (s, 3F, CF_3), -114.5 (s, 2F, CF_2). GC-MS m/z 252 (M^+).



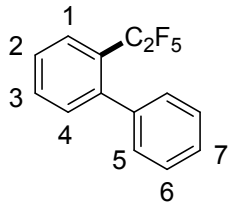
1,3-Dimethyl-5-(perfluoroethyl)benzene (3b)

Obtained as a yellow oil in 74% yield (83 mg). R_f (*n*-pentane) = 0.79. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.19 (m, 3H, H_1, H_2), 2.40 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.5 (s), 133.5 (t, J = 1.6 Hz), 126.1 (s), 124.0 (t, J = 6.2 Hz), 119.2 (qt, J_{CF} = 286.8, 39.4 Hz, CF_3), 113.5 (tq, J_{CF} = 254.5, 38.4 Hz, CF_2), 21.3 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.7 (s, 3F, CF_3), -114.6 (s, 2F, CF_2). IR (KBr): ν 2924, 2851, 1456, 1383, 1257, 1200, 1111, 1036, 979, 857, 843, 8251, 698, 647 cm^{-1}. GC-MS m/z 224 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_9F_5$: 224.0624; found: 224.0622.



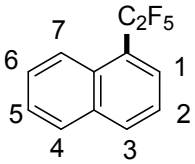
4-(Perfluoroethyl)biphenyl (3c) [3]

Obtained as a white solid in 92% yield (125 mg). R_f (*n*-pentane) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.67 (m, 4H, H_4, H_5), 7.66 – 7.59 (m, 2H, H_3), 7.55 – 7.46 (m, 2H, H_2), 7.47 – 7.39 (m, 1H, H_1). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9 (t, J = 1.7 Hz), 139.7 (s), 129.0 (s), 128.3 (s), 127.5 (s), 127.4 (s), 127.3 (s), 126.9 (t, J = 6.7 Hz), 119.2 (qt, J_{CF} = 286.8, 39.4 Hz, CF_3), 113.6 (tq, J_{CF} = 254.5, 38.4 Hz, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.7 (s, 3F, CF_3), -114.7 (s, 2F, CF_2). GC-MS m/z 272 (M^+).



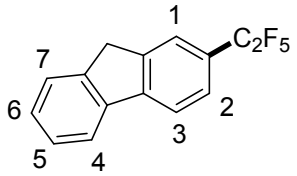
2-(Perfluoroethyl)biphenyl (3d)

Obtained as a colourless oil in 39% yield (53 mg). R_f (*n*-pentane) = 0.90. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.8 Hz, 1H, H_1), 7.58 – 7.45 (m, 2H, H_2, H_3), 7.40 – 7.32 (m, 3H, H_4, H_5), 7.31 – 7.20 (m, 3H, H_6, H_7). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (t, *J* = 2.4 Hz), 140.4 (s), 132.8 (s), 131.1 (s), 129.0 (s), 127.9 (td, *J* = 7.7, 1.3 Hz), 127.5 (s), 127.3 (s), 127.2 (s), 126.3 (t, *J* = 22.1 Hz), 119.1 (qt, J_{CF} = 288.9, 40.4 Hz, CF_3), 114.2 (tq, J_{CF} = 258.5, 39.4 Hz, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.6 (s, 3F, CF_3), -106.5 (s, 2F, CF_2). IR (KBr): ν 2917, 2849, 1599, 1483, 1443, 1332, 1290, 1201, 1151, 1118, 1080, 1056, 1009, 968, 954, 763, 734, 701, 670, 650 cm^{-1}. GC-MS m/z 272 (M^+). HRMS (EI) m/z: calcd. for $C_{14}H_9F_5$: 272.0624; found: 272.0619.



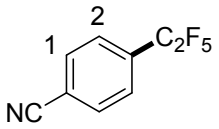
1-(Perfluoroethyl)naphthalene (3e) [4]

Obtained as a colourless oil in 76% yield (93 mg). R_f (*n*-pentane) = 0.87. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.5 Hz, 1H, H_1), 8.06 (d, *J* = 8.2 Hz, 1H, H_7), 7.93 (d, *J* = 8.0 Hz, 1H, H_3), 7.85 (d, *J* = 7.4 Hz, 1H, H_4), 7.67 – 7.48 (m, 3H, H_2, H_5, H_6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1 (s), 133.3 (t, *J* = 1.3 Hz), 129.9 (t, *J* = 1.4 Hz), 129.0 (s), 127.6 (t, *J* = 1.2 Hz), 127.4 (td, *J* = 9.6, 1.0 Hz), 126.4 (s), 125.7 (s), 124.7 (tq, *J* = 6.1, 2.0 Hz), 124.3 (s), 119.6 (qt, J_{CF} = 287.9, 39.4 Hz, CF_3), 115.2 (tq, J_{CF} = 255.5, 39.4 Hz, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.4 (s, 3F, CF_3), -108.3 (s, 2F, CF_2). GC-MS m/z 246 (M^+).



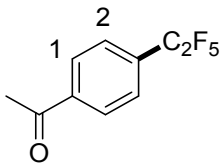
2-(Perfluoroethyl)-9*H*-fluorene (3f)

Obtained as a white solid in 78% yield (111 mg). R_f (*n*-pentane) = 0.82. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.81 (m, 2H, H_2, H_3), 7.77 (s, 1H, H_1), 7.69 – 7.52 (m, 2H, H_4, H_7), 7.48 – 7.28 (m, 2H, H_5, H_6), 3.96 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3 (t, J = 1.7 Hz), 143.8 (s), 143.5 (s), 140.3 (s), 128.0 (s), 127.1 (s), 126.6 (t, J = 23.7 Hz), 125.3 (s), 125.2 (s), 123.1 (td, J = 6.4, 0.6 Hz), 120.7 (s), 119.9 (s), 119.3 (qt, J_{CF} = 286.8, 40.4 Hz, CF_3), 113.9 (tq, J_{CF} = 254.5, 38.4 Hz, CF_2), 36.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.7 (s, 3F, CF_3), -113.8 (s, 2F, CF_2). IR (KBr): ν 2927, 1467, 1427, 1332, 1300, 1229, 1203, 1182, 1162, 1148, 1121, 1085, 1005, 995, 954, 884, 867, 838, 773, 742, 665, 647 cm^{-1}. GC-MS m/z 284 (M^+). HRMS (EI) m/z: calcd. for $C_{15}H_9F_5$: 284.0624; found: 284.0626.



4-(Perfluoroethyl)benzonitrile (3g) [4]

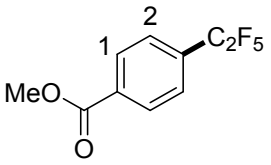
Obtained as a yellow oil in 39% yield (40 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.80. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.3 Hz, 2H, H_1), 7.74 (d, J = 8.3 Hz, 2H, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.9 (s), 132.6 (s), 127.4 (td, J = 6.3, 1.0 Hz), 126.9 (s), 121.8 – 116.3 (m, CF_3), 116.3 (t, J = 1.8 Hz), 116.6 – 109.8 (m, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.49 (s, 3F, CF_3), -115.74 (s, 2F, CF_2). GC-MS m/z 221 (M^+).



1-(4-(Perfluoroethyl)phenyl)ethanone (3h) [4]

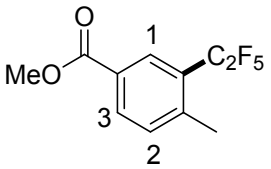
Obtained as a yellow oil in 62% yield (74 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.1 Hz, 2H, H_1), 7.72 (d, J = 8.1 Hz, 2H, H_2), 2.65 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0 (s), 139.8 (t, J = 1.5 Hz), 132.8 (t, J = 23.9 Hz), 128.5 (s), 126.9 (td, J = 6.3, 1.0 Hz), 119.3 (qt, J_{CF} = 286.8, 40.4 Hz, CF_3), 113.9 (tq, J_{CF}

= 254.5, 38.4 Hz, CF_2), 26.8 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.6 (s, 3F, CF_3), -115.4 (s, 2F, CF_2). GC-MS m/z 238 (M^+).



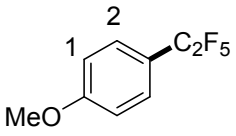
Methyl 4-(perfluoroethyl)benzoate (3i) [3]

Obtained as a yellow oil in 76% yield (96 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.87. ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.5 Hz, 2H, H_1), 7.69 (d, J = 8.2 Hz, 2H, H_2), 3.96 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (s), 133.5 (t, J = 1.6 Hz), 132.8 (t, J = 23.8 Hz), 129.9 (s), 126.7 (td, J = 6.3, 1.0 Hz), 118.9 (qt, J_{CF} = 286.8, 39.4 Hz, CF_3), 113.1 (tq, J_{CF} = 255.5, 38.4 Hz, CF_2), 52.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.6 (s, 3F, CF_3), -115.4 (s, 2F, CF_2). GC-MS m/z 254 (M^+).



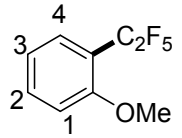
Methyl 4-methyl-3-(perfluoroethyl)benzoate (3j)

Obtained as a yellow oil in 68% yield (91 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.83. ^1H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H, H_1), 8.07 (d, J = 8.0 Hz, 1H, H_3), 7.36 (d, J = 8.0 Hz, 1H, H_2), 3.93 (s, 3H, OCH_3), 2.54 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8 (s), 143.1 (t, J = 2.1 Hz), 132.9 (s), 132.6 (t, J = 1.1 Hz), 129.4 (td, J = 8.9, 1.0 Hz), 128.5 (s), 127.2 (t, J = 22.5 Hz), 119.4 (qt, J_{CF} = 287.9, 39.4 Hz, CF_3), 114.4 (tq, J_{CF} = 256.5, 39.4 Hz, CF_2), 52.3 (s), 20.5 (tt, J = 3.8, 2.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.2 (s, 3F, CF_3), -110.5 (s, 2F, CF_2). IR (KBr): ν 2956, 1727, 1617, 1437, 1312, 1281, 1243, 1197, 1157, 1131, 1119, 1078, 1037, 1014, 995, 962, 922, 852, 789, 760, 681 cm^{-1}. GC-MS m/z 268 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_9F_5O_2$: 268.0523; found: 268.0517.



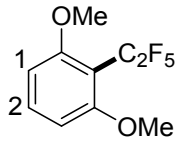
1-Methoxy-4-(perfluoroethyl)benzene (3k) [2]

Obtained as a colourless oil in 87% yield (98 mg). R_f (*n*-pentane) = 0.48. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.6 Hz, 2H, H_2), 6.99 (d, *J* = 8.4 Hz, 2H, H_1), 3.86 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (t, *J* = 1.6 Hz), 128.0 (td, *J* = 6.4, 1.1 Hz), 120.7 (s), 119.2 (qt, J_{CF} = 284.2, 40.1 Hz, CF_3), 114.1 (s), 113.6 (tq, J_{CF} = 251.5, 38.2 Hz, CF_2), 55.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -85.0 (s, 3F, CF_3), -113.8 (s, 2F, CF_2). GC-MS m/z 226 (M^+).



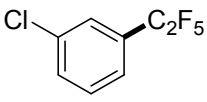
1-Methoxy-2-(perfluoroethyl)benzene (3l) [4]

Obtained as a yellow oil in 61% yield (69 mg). R_f (*n*-pentane) = 0.63. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (m, 2H, H_3, H_4), 7.13 – 6.95 (m, 2H, H_1, H_2), 3.87 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3 (t, *J* = 2.7 Hz), 133.5 (t, *J* = 1.4 Hz), 128.8 (td, *J* = 8.6, 0.7 Hz), 120.9 (t, *J* = 39.2 Hz), 120.3 (s), 119.5 (qt, J_{CF} = 287.9, 39.4 Hz, CF_3), 113.7 (tq, J_{CF} = 256.5, 40.4 Hz, CF_2), 112.5 (s), 55.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.9 (s, 3F, CF_3), -111.8 (s, 2F, CF_2). GC-MS m/z 226 (M^+).



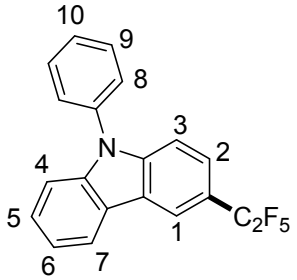
1,3-Dimethoxy-2-(perfluoroethyl)benzene (3m)

Obtained as a yellow oil in 72% yield (92 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.76. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, *J* = 8.4 Hz, 1H, H_2), 6.62 (d, *J* = 8.4 Hz, 2H, H_1), 3.83 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5 (t, *J* = 2.2 Hz), 133.3 (s), 119.8 (qt, J_{CF} = 288.9, 39.4 Hz, CF_3), 114.2 (tq, J_{CF} = 258.6, 40.4 Hz, CF_2), 105.3 (s), 104.2 (s), 56.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.8 (s, 3F, CF_3), -107.2 (s, 2F, CF_2). IR (KBr): ν 2946, 2846, 1595, 1478, 1435, 1346, 1299, 1258, 1225, 1193, 1137, 1112, 1090, 1053, 1022, 957, 922, 903, 883, 784, 757, 722, 683, 650 cm^{-1}. GC-MS m/z 256 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_9F_5O_2$: 256.0523; found: 256.0528.



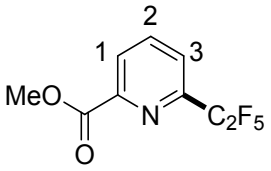
1-Chloro-3-(perfluoroethyl)benzene (3n) [5]

Quantitative ^{19}F NMR analysis of the reaction mixture indicated that **3n** was produced in 67% yield. Characterization of **3n** in reaction solution: ^{19}F NMR (unlocked) δ -84.6 (s, 3F, CF_3), -114.5 (s, 2F, CF_2). GC-MS m/z 230 (M^+).



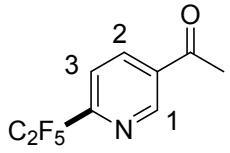
3-(Perfluoroethyl)-9-phenyl-9*H*-carbazole (3o)

Obtained as a yellow oil in 83% yield (150 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.70. ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H, H_1), 8.22 (d, J = 7.8 Hz, 1H, H_2), 7.70 – 7.60 (m, 3H, H_3, H_4, H_7), 7.61 – 7.42 (m, 6H, H_5, H_6, H_8, H_9), 7.38 (t, J = 7.4 Hz, 1H, H_{10}). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (s), 141.7 (s), 136.9 (s), 130.1 (s), 128.2 (s), 127.2 (s), 126.9 (s), 123.8 (t, J = 6.1 Hz), 123.3 (s), 122.8 (s), 120.8 (s), 120.6 (s), 119.9 (t, J = 24.2 Hz), 119.2 (t, J = 6.8 Hz), 119.5 (qt, J_{CF} = 286.8, 41.4 Hz, CF_3), 114.4 (tq, J_{CF} = 253.5, 38.4 Hz, CF_2), 110.2 (s), 109.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.6 (s, 3F, CF_3), -112.4 (s, 2F, CF_2). IR (KBr): ν 1632, 1599, 1503, 1456, 1436, 1365, 1333, 1320, 1257, 1237, 1198, 1146, 1121, 1109, 1083, 978, 939, 745, 732, 698, 672 cm^{-1}. GC-MS m/z 361 (M^+). HRMS (EI) m/z: calcd. for $C_{20}H_{12}F_5N$: 361.0890; found: 361.0887.



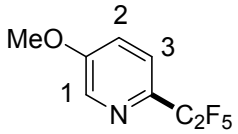
Methyl 6-(perfluoroethyl)picolinate (3p) [6]

Obtained as a yellow oil in 65% yield (83 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.61. ^1H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.9 Hz, 1H, H_1), 8.06 (t, J = 7.7 Hz, 1H, H_2), 7.88 (d, J = 7.9 Hz, 1H, H_3), 4.01 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7 (s), 148.7 (s), 147.9 (t, J = 26.0 Hz), 138.6 (s), 127.5 (t, J = 1.3 Hz), 124.9 (td, J = 4.3, 1.0 Hz), 118.8 (qt, J_{CF} = 287.9, 37.4 Hz, CF_3), 110.9 (tq, J_{CF} = 256.5, 38.4 Hz, CF_2), 53.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.1 (s, 3F, CF_3), -117.2 (s, 2F, CF_2). GC-MS m/z 255 (M^+).



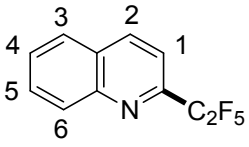
1-(6-(Perfluoroethyl)pyridin-3-yl)ethanone (3q)

Obtained as a colourless oil in 51% yield (61 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.38. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H, H_1), 8.42 (dd, J = 8.2, 2.1 Hz, 1H, H_2), 7.84 (d, J = 8.2 Hz, 1H, H_3), 2.69 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.5 (s), 151.1 (t, J = 25.8 Hz), 149.82 (s), 136.98 (s), 134.05 (t, J = 1.4 Hz), 122.08 (td, J = 4.3, 0.9 Hz), 118.7 (qt, J_{CF} = 287.9, 37.4 Hz, CF_3), 111.0 (tq, J_{CF} = 256.5, 38.4 Hz, CF_2), 26.94 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.0 (d, J = 1.8 Hz, 3F, CF_3), -117.4 (s, 2F, CF_2). IR (KBr): ν 2922, 1698, 1593, 1427, 1381, 1359, 1333, 1309, 1270, 1206, 1161, 1112, 1081, 1022, 983, 961, 850, 736, 648, 636 cm^{-1}. GC-MS m/z 239 (M^+). HRMS (EI) m/z: calcd. for $C_9H_6F_5NO$: 239.0370; found: 239.0371.



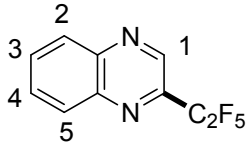
5-Methoxy-2-(perfluoroethyl)pyridine (3r)

Obtained as a colourless oil in 53% yield (60 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H, H_1), 7.63 (d, J = 8.7 Hz, 1H, H_3), 7.30 (dd, J = 8.7, 2.7 Hz, 1H, H_2), 3.92 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6 (t, J = 1.4 Hz), 139.4 (t, J = 26.2 Hz), 138.3 (s), 122.8 (td, J = 4.4, 0.9 Hz), 120.4 (s), 119.0 (qt, J_{CF} = 287.9, 38.4 Hz, CF_3), 111.4 (tq, J_{CF} = 254.5, 37.4 Hz, CF_2), 55.8 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.5 (s, 3F, CF_3), -116.3 (s, 2F, CF_2). IR (KBr): ν 2930, 1688, 1583, 1437, 1371, 1379, 1343, 1319, 1260, 1226, 1151, 1122, 1091, 1032, 963, 971, 860, 746, 647, 626 cm^{-1}. GC-MS m/z 227 (M^+). HRMS (EI) m/z: calcd. for $C_8H_6F_5NO$: 227.0370; found: 227.0366.



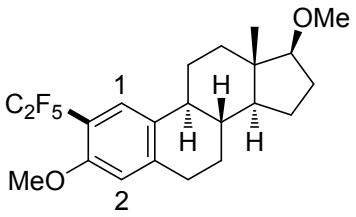
2-(Perfluoroethyl)quinoline (3s) [4]

Obtained as a orange oil in 80% yield (99 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.70. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.5, 3.7 Hz, 1H, H_2), 8.24 (d, *J* = 8.5 Hz, 1H, H_1), 7.90 (d, *J* = 8.2 Hz, 1H, H_6), 7.84 – 7.79 (m, 1H, H_5), 7.75 (d, *J* = 8.6 Hz, 1H, H_3), 7.67 (t, *J* = 7.5 Hz, 1H, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5 (t, *J* = 25.4 Hz), 147.4 (s), 137.8 (s), 130.7 (s), 130.3 (s), 128.7 (s), 128.6 (s), 127.6 (s), 119.1 (qt, J_{CF} = 287.9, 38.4 Hz, CF_3), 117.8 (td, *J* = 3.8, 1.1 Hz), 111.4 (tq, J_{CF} = 256.5, 38.4 Hz, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -82.8 (t, *J* = 1.8 Hz, 3F, CF_3), -116.6 (s, 2F, CF_2). GC-MS m/z 247 (M^+).



2-(Perfluoroethyl)quinoxaline (3t) [6]

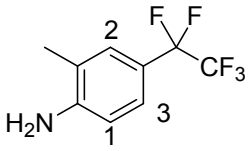
Obtained as a yellow oil in 70% yield (87 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.85. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H, H_1), 8.28 – 8.19 (m, 2H, H_2, H_5), 7.97 – 7.89 (m, 2H, H_3, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6 (t, *J* = 1.4 Hz), 142.5 (t, *J* = 25.9 Hz), 141.7 (ddd, *J* = 5.4, 3.0, 1.1 Hz), 141.1 (s), 132.5 (s), 131.5 (s), 130.2 (s), 129.5 (s), 118.8 (qt, J_{CF} = 287.9, 36.4 Hz, CF_3), 111.1 (tq, J_{CF} = 257.6, 38.4 Hz, CF_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -82.9 – -82.9 (m, 3F, CF_3), -117.0 (s, 2F, CF_2). GC-MS m/z 248 (M^+).



(8R,9S,13S,14S,17S)-3,17-Dimethoxy-13-methyl-2-(perfluoroethyl)-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthrene (3u)

Obtained as a white solid in 55% yield (115 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.89. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H, H_1), 6.71 (s, 1H, H_2), 3.82 (s, 3H, OCH_3), 3.38 (s, 3H, OCH_3), 3.32 (t, *J* = 8.3 Hz, 1H, CH), 3.02 – 2.78 (m, 2H, CH_2), 2.39 – 2.25 (m, 1H, CH), 2.22 – 2.15 (m, 1H, CH), 2.13 – 2.01 (m, 2H, CH_2), 1.92 – 1.88 (m, 1H, CH), 1.77 – 1.65 (m, 1H, CH), 1.59 – 1.17 (m, 7H, CH_2), 0.80 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9 (t, *J* = 2.5 Hz), 142.7 (s), 132.6 (s), 125.7 (t, *J* = 8.4 Hz), 119.5 (qt, J_{CF} = 287.9, 40.4 Hz, CF_3), 114.0 (tq, J_{CF} = 257.6, 38.4 Hz, CF_2), 113.9 (t, *J* = 22.4 Hz), 112.8 (s), 90.7 (s),

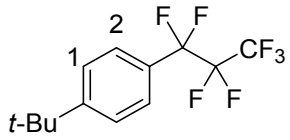
57.9 (s), 55.9 (s), 50.2 (s), 43.7 (s), 43.2 (s), 38.4 (s), 37.9 (s), 29.9 (s), 27.7 (s), 26.9 (s), 26.3 (s), 23.0 (s), 11.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.9 (t, J = 1.9 Hz, 3F, CF_3), -111.3 (s, 2F, CF_2). IR (KBr): ν 2930, 2869, 1617, 1506, 1464, 1409, 1326, 1277, 1240, 1193, 1146, 1133, 1102, 1070, 1029, 996, 975, 961, 901, 864, 753, 730, 649 cm^{-1}. GC-MS m/z 418 (M^+). HRMS (EI) m/z: calcd. for $C_{22}H_{27}F_5O_2$: 418.1931; found: 418.1933.



2-Methyl-4-(perfluoroethyl)aniline (3v)

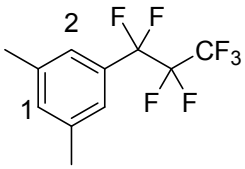
Obtained as a yellow oil in 53% yield (60 mg). R_f (*n*-pentane/diethyl ether 10:3) = 0.60. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.23 (m, 2H, H_2, H_3), 6.70 (d, J = 9.0 Hz, 1H, H_1), 3.90 (s, 2H, NH_2), 2.19 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8 (t, J = 1.5 Hz), 130.0 (s), 128.5 (td, J = 6.3, 1.0 Hz), 125.5 (t, J = 6.0 Hz), 123.7 – 110.6 (m, CF_2CF_3), 115.9 (s), 114.10 (s), 17.3 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.6 (s, 3F, CF_3), -113.8 (s, 2F, CF_2). GC-MS m/z 225 (M^+). HRMS (EI) m/z: calcd. for $C_9H_8F_5N$: 225.0577; found: 225.0575.

Data for compounds 4



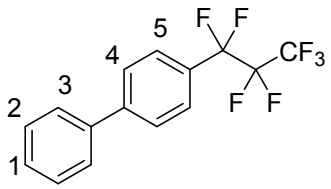
1-*tert*-Butyl-4-(perfluoropropyl)benzene (4a)

Obtained as a colourless oil in 86% yield (130 mg). R_f (*n*-pentane) = 0.94. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.50 (m, 4H, H_1, H_2), 1.38 (s, 9H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4 (t, *J* = 1.7 Hz), 126.5 (t, *J* = 6.5 Hz), 125.8 (t, *J* = 21.9 Hz), 125.6 (s), 118.1 (qt, *J* = 288.6, 34.4 Hz), 115.4 (tt, *J* = 255.3, 30.7 Hz), 108.8 (tq, *J* = 264.7, 37.8 Hz), 34.9 (s), 31.1 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.1 (t, *J* = 9.9 Hz, 3F, CF_3), -111.4 (q, *J* = 9.8 Hz, 2F, CF_2), -126.5 (s, 2F, CF_2). IR (KBr): ν 2967, 1614, 1348, 1270, 1228, 1204, 1179, 1113, 1071, 1040, 1015, 931, 902, 828, 724, 678, 650 cm^{-1}. GC-MS m/z 302 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_{13}F_7$: 302.0905; found: 302.0901.



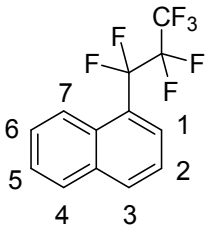
1,3-dimethyl-5-(perfluoropropyl)benzene (4b)

Obtained as a colourless oil in 73% yield (100 mg). R_f (*n*-pentane) = 0.93. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (s, 3H, H_1, H_2), 2.38 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (s), 132.8 (t, *J* = 24.2 Hz), 129.8 (s), 126.9 (t, *J* = 6.4 Hz), 117.9 (qt, *J* = 288.9, 33.9 Hz), 114.9 (tt, *J* = 255.3, 30.7 Hz), 108.6 (tq, *J* = 265.1, 37.7 Hz), 52.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, *J* = 10.0 Hz, 3F, CF_3), -111.4 (q, *J* = 10.0 Hz, 2F, CF_2), -126.4 (s, 2F, CF_2). IR (KBr): ν 2921, 2174, 2153, 1456, 1383, 1257, 1238, 1123, 1046, 981, 857, 833, 8251, 699, 637 cm^{-1}. GC-MS m/z 274 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_9F_7$: 274.0592; found: 274.0591.



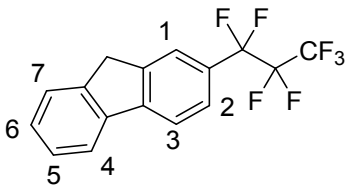
4-(perfluoropropyl)biphenyl (4c) [7]

Obtained as a white solid in 93% yield (150 mg). R_f (*n*-pentane) = 0.83. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.61 (m, 6H, H_3, H_4, H_5), 7.53 – 7.42 (m, 3H, H_1, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9 (t, *J* = 1.6 Hz), 139.7 (s), 129.0 (s), 128.3 (s), 118.1 (qt, *J* = 288.8, 34.5 Hz), 115.4 (tt, *J* = 255.8, 31.2 Hz), 108.8 (tq, *J* = 265.7, 38.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, *J* = 9.9 Hz, 3F, CF_3), -111.6 (q, *J* = 9.8 Hz, 2F, CF_2), -126.4 (s, 2F, CF_2). GC-MS m/z 322 (M^+).



1-(Perfluoropropyl)naphthalene (4e)

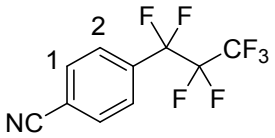
Obtained as a colourless oil in 41% yield (61 mg). R_f (*n*-pentane) = 0.83. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.3 Hz, 1H, H_1), 8.06 (d, *J* = 8.2 Hz, 1H, H_7), 7.93 (d, *J* = 7.8 Hz, 1H, H_3), 7.83 (d, *J* = 7.4 Hz, 1H, H_4), 7.64 – 7.54 (m, 3H, H_2, H_5, H_6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1 (s), 133.4 (s), 130.2 (s), 129.0 (s), 127.8 (t, *J* = 9.9 Hz), 127.6 (s), 126.4 (s), 125.7 (s), 124.8 (tt, *J* = 6.3, 3.3 Hz), 124.2 (s), 118.3 (qt, *J* = 295.1, 33.2 Hz), 117.2 (tt, *J* = 257.1, 32.6 Hz), 109.4 (tq, *J* = 264.9, 37.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.9 (t, *J* = 10.4 Hz, 3F, CF_3), -105.3 (q, *J* = 10.3 Hz, 2F, CF_2), -124.7 (s, 2F, CF_2). IR (KBr): ν 3058, 1580, 1515, 1341, 1287, 1252, 1226, 1204, 1178, 1126, 1110, 1071, 1061, 1029, 995, 927, 913, 890, 861, 812, 794, 771, 741, 693, 527 cm^{-1}. GC-MS m/z 296 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_7F_7$: 296.0436; found: 296.0430.



2-(Perfluoropropyl)-9*H*-fluorene (4f)

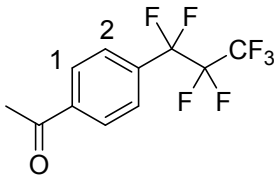
Obtained as a white solid in 88% yield (147 mg). R_f (*n*-pentane) = 0.74. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.80 (m, 2H, H_2, H_3), 7.76 (s, 1H, H_1), 7.67 – 7.54 (m, 2H, H_4, H_7), 7.49 – 7.34 (m, 2H, H_5, H_6), 3.94 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4 (t, *J* = 1.7 Hz), 143.9 (s), 143.4 (s), 140.2 (s), 128.0 (s), 127.1 (s), 126.7 (t, *J* = 24.1 Hz), 125.6 (t, *J* = 6.6 Hz), 125.2 (s), 123.4 (t, *J* = 6.7 Hz), 120.7 (s), 119.8 (s), 118.2 (qt, *J* = 288.8, 34.5 Hz), 115.4 (tt, *J*

= 255.9, 30.9 Hz), 108.9 (tq, *J* = 264.7, 37.8 Hz), 36.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, *J* = 9.9 Hz, 3F, CF_3), -110.6 (q, *J* = 9.9 Hz, 2F, CF_2), -126.2 (s, 2F, CF_2). IR (KBr): ν 2930, 1424, 1352, 1274, 1230, 1192, 1175, 1147, 1115, 1070, 903, 832, 813, 772, 727, 649 cm^{-1}. GC-MS m/z 334 (M^+). HRMS (EI) m/z: calcd. for $C_{16}H_9F_7$: 334.0592; found: 334.0588.



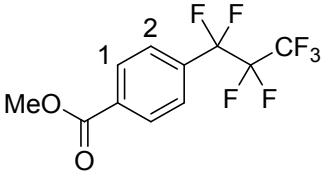
4-(Perfluoropropyl)benzonitrile (4g) [8]

Obtained as a yellow oil in 52% yield (71 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.70. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 2H, H_1), 7.73 (d, *J* = 8.3 Hz, 2H, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.0 (t, *J* = 25.0 Hz), 132.5 (s), 127.7 (tt, *J* = 6.5, 1.5 Hz), 117.4 (s), 116.4 (t, *J* = 1.9 Hz), 118.1 (qt, *J* = 288.5, 34.4 Hz), 115.3 (tt, *J* = 255.7, 30.6 Hz), 108.5 (tq, *J* = 264.7, 37.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.9 (t, *J* = 9.8 Hz, 3F, CF_3), -112.7 (q, *J* = 9.8 Hz, 2F, CF_2), -126.2 (s, 2F, CF_2). GC-MS m/z 271 (M^+).



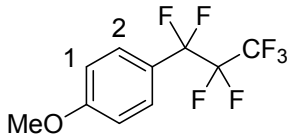
1-(4-(Perfluoropropyl)phenyl)ethanone (4h)

Obtained as a yellow oil in 71% yield (102 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.64. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.3 Hz, 2H, H_1), 7.70 (d, *J* = 8.3 Hz, 2H, H_2), 2.65 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9 (s), 139.8 (s), 132.8 (t, *J* = 24.2 Hz), 128.4 (s), 127.2 (t, *J* = 6.4 Hz), 117.9 (qt, *J* = 288.6, 34.0 Hz), 114.9 (tt, *J* = 256.7, 31.4 Hz), 108.6 (tq, *J* = 265.4, 38.2 Hz), 26.7 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, *J* = 9.8 Hz, 3F, CF_3), -112.3 (q, *J* = 9.7 Hz, 2F, CF_2), -126.4 (s, 2F, CF_2). IR (KBr): ν 2950, 1692, 1348, 1266, 1231, 1182, 1118, 902, 827, 722, 649 cm^{-1}. GC-MS m/z 288 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_7F_7O$: 288.0385; found: 288.0382.



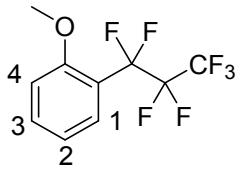
Methyl 4-(perfluoropropyl)benzoate (4i) [8]

Obtained as a yellow oil in 78% yield (118 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.76. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.1 Hz, 2H, H_1), 7.67 (d, *J* = 8.3 Hz, 2H, H_2), 3.96 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8 (s), 133.6 (t, *J* = 3.7 Hz), 132.8 (t, *J* = 24.3 Hz), 129.8 (s), 126.9 (t, *J* = 6.5 Hz), 117.9 (qt, *J* = 288.7, 32.7 Hz), 114.9 (tt, *J* = 256.6, 31.3 Hz), 108.6 (tq, *J* = 265.2, 38.1 Hz), 52.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, *J* = 9.8 Hz, 3F, CF_3), -112.3 (q, *J* = 9.8 Hz, 2F, CF_2), -126.4 (s, 2F, CF_2). GC-MS m/z 304 (M^+).



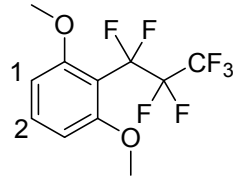
1-Methoxy-4-(perfluoropropyl)benzene (4k) [8]

Obtained as a yellow oil in 87% yield (120 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.81. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H, H_2), 6.99 (d, *J* = 7.9 Hz, 2H, H_1), 3.86 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (t, *J* = 1.6 Hz), 128.3 (t, *J* = 6.5 Hz), 120.7 (t, *J* = 24.7 Hz), 117.9 (qt, *J* = 288.6, 34.0 Hz), 114.9 (tt, *J* = 256.7, 31.4 Hz), 108.6 (tq, *J* = 265.4, 38.2 Hz), 114.0 (s), 55.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.1 (t, *J* = 9.8 Hz, 3F, CF_3), -110.7 (q, *J* = 9.8 Hz, 2F, CF_2), -126.5 (s, 2F, CF_2). GC-MS m/z 276 (M^+).



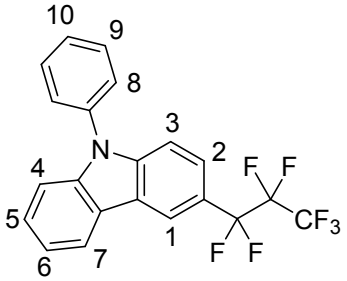
1-Methoxy-2-(perfluoropropyl)benzene (4l) [9]

Obtained as a yellow oil in 70% yield (97 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.89. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.47 (m, 2H, H_1, H_2), 7.06 – 7.01 (m, 2H, H_3, H_4), 3.87 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4 (t, *J* = 2.6 Hz), 133.6 (s), 129.1 (t, *J* = 8.9 Hz), 120.3 (s), 116.9 (t, *J* = 22.7 Hz), 117.9 (qt, *J* = 288.6, 34.0 Hz), 114.9 (tt, *J* = 256.7, 31.4 Hz), 108.6 (tq, *J* = 265.4, 38.2 Hz), 55.90 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.5 (t, *J* = 9.6 Hz, 3F, CF_3), -108.6 (q, *J* = 9.6 Hz, 2F, CF_2), -125.8 (s, 2F, CF_2). GC-MS m/z 276 (M^+).



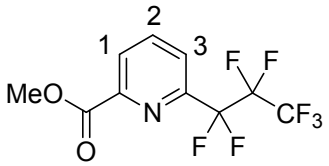
1,3-Dimethoxy-2-(perfluoropropyl)benzene (4m)

Obtained as a yellow oil in 53% yield (81 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.79. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, *J* = 8.2 Hz, 1H, H_2), 6.62 (d, *J* = 8.4 Hz, 2H, H_1), 3.82 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.6 (t, *J* = 2.2 Hz), 133.4 (s), 117.8 (qt, *J* = 288.5, 34.1 Hz), 114.9 (tt, *J* = 255.6, 31.5 Hz), 109.6 (tq, *J* = 265.4, 38.2 Hz), 105.3 (s), 104.7 (s), 56.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.7 (t, *J* = 9.3 Hz, 3F, CF_3), -104.1 (q, *J* = 10.5 Hz, 2F, CF_2), -126.7 (s, 2F, CF_2). IR (KBr): ν 2946, 2846, 1595, 1478, 1435, 1346, 1299, 1258, 1225, 1193, 1137, 1112, 1090, 1053, 1022, 957, 922, 903, 883, 784, 757, 722, 683, 650 cm^{-1}. GC-MS m/z 306 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_9F_7O_2$: 306.0491; found: 306.0485.



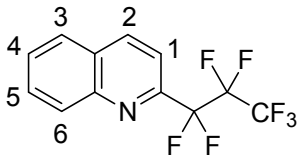
3-(Perfluoropropyl)-9-phenyl-9*H*-carbazole (4o)

Obtained as a white solid in 91% yield (187 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.85. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H, H_1), 8.26 (d, *J* = 7.8 Hz, 1H, H_2), 7.70 – 7.66 (m, 3H, H_3, H_4, H_7), 7.64 – 7.47 (m, 6H, H_5, H_6, H_8, H_9), 7.43 – 7.40 (t, *J* = 7.3 Hz, 1H, H_{10}). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (s), 141.7 (s), 137.0 (s), 130.1 (s), 128.2 (s), 127.2 (s), 127.0 (s), 124.1 (t, *J* = 6.3 Hz), 123.3 (s), 122.8 (s), 120.9 (s), 120.6 (s), 120.0 (t, *J* = 24.6 Hz), 119.5 (t, *J* = 6.9 Hz), 117.9 (qt, *J* = 288.6, 34.0 Hz), 116.2 (tt, *J* = 251.3, 30.7 Hz), 110.3 (s), 109.9 (s), 109.1 (tq, *J* = 263.0, 37.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.9 (t, *J* = 9.9 Hz, 3F, CF_3), -109.2 (q, *J* = 9.9 Hz, 2F, CF_2), -126.0 (s, 2F, CF_2). IR (KBr): ν 1631, 1600, 1502, 1455, 1437, 1345, 1323, 1302, 1254, 1231, 1195, 1176, 1107, 1063, 1026, 1012, 948, 932, 908, 883, 814, 790, 761, 730, 697, 689, 641 cm^{-1}. GC-MS m/z 411 (M^+). HRMS (EI) m/z: calcd. for $C_{21}H_{12}F_7N$: 411.0858; found: 411.0857.



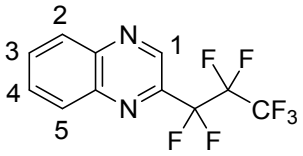
Methyl 6-(perfluoropropyl)picolinate (4p)

Obtained as a yellow oil in 73% yield (111 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.55. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.9 Hz, 1H, H_1), 8.06 (t, *J* = 7.9 Hz, 1H, H_2), 7.85 (d, *J* = 7.9 Hz, 1H, H_3), 4.01 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7 (s), 148.7 (s), 147.9 (t, *J* = 26.0 Hz), 138.5 (s), 127.5 (s), 125.2 (t, *J* = 4.4 Hz), 117.8 (qt, *J* = 288.9, 33.8 Hz), 112.5 (tt, *J* = 258.1, 30.9 Hz), 108.8 (tq, *J* = 266.9, 38.4 Hz), 53.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.2 (t, *J* = 9.3 Hz, 3F, CF_3), -114.7 (q, *J* = 9.3 Hz, 2F, CF_2), -126.2 (s, 2F, CF_2). IR (KBr): ν 2986, 1731, 1588, 1441, 1352, 1323, 1208, 1103, 1085, 1059, 984, 946, 904, 829, 769, 724, 649 cm^{-1}. GC-MS m/z 305 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_6F_7NO_2$: 305.0287; found: 305.0282.



2-(Perfluoropropyl)quinoline (4s) [10]

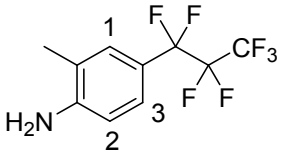
Obtained as a orange oil in 70% yield (104 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.85. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.33 (m, 1H, H_2), 8.25 (d, *J* = 8.6 Hz, 1H, H_1), 7.92 – 7.89 (m, 1H, H_6), 7.85 – 7.80 (m, 1H, H_5), 7.73 (d, *J* = 8.5 Hz, 1H, H_3), 7.71 – 7.65 (m, 1H, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5 (t, *J* = 25.0 Hz), 147.4 (s), 137.7 (s), 130.7 (s), 130.3 (s), 128.7 (s), 128.6 (t, *J* = 1.2 Hz), 127.6 (s), 118.2 (t, *J* = 4.1 Hz), 118.0 (qt, *J* = 288.6, 33.2 Hz), 113.0 (tt, *J* = 257.8, 30.6 Hz), 108.8 (tq, *J* = 266.9, 38.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.1 (q, *J* = 9.2 Hz, 3F, CF_3), -114.4 (q, *J* = 9.2 Hz, 2F, CF_2), -126.1 (s, 2F, CF_2). GC-MS m/z 297 (M^+).



2-(Perfluoropropyl)quinoxaline (4t)

Obtained as a yellow oil in 67% yield (100 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H, H_1), 8.32 – 8.17 (m, 2H, H_2, H_5), 8.00 – 7.87 (m, 2H, H_3, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5 (t, *J* = 1.3 Hz), 142.5 (t, *J* = 25.7 Hz), 141.9 (tt, *J* = 4.4, 1.3 Hz), 141.2 (s), 132.6 (s), 131.5 (s), 130.2 (s), 129.5 (s), 117.8 (qt, *J* = 288.9, 33.7 Hz), 112.7 (tt, *J* = 259.4, 31.2 Hz), 108.9 (tq, *J* = 266.9, 36.4 Hz). ^{19}F NMR (376 MHz,

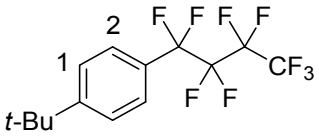
$CDCl_3$) δ -80.0 (dd, J = 17.2, 8.6 Hz, 3F, CF_3), -114.8 (qd, J = 9.3, 3.2 Hz, 2F, CF_2), -126.0 (s, 2F, CF_2). IR (KBr): ν 2918, 2038, 1727, 1570, 1494, 1470, 1352, 1300, 1264, 1229, 1205, 1183, 1152, 1118, 1083, 1055, 1010, 976, 920, 903, 854, 839, 798, 763, 743, 650 cm^{-1}. GC-MS m/z 298 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_5F_7N_2$: 298.0341; found: 298.0334.



2-Methyl-4-(perfluoropropyl)aniline (4v)

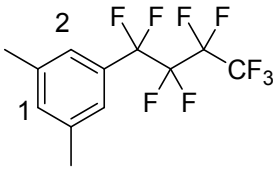
Obtained as a yellow oil in 61% yield (84 mg). R_f (*n*-pentane/diethyl ether 10:3) = 0.54. ^1H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.21 (m, 2H, H_1, H_2), 6.70 (d, J = 8.6 Hz, 1H, H_3), 3.91 (s, 2H, NH_2), 2.19 (s, 3H, CH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8 (t, J = 1.5 Hz), 130.0 (s), 128.7 (tt, J = 6.5, 1.2 Hz), 125.7 (tt, J = 6.8, 1.3 Hz), 121.7 (s), 120.5 – 110.8 (m, $CF_2CF_2CF_3$), 114.0 (s), 17.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.0 (t, J = 10.0 Hz, 3F, CF_3), -110.2 (q, J = 10.0 Hz, 2F, CF_2), -126.5 (s, 2F, CF_2). GC-MS m/z 275 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_8F_7N$: 275.0545; found: 275.0543.

Data for compounds 5



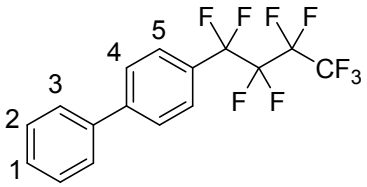
1-*tert*-Butyl-4-(perfluorobutyl)benzene (5a) [8]

Obtained as a colourless oil in 84% yield (148 mg). R_f (*n*-pentane) = 0.90. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.52 (m, 4H, H_1, H_2), 1.37 (s, 9H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4 (t, *J* = 1.6 Hz), 126.6 (t, *J* = 6.5 Hz), 125.9 (t, *J* = 24.4 Hz), 125.6 (s), 122.0 – 102.3 (m, $CF_2CF_2CF_2CF_3$), 34.9 (s), 31.1 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 – -81.1 (m, 3F, CF_3), -110.6 (td, *J* = 13.3, 2.3 Hz, 2F, CF_2), -122.8 (h, *J* = 9.7 Hz, 2F, CF_2), -125.5 – -125.8 (m, 2F, CF_2). GC-MS m/z 352 (M^+).



1,3-Dimethyl-5-(perfluorobutyl)benzene (5b)

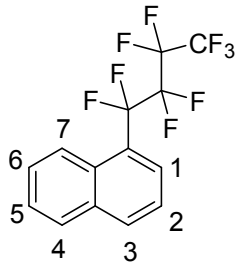
Obtained as a colourless oil in 80% yield (130 mg). R_f (*n*-pentane) = 0.90. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (s, 3H, H_1, H_2), 2.38 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4 (s), 133.5 (t, *J* = 1.7 Hz), 128.7 (t, *J* = 23.8 Hz), 124.4 (tt, *J* = 6.6, 1.4 Hz), 120.0 – 101.3 (m, $CF_2CF_2CF_2CF_3$). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.1 (tt, *J* = 9.9, 3.0 Hz, 3F, CF_3), -110.7 (t, *J* = 13.3 Hz, 2F, CF_2), -122.7 (h, *J* = 9.8 Hz, 2F, CF_2), -125.5 – -125.8 (m, 2F, CF_2). IR (KBr): ν 2921, 2174, 2153, 1352, 1213, 1132, 1029, 882, 858, 804, 780 cm^{-1}. GC-MS m/z 324 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_9F_9$: 324.0561; found: 324.0556.



4-(Perfluorobutyl)biphenyl (5c) [8]

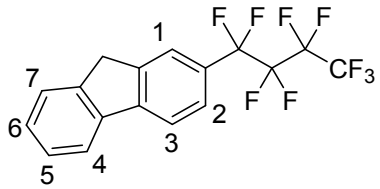
Obtained as a white solid in 97% yield (180 mg). R_f (*n*-pentane) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.67 (m, 4H, H_4, H_5), 7.65 – 7.64 (m, 2H, H_3), 7.55 – 7.49 (m, 2H, H_2), 7.47 – 7.42 (m, 1H, H_1). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9 (t, *J* = 1.6 Hz), 139.7 (s), 129.0 (s), 128.4 (s), 127.5 – 127.1 (m), 123.4 – 100.2 (m, $CF_2CF_2CF_2CF_3$). ^{19}F NMR (376 MHz,

$CDCl_3$) δ -81.1 – -81.2 (m, 3F, CF_3), -110.8 (t, J = 13.4 Hz, 2F, CF_2), -122.7 (dd, J = 19.5, 9.7 Hz, 2F, CF_2), -124.2 – -127.0 (m, 2F, CF_2). GC-MS m/z 372 (M^+).



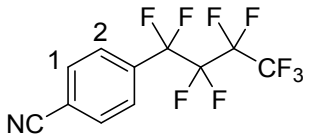
1-(Perfluorobutyl)naphthalene (5e)

Obtained as a yellow oil in 44% yield (76 mg). R_f (*n*-pentane) = 0.81. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.9 Hz, 1H, H_1), 8.09 (d, J = 8.2 Hz, 1H, H_7), 7.96 (d, J = 7.9 Hz, 1H, H_3), 7.86 (d, J = 7.3 Hz, 1H, H_4), 7.66 – 7.56 (m, 3H, H_2, H_5, H_6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1 (s), 133.4 (t, J = 1.3 Hz), 130.3 (t, J = 1.6 Hz), 129.0 (s), 127.9 (t, J = 9.9 Hz), 127.6 (t, J = 1.2 Hz), 126.7 (s), 126.4 (s), 124.8 (tt, J = 6.4, 3.3 Hz), 124.2 (s), 121.9 – 108.0 (m, $CF_2CF_2CF_2CF_3$). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, J = 9.8, 2.8 Hz, 3F, CF_3), -104.6 (t, J = 14.3 Hz, 2F, CF_2), -121.0 – -121.2 (m, 2F, CF_2), -125.4 – -125.7 (m, 2F, CF_2). IR (KBr): ν 2916, 2848, 1580, 1516, 1349, 1278, 1230, 1193, 1077, 976, 951, 923, 880, 785, 768, 737, 727, 669, 621, 535, 517 cm^{-1}. GC-MS m/z 346 (M^+). HRMS (EI) m/z: calcd. for $C_{14}H_7F_9$: 346.0404; found: 346.0400.



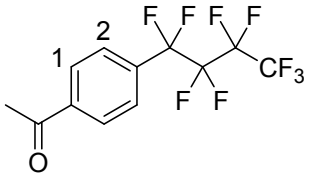
2-(Perfluorobutyl)-9*H*-fluorene (5f) [11]

Obtained as a white solid in 95% yield (182 mg). R_f (*n*-pentane) = 0.68. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.80 (m, 2H, H_2, H_3), 7.76 (s, 1H, H_1), 7.66 – 7.56 (m, 2H, H_4, H_7), 7.47 – 7.35 (m, 2H, H_5, H_6), 3.95 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4 (t, J = 1.7 Hz), 143.9 (s), 143.4 (s), 140.2 (s), 128.0 (s), 127.1 (s), 126.8 (t, J = 24.0 Hz), 125.7 (tt, J = 6.8, 1.4 Hz), 125.2 (s), 123.5 (tt, J = 6.7, 1.3 Hz), 120.7 (s), 119.8 (s), 121.4 – 105.7 (m, $CF_2CF_2CF_2CF_3$), 36.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (tt, J = 9.7, 2.8 Hz, 3F, CF_3), -109.9 (td, J = 13.3, 2.4 Hz, 2F, CF_2), -122.6 (dd, J = 19.5, 9.8 Hz, 2F, CF_2), -125.5 – -125.6 (m, 2F, CF_2). GC-MS m/z 384 (M^+).



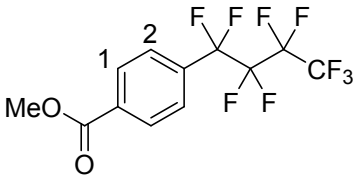
4-(Perfluorobutyl)benzonitrile (5g) [8]

Obtained as a yellow oil in 35% yield (56 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 2H, H_1), 7.73 (d, *J* = 8.3 Hz, 2H, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.2 (t, *J* = 24.5 Hz), 132.5 (s), 127. 8 (tt, *J* = 6.7, 1.6 Hz), 117.4 (s), 120.5 – 112.2 (m, $CF_2CF_2CF_2CF_3$), 116.4 (t, *J* = 1.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (tt, *J* = 9.7, 2.6 Hz, 3F, CF_3), -111.9 (t, *J* = 13.3 Hz, 2F, CF_2), -122.5 – -122.7 (m, 2F, CF_2), -125.4 – -125.6 (m, 2F, CF_2). GC-MS m/z 321 (M^+).



1-(4-(Perfluorobutyl)phenyl)ethanone (5h) [8]

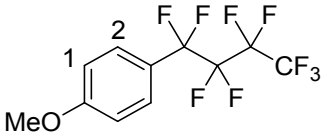
Obtained as a yellow oil in 65% yield (110 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.60. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.9 Hz, 2H, H_1), 7.73 (d, *J* = 7.8 Hz, 2H, H_2), 2.67 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9 (s), 139.8 (t, *J* = 1.5 Hz), 132.9 (t, *J* = 24.2 Hz), 128.4 (s), 127.3 (t, *J* = 6.5 Hz), 122.8 – 102.8 (m, $CF_2CF_2CF_2CF_3$), 26.7 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.1 (tt, *J* = 9.7, 2.5 Hz, 3F, CF_3), -111.5 (t, *J* = 13.0 Hz, 2F, CF_2), -122.7 (d, *J* = 7.7 Hz, 2F, CF_2), -125.5 – -125.6 (m, 2F, CF_2). GC-MS m/z 338 (M^+).



Methyl 4-(perfluorobutyl)benzoate (5i) [8]

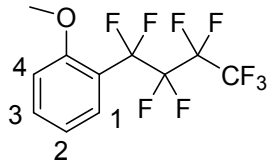
Obtained as a yellow oil in 80% yield (142 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.9 Hz, 2H, H_1), 7.67 (d, *J* = 7.7 Hz, 2H, H_2), 3.95 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8 (s), 133.6 (t, *J* = 1.6 Hz), 132.9 (t, *J* = 24.2 Hz), 129.8 (s), 126.9 (t, *J* = 6.5 Hz), 124.5 – 101.7 (m, $CF_2CF_2CF_2CF_3$), 52.5 (s). ^{19}F NMR

(376 MHz, $CDCl_3$) δ -81.2 (tt, J = 9.5, 2.8 Hz, 3F, CF_3), -111.5 (t, J = 13.3 Hz, 2F, CF_2), -122.8 (d, J = 8.8 Hz, 2F, CF_2), -125.6 – -125.7 (m, 2F, CF_2). GC-MS m/z 354 (M^+).



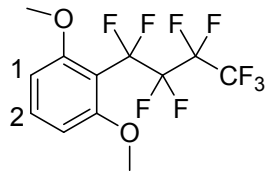
1-Methoxy-4-(perfluorobutyl)benzene (5k) [8]

Obtained as a yellow oil in 93% yield (152 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.78. ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 7.9 Hz, 2H, H_2), 6.99 (d, J = 7.5 Hz, 2H, H_1), 3.86 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (t, J = 1.6 Hz), 128.4 (t, J = 6.6 Hz), 120.8 (t, J = 24.8 Hz), 122.8 – 107.2 (m, $CF_2CF_2CF_2CF_3$), 113.9 (s), 55.3 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.2 (t, J = 9.7 Hz, 3F, CF_3), -110.0 (t, J = 13.3 Hz, 2F, CF_2), -122.9 (dd, J = 17.4, 9.3 Hz, 2F, CF_2), -124.6 – -126.8 (m, 2F, CF_2). GC-MS m/z 326 (M^+).



1-Methoxy-2-(perfluorobutyl)benzene (5l) [8]

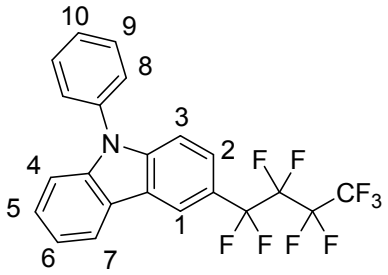
Obtained as a yellow oil in 61% yield (99 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.94. ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.47 (m, 2H, H_1, H_2), 7.08 – 6.99 (m, 2H, H_3, H_4), 3.87 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5 (t, J = 2.8 Hz), 133.6 (t, J = 1.4 Hz), 129.2 (t, J = 8.9 Hz), 120.3 (s), 119.6 – 112.8 (m, $CF_2CF_2CF_2CF_3$), 112.5 (s), 112.4 (s), 55.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (tt, J = 10.1, 2.7 Hz, 3F, CF_3), -107.9 (t, J = 13.7 Hz, 2F, CF_2), -122.0 – -122.2 (m, 2F, CF_2), -126.0 – -126.2 (m, 2F, CF_2). GC-MS m/z 326 (M^+).



1,3-Dimethoxy-2-(perfluorobutyl)benzene (5m)

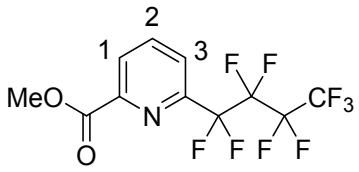
Obtained as a yellow oil in 39% yield (69 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.48. ^1H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, J = 8.4 Hz, 1H, H_2), 6.62 (d, J = 8.4 Hz, 2H, H_1), 3.83 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7 (t, J = 2.4 Hz), 133.5 (s), 123.3 – 106.9 (m, $CF_2CF_2CF_2CF_3$), 105.4 (s), 104.8 (s), 56.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.1 (ddd, J =

12.5, 6.8, 2.7 Hz, 3F, CF_3), -111.1 (t, J = 13.4 Hz, 2F, CF_2), -122.7 (dd, J = 18.8, 9.3 Hz, 2F, CF_2), -125.6 (td, J = 13.0, 2.5 Hz, 2F, CF_2). IR (KBr): ν 2970, 2856, 1585, 1488, 1475, 1366, 1279, 1248, 1235, 1173, 1167, 1162, 1093, 1013, 1042, 967, 932, 973, 843, 774, 759, 732, 684, 653 cm^{-1}. GC-MS m/z 356 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_9F_9O_2$: 356.0459; found: 356.0452.



3-(perfluorobutyl)-9-phenyl-9*H*-carbazole (5o)

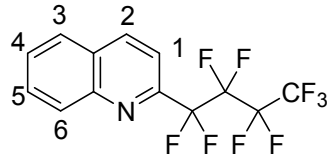
Obtained as a white solid in 96% yield (221 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.85. ^1H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H, H_1), 8.28 (d, J = 7.7 Hz, 1H, H_2), 7.87 – 7.33 (m, 10H, H_3, H_4, H_5, H_6, H_7, H_8, H_9, H_{10}). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (s), 141.7 (s), 137.0 (s), 130.1 (s), 128.2 (s), 127.2 (s), 127.0 (s), 124.2 (t, J = 6.3 Hz), 123.3 (s), 122.9 (s), 120.9 (s), 120.6 (s), 120.1 (t, J = 24.4 Hz), 119.6 (t, J = 6.9 Hz), 123.8 – 105.5 (m, *$CF_2CF_2CF_2CF_3$*), 110.3 (s), 109.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (t, J = 9.6 Hz, 3F, CF_3), -108.4 (t, J = 13.3 Hz, 2F, CF_2), -122.3 (dd, J = 17.7, 8.8 Hz, 2F, CF_2), -125.4 (t, J = 12.6 Hz, 2F, CF_2). IR (KBr): ν 1599, 1503, 1459, 1437, 1350, 1323, 1258, 1234, 1203, 1131, 1078, 904, 871, 761, 728, 717, 697, 649, 604 cm^{-1}. GC-MS m/z 461 (M^+). HRMS (EI) m/z: calcd. for $C_{22}H_{12}F_9N$: 461.0826; found: 461.0821.



Methyl 6-(perfluorobutyl)picolinate (5p)

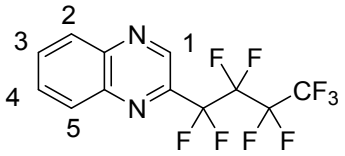
Obtained as a colourless oil in 68% yield (121 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.29. ^1H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, J = 7.8 Hz, 1H, H_1), 8.06 (t, J = 7.9 Hz, 1H, H_2), 7.86 (d, J = 7.9 Hz, 1H, H_3), 4.02 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7 (s), 148.7 (s), 148.1 (t, J = 26.0 Hz), 138.4 (s), 127.5 (t, J = 1.3 Hz), 125.3 (t, J = 4.5 Hz), 121.3 – 107.2 (m, *$CF_2CF_2CF_2CF_3$*), 53.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, J = 9.7, 2.5 Hz, 3F, CF_3),

-113.9 (td, J = 13.0, 2.2 Hz, 2F, CF_2), -122.4 – -122.5 (m, 2F, CF_2), -125.5 – -125.6 (m, 2F, CF_2). IR (KBr): ν 2996, 1741, 1688, 1451, 1362, 1333, 1218, 1113, 1095, 1060, 974, 956, 914, 839, 779, 734, 659 cm^{-1}. GC-MS m/z 355 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_6F_9NO_2$: 355.0255; found: 355.0258.



2-(Perfluorobutyl)quinoline (5s) [12]

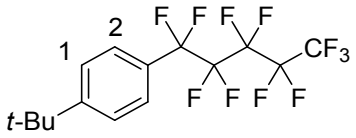
Obtained as a orange oil in 68% yield (118 mg). R_f (n-pentane/diethyl ether 10:1) = 0.74. ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 8.6 Hz, 1H, H_2), 8.26 (d, J = 8.6 Hz, 1H, H_1), 7.92 (d, J = 8.2 Hz, 1H, H_6), 7.83 (ddd, J = 8.5, 6.9, 1.4 Hz, 1H, H_5), 7.74 (d, J = 8.6 Hz, 1H, H_3), 7.71 – 7.65 (m, 1H, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.5 (t, J = 25.4 Hz), 147.4 (s), 137.7 (s), 130.7 (s), 130.3 (s), 128.7 (s), 128.6 (s), 127.6 (s), 118.2 (t, J = 3.9 Hz), 122.9 – 105.7 (m, $CF_2CF_2CF_2CF_3$). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, J = 9.7, 2.5 Hz, 3F, CF_3), -113.6 (td, J = 12.8, 2.4 Hz, 2F, CF_2), -122.3 – -122.4 (m, 2F, CF_2), -125.5 – -125.6 (m, 2F, CF_2). GC-MS m/z 347 (M^+).



2-(Perfluorobutyl)quinoxaline (5t)

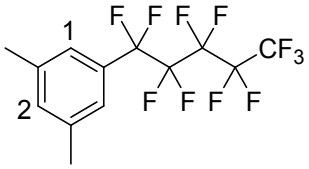
Obtained as a colourless oil in 68% yield (118 mg). R_f (n-pentane/diethyl ether 10:1) = 0.62. ^1H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H, H_1), 8.33 – 8.16 (m, 2H, H_2, H_5), 7.96 – 7.88 (m, 2H, H_3, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5 (s), 142.6 (t, J = 25.7 Hz), 141.9 (t, J = 4.4 Hz), 132.5 (s), 131.5 (s), 130.2 (s), 129.5 (s), 129.2 (s), 123.4 – 103.5 (m, $CF_2CF_2CF_2CF_3$). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, J = 9.7, 2.6 Hz, 3F, CF_3), -114.0 (td, J = 12.8, 2.7 Hz, 2F, CF_2), -122.3 – -122.4 (m, 2F, CF_2), -125.4 – -125.5 (m, 2F, CF_2). IR (KBr): ν 1586, 1571, 1497, 1470, 1405, 1354, 1301, 1236, 1201, 1135, 1097, 1017, 904, 883, 843, 830, 812, 762, 733, 664, 649 cm^{-1}. GC-MS m/z 348 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_5F_9N_2$: 348.0309; found: 348.0306.

Data for compounds 6



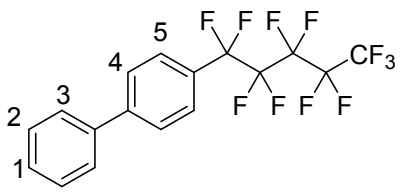
1-*tert*-Butyl-4-(perfluoropentyl)benzene (6a)

Obtained as a colorless oil in 89% yield (179 mg). R_f (*n*-pentane) = 0.85. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.48 (m, 4H, H_1, H_2), 1.36 (s, 9H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4 (t, *J* = 1.6 Hz), 126.6 (tt, *J* = 6.5, 1.3 Hz), 126.0 (t, *J* = 24.2 Hz), 125.5 (s), 121.5 – 103.8 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 34.9 (s), 31.0 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.6 – -81.5 (m, 3F, CF_3), -110.5 – -110.6 (m, 2F, CF_2), -122.1 (d, *J* = 12.3 Hz, 2F, CF_2), -122.3 – -122.4 (m, 2F, CF_2), -126.2 – -126.4 (m, 2F, CF_2). IR (KBr): ν 2967, 1615, 1464, 1412, 1359, 1300, 1232, 1198, 1140, 1105, 1075, 1053, 1053, 905, 858, 839, 823, 724, 692, 650 cm^{-1}. GC-MS m/z 402 (M^+). HRMS (EI) m/z: calcd. for $C_{15}H_{13}F_{11}$: 402.0842; found: 402.0844.



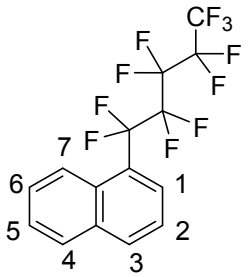
1,3-Dimethyl-5-(perfluoropentyl)benzene (6b)

Obtained as a colorless oil in 78% yield (146 mg). R_f (*n*-pentane) = 0.85. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (s, 2H, H_1), 7.22 (s, 1H, H_2), 2.40 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4 (s), 133.5 (t, *J* = 1.6 Hz), 128.9 (t, *J* = 23.7 Hz), 124.4 (tt, *J* = 6.5, 1.3 Hz), 120.2 – 104.6 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 21.0 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (tt, *J* = 9.9, 2.6 Hz, 3F, CF_3), -110.6 (t, *J* = 14.6 Hz, 2F, CF_2), -122.0 – -122.1 (m, 2F, CF_2), -122.4 – -122.5 (m, 2F, CF_2), -126.3 – -126.4 (m, 2F, CF_2). IR (KBr): ν 2979, 1357, 1323, 1237, 1197, 1143, 1112, 1078, 904, 873, 859, 783, 767, 722, 680, 649 cm^{-1}. GC-MS m/z 374 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_9F_{11}$: 374.0529; found: 374.0526.



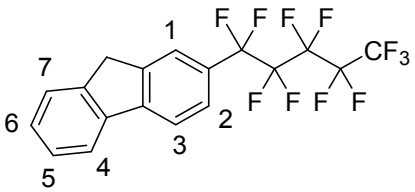
4-(Perfluoropentyl)biphenyl (6c)

Obtained as a white solid in 81% yield (171 mg). R_f(*n*-pentane) = 0.80. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.62 (m, 6H, H_3, H_4, H_5), 7.55 – 7.39 (m, 3H, H_1, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.9 (s), 139.7 (s), 129.0 (s), 128.3 (s), 127.9 – 126.3 (m), 123.6 – 101.3 (m, *$CF_2CF_2CF_2CF_2CF_3$*). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, *J* = 9.9, 2.5 Hz, 3F, CF_3), -110.6 (t, *J* = 14.4 Hz, 2F, CF_2), -122.0 (s, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.2 – -126.3 (m, 2F, CF_2). IR (KBr): ν 1615, 1489, 1408, 1360, 1298, 1232, 1197, 1140, 1105, 1077, 1055, 1009, 967, 905, 859, 809, 790, 768, 729, 650, 633 cm^{-1}. GC-MS m/z 422 (M^+). HRMS (EI) m/z: calcd. for $C_{17}H_9F_{11}$: 422.0529; found: 422.0527.



1-(Perfluoropentyl)naphthalene (6e)

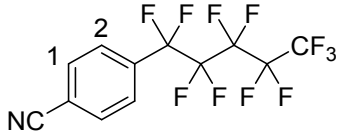
Obtained as a colourless oil in 37% yield (73 mg). R_f(*n*-pentane) = 0.81. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.5 Hz, 1H, H_1), 8.05 (d, *J* = 8.2 Hz, 1H, H_7), 7.92 (d, *J* = 8.0 Hz, 1H, H_3), 7.83 (d, *J* = 7.4 Hz, 1H, H_4), 7.69 – 7.48 (m, 3H, H_2, H_5, H_6). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.1 (s), 133.4 (s), 130.3 (s), 128.9 (s), 128.0 (t, *J* = 9.9 Hz), 127.6 (s), 126.4 (s), 124.8 (tt, *J* = 6.2, 3.2 Hz), 124.6 (s), 124.2 (s), 122.4 – 105.0 (m, *$CF_2CF_2CF_2CF_2CF_3$*). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 (tt, *J* = 10.0, 2.6 Hz, 3F, CF_3), -104.5 (t, *J* = 15.2 Hz, 2F, CF_2), -120.3 – -120.4 (m, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.0 – -126.1 (m, 2F, CF_2). IR (KBr): ν 2251, 2012, 2001, 1939, 1515, 1349, 1238, 1190, 1142, 1102, 903, 856, 827, 778, 718, 650, 621 cm^{-1}. GC-MS m/z 396 (M^+). HRMS (EI) m/z: calcd. for $C_{15}H_7F_{11}$: 396.0372; found: 396.0369.



2-(Perfluoropentyl)-9*H*-fluorene (6f)

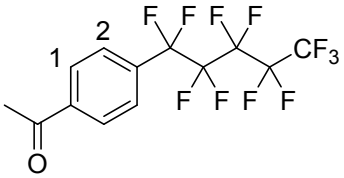
Obtained as a white solid in 75% yield (163 mg). R_f(*n*-pentane) = 0.70. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.80 (m, 2H, H_2, H_3), 7.76 (s, 1H, H_1), 7.60 (t, *J* = 7.6 Hz, 2H, H_4, H_7), 7.47

– 7.33 (m, 2H, H_5, H_6), 3.96 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4 (s), 143.8 (s), 143.4 (s), 140.2 (s), 128.0 (s), 127.1 (s), 126.8 (s), 125.7 (t, *J* = 6.6 Hz), 125.2 (s), 123.5 (t, *J* = 6.6 Hz), 120.7 (s), 119.8 (s), 119.5 – 104.9 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 36.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 (tt, *J* = 9.9, 2.5 Hz, 3F, CF_3), -109.7 (t, *J* = 14.4 Hz, 2F, CF_2), -121.8 – -121.9 (m, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.2 – -126.3 (m, 2F, CF_2). IR (KBr): ν 2967, 2153, 1964, 1618, 1427, 1360, 1237, 1199, 1141, 1102, 905, 841, 803, 782, 729, 692, 650 cm^{-1}. GC-MS m/z 434 (M^+). HRMS (EI) m/z: calcd. for $C_{18}H_9F_{11}$: 434.0529; found: 434.0524.



4-(Perfluoropentyl)benzonitrile (6g)

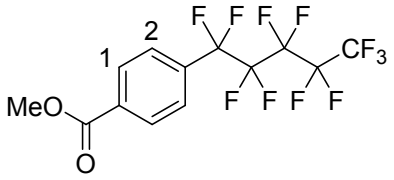
Obtained as a yellow oil in 39% yield (72 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.87. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.3 Hz, 2H, H_1), 7.73 (d, *J* = 8.3 Hz, 2H, H_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.2 (t, *J* = 24.6 Hz), 132.5 (s), 127.7 (t, *J* = 6.5 Hz), 117.4 (s), 116.3 (t, *J* = 1.6 Hz), 123.8 – 105.5 (m, *$CF_2CF_2CF_2CF_2CF_3$*). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.4 – -81.2 (m, 3F, CF_3), -111.7 (t, *J* = 14.3 Hz, 2F, CF_2), -121.9 (d, *J* = 2.6 Hz, 2F, CF_2), -122.1 – -122.3 (m, 2F, CF_2), -125.5 – -127.2 (m, 2F, CF_2). IR (KBr): ν 1616, 1479, 1428, 1240, 902, 859,823, 800, 783, 722, 649 cm^{-1}. GC-MS m/z 371 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_4F_{11}N$: 371.0168; found: 371.0161.



1-(4-(Perfluoropentyl)phenyl)ethanone (6h)

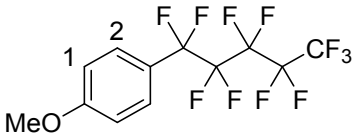
Obtained as a yellow oil in 70% yield (136 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.55. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4 Hz, 2H, H_1), 7.70 (d, *J* = 8.3 Hz, 2H, H_2), 2.65 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9 (s), 139.8 (t, *J* = 1.5 Hz), 132.9 (t, *J* = 24.1 Hz), 128.4 (s), 127.3 (t, *J* = 6.5 Hz), 120.8 – 100.5 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 26.7 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 – -80.9 (m, 3F, CF_3), -111.3 (t, *J* = 14.2 Hz, 2F, CF_2), -122.0 – -122.1 (m, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.2 – -126.3 (m, 2F, CF_2). IR (KBr): ν 2918, 2849, 1694, 1409, 1359, 1298, 1263, 1231, 1198, 1140, 1106, 1083, 1051,

1018, 906, 861, 730, 689, 659 cm^{-1}. GC-MS m/z 388 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_7F_{11}O$: 388.0321; found: 388.0322.



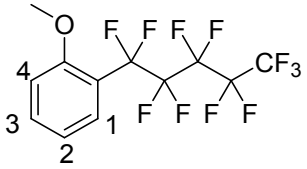
Methyl 4-(perfluoropentyl)benzoate (6i)

Obtained as a yellow oil in 65% yield (131 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.74. ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.7 Hz, 2H, H_1), 7.68 (d, *J* = 8.4 Hz, 2H, H_2), 3.96 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8 (s), 133.6 (t, *J* = 1.5 Hz), 132.9 (t, *J* = 24.1 Hz), 129.8 (s), 127.0 (tt, *J* = 6.5, 1.4 Hz), 124.5 – 104.9 (m, $CF_2CF_2CF_2CF_2CF_3$), 52.5 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 (tt, *J* = 9.7, 2.6 Hz, 3F, CF_3), -111.2 (t, *J* = 14.2 Hz, 2F, CF_2), -122.0 – -122.1 (m, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.2 – -126.3 (m, 2F, CF_2). IR (KBr): ν 2975, 1769, 1678, 1240, 1106, 902, 874, 869, 785, 767, 722, 649 cm^{-1}. GC-MS m/z 404 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_7F_{11}O_2$: 404.0270; found: 404.0268.



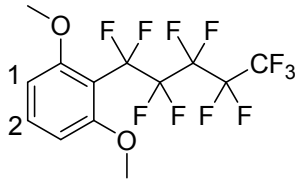
1-Methoxy-4-(perfluoropentyl)benzene (6k)

Obtained as a colourless oil in 85% yield (160 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.84. ^1H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.7 Hz, 2H, H_2), 6.99 (d, *J* = 8.8 Hz, 2H, H_1), 3.86 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3 (t, *J* = 1.6 Hz), 128.4 (t, *J* = 6.6 Hz), 120.9 (t, *J* = 24.8 Hz), 122.8 – 106.2 (m, $CF_2CF_2CF_2CF_2CF_3$), 113.9 (s), 55.3 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 – -81.0 (m, 3F, CF_3), -109.8 (t, *J* = 14.0 Hz, 2F, CF_2), -118.9 – -124.1 (m, 4F, CF_2CF_2), -124.9 – -128.0 (m, 2F, CF_2). IR (KBr): ν 2936, 1615, 1518, 1359, 1310, 1238, 1199, 1180, 1142, 1102, 1030, 903, 856, 835, 775, 694, 649, 622, 554 cm^{-1}. GC-MS m/z 376 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_7F_{11}O$: 376.0321; found: 376.0320.



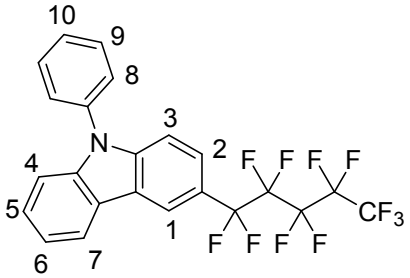
1-Methoxy-2-(perfluoropentyl)benzene (6l)

Obtained as a yellow oil in 69% yield (130 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.71. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.46 (m, 2H, H_1, H_2), 7.09 – 6.99 (m, 2H, H_3, H_4), 3.87 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5 (t, J = 2.8 Hz), 133.5 (t, J = 1.3 Hz), 129.2 (t, J = 8.9 Hz), 120.2 (s), 117.0 (t, J = 22.7 Hz), 123.6 – 104.0 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 112.4 (s), 55.8 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.0 (tt, J = 10.0, 2.7 Hz, 3F, CF_3), -107.8 (t, J = 14.6 Hz, 2F, CF_2), -121.4 – -121.5 (m, 2F, CF_2), -122.7 – -122.8 (m, 2F, CF_2), -126.1 – -126.3 (m, 2F, CF_2). IR (KBr): ν 2969, 1605, 1496, 1466, 1263, 1238, 1198, 1141, 1064, 1027, 903, 873, 859, 723, 650 cm^{-1}. GC-MS m/z 376 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_7F_{11}O$: 376.0321; found: 376.0316.



1,3-Dimethoxy-2-(perfluoropentyl)benzene (6m)

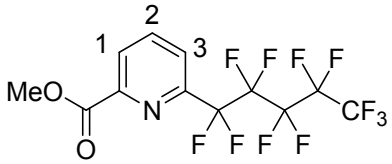
Obtained as a white solid in 50% yield (102 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.67. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (t, J = 8.5 Hz, 1H, H_2), 6.62 (d, J = 8.4 Hz, 2H, H_1), 3.82 (s, 6H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7 (t, J = 2.3 Hz), 133.4 (s), 122.7 – 109.4 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 106.2 (s), 105.3 (s), 56.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, J = 10.0, 2.7 Hz, 3F, CF_3), -103.3 (t, J = 14.7 Hz, 2F, CF_2), -122.0 – -122.2 (m, 2F, CF_2), -123.0 – -123.1 (m, 2F, CF_2), -126.0 – -126.2 (m, 2F, CF_2). IR (KBr): ν 2964, 1596, 1478, 1435, 1259, 1238, 1138, 1092, 902, 847, 797, 722, 649 cm^{-1}. GC-MS m/z 406 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_9F_{11}O_2$: 406.0427; found: 406.0423.



3-(Perfluoropentyl)-9-phenyl-9*H*-carbazole (6o)

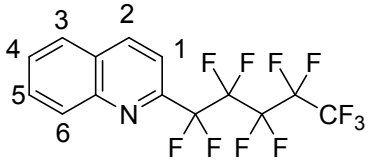
Obtained as a white solid in 86% yield (220 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.80. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 – 8.40 (m, 1H, H_1), 8.34 – 8.15 (m, 1H, H_2), 7.47 – 7.37 (m,

3H, H_3, H_4, H_7), 7.63 – 7.27 (m, 7H, H_5, H_6, H_8, H_9, H_{10}). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (s), 141.7 (s), 137.0 (s), 130.1 (s), 128.1 (s), 127.2 (s), 127.0 (s), 124.2 (s), 123.3 (s), 123.2 (s), 122.8 (s), 120.7 (s), 120.6 (s), 119.6 (s), 120.5 – 105.2 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 110.2 (s), 109.9 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 (t, *J* = 10.0 Hz, 3F, CF_3), -108.3 (t, *J* = 14.3 Hz, 2F, CF_2), -121.6 – -121.7 (m, 2F, CF_2), -122.1 – -122.2 (m, 2F, CF_2), -126.1 – -126.2 (m, 2F, CF_2). IR (KBr): ν 3066, 1631, 1599, 1503, 1459, 1437, 1360, 1335, 1323, 1226, 1194, 1138, 1101, 1068, 905, 857, 837, 782, 744, 733, 713, 705, 641, 585 cm^{-1}. GC-MS m/z 511 (M^+). HRMS (EI) m/z: calcd. for $C_{23}H_{12}F_{11}N$: 511.0794; found: 511.0788.



Methyl 6-(perfluoropentyl)picolinate (6p)

Obtained as a yellow oil in 70% yield (142 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.9 Hz, 1H, H_1), 8.06 (t, *J* = 7.9 Hz, 1H, H_2), 7.86 (d, *J* = 7.9 Hz, 1H, H_3), 4.01 (s, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.7 (s), 148.7 (s), 148.1 (t, *J* = 26.1 Hz), 138.4 (s), 127.5 (t, *J* = 1.2 Hz), 125.3 (t, *J* = 4.4 Hz), 119.9 – 104.7 (m, *$CF_2CF_2CF_2CF_2CF_3$*), 53.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.9 (tt, *J* = 9.9, 2.5 Hz, 3F, CF_3), -113.8 (t, *J* = 13.6 Hz, 2F, CF_2), -121.7 – -121.8 (m, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.2 – -126.3 (m, 2F, CF_2). IR (KBr): ν 2976, 1729, 1688, 1451, 1362, 1333, 1239, 1203, 1142, 1060, 974, 956, 914, 849, 779, 734, 649 cm^{-1}. GC-MS m/z 405 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_6F_{11}NO_2$: 405.0223; found: 405.0216.



2-(Perfluoropentyl)quinoline (6s) [13]

Obtained as a orange oil in 56% yield (111 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.6 Hz, 1H, H_2), 8.26 (d, *J* = 8.6 Hz, 1H, H_1), 7.91 (d, *J* = 8.2 Hz, 1H, H_6), 7.84 – 7.80 (m, 1H, H_5), 7.76 – 7.63 (m, 2H, H_3, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7 (t, *J* = 25.7 Hz), 147.4 (s), 137.7 (s), 130.7 (s), 130.3 (s), 128.7 (s), 128.6 (t, *J* = 1.2 Hz), 127.6 (s), 118.2 (t, *J* = 4.1 Hz), 121.3 – 104.9 (m, *$CF_2CF_2CF_2CF_2CF_3$*).

^{19}F NMR (376 MHz, $CDCl_3$) δ -80.7 – -81.0 (m, 3F, CF_3), -113.5 (t, *J* = 13.7 Hz, 2F, CF_2), -121.7 (dd, *J* = 11.6, 2.2 Hz, 2F, CF_2), -122.2 – -122.3 (m, 2F, CF_2), -126.1 – -126.4 (m, 2F, CF_2). GC-MS m/z 397 (M^+).

2-(Perfluoropentyl)quinoxaline (6t)

Obtained as a yellow oil in 62% yield (123 mg). R_f (*n*-pentane/diethyl ether 10:1) = 0.77. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H, H_1), 8.29 – 8.19 (m, 2H, H_2, H_5), 7.96 – 7.89 (m, 2H, H_3, H_4). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5 (t, *J* = 1.4 Hz), 142.7 (t, *J* = 25.7 Hz), 141.9 (t, *J* = 4.6 Hz), 141.2 (s), 132.5 (s), 131.5 (s), 130.2 (s), 129.5 (s), 121.3 – 107.6 (m, *$CF_2CF_2CF_2CF_2CF_3$*). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.8 (tt, *J* = 9.8, 2.3 Hz, 3F, CF_3), -113.9 – -114.0 (m, 2F, CF_2), -121.6 – -121.7 (m, 2F, CF_2), -122.1 – -122.2 (m, 2F, CF_2), -126.1 – -126.3 (m, 2F, CF_2). IR (KBr): ν 1596, 1581, 1487, 1480, 1415, 1354, 1239, 1204, 1144, 1110, 903, 722, 649, 549 cm^{-1}. GC-MS m/z 398 (M^+). HRMS (EI) m/z: calcd. for $C_{13}H_5F_{11}N_2$: 398.0277; found: 398.0279.

Crystal Structure Analyses.

The suitable crystals of **1a** and **1b** were mounted on quartz fibers and X-ray data collected on a Bruker AXS APEX diffractometer, equipped with a CCD detector at -50 ºC, using MoKα radiation (λ 0.71073 Å). The data was corrected for Lorentz and polarisation effect with the **SMART** suite of programs and for absorption effects with SADABS.[14] Structure solution and refinement were carried out with the SHELXTL suite of programs.[14] The structure was solved by direct methods to locate the heavy atoms, followed by difference maps for the light non-hydrogen atoms. Because of disordered $CF_3CF_2CO_2^-$ groups in lattice in **1a**, their thermal parameters seem abnormal.

Crystallographic data for structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publications nos. 1427126, and 1427127.

Table 1. Selected crystal data, data collection and refinement parameters of complexes **1a–b**.

Complexes	**1a** (CCDC-1427126)	**1b** (CCDC-1427127)
Formula	$C_{27}H_{16}CuF_5N_4O_2$	$C_{34}H_{22}CuF_7N_4O_2$
formula weight	586.99	715.11
Crystal size/mm	0.50 × 0.40 × 0.20	0.50 × 0.40 × 0.20
temperature/K	173(2)	293(2)
Crystal system	Monoclinic	Orthorhombic
space group	P21/n	Ibam
a/Å	12.346(3)	15.422(3)
b/Å	9.3473(19)	17.640(4)
c/Å	20.554(4)	21.739(4)
α/º	90	90
β/º	99.01(3)	90
γ/º	90	90
V/Å^3	2342.7(9)	5914(2)
Z	4	8
D_c/g cm^{-3}	1.664	1.606
radiation used	Mo-Kα	Mo-Kα
μ/mm^{-1}	1.008	0.824
θ range/º	3.01 to 27.48	3.03 to 27.48
No. of unique reflections Measured	5362	3485
max., min. transmission	1.00 and 0.25	1.00 and 0.25
final *R* indices [$I>2\sigma(I)$] [a, b]	R_1 = 0.0719	R_1 = 0.0555
	wR_2 = 0.2062	wR_2 = 0.1485
R indices (all data)	R_1 = 0.0812	R_1 = 0.0493
	wR_2 = 0.2142	wR_2 = 0.1447
goodness-of-fit on F^2 [c]	1.684	1.268
large diff peak and hole, e·Å^{-3}	1.677 and -1.395	1.024 and -0.790

[a] $R = (\Sigma||F_o| - |F_c||)\Sigma|F_o|$. [b] $wR_2 = [(\Sigma\omega(|F_o| - |F_c|)^2/\Sigma\omega|F_o|^2]^{1/2}$. [c] GoF = $[(\Sigma\omega(|F_o| - |F_c|)^2/(N_{obs}-N_{param})]^{1/2}$

Computational studies

Table S1. Computed energy parameters of important TSs and intermediates.

system	B3LYP/6-31G*			B3LYP/6-311+G**	
	SCF Energy (Hartree)	G_{corr} (Hartree)	gcp-D3 (Hartree)	SCF Energy (Hartree)	ΔG_{rel} (kcal/mol)
a	-2103.42282	0.31539	0.02361	-2104.00648	0.0
TS_1	-2103.36893	0.31322	0.01880	-2103.95547	27.6
b	-2103.40032	0.30976	0.01642	-2103.98744	3.9
a'	-1531.80810	0.15845	0.04418	-1532.23619	1.0
TS_1'	-1531.74535	0.15650	0.03895	-1532.17447	35.3
b'	-1531.79051	0.15181	0.03895	-1532.22360	1.5
c	-1914.81653	0.30420	0.01167	-1915.33828	-4.1
d	-1678.47102	0.21765	0.04602	-1678.93245	10.9
TS_2	-1678.44232	0.22449	0.03239	-1678.89956	27.3
e	-1678.45594	0.22698	0.03127	-1678.90654	23.8
TS_3	-1678.45150	0.22700	0.02562	-1678.90061	24.0
f	-1678.56273	0.22499	0.03875	-1679.01089	
CO_2	-188.58094	-0.00615	0.00274	-188.64827	
PhI	-335.26038	0.05432	-0.00035	-335.35663	
Phen	-571.61038	0.13629	-0.00857	-571.75997	

Table S2. Cartesian coordinates (Å) of optimized geometries of the stationary points and transition states.

a

Number of imaginary frequencies : 0

Electronic energy= -2103.42282136 (hartree/particle)

Coordinates

At No.	x	y	z
7	-2.550966000	-1.483784000	0.170135000
7	-2.049163000	1.134931000	-0.459384000
6	-2.779057000	-2.750190000	0.481432000
6	-4.042044000	-3.237574000	0.872663000
6	-5.101217000	-2.353098000	0.930303000
6	-5.944448000	-0.018048000	0.629778000
6	-5.698029000	1.279480000	0.296643000
6	-4.097263000	3.048753000	-0.441714000
6	-2.810071000	3.391230000	-0.802881000
6	-1.808486000	2.402675000	-0.798774000
6	-3.577606000	-0.606664000	0.227873000
6	-4.894046000	-0.994961000	0.602305000
6	-4.383688000	1.712378000	-0.085815000
6	-3.313751000	0.778357000	-0.115002000
1	-1.922538000	-3.418691000	0.417734000
1	-4.168760000	-4.287459000	1.118417000
1	-6.093779000	-2.686696000	1.223418000
1	-6.942985000	-0.335732000	0.919140000
1	-6.497867000	2.015478000	0.314883000
1	-4.894053000	3.788491000	-0.429034000
1	-2.554198000	4.406884000	-1.087171000
1	-0.780193000	2.615474000	-1.076586000
29	-0.422531000	-0.212767000	-0.396383000
7	0.504645000	-2.023653000	-1.178199000
7	0.895295000	-0.775727000	1.217642000
6	0.329123000	-2.595331000	-2.362941000
6	1.187366000	-3.585480000	-2.875627000
6	2.264021000	-3.991117000	-2.111833000
6	3.581082000	-3.760644000	0.001337000
6	3.764939000	-3.151726000	1.205268000
6	3.040340000	-1.450192000	2.887066000
6	2.151527000	-0.456410000	3.244825000
6	1.091667000	-0.149791000	2.372447000
6	1.567113000	-2.401369000	-0.426336000

6	2.482536000	-3.399549000	-0.848888000
6	2.869892000	-2.125535000	1.659382000
6	1.768738000	-1.746512000	0.849316000
1	-0.529498000	-2.255090000	-2.936048000
1	0.995384000	-4.013553000	-3.854434000
1	2.950073000	-4.753831000	-2.471715000
1	4.271412000	-4.527099000	-0.341393000
1	4.604203000	-3.423903000	1.840028000
1	3.876441000	-1.711724000	3.530756000
1	2.261139000	0.093177000	4.174103000
1	0.385361000	0.638203000	2.617338000
6	2.503428000	2.769567000	-0.855639000
6	2.364309000	3.101104000	0.642064000
9	3.805464000	2.986485000	-1.183219000
9	1.746918000	3.700204000	-1.519178000
6	2.051453000	1.306108000	-1.187551000
8	2.927151000	0.440386000	-1.138469000
8	0.804258000	1.222406000	-1.411319000
9	1.081061000	2.965257000	1.047446000
9	3.118443000	2.278875000	1.391383000
9	2.741041000	4.365718000	0.901837000

……

TS_1

Number of imaginary frequencies : 1

Electronic energy= -2103.36893469 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	1.453171000	-1.354017000	-1.181162000
7	2.142489000	0.232808000	0.931434000
6	1.104263000	-2.121656000	-2.202918000
6	2.020522000	-2.910292000	-2.925614000
6	3.351116000	-2.884155000	-2.557257000
6	5.121639000	-1.982923000	-1.036911000
6	5.467837000	-1.174804000	0.003722000
6	4.805522000	0.459782000	1.775665000
6	3.803200000	1.182308000	2.388658000
6	2.477465000	1.041581000	1.933678000
6	2.753389000	-1.320616000	-0.808353000
6	3.758008000	-2.074439000	-1.473799000
6	4.482568000	-0.396323000	0.699317000
6	3.120389000	-0.470739000	0.306963000

1	0.049662000	-2.111428000	-2.468189000
1	1.676190000	-3.518938000	-3.755935000
1	4.091461000	-3.474771000	-3.091327000
1	5.875017000	-2.567206000	-1.558944000
1	6.503610000	-1.102953000	0.325753000
1	5.839351000	0.543029000	2.101979000
1	4.015686000	1.858109000	3.210802000
1	1.663699000	1.603511000	2.377568000
29	0.127659000	0.035923000	0.162156000
7	-1.084230000	-1.321155000	1.394823000
7	-1.722852000	-0.290689000	-1.046137000
6	-0.764599000	-1.815286000	2.584614000
6	-1.604271000	-2.681088000	3.309295000
6	-2.824556000	-3.032493000	2.766174000
6	-4.458902000	-2.814752000	0.883765000
6	-4.792348000	-2.269733000	-0.319567000
6	-4.200122000	-0.787503000	-2.249087000
6	-3.282410000	0.057628000	-2.839876000
6	-2.048196000	0.281036000	-2.198237000
6	-2.278775000	-1.658882000	0.849076000
6	-3.199223000	-2.518088000	1.505417000
6	-3.890887000	-1.391442000	-1.009823000
6	-2.624978000	-1.097287000	-0.440423000
1	0.196210000	-1.506471000	2.988135000
1	-1.289835000	-3.051801000	4.279678000
1	-3.504537000	-3.693045000	3.298380000
1	-5.149144000	-3.475540000	1.401775000
1	-5.754135000	-2.488201000	-0.776621000
1	-5.161538000	-0.986186000	-2.716318000
1	-3.495830000	0.552228000	-3.782083000
1	-1.308666000	0.956430000	-2.614122000
6	0.004671000	2.524318000	-0.213092000
6	-0.835459000	3.707220000	-0.689674000
9	0.464542000	1.974952000	-1.457421000
9	1.138520000	3.104336000	0.340880000
6	-1.276613000	1.894285000	1.648831000
8	-2.380522000	1.740131000	1.232812000
8	-0.469917000	2.000895000	2.524582000
9	-0.163452000	4.559692000	-1.502728000
9	-1.914686000	3.276345000	-1.383870000
9	-1.280631000	4.434753000	0.356675000

…….

b

Number of imaginary frequencies : 0
Electronic energy= -2103.40032434 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	1.383965000	-1.726549000	0.345311000
7	2.051995000	0.793329000	1.250047000
6	1.069160000	-2.951975000	-0.063945000
6	2.019903000	-3.954848000	-0.317876000
6	3.357503000	-3.653298000	-0.153829000
6	5.104255000	-1.973363000	0.425978000
6	5.435754000	-0.707403000	0.799314000
6	4.733010000	1.596296000	1.441868000
6	3.709640000	2.490380000	1.683543000
6	2.381502000	2.036247000	1.577464000
6	2.694840000	-1.419626000	0.527780000
6	3.731062000	-2.360163000	0.270142000
6	4.421858000	0.270731000	1.070261000
6	3.046816000	-0.081304000	0.966913000
1	0.009150000	-3.144323000	-0.209016000
1	1.696623000	-4.938203000	-0.644873000
1	4.128385000	-4.393639000	-0.353107000
1	5.875800000	-2.711189000	0.220835000
1	6.478007000	-0.413551000	0.895985000
1	5.774429000	1.897703000	1.524980000
1	3.910656000	3.521245000	1.958232000
1	1.553788000	2.716336000	1.765288000
29	-0.003781000	-0.047386000	-0.134140000
7	-1.330757000	0.015647000	1.508706000
7	-1.999167000	-1.107598000	-0.878541000
6	-0.980414000	0.476324000	2.709469000
6	-1.868731000	0.550441000	3.795202000
6	-3.178317000	0.142557000	3.620291000
6	-4.929957000	-0.778192000	2.091006000
6	-5.290198000	-1.228165000	0.856325000
6	-4.638936000	-1.803358000	-1.495467000
6	-3.642487000	-1.881288000	-2.450743000
6	-2.327400000	-1.523764000	-2.094975000
6	-2.605483000	-0.431861000	1.337403000
6	-3.582898000	-0.361734000	2.366226000
6	-4.324853000	-1.335586000	-0.200569000
6	-2.974223000	-0.973228000	0.047974000
1	0.051650000	0.799015000	2.799793000

1	-1.521552000	0.939844000	4.747002000
1	-3.899040000	0.206022000	4.431695000
1	-5.664031000	-0.710114000	2.889792000
1	-6.317306000	-1.521335000	0.653979000
1	-5.661494000	-2.090584000	-1.728099000
1	-3.855173000	-2.223927000	-3.458632000
1	-1.511519000	-1.564466000	-2.810867000
6	0.721727000	0.597138000	-1.875265000
6	0.106971000	1.785250000	-2.602788000
9	0.596033000	-0.458217000	-2.820005000
9	2.094440000	0.873522000	-1.861975000
6	-1.631571000	3.229852000	0.354415000
8	-2.547655000	2.887425000	-0.284081000
8	-0.746507000	3.598784000	1.026599000
9	0.681465000	2.070317000	-3.793236000
9	-1.208058000	1.575977000	-2.838566000
9	0.205135000	2.911236000	-1.844936000

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a'

Number of imaginary frequencies : 0

Electronic energy= -1531.80809718 (hartree/particle)

…….

Coordinates

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At No.	x	y	z
7	1.312716000	1.079069000	0.129510000
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6	0.853497000	2.322588000	0.196036000
6	1.714177000	3.439947000	0.139914000
6	3.074936000	3.240296000	0.012640000
6	4.979671000	1.609850000	-0.189154000
6	5.408189000	0.316523000	-0.250504000
6	4.870722000	-2.133312000	-0.245342000
6	3.909948000	-3.123330000	-0.176976000
6	2.557809000	-2.755507000	-0.050600000
6	2.642053000	0.867595000	0.005732000
6	3.584437000	1.922259000	-0.058779000
6	4.479055000	-0.777105000	-0.187146000
6	3.093968000	-0.504307000	-0.059528000
1	-0.225837000	2.411195000	0.296726000
1	1.297248000	4.440213000	0.197499000
1	3.761089000	4.082330000	-0.032875000
1	5.693215000	2.428150000	-0.237959000
1	6.466409000	0.090244000	-0.348860000

1	5.923839000	-2.383768000	-0.343382000
1	4.177641000	-4.173871000	-0.218891000
1	1.779136000	-3.509997000	0.005405000
6	-3.914301000	-0.332618000	0.530665000
6	-4.693467000	0.190814000	-0.694073000
9	-4.183072000	-1.659547000	0.629817000
9	-4.429900000	0.283848000	1.632785000
29	0.216871000	-0.799137000	0.190824000
6	-2.389380000	-0.043946000	0.437284000
8	-1.662930000	-1.091892000	0.343521000
8	-2.060584000	1.144001000	0.457325000
9	-5.966328000	-0.241966000	-0.664912000
9	-4.707893000	1.527995000	-0.735183000
9	-4.121922000	-0.266179000	-1.826285000

……

TS_1'

Number of imaginary frequencies : 1

Electronic energy= -1531.74534814 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	1.212206000	-1.360956000	-0.035848000
7	0.892296000	1.336739000	-0.245428000
6	1.335398000	-2.679558000	0.062031000
6	2.583092000	-3.306927000	0.249009000
6	3.720237000	-2.527988000	0.335900000
6	4.742064000	-0.235456000	0.313745000
6	4.583265000	1.114604000	0.210558000
6	3.066576000	3.088160000	-0.091385000
6	1.783410000	3.566387000	-0.269812000
6	0.716629000	2.650821000	-0.340469000
6	2.318863000	-0.582020000	0.045274000
6	3.615075000	-1.121427000	0.234422000
6	3.284221000	1.695986000	0.018969000
6	2.149237000	0.851537000	-0.065320000
1	0.413055000	-3.249990000	-0.011556000
1	2.633830000	-4.388171000	0.322857000
1	4.697109000	-2.981869000	0.481654000
1	5.729759000	-0.664540000	0.459119000
1	5.442295000	1.777082000	0.272575000
1	3.912247000	3.768408000	-0.032502000
1	1.584092000	4.629414000	-0.354787000
1	-0.306602000	2.987787000	-0.472748000

6	-2.622423000	-0.350041000	0.633862000
6	-3.406216000	0.882695000	0.183272000
9	-3.531000000	-1.205746000	1.177932000
9	-1.843556000	0.098149000	1.727228000
29	-0.523218000	-0.178311000	-0.309797000
6	-2.040042000	-1.640915000	-0.967676000
8	-1.909367000	-0.966681000	-1.979023000
8	-2.090173000	-2.749947000	-0.511921000
9	-4.064643000	1.490300000	1.190610000
9	-2.555662000	1.808720000	-0.345002000
9	-4.298915000	0.559720000	-0.761689000

……

b'

Number of imaginary frequencies : 0

Electronic energy= -1531.79050834 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	1.098681000	1.393079000	0.020952000
7	1.248045000	-1.306049000	-0.092342000
6	1.004549000	2.720087000	0.066101000
6	2.133897000	3.559535000	0.110425000
6	3.393390000	2.993085000	0.108694000
6	4.793560000	0.912298000	0.053449000
6	4.867999000	-0.448350000	0.003510000
6	3.690736000	-2.665733000	-0.103232000
6	2.495083000	-3.355433000	-0.153154000
6	1.285612000	-2.629741000	-0.147043000
6	2.332585000	0.823367000	0.014192000
6	3.525391000	1.586975000	0.059382000
6	3.679759000	-1.252755000	-0.046949000
6	2.411593000	-0.619787000	-0.042681000
1	-0.001641000	3.127088000	0.066111000
1	1.999503000	4.635514000	0.146187000
1	4.284941000	3.613972000	0.144113000
1	5.698565000	1.512745000	0.090116000
1	5.833695000	-0.946896000	0.000181000
1	4.640551000	-3.194563000	-0.107352000
1	2.472628000	-4.439500000	-0.197759000
1	0.323097000	-3.131953000	-0.189983000
6	-2.398359000	-0.373147000	0.020634000
6	-2.673501000	-1.870730000	0.127516000
9	-3.130341000	0.188621000	1.079333000

9	-3.093747000	0.028443000	-1.130992000
29	-0.516906000	0.127510000	-0.006405000
6	-3.641470000	2.713309000	-0.159255000
8	-4.782144000	2.470978000	-0.181775000
8	-2.510633000	3.021392000	-0.141690000
9	-3.976650000	-2.206986000	0.105988000
9	-2.071364000	-2.531736000	-0.898703000
9	-2.144662000	-2.365035000	1.272378000

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c

Number of imaginary frequencies : 0

Electronic energy= -1914.81652937 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	-1.110841000	-1.420158000	0.929564000
7	-1.959293000	-0.283072000	-1.434807000
6	-0.705824000	-2.017201000	2.047319000
6	-1.579826000	-2.622160000	2.965648000
6	-2.937269000	-2.580606000	2.711880000
6	-4.803446000	-1.842869000	1.233765000
6	-5.226143000	-1.198376000	0.112174000
6	-4.691086000	0.049456000	-1.979499000
6	-3.733734000	0.568676000	-2.828168000
6	-2.377548000	0.370447000	-2.510523000
6	-2.440937000	-1.395308000	0.652593000
6	-3.405216000	-1.951339000	1.539051000
6	-4.285946000	-0.633245000	-0.812772000
6	-2.889119000	-0.754702000	-0.569984000
1	0.366057000	-2.002600000	2.227756000
1	-1.184521000	-3.098630000	3.857384000
1	-3.651463000	-3.019633000	3.404142000
1	-5.519604000	-2.271904000	1.930065000
1	-6.287286000	-1.100226000	-0.103089000
1	-5.751366000	0.163642000	-2.191603000
1	-4.008040000	1.110743000	-3.727817000
1	-1.601145000	0.760553000	-3.165377000
29	0.132857000	0.175694000	0.026640000
7	1.488637000	-0.805359000	-1.270656000
7	2.171528000	0.029699000	1.226305000
6	1.141507000	-1.292984000	-2.460379000
6	2.063063000	-1.845816000	-3.365332000

6	3.402190000	-1.880390000	-3.022099000
6	5.177538000	-1.355056000	-1.340375000
6	5.530102000	-0.836263000	-0.130726000
6	4.846249000	0.214692000	2.039142000
6	3.824642000	0.676906000	2.847958000
6	2.494860000	0.561131000	2.399204000
6	2.797226000	-0.872706000	-0.903871000
6	3.805589000	-1.382590000	-1.765137000
6	4.536797000	-0.330162000	0.773723000
6	3.166088000	-0.377922000	0.403932000
1	0.083117000	-1.235691000	-2.695472000
1	1.716417000	-2.224073000	-4.321891000
1	4.146556000	-2.282313000	-3.704894000
1	5.934897000	-1.744395000	-2.016000000
1	6.573646000	-0.802272000	0.172181000
1	5.883687000	0.270524000	2.359789000
1	4.030375000	1.113545000	3.820346000
1	1.663250000	0.918747000	2.998856000
6	-0.607709000	1.911279000	0.667412000
6	-0.374238000	3.168002000	-0.160485000
9	-0.103945000	2.250132000	1.942865000
9	-2.000545000	1.875023000	0.849267000
9	-0.895715000	4.296974000	0.374920000
9	0.949999000	3.389536000	-0.331717000
9	-0.921407000	3.032308000	-1.394944000

……

d

Number of imaginary frequencies : 0

Electronic energy= -1678.47101688 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	-3.889155000	0.186265000	-0.098349000
7	-1.552223000	1.554643000	-0.062365000
6	-5.015557000	-0.512424000	-0.114885000
6	-6.287563000	0.094798000	-0.061210000
6	-6.370544000	1.471401000	0.009189000
6	-5.169863000	3.675455000	0.096547000
6	-3.994042000	4.365424000	0.110059000
6	-1.487845000	4.351473000	0.069294000
6	-0.319295000	3.617753000	0.017033000
6	-0.396074000	2.214108000	-0.047710000

6	-3.957467000	1.534596000	-0.028577000
6	-5.184778000	2.241637000	0.026791000
6	-2.731995000	3.681875000	0.056719000
6	-2.709938000	2.266134000	-0.011855000
1	-4.904746000	-1.591162000	-0.174545000
1	-7.179907000	-0.522569000	-0.076687000
1	-7.334870000	1.971434000	0.051044000
1	-6.118661000	4.203806000	0.138199000
1	-3.991909000	5.450786000	0.162281000
1	-1.463935000	5.436968000	0.120462000
1	0.651949000	4.101086000	0.025532000
1	0.502408000	1.605630000	-0.086495000
6	4.439549000	-0.126427000	0.079955000
6	5.030712000	0.056297000	-1.173879000
6	5.052650000	0.379116000	1.230376000
6	6.233558000	0.749989000	-1.279237000
1	4.558296000	-0.340204000	-2.066132000
6	6.255389000	1.073313000	1.127793000
1	4.597913000	0.232639000	2.204191000
6	6.853161000	1.265545000	-0.128767000
1	6.696369000	0.894468000	-2.250301000
1	6.735271000	1.467578000	2.017918000
29	-1.708427000	-0.490784000	-0.148837000
53	2.591998000	-1.175855000	0.235843000
6	-1.124058000	-2.349699000	-0.237186000
9	-0.076549000	-2.675893000	0.649954000
6	-2.201338000	-3.382863000	0.088763000
9	-0.651480000	-2.727006000	-1.493910000
9	-2.676921000	-3.196817000	1.341015000
9	-3.258031000	-3.239035000	-0.760229000
9	-1.793423000	-4.661803000	-0.005280000
6	8.087332000	1.986863000	-0.236356000
7	9.086522000	2.576434000	-0.323568000

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TS_2

Number of imaginary frequencies : 1

Electronic energy= -1678.44232142 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
7	-0.982138000	1.760967000	0.372216000
7	-2.004436000	-0.769874000	0.399465000
6	-0.477705000	2.985348000	0.288871000

6	-1.271801000	4.142015000	0.176758000
6	-2.645294000	4.006056000	0.154780000
6	-4.633470000	2.488721000	0.198312000
6	-5.142543000	1.226617000	0.254745000
6	-4.758095000	-1.242982000	0.370723000
6	-3.861419000	-2.291667000	0.428072000
6	-2.484547000	-2.007330000	0.433948000
6	-2.328687000	1.612545000	0.320050000
6	-3.216449000	2.716501000	0.224287000
6	-4.277086000	0.084025000	0.329311000
6	-2.870700000	0.271833000	0.354555000
1	0.606145000	3.058587000	0.310962000
1	-0.798622000	5.116441000	0.113248000
1	-3.292906000	4.875696000	0.078451000
1	-5.294661000	3.348467000	0.130543000
1	-6.216498000	1.062253000	0.234589000
1	-5.829694000	-1.424156000	0.353948000
1	-4.197961000	-3.322604000	0.459543000
1	-1.749341000	-2.805475000	0.463989000
6	2.089599000	-0.076734000	0.604890000
6	2.291718000	1.147220000	1.264505000
6	3.029846000	-0.550651000	-0.322715000
6	3.379834000	1.943856000	0.916748000
1	1.611821000	1.469962000	2.044871000
6	4.115621000	0.245295000	-0.658233000
1	2.887147000	-1.506625000	-0.808943000
6	4.300404000	1.501901000	-0.047757000
1	3.534946000	2.897445000	1.412675000
1	4.826125000	-0.098399000	-1.403365000
29	0.055630000	-0.270683000	0.077975000
53	1.141997000	-1.720456000	2.119755000
6	0.177032000	-0.326828000	-1.955193000
9	1.262520000	0.324531000	-2.512205000
6	0.143521000	-1.700092000	-2.621448000
9	-0.953428000	0.330216000	-2.445696000
9	1.222465000	-2.435478000	-2.255942000
9	-0.956723000	-2.387783000	-2.233149000
9	0.131849000	-1.652324000	-3.967676000
6	5.427487000	2.315010000	-0.388479000
7	6.342378000	2.981187000	-0.661277000

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e

Number of imaginary frequencies : 0

Electronic energy= -1678.45594074 (hartree/particle)

Coordinates

At No.	x	y	z
7	0.743714000	1.500344000	-0.307916000
7	1.677883000	-0.605632000	1.134463000
6	0.274819000	2.511093000	-1.032098000
6	0.954365000	3.734171000	-1.152228000
6	2.159980000	3.898626000	-0.498509000
6	3.933133000	2.923095000	0.975367000
6	4.407781000	1.866900000	1.693485000
6	4.125476000	-0.492674000	2.489465000
6	3.357936000	-1.640186000	2.504497000
6	2.134640000	-1.653626000	1.808187000
6	1.926989000	1.641745000	0.342717000
6	2.683128000	2.839792000	0.274477000
6	3.671695000	0.637262000	1.773649000
6	2.426208000	0.524015000	1.105019000
1	-0.669355000	2.342187000	-1.538353000
1	0.526629000	4.525288000	-1.758471000
1	2.713786000	4.830530000	-0.575034000
1	4.498534000	3.848782000	0.914209000
1	5.358502000	1.936678000	2.214875000
1	5.075703000	-0.448265000	3.015210000
1	3.680428000	-2.527779000	3.038626000
1	1.512777000	-2.541004000	1.792662000
6	-1.064524000	-2.098367000	0.055948000
9	-1.931138000	-2.418932000	-0.920049000
9	-0.010353000	-2.965321000	0.008690000
6	-1.744801000	-2.382906000	1.417483000
29	-0.119487000	-0.367961000	-0.224197000
53	1.029848000	-1.005554000	-2.634589000
6	-1.886319000	0.373582000	0.199826000
6	-2.128597000	1.031725000	1.404500000
6	-2.769674000	0.468816000	-0.872527000
6	-3.263142000	1.833109000	1.527393000
6	-3.904700000	1.274988000	-0.754300000
6	-4.152911000	1.961941000	0.445676000
1	-1.451313000	0.929732000	2.246979000
1	-2.584874000	-0.075658000	-1.794380000
1	-3.465078000	2.361235000	2.454484000
1	-4.601631000	1.366449000	-1.581829000
9	-2.993189000	-1.910976000	1.463627000
9	-1.794948000	-3.706966000	1.639862000

9	-1.032744000	-1.825923000	2.421676000
6	-5.314257000	2.794081000	0.571297000
7	-6.252018000	3.474866000	0.674273000

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TS_3

Number of imaginary frequencies : 1

Electronic energy= -1678.45149746 (hartree/particle)

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Coordinates

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At No.	x	y	z
7	-1.011058000	-0.014700000	1.572120000
7	-1.797185000	0.072053000	-1.043086000
6	-0.621359000	-0.132074000	2.834196000
6	-1.518708000	-0.244981000	3.912821000
6	-2.873841000	-0.240862000	3.652059000
6	-4.714085000	-0.168656000	1.960856000
6	-5.103331000	-0.115895000	0.656861000
6	-4.494964000	-0.016951000	-1.765531000
6	-3.507194000	0.037481000	-2.727968000
6	-2.163046000	0.077625000	-2.320088000
6	-2.338750000	-0.038388000	1.300631000
6	-3.324162000	-0.145601000	2.316908000
6	-4.135999000	-0.037578000	-0.400320000
6	-2.753733000	0.009840000	-0.083604000
1	0.450781000	-0.146803000	3.007090000
1	-1.137104000	-0.334458000	4.924555000
1	-3.599188000	-0.322676000	4.457386000
1	-5.451565000	-0.240455000	2.755632000
1	-6.156862000	-0.143857000	0.392575000
1	-5.545076000	-0.052792000	-2.043422000
1	-3.746885000	0.045202000	-3.785873000
1	-1.361519000	0.110017000	-3.049269000
6	0.953877000	1.878127000	-1.073984000
9	2.163095000	2.441826000	-1.312256000
9	0.371027000	1.727215000	-2.304968000
29	0.195968000	-0.048594000	-0.397820000
53	0.280371000	-2.702599000	-0.780058000
6	2.101110000	0.267931000	-0.106019000
6	2.497392000	0.653967000	1.175169000
6	3.020622000	-0.269947000	-1.013343000
6	3.804571000	0.402773000	1.593957000
6	4.323261000	-0.513022000	-0.597790000
6	4.723060000	-0.186060000	0.712930000

1	1.809484000	1.153981000	1.845240000
1	2.716217000	-0.539882000	-2.017894000
1	4.118526000	0.677794000	2.596077000
1	5.035734000	-0.966151000	-1.279631000
6	6.069249000	-0.429847000	1.138500000
7	7.162897000	-0.622408000	1.486253000
6	0.169866000	2.964780000	-0.299257000
9	-1.121042000	2.643914000	-0.129824000
9	0.719632000	3.154087000	0.912790000
9	0.218300000	4.127007000	-0.969248000

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f

Number of imaginary frequencies : 0

Electronic energy= -1678.56272726 (hartree/particle)

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Coordinates

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At No.	x	y	z
7	2.293909000	0.637002000	1.264984000
7	2.108272000	0.541514000	-1.436493000
6	2.367737000	0.702014000	2.588902000
6	3.317798000	-0.021853000	3.335043000
6	4.214020000	-0.835007000	2.669059000
6	5.050312000	-1.741884000	0.483983000
6	4.955430000	-1.791387000	-0.875039000
6	3.822824000	-1.036936000	-2.982997000
6	2.842311000	-0.265473000	-3.576075000
6	2.000984000	0.514625000	-2.760074000
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6	4.160504000	-0.923924000	1.259638000
6	3.963174000	-1.026424000	-1.576768000
6	3.067769000	-0.209661000	-0.842308000
1	1.646929000	1.351664000	3.077415000
1	3.333576000	0.067424000	4.416282000
1	4.960285000	-1.407120000	3.214262000
1	5.805374000	-2.324482000	1.004887000
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1	4.489002000	-1.650972000	-3.583571000
1	2.711281000	-0.250715000	-4.653068000
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6	-1.263301000	-2.037503000	-0.442167000
9	-1.118138000	-3.276683000	-0.997866000
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29	0.907852000	1.600607000	-0.043941000

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6	-2.717812000	-1.661726000	-0.328854000
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6	-4.435842000	0.027459000	-0.196639000
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7	-7.921917000	-0.363886000	0.142005000
6	-0.516405000	-2.088090000	0.911061000
9	-0.560744000	-0.892612000	1.518852000
9	-1.081055000	-3.001606000	1.715832000
9	0.772666000	-2.422320000	0.728013000

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CO_2

Number of imaginary frequencies : 0

Electronic energy= -188.580935190 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
6	0.000112000	-0.000171000	-0.000121000
8	0.947518000	0.148234000	-0.667088000
8	-0.947602000	-0.148106000	0.667179000

……

PhI

Number of imaginary frequencies : 0

Electronic energy= -335.260375592 (hartree/particle)

……

Coordinates

……

At No.	x	y	z
6	0.048331000	-0.000022000	-0.000235000
6	-0.638028000	-1.215873000	-0.000303000
6	-0.637917000	1.215882000	-0.000273000
6	-2.030880000	-1.214618000	-0.000190000
1	-0.099093000	-2.156651000	-0.000418000
6	-2.030762000	1.214779000	-0.000171000

1	-0.098904000	2.156615000	-0.000498000
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1	-2.575171000	-2.153444000	-0.000127000
1	-2.574925000	2.153681000	-0.000212000
53	2.185740000	-0.000022000	0.000096000
6	-4.169534000	0.000148000	0.000153000
7	-5.332706000	-0.000223000	0.000474000

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Phen

Number of imaginary frequencies : 0

Electronic energy= -571.610381147 (hartree/particle)

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Coordinates

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At No.	x	y	z
7	1.380909000	-1.563576000	-0.000096000
7	-1.380902000	-1.563580000	0.000068000
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6	3.482224000	-0.372873000	0.000055000
6	2.829090000	0.841425000	0.000088000
6	0.680411000	2.101705000	0.000026000
6	-0.680408000	2.101699000	-0.000032000
6	-2.829082000	0.841435000	-0.000037000
6	-3.482221000	-0.372880000	0.000029000
6	-2.703618000	-1.548732000	0.000115000
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6	1.416909000	0.870694000	0.000011000
6	-1.416915000	0.870696000	-0.000052000
6	-0.729345000	-0.377906000	-0.000104000
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1	-3.193534000	-2.522176000	0.000219000

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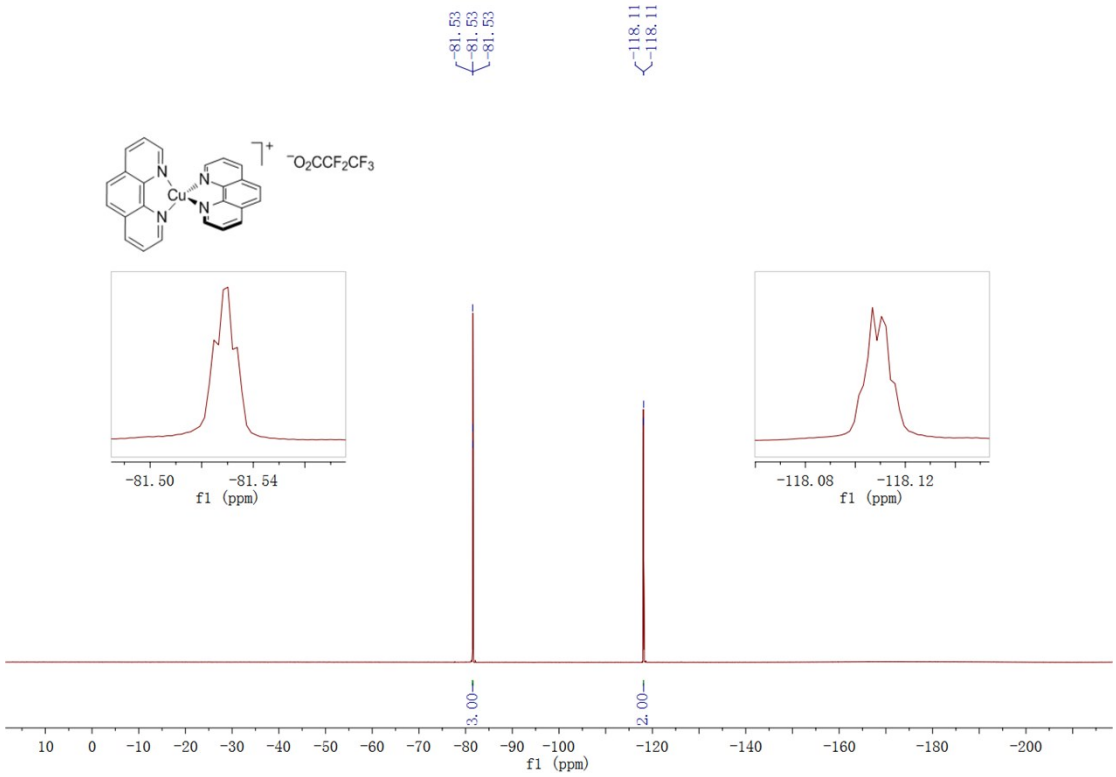
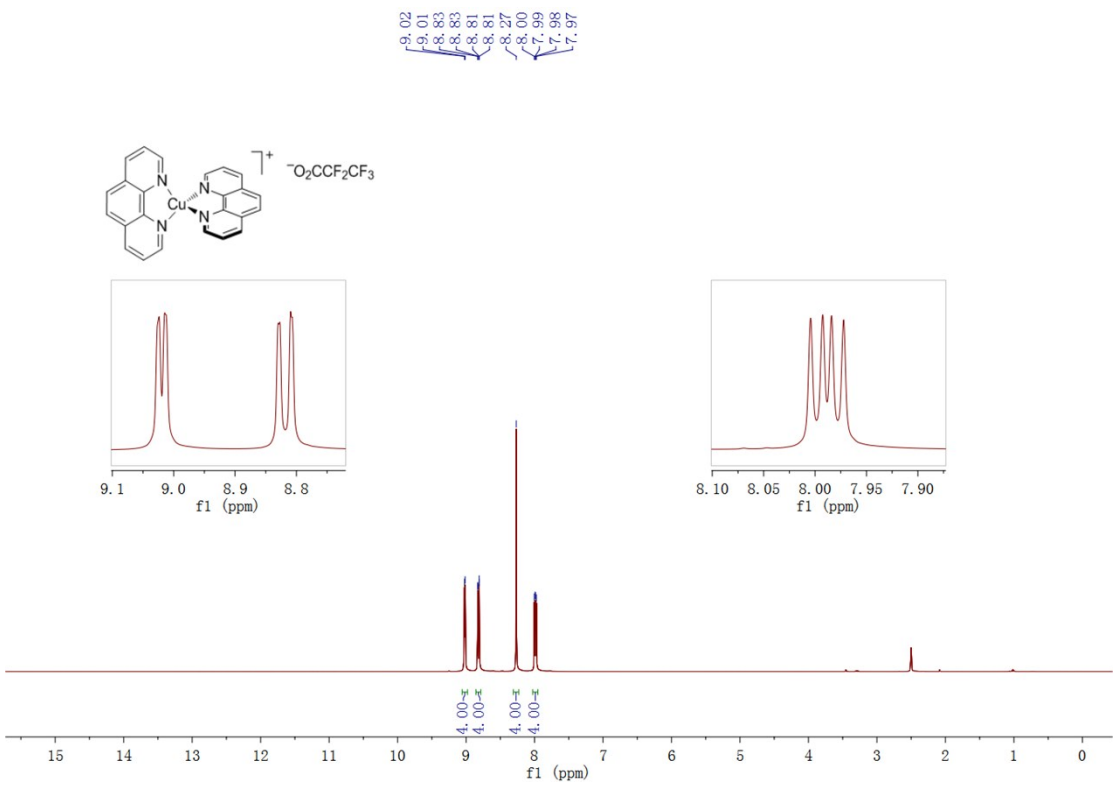
Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra

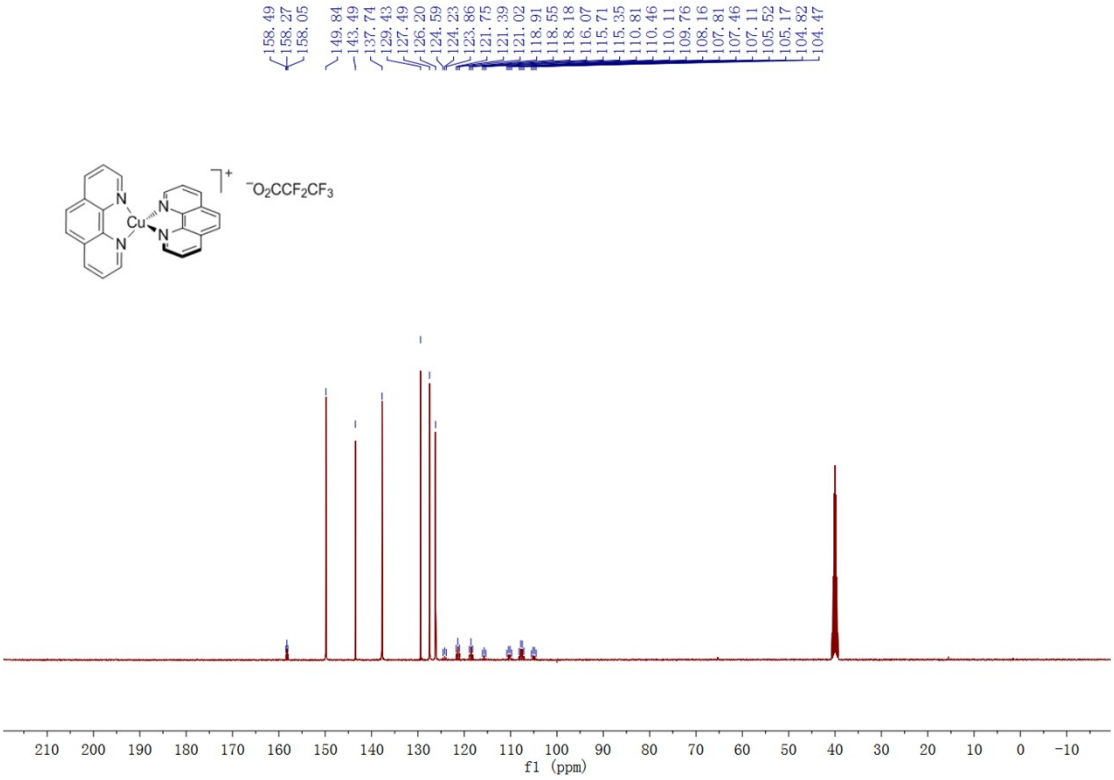
^{19}F NMR spectrum of **1a** in DMSO-d_6



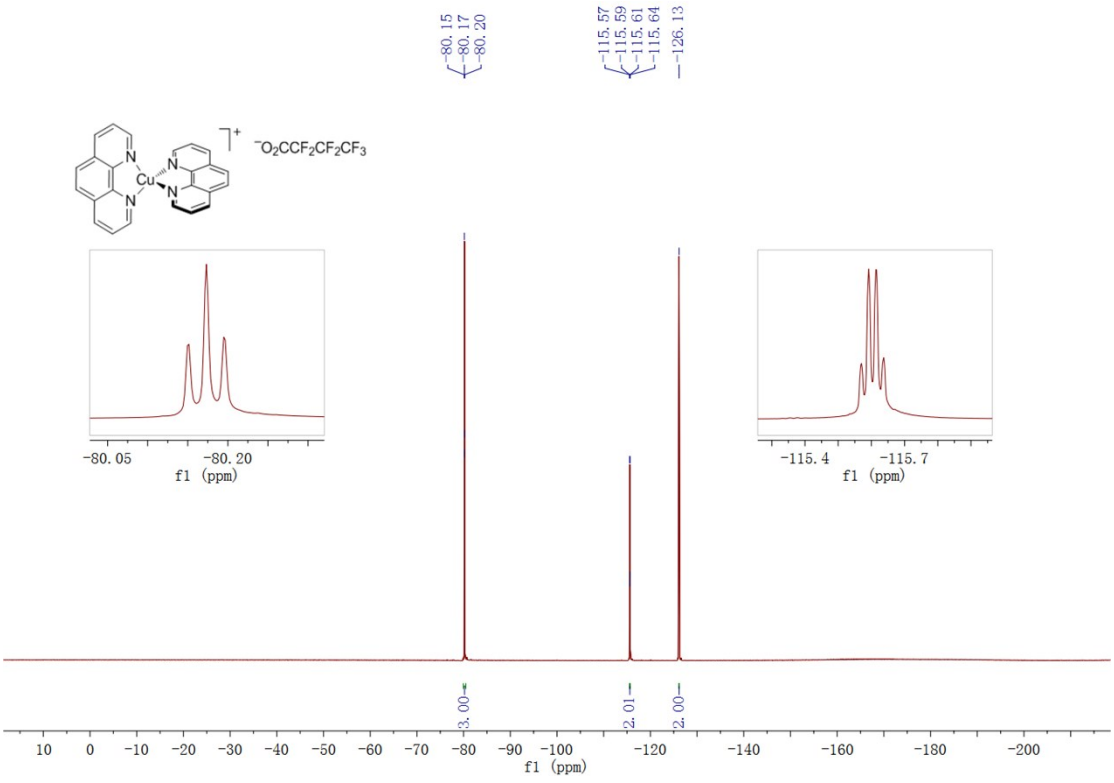
^{1}H NMR spectrum of **1a** in DMSO-d_6



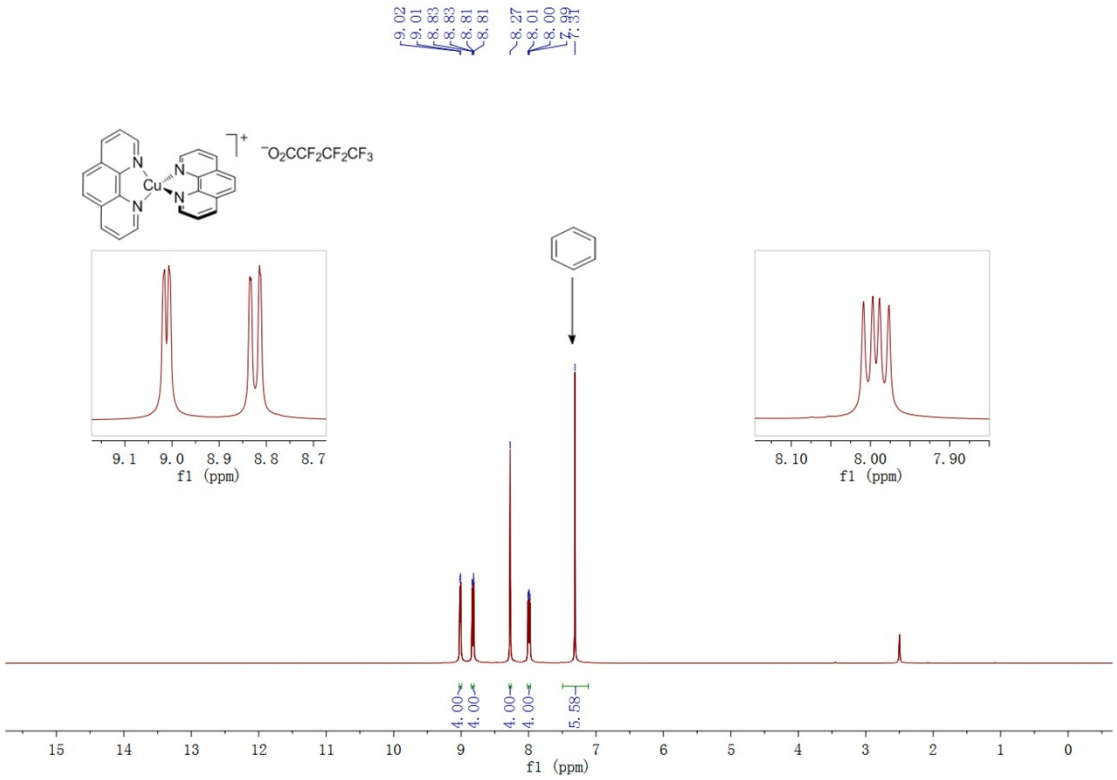
^{13}C NMR spectrum of **1a** in DMSO-d_6



^{19}F NMR spectrum of **1b** in DMSO-d_6



^{1}H NMR spectrum of **1b** in DMSO-d_6



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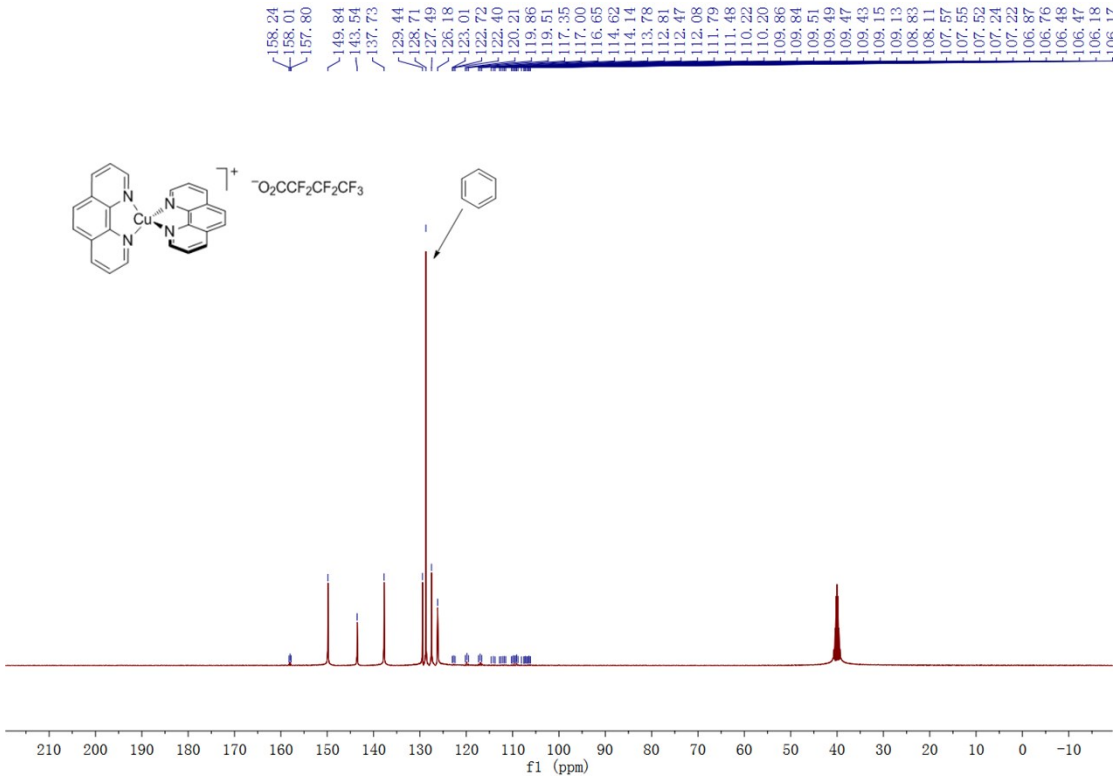

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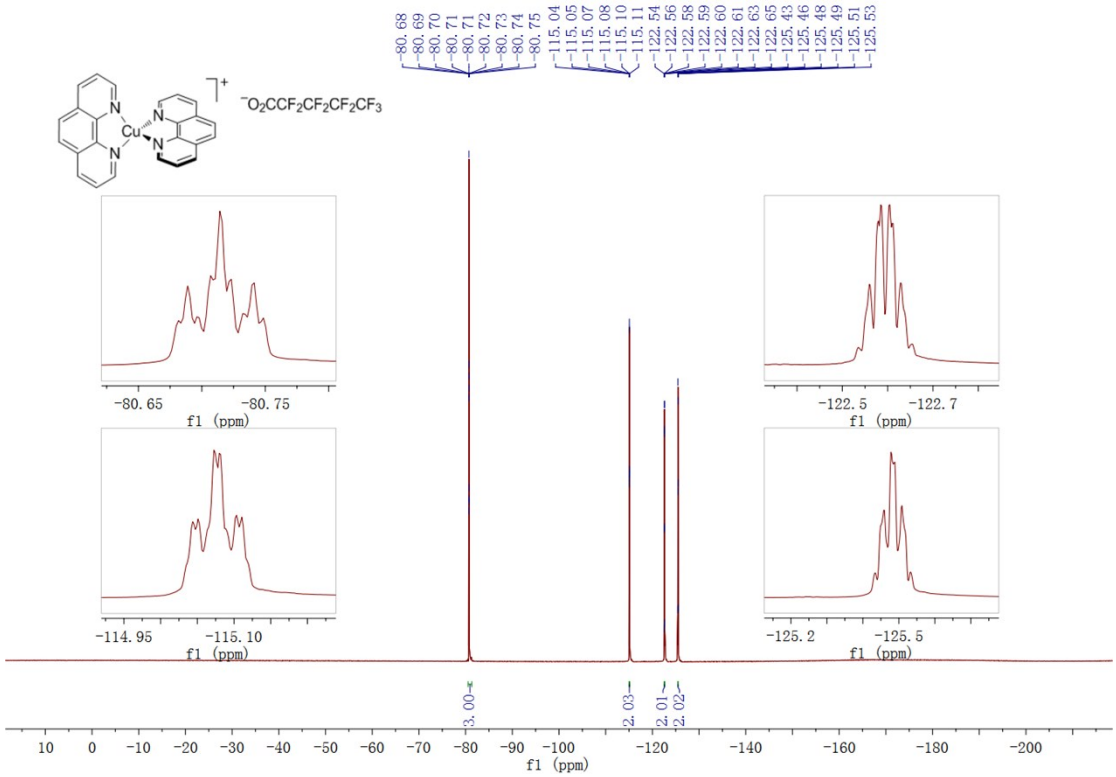

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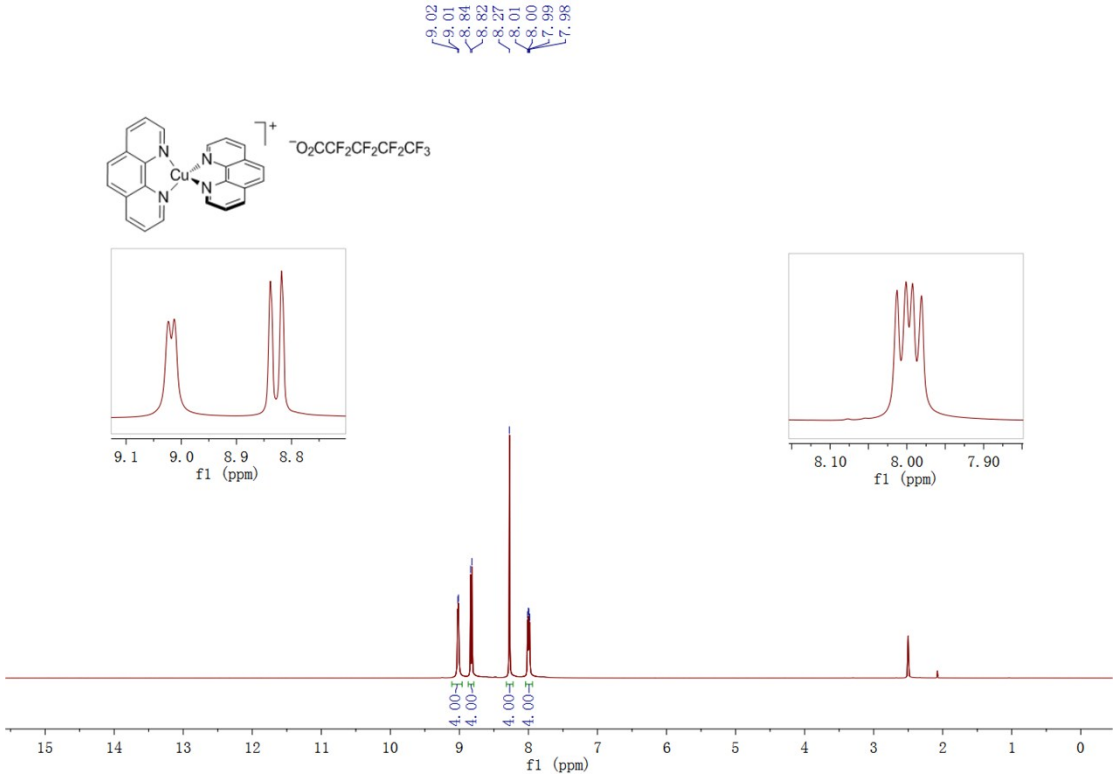
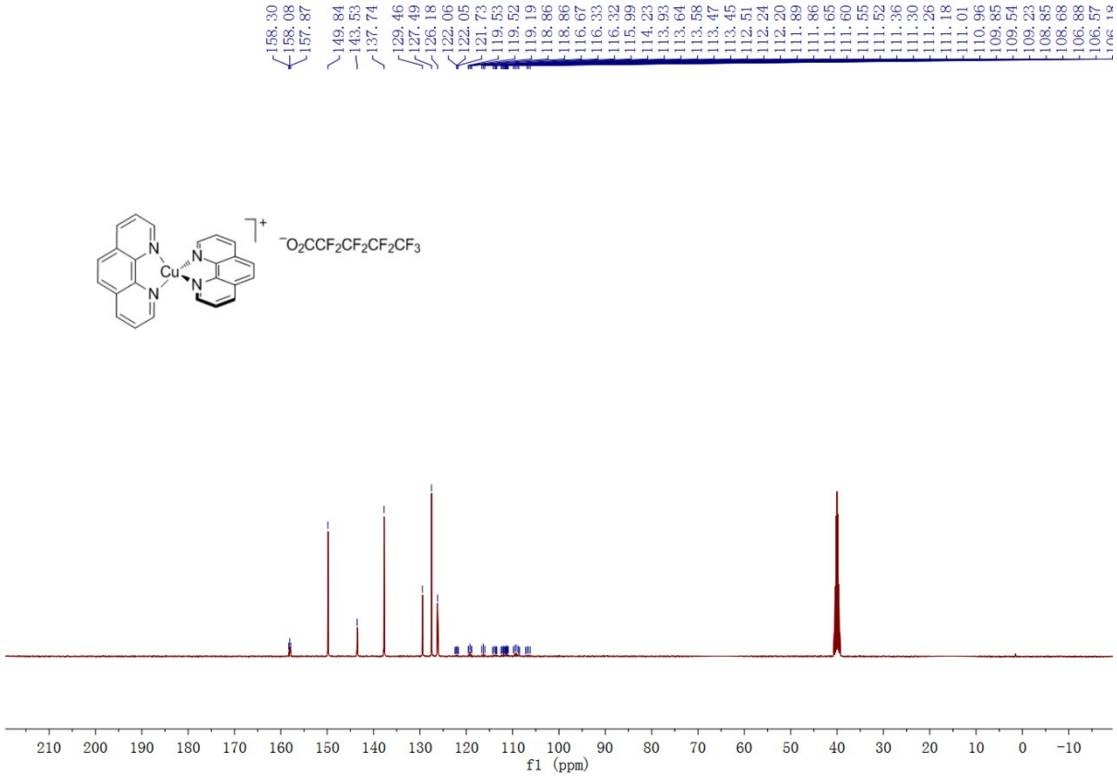


^{13}C NMR spectrum of **1c** in DMSO-d_6



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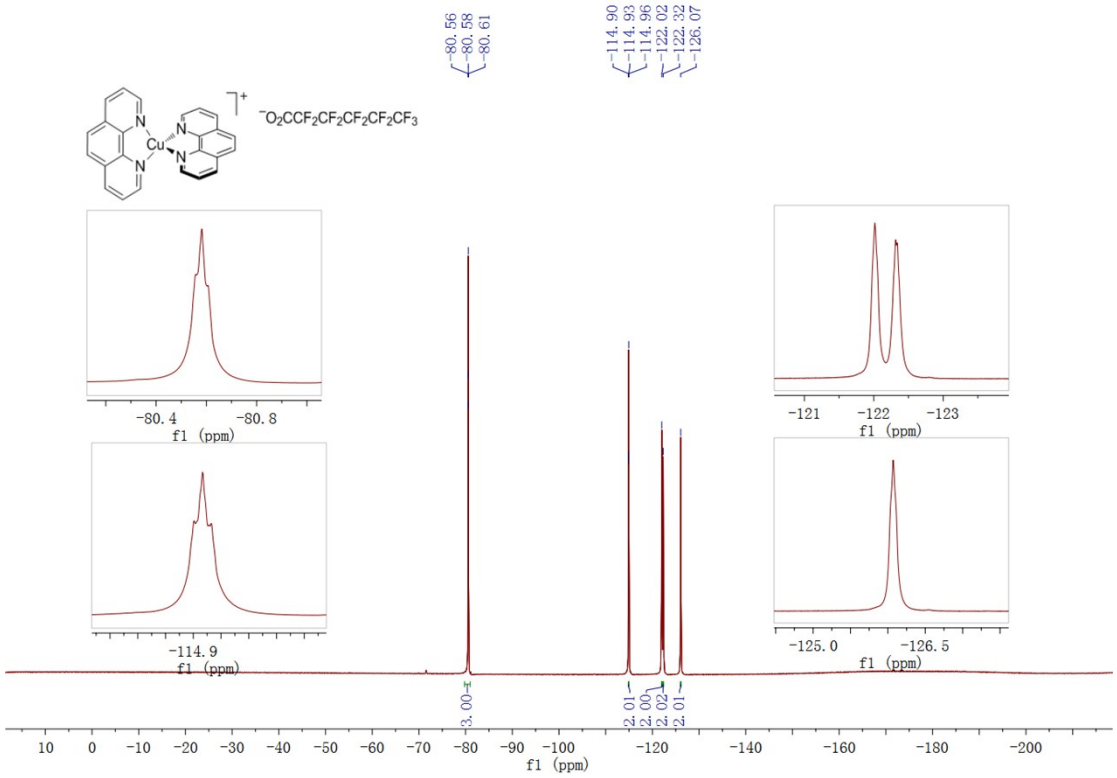

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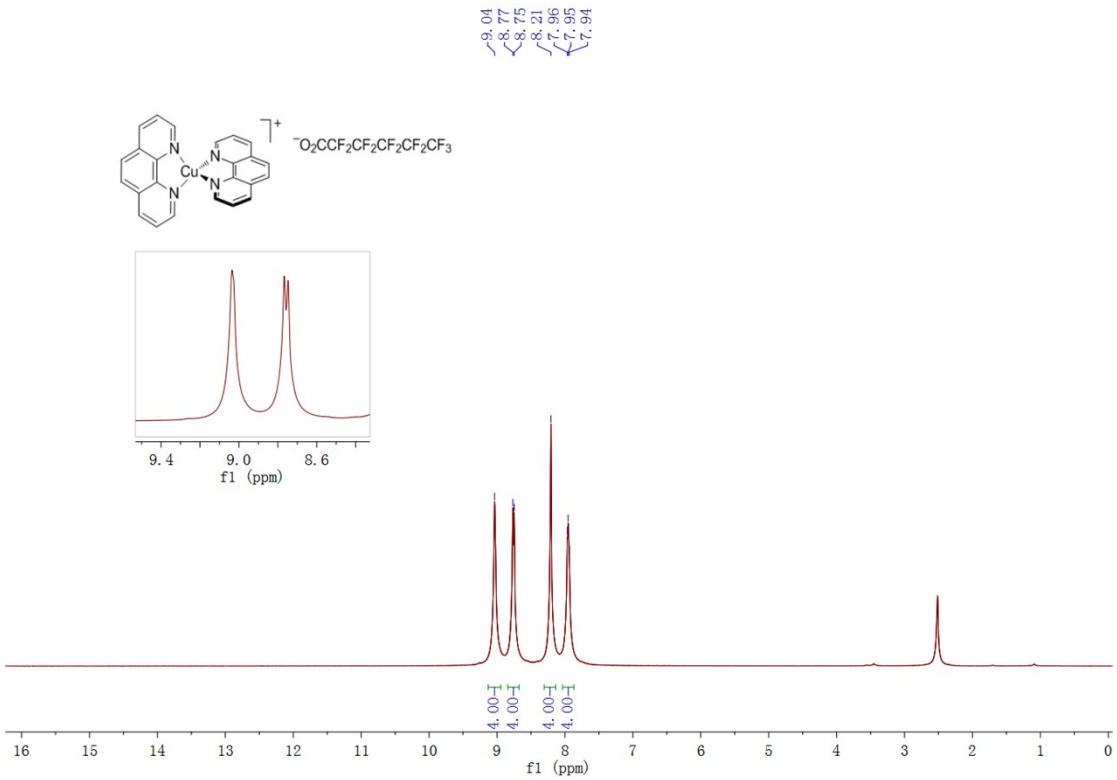
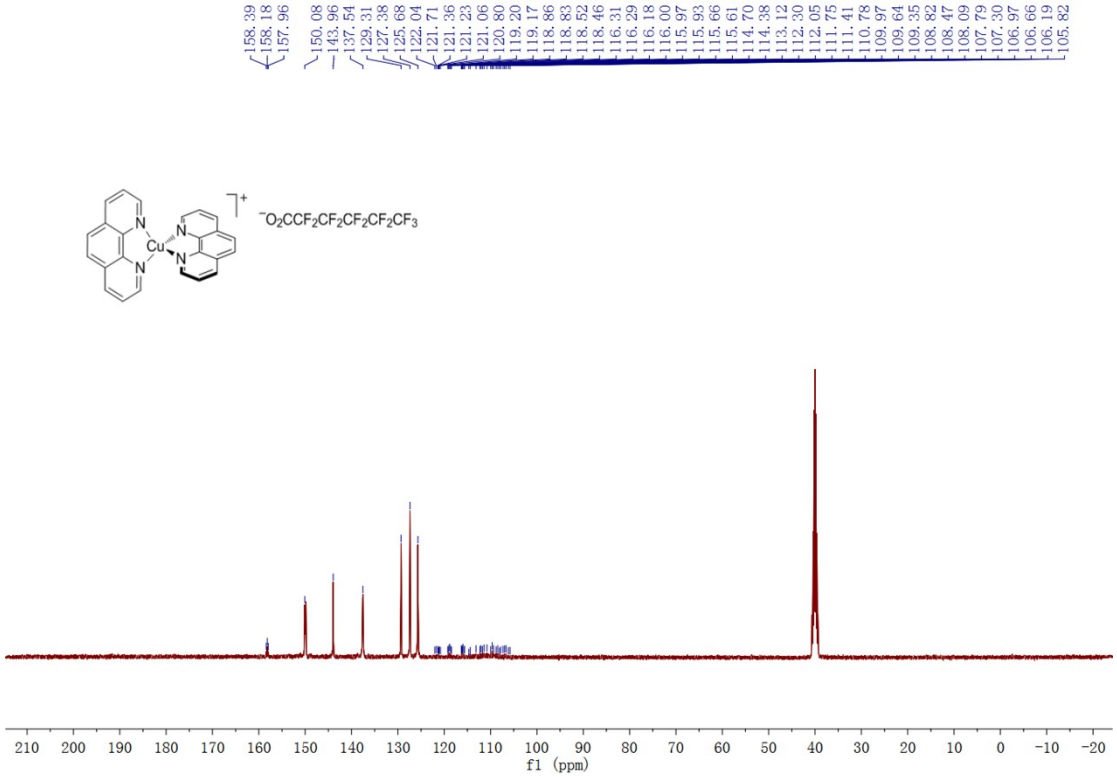
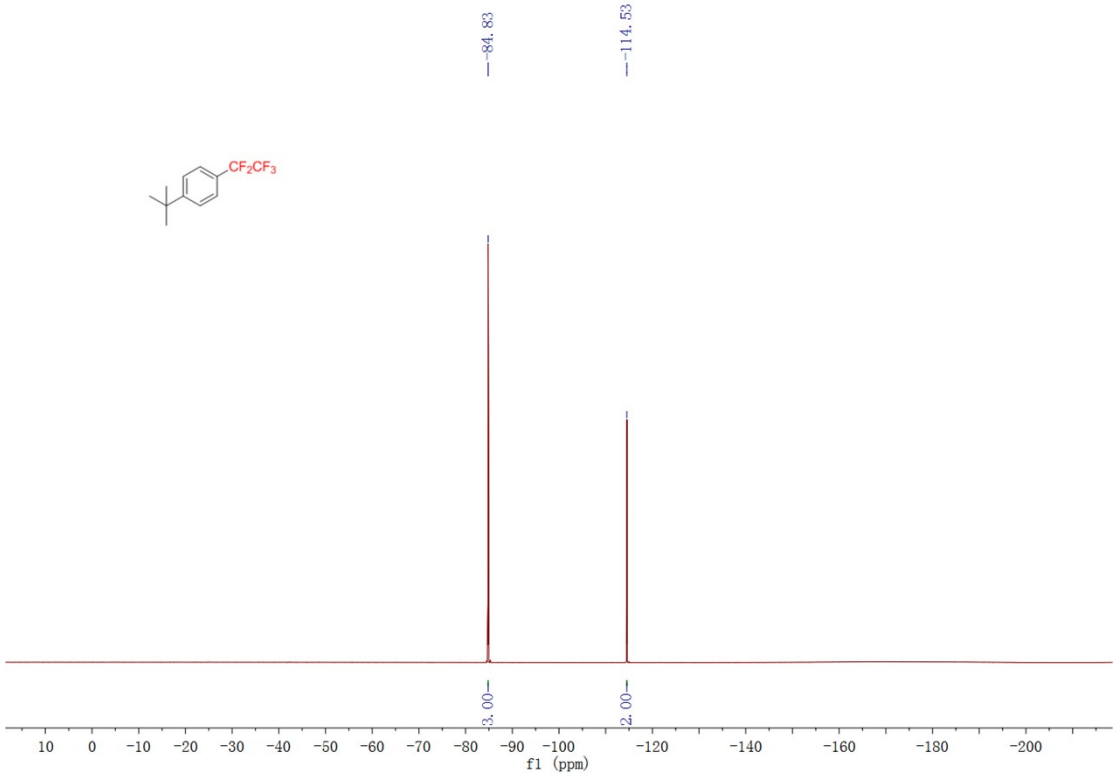


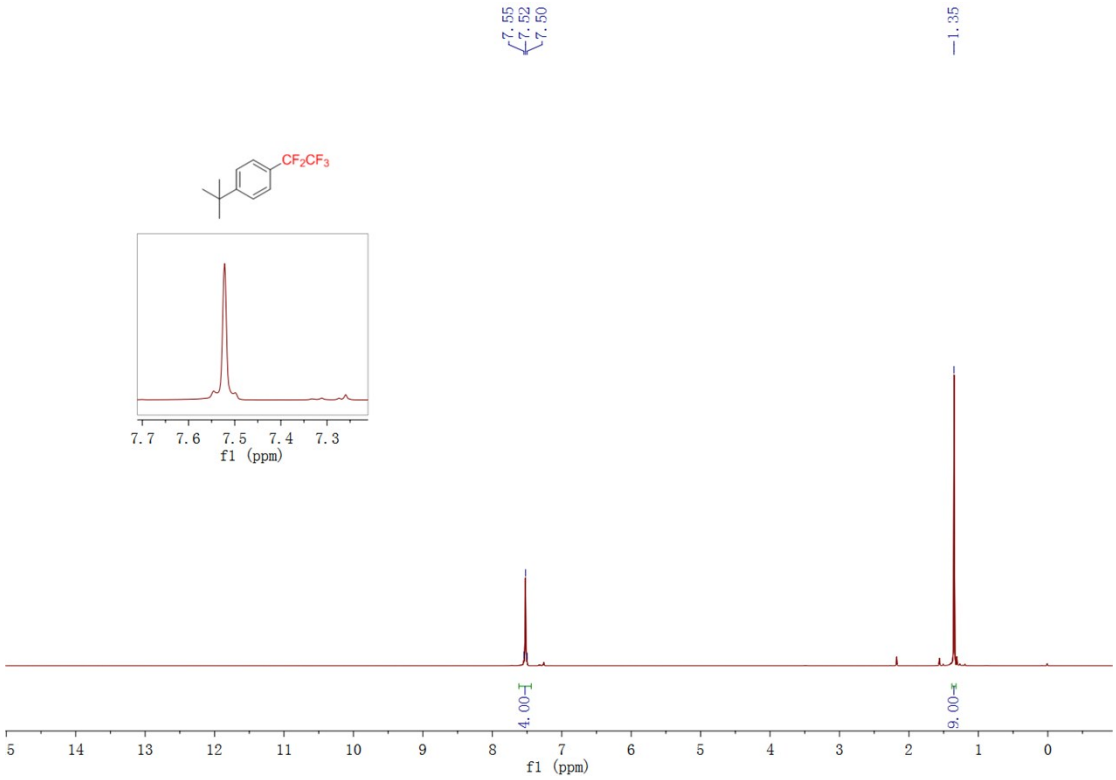
^{13}C NMR spectrum of **1d** in DMSO-d_6



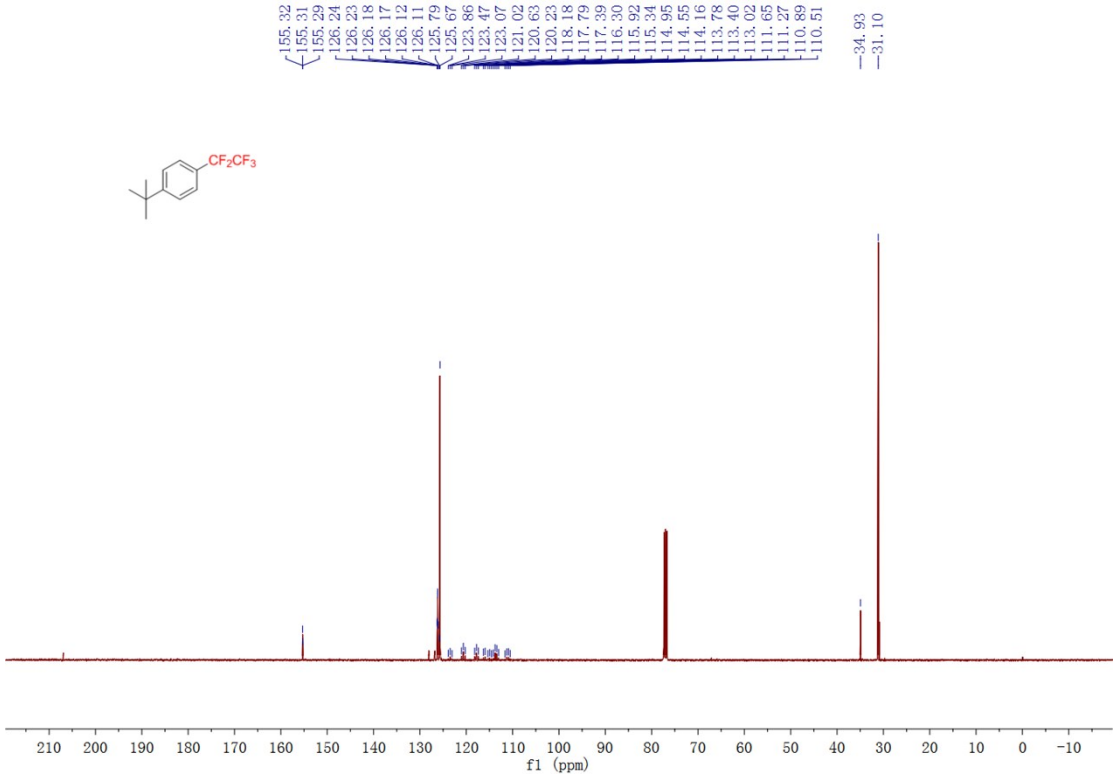
^{19}F NMR spectrum of **3a** in $CDCl_3$



^{1}H NMR spectrum of **3a** in $CDCl_3$



^{13}C NMR spectrum of **3a** in $CDCl_3$



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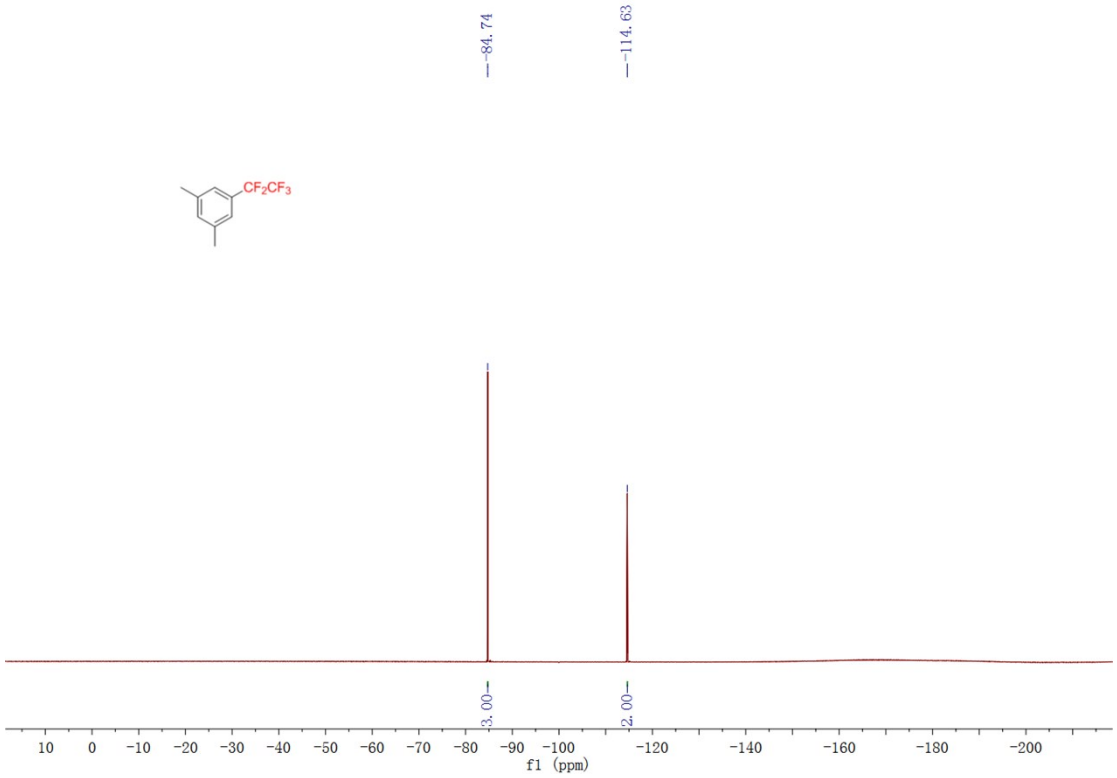

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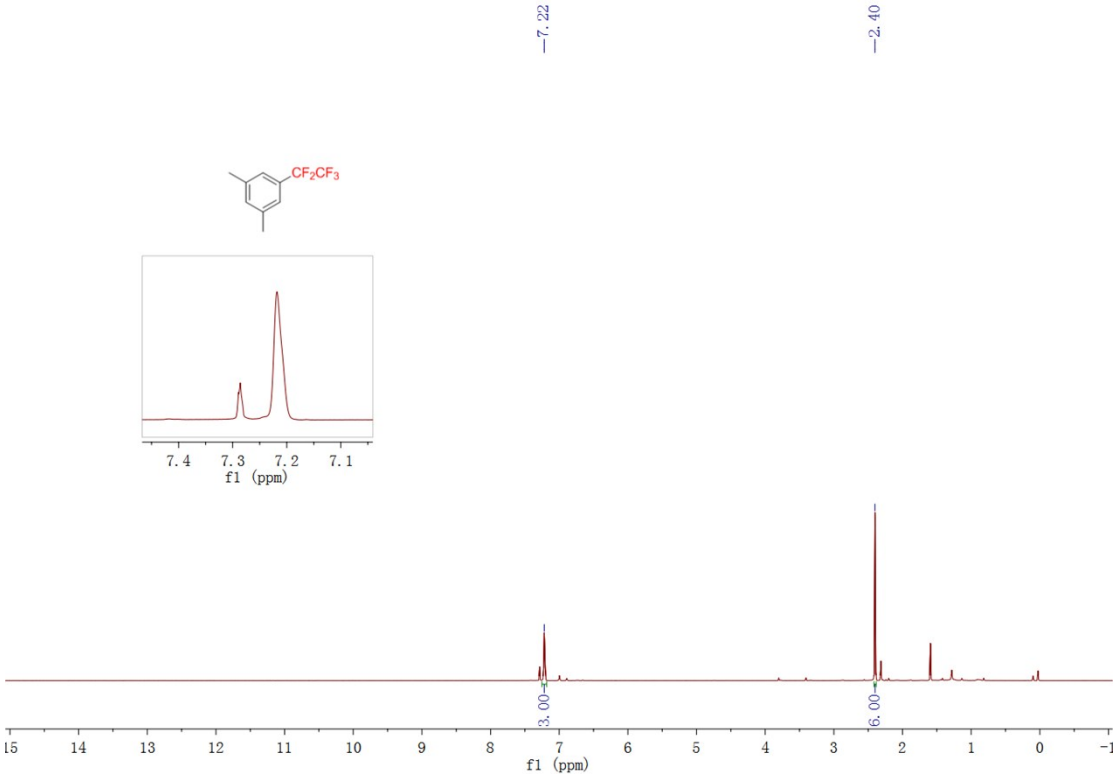

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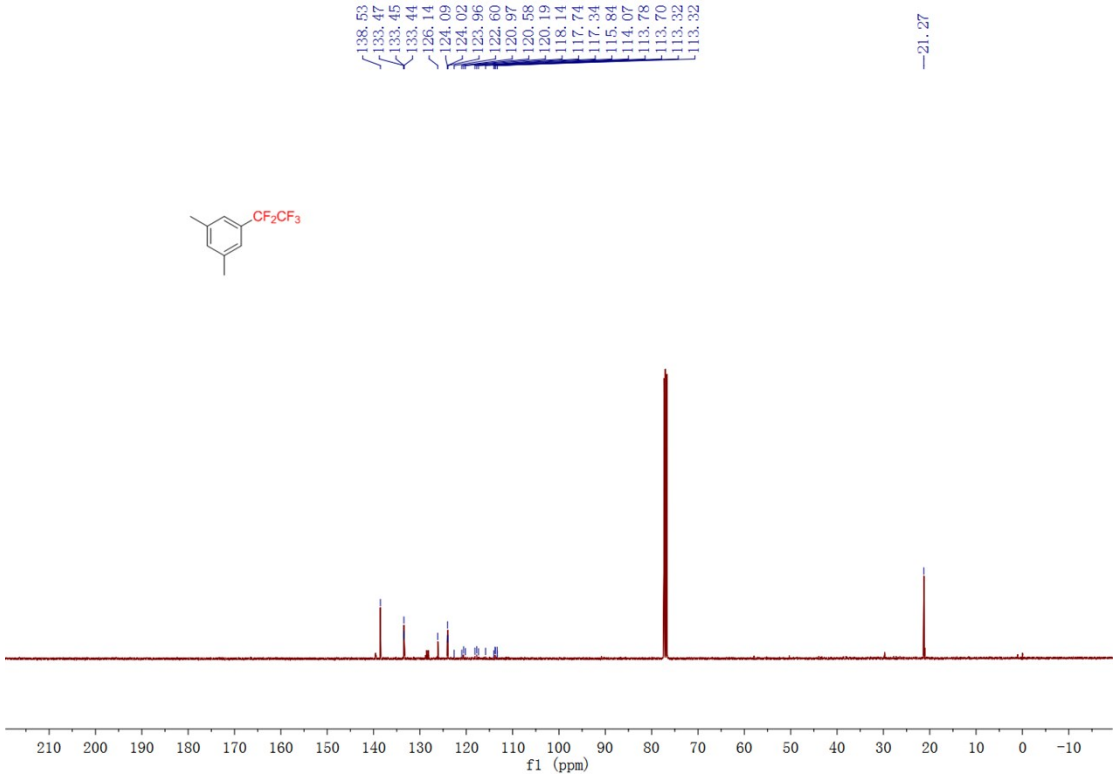

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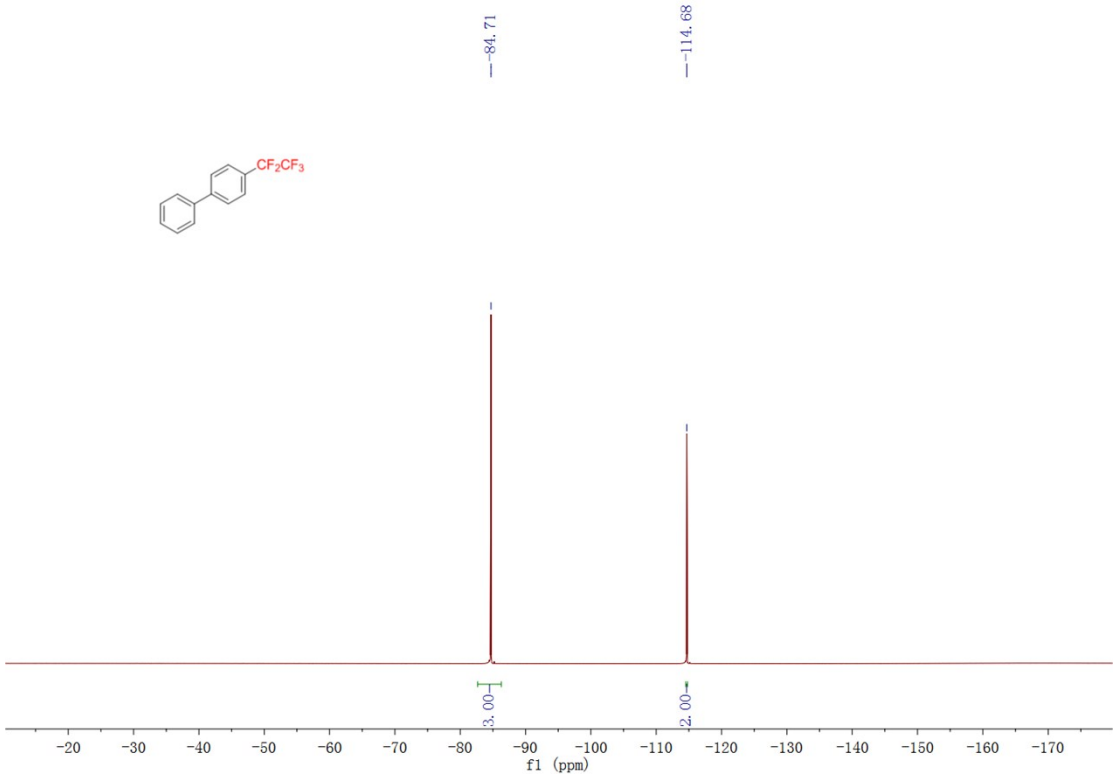

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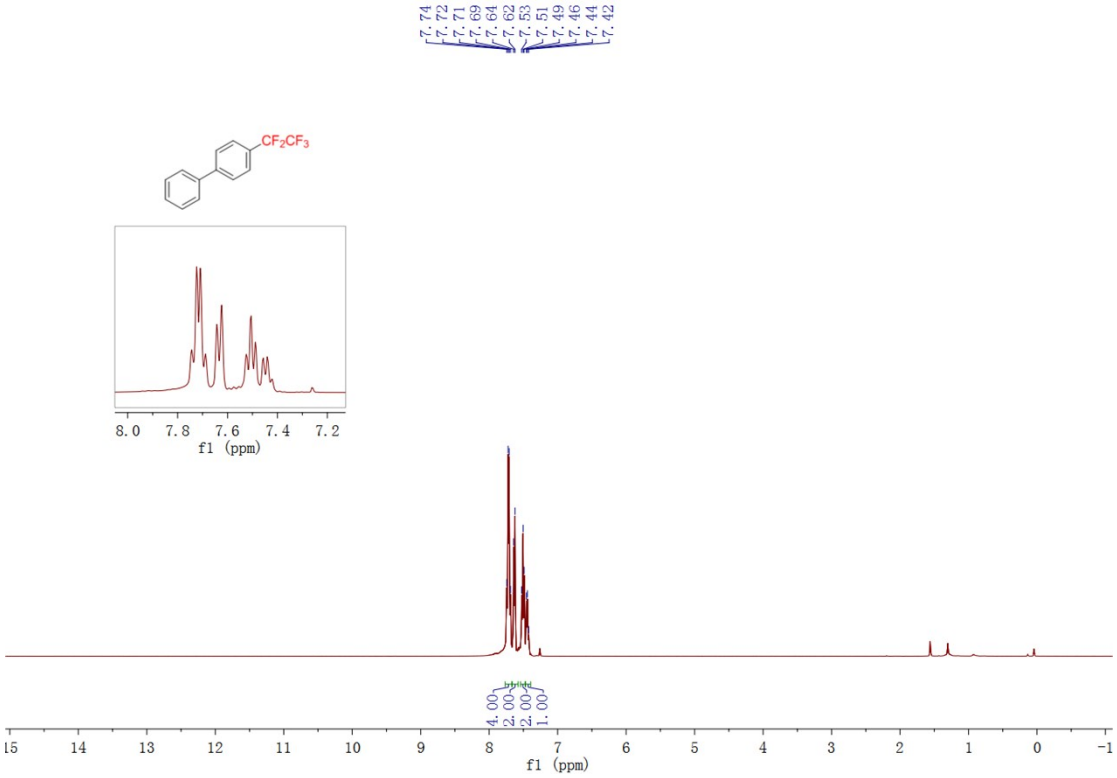

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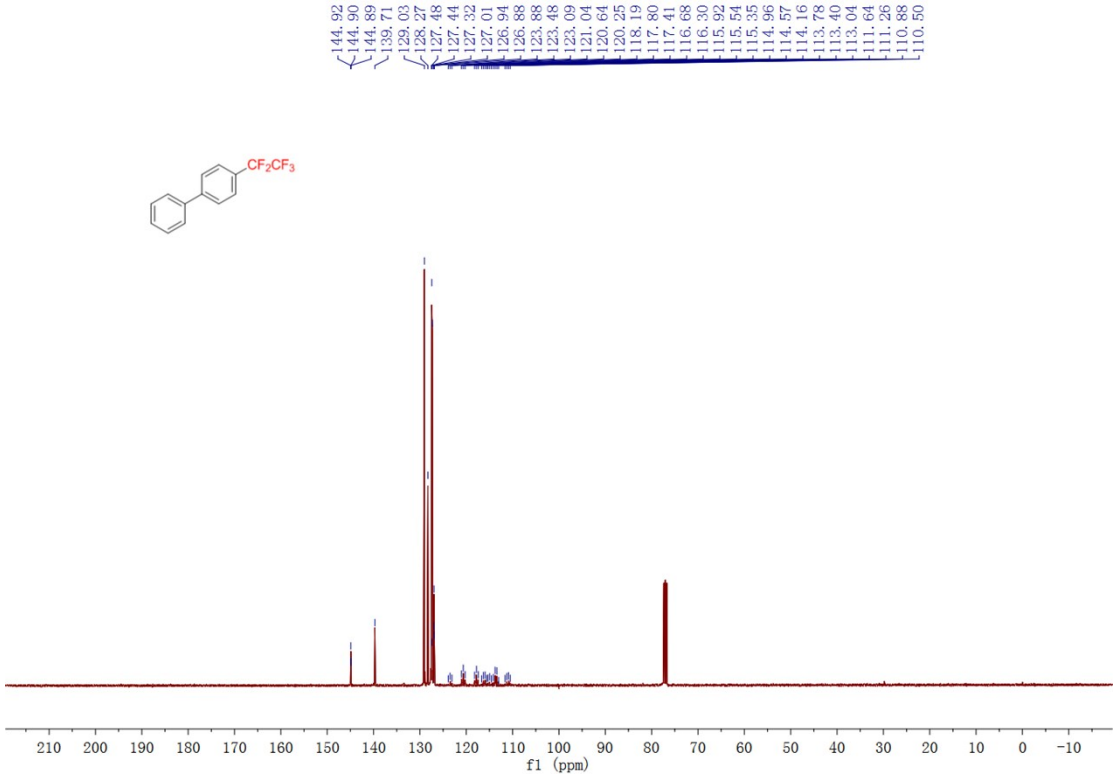

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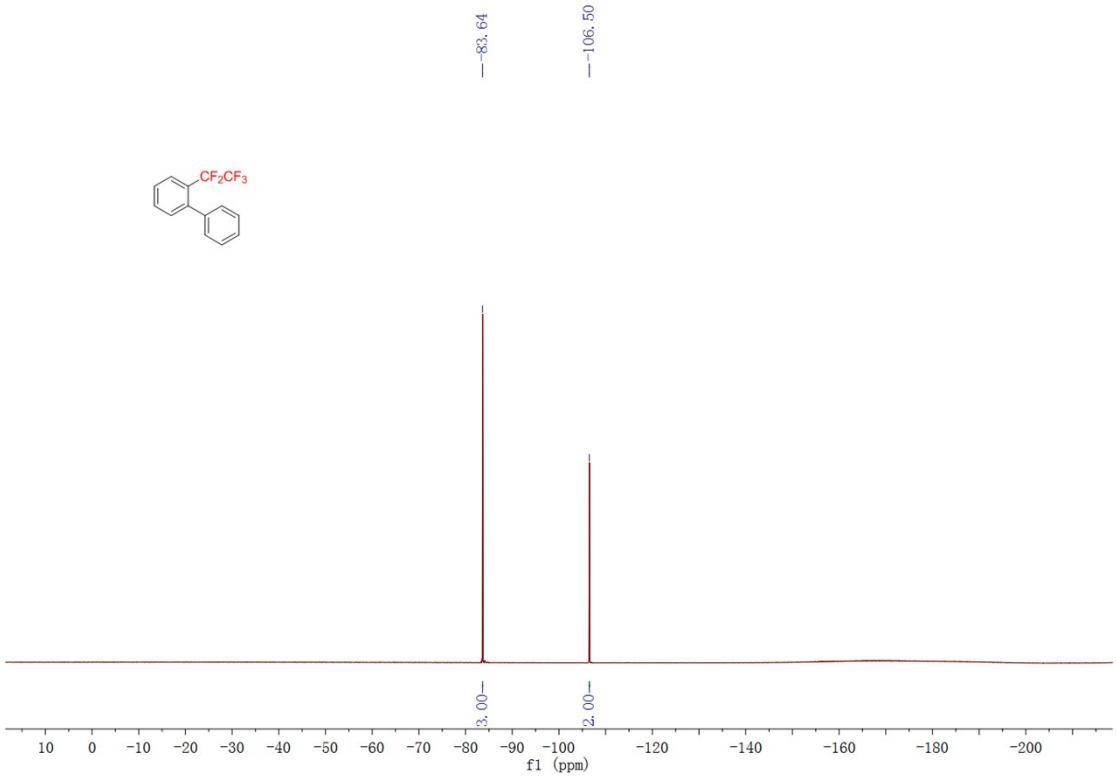

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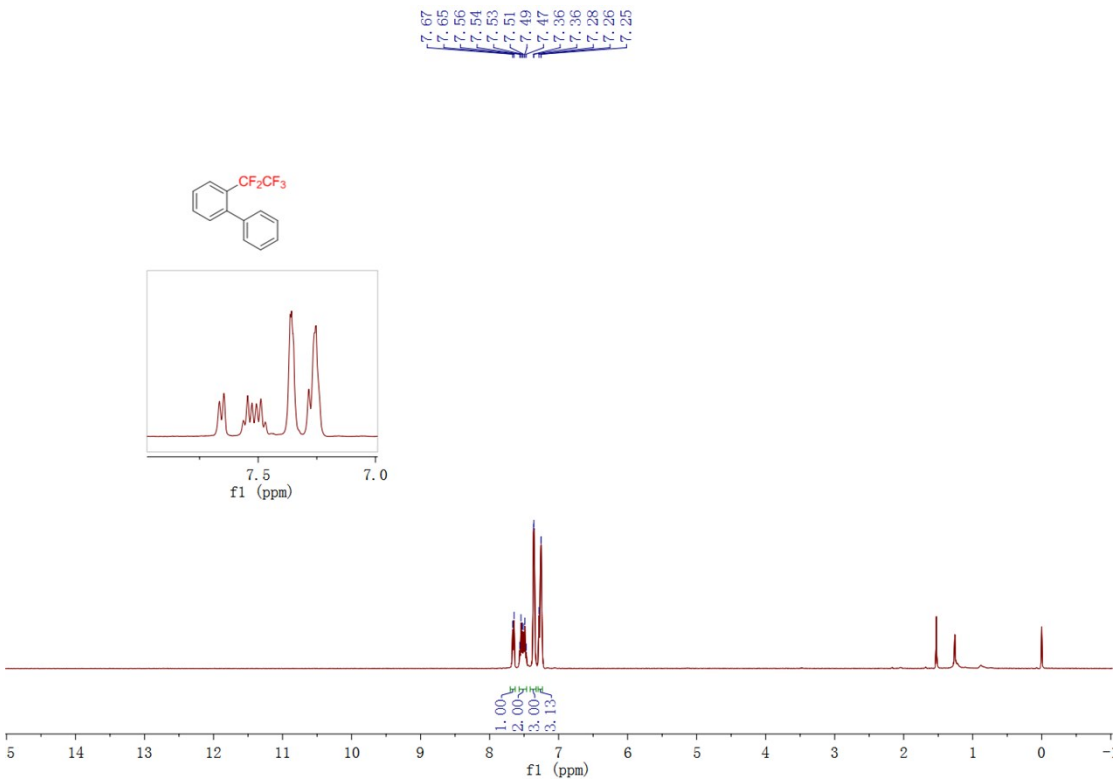

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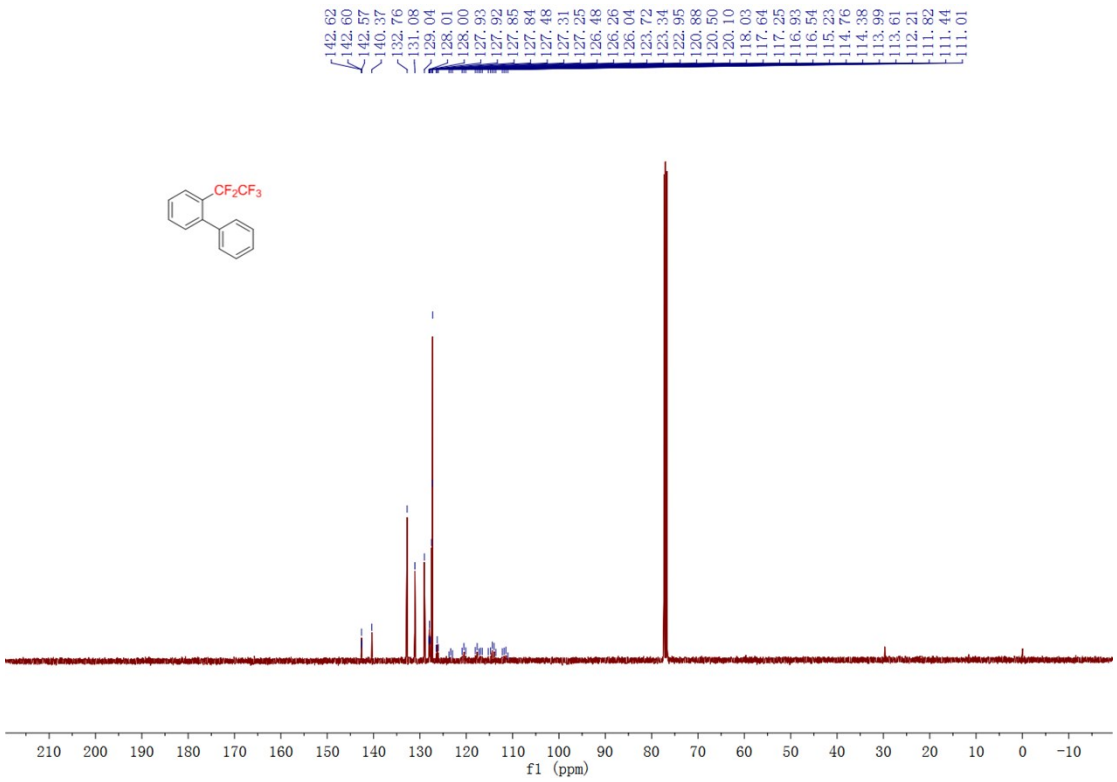

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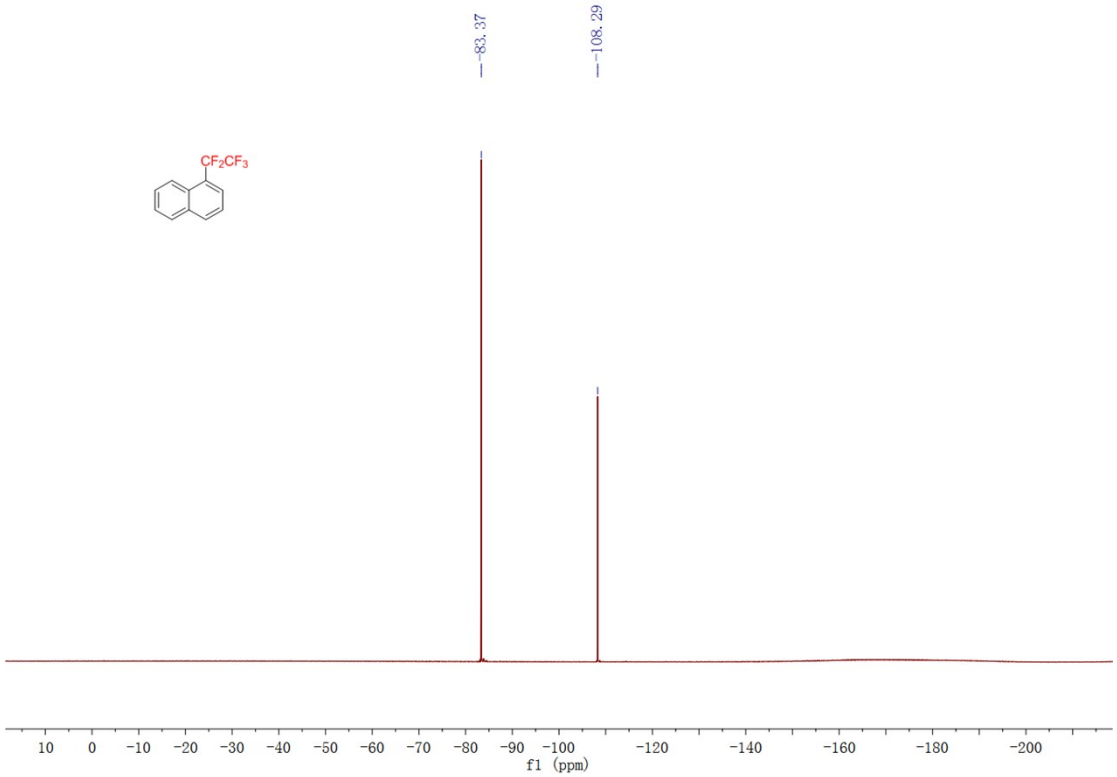

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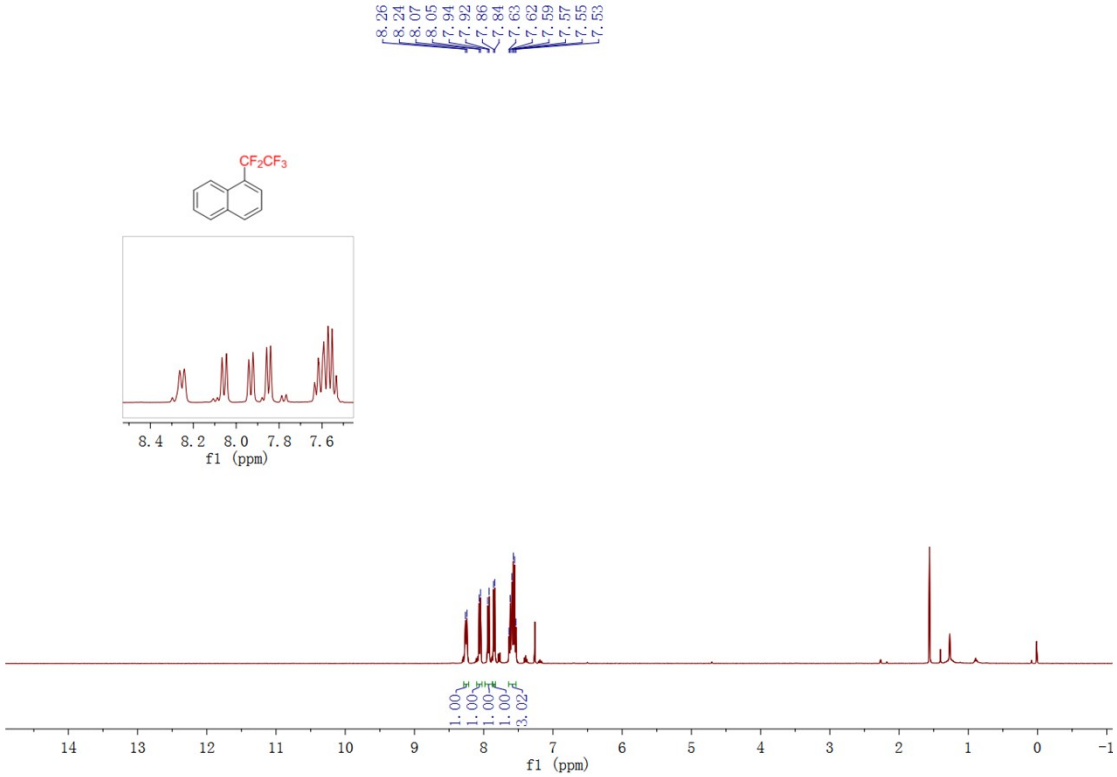

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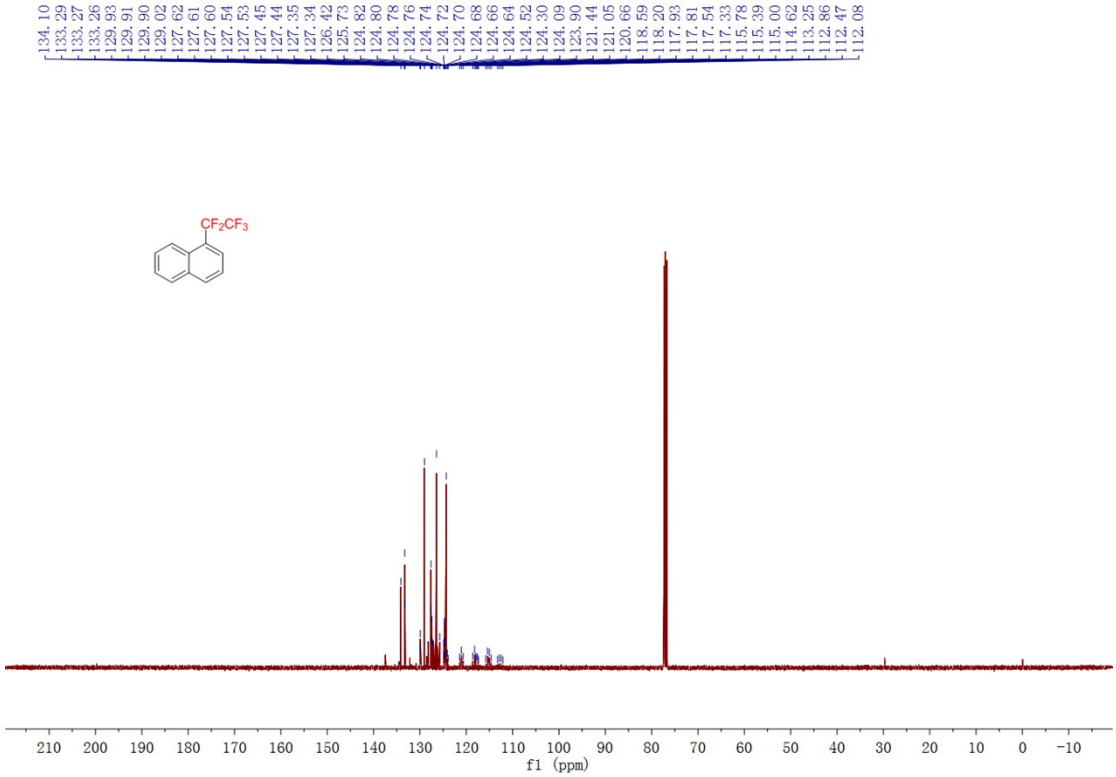

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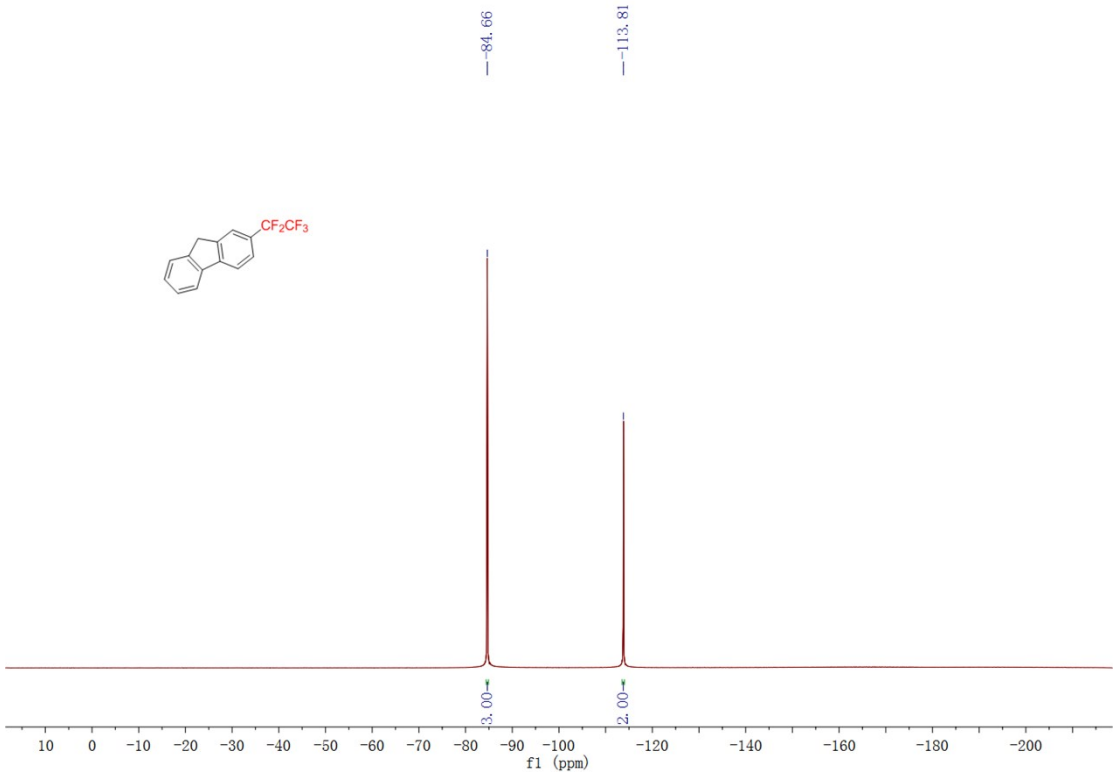

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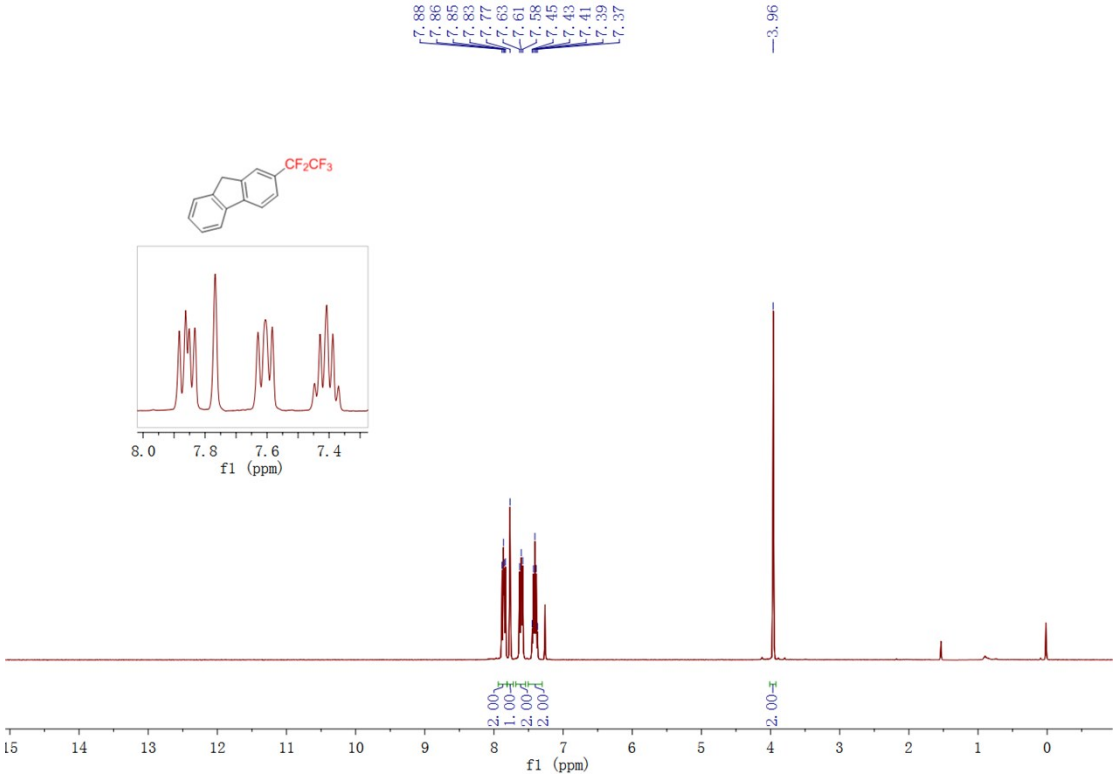

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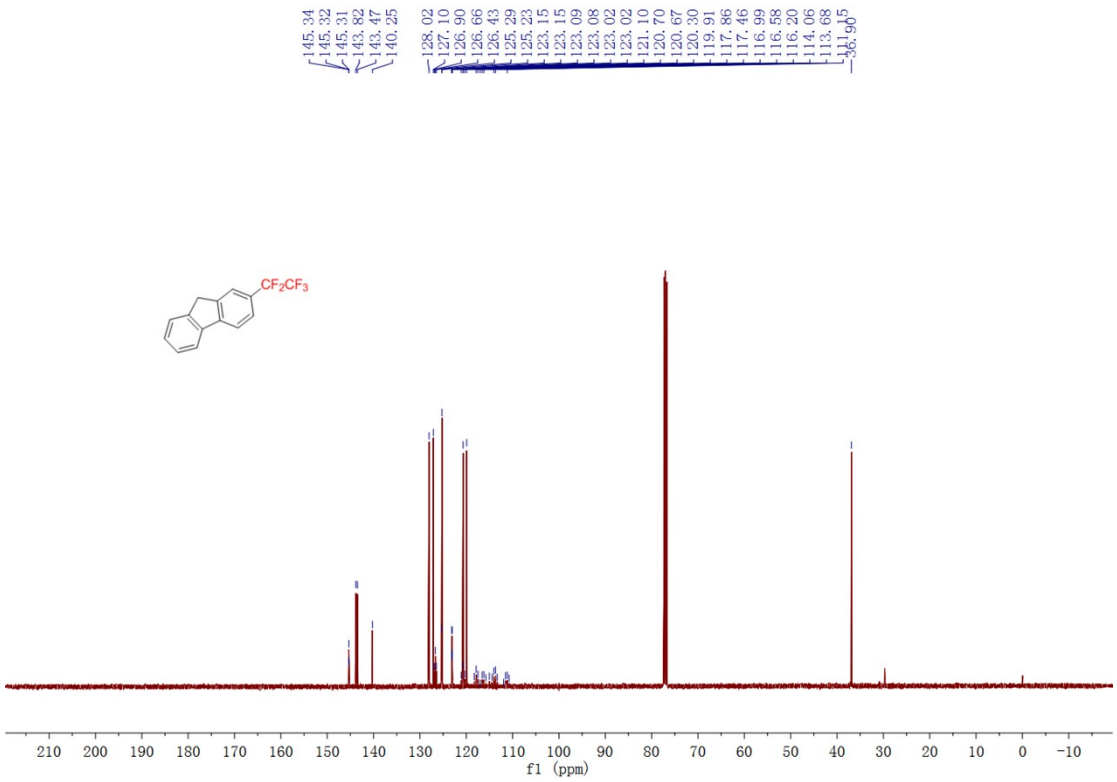
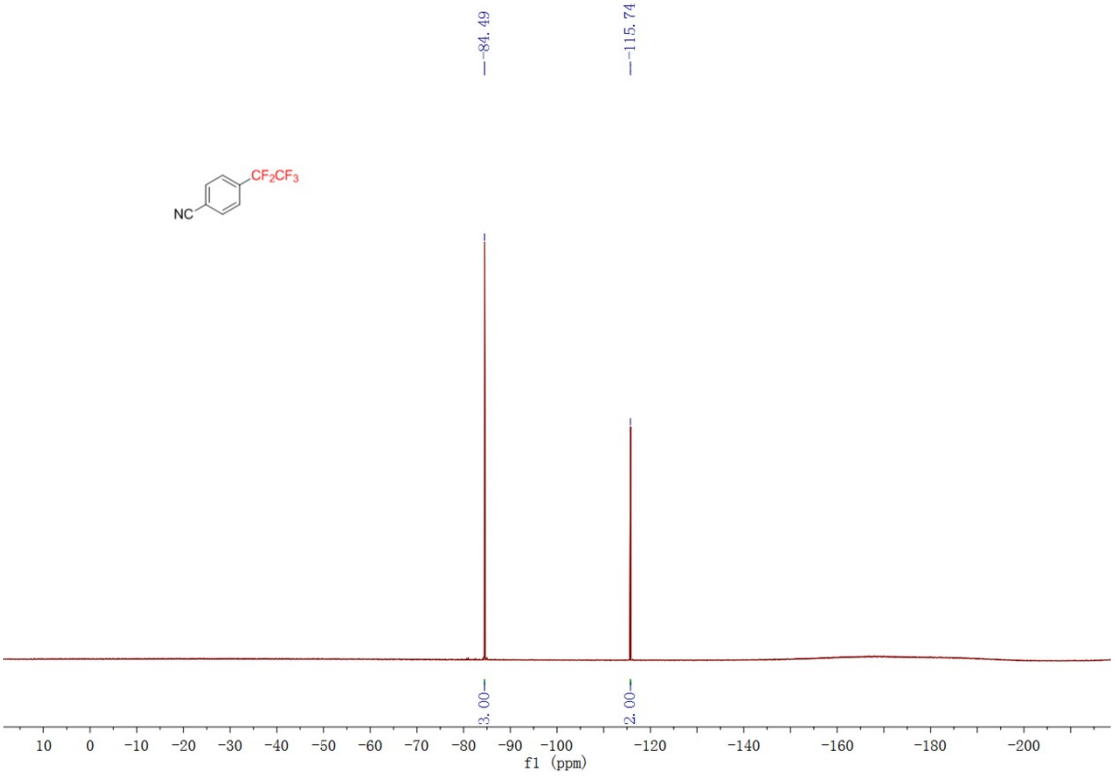


^{19}F NMR spectrum of **3g** in $CDCl_3$



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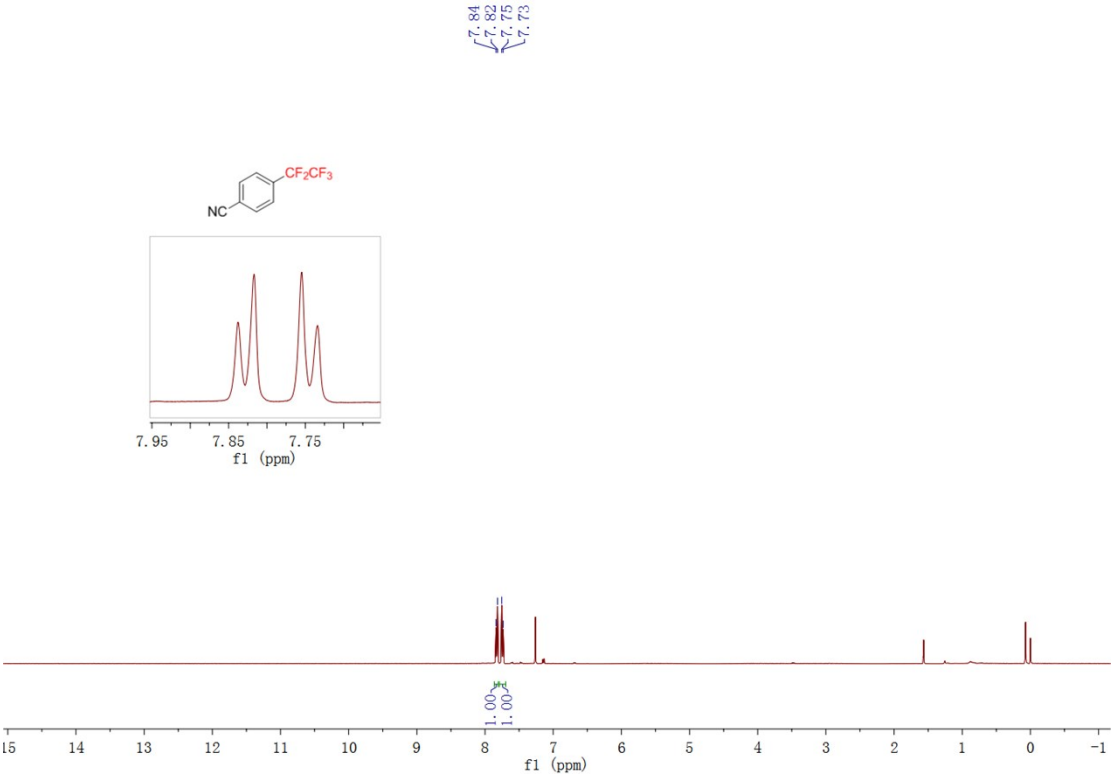

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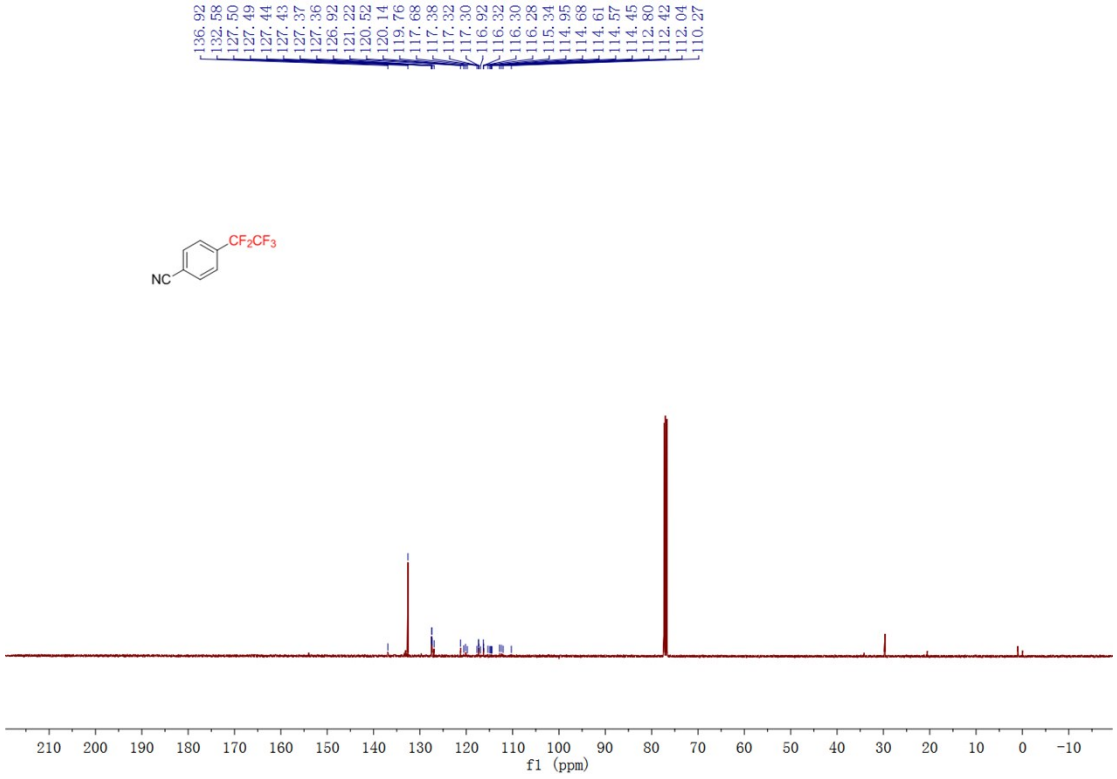

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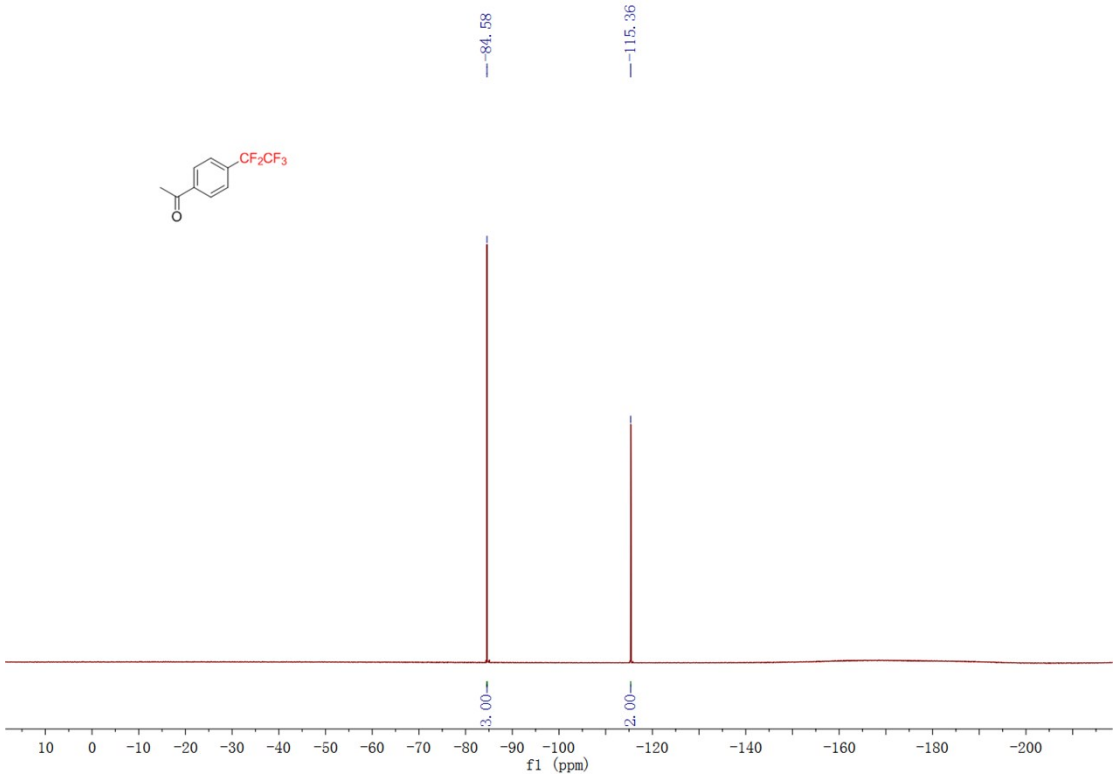

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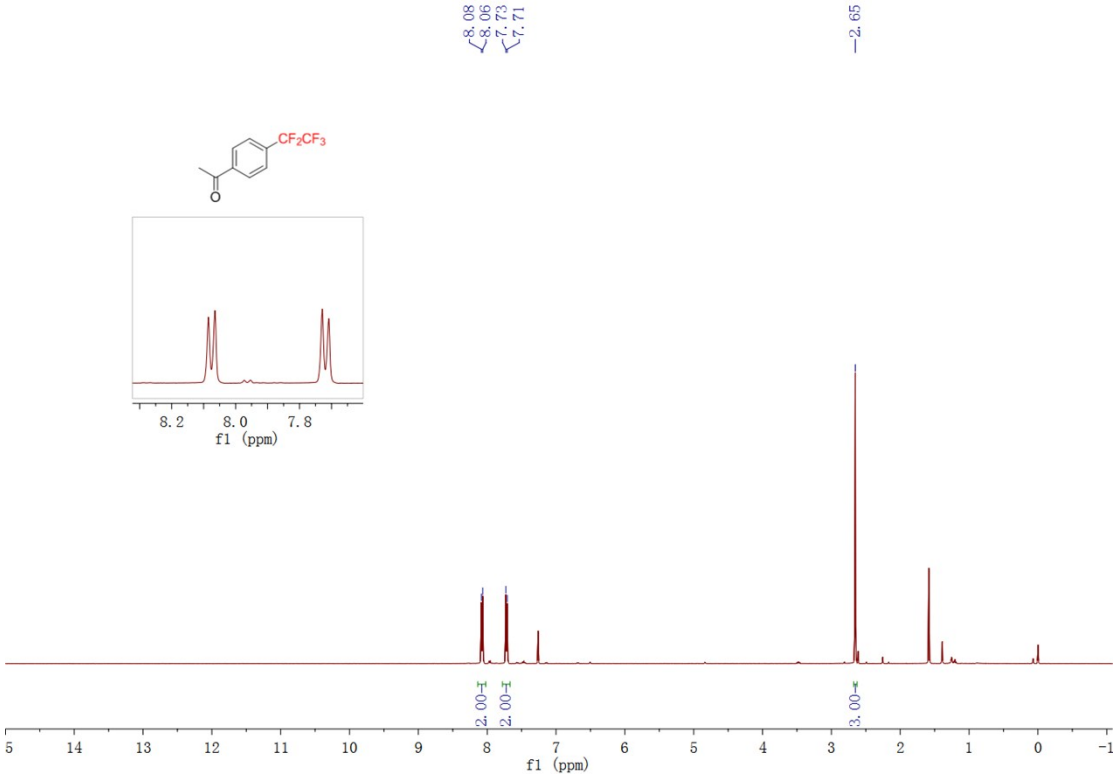

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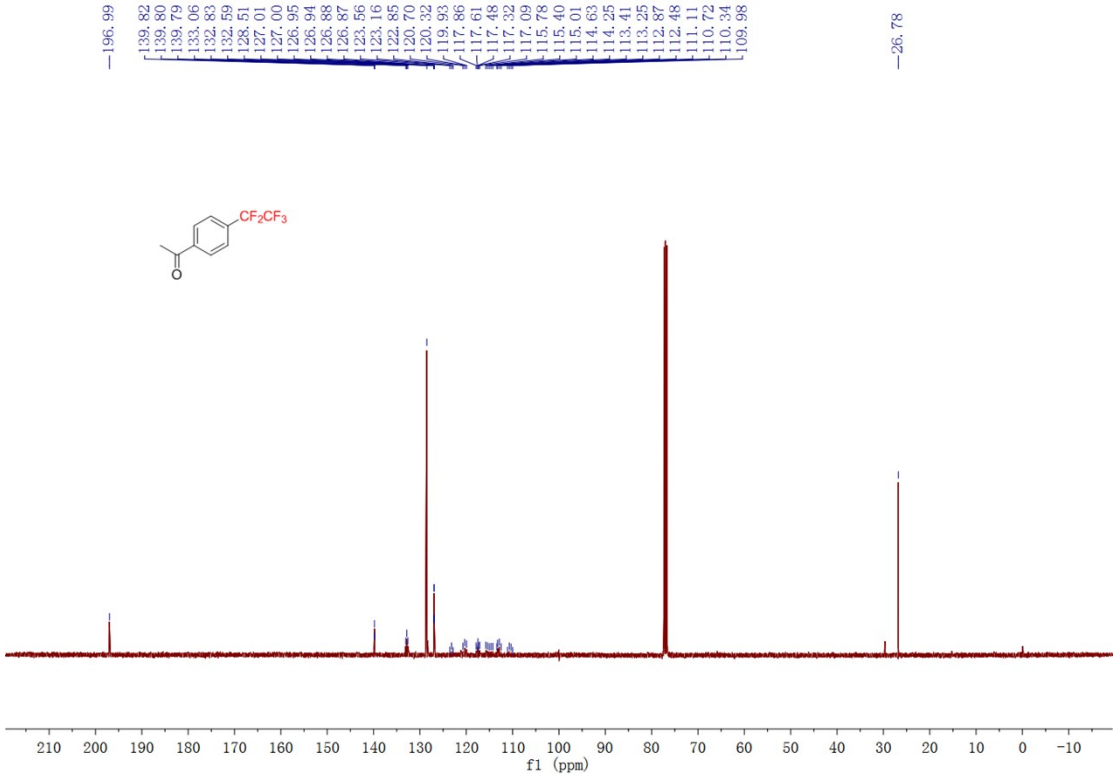
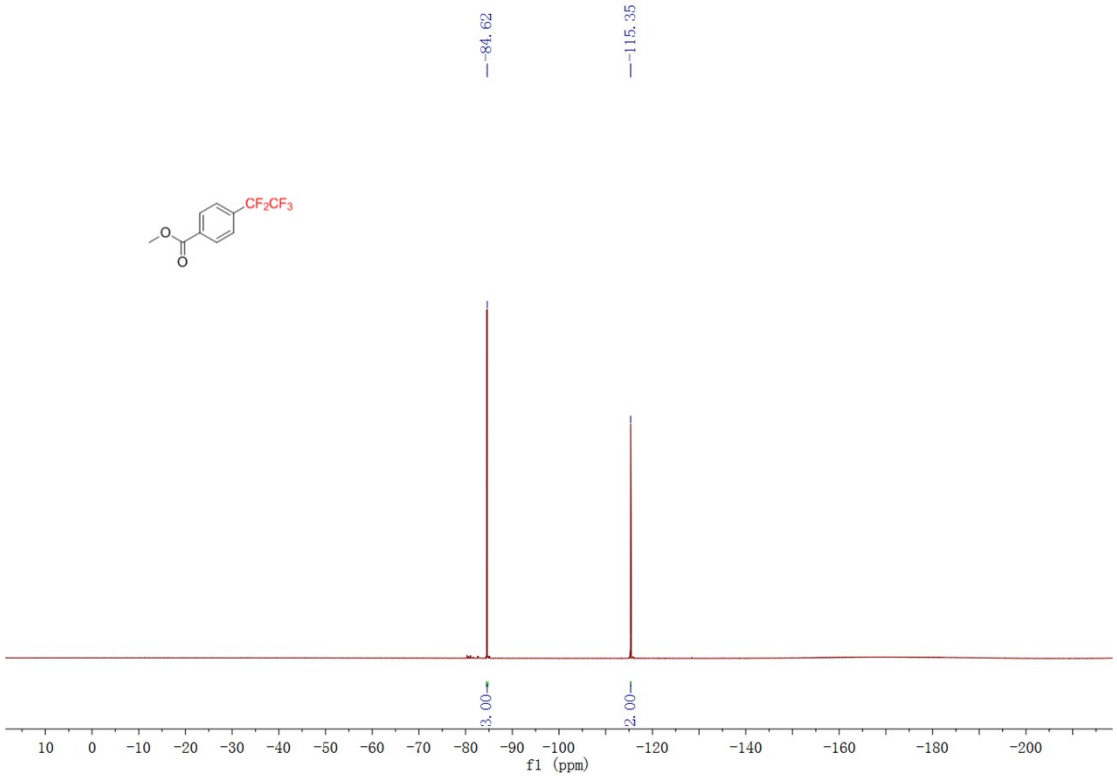
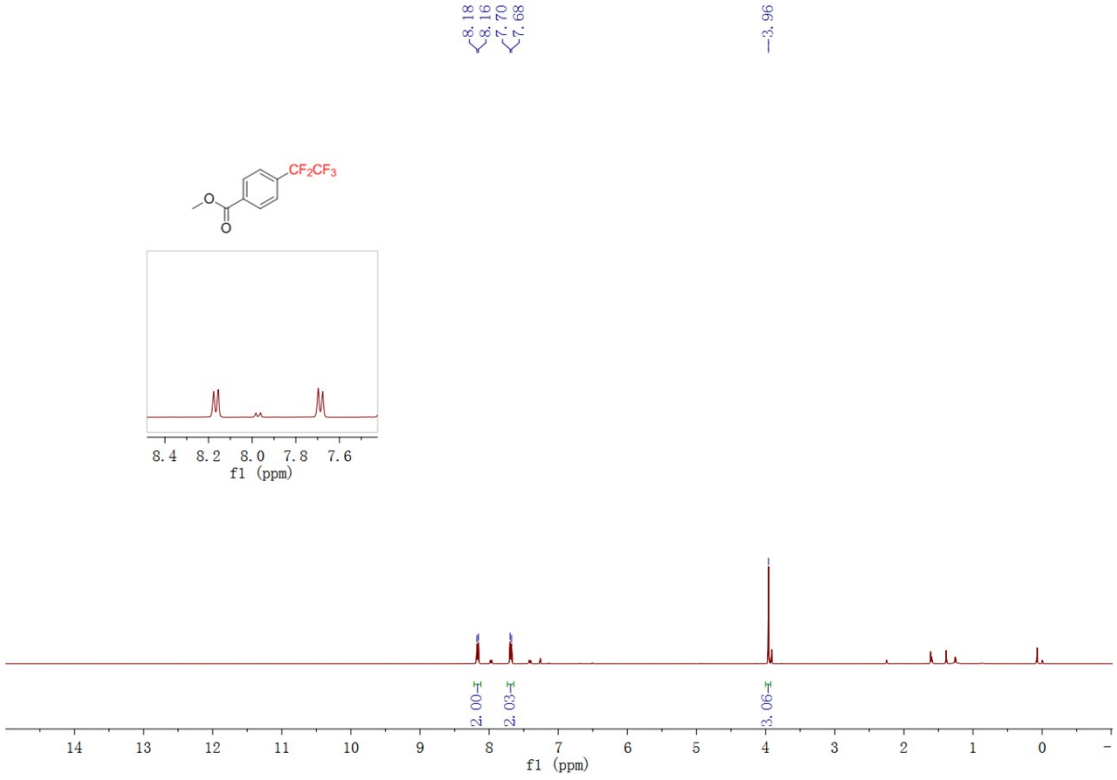


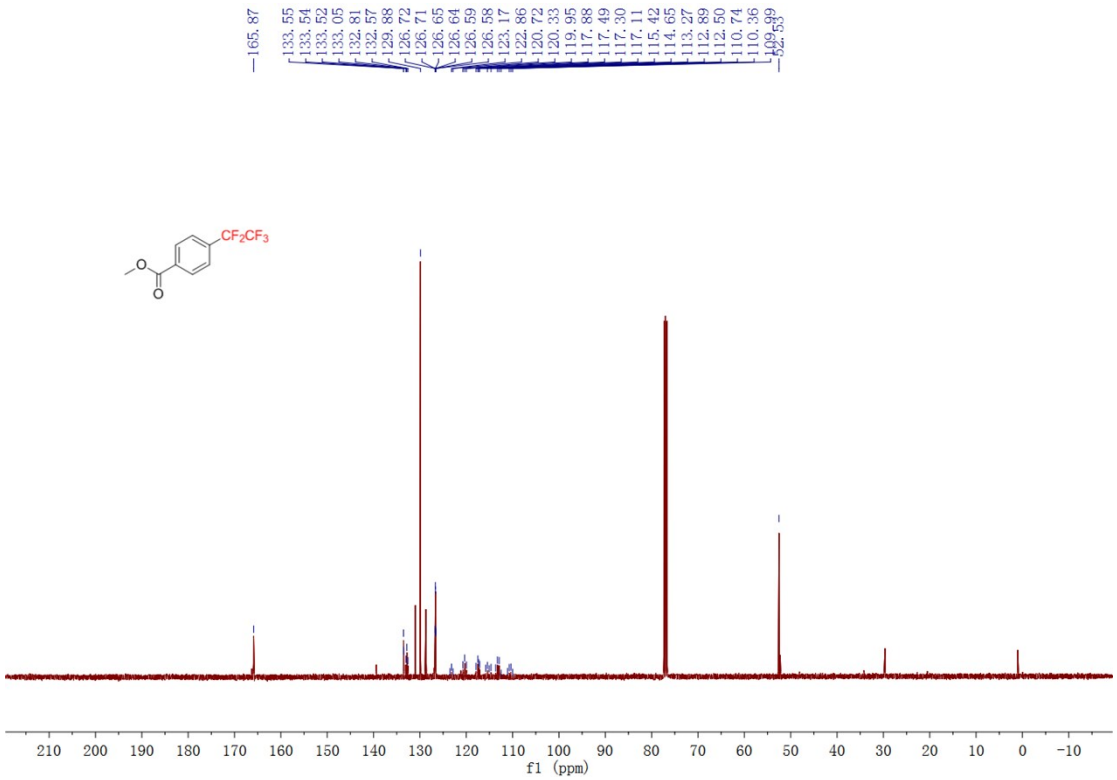
^{19}F NMR spectrum of **3i** in $CDCl_3$



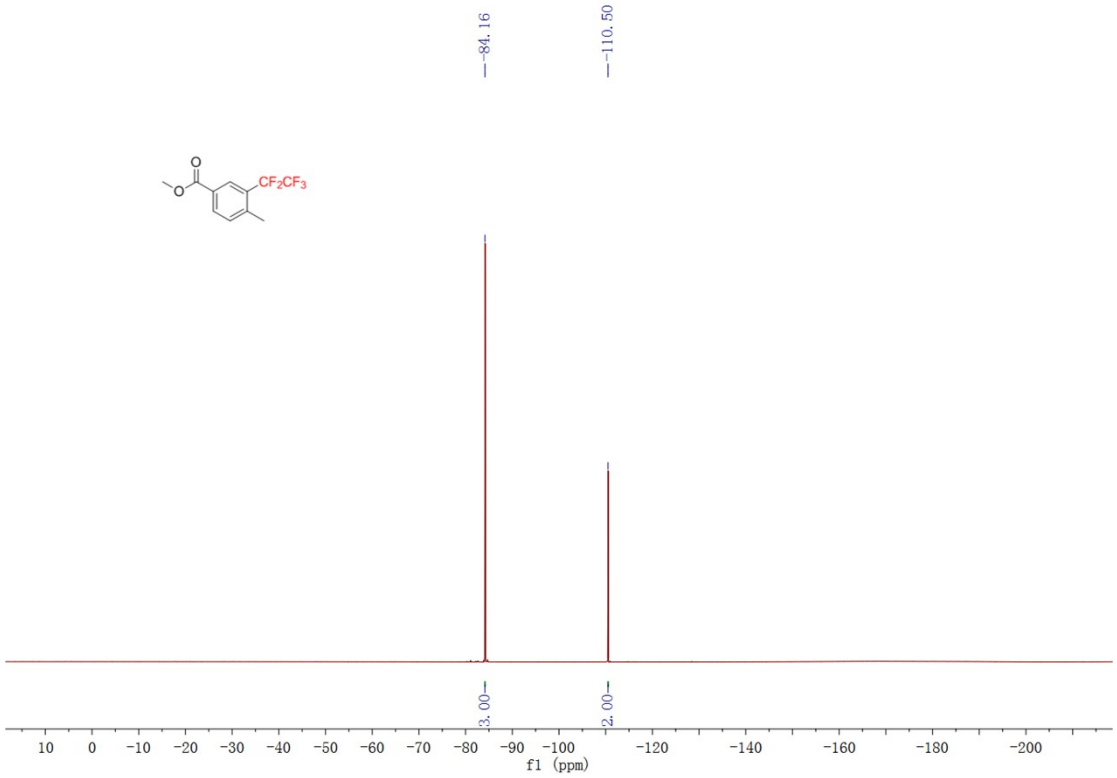
^{1}H NMR spectrum of **3i** in $CDCl_3$



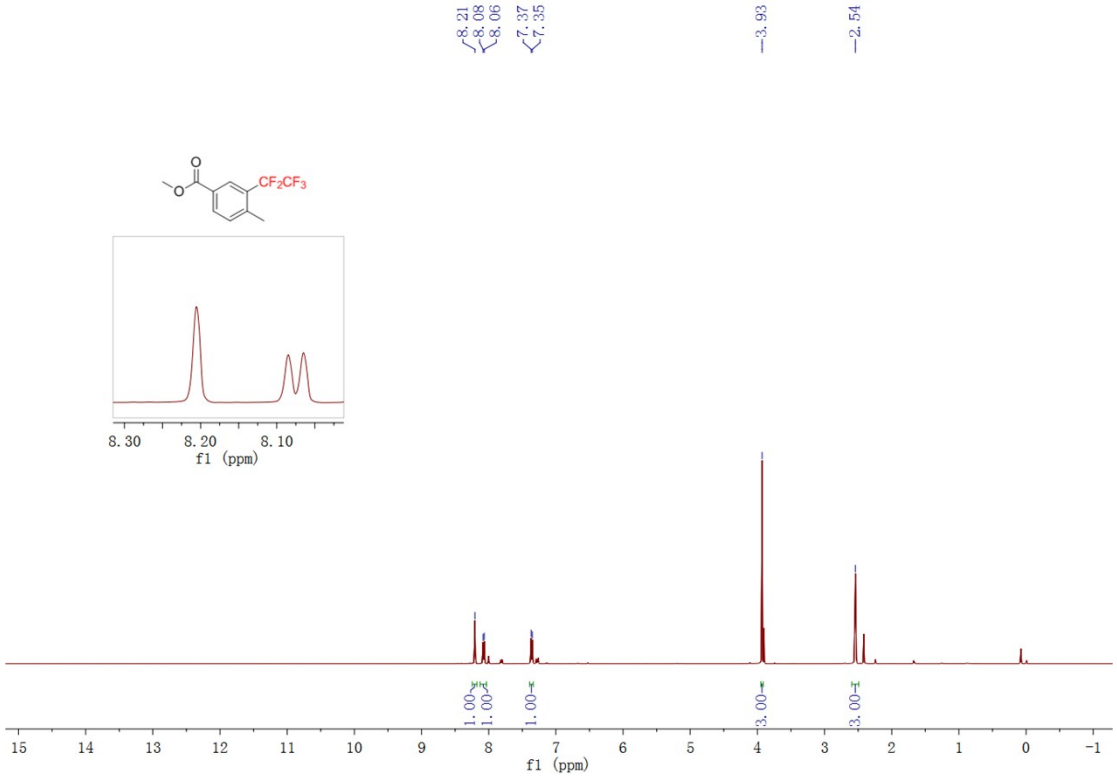
^{13}C NMR spectrum of **3i** in $CDCl_3$



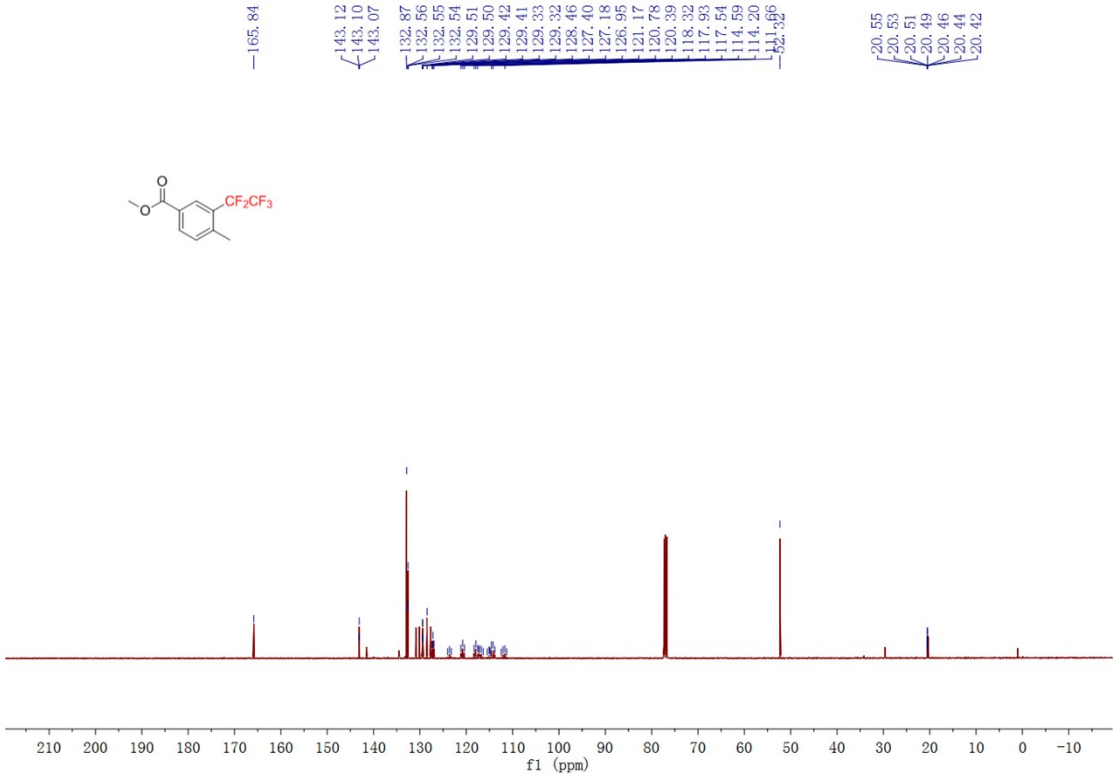
^{19}F NMR spectrum of **3j** in $CDCl_3$



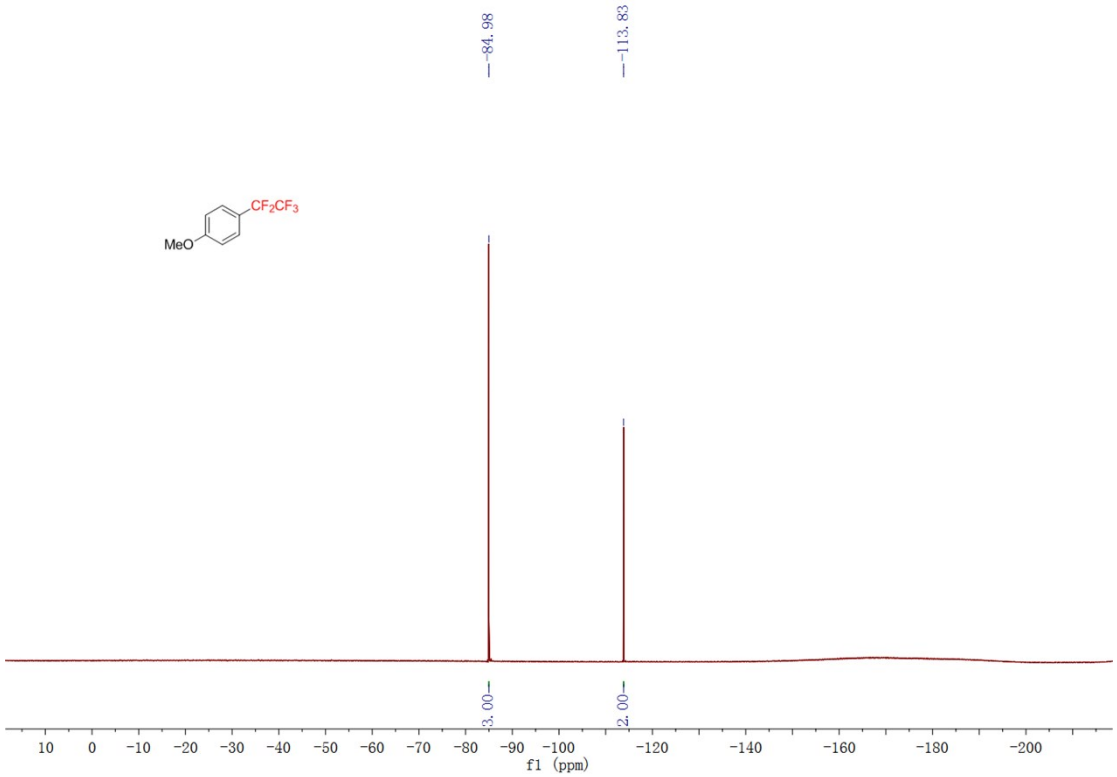
^{1}H NMR spectrum of **3j** in $CDCl_3$



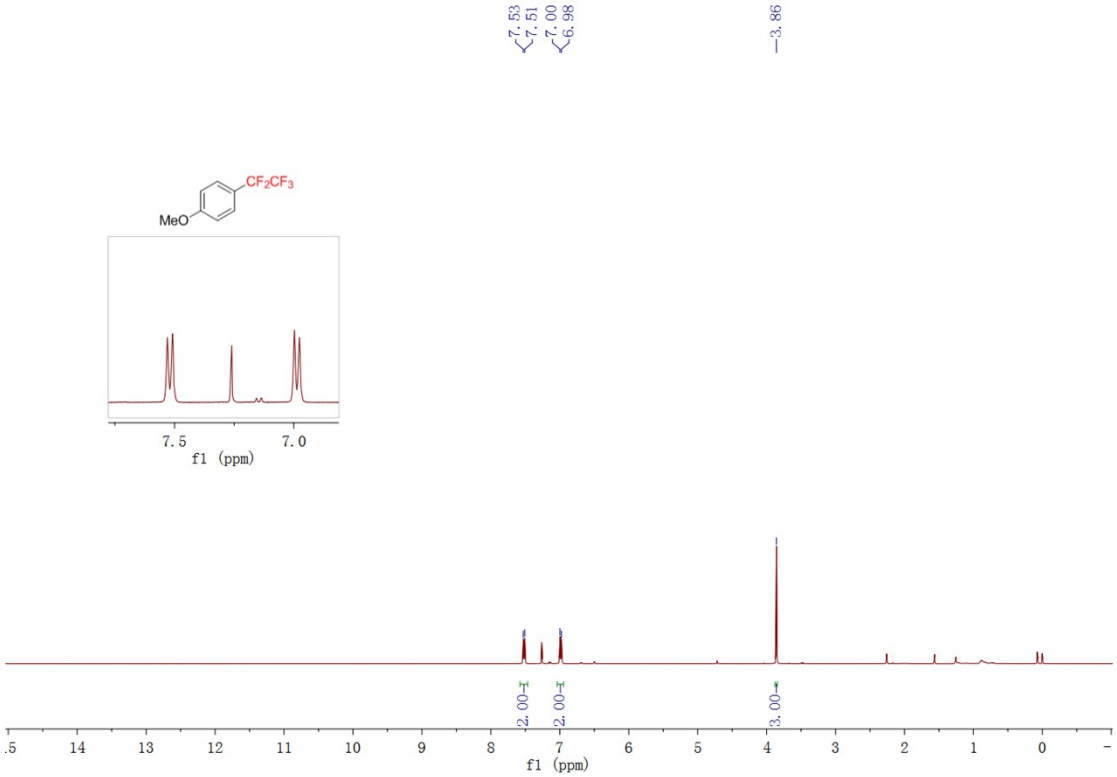
^{13}C NMR spectrum of **3j** in $CDCl_3$



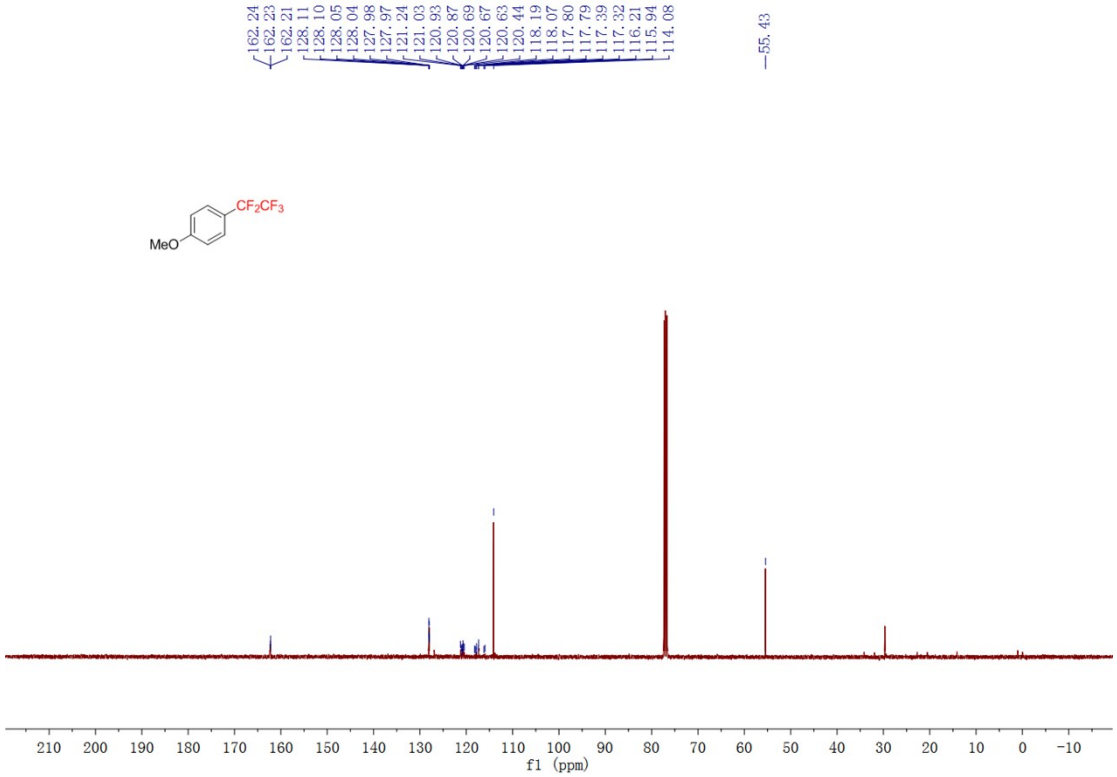
^{19}F NMR spectrum of **3k** in $CDCl_3$



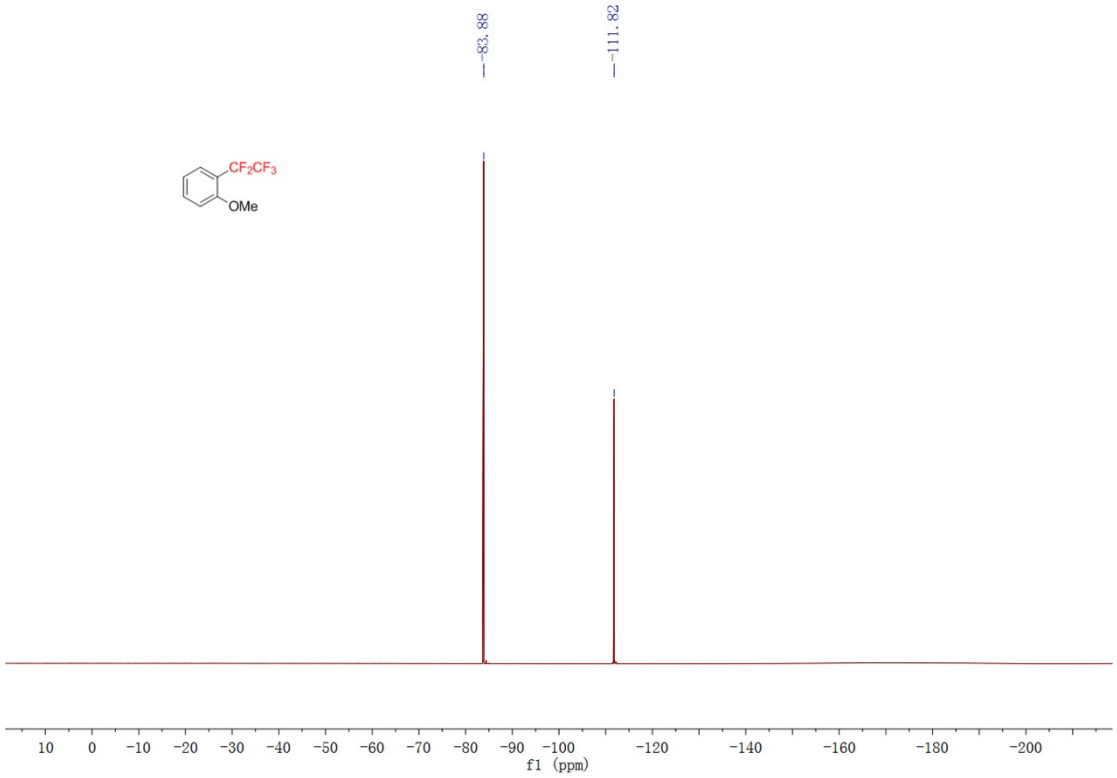
^{1}H NMR spectrum of **3k** in $CDCl_3$



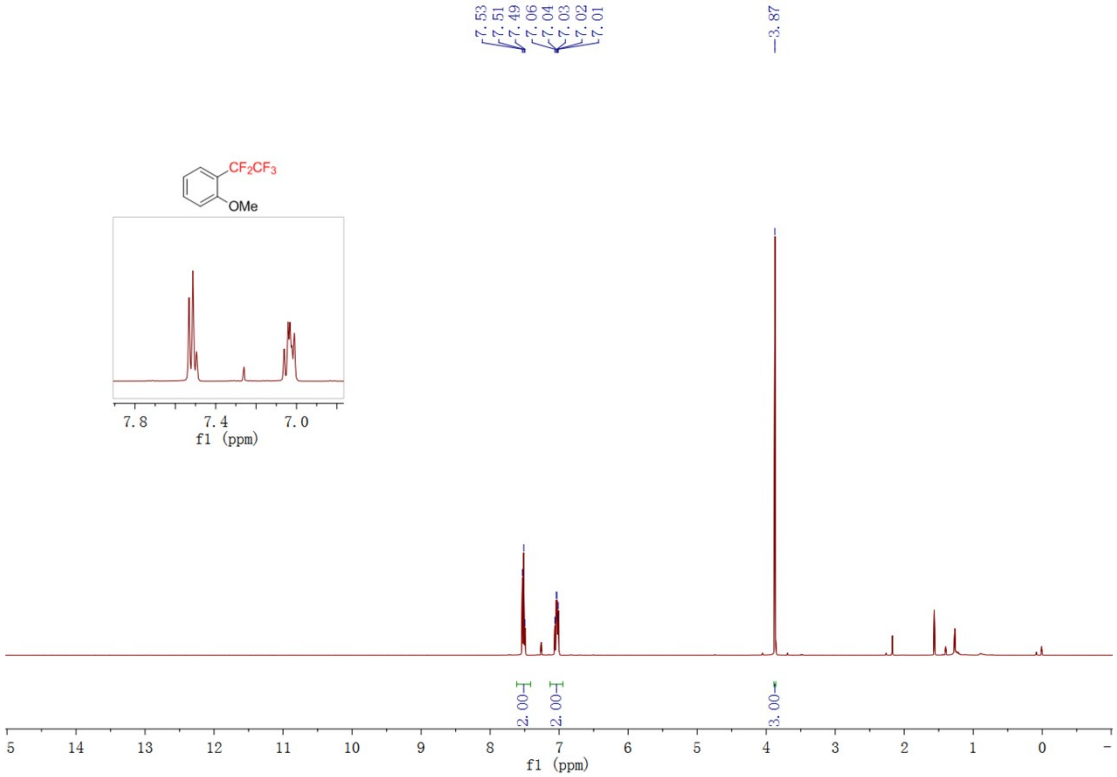
^{13}C NMR spectrum of **3k** in $CDCl_3$



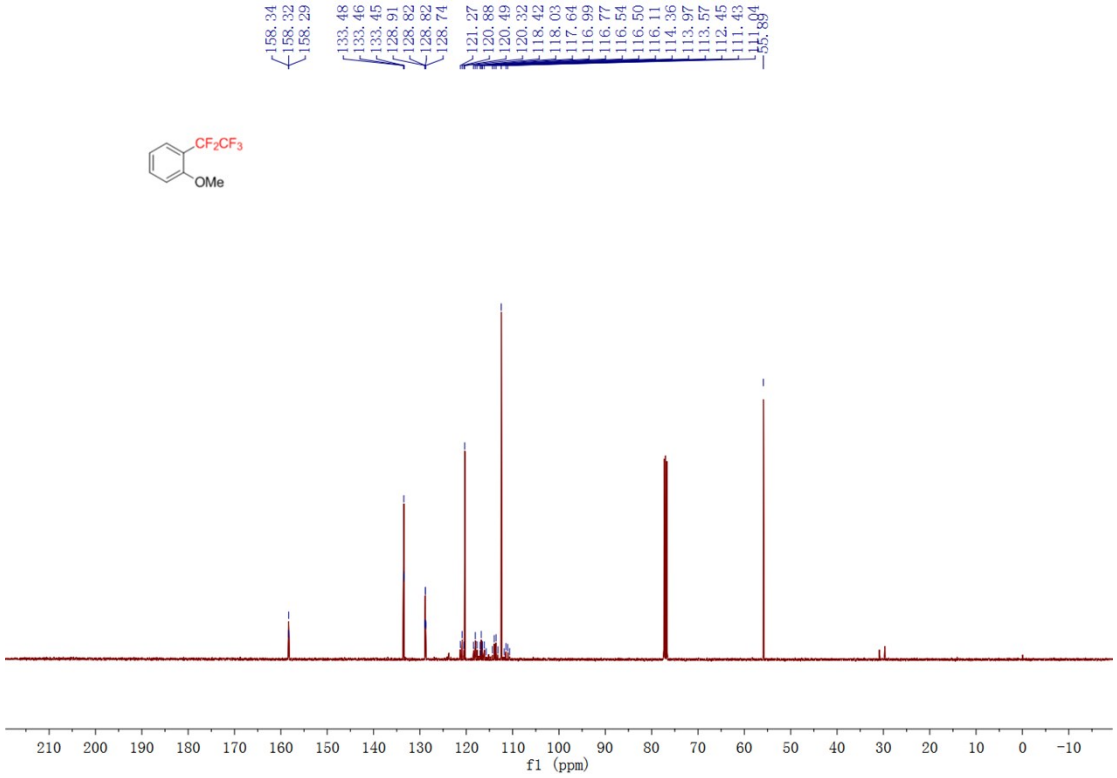
^{19}F NMR spectrum of **3l** in $CDCl_3$



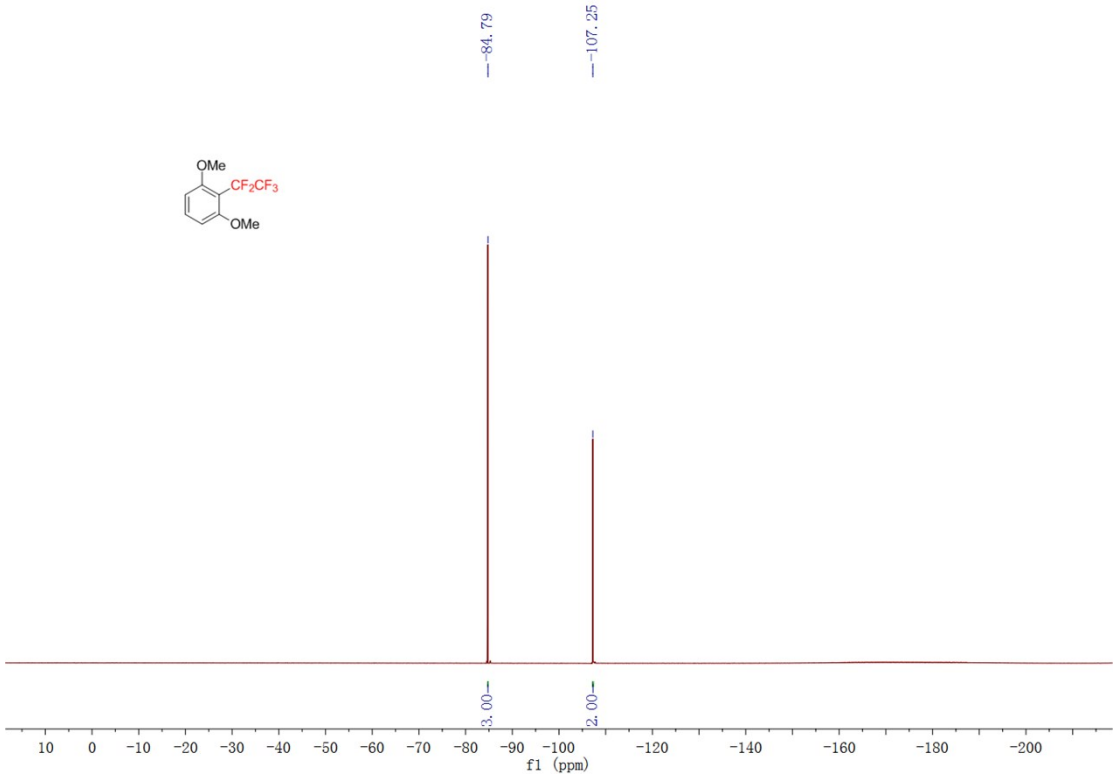
^{1}H NMR spectrum of **3l** in $CDCl_3$



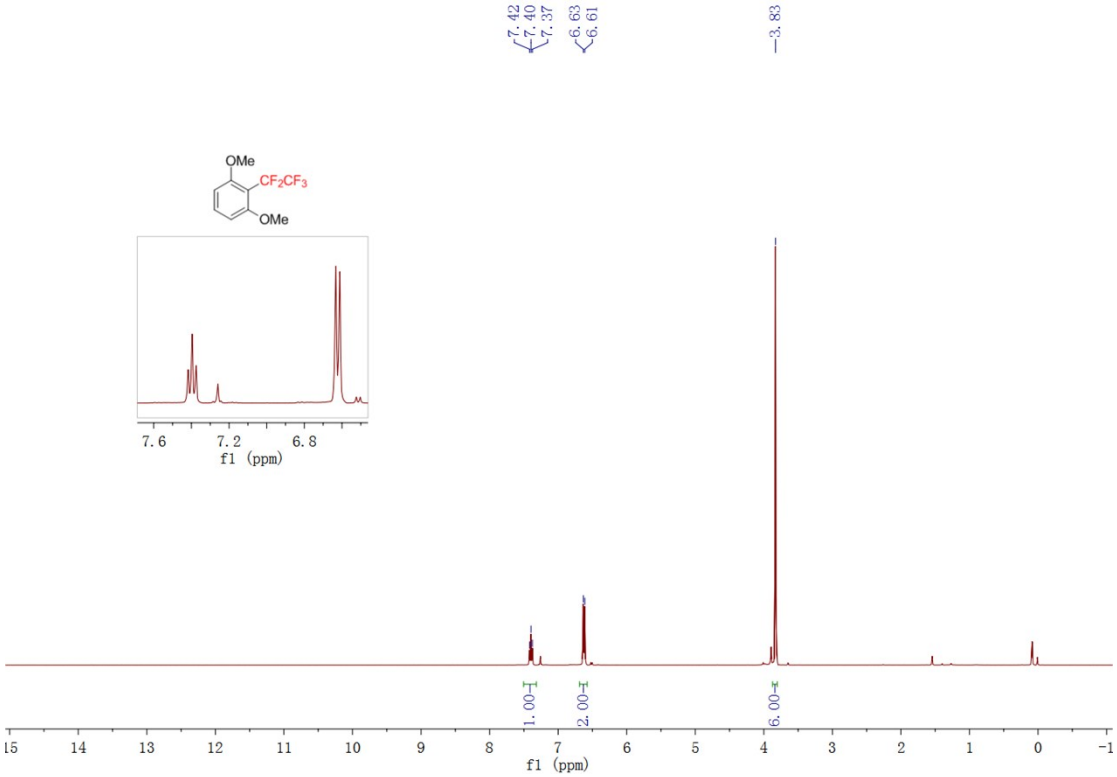
^{13}C NMR spectrum of **3l** in $CDCl_3$



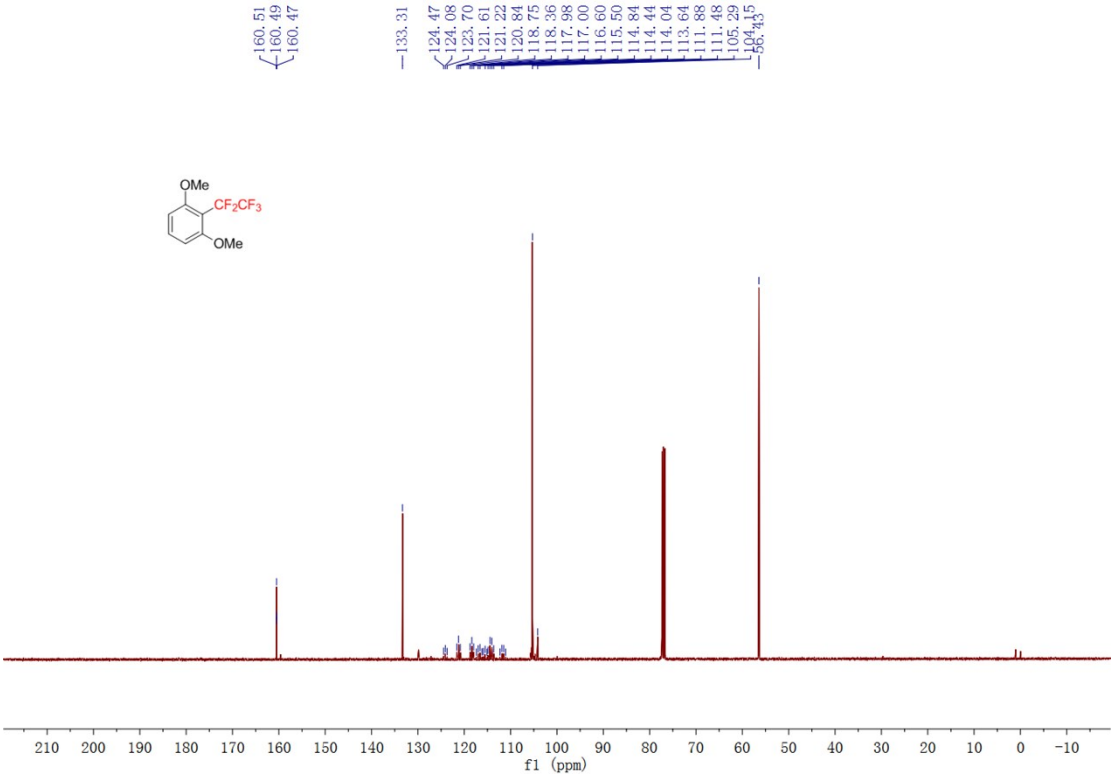
^{19}F NMR spectrum of **3m** in $CDCl_3$



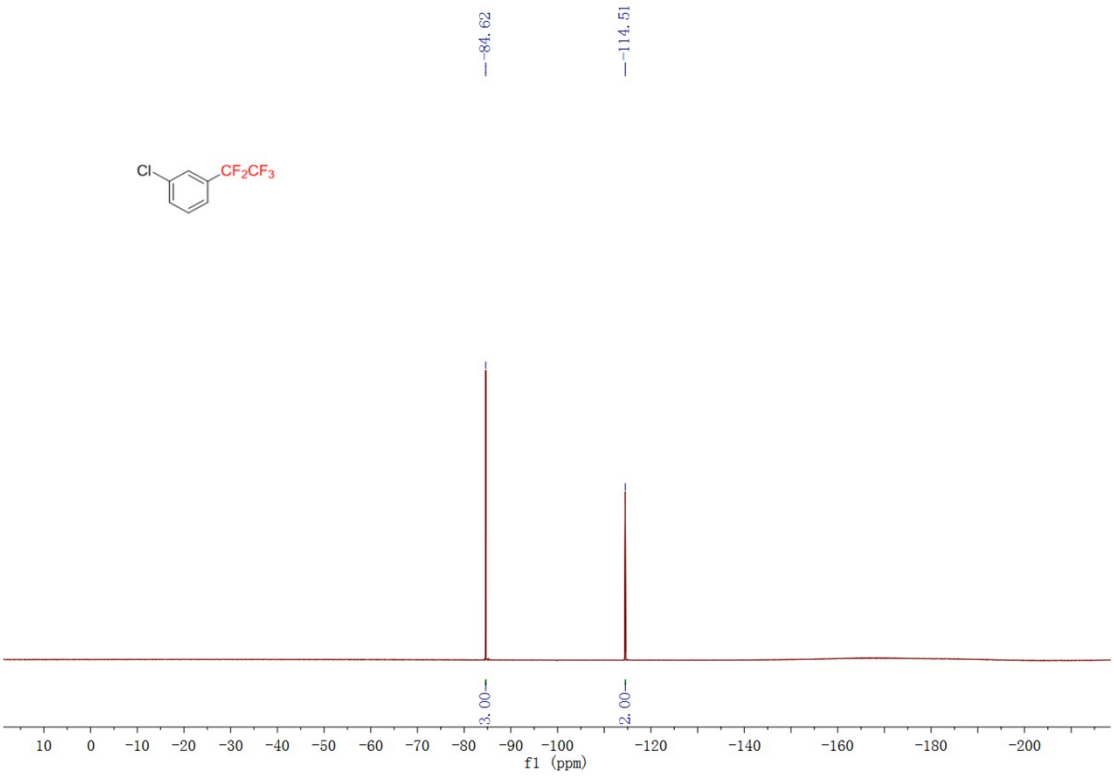
^{1}H NMR spectrum of **3m** in $CDCl_3$



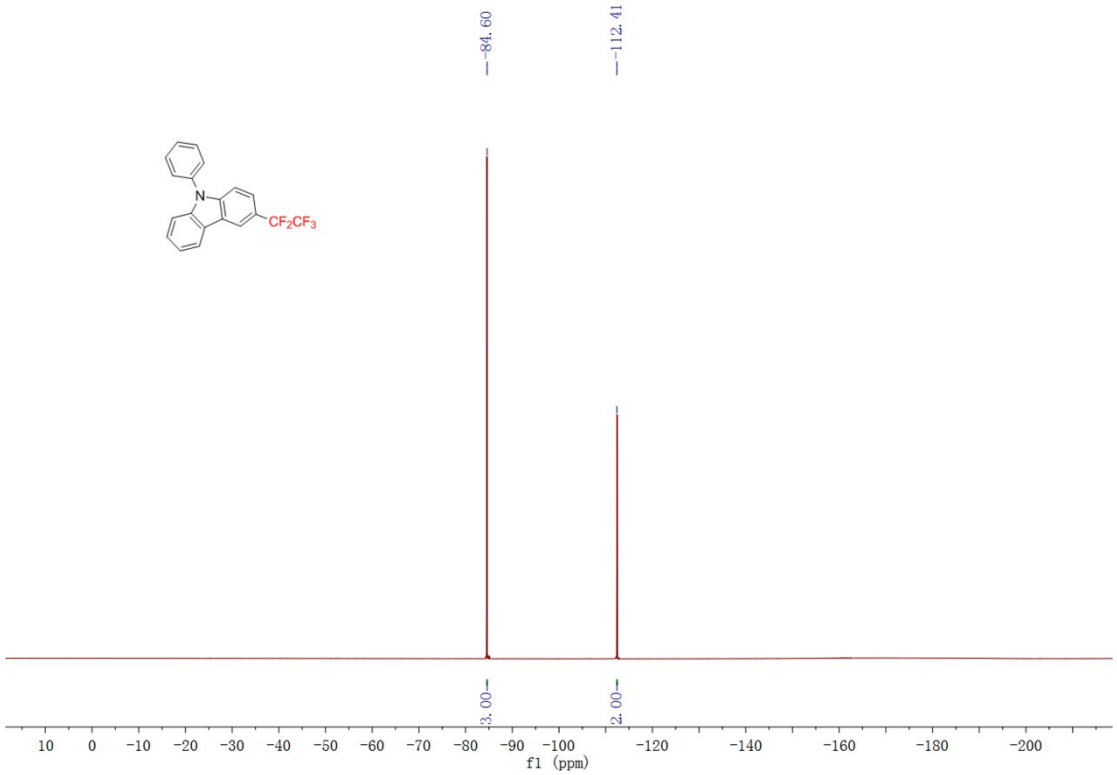
^{13}C NMR spectrum of **3m** in $CDCl_3$



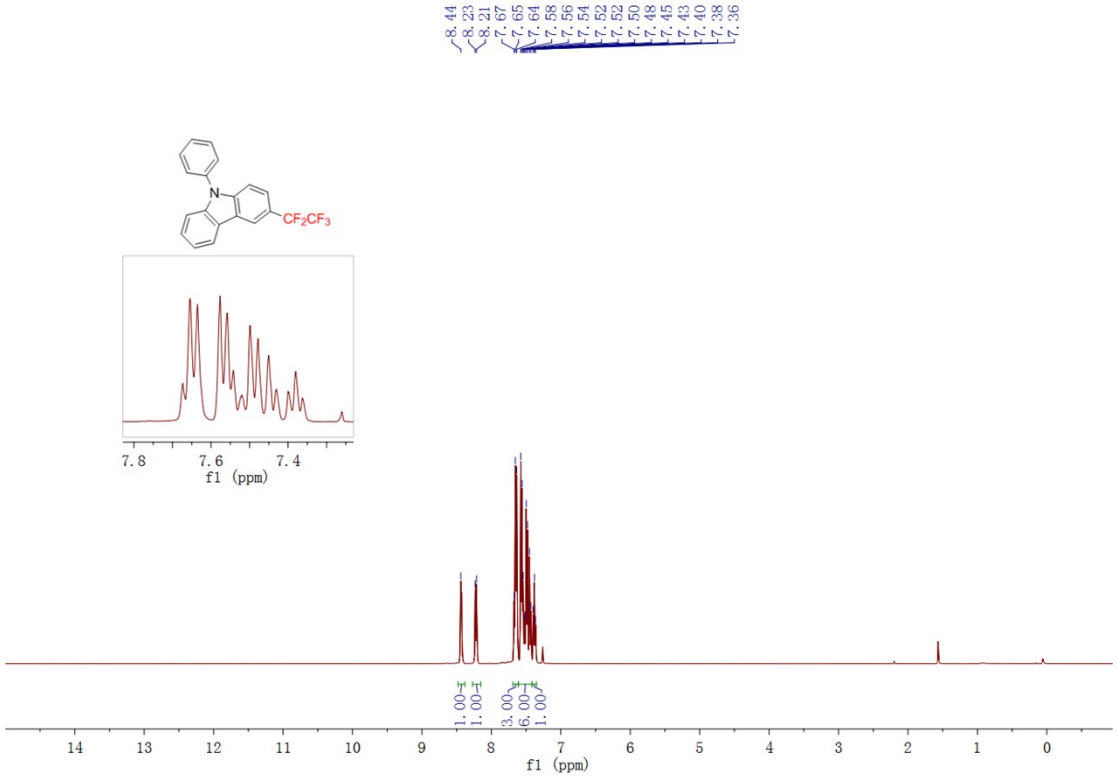
^{19}F NMR spectrum of **3n** (unlocked)



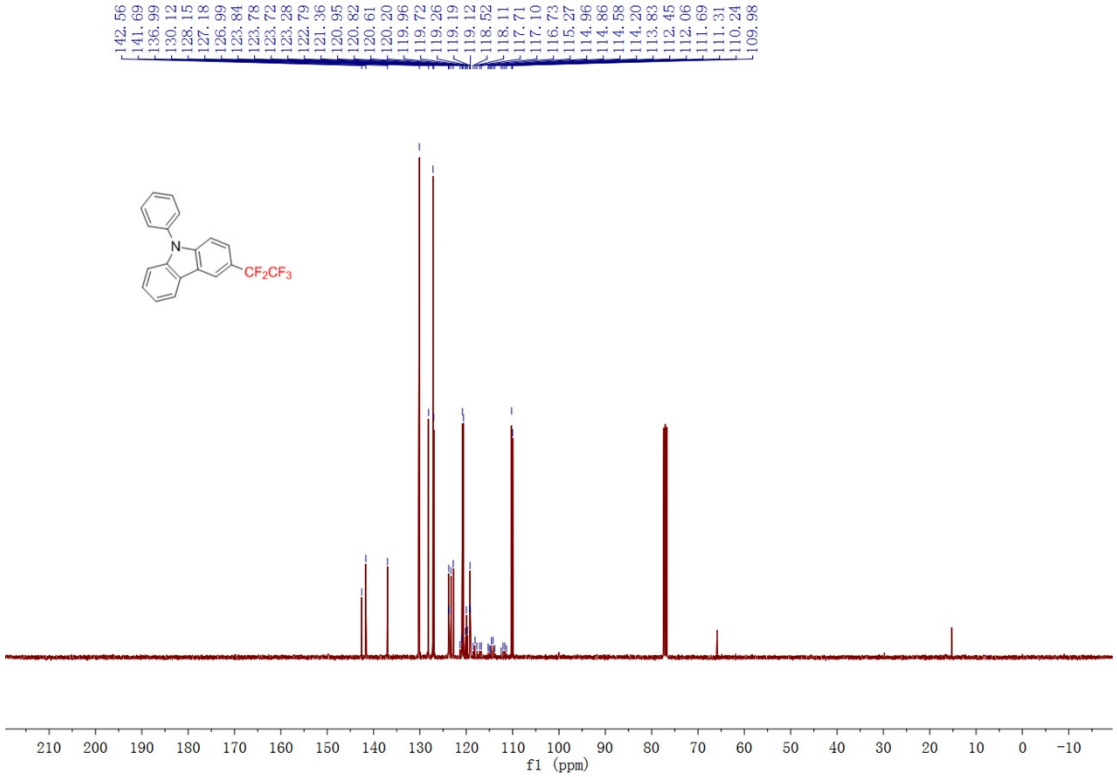
^{19}F NMR spectrum of **3o** in $CDCl_3$



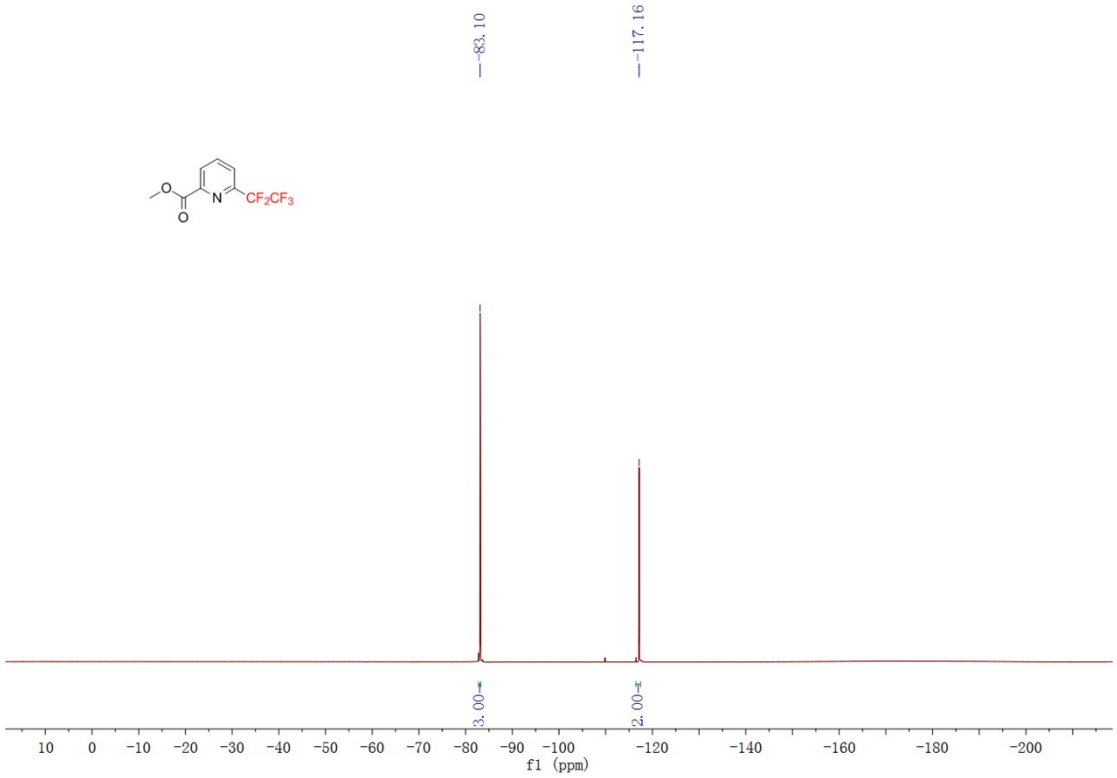
^{1}H NMR spectrum of **3o** in $CDCl_3$



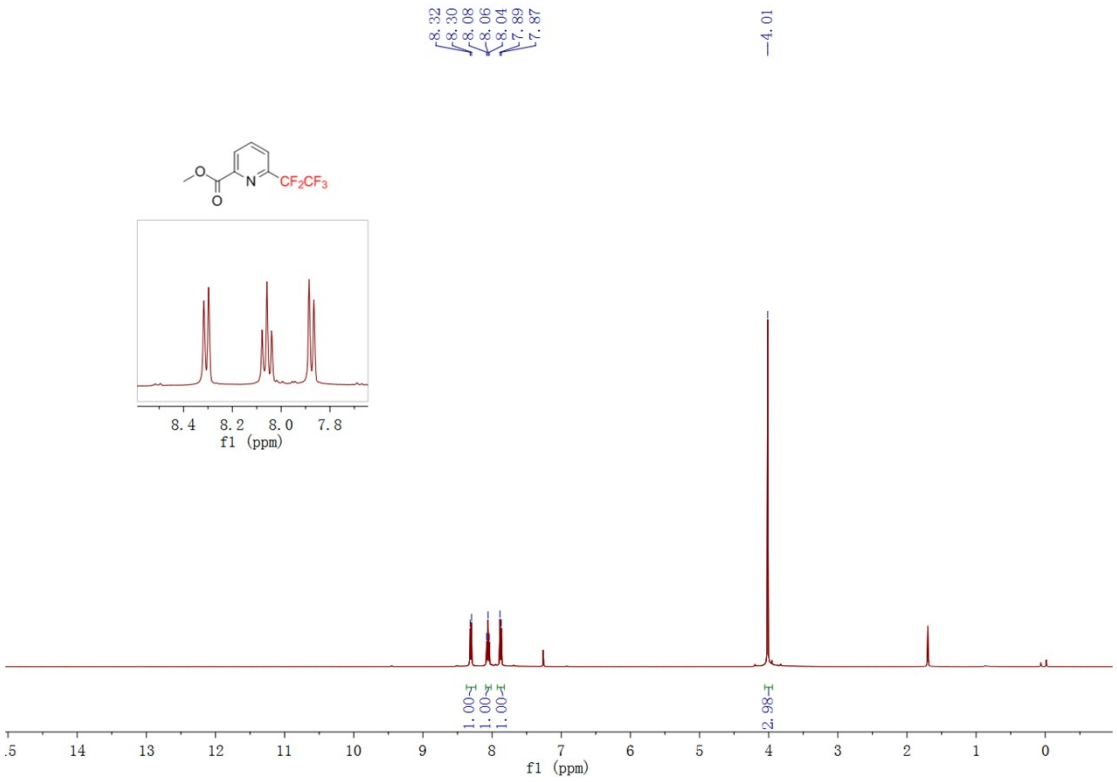
^{13}C NMR spectrum of **3o** in $CDCl_3$



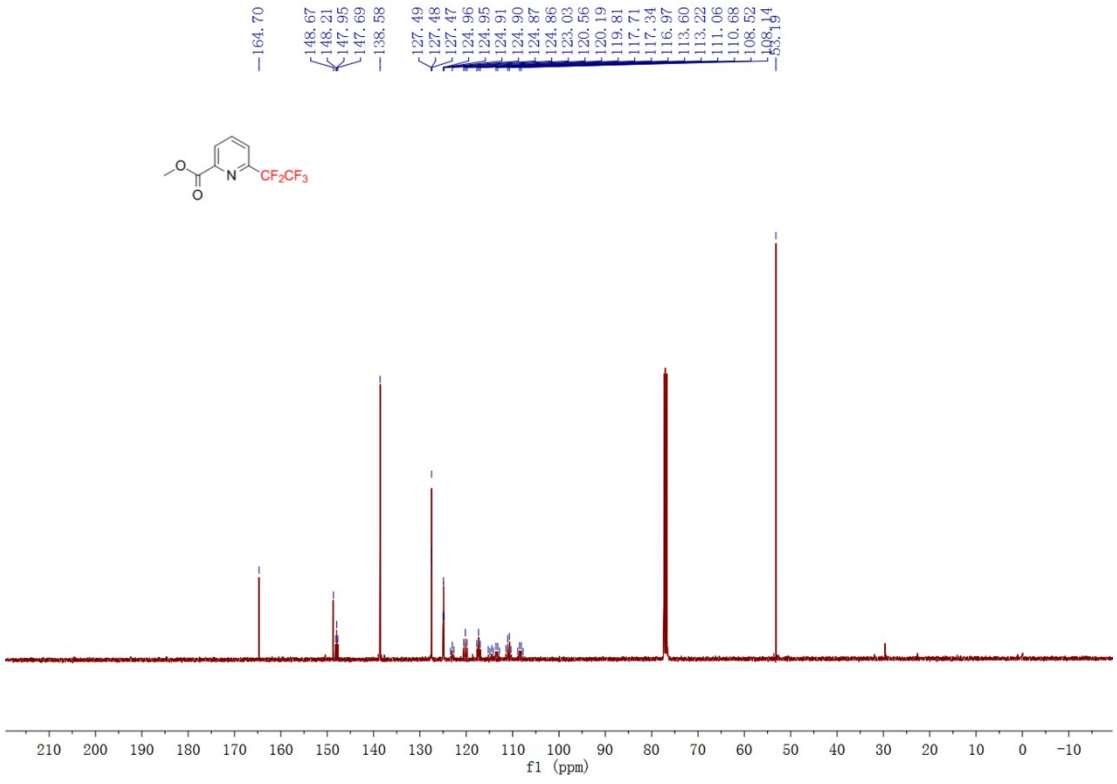
^{19}F NMR spectrum of **3p** in $CDCl_3$



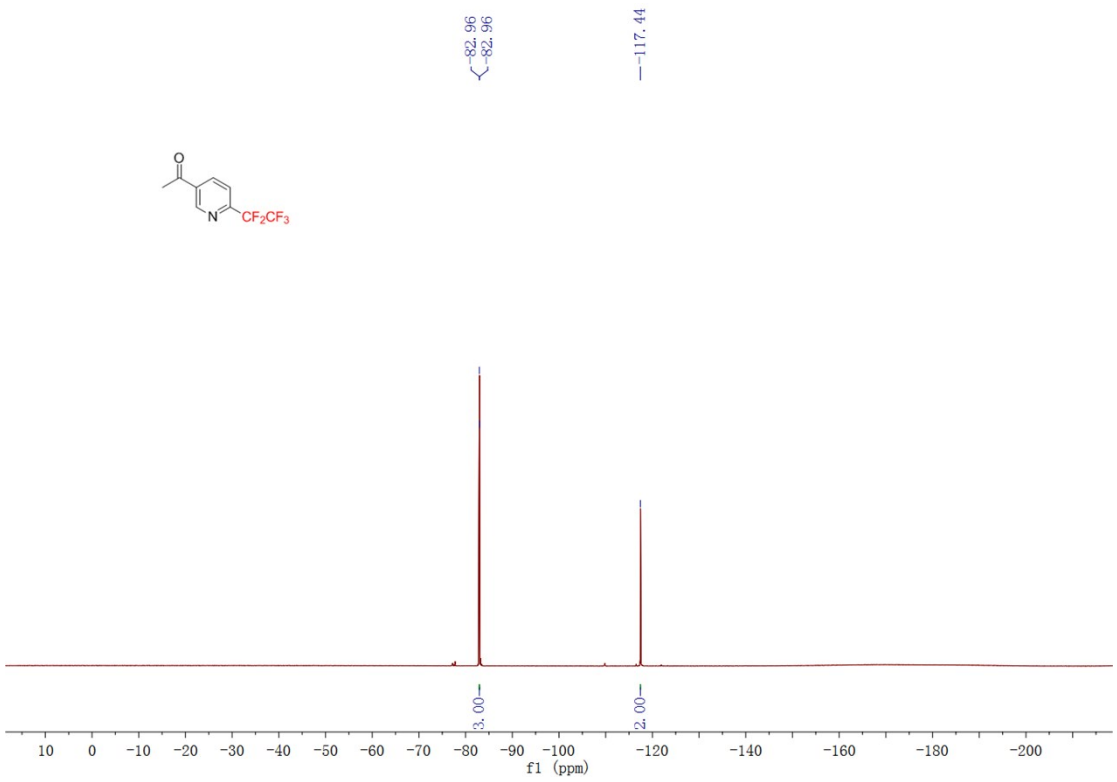
^{1}H NMR spectrum of **3p** in $CDCl_3$



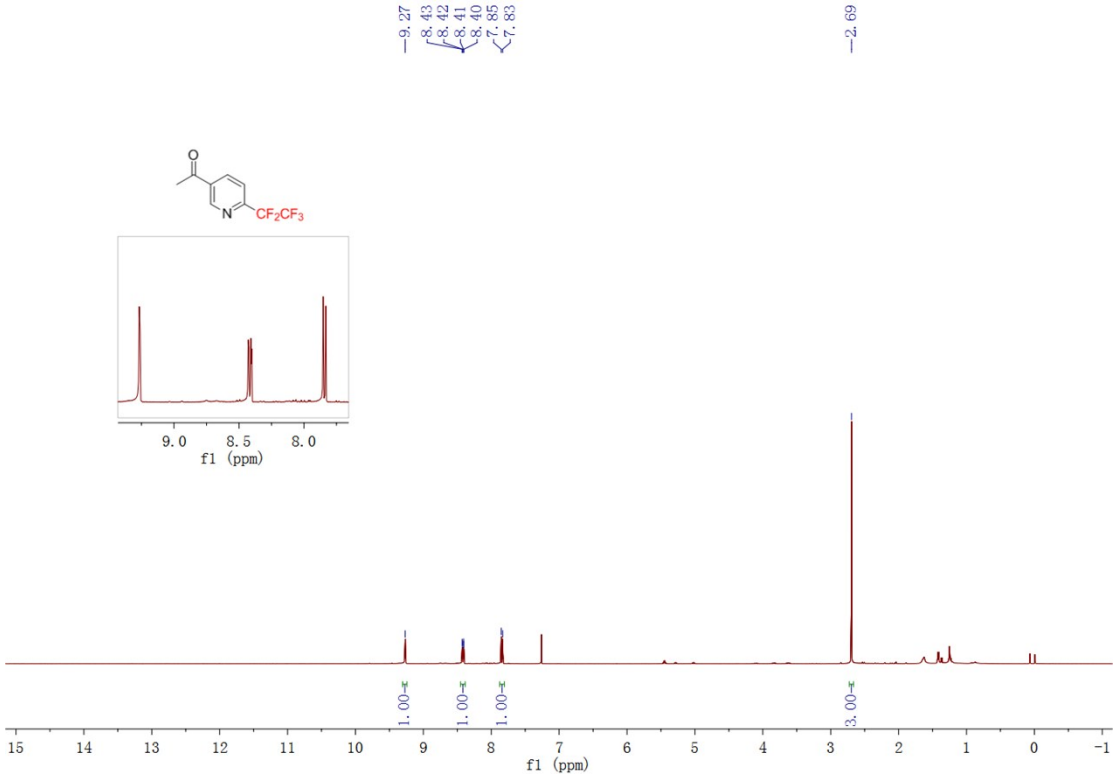
^{13}C NMR spectrum of **3p** in $CDCl_3$



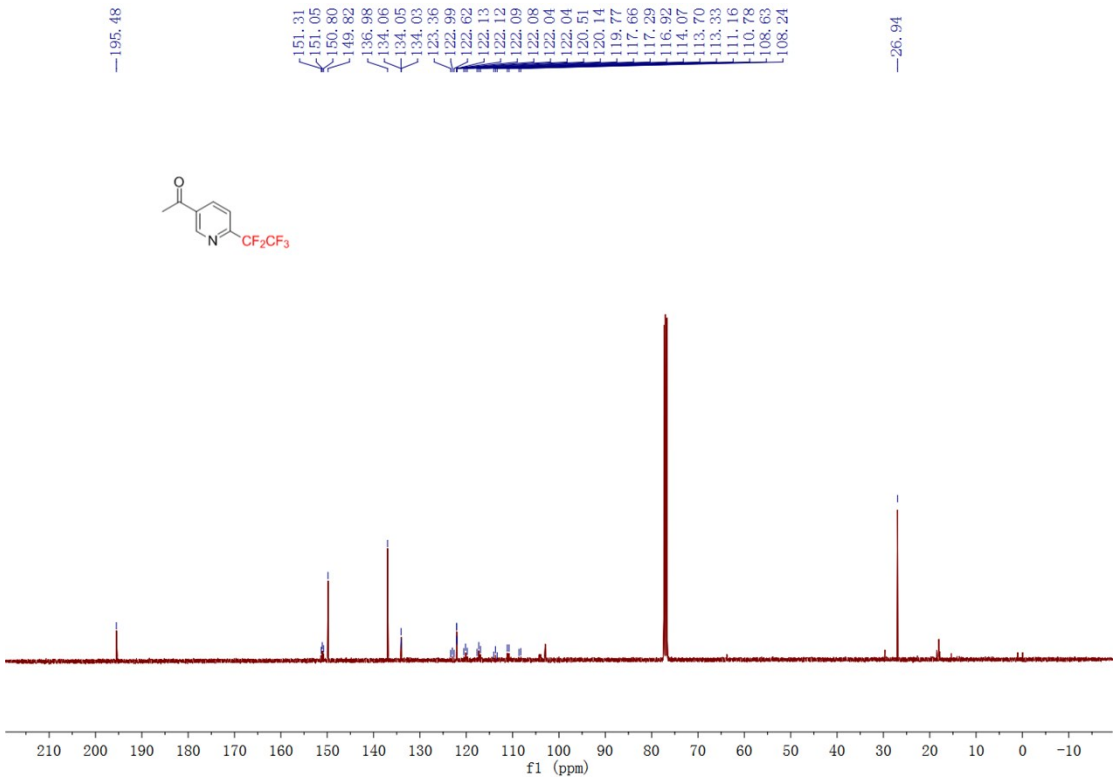
^{19}F NMR spectrum of **3q** in $CDCl_3$



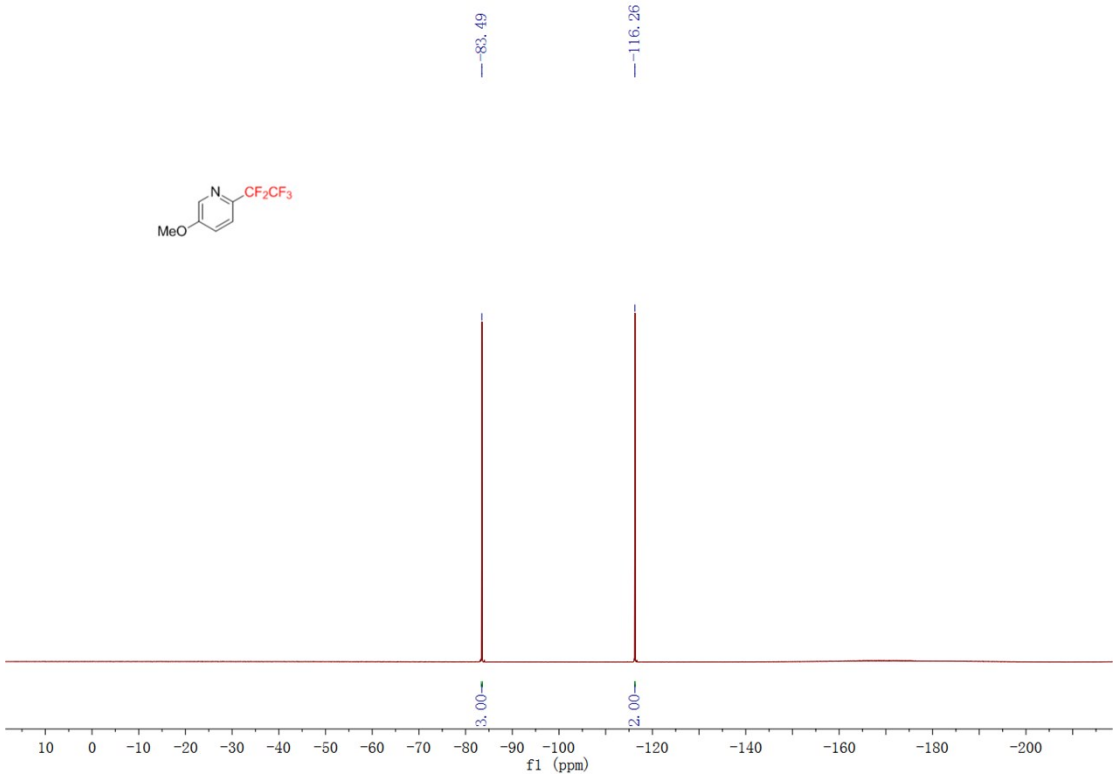
^{1}H NMR spectrum of **3q** in $CDCl_3$



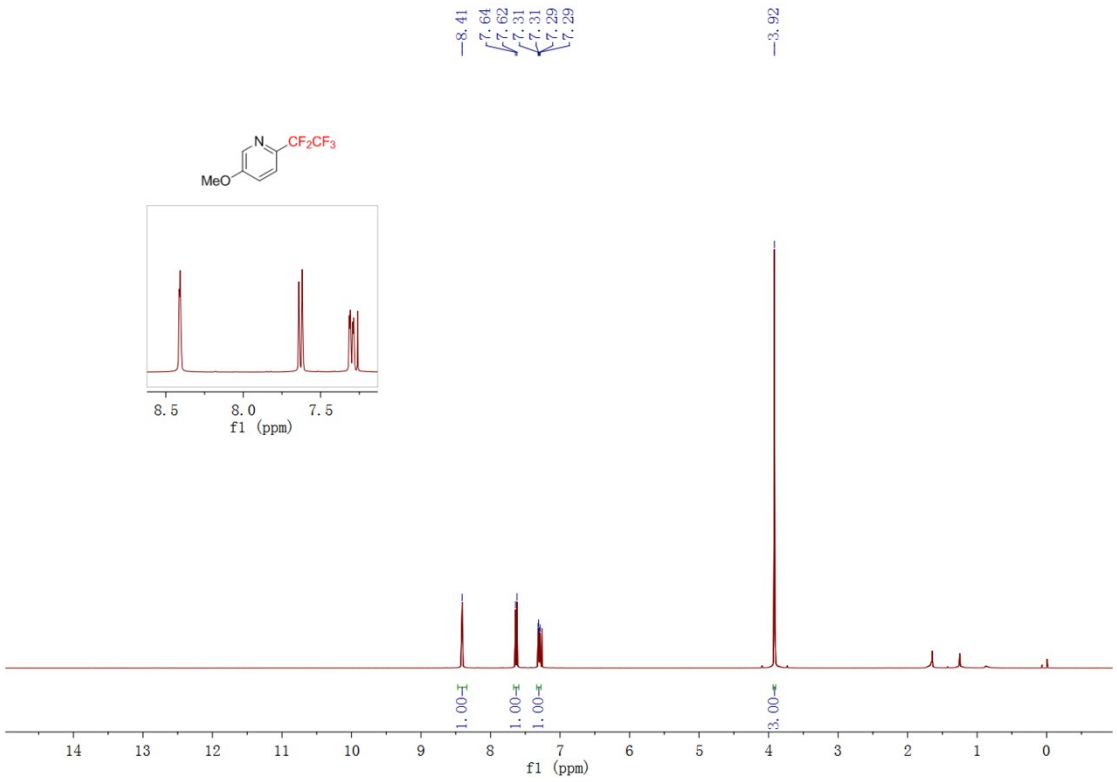
^{13}C NMR spectrum of **3q** in $CDCl_3$



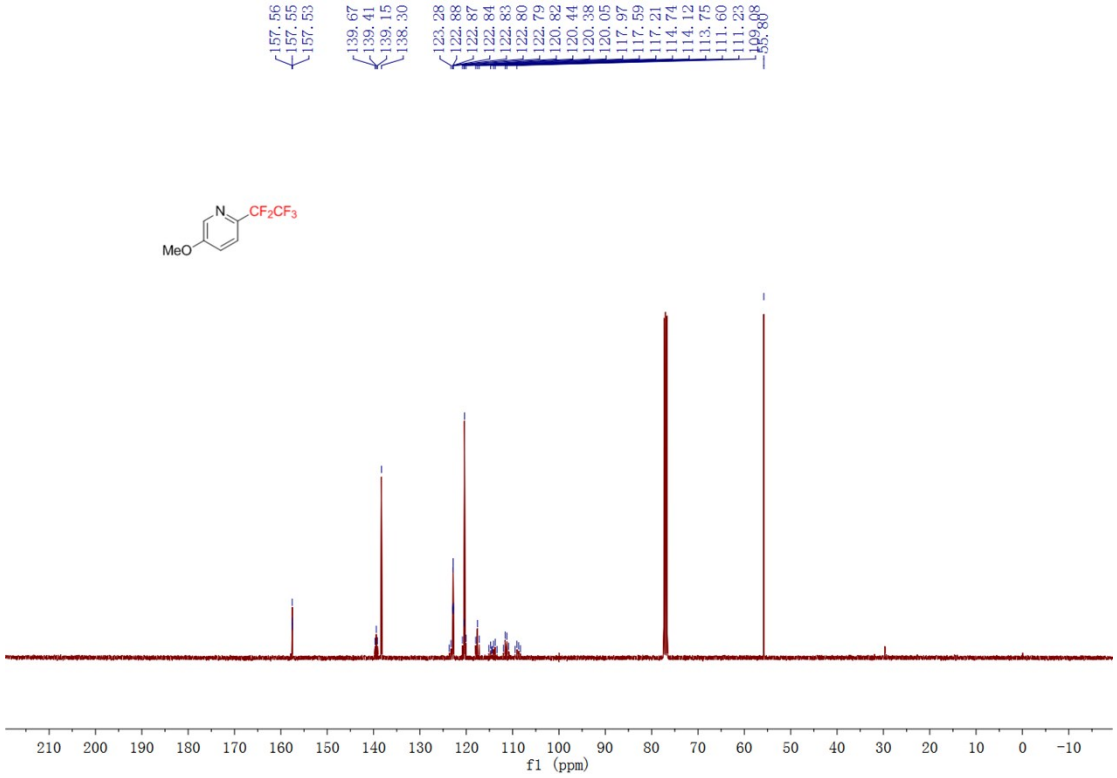
^{19}F NMR spectrum of **3r** in $CDCl_3$



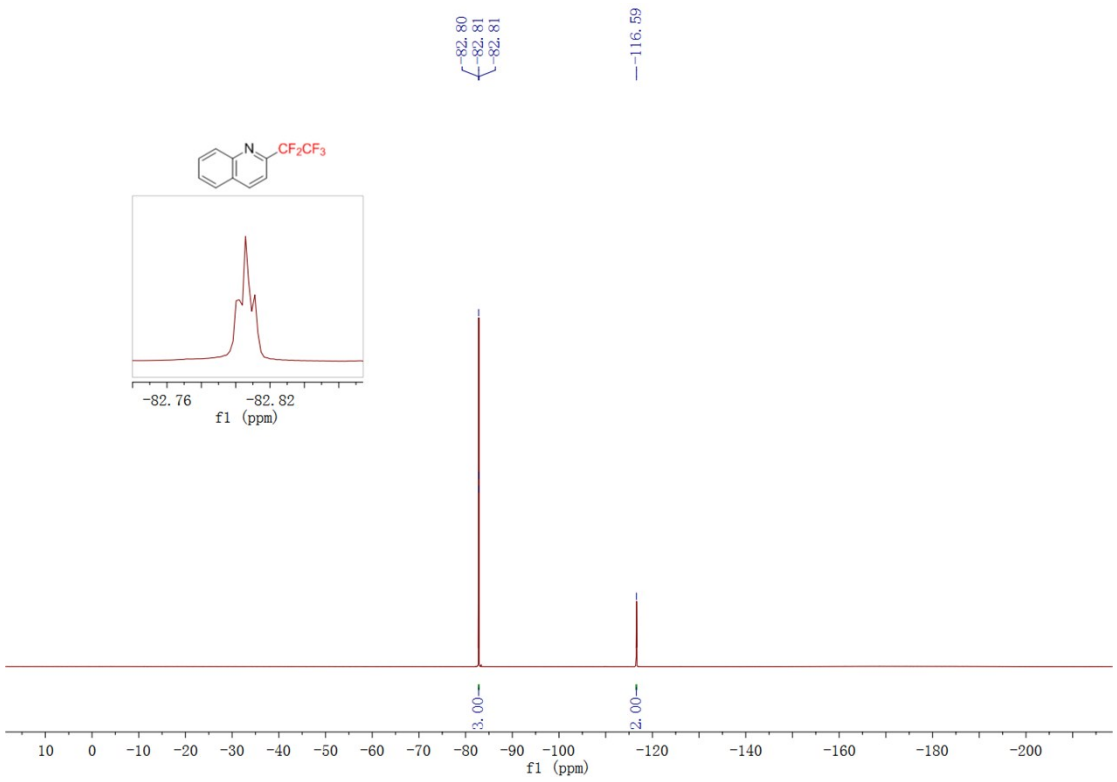
^{1}H NMR spectrum of **3r** in $CDCl_3$



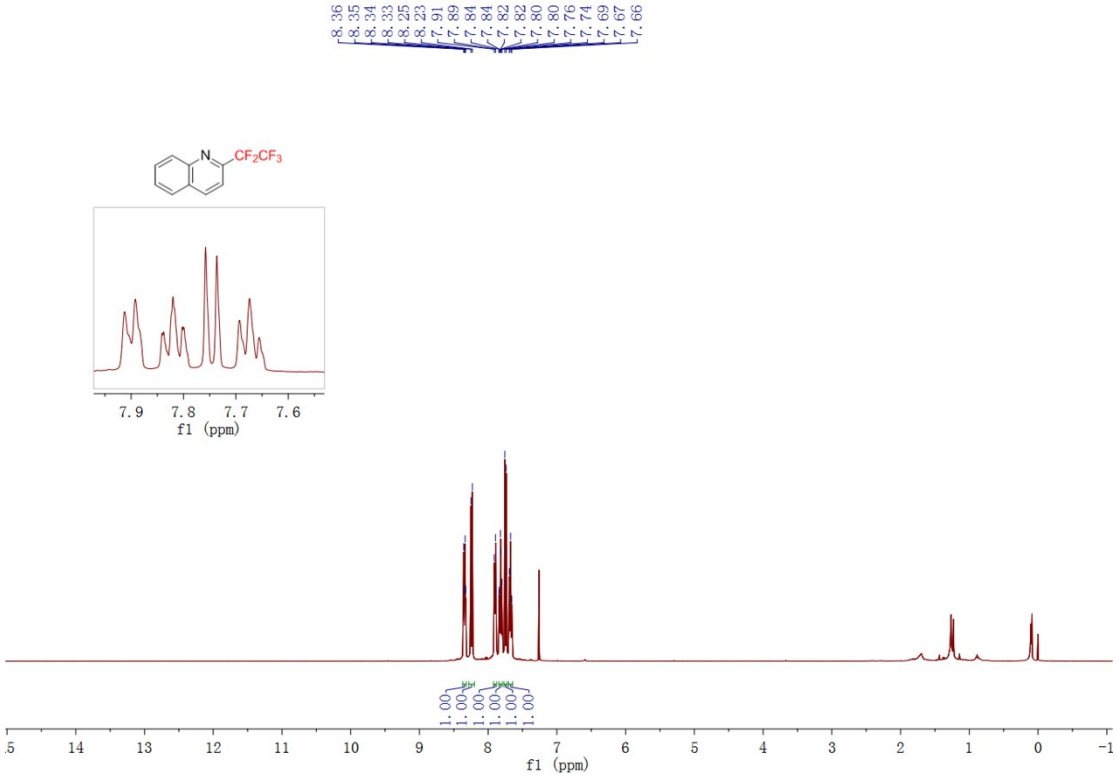
^{13}C NMR spectrum of **3r** in $CDCl_3$



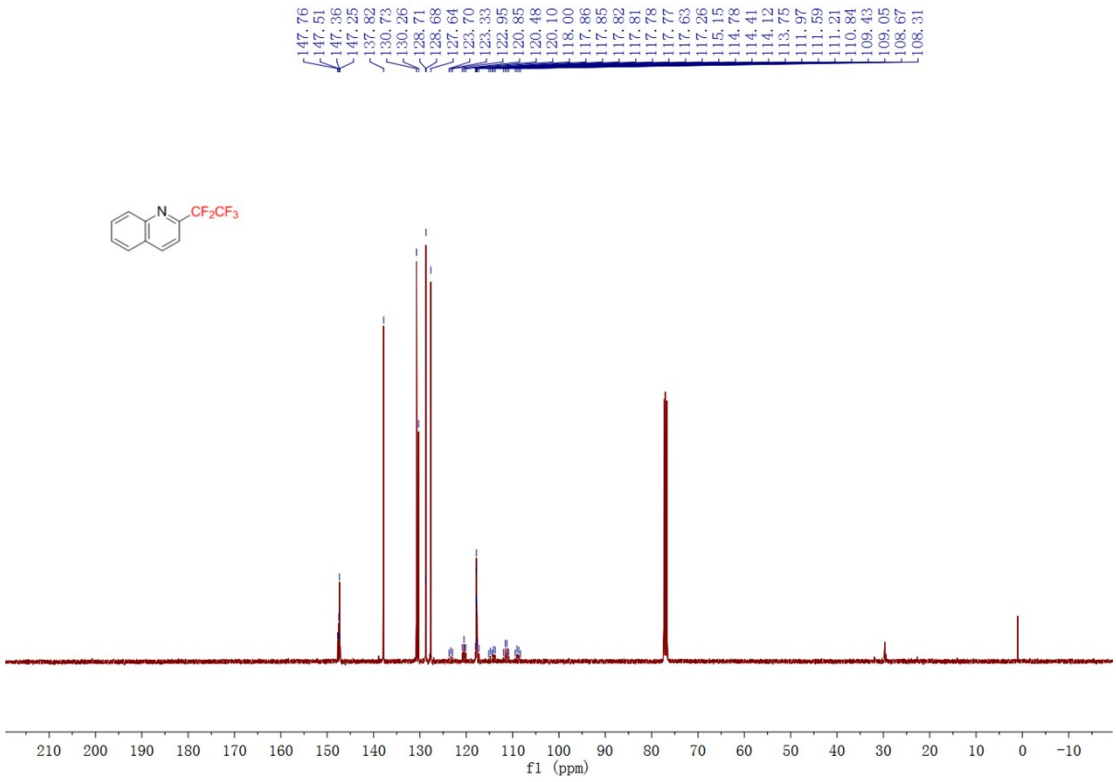
^{19}F NMR spectrum of **3s** in $CDCl_3$



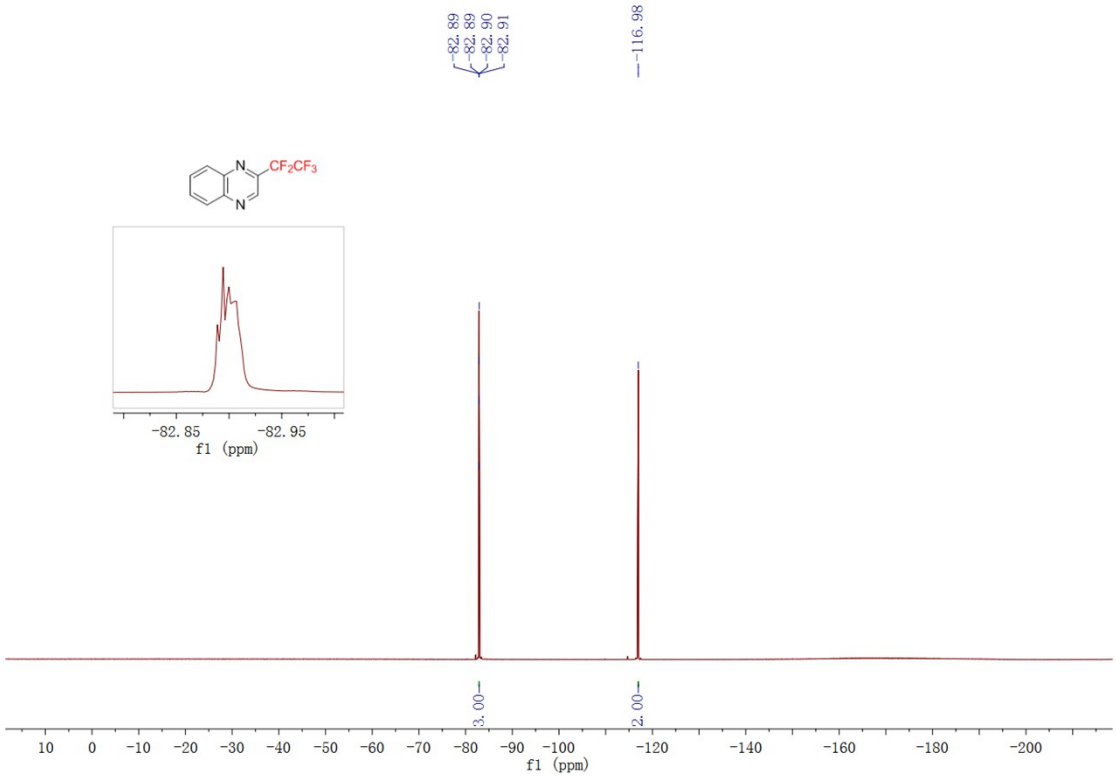
^{1}H NMR spectrum of **3s** in $CDCl_3$



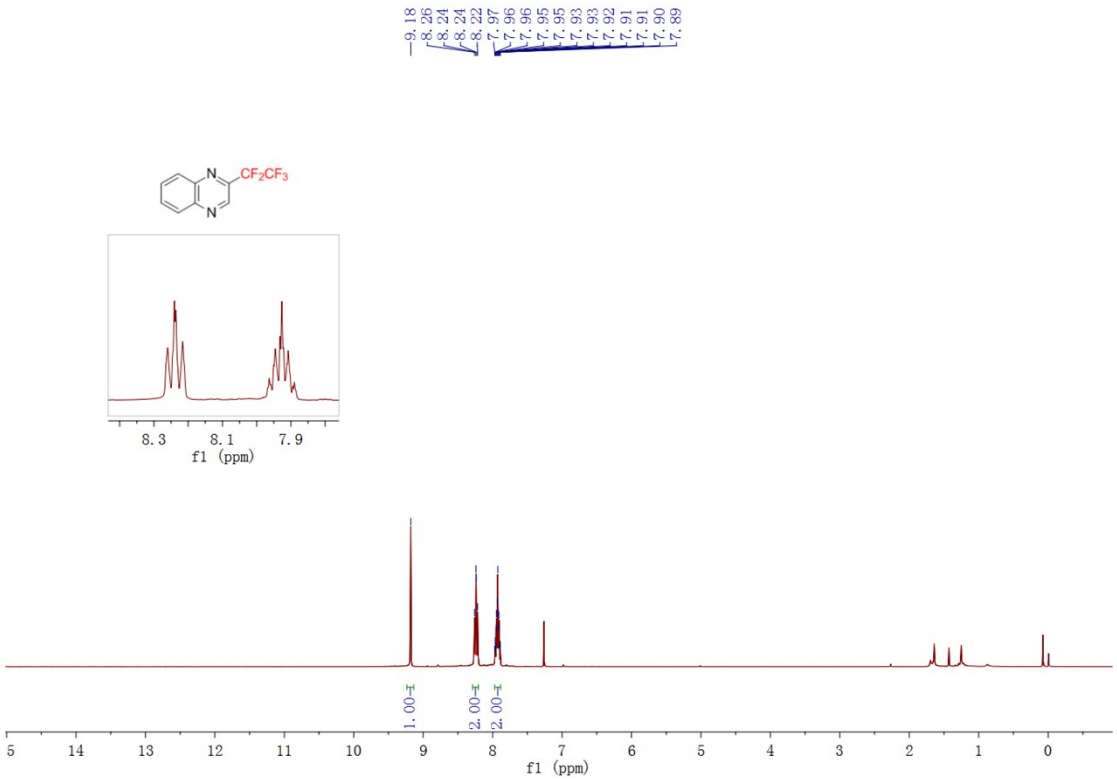
^{13}C NMR spectrum of **3s** in $CDCl_3$



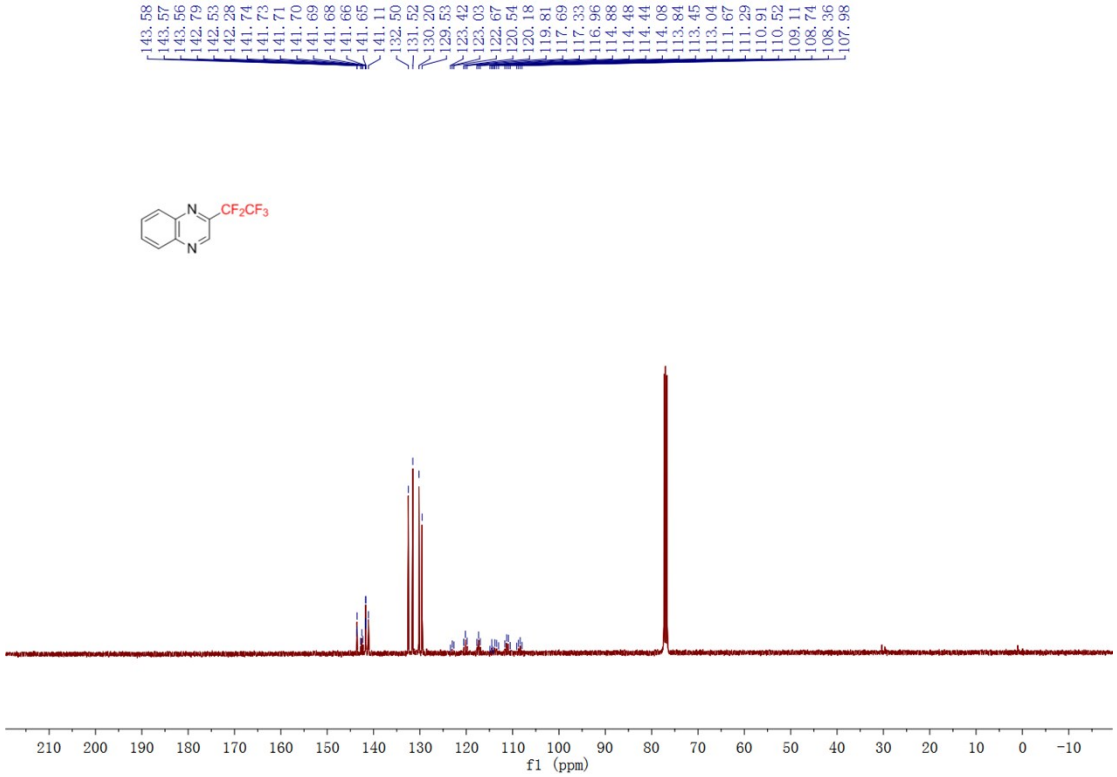
^{19}F NMR spectrum of **3t** in $CDCl_3$



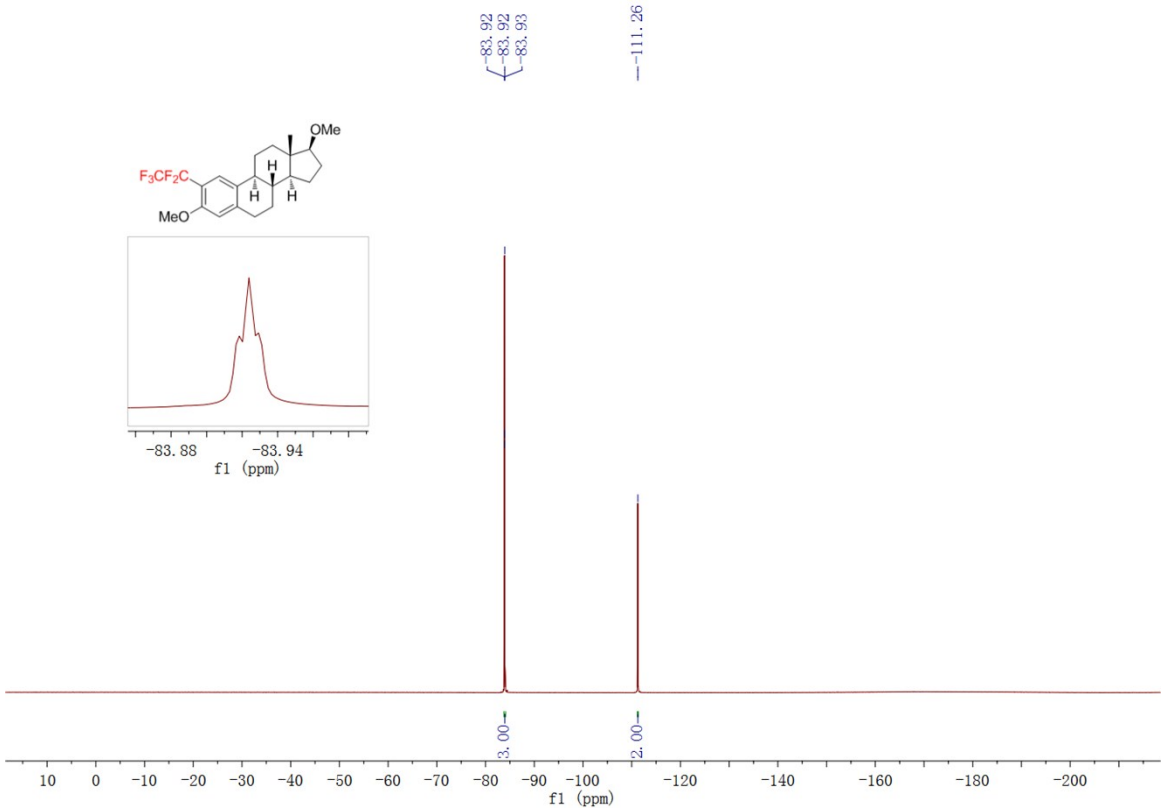
^{1}H NMR spectrum of **3t** in $CDCl_3$



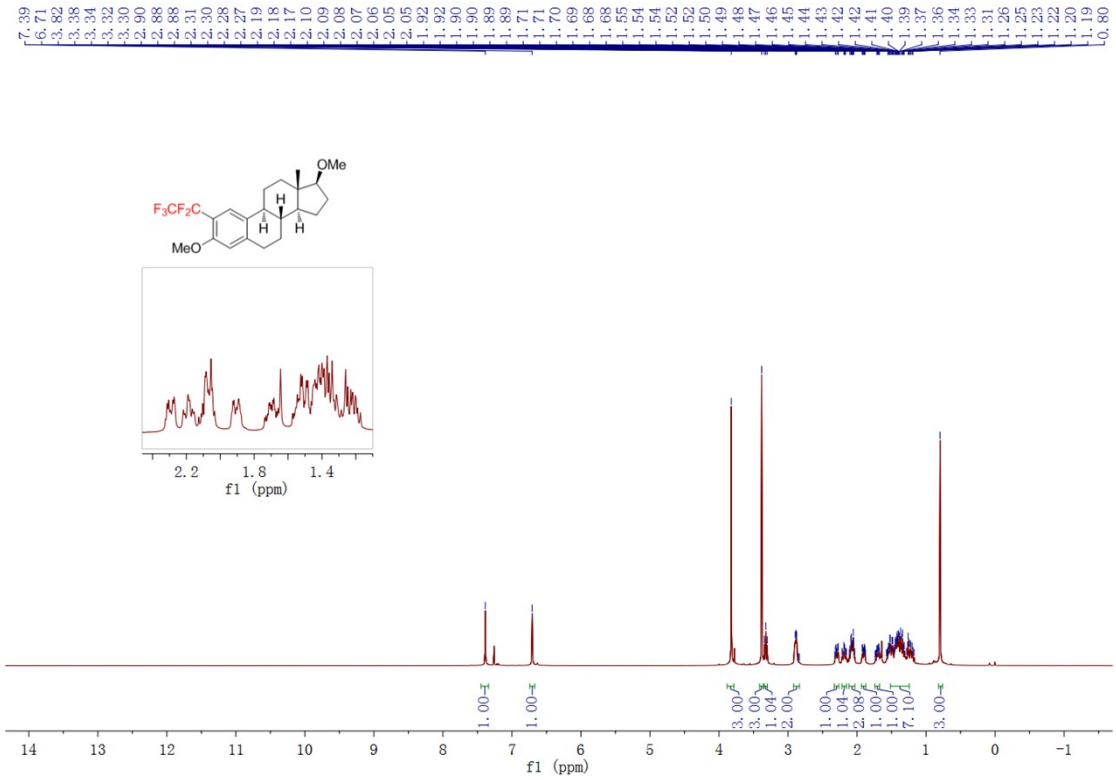
^{13}C NMR spectrum of **3t** in $CDCl_3$



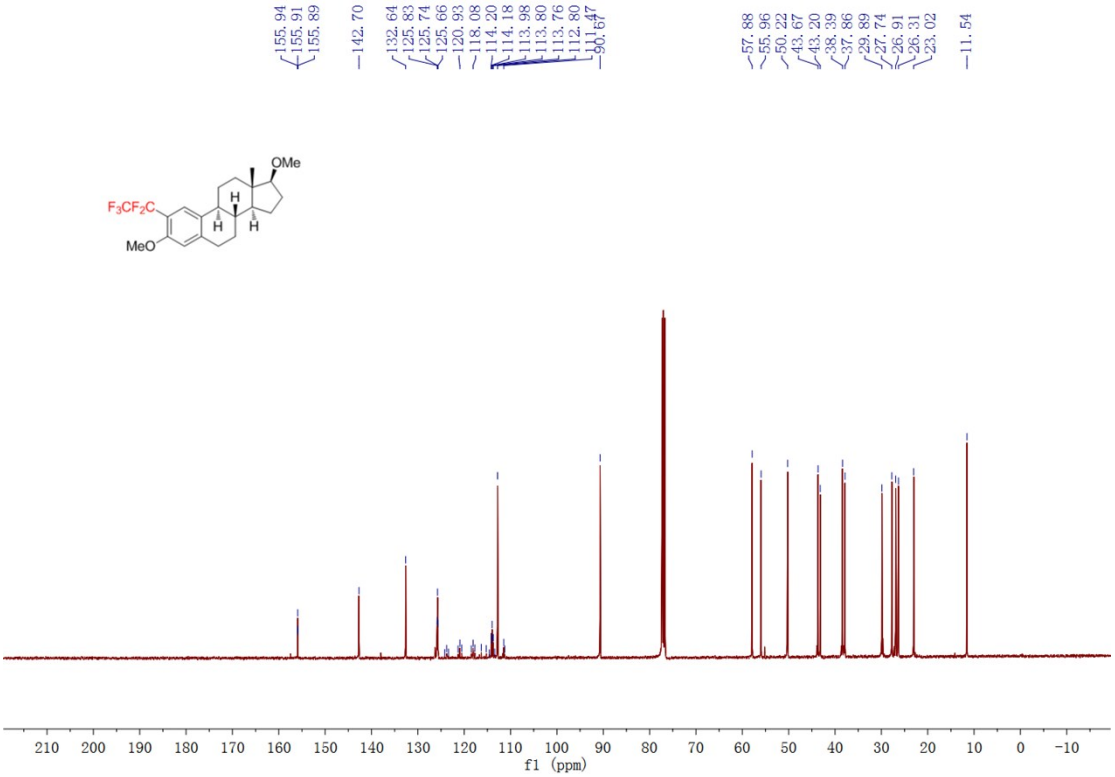
^{19}F NMR spectrum of **3u** in $CDCl_3$



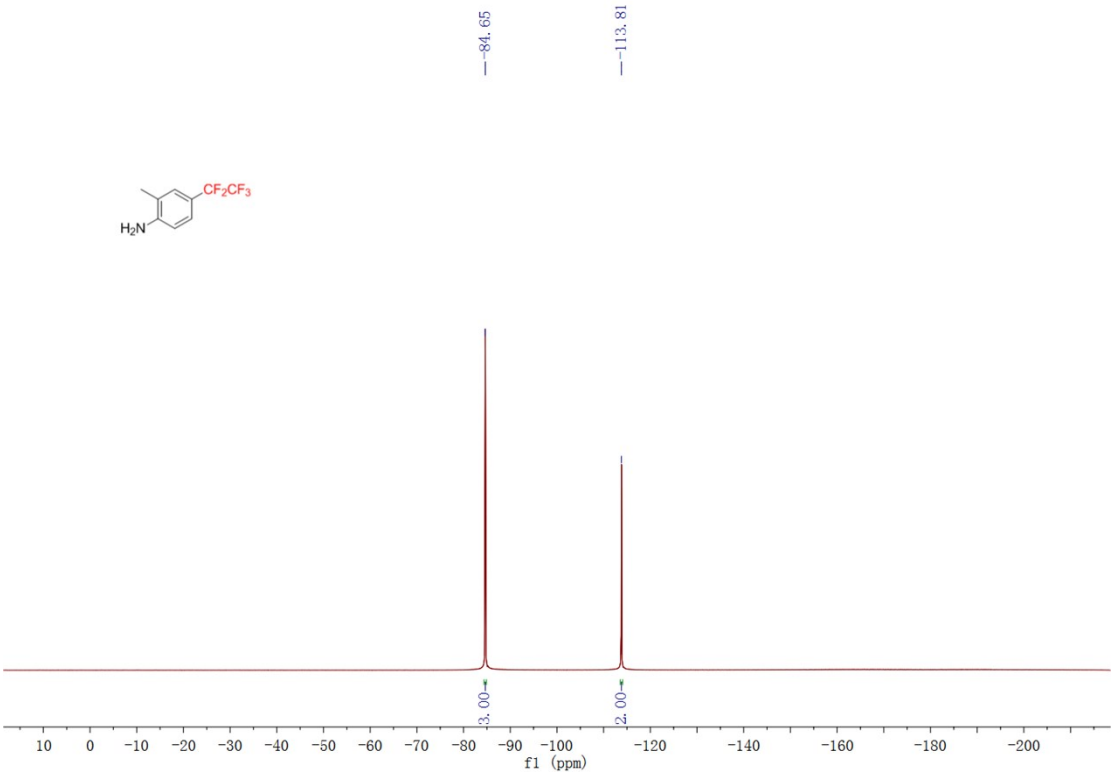
^{1}H NMR spectrum of **3u** in $CDCl_3$



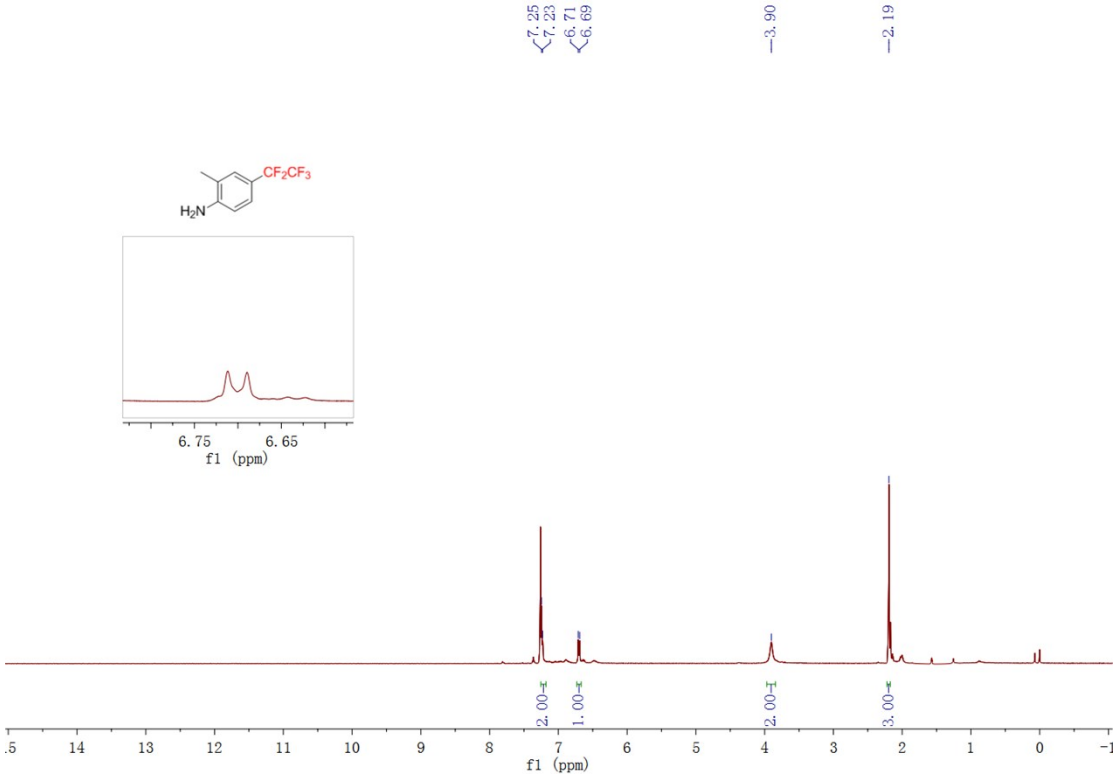
^{13}C NMR spectrum of **3u** in $CDCl_3$



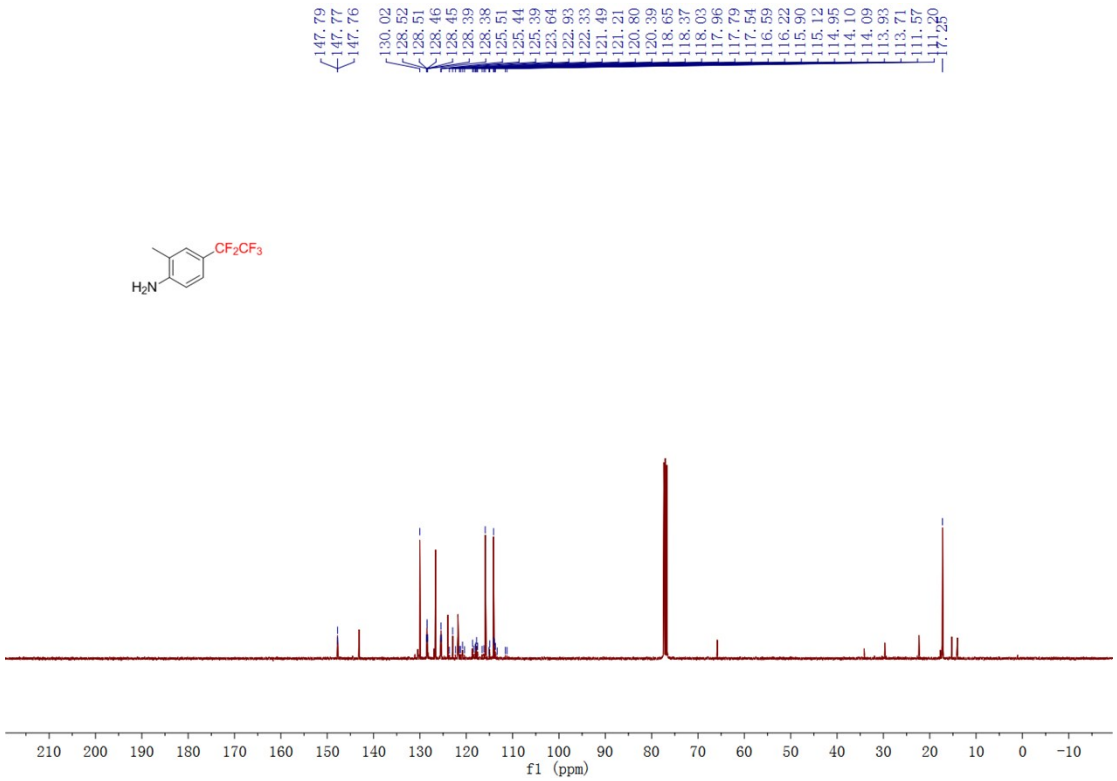
^{19}F NMR spectrum of **3v** in $CDCl_3$



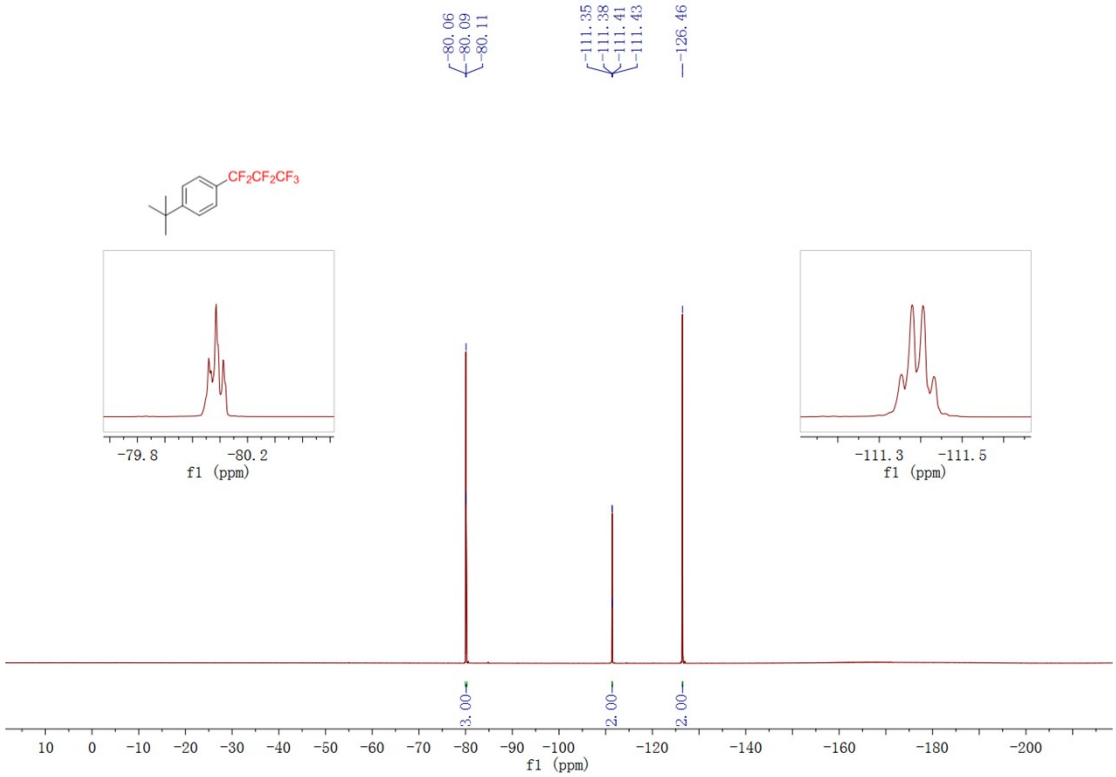
^{1}H NMR spectrum of **3v** in $CDCl_3$



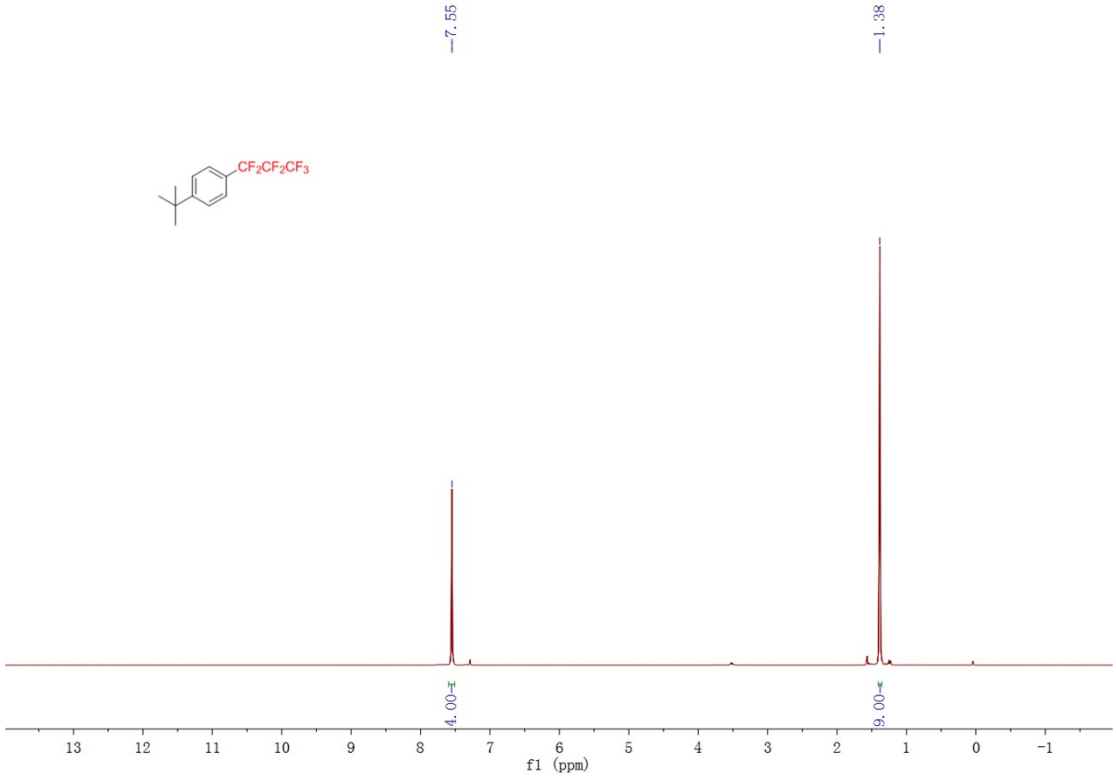
^{13}C NMR spectrum of **3v** in $CDCl_3$



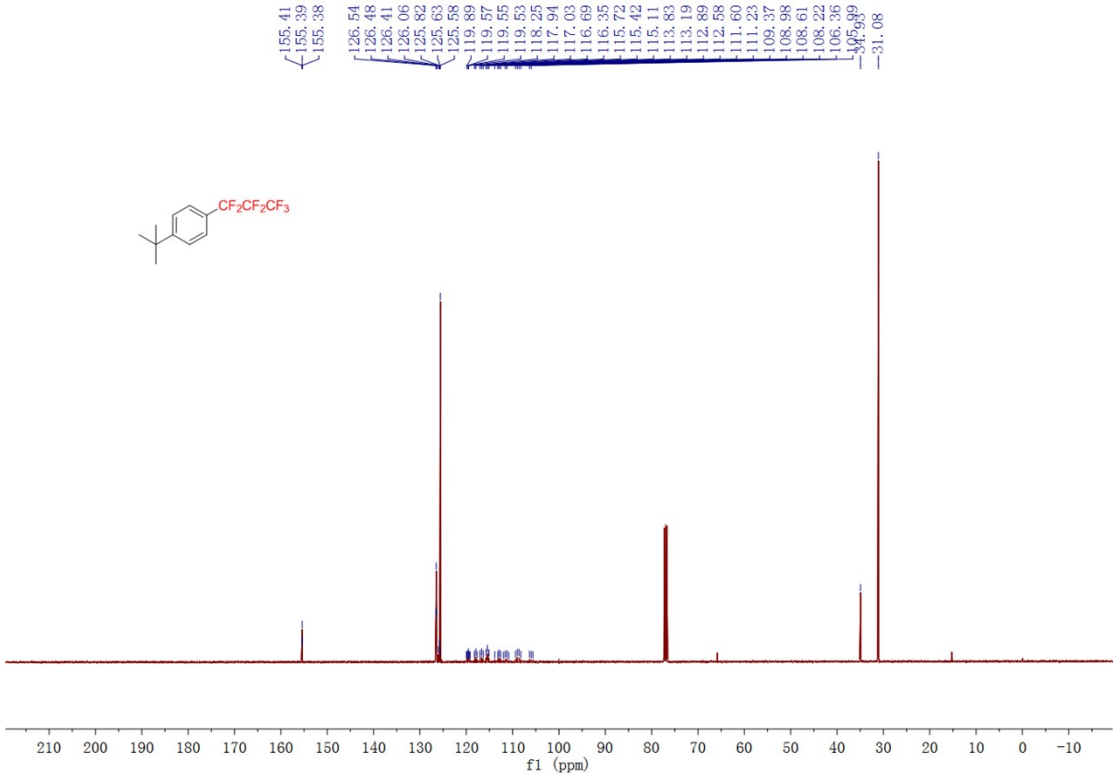
^{19}F NMR spectrum of **4a** in $CDCl_3$



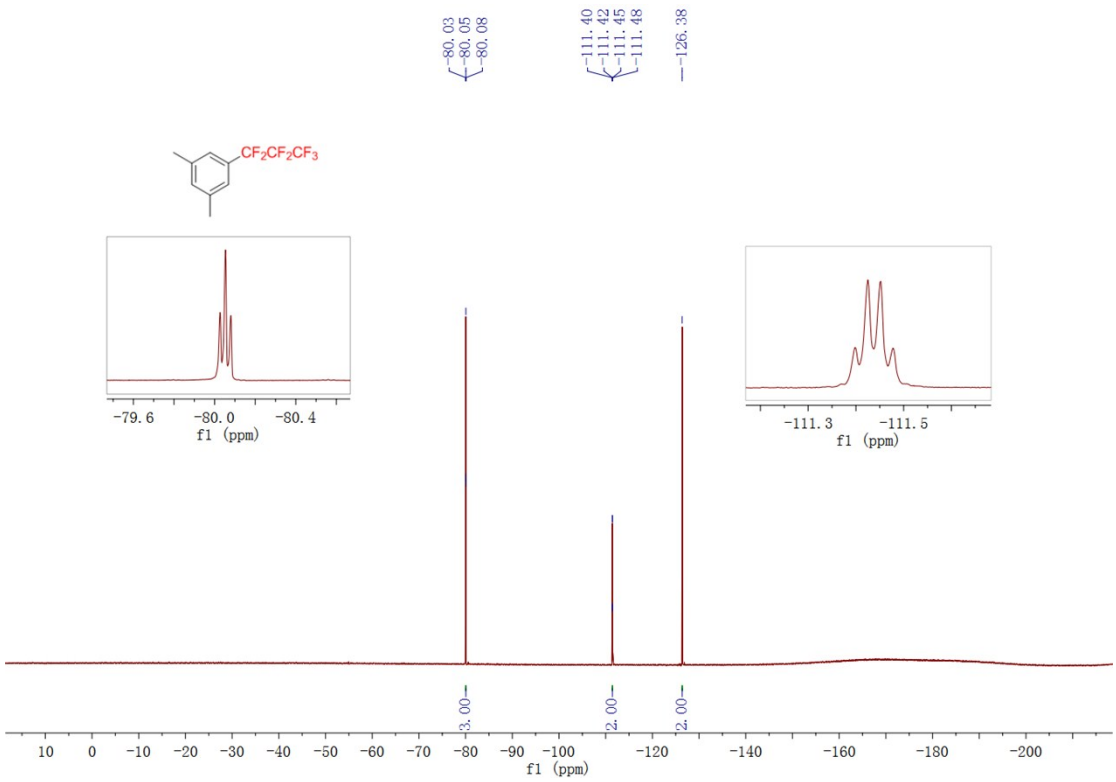
^{1}H NMR spectrum of **4a** in $CDCl_3$



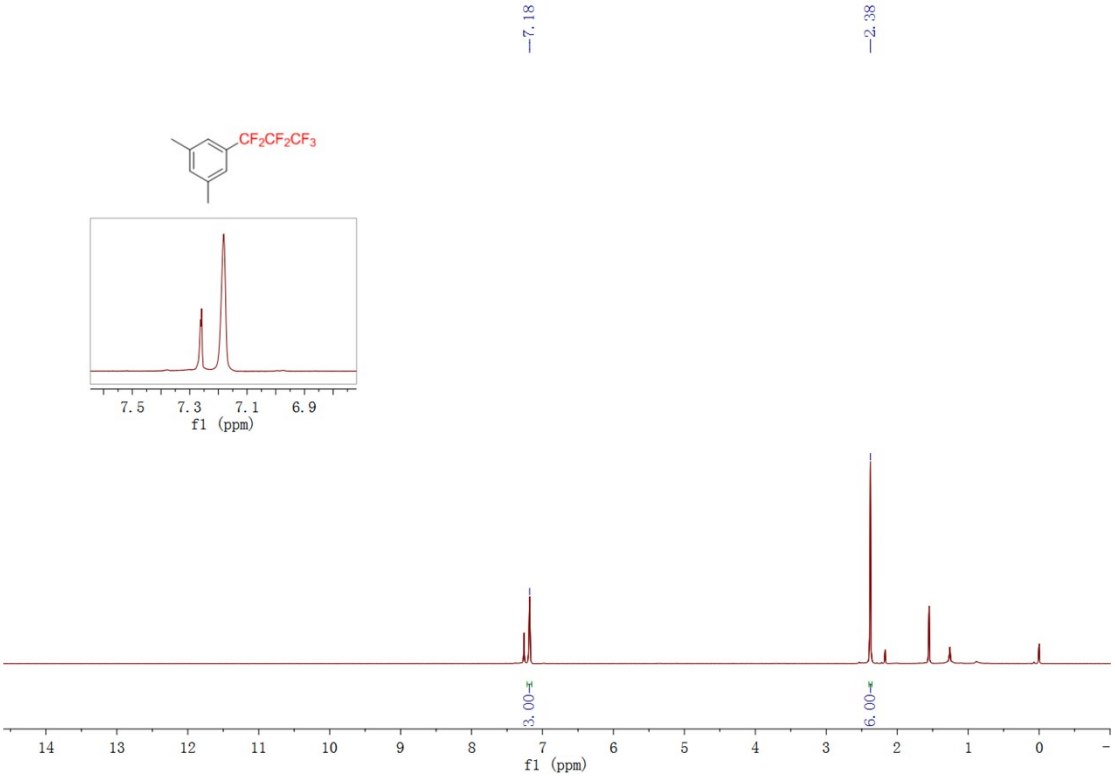
^{13}C NMR spectrum of **4a** in $CDCl_3$



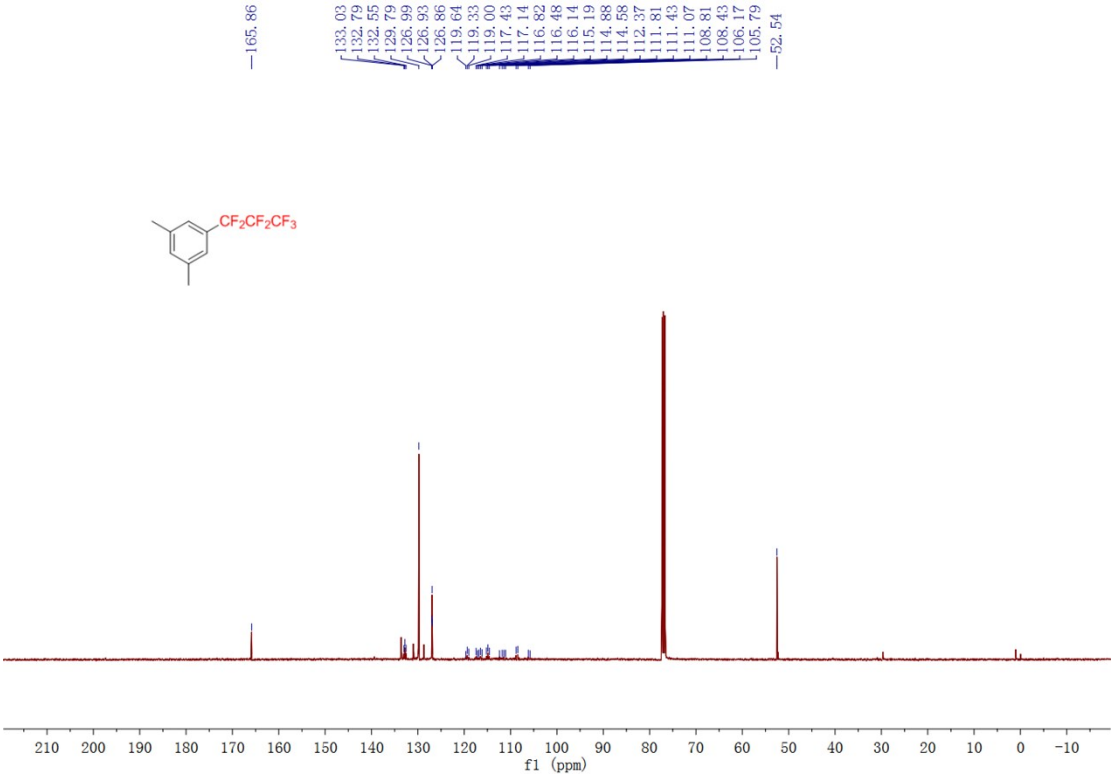
^{19}F NMR spectrum of **4b** in $CDCl_3$



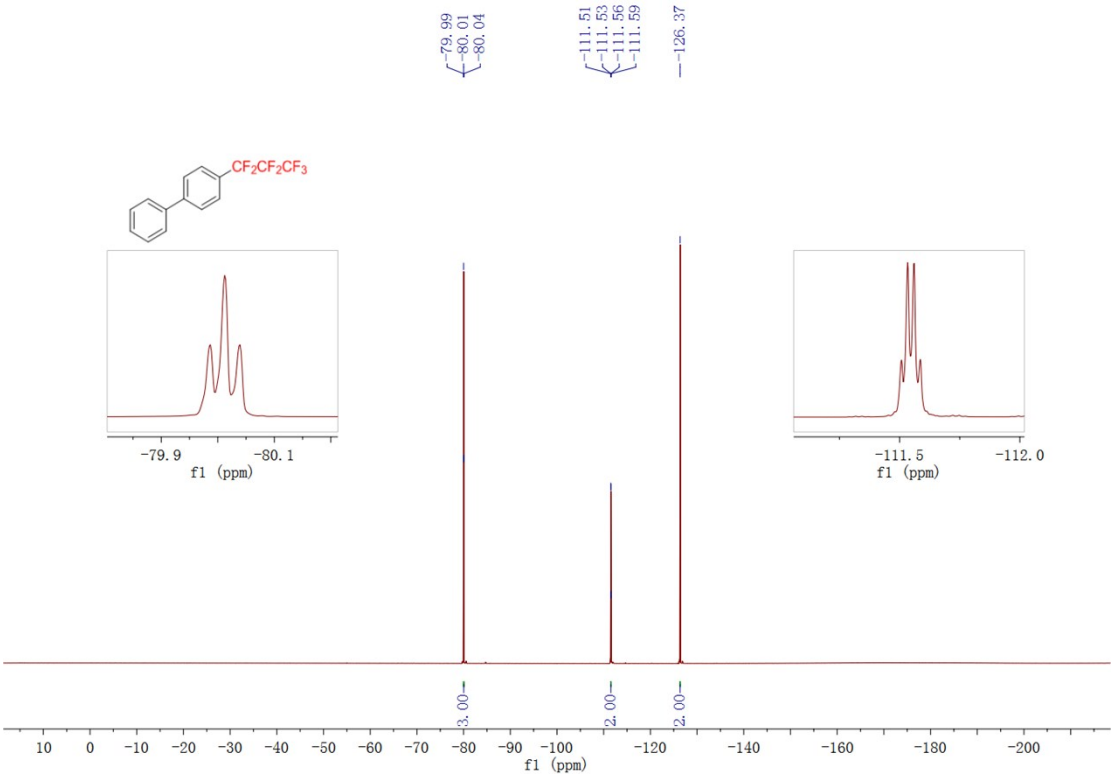
^{1}H NMR spectrum of **4b** in $CDCl_3$



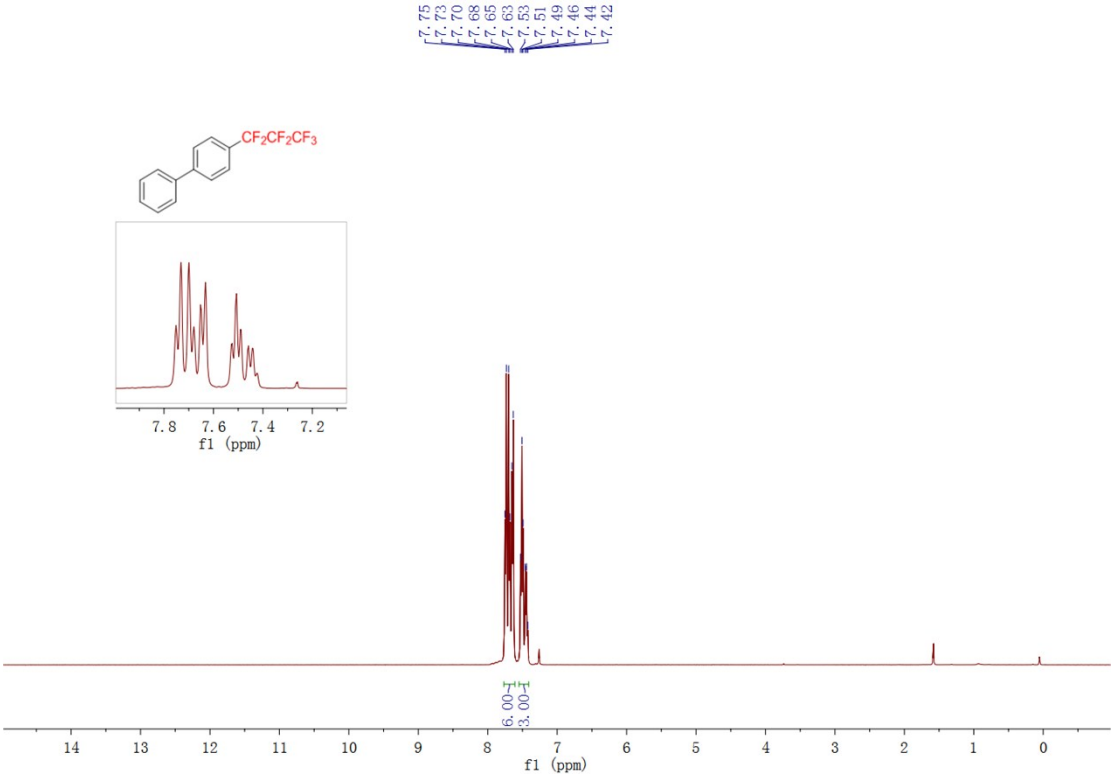
^{13}C NMR spectrum of **4b** in $CDCl_3$



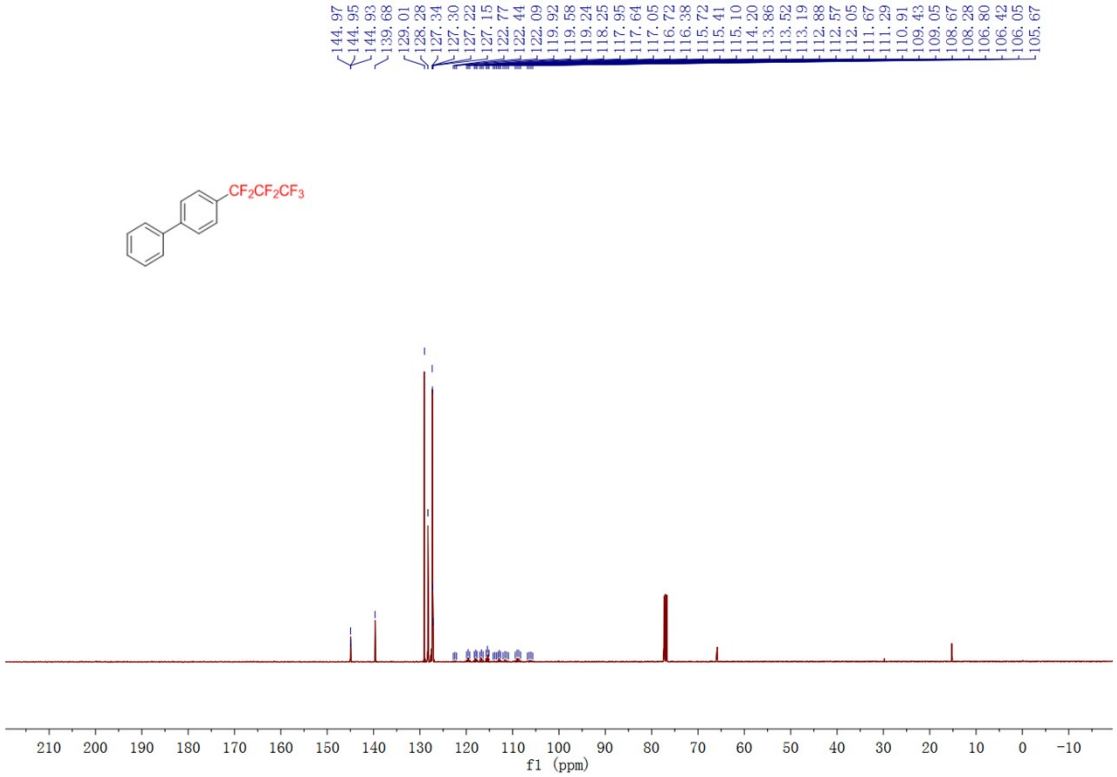
^{19}F NMR spectrum of **4c** in $CDCl_3$



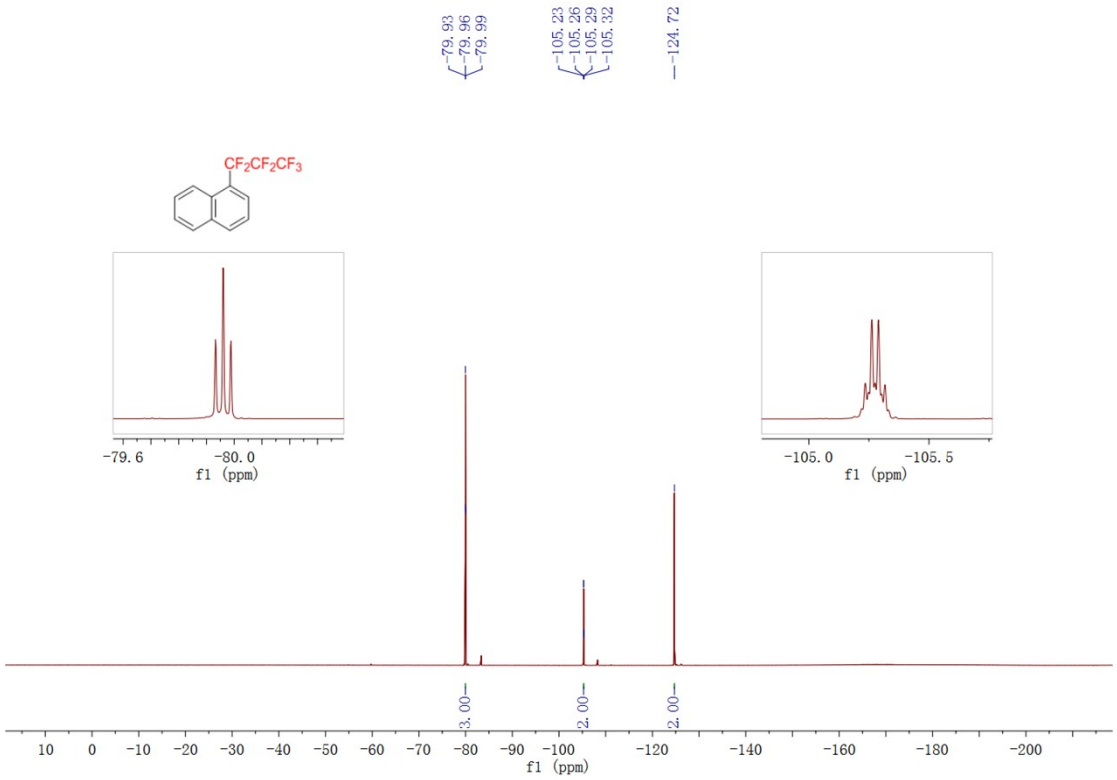
^{1}H NMR spectrum of **4c** in $CDCl_3$



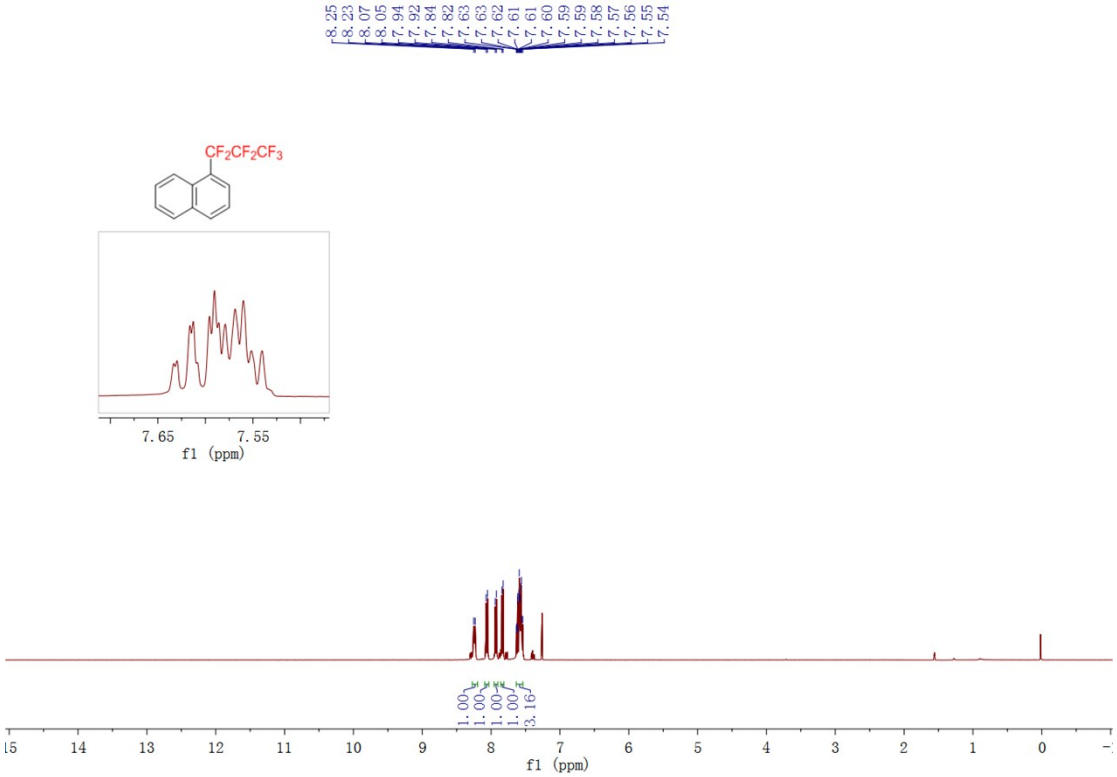
^{13}C NMR spectrum of **4c** in $CDCl_3$



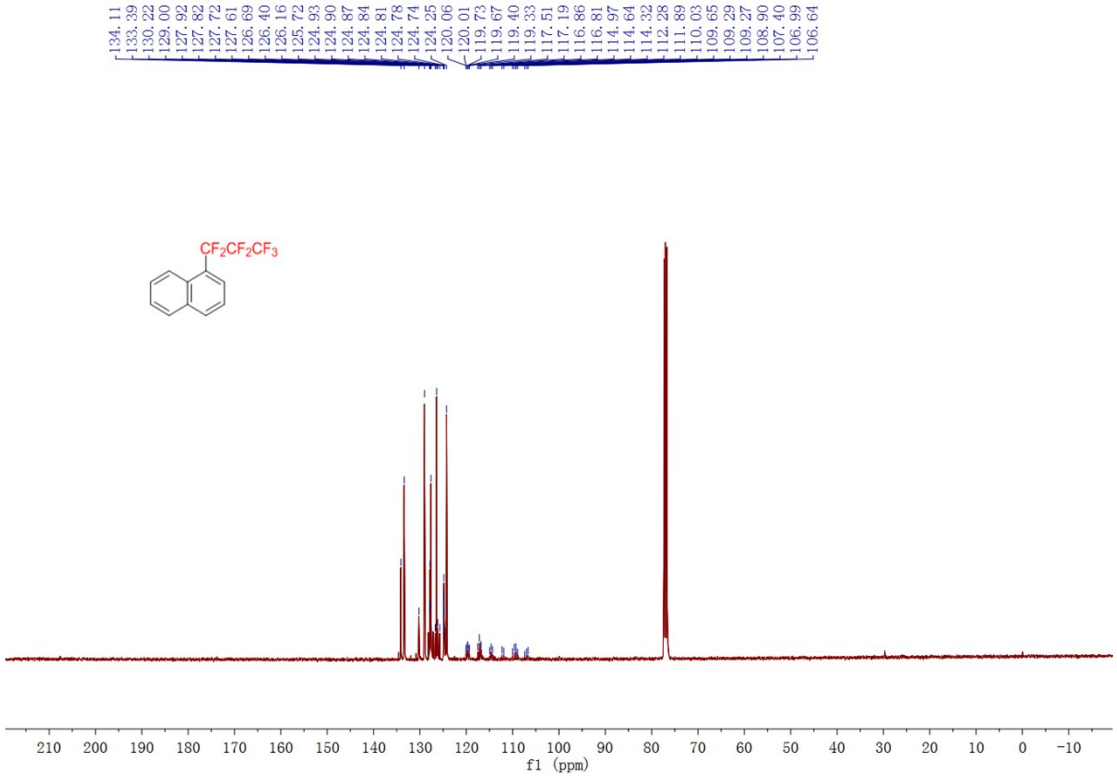
^{19}F NMR spectrum of **4e** in $CDCl_3$



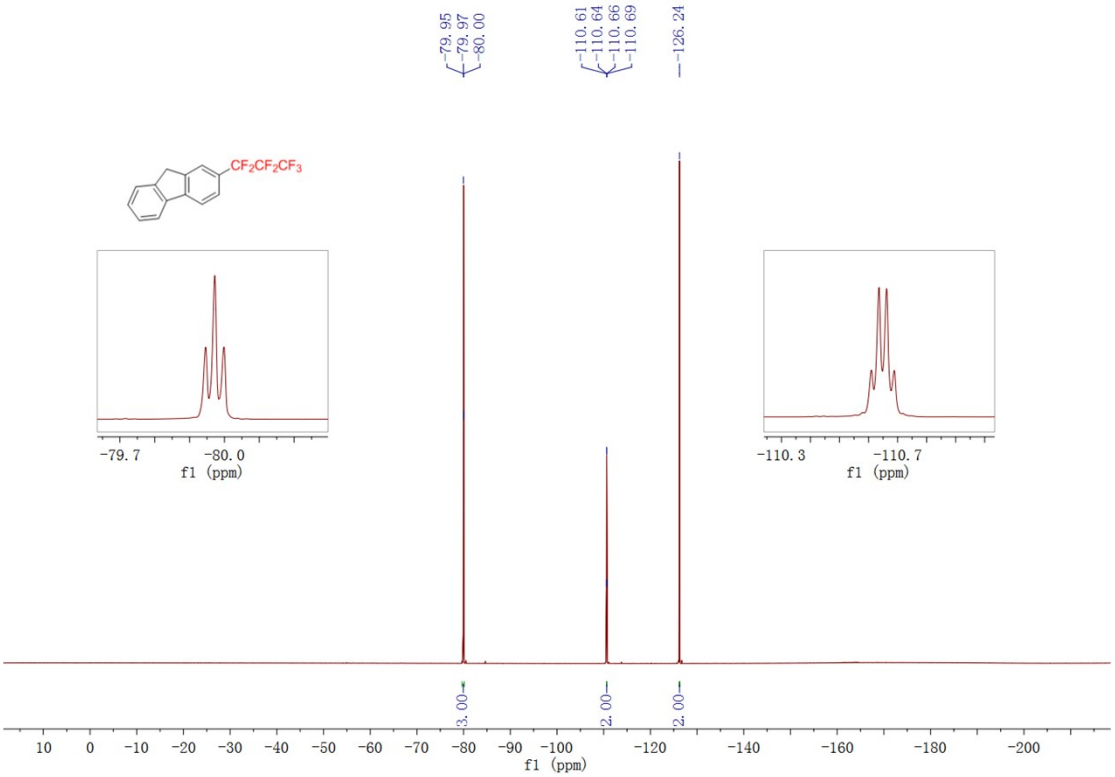
^{1}H NMR spectrum of **4e** in $CDCl_3$



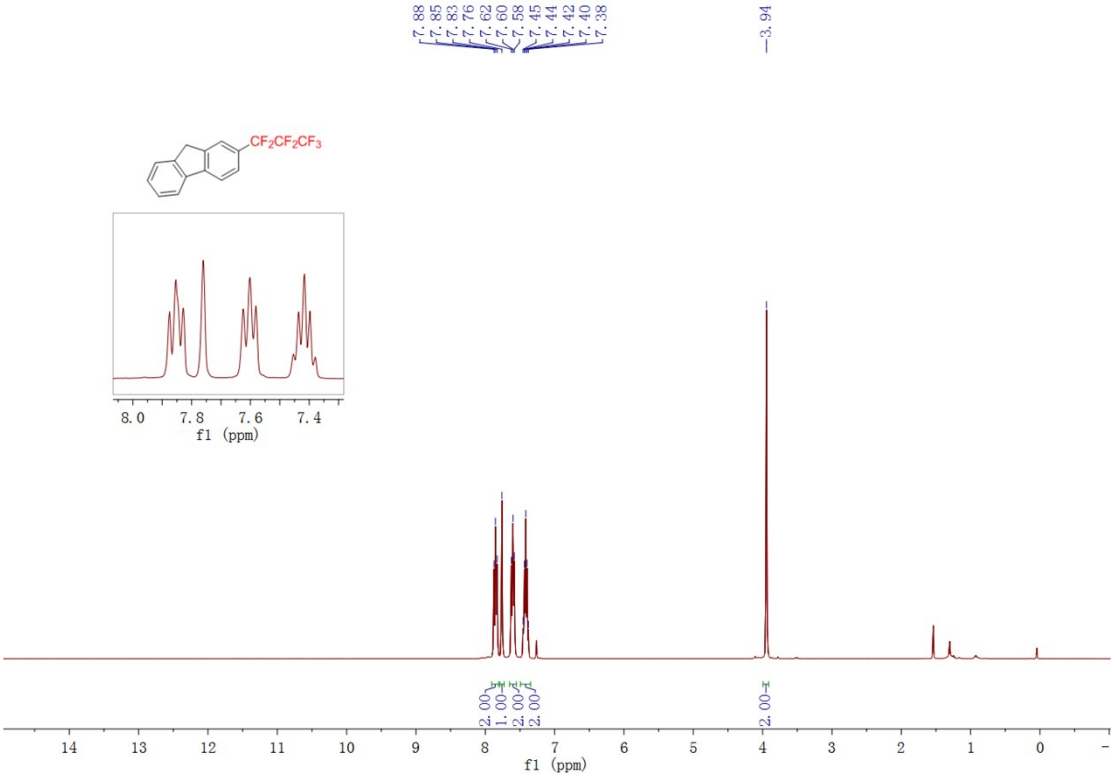
^{13}C NMR spectrum of **4e** in $CDCl_3$



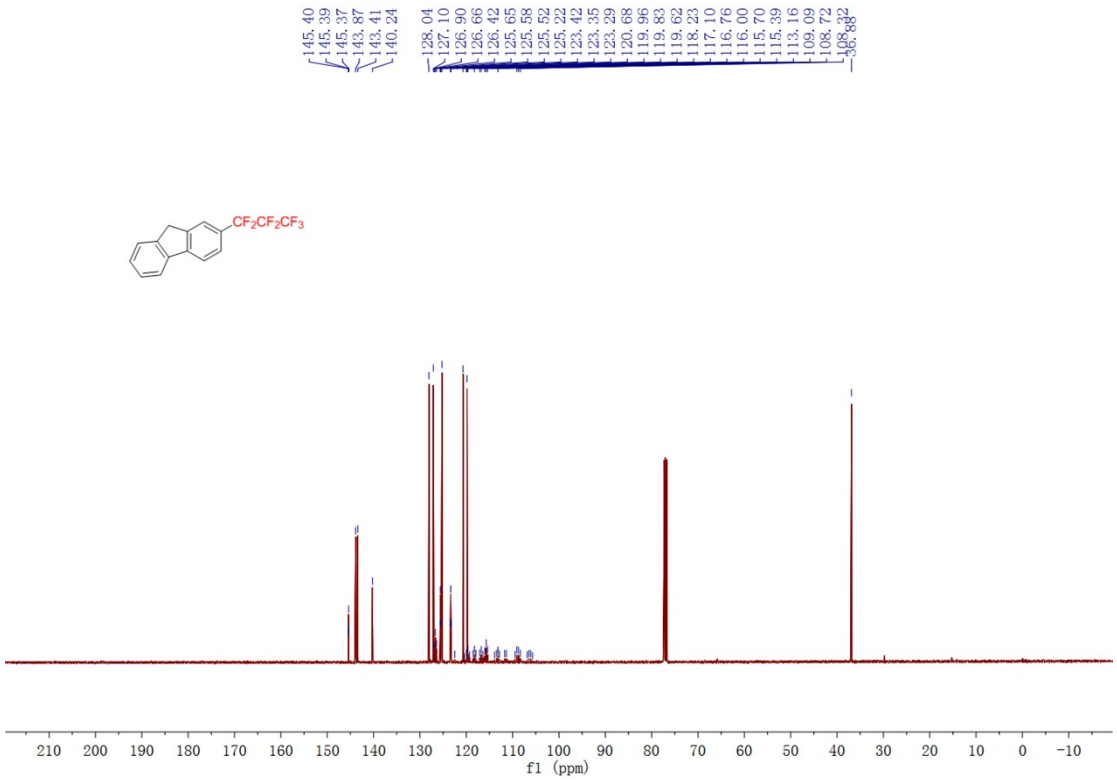
^{19}F NMR spectrum of **4f** in $CDCl_3$



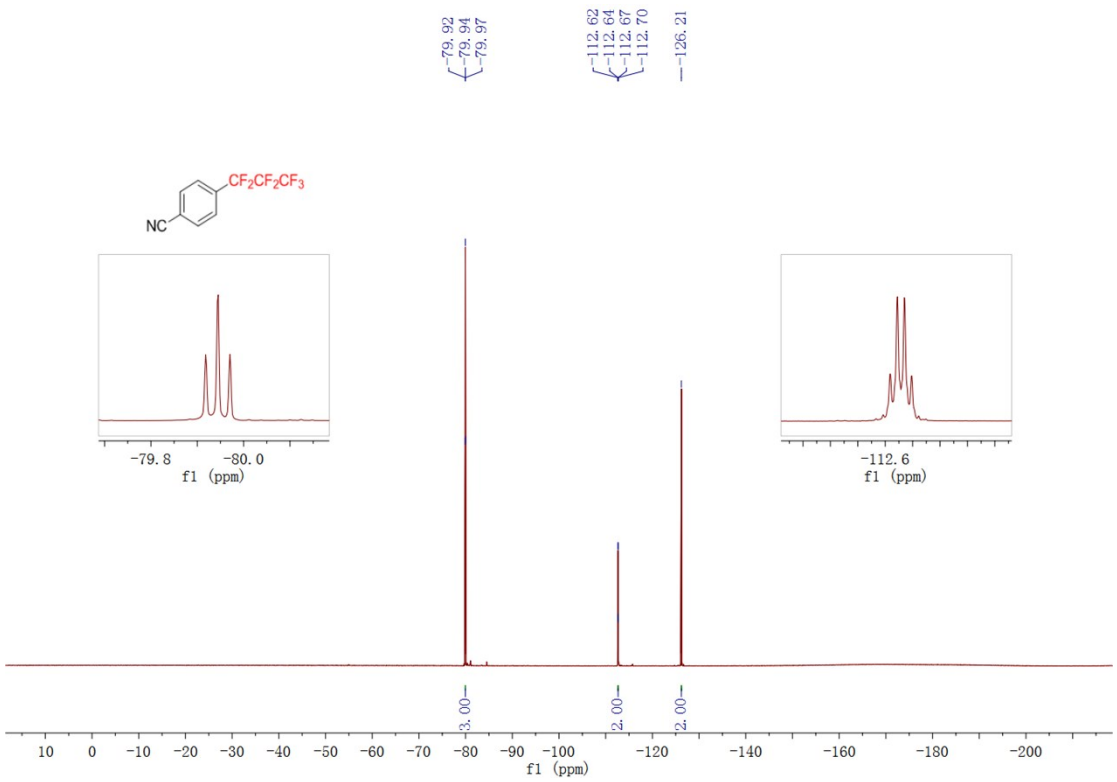
^{1}H NMR spectrum of **4f** in $CDCl_3$



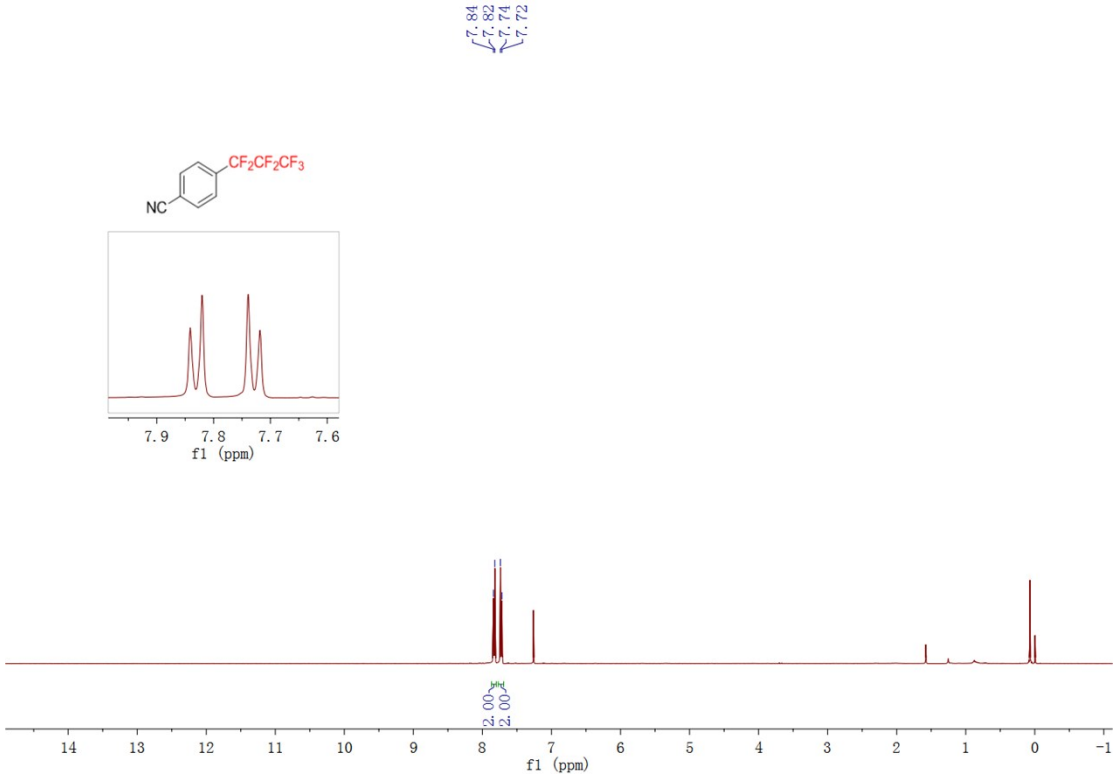
^{13}C NMR spectrum of **4f** in $CDCl_3$



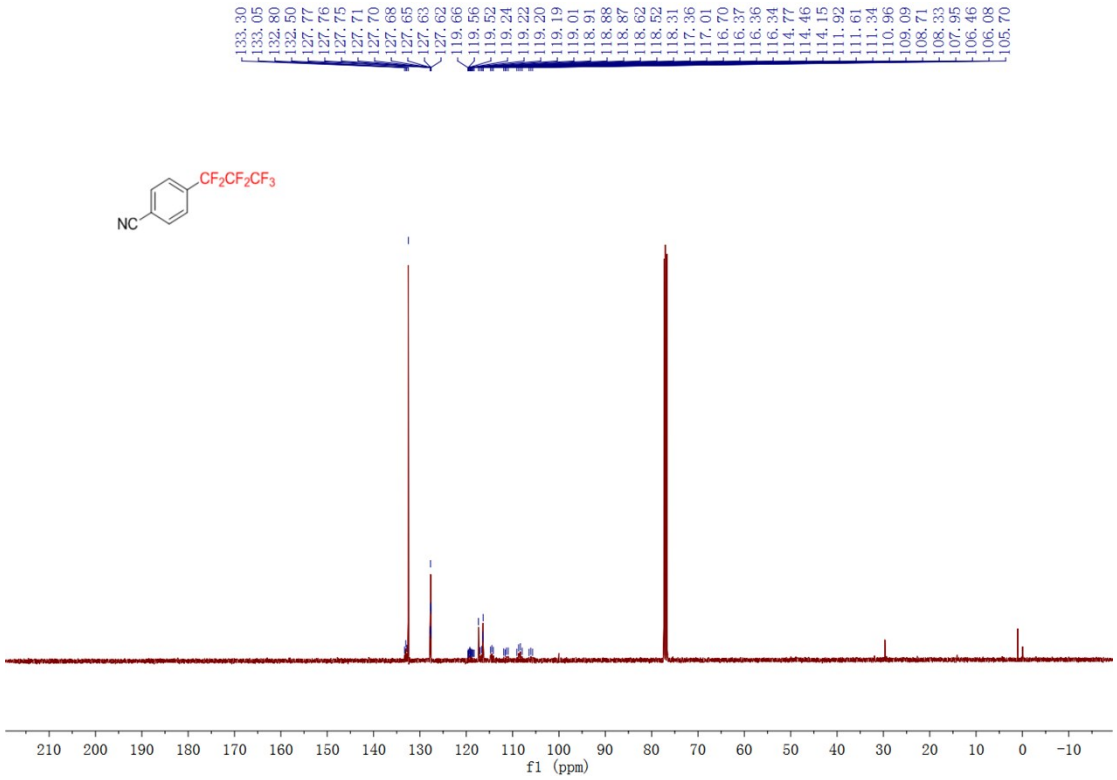
^{19}F NMR spectrum of **4g** in $CDCl_3$



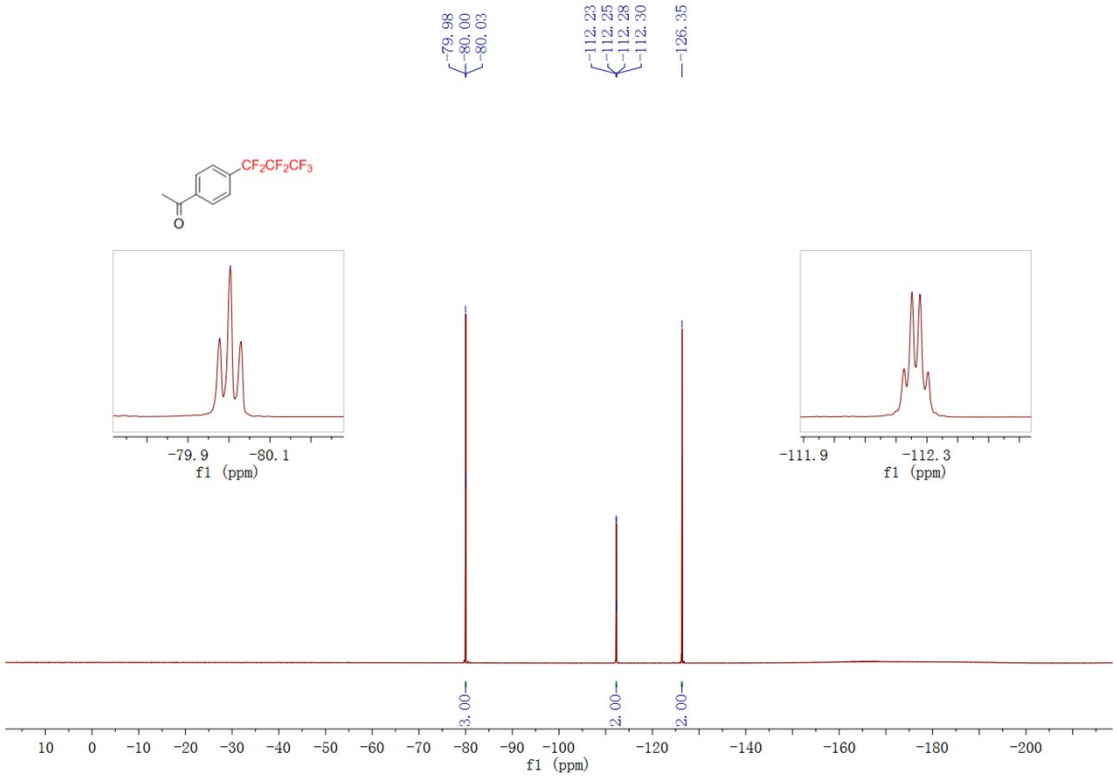
^{1}H NMR spectrum of **4g** in $CDCl_3$



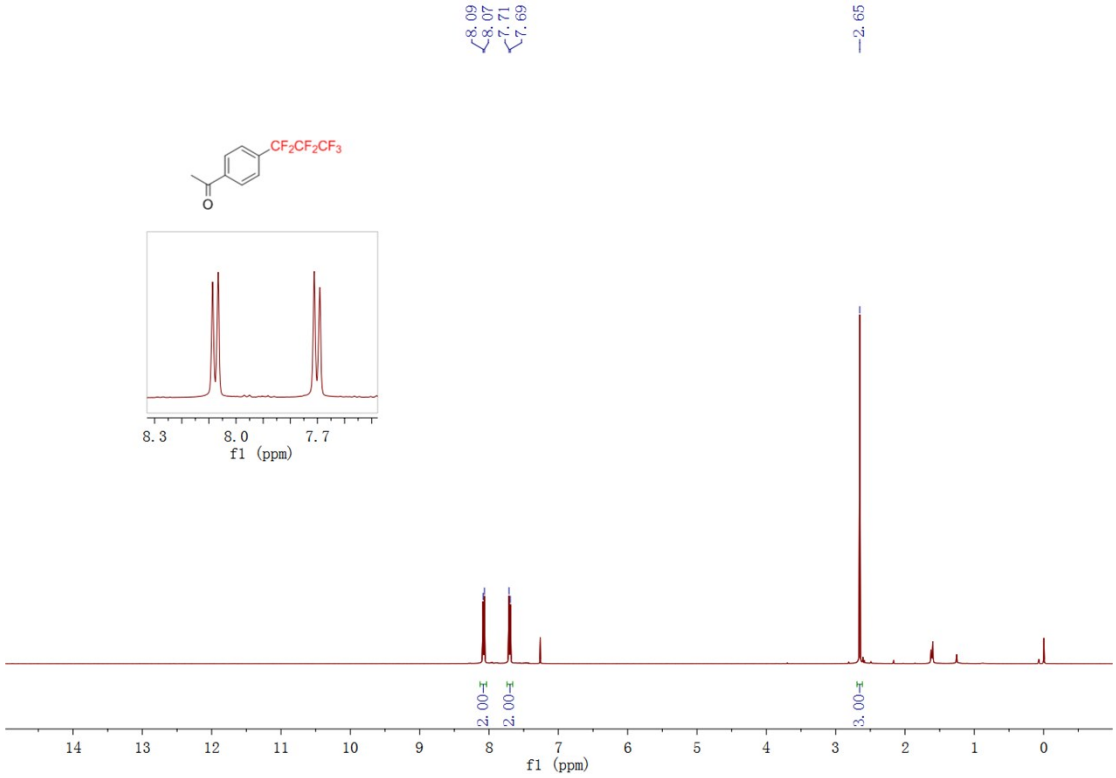
^{13}C NMR spectrum of **4g** in $CDCl_3$



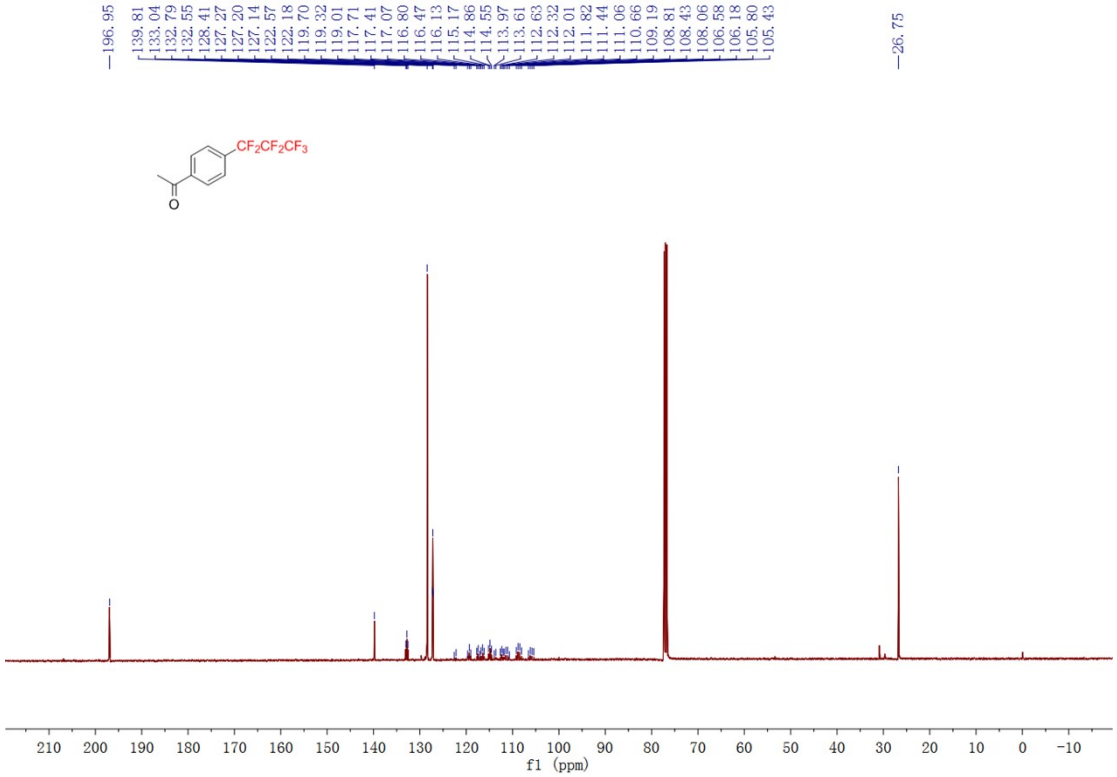
^{19}F NMR spectrum of **4h** in $CDCl_3$



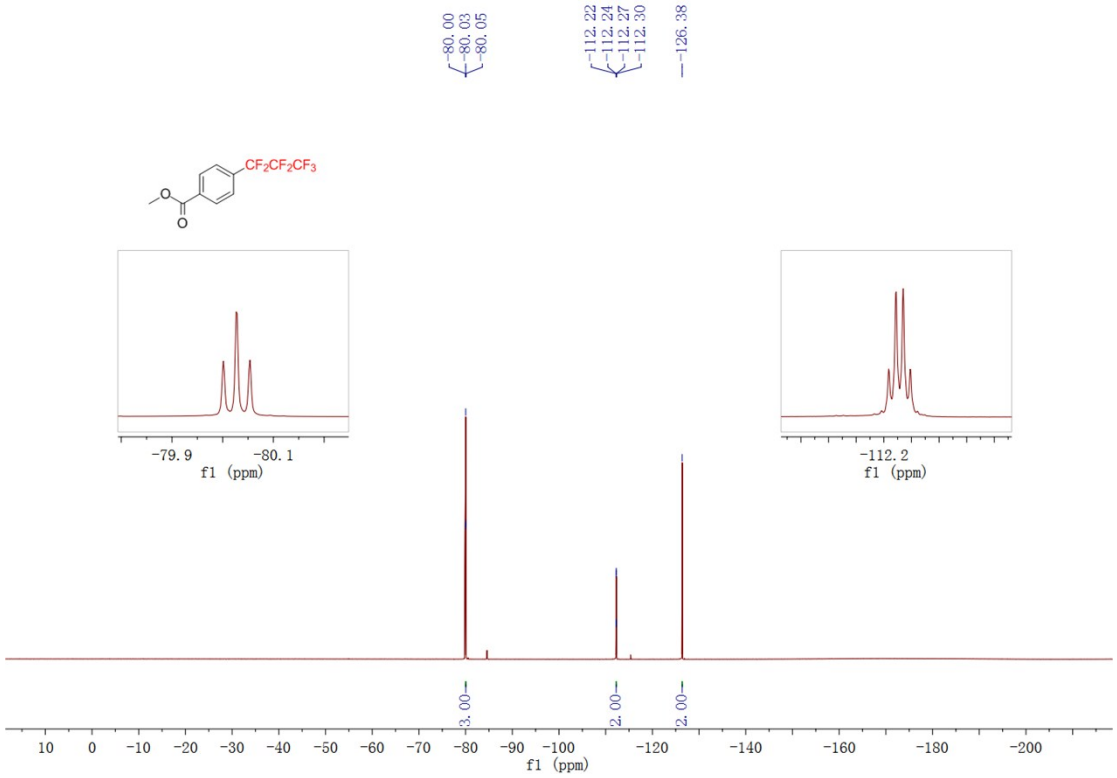
^{1}H NMR spectrum of **4h** in $CDCl_3$



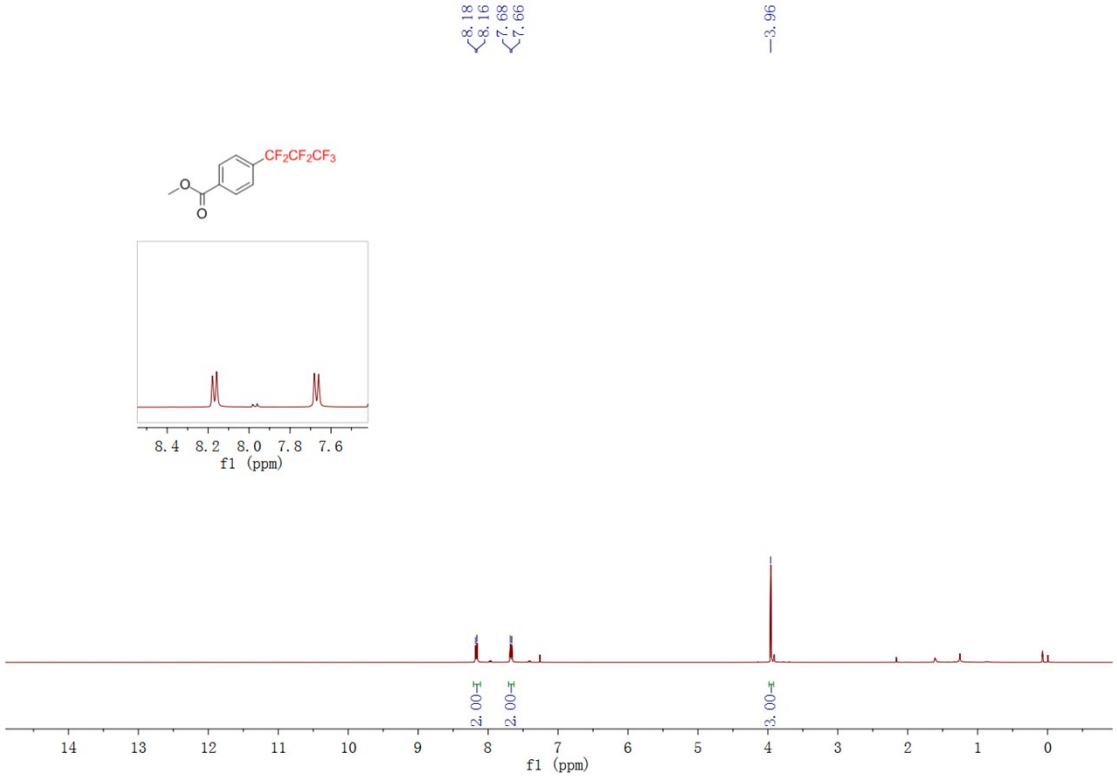
^{13}C NMR spectrum of **4h** in $CDCl_3$



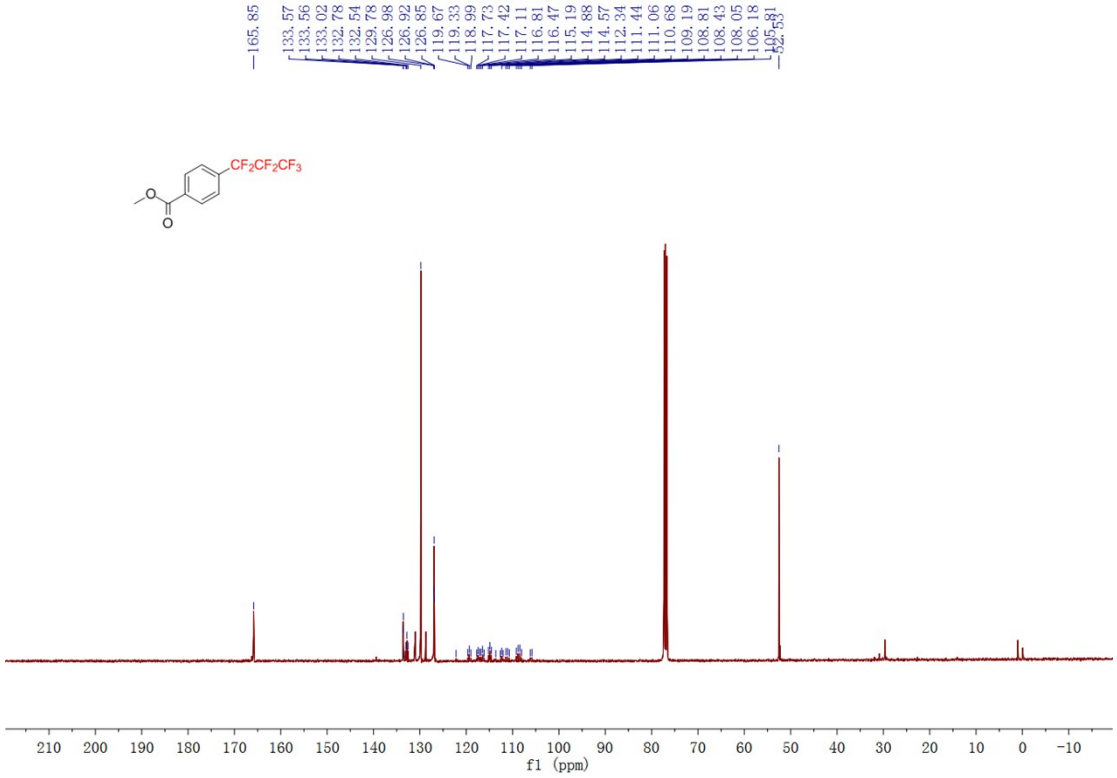
^{19}F NMR spectrum of **4i** in $CDCl_3$



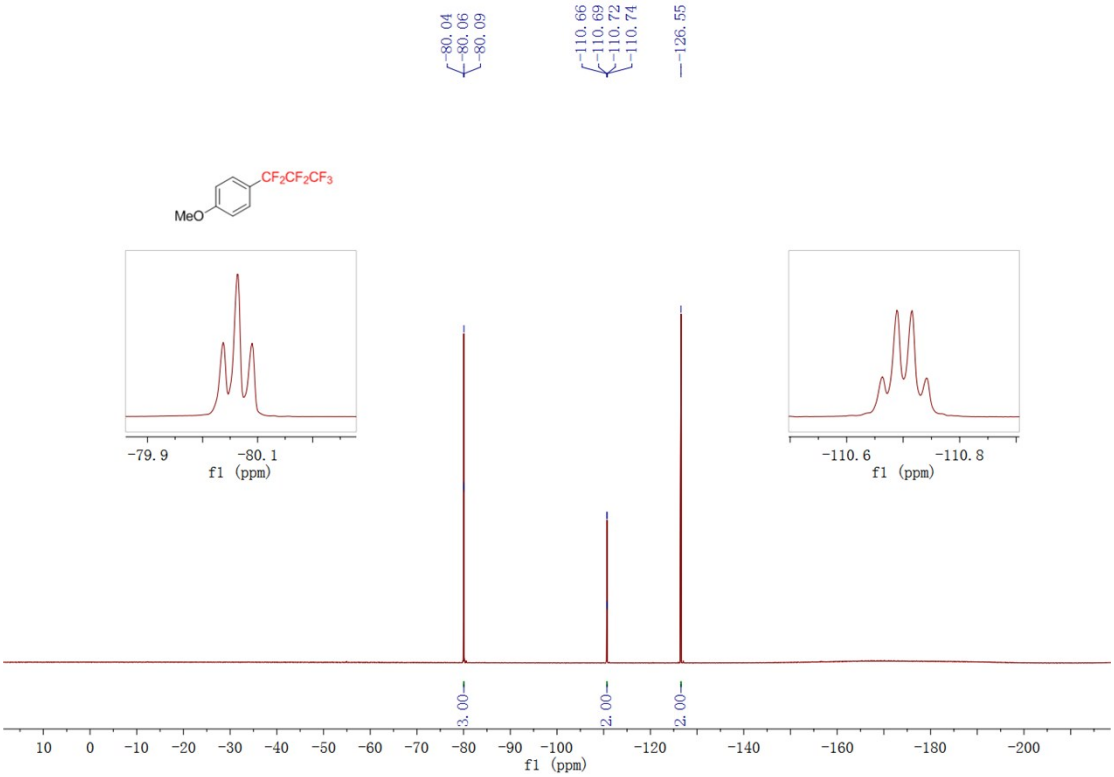
^{1}H NMR spectrum of **4i** in $CDCl_3$



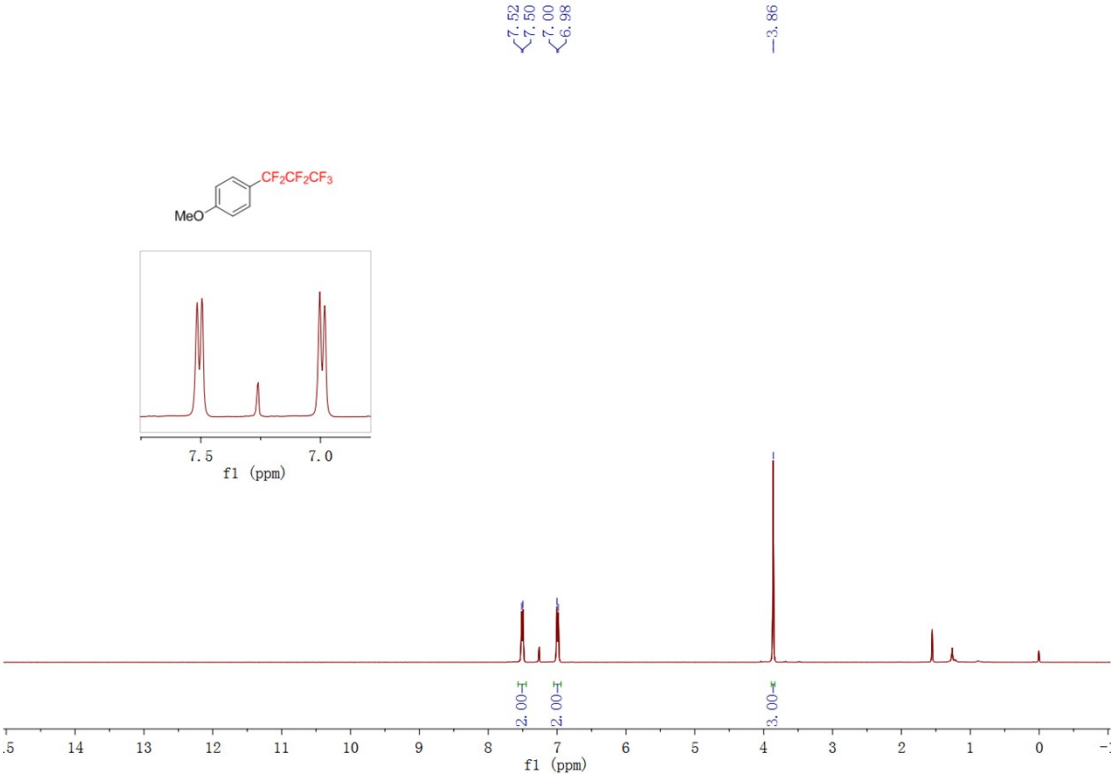
^{13}C NMR spectrum of **4i** in $CDCl_3$



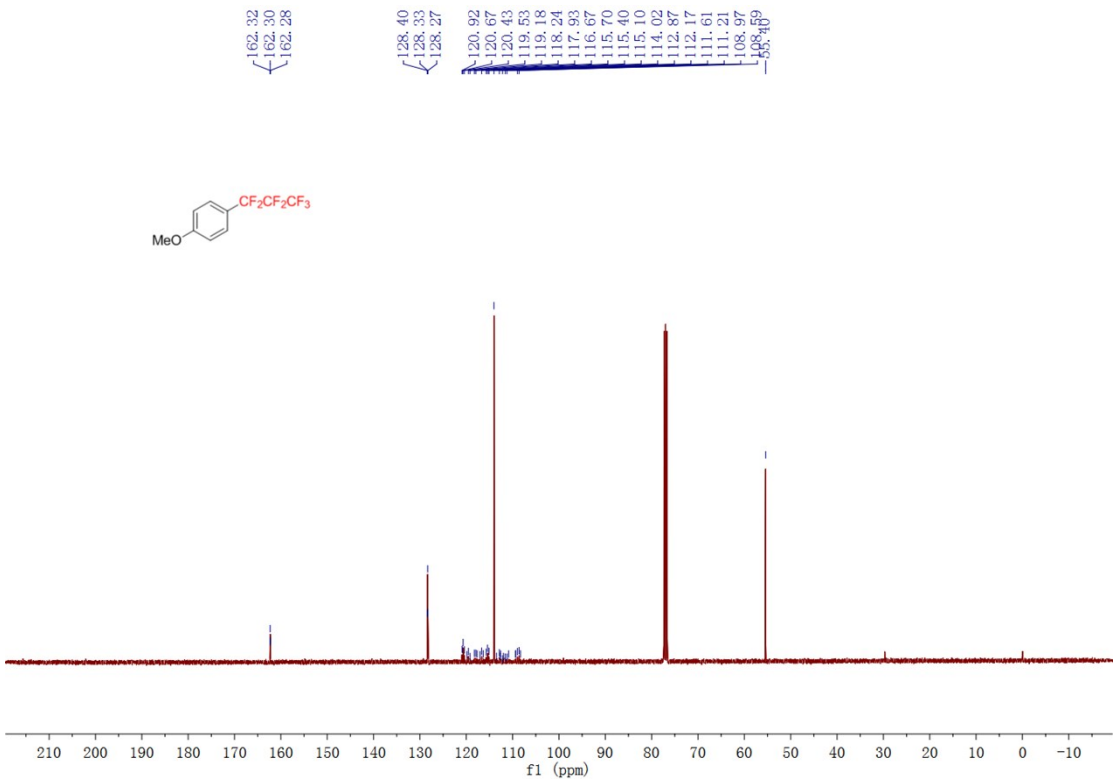
^{19}F NMR spectrum of **4k** in $CDCl_3$



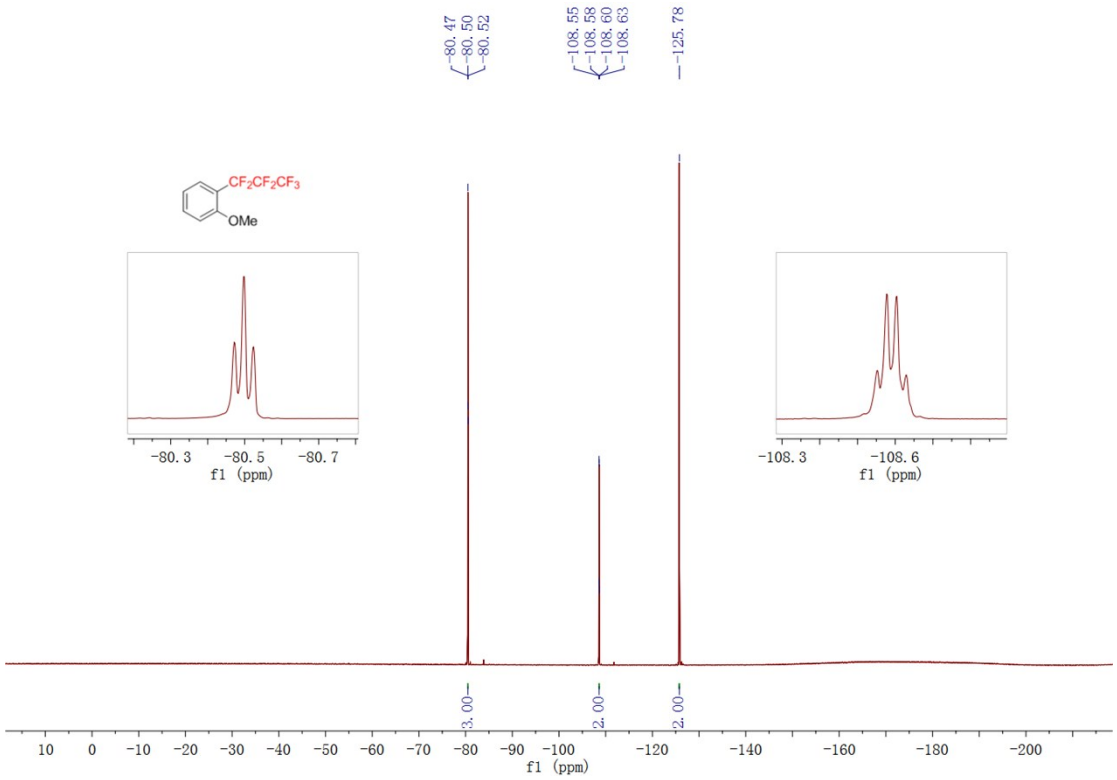
^{1}H NMR spectrum of **4k** in $CDCl_3$



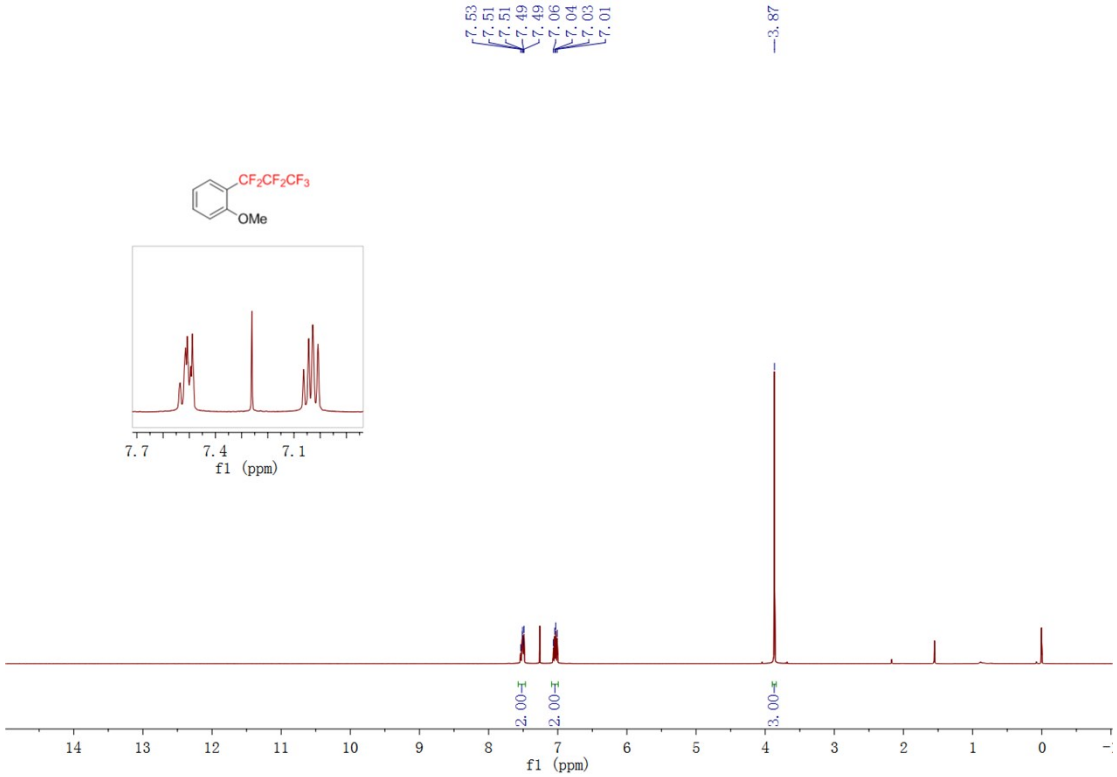
^{13}C NMR spectrum of **4k** in $CDCl_3$



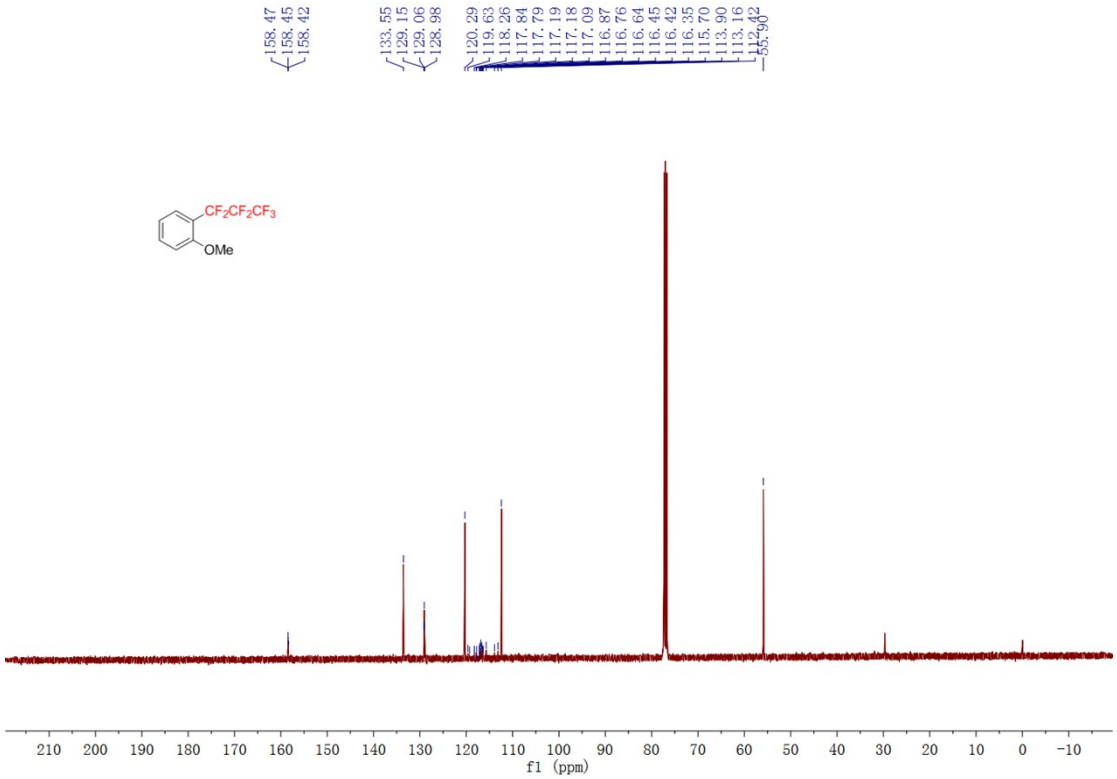
^{19}F NMR spectrum of **4l** in $CDCl_3$



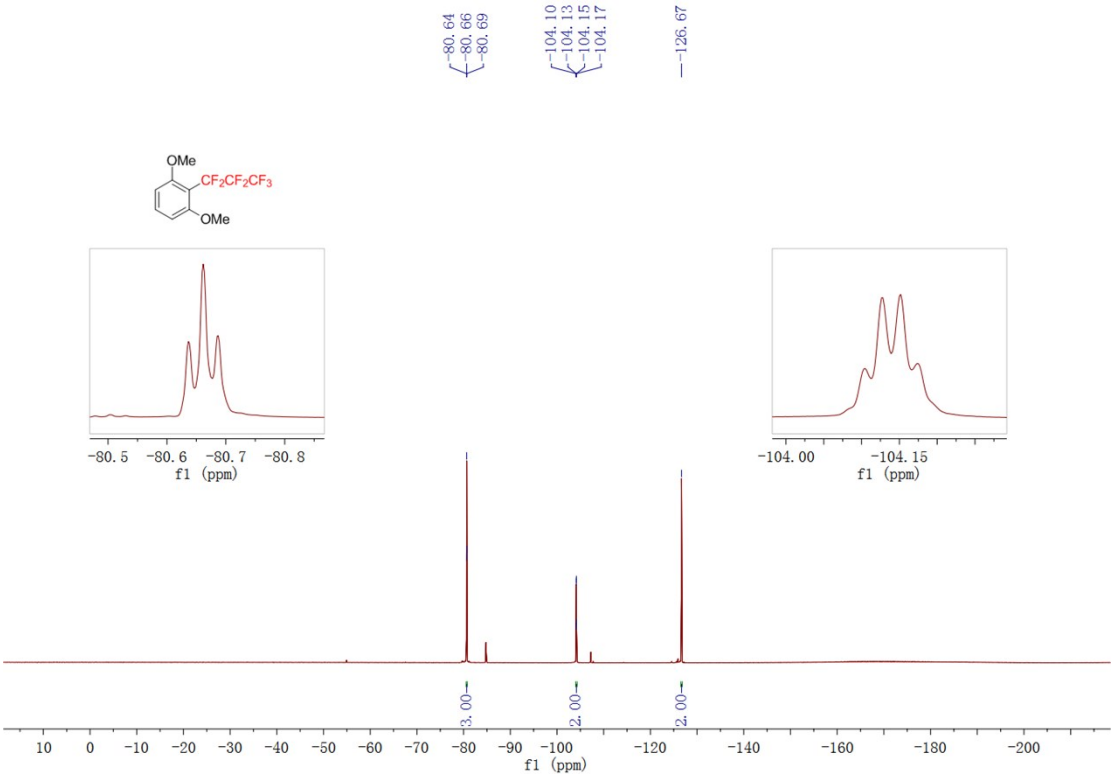
^{1}H NMR spectrum of **4l** in $CDCl_3$



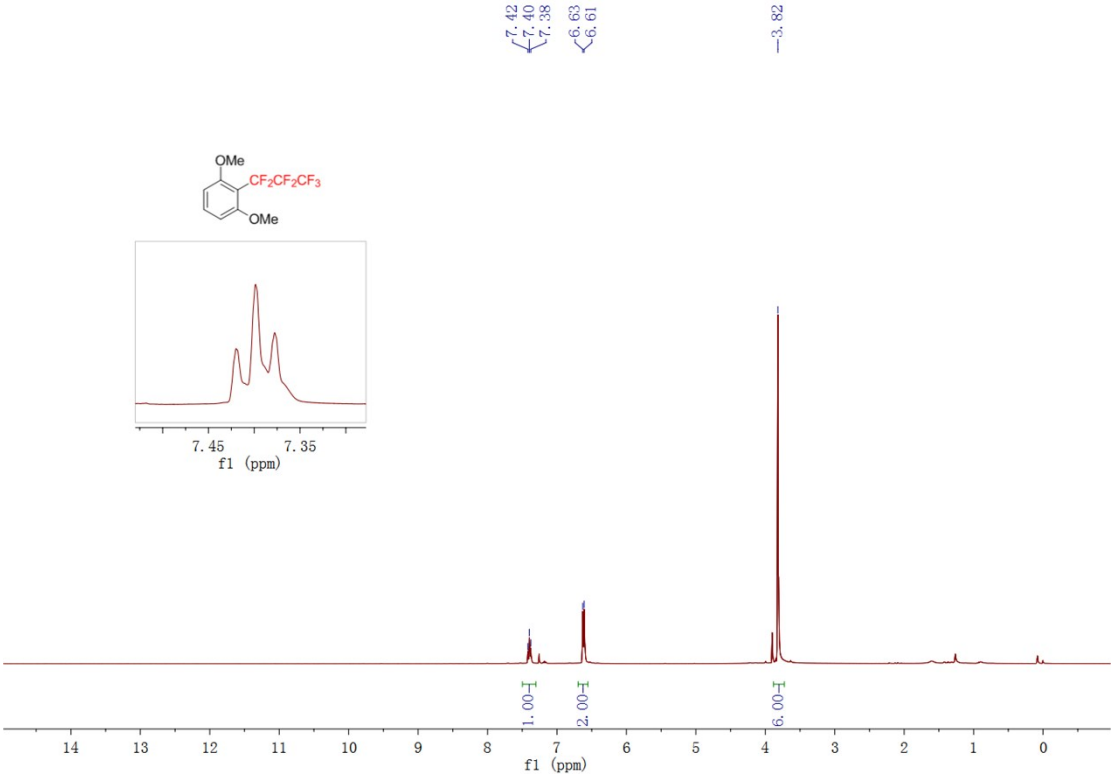
^{13}C NMR spectrum of **4l** in $CDCl_3$



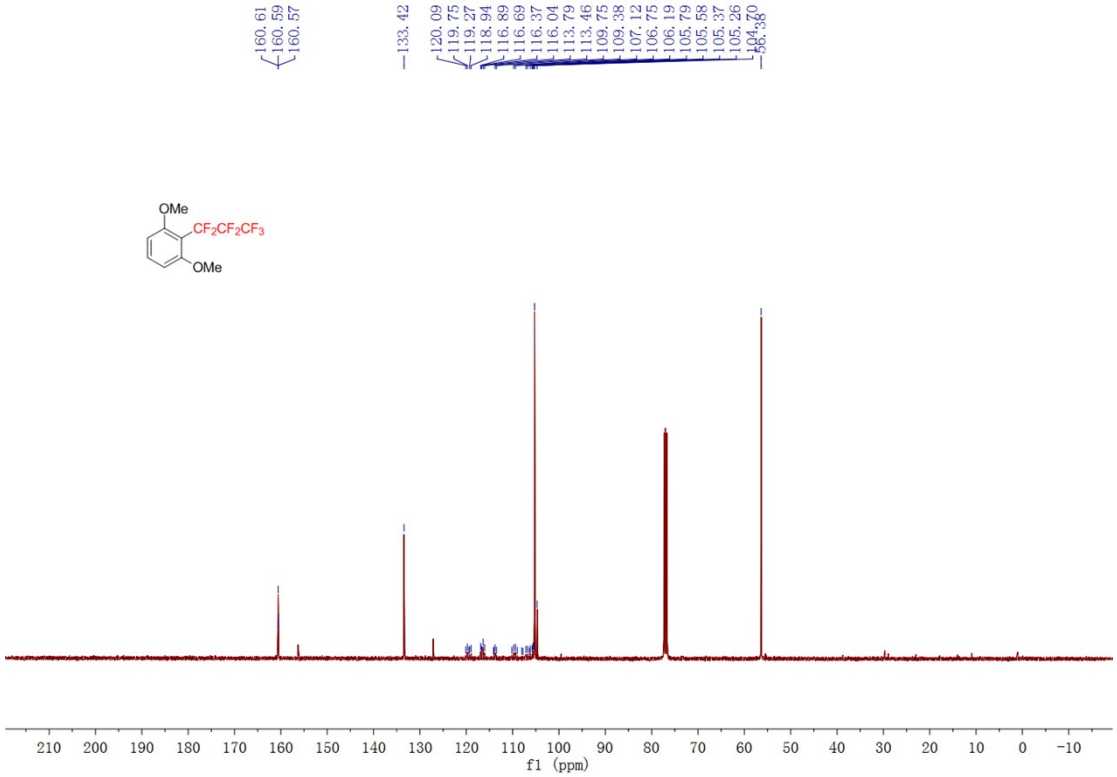
^{19}F NMR spectrum of **4m** in $CDCl_3$



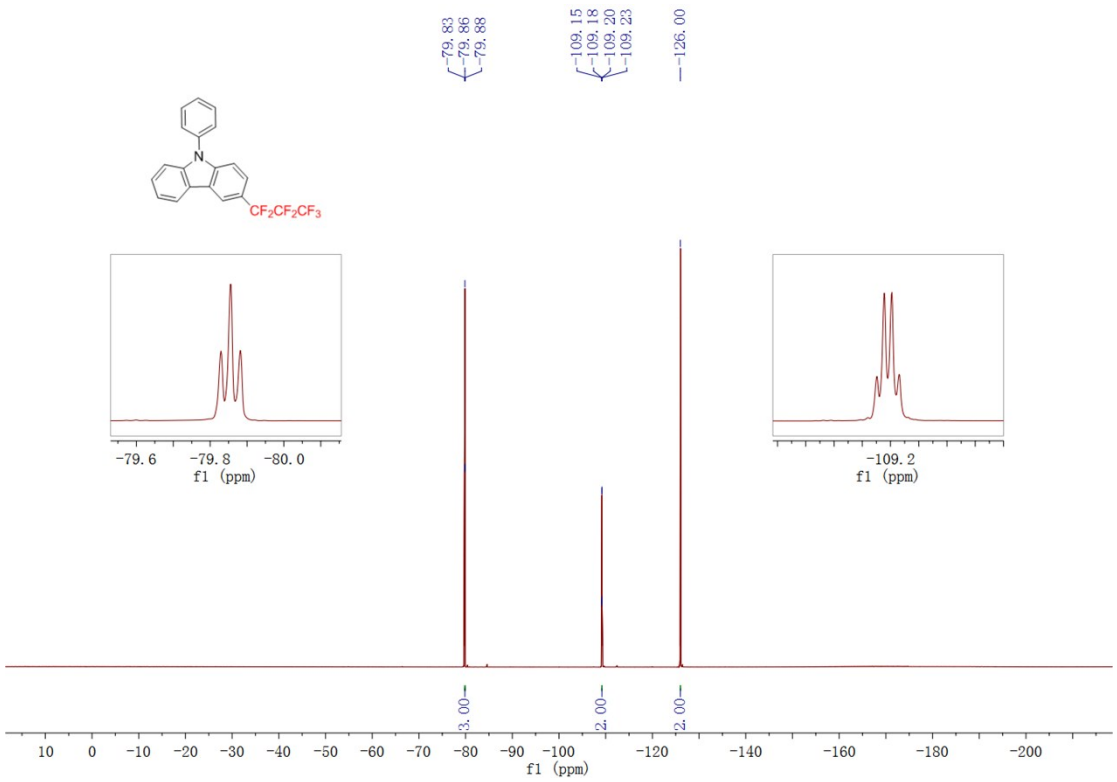
^{1}H NMR spectrum of **4m** in $CDCl_3$



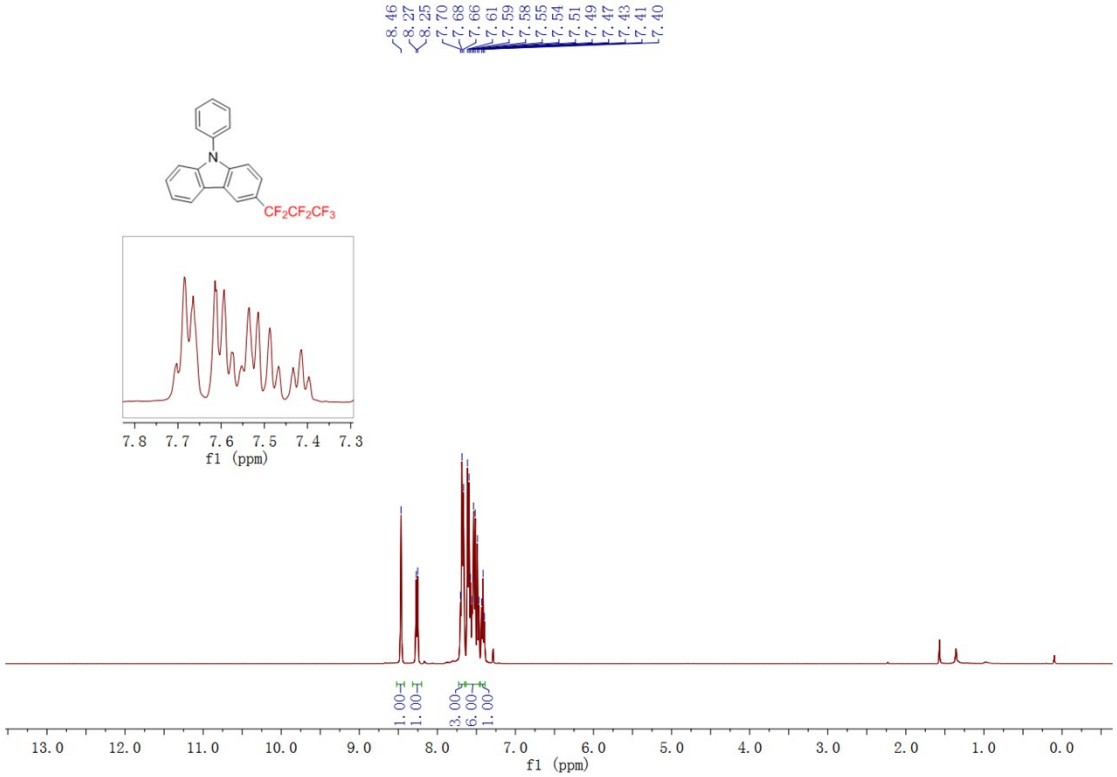
^{13}C NMR spectrum of **4m** in $CDCl_3$



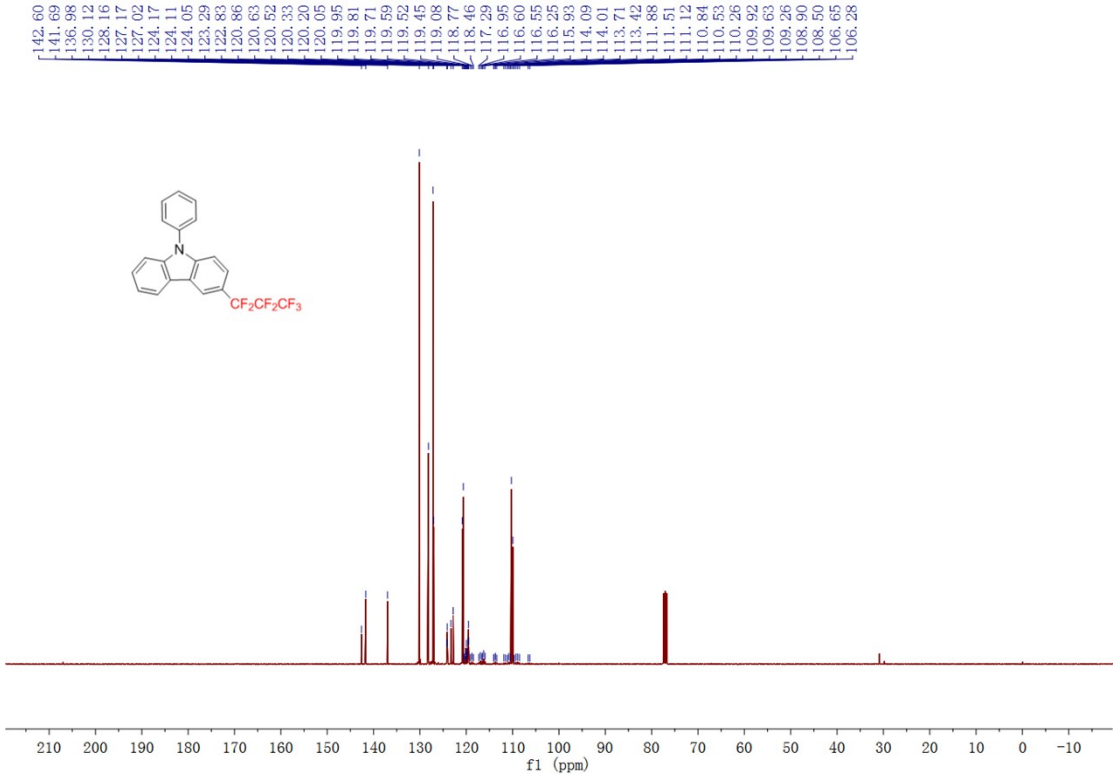
^{19}F NMR spectrum of **4o** in $CDCl_3$



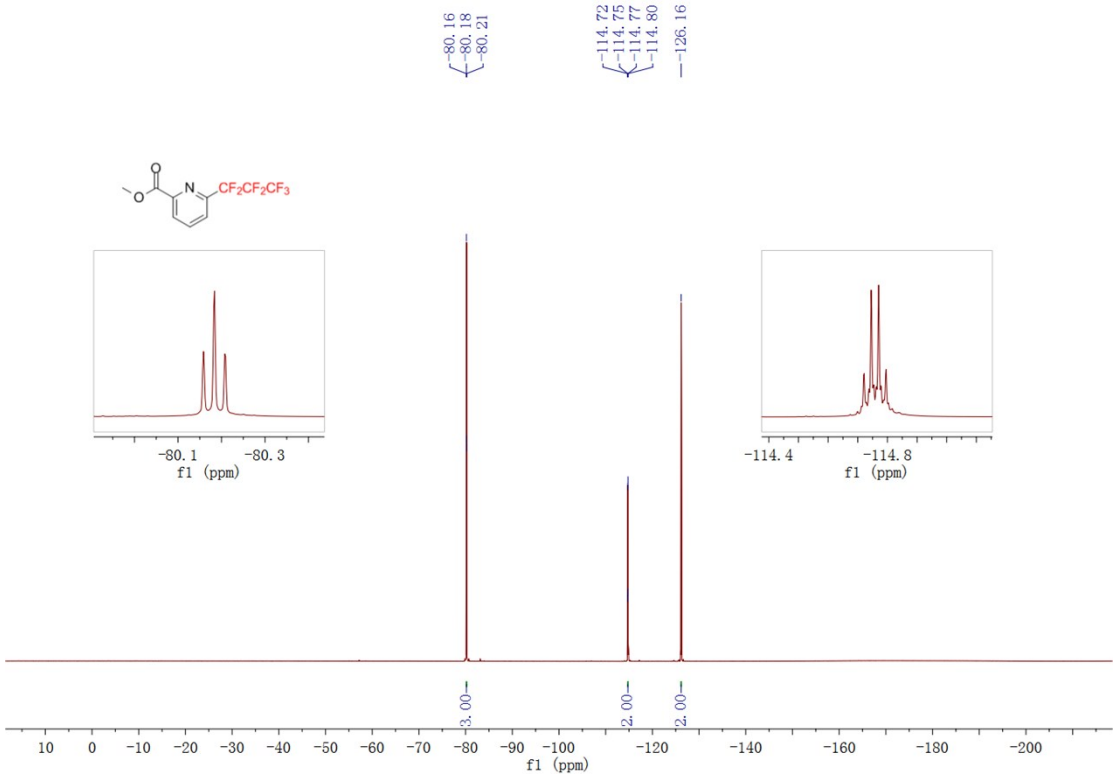
^{1}H NMR spectrum of **4o** in $CDCl_3$



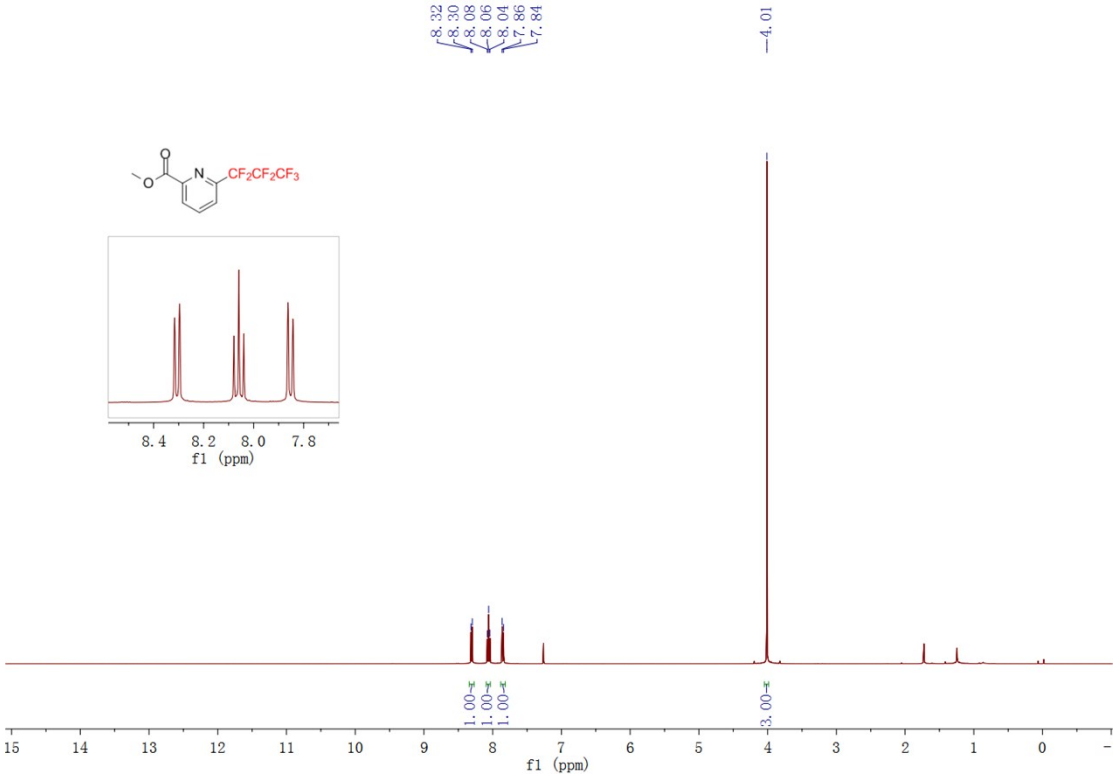
^{13}C NMR spectrum of **4o** in $CDCl_3$



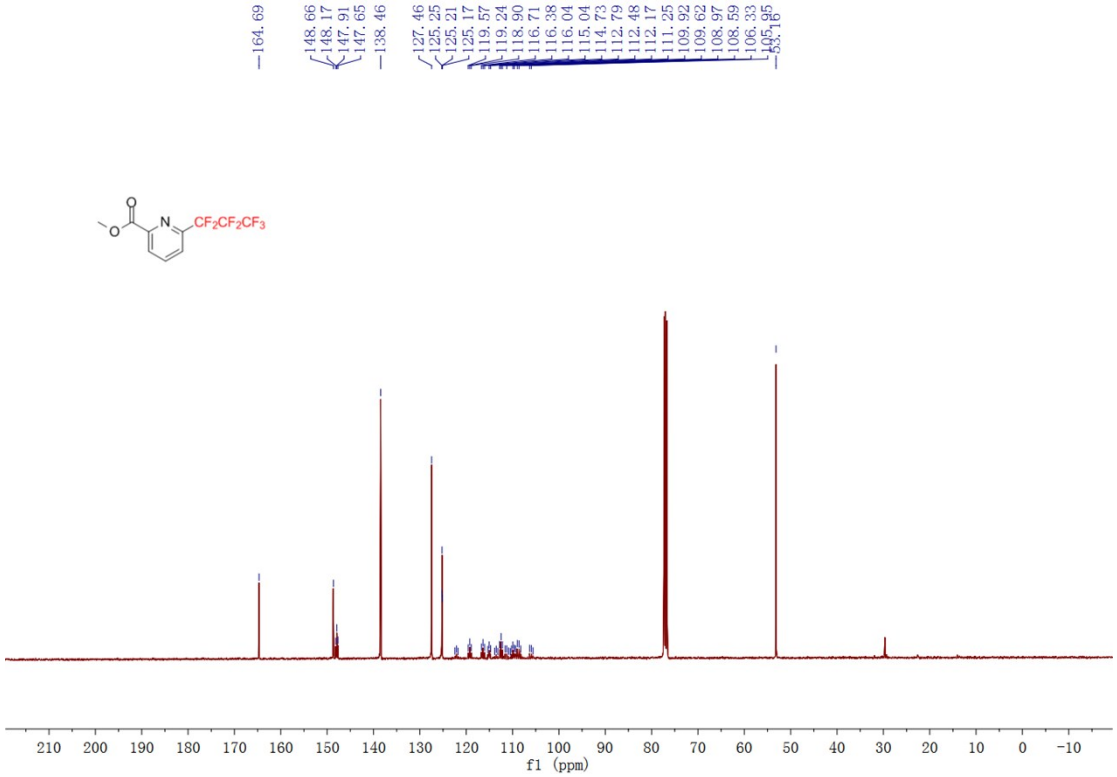
^{19}F NMR spectrum of **4p** in $CDCl_3$



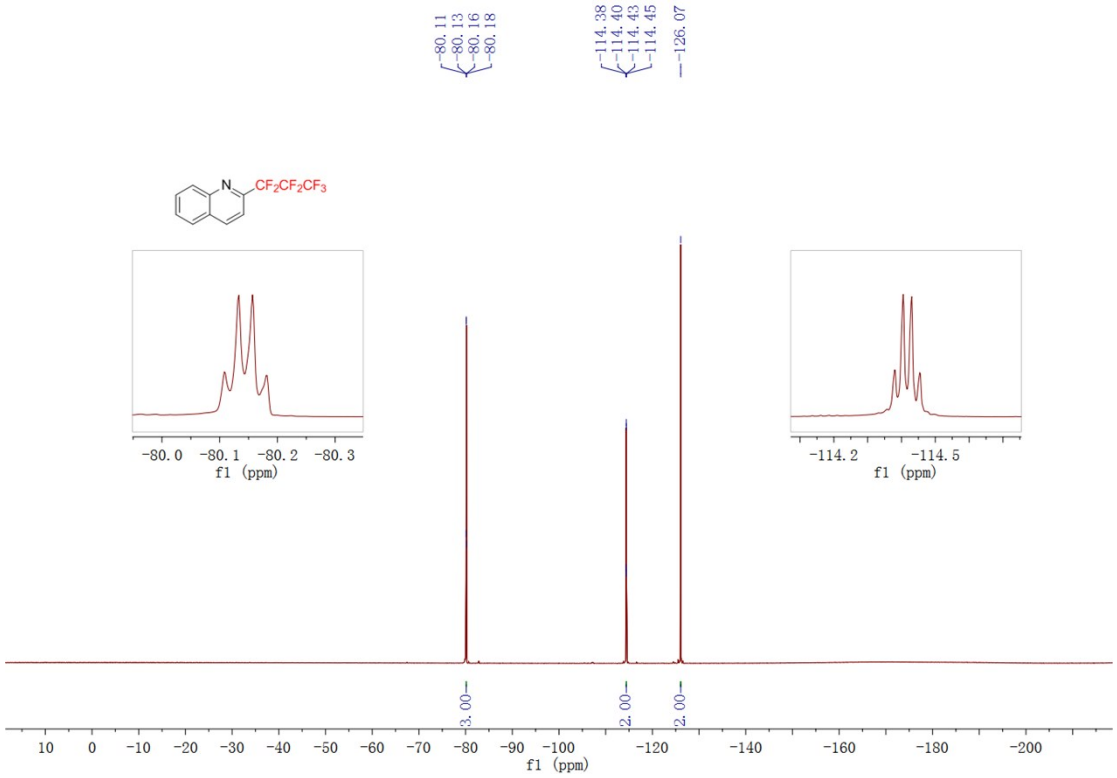
^{1}H NMR spectrum of **4p** in $CDCl_3$



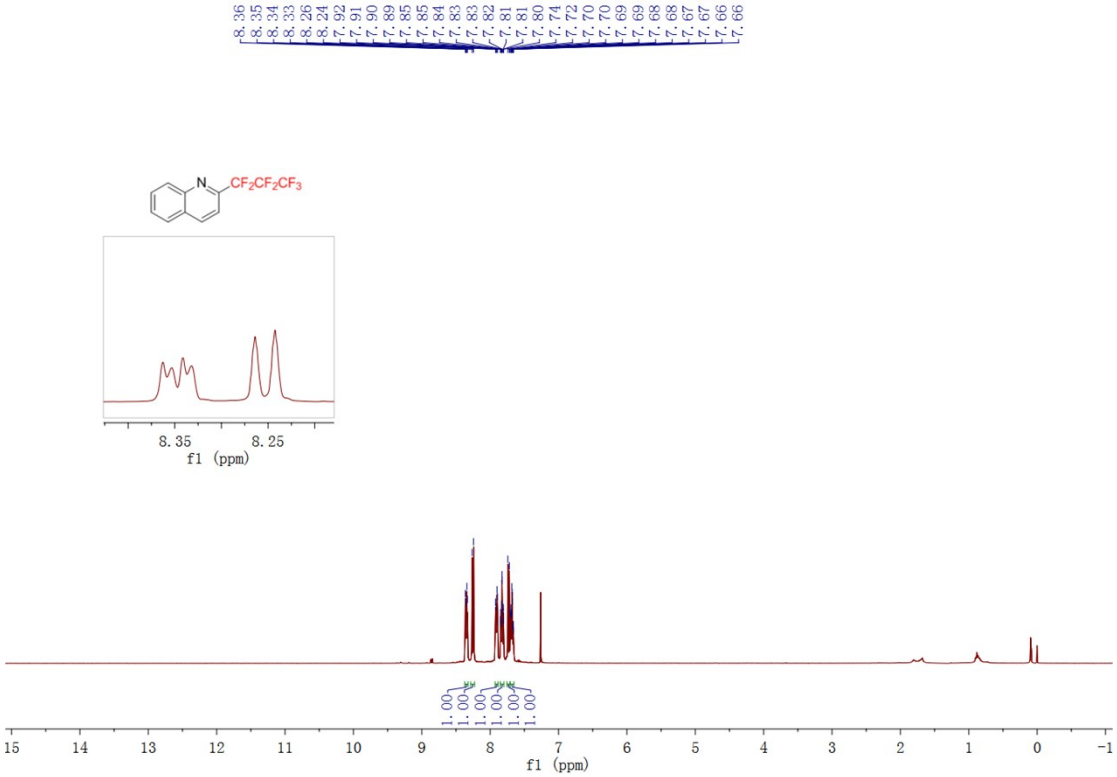
^{13}C NMR spectrum of **4p** in $CDCl_3$



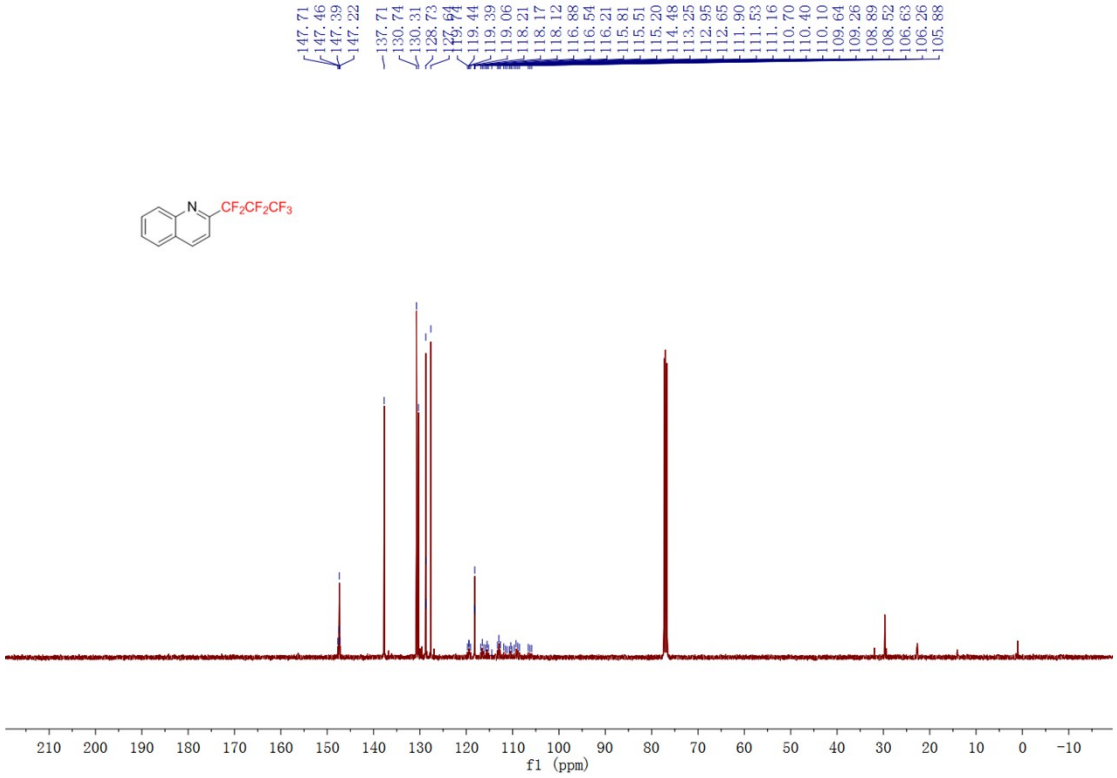
^{19}F NMR spectrum of **4s** in $CDCl_3$



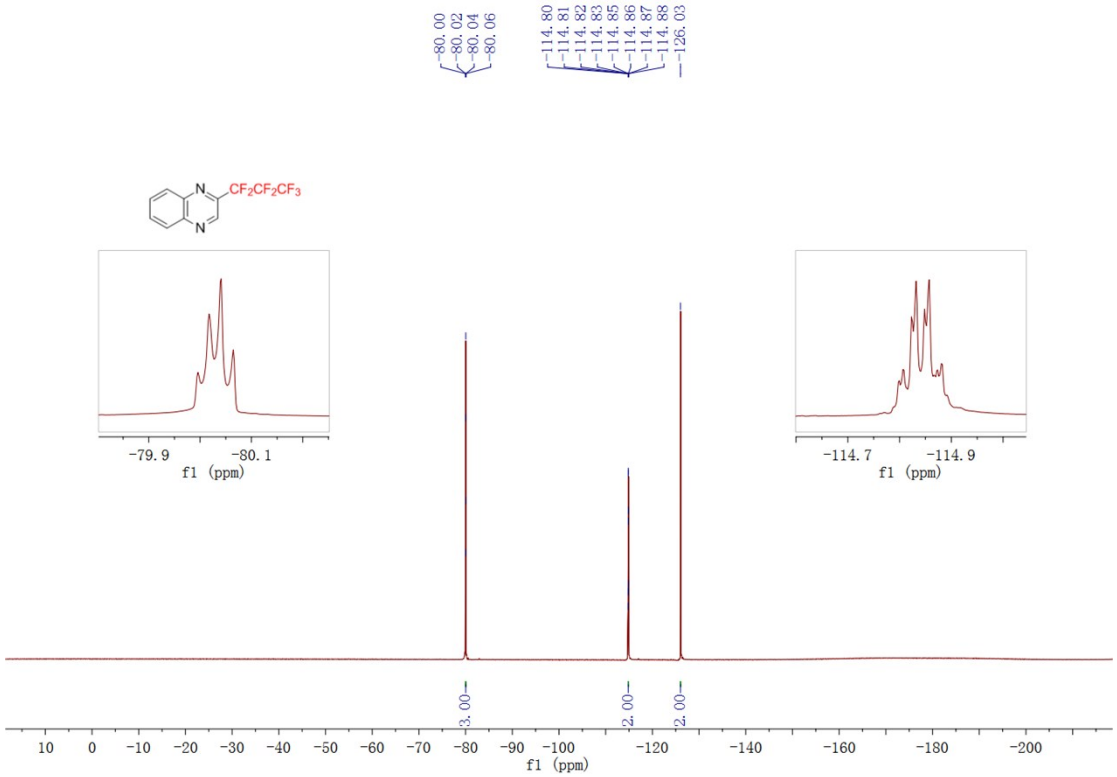
^{1}H NMR spectrum of **4s** in $CDCl_3$



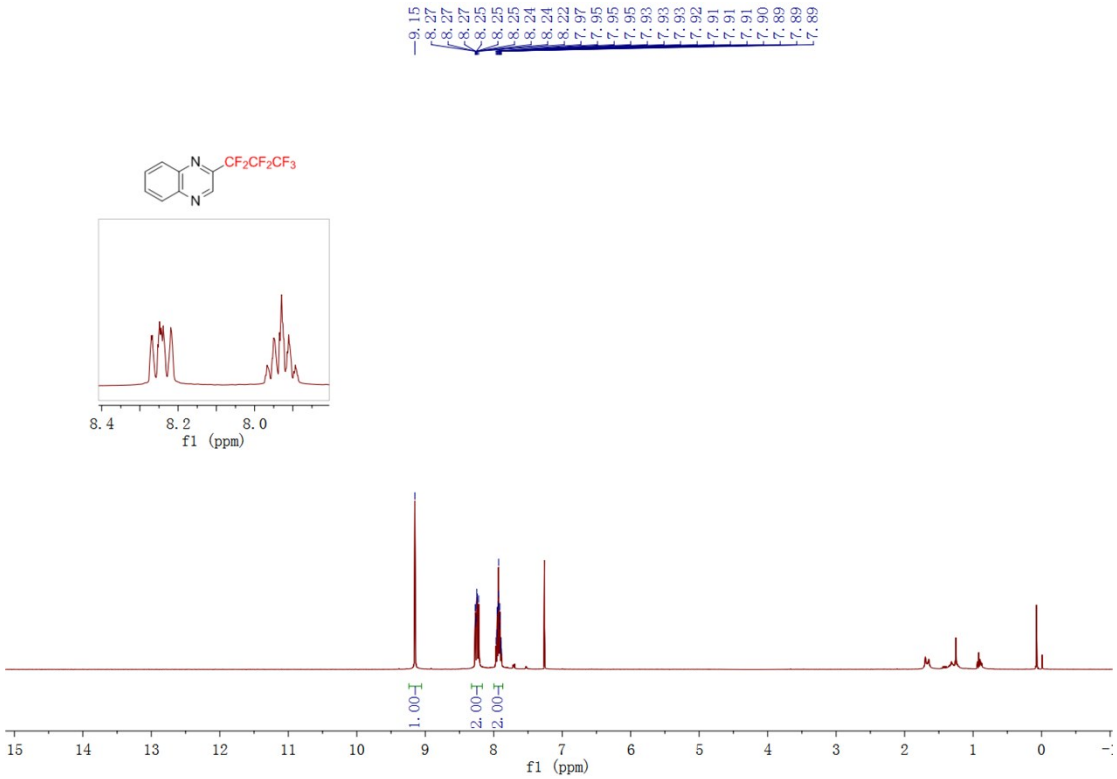
^{13}C NMR spectrum of **4s** in $CDCl_3$



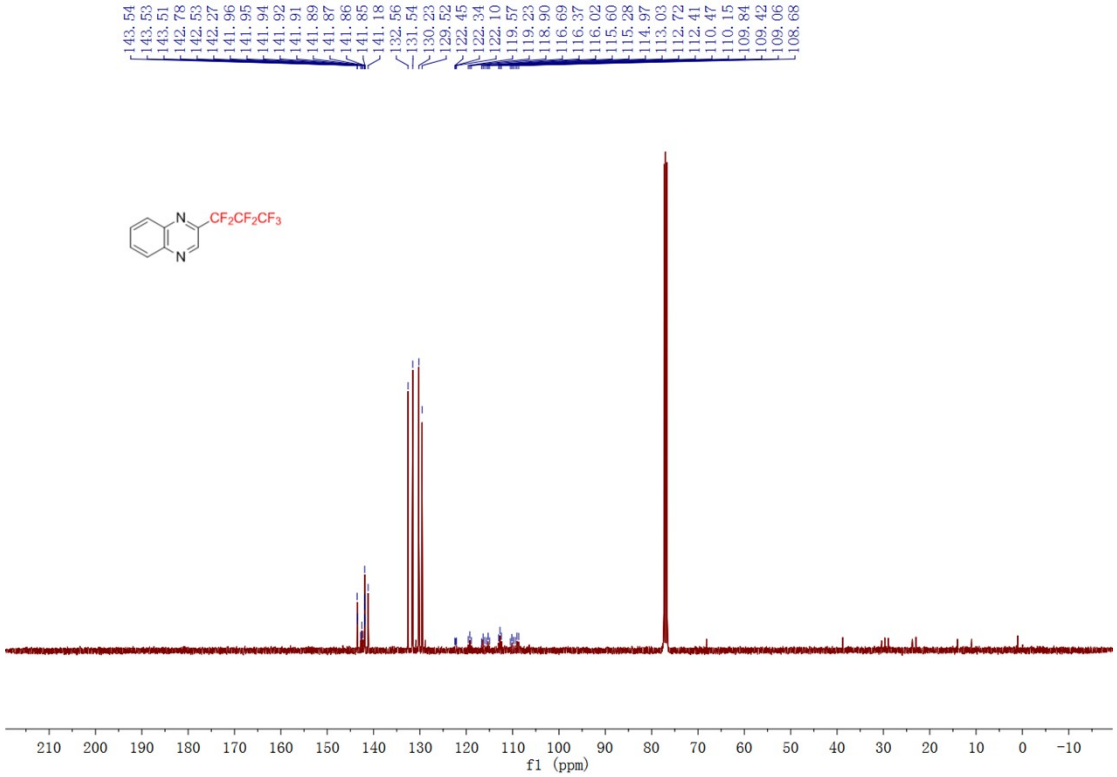
^{19}F NMR spectrum of **4t** in $CDCl_3$



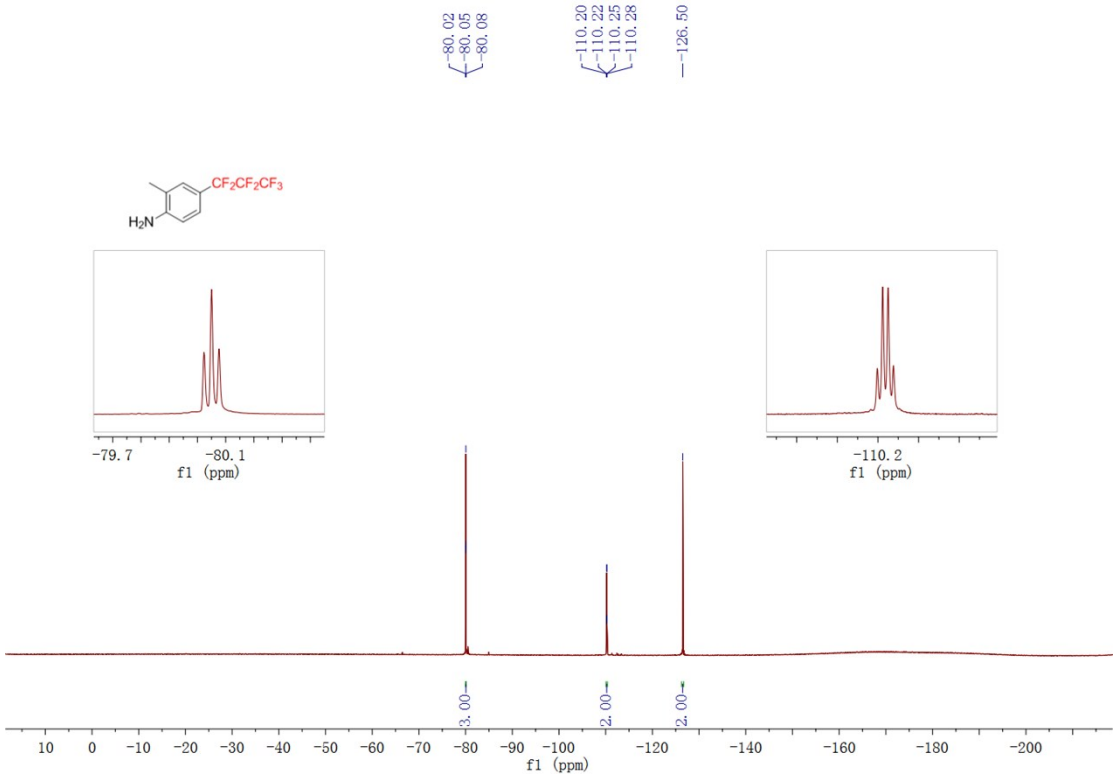
^{1}H NMR spectrum of **4t** in $CDCl_3$



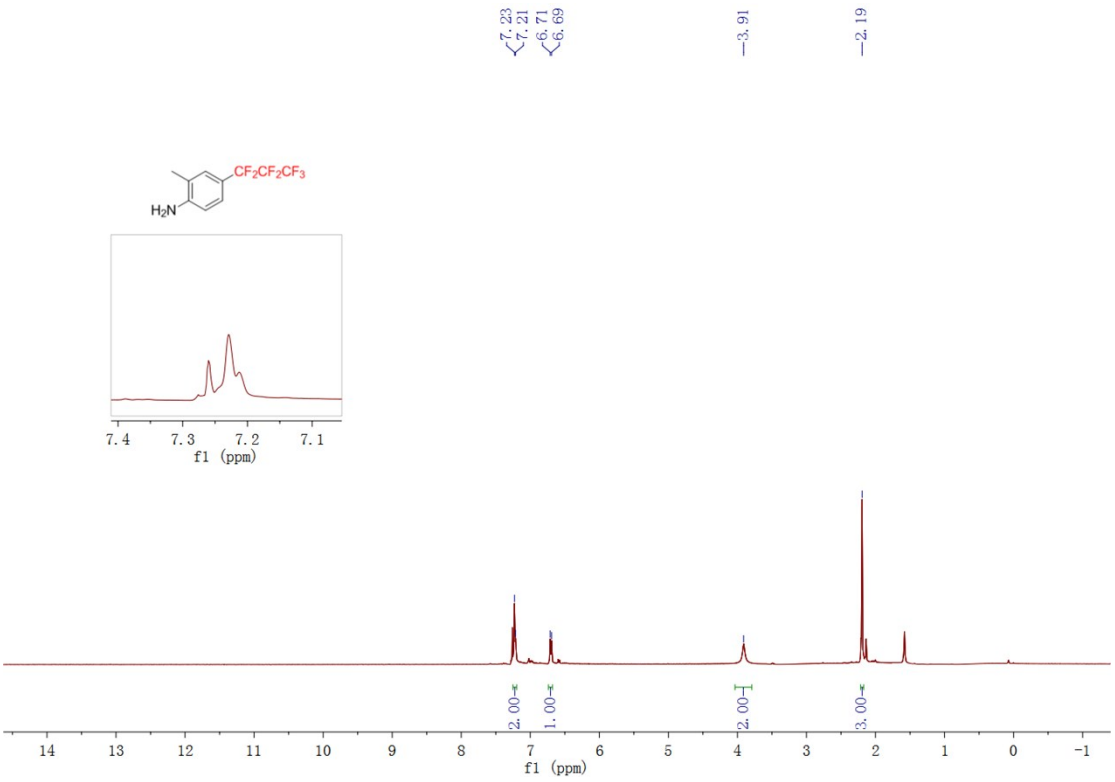
^{13}C NMR spectrum of **4t** in $CDCl_3$



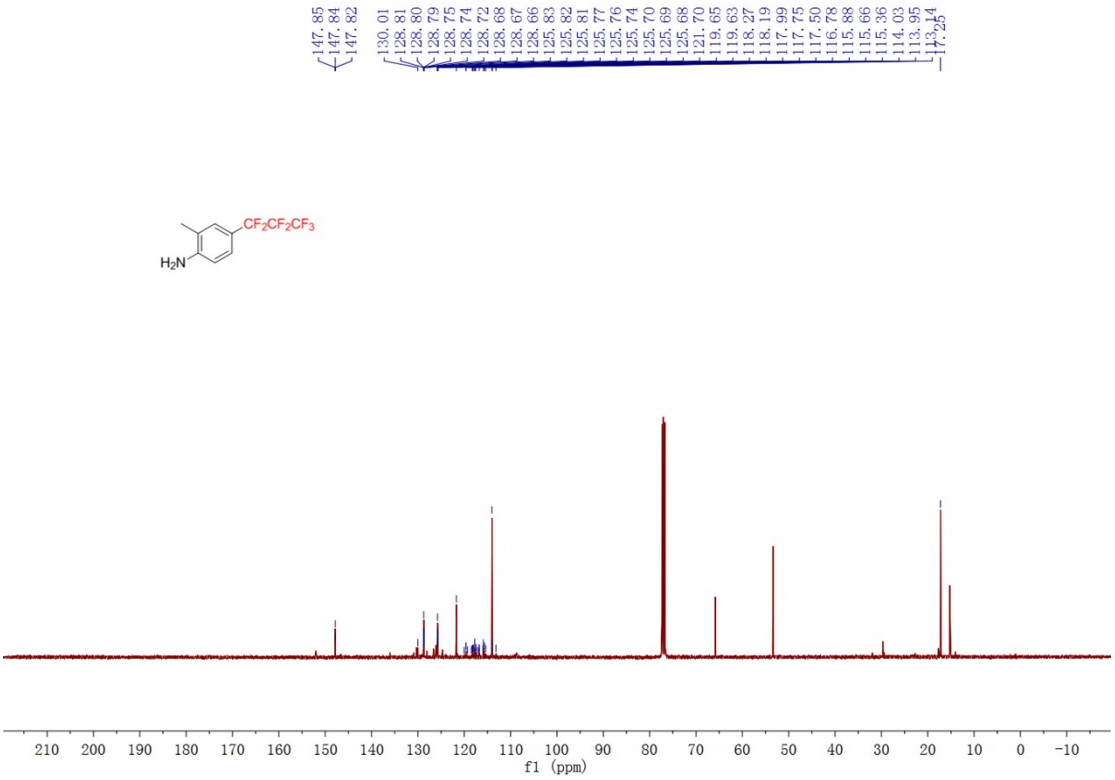
^{19}F NMR spectrum of **4v** in $CDCl_3$



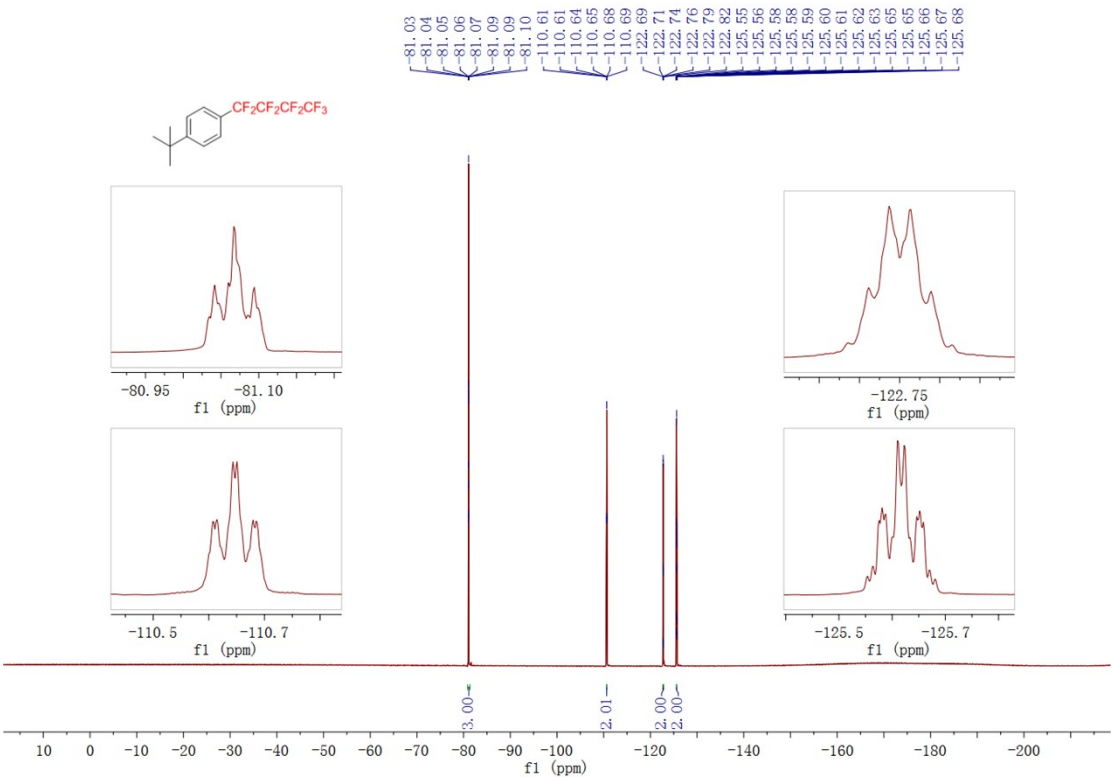
^{1}H NMR spectrum of **4v** in $CDCl_3$



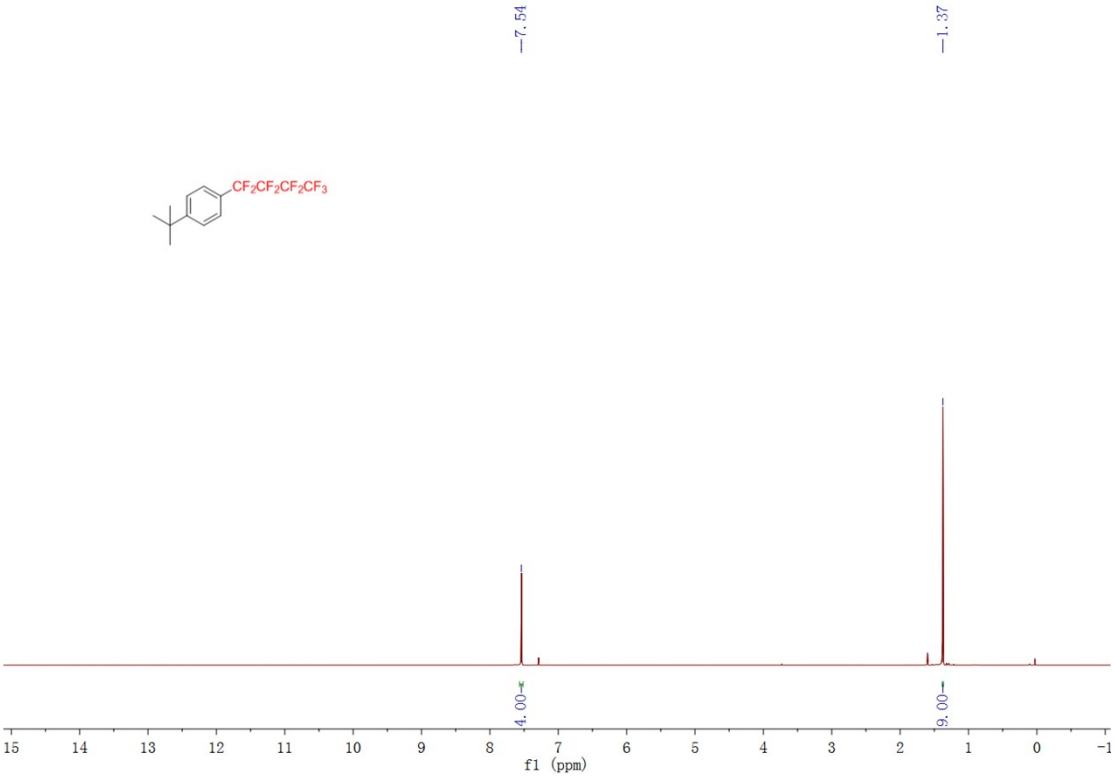
^{13}C NMR spectrum of **4v** in $CDCl_3$



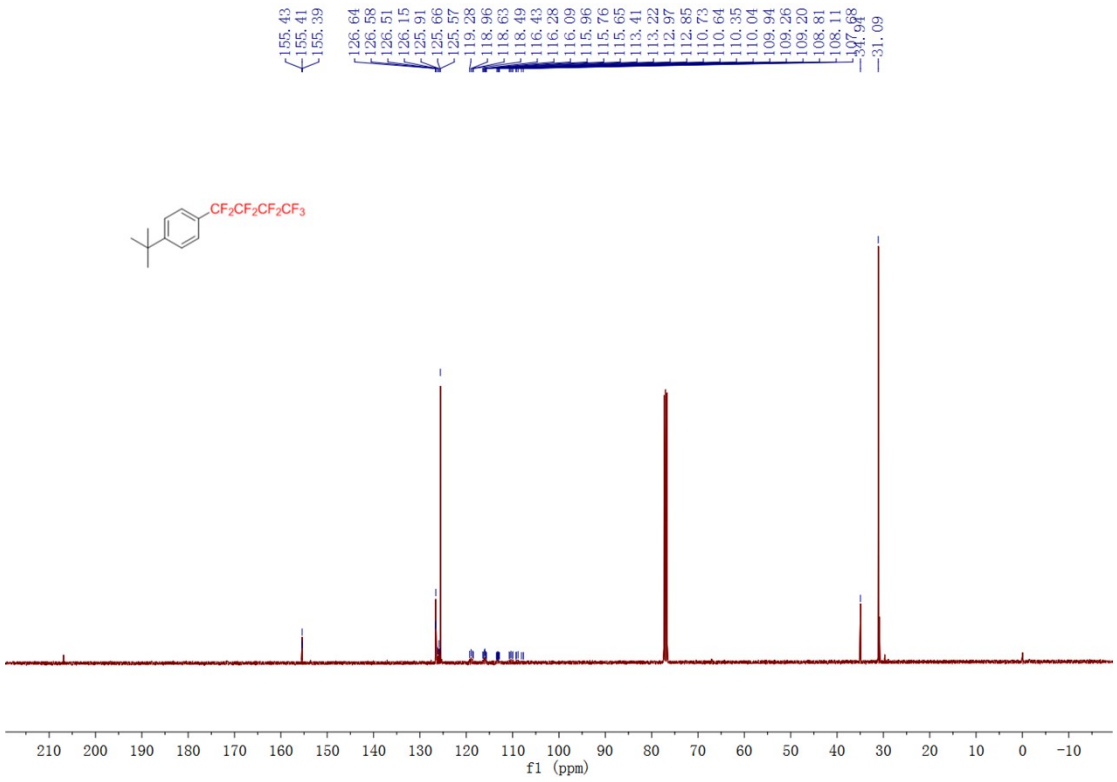
^{19}F NMR spectrum of **5a** in $CDCl_3$



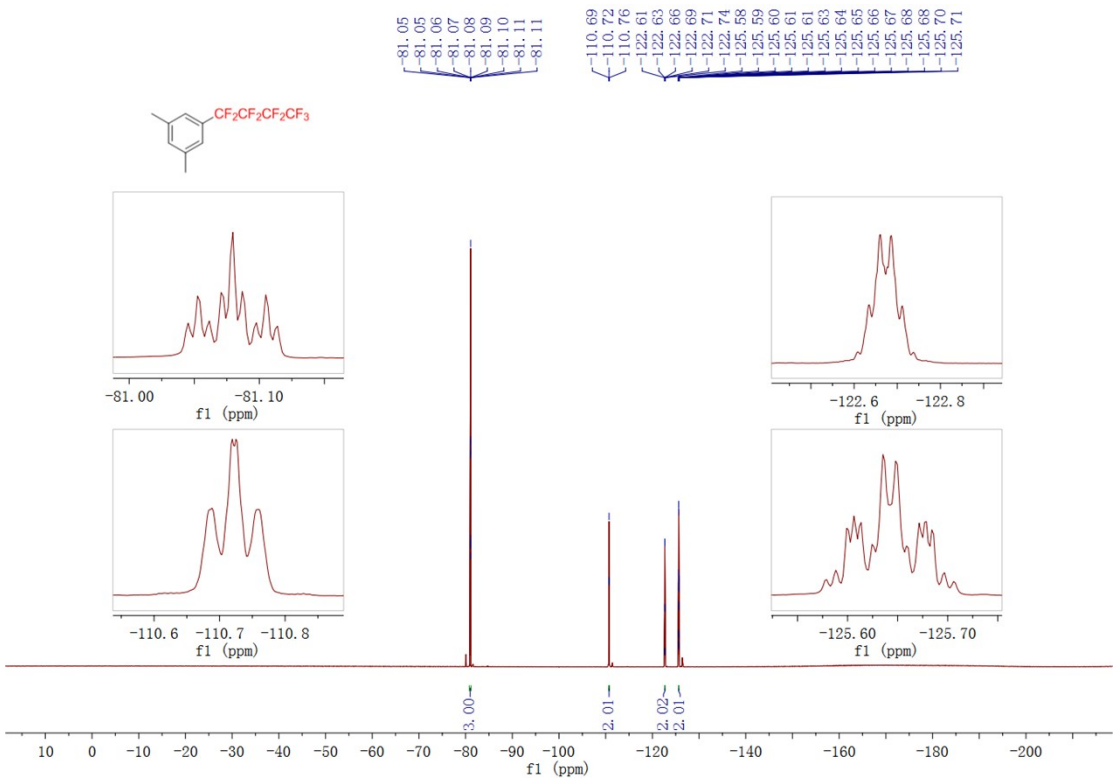
^{1}H NMR spectrum of **5a** in $CDCl_3$



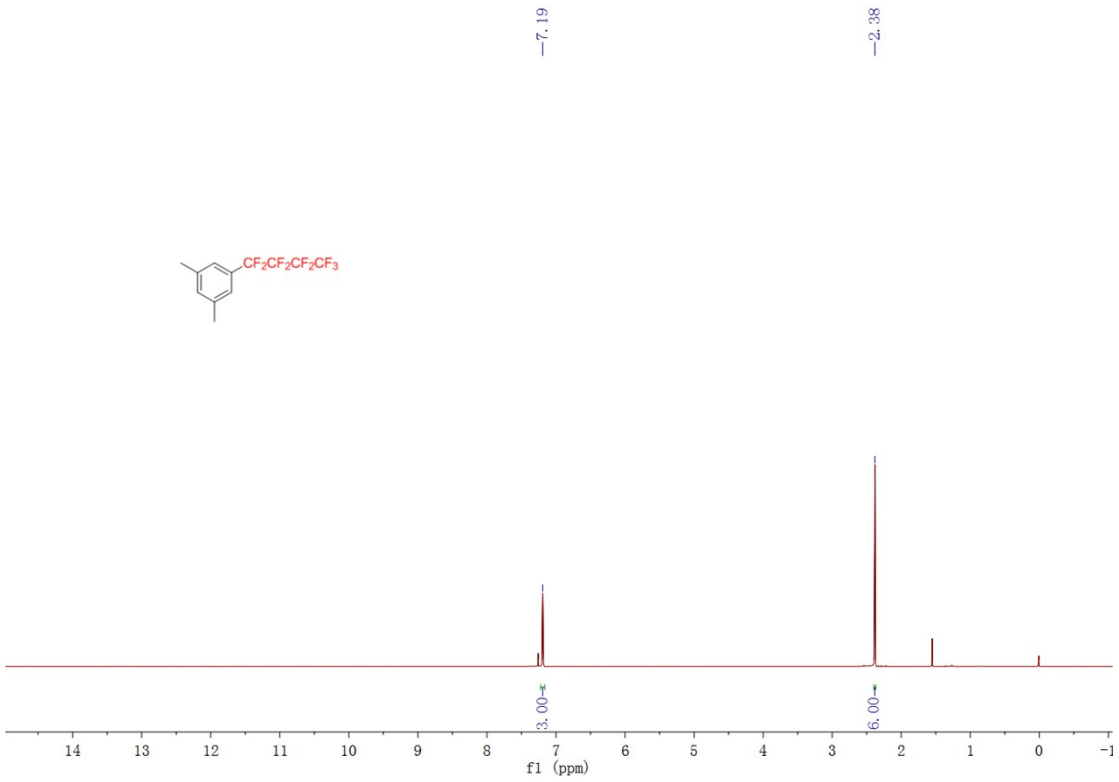
^{13}C NMR spectrum of **5a** in $CDCl_3$



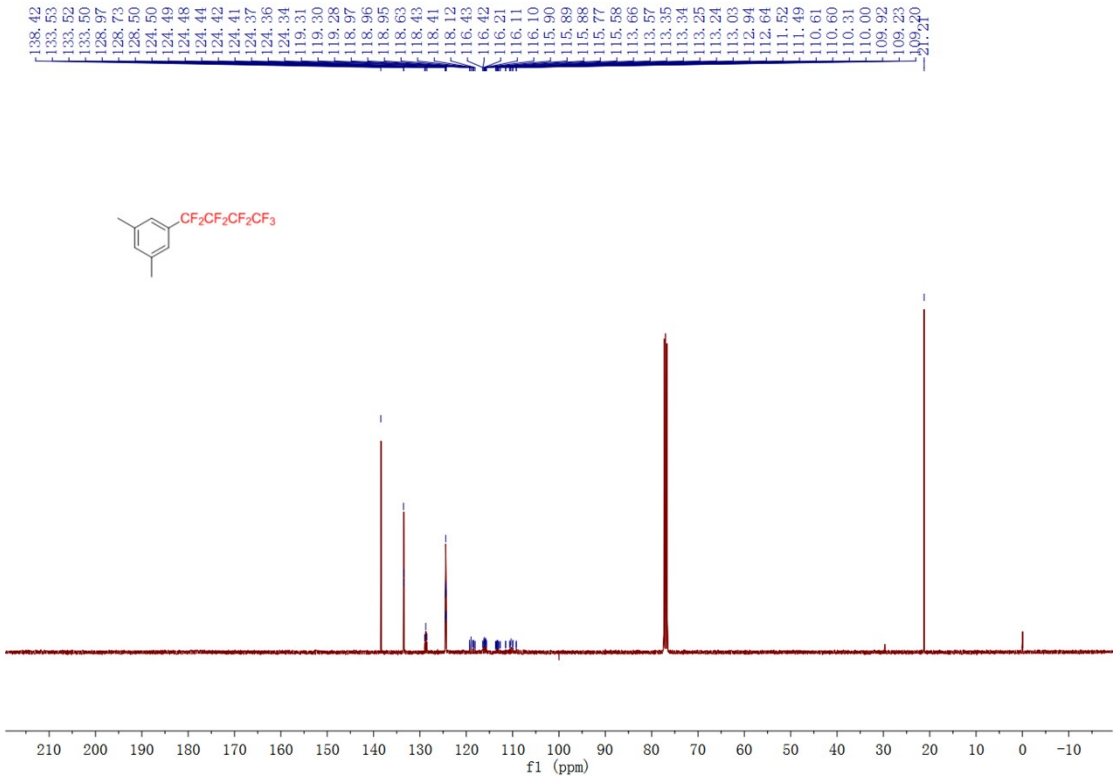
^{19}F NMR spectrum of **5b** in $CDCl_3$



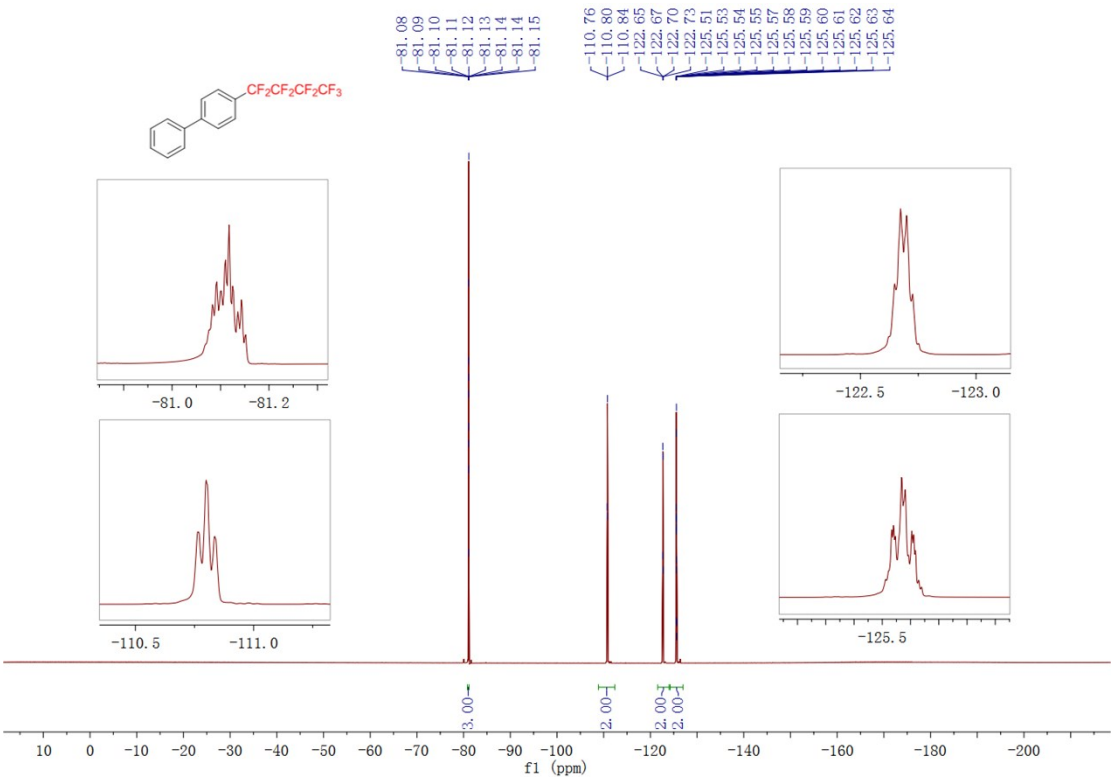
^{1}H NMR spectrum of **5b** in $CDCl_3$



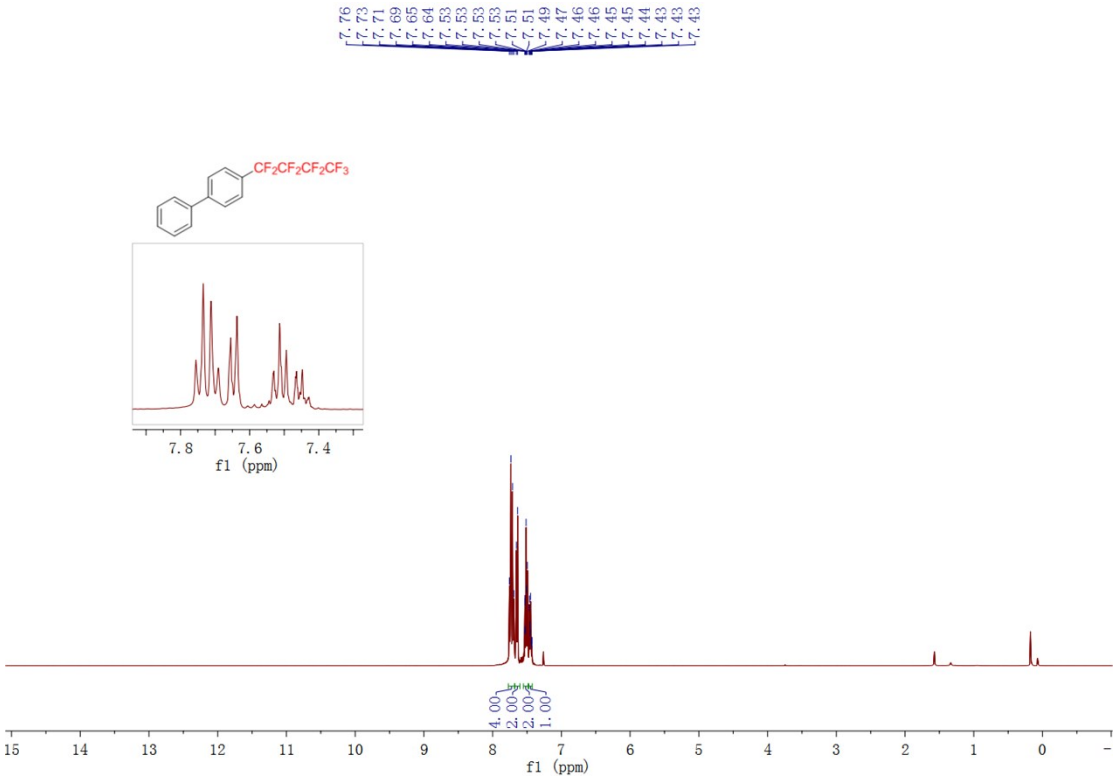
^{13}C NMR spectrum of **5b** in $CDCl_3$



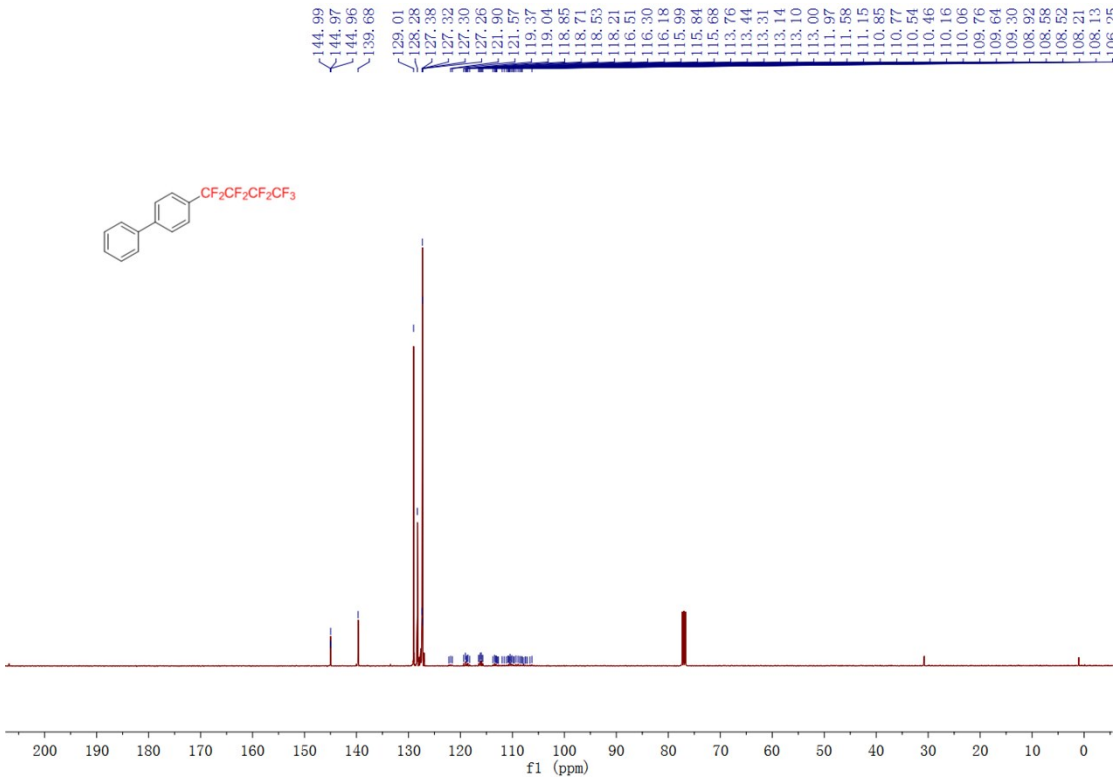
^{19}F NMR spectrum of **5c** in $CDCl_3$



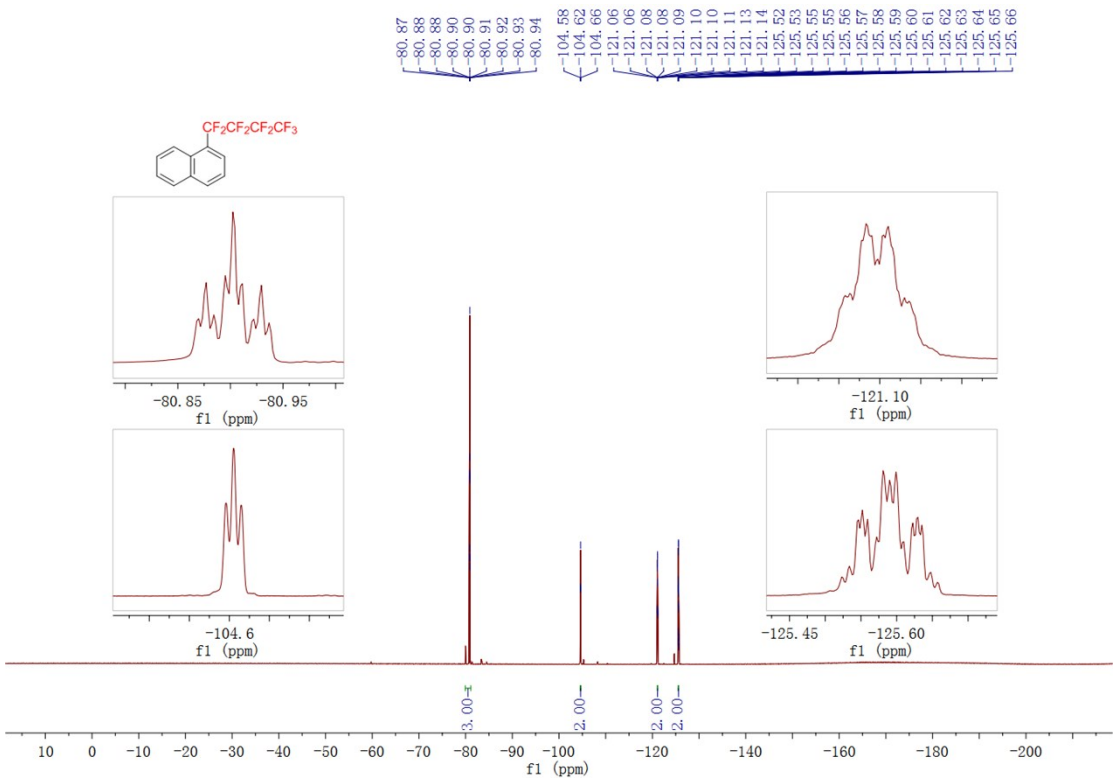
^{1}H NMR spectrum of **5c** in $CDCl_3$



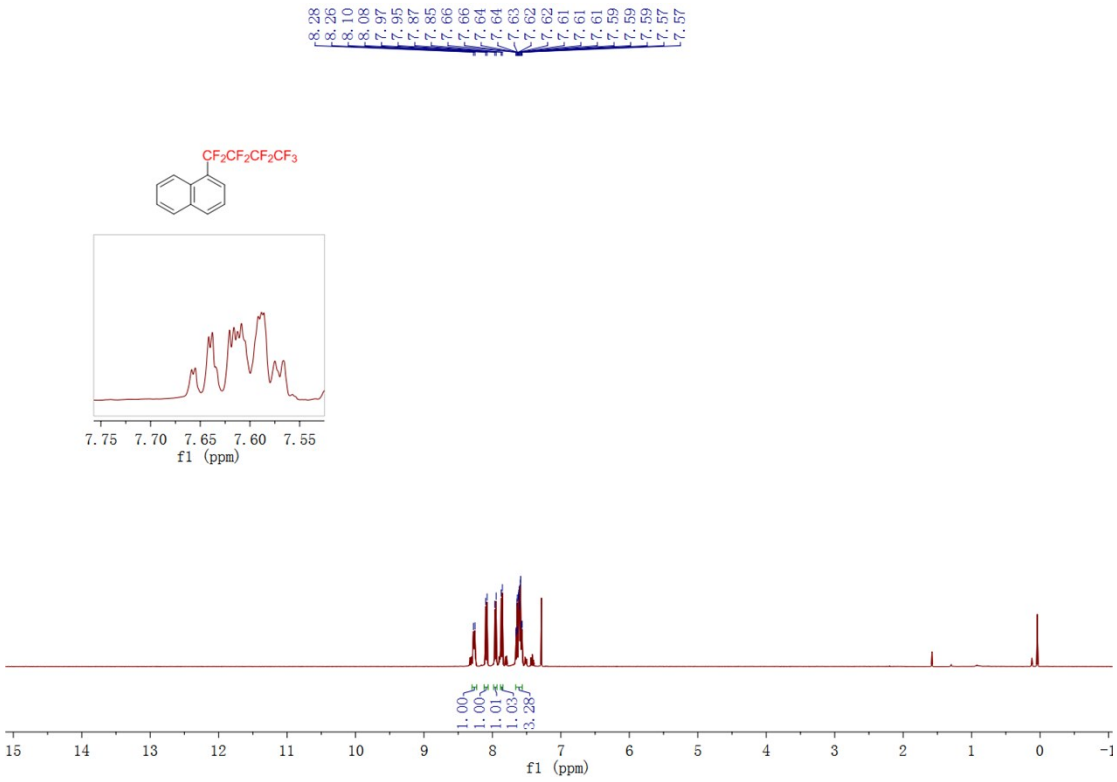
^{13}C NMR spectrum of **5c** in $CDCl_3$



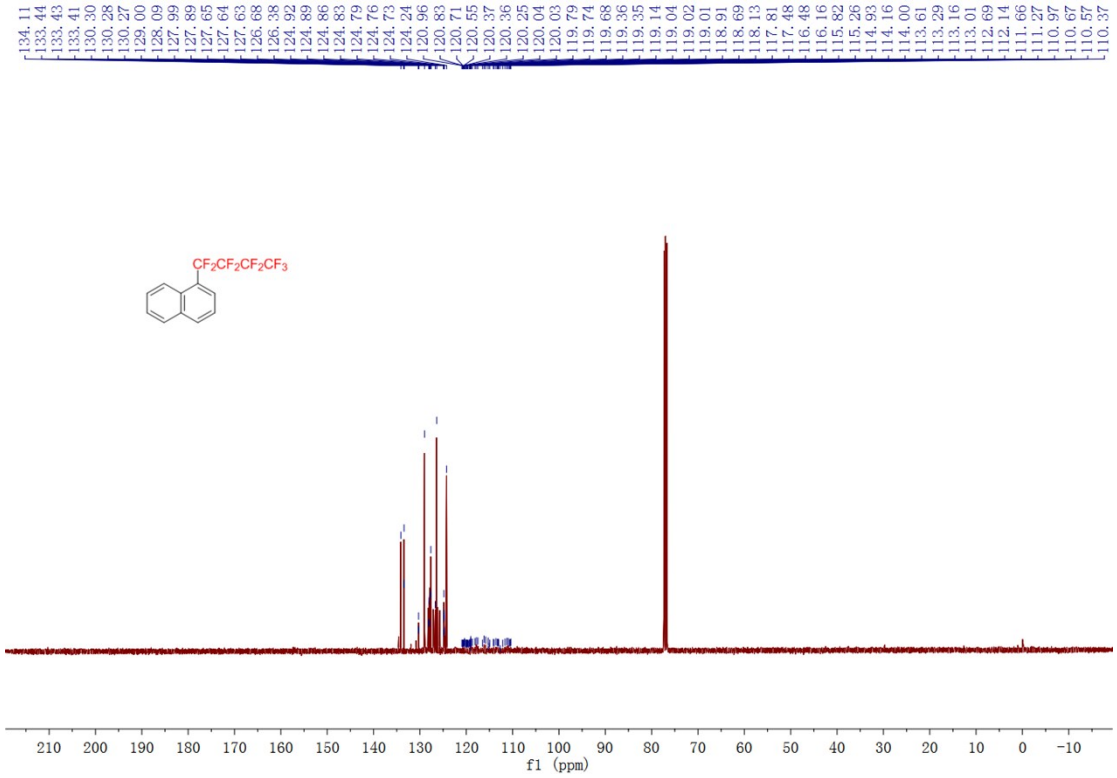
^{19}F NMR spectrum of **5e** in $CDCl_3$



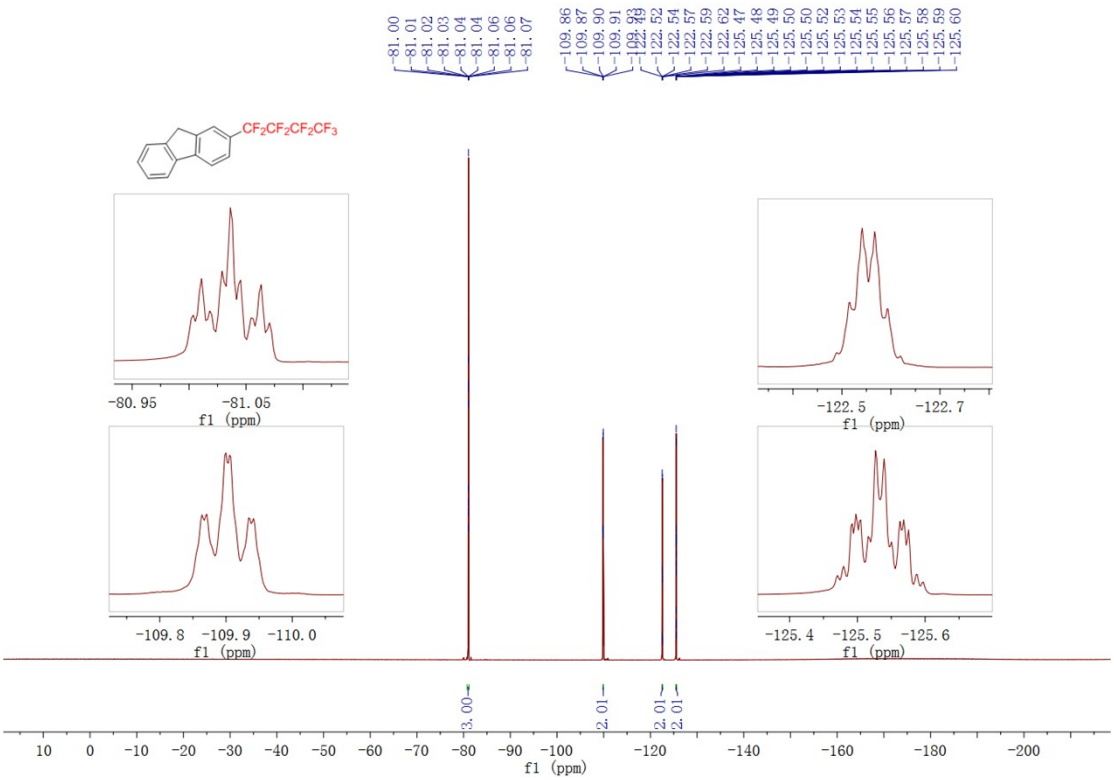
^{1}H NMR spectrum of **5e** in $CDCl_3$



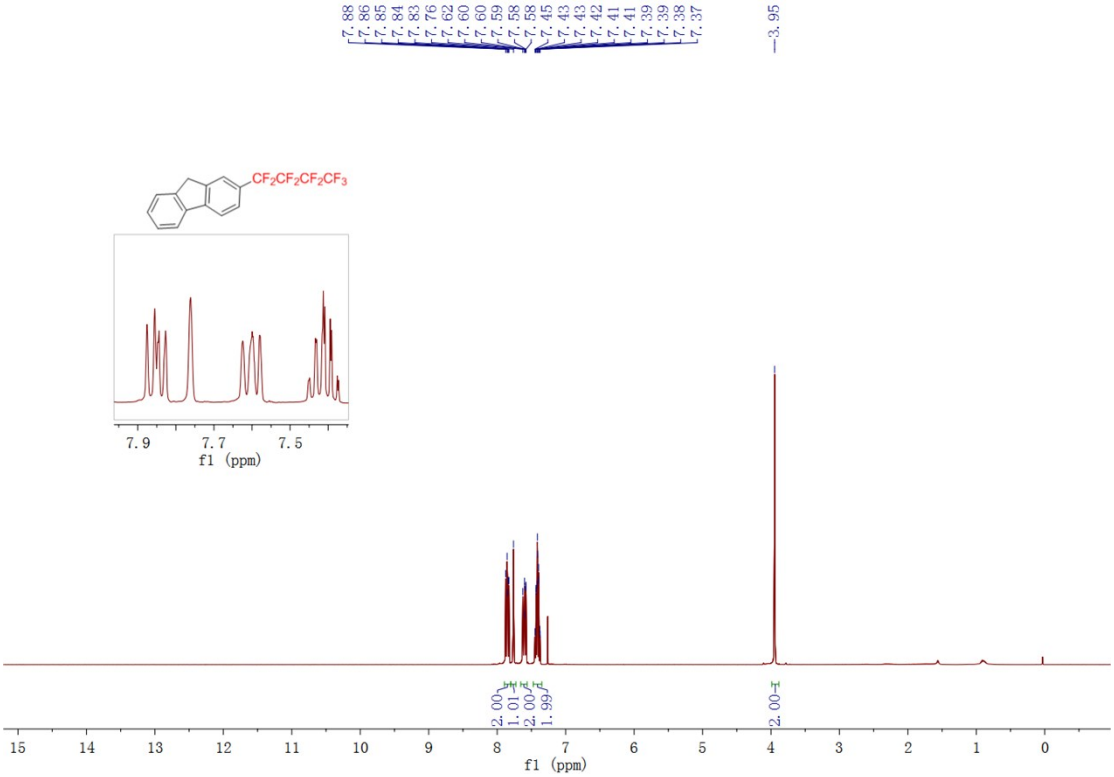
^{13}C NMR spectrum of **5e** in $CDCl_3$



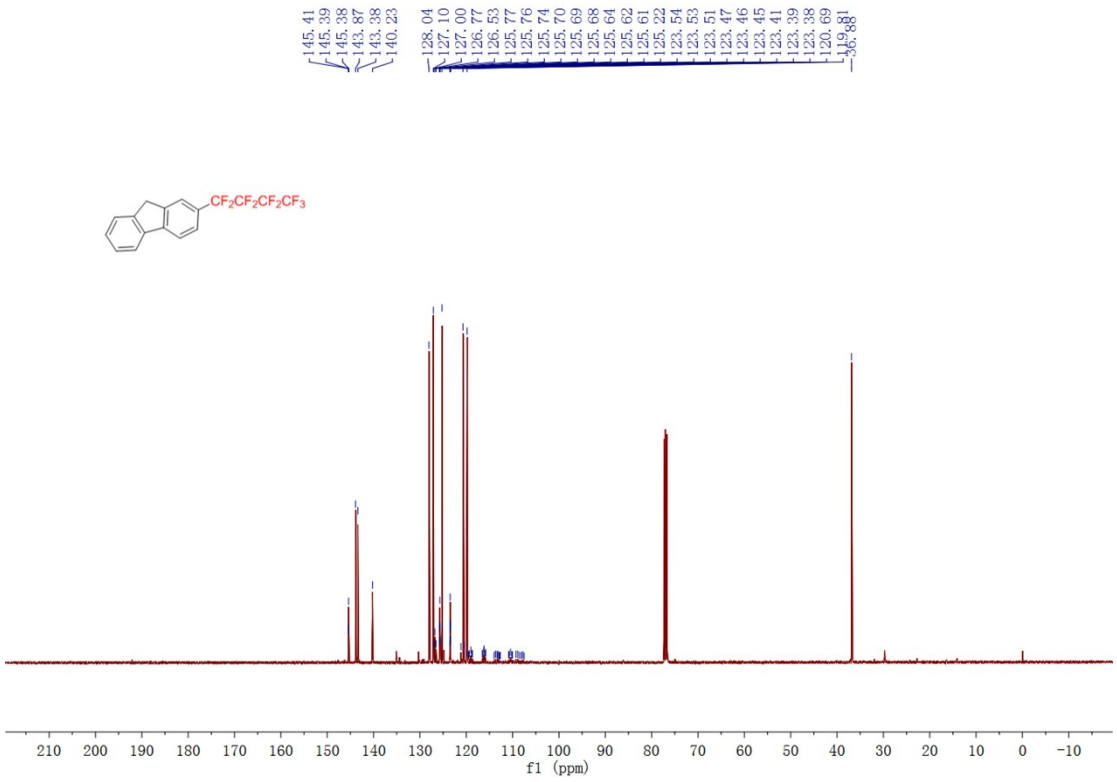
^{19}F NMR spectrum of **5f** in $CDCl_3$



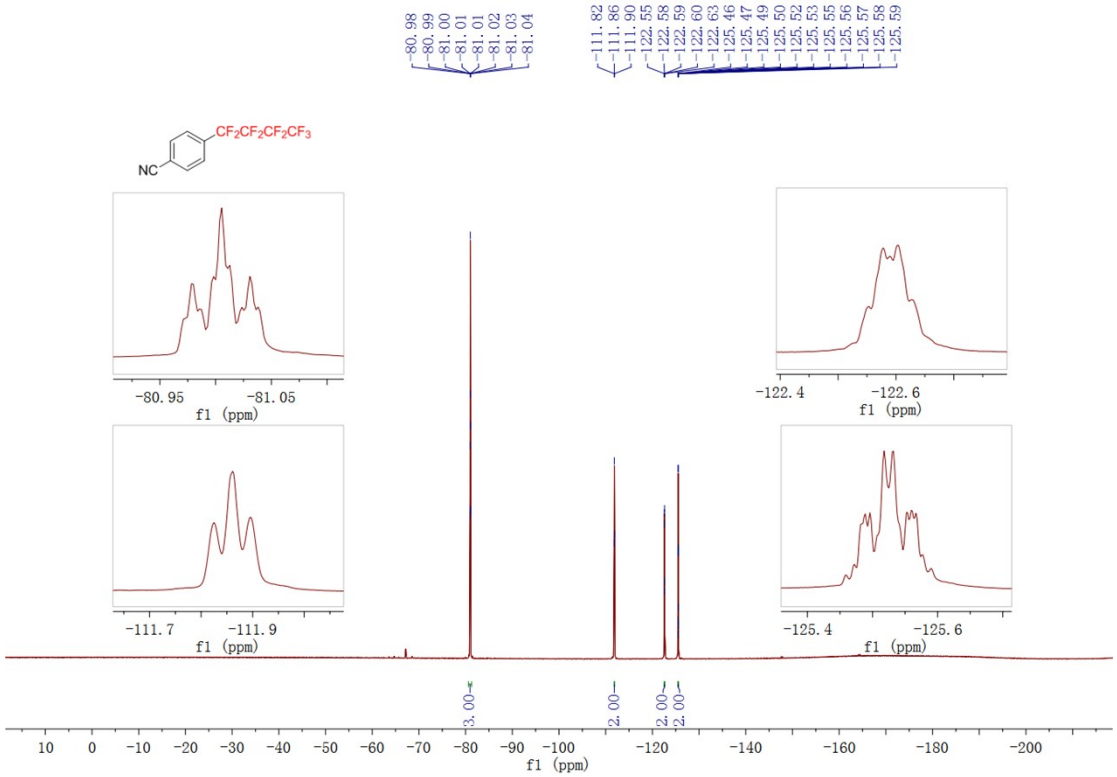
^{1}H NMR spectrum of **5f** in $CDCl_3$



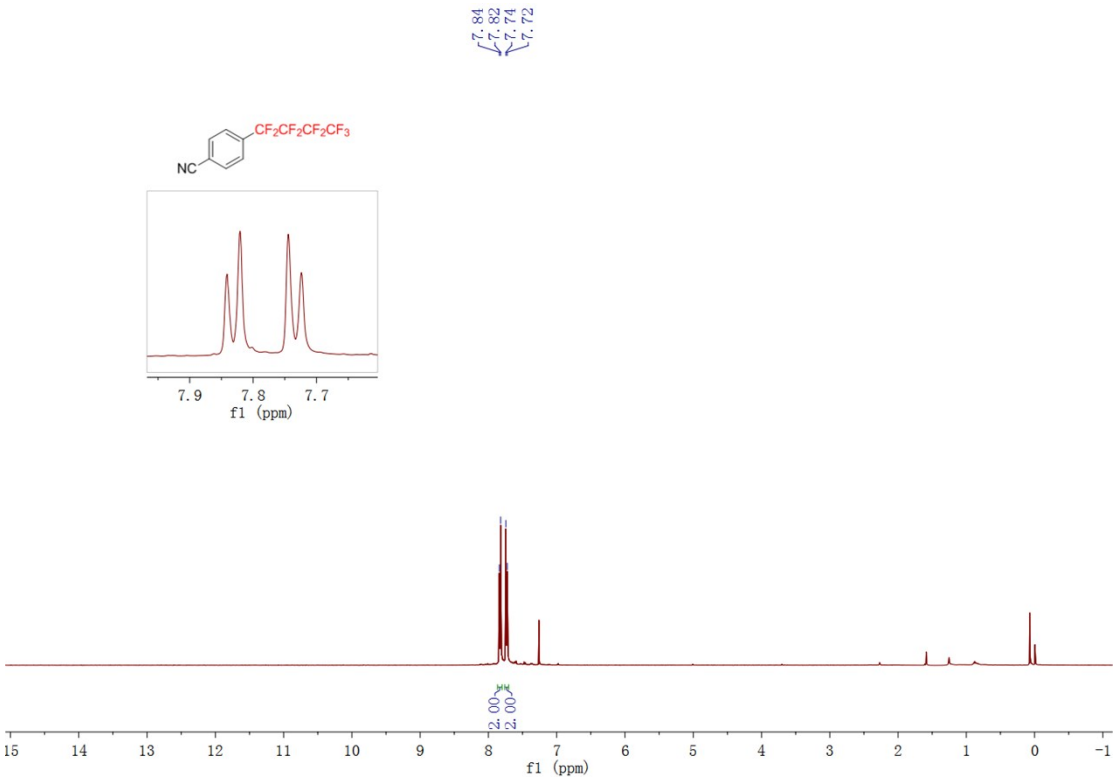
^{13}C NMR spectrum of **5f** in $CDCl_3$



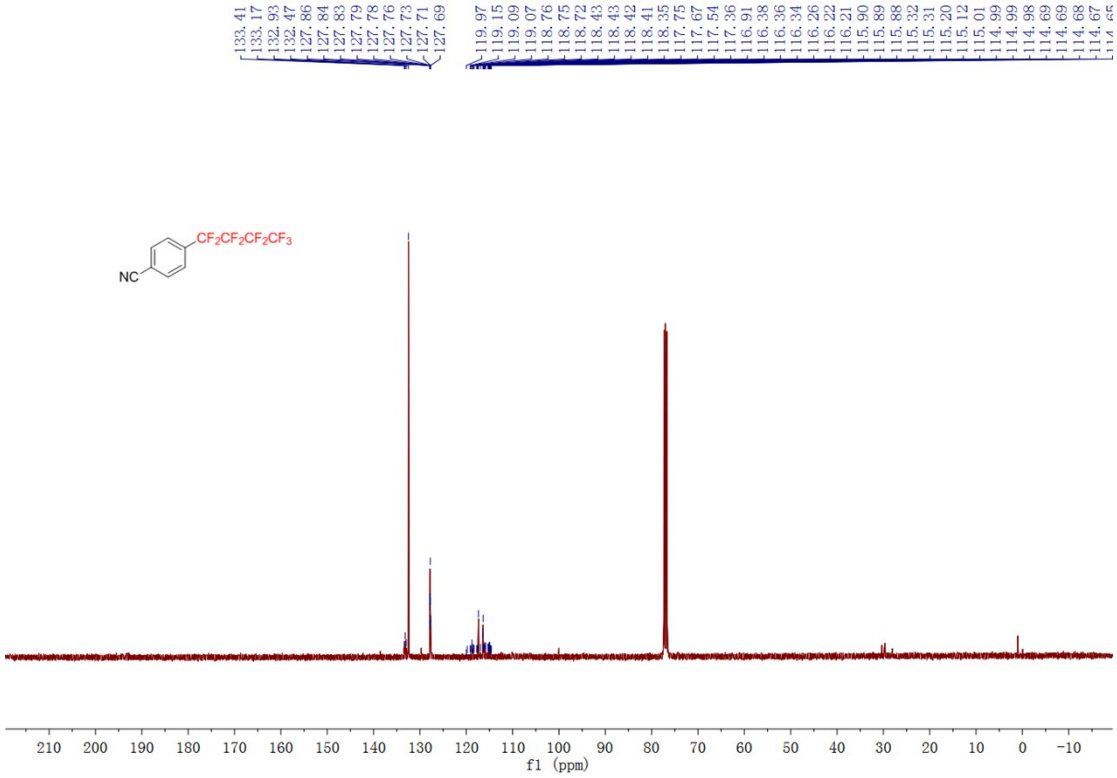
^{19}F NMR spectrum of **5g** in $CDCl_3$



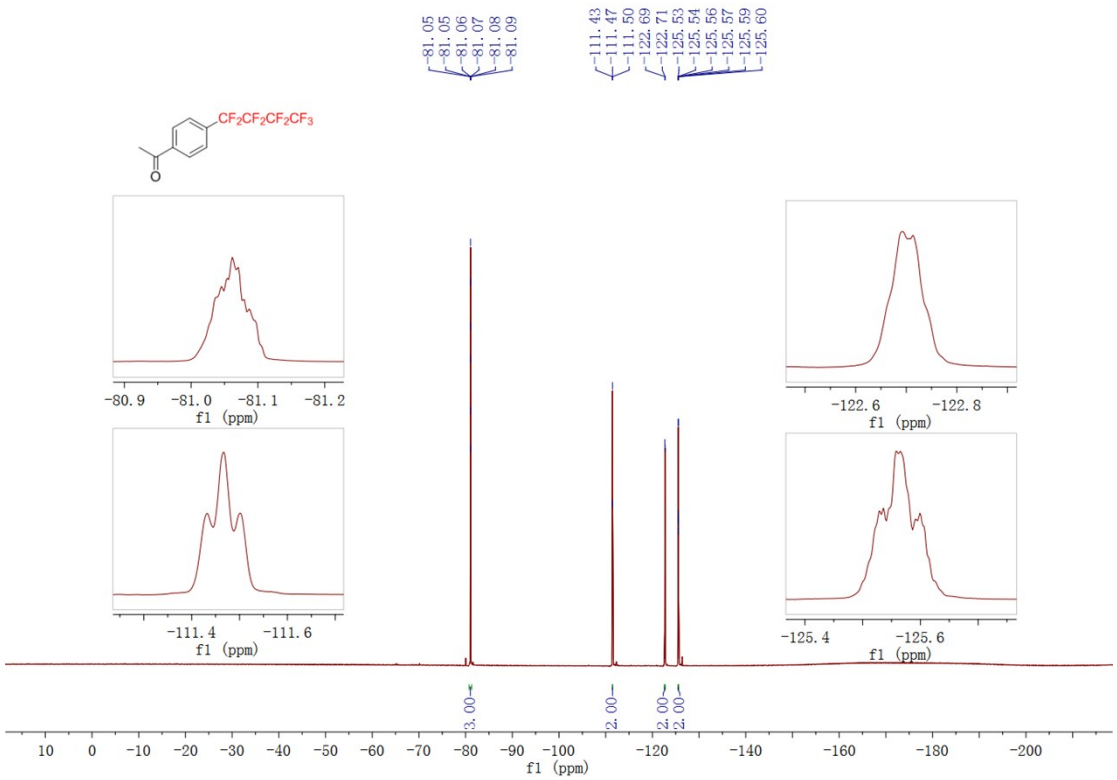
^{1}H NMR spectrum of **5g** in $CDCl_3$



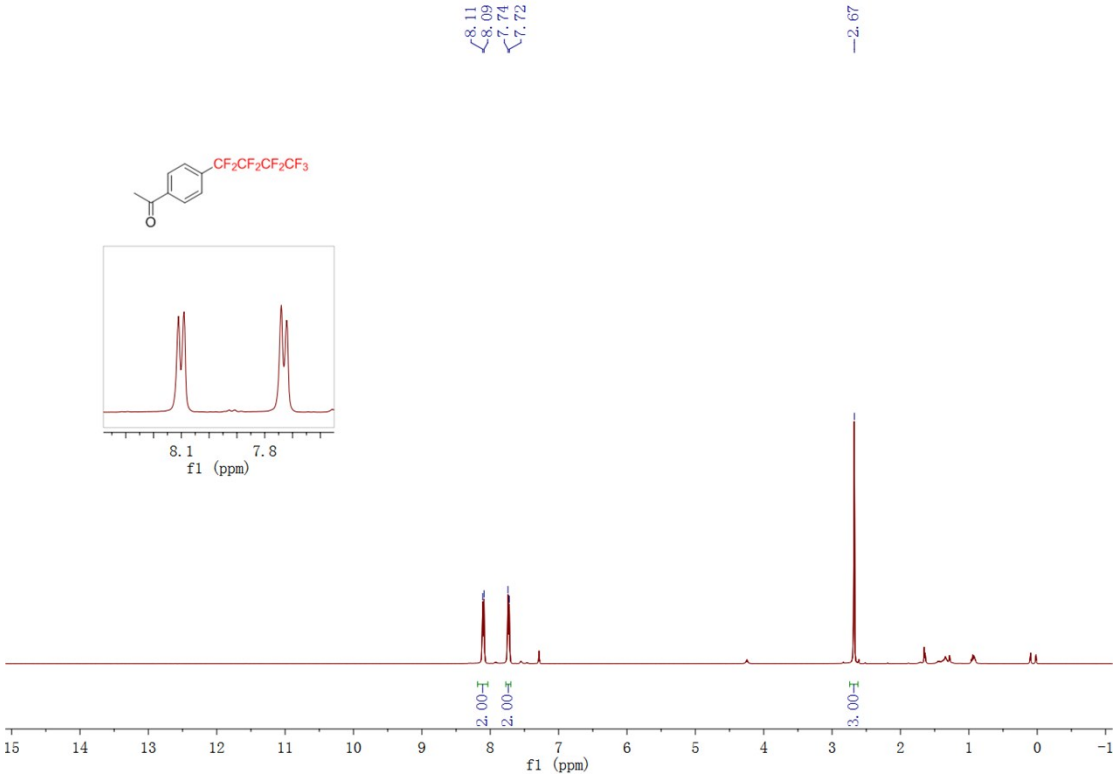
^{13}C NMR spectrum of **5g** in $CDCl_3$



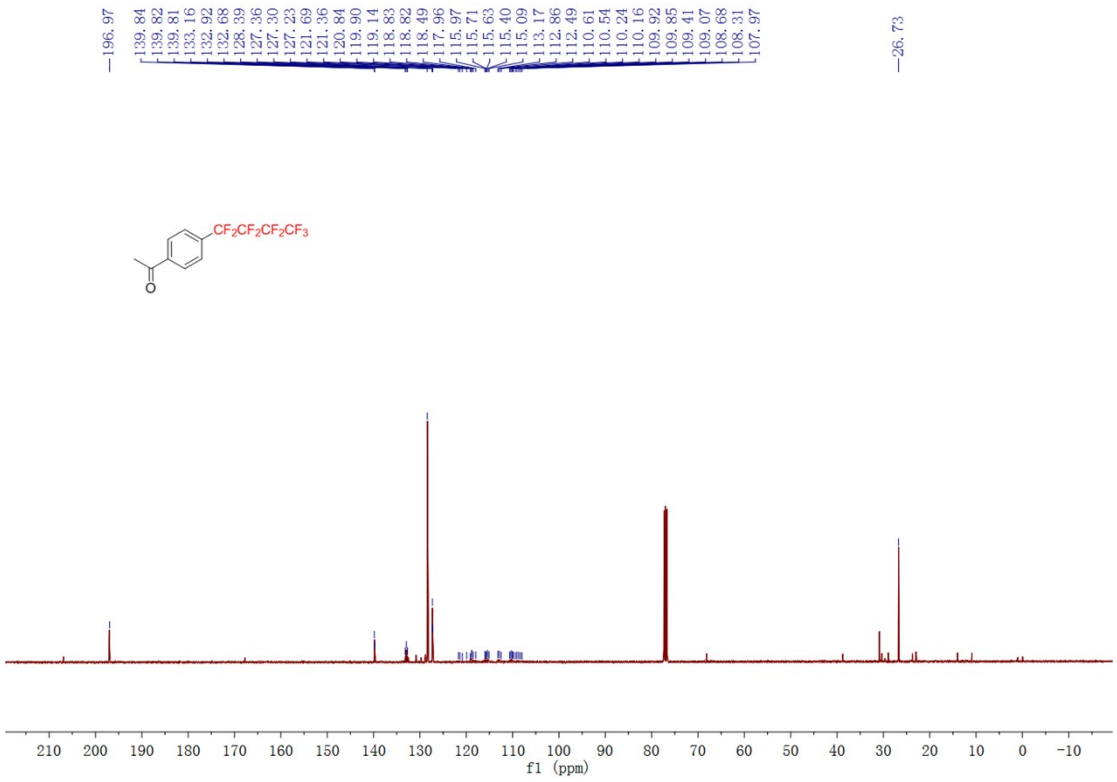
^{19}F NMR spectrum of **5h** in $CDCl_3$



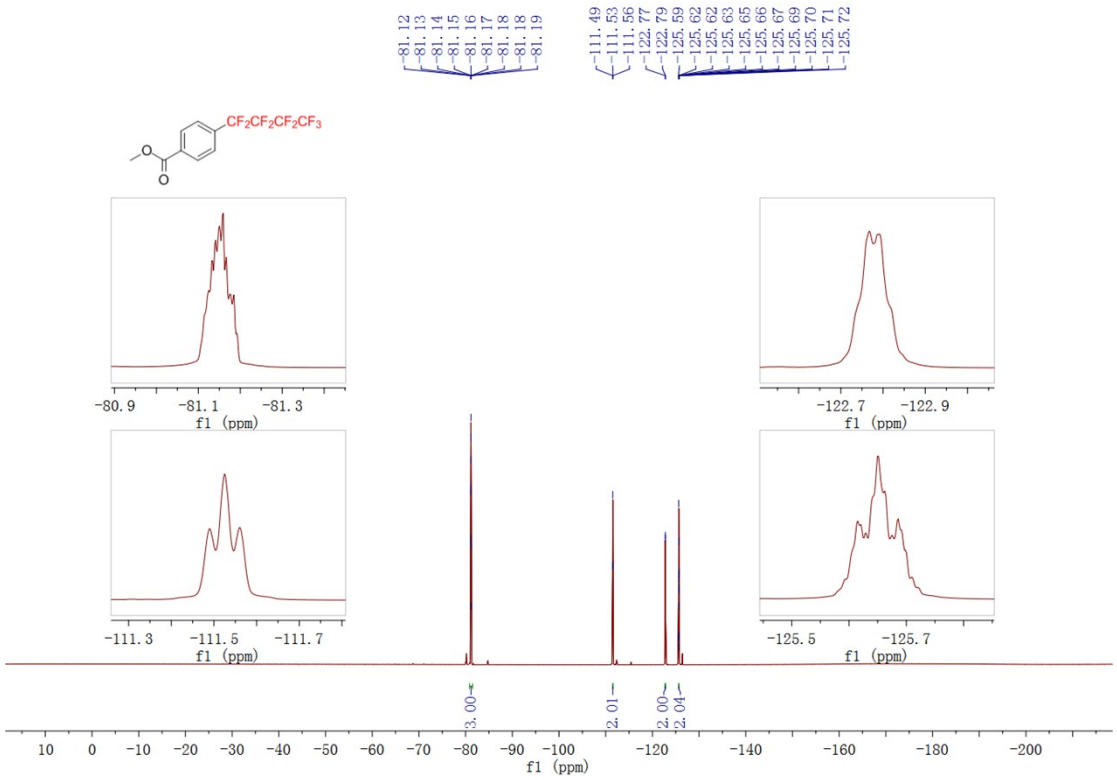
^{1}H NMR spectrum of **5h** in $CDCl_3$



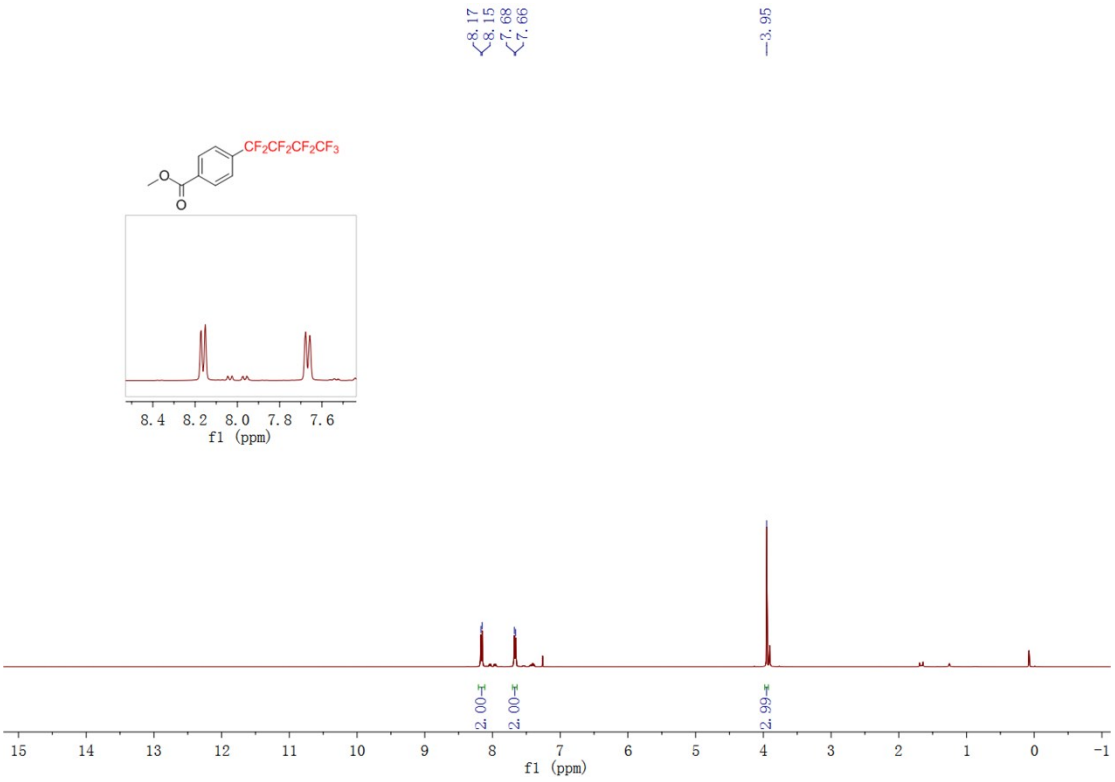
^{13}C NMR spectrum of **5h** in $CDCl_3$



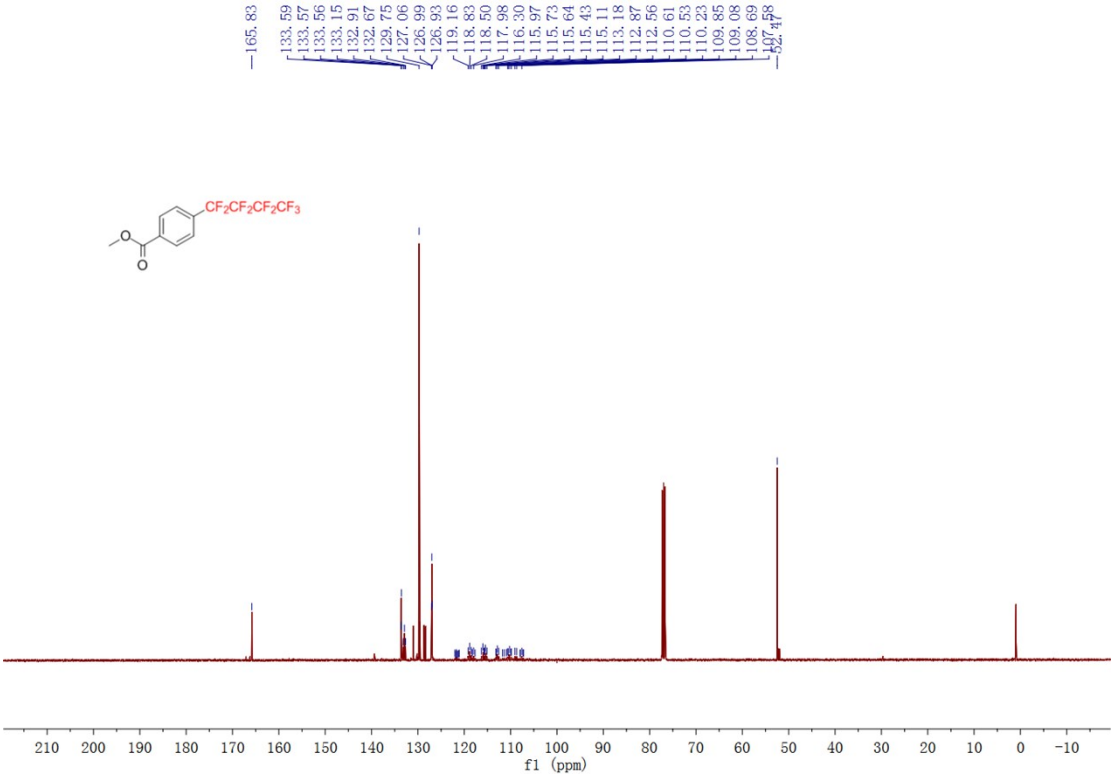
^{19}F NMR spectrum of **5i** in $CDCl_3$



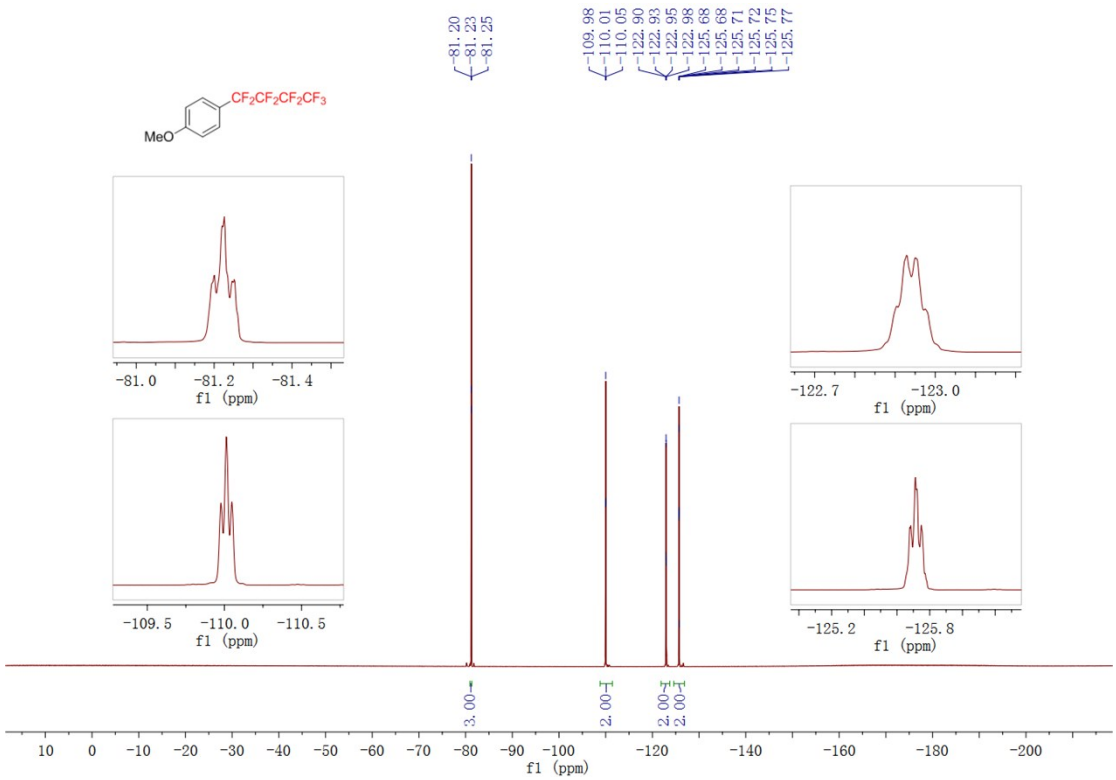
^{1}H NMR spectrum of **5i** in $CDCl_3$



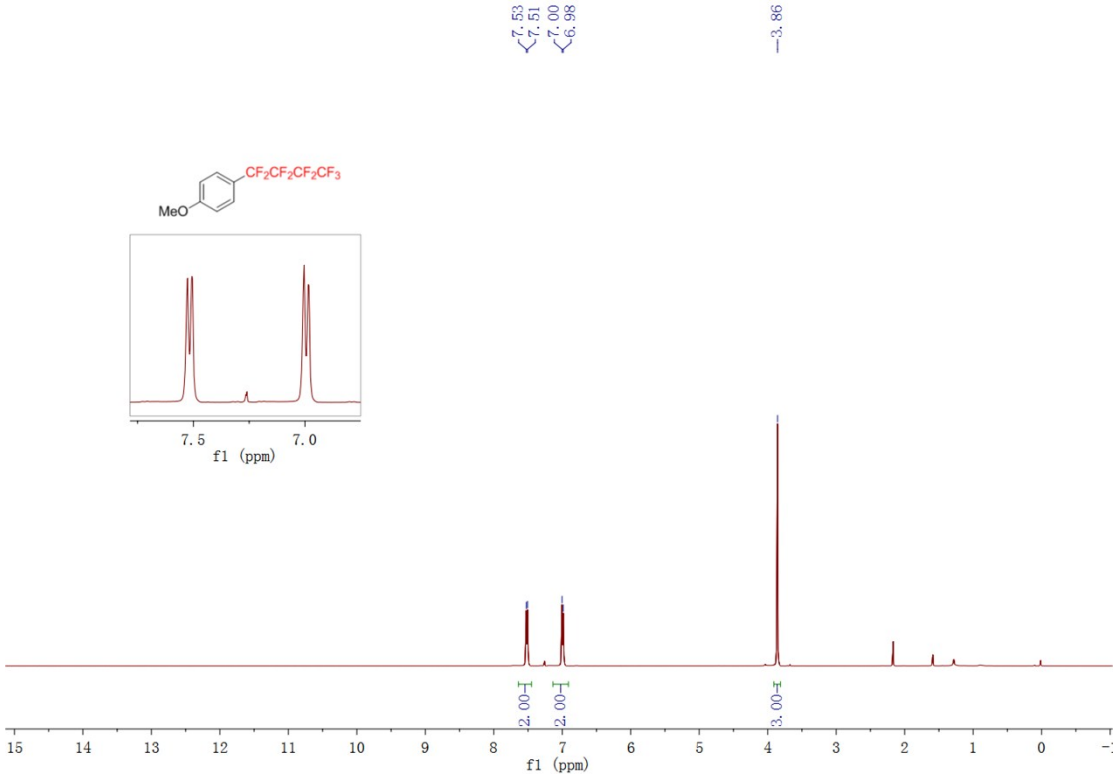
^{13}C NMR spectrum of **5i** in $CDCl_3$



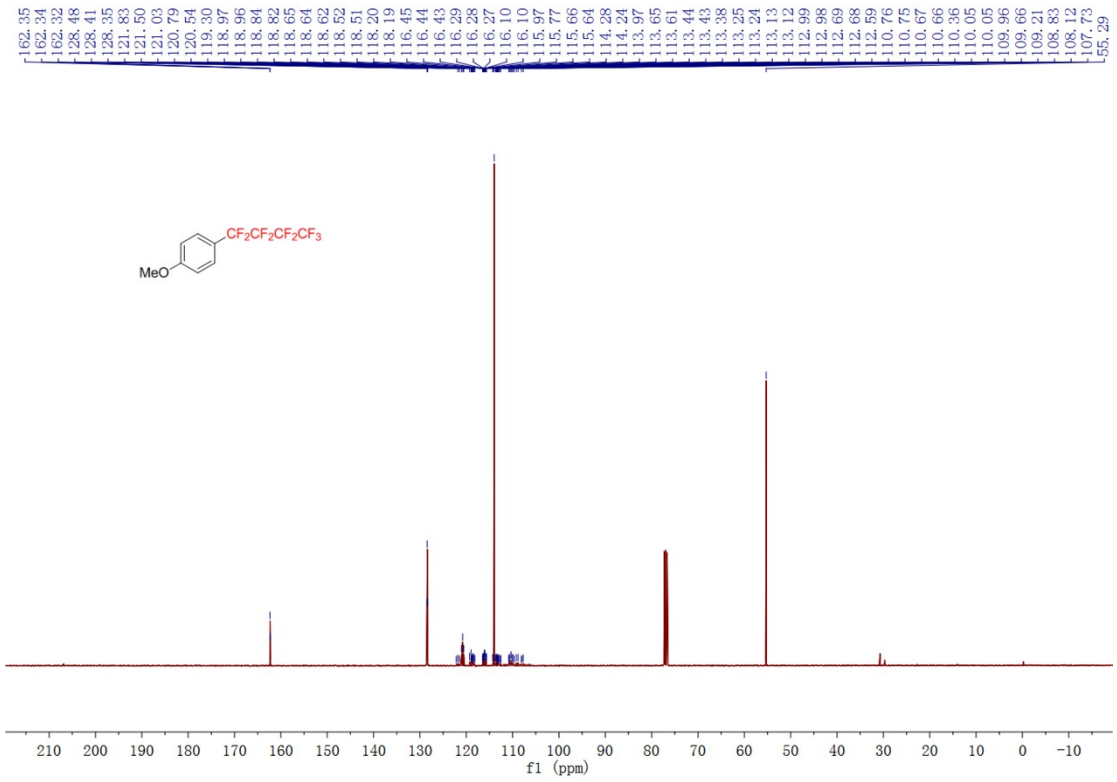
^{19}F NMR spectrum of **5k** in $CDCl_3$



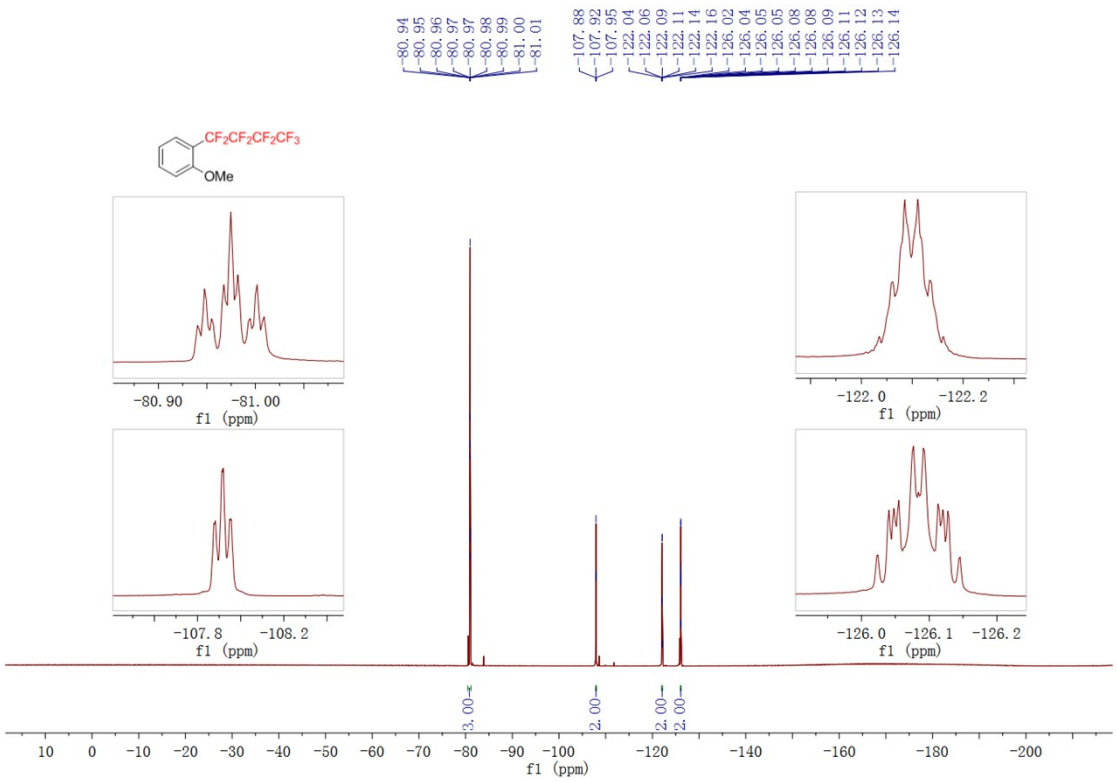
^{1}H NMR spectrum of **5k** in $CDCl_3$



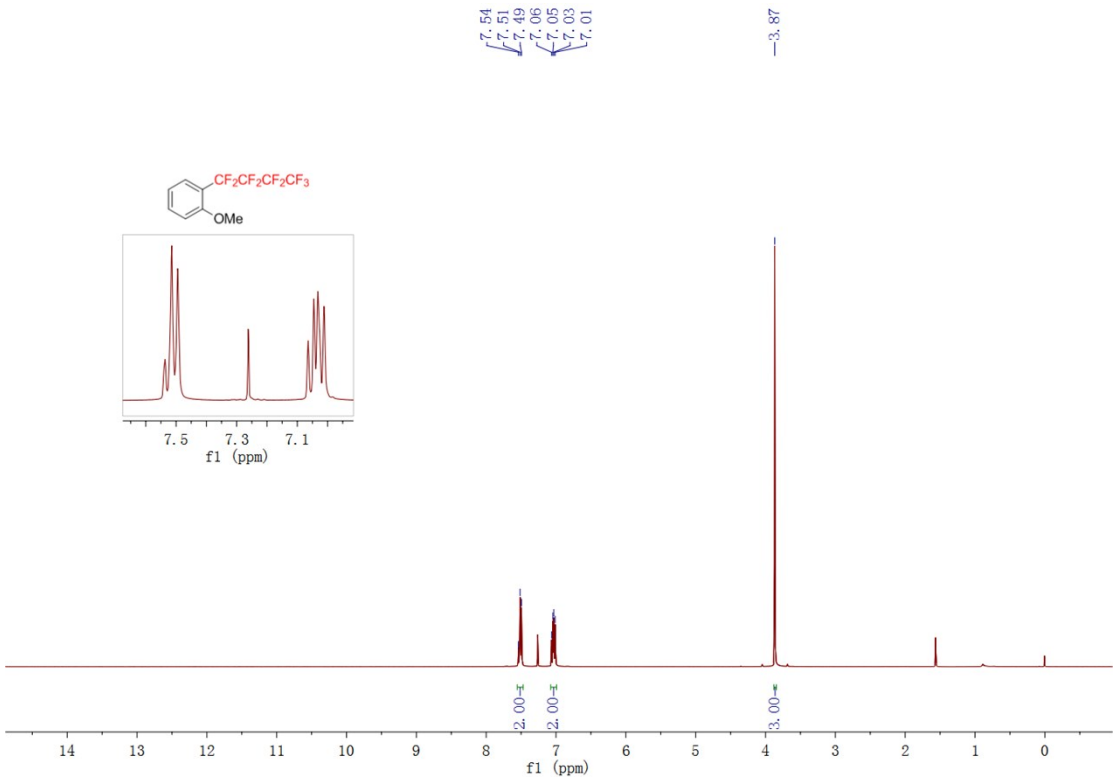
^{13}C NMR spectrum of **5k** in $CDCl_3$



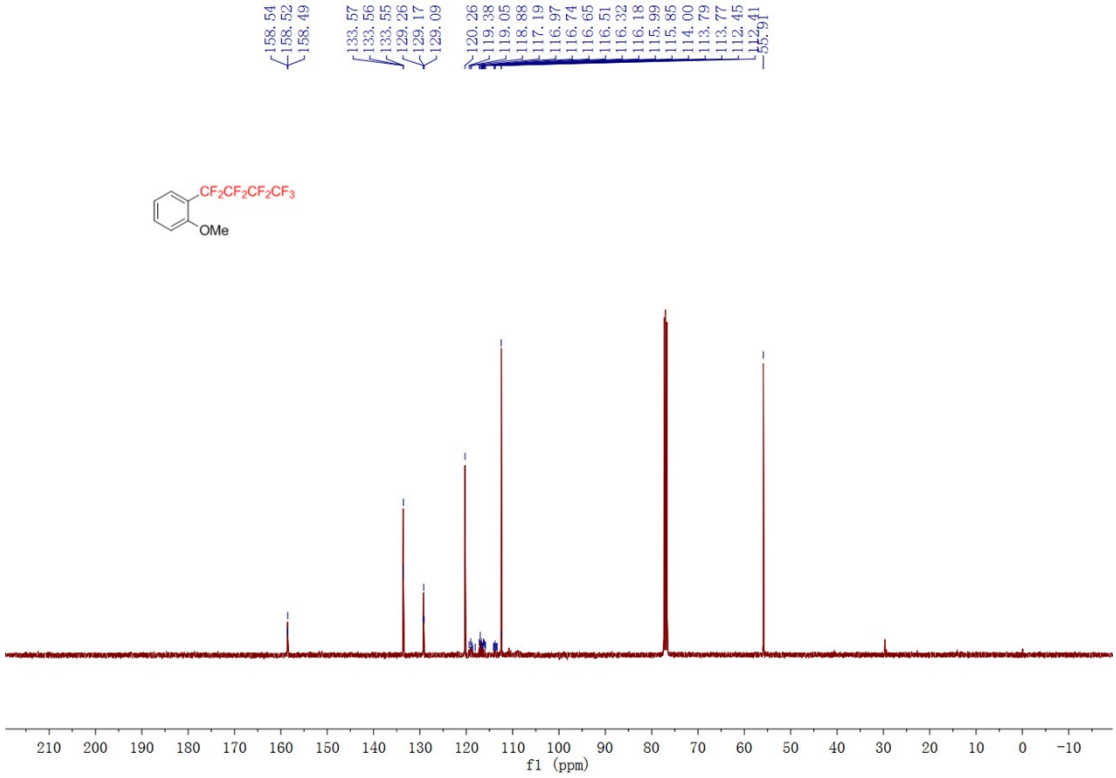
^{19}F NMR spectrum of **5l** in $CDCl_3$



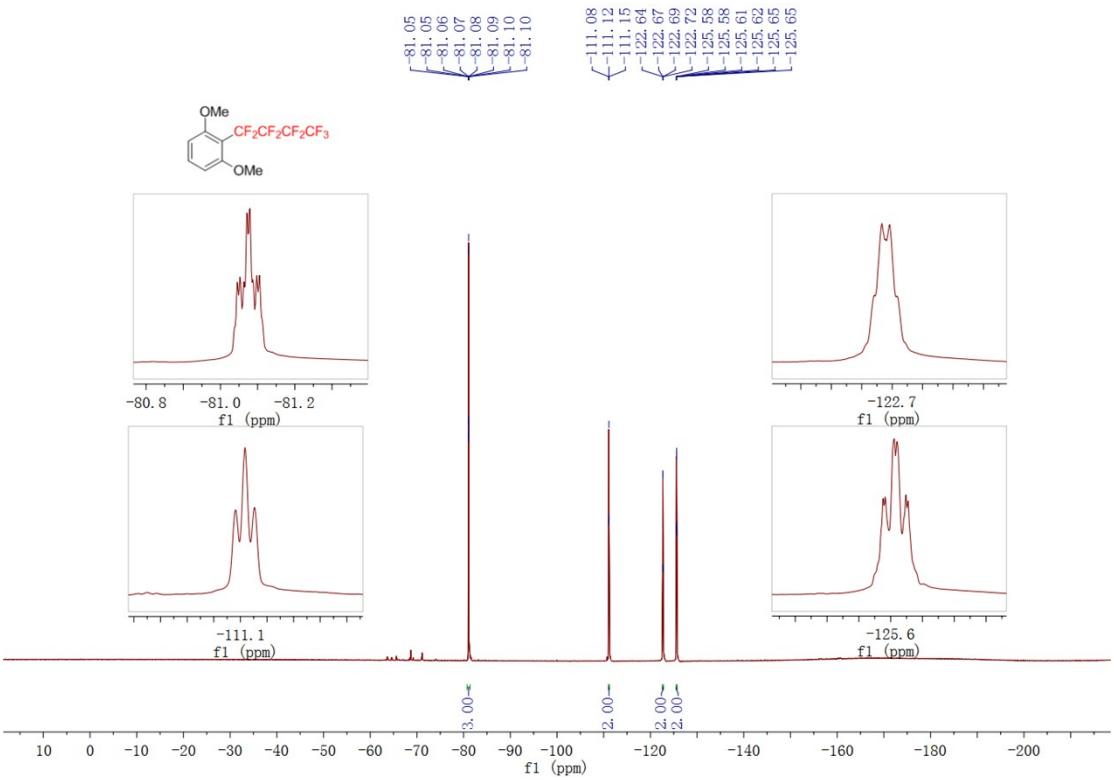
^{1}H NMR spectrum of **5l** in $CDCl_3$



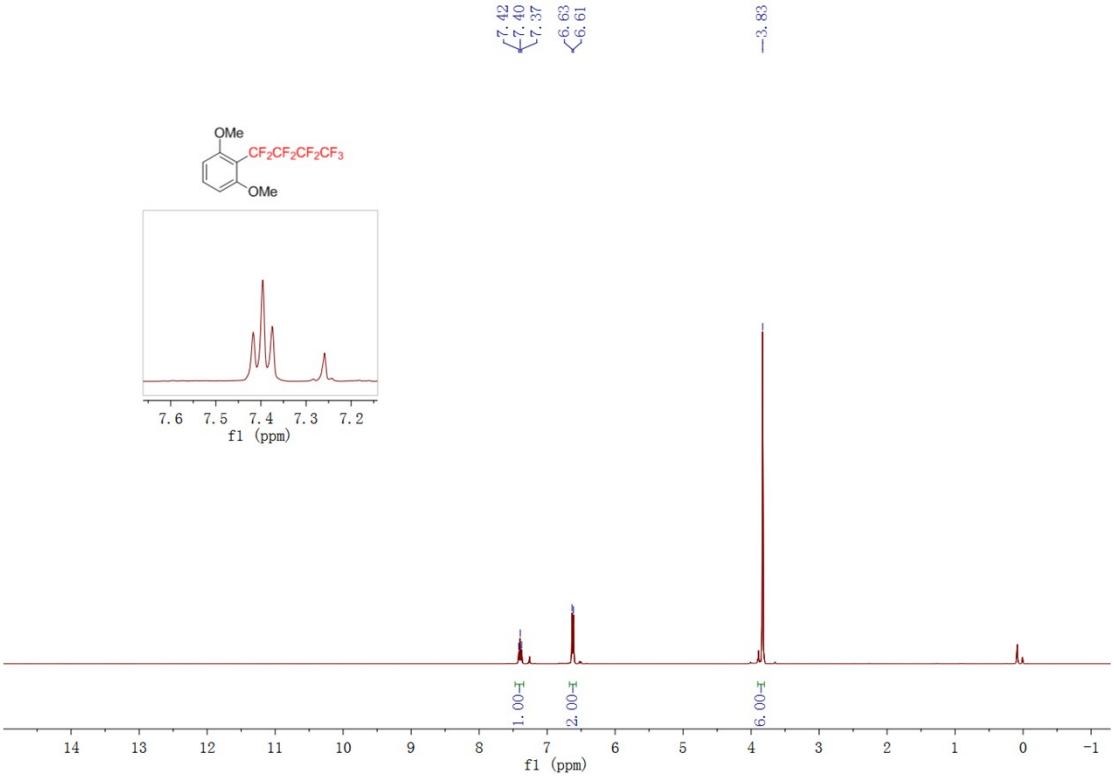
^{13}C NMR spectrum of **5l** in $CDCl_3$



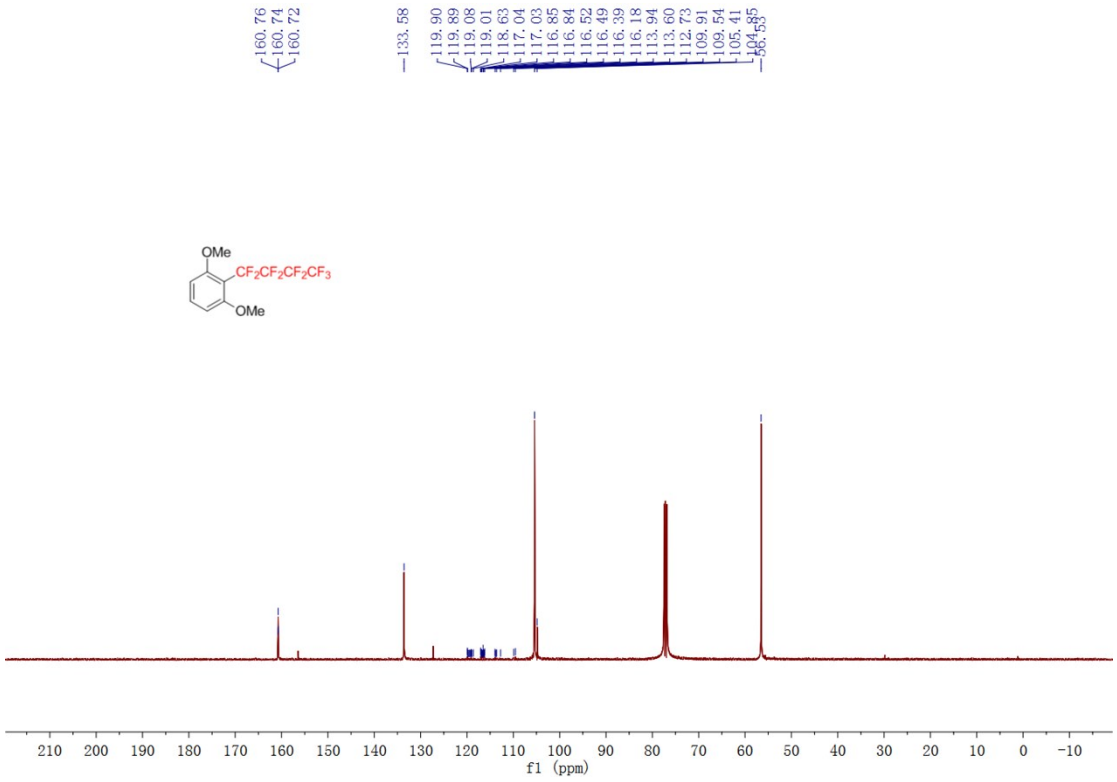
^{19}F NMR spectrum of **5m** in $CDCl_3$



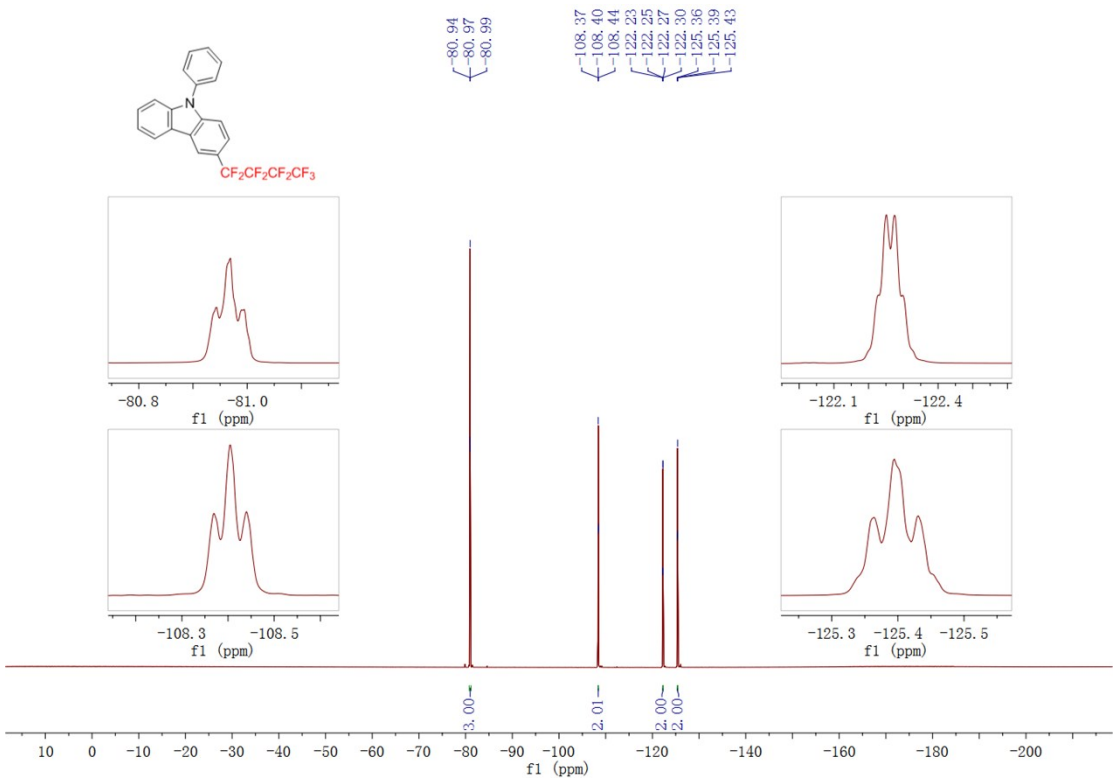
^{1}H NMR spectrum of **5m** in $CDCl_3$



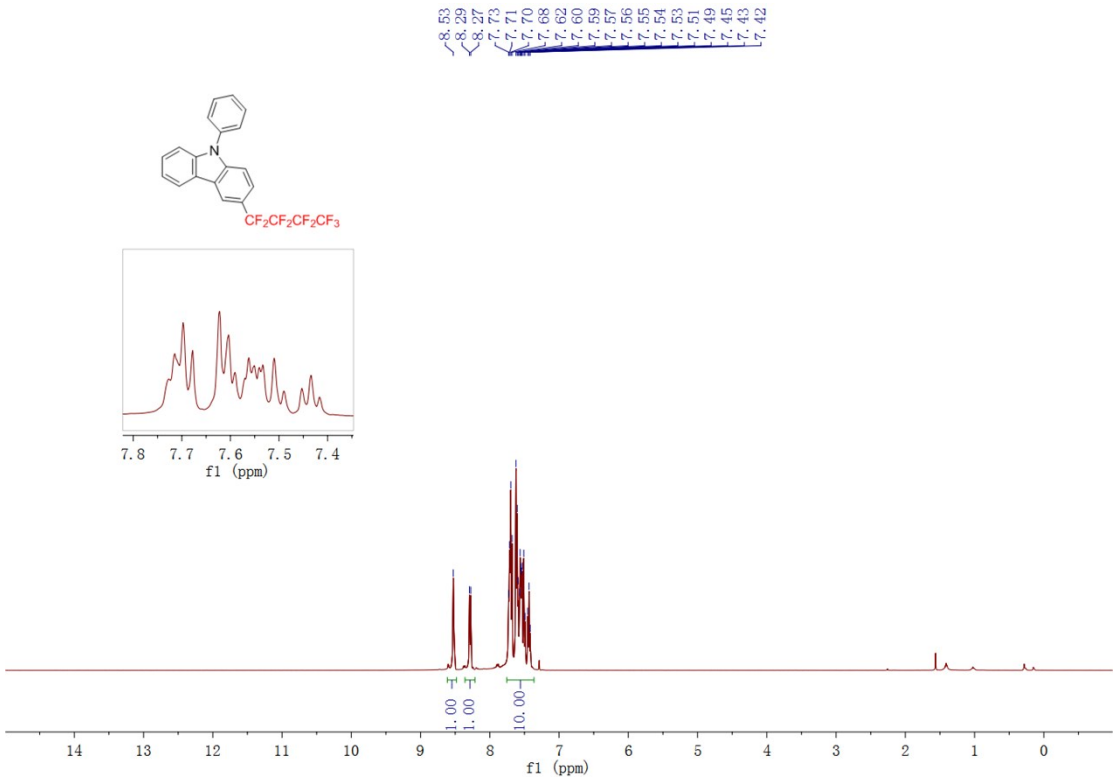
^{13}C NMR spectrum of **5m** in $CDCl_3$



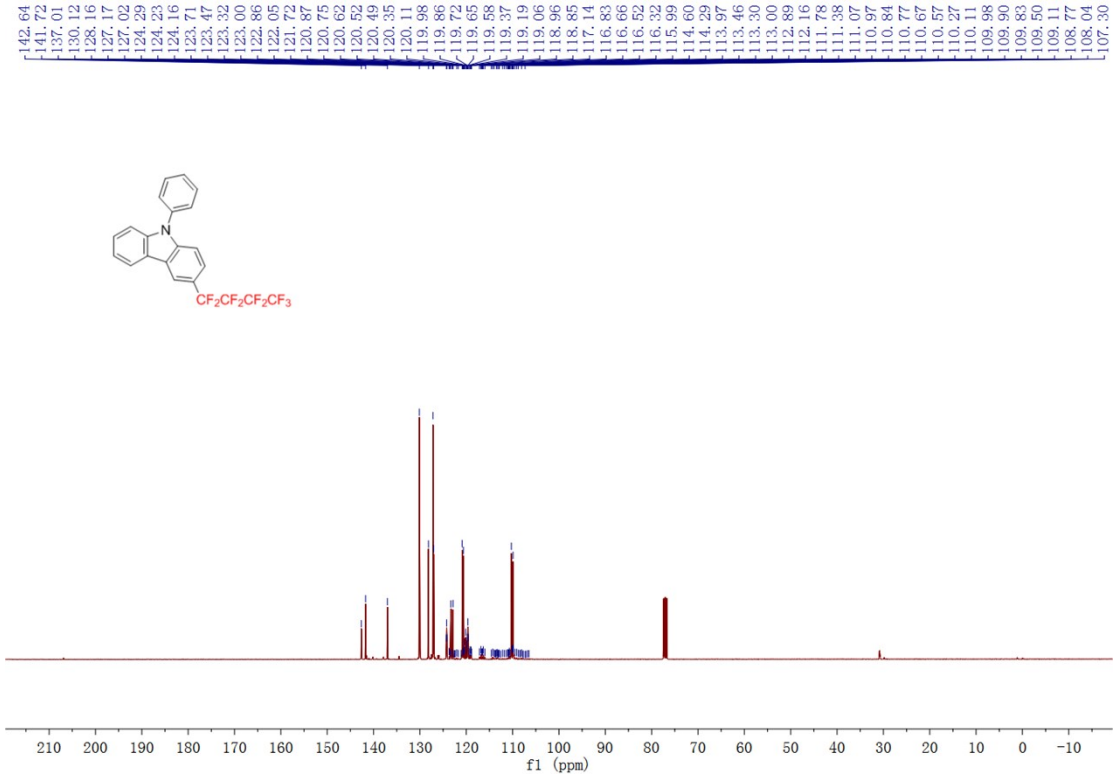
^{19}F NMR spectrum of **5o** in $CDCl_3$



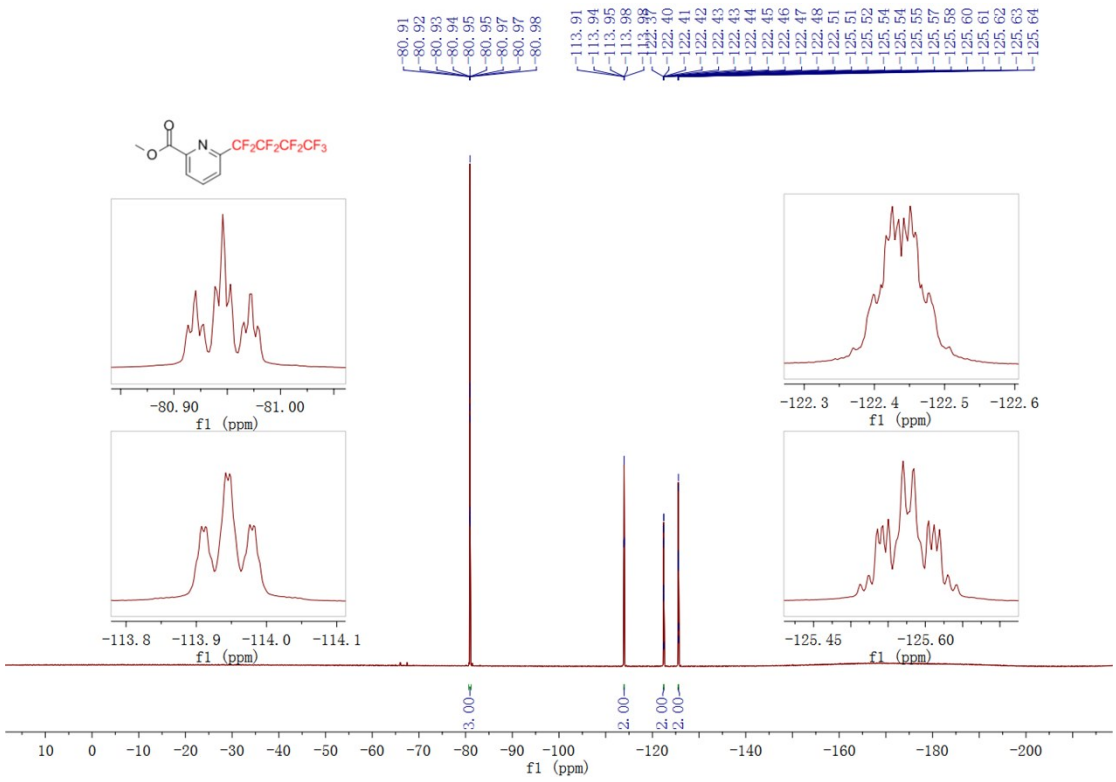
^{1}H NMR spectrum of **5o** in $CDCl_3$



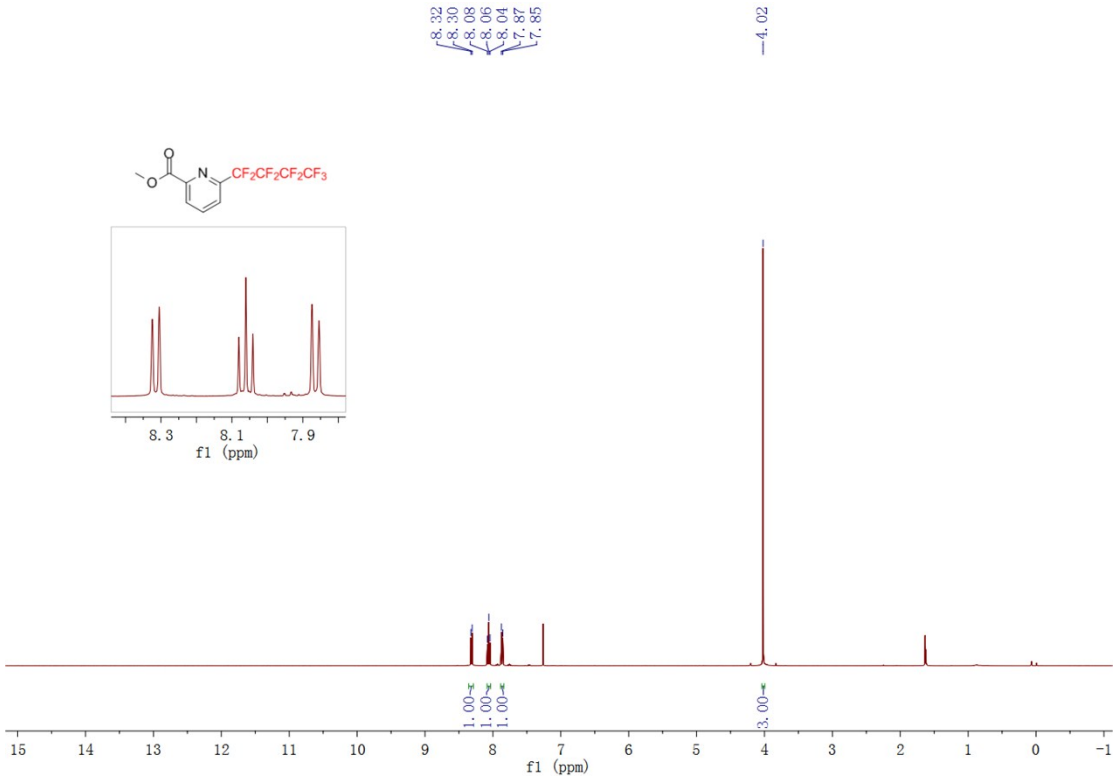
^{13}C NMR spectrum of **5o** in $CDCl_3$



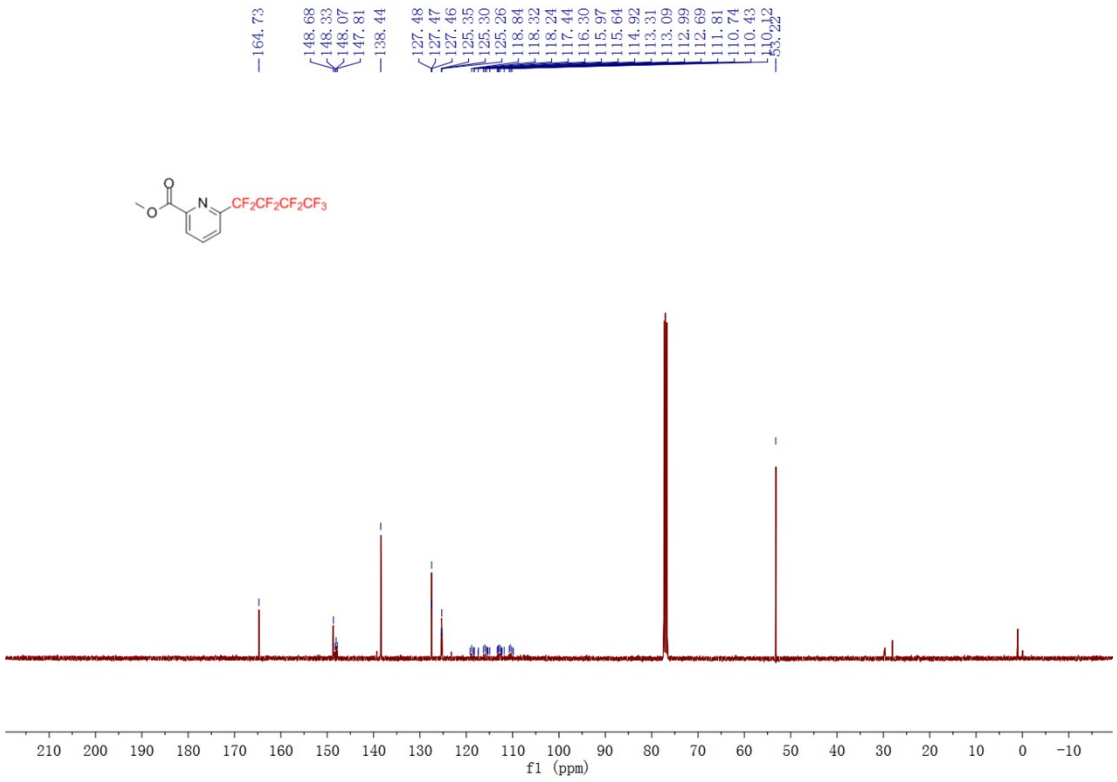
^{19}F NMR spectrum of **5p** in $CDCl_3$



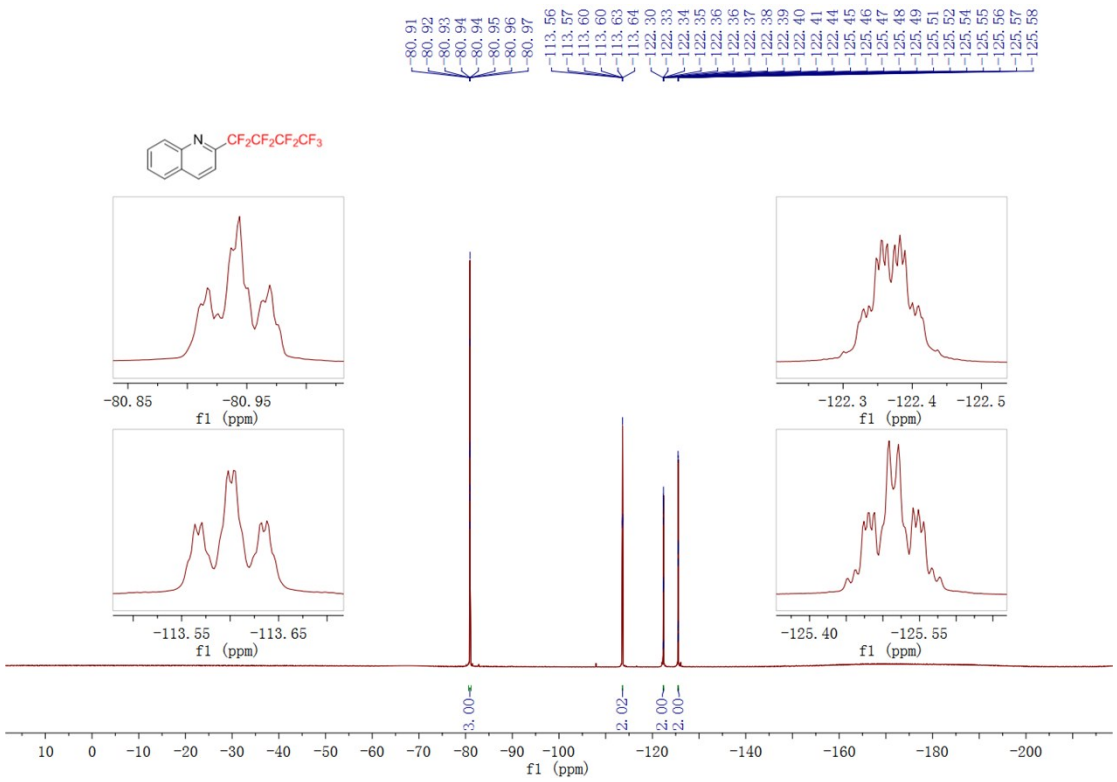
^{1}H NMR spectrum of **5p** in $CDCl_3$



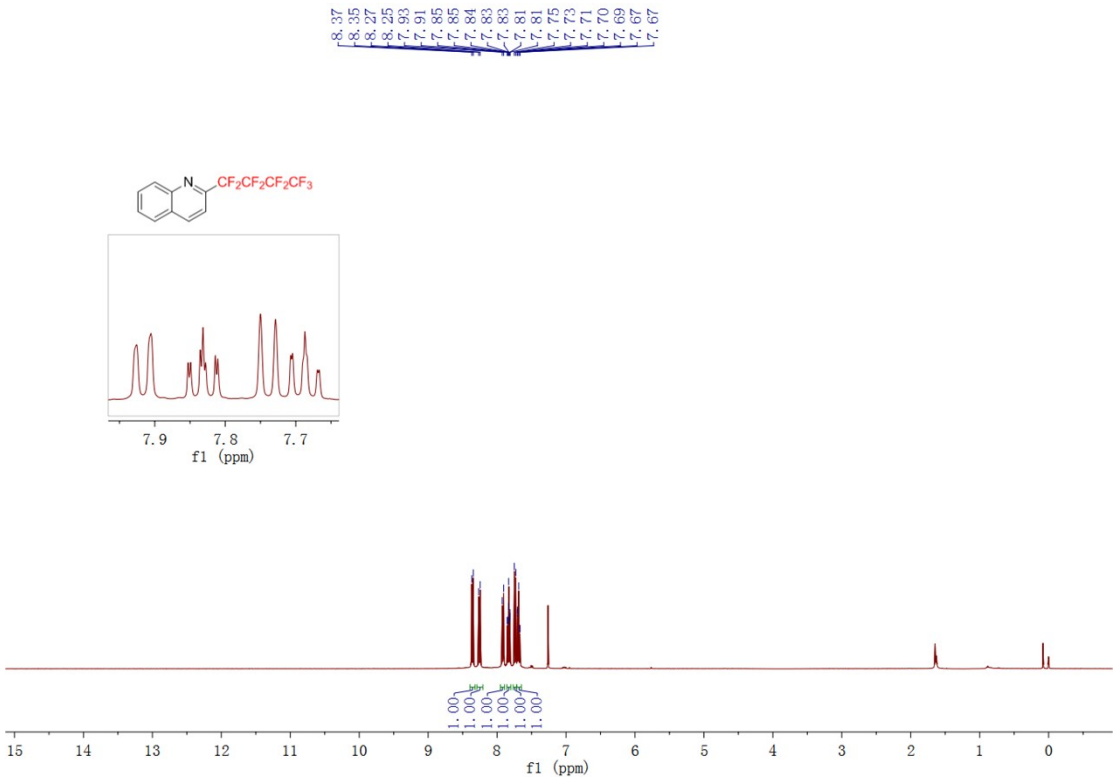
^{13}C NMR spectrum of **5p** in $CDCl_3$



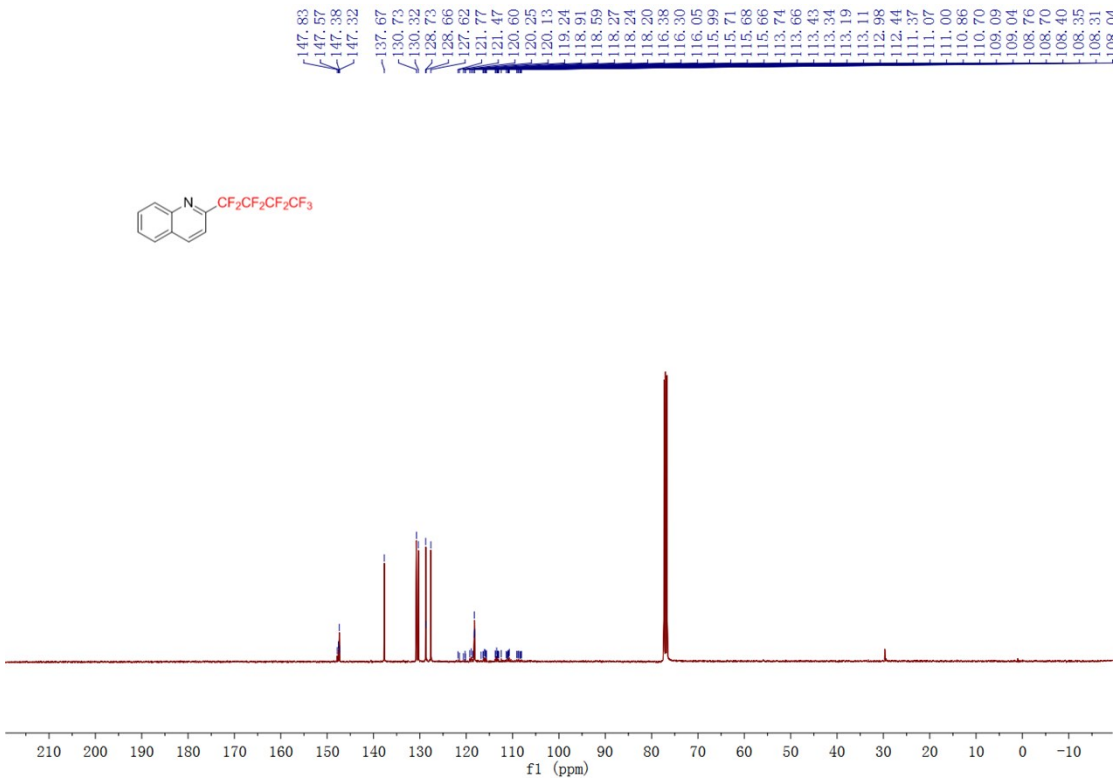
^{19}F NMR spectrum of **5s** in $CDCl_3$



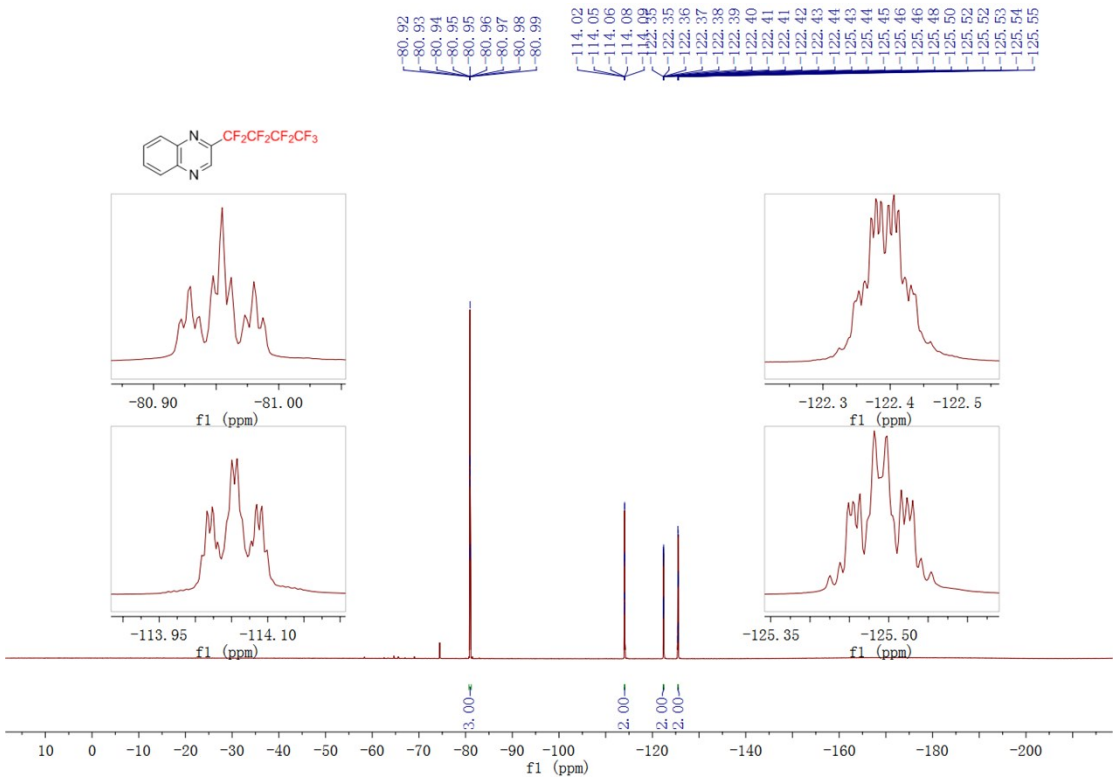
^{1}H NMR spectrum of **5s** in $CDCl_3$



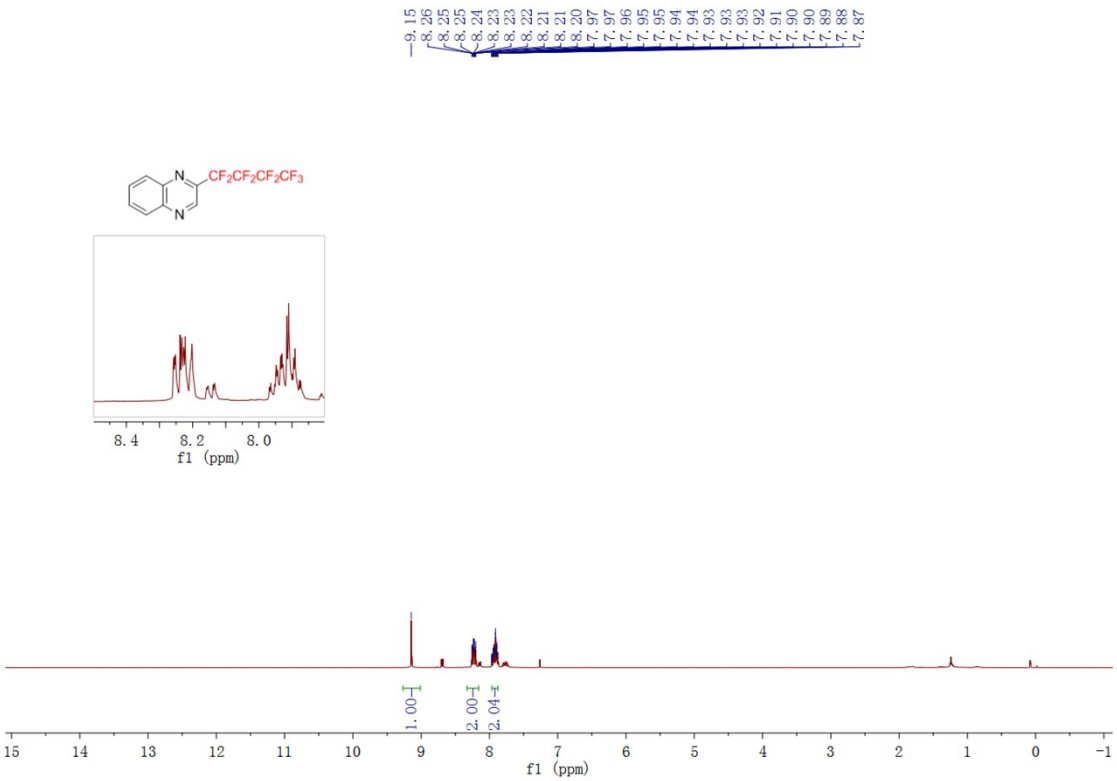
^{13}C NMR spectrum of **5s** in $CDCl_3$



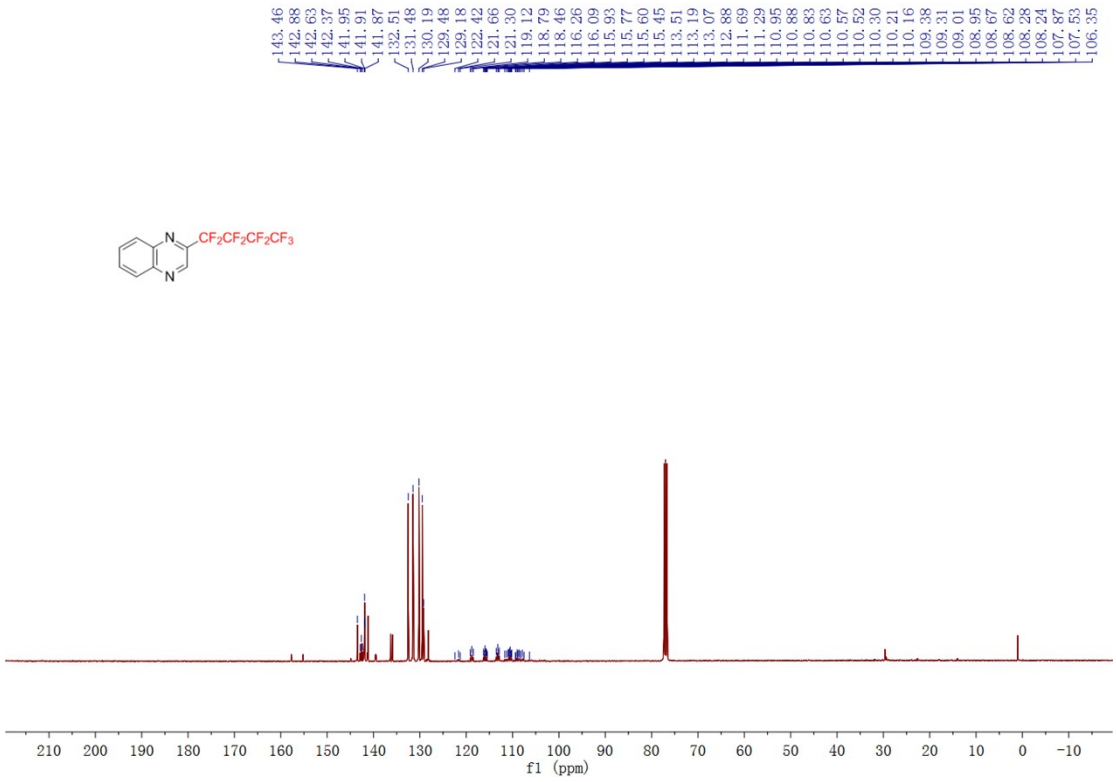
^{19}F NMR spectrum of **5t** in $CDCl_3$



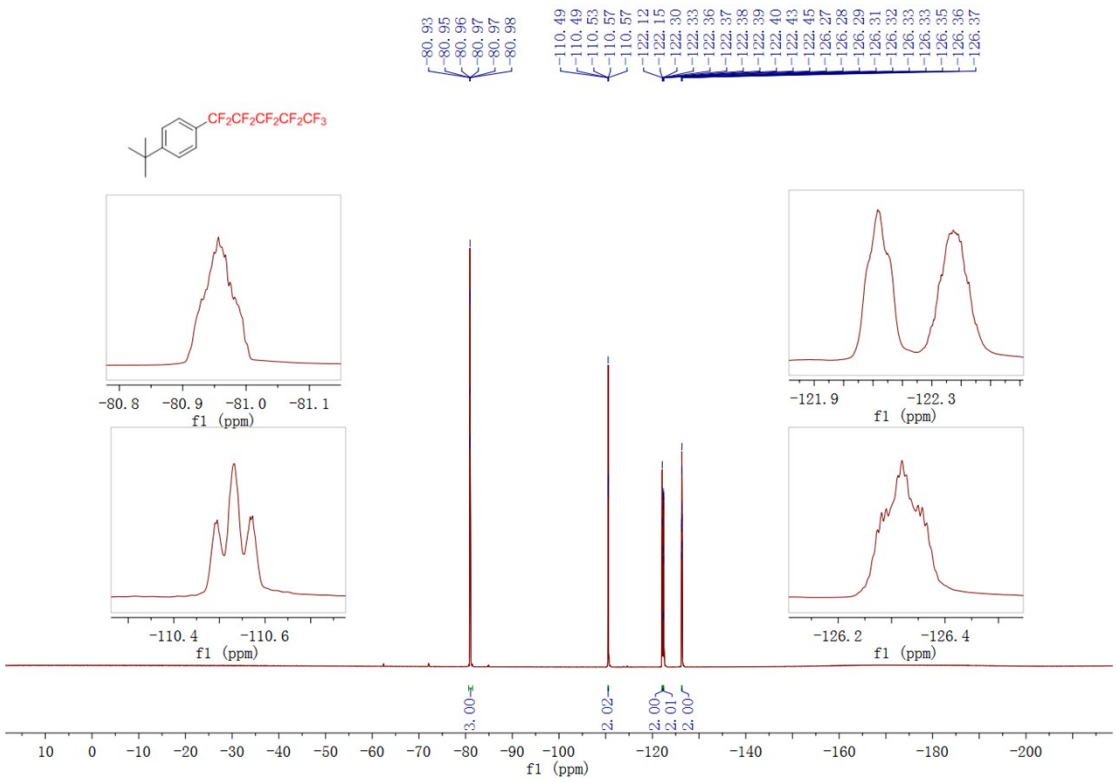
^{1}H NMR spectrum of **5t** in $CDCl_3$



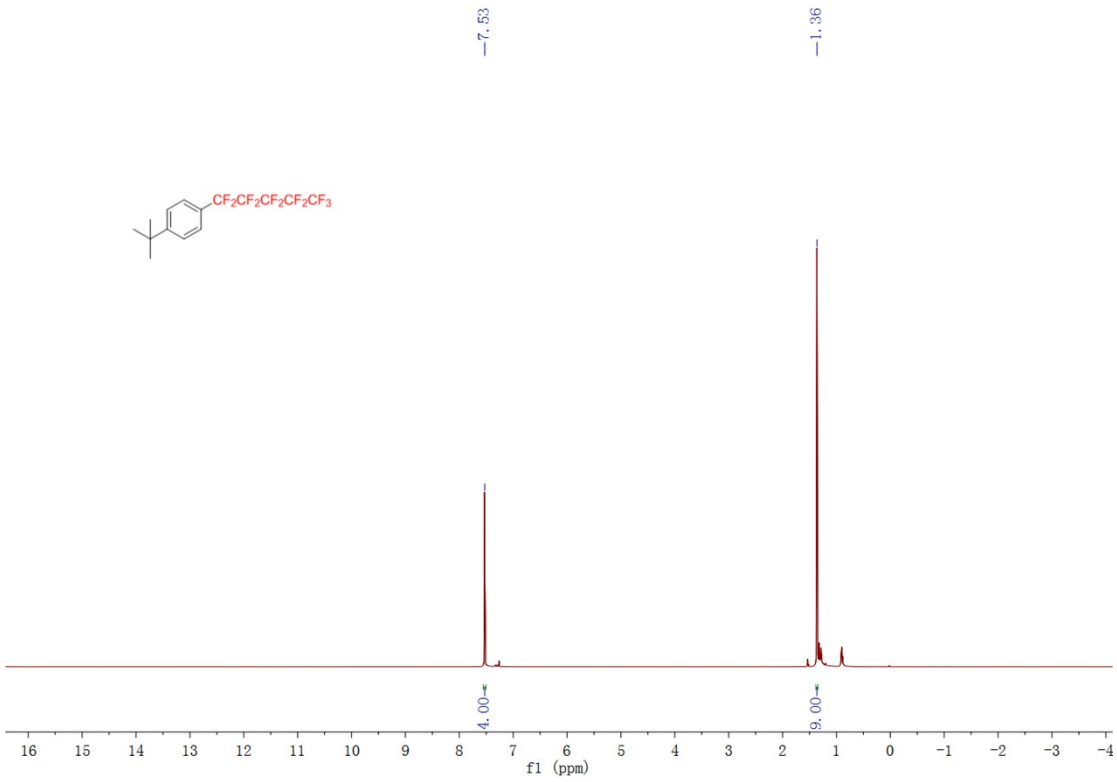
^{13}C NMR spectrum of **5t** in $CDCl_3$



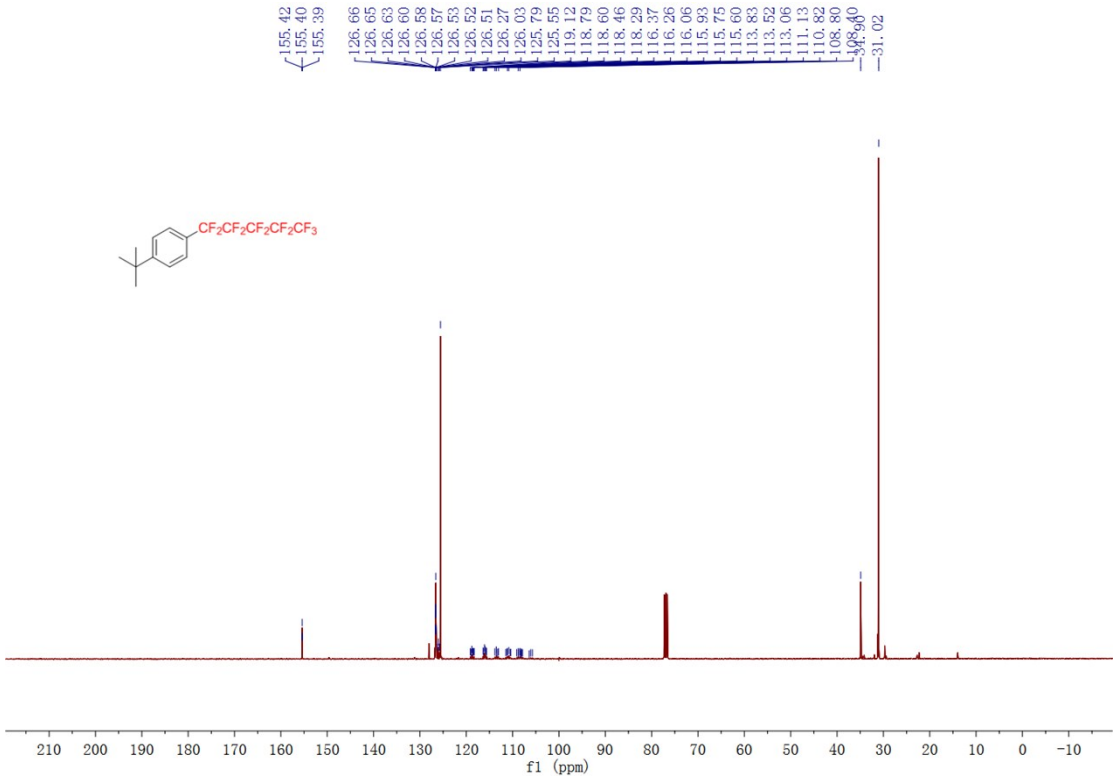
^{19}F NMR spectrum of **6a** in $CDCl_3$



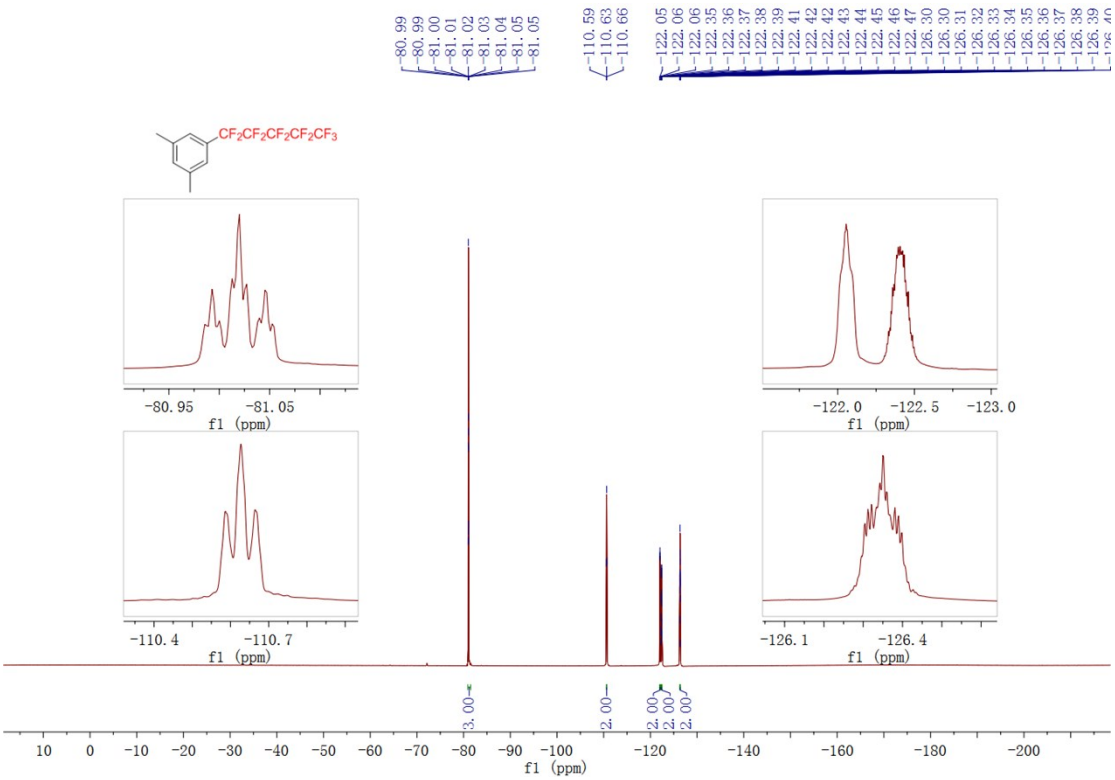
^{1}H NMR spectrum of **6a** in $CDCl_3$



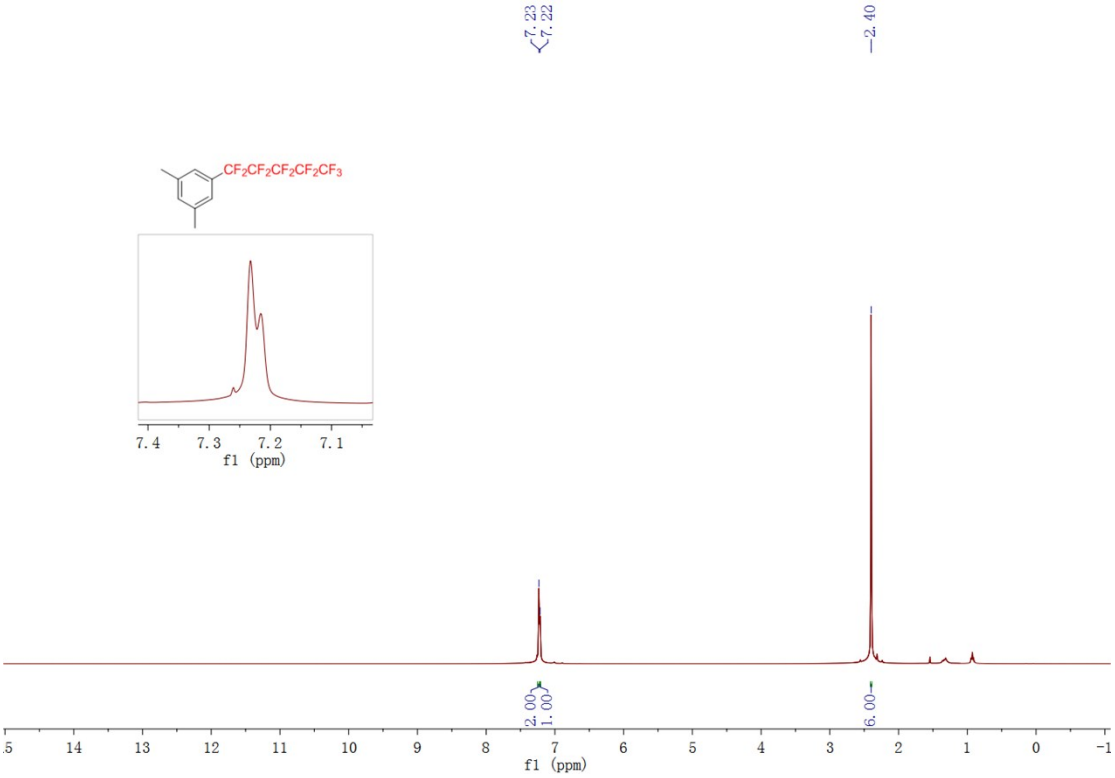
^{13}C NMR spectrum of **6a** in $CDCl_3$



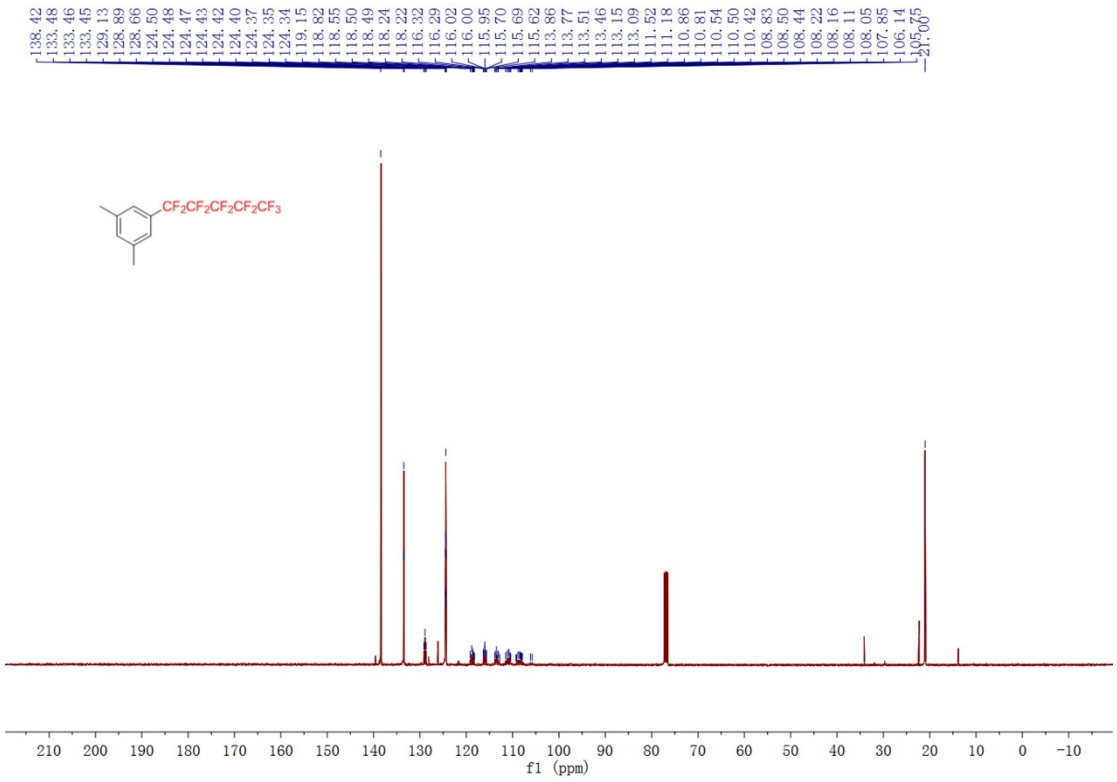
^{19}F NMR spectrum of **6b** in $CDCl_3$



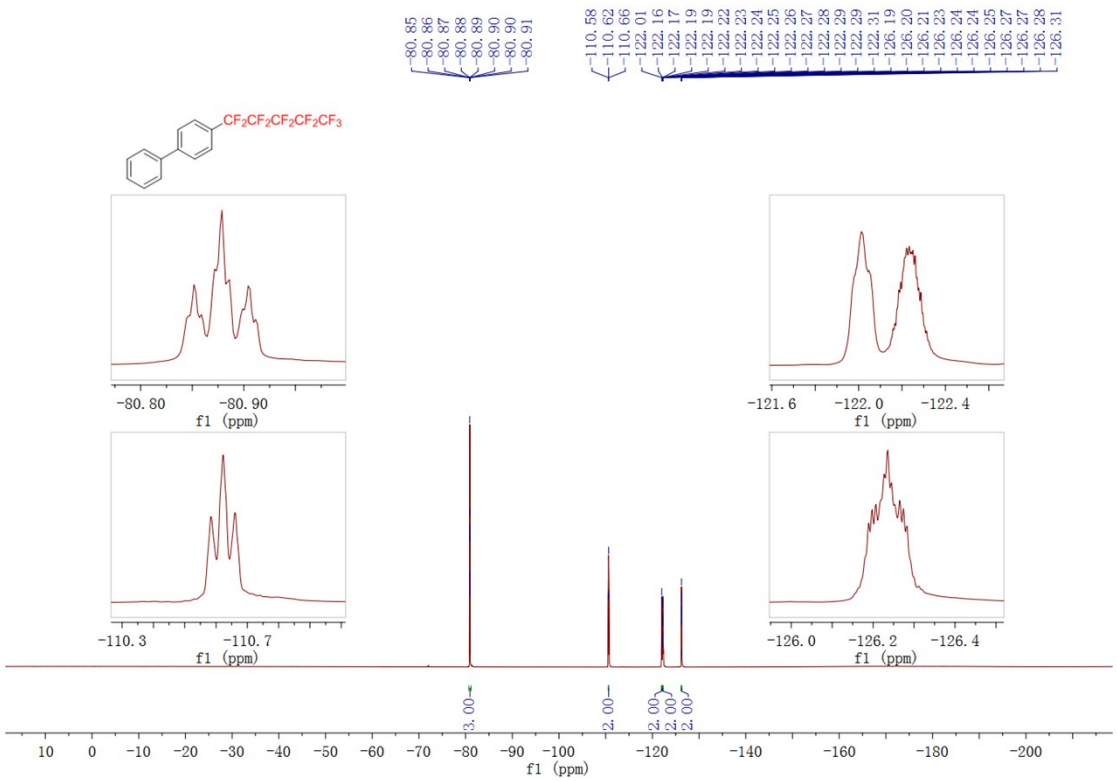
^{1}H NMR spectrum of **6b** in $CDCl_3$



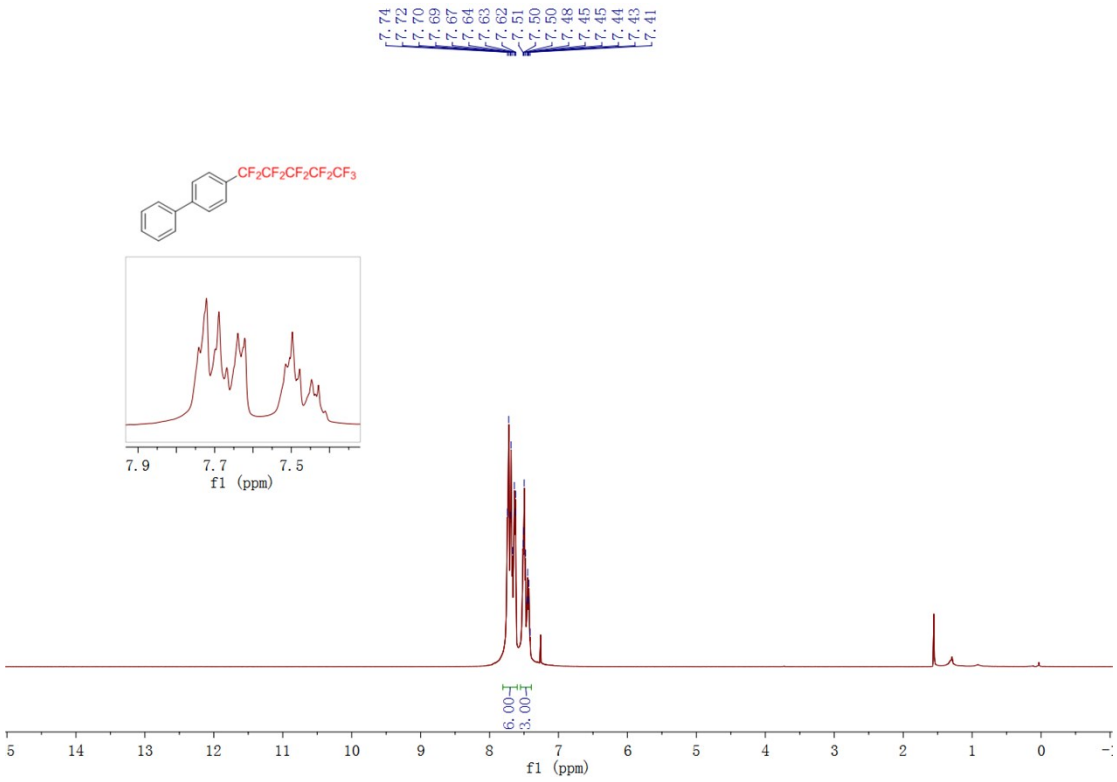
^{13}C NMR spectrum of **6b** in $CDCl_3$



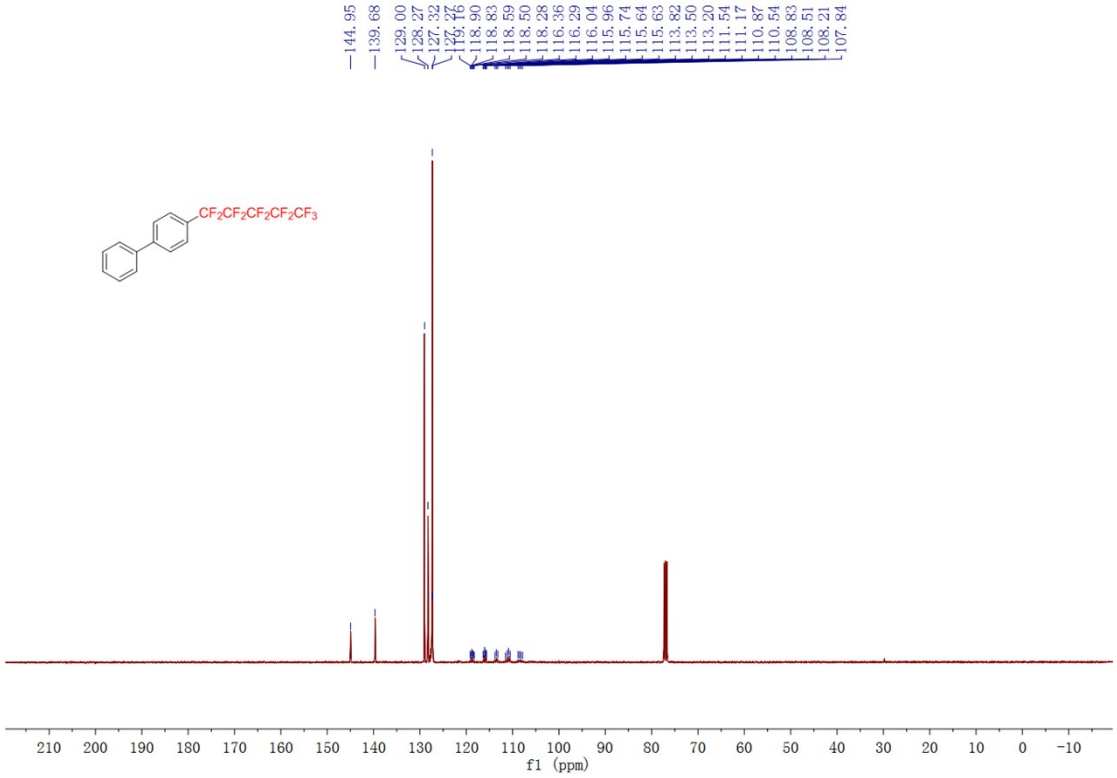
^{19}F NMR spectrum of **6c** in $CDCl_3$



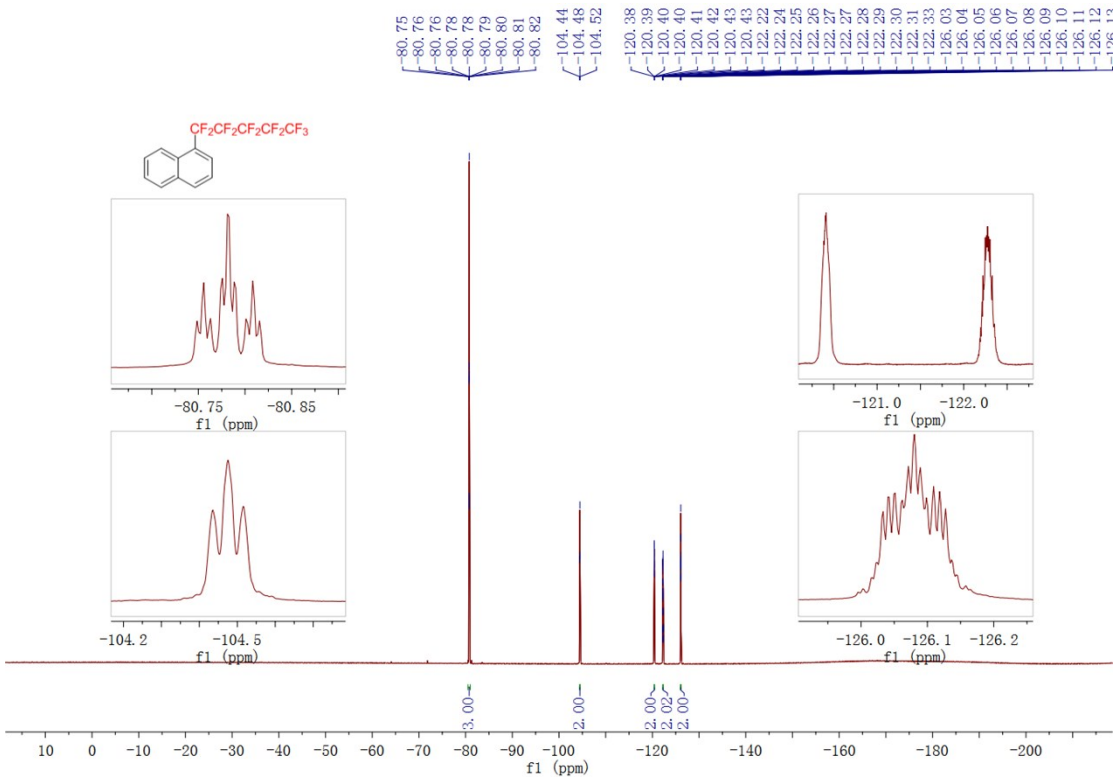
^{1}H NMR spectrum of **6c** in $CDCl_3$



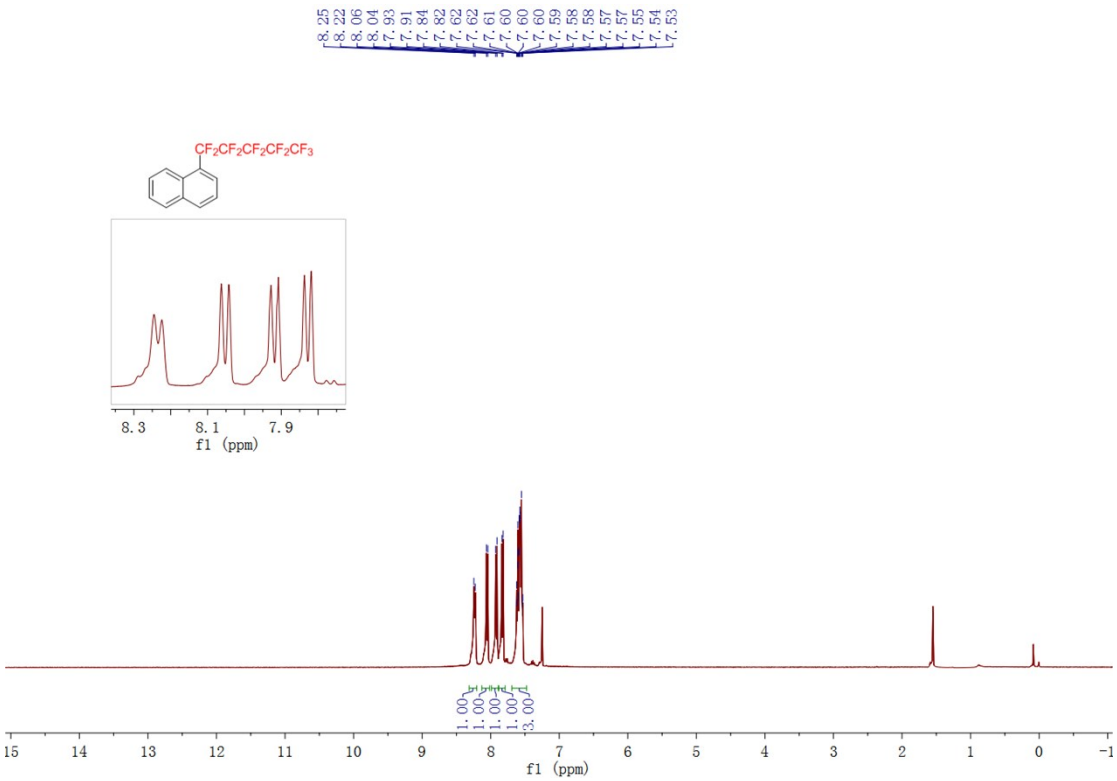
^{13}C NMR spectrum of **6c** in $CDCl_3$



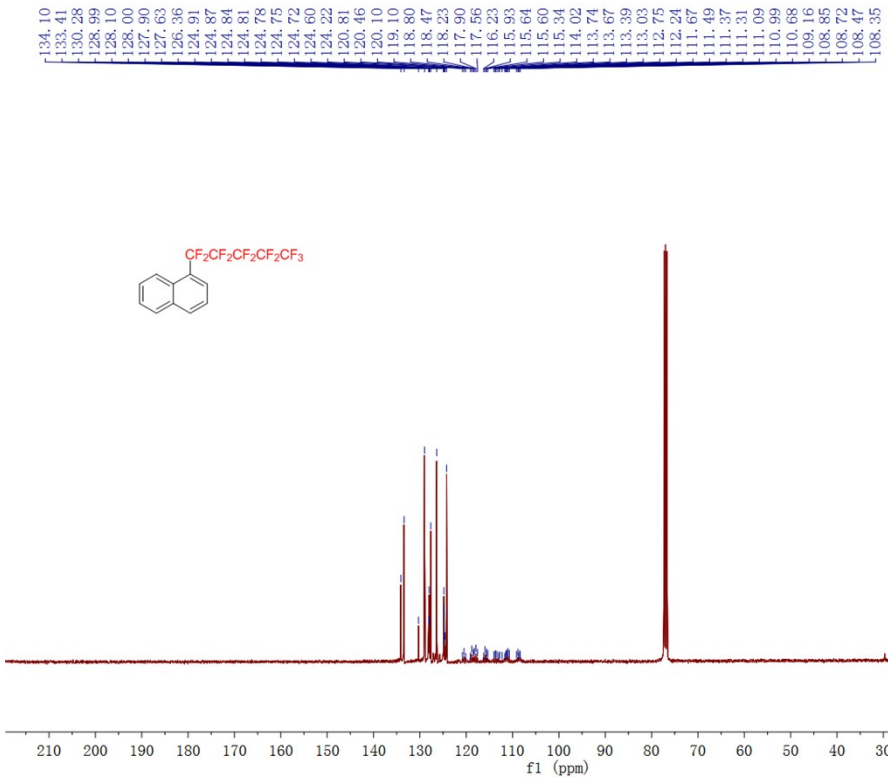
^{19}F NMR spectrum of **6e** in $CDCl_3$



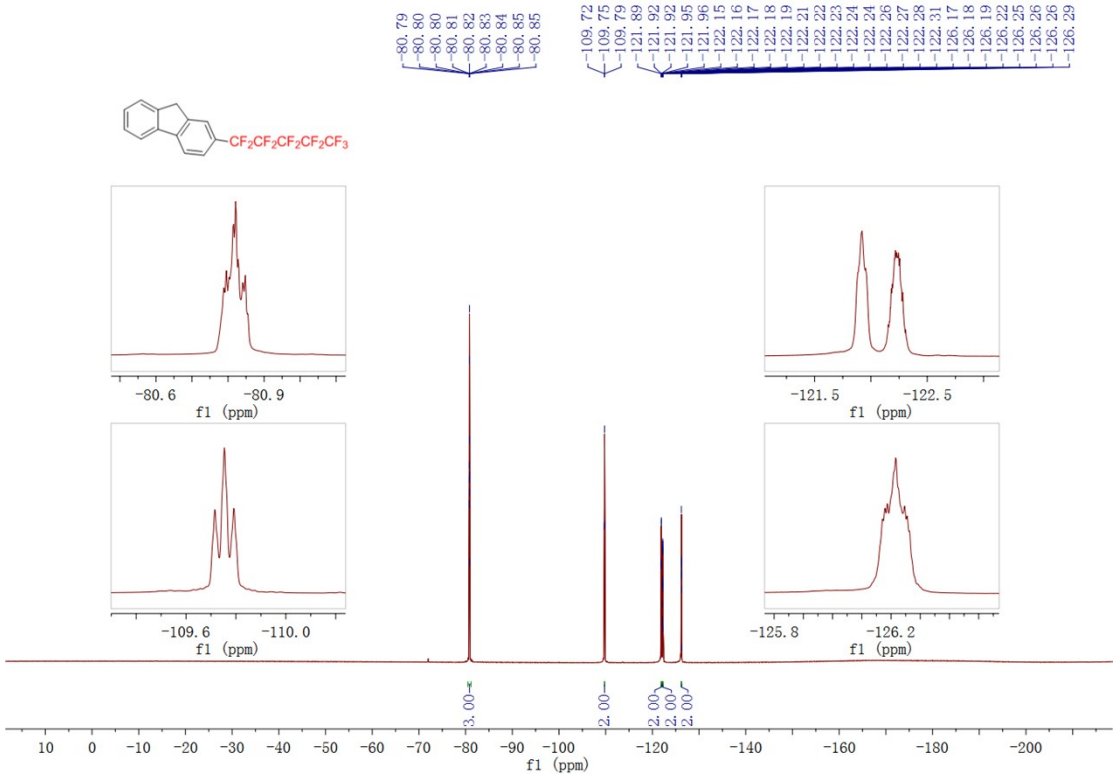
^{1}H NMR spectrum of **6e** in $CDCl_3$



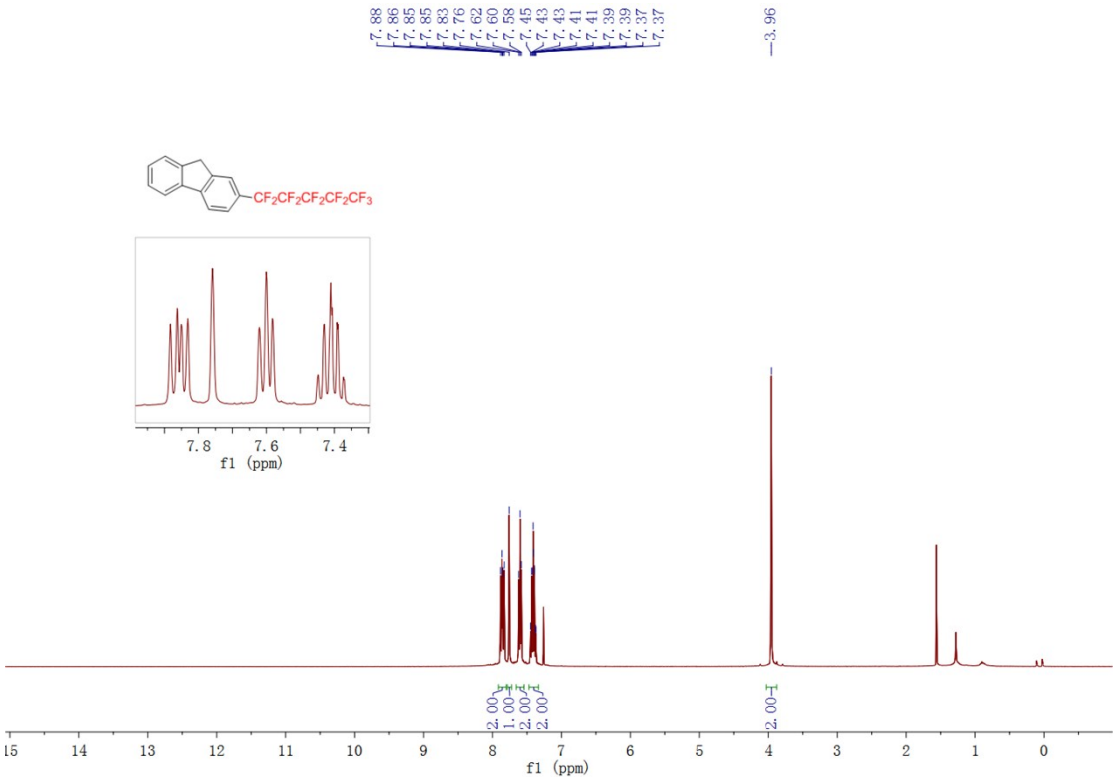
^{13}C NMR spectrum of **6e** in $CDCl_3$



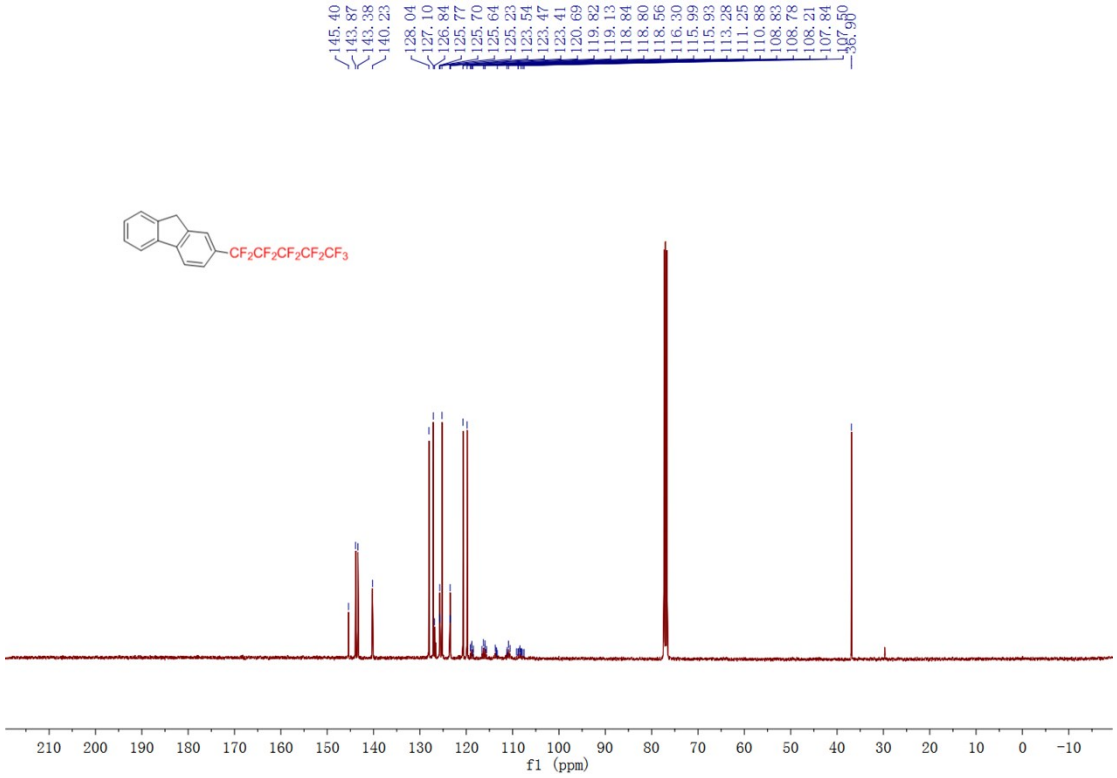
^{19}F NMR spectrum of **6f** in $CDCl_3$



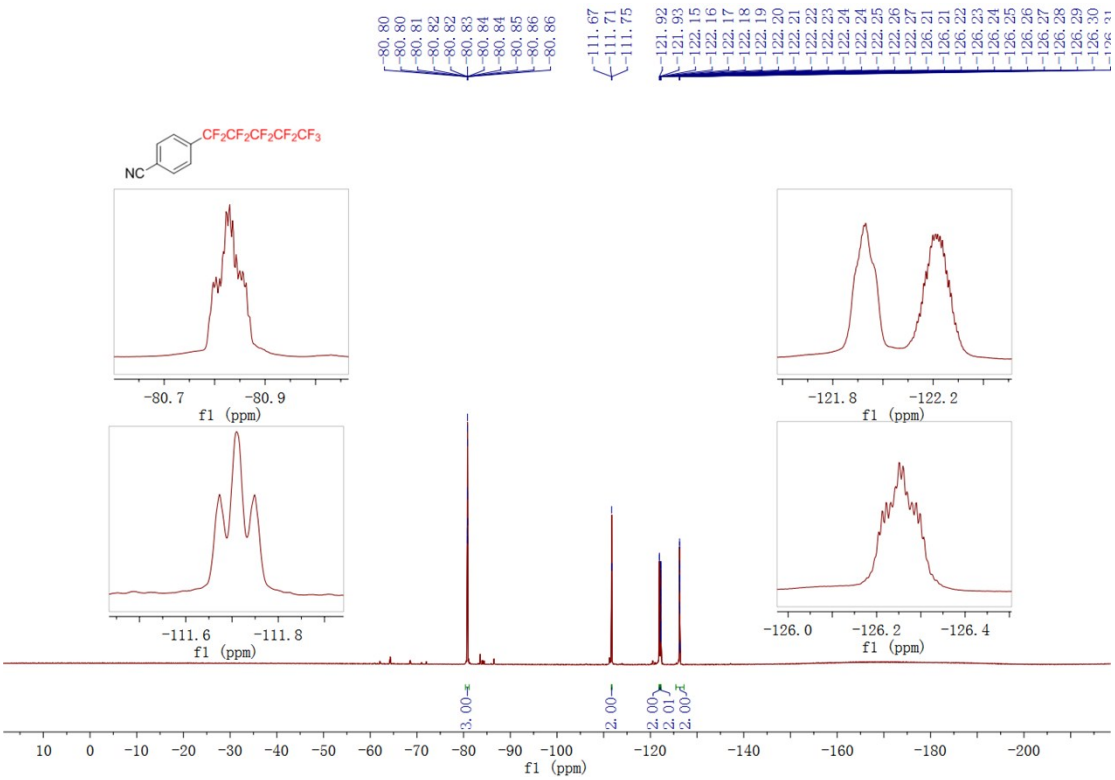
^{1}H NMR spectrum of **6f** in $CDCl_3$



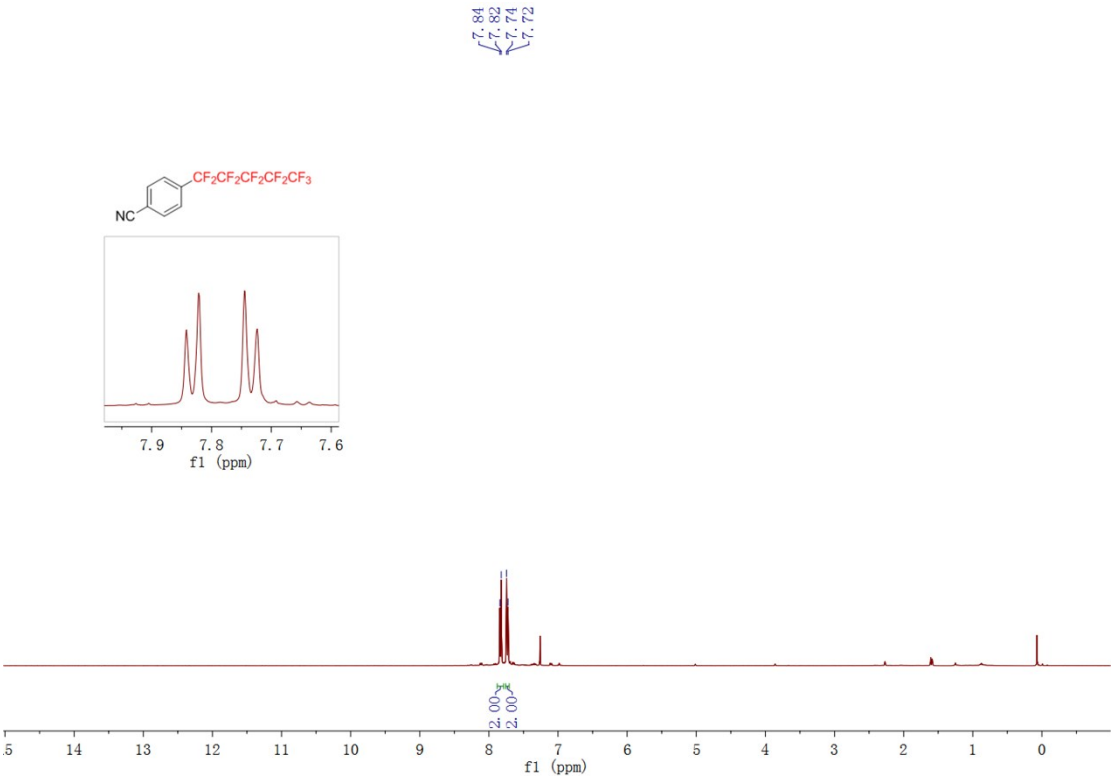
^{13}C NMR spectrum of **6f** in $CDCl_3$



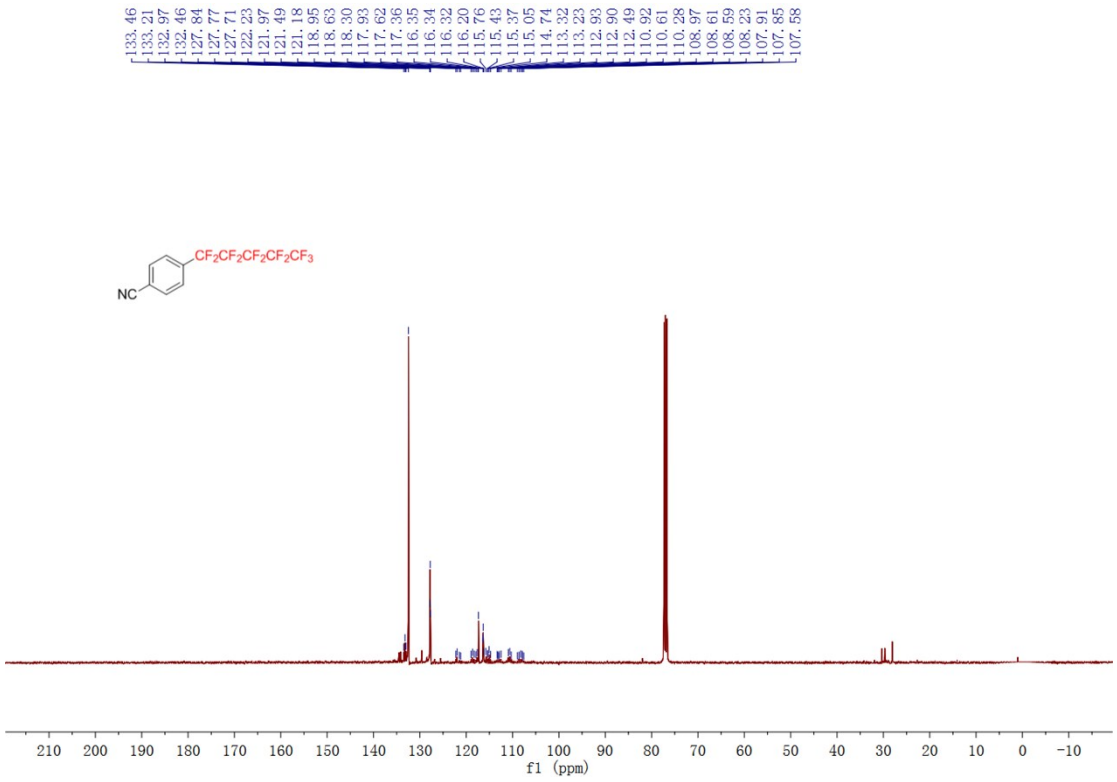
^{19}F NMR spectrum of **6g** in $CDCl_3$



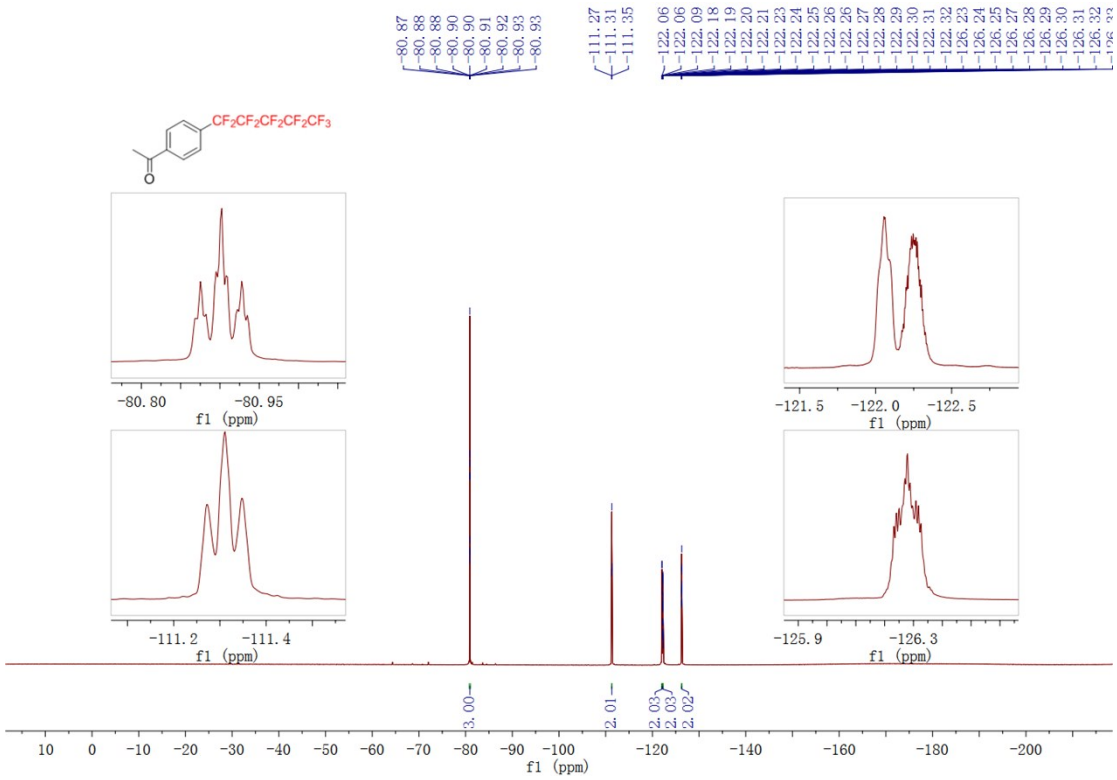
^{1}H NMR spectrum of **6g** in $CDCl_3$



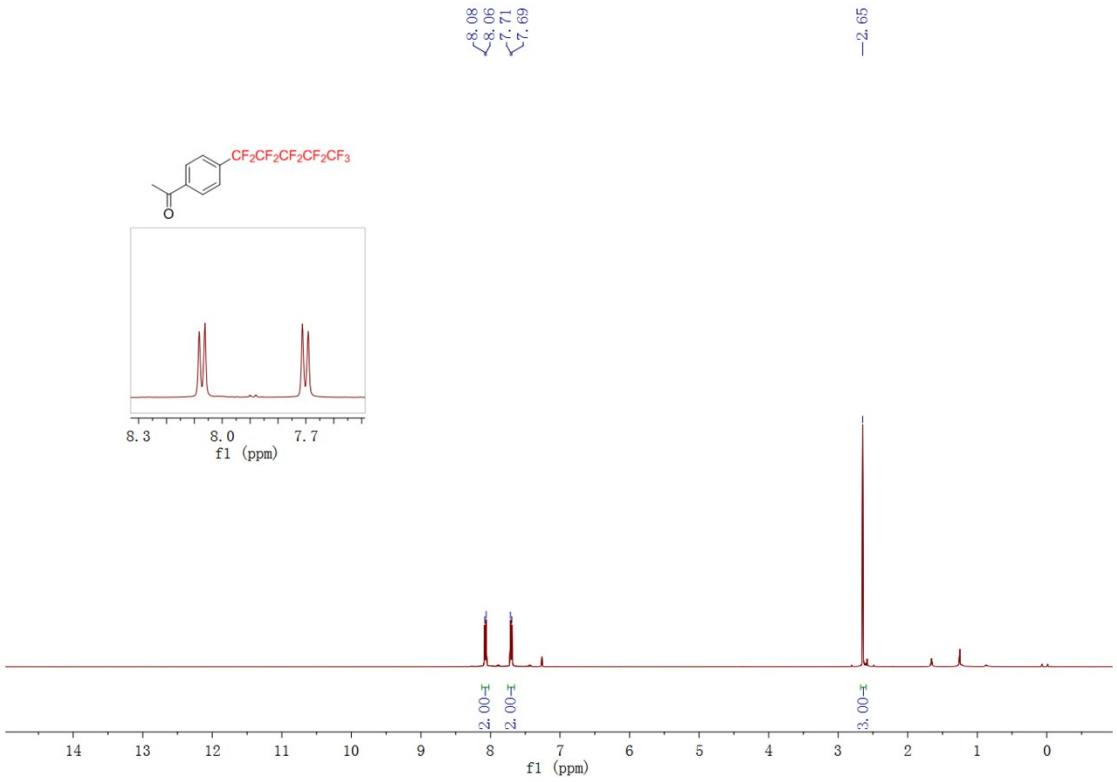
^{13}C NMR spectrum of **6g** in $CDCl_3$



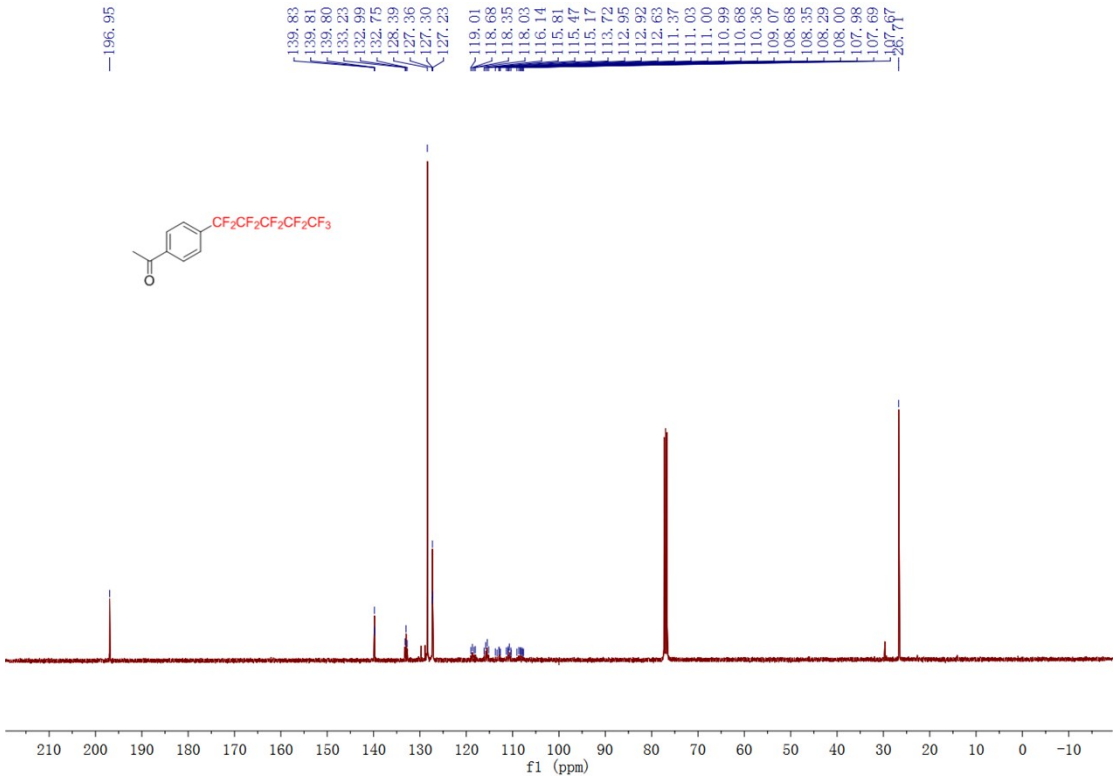
^{19}F NMR spectrum of **6h** in $CDCl_3$



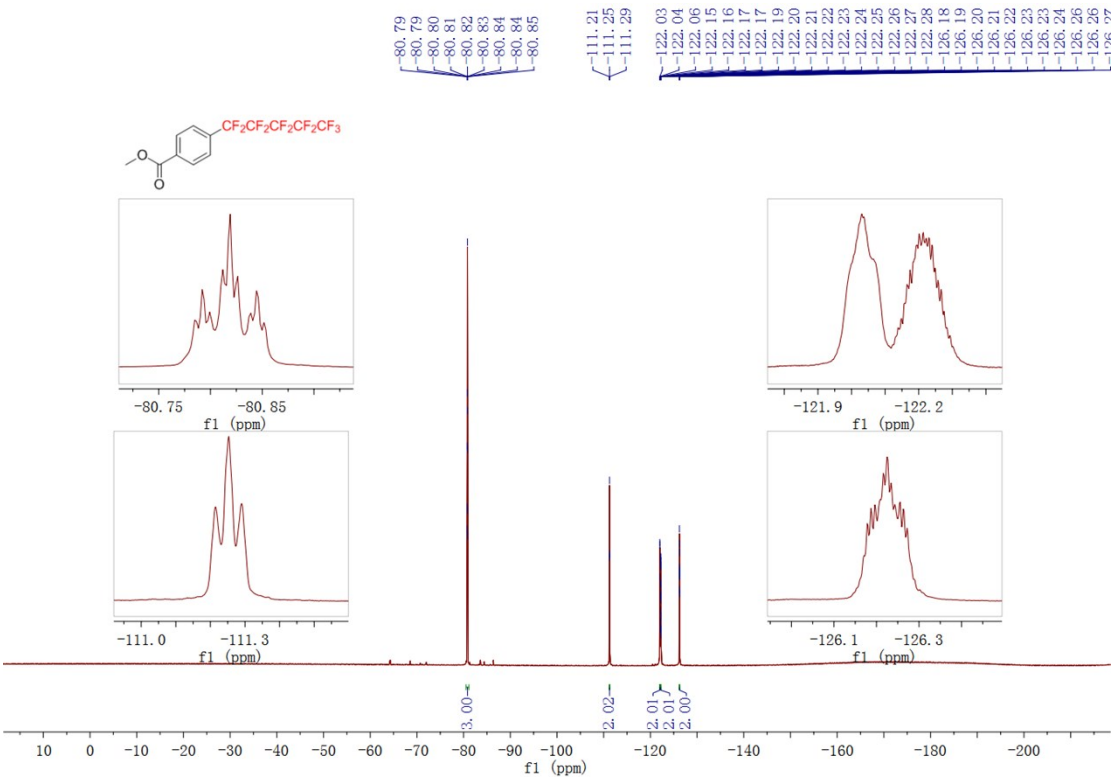
^{1}H NMR spectrum of **6h** in $CDCl_3$



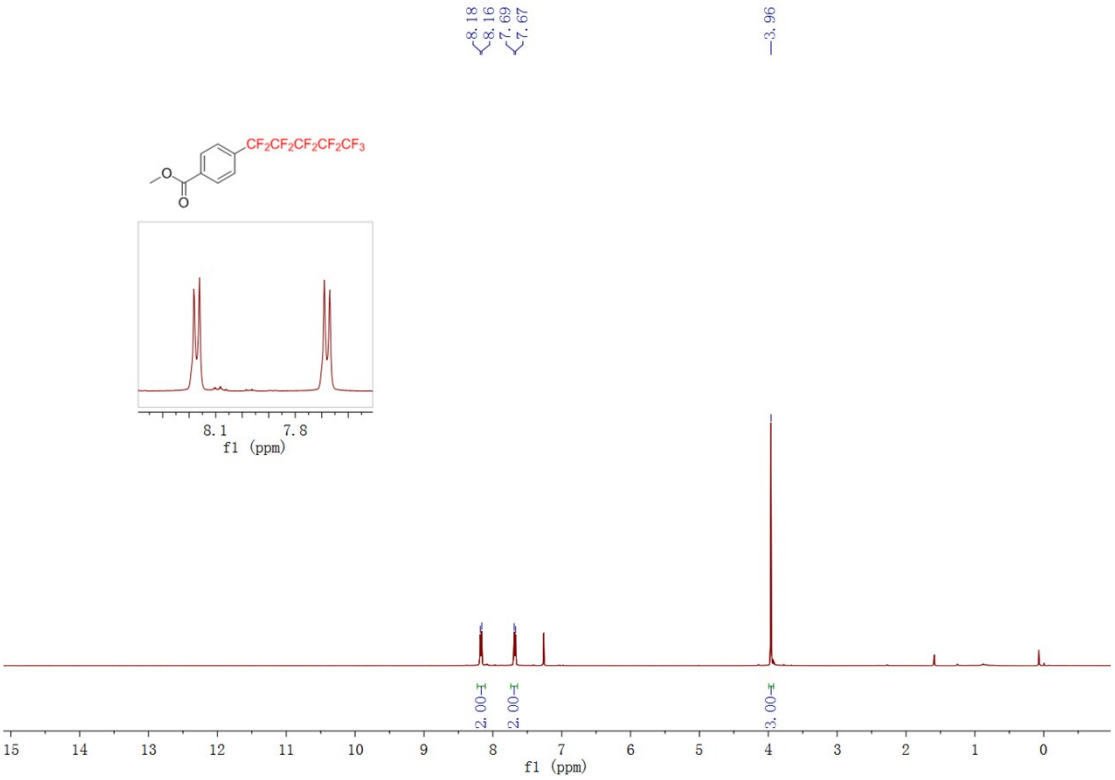
^{13}C NMR spectrum of **6h** in $CDCl_3$



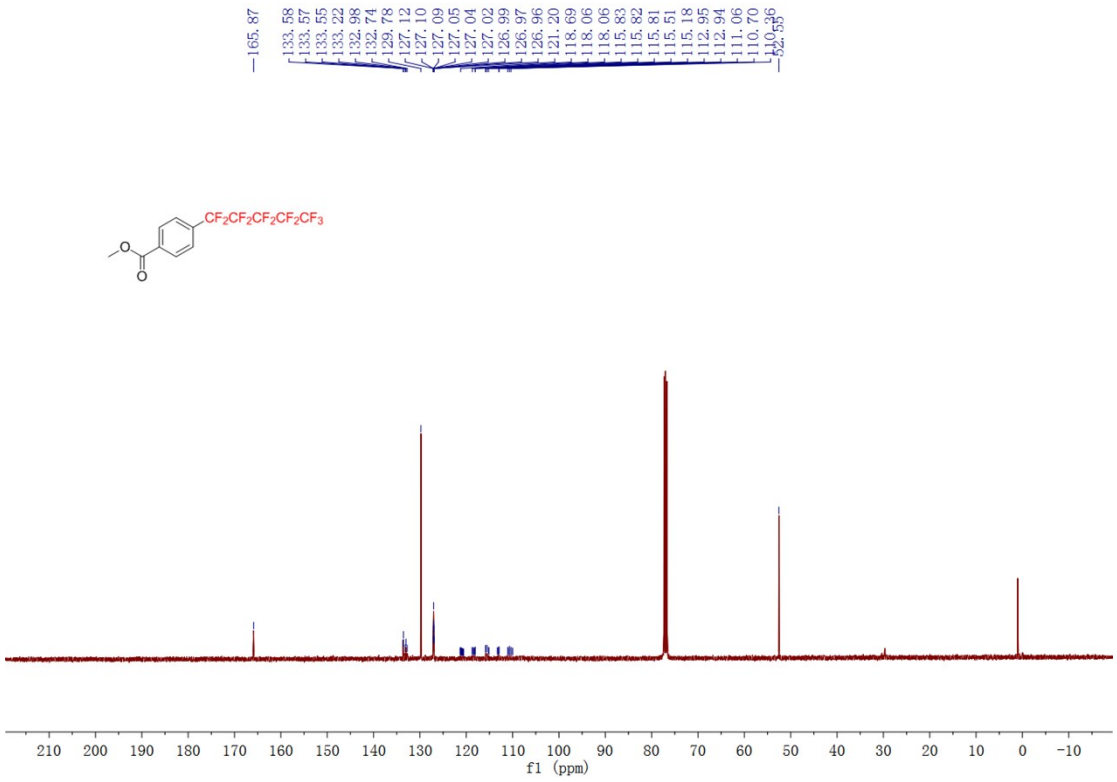
^{19}F NMR spectrum of **6i** in $CDCl_3$



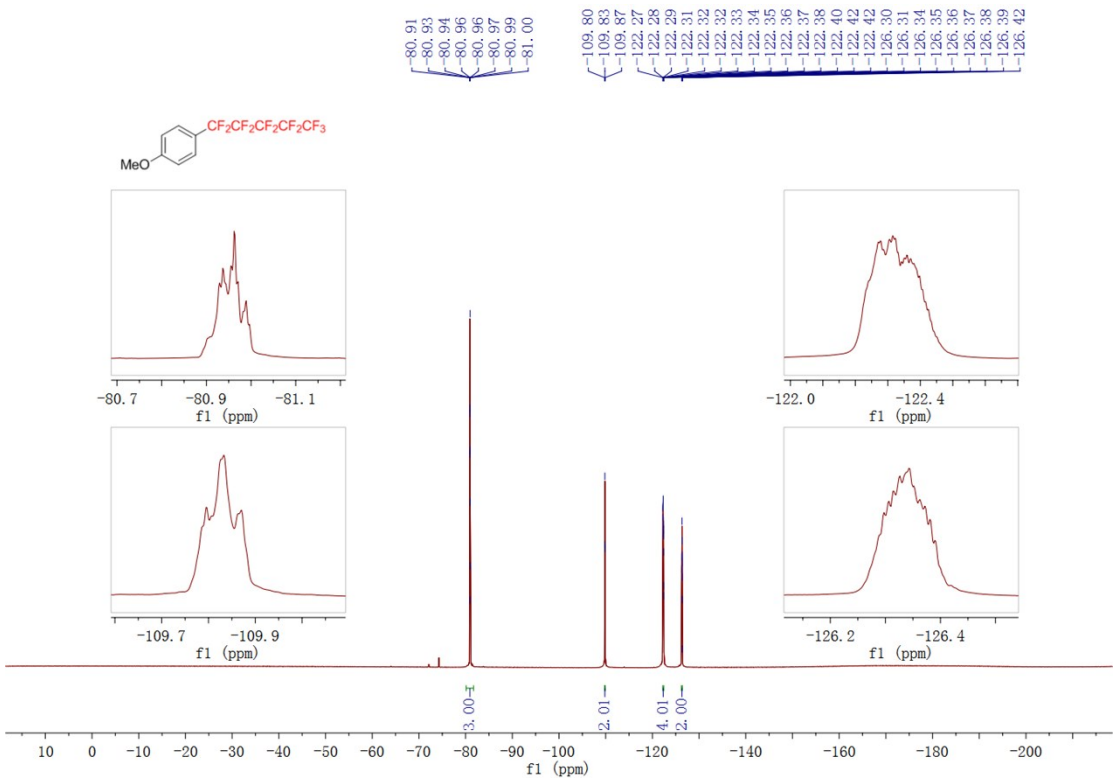
^{1}H NMR spectrum of **6i** in $CDCl_3$



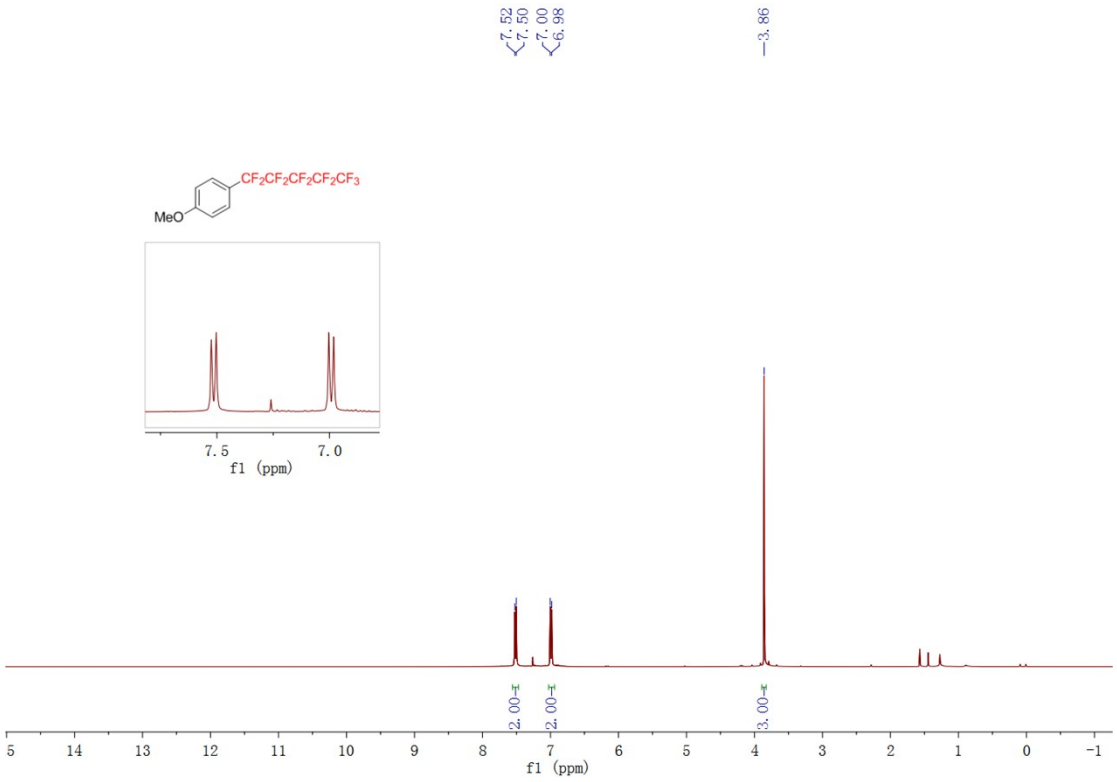
^{13}C NMR spectrum of **6i** in $CDCl_3$



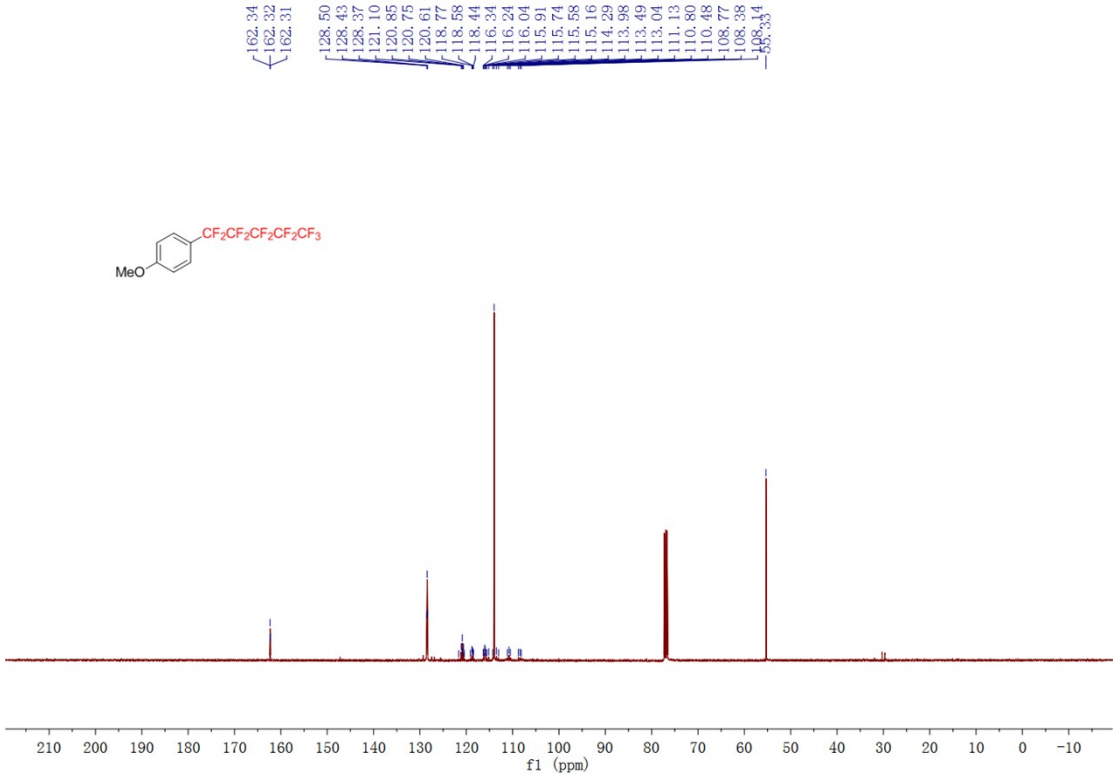
^{19}F NMR spectrum of **6k** in $CDCl_3$



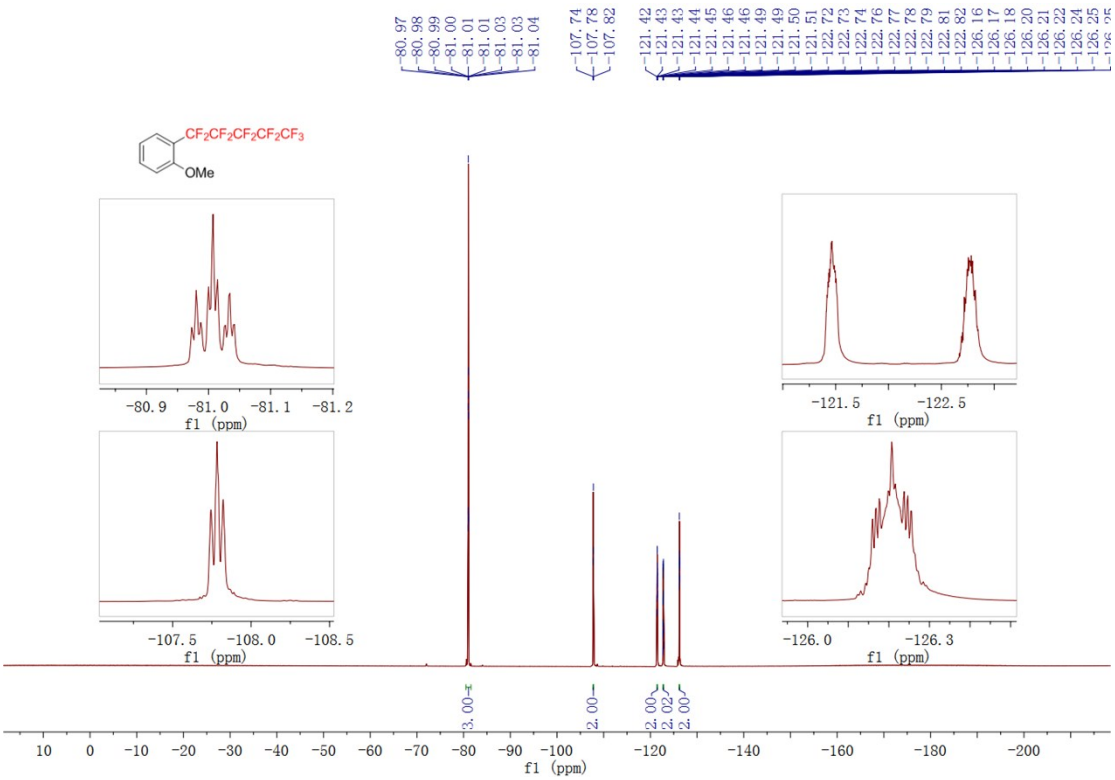
^{1}H NMR spectrum of **6k** in $CDCl_3$



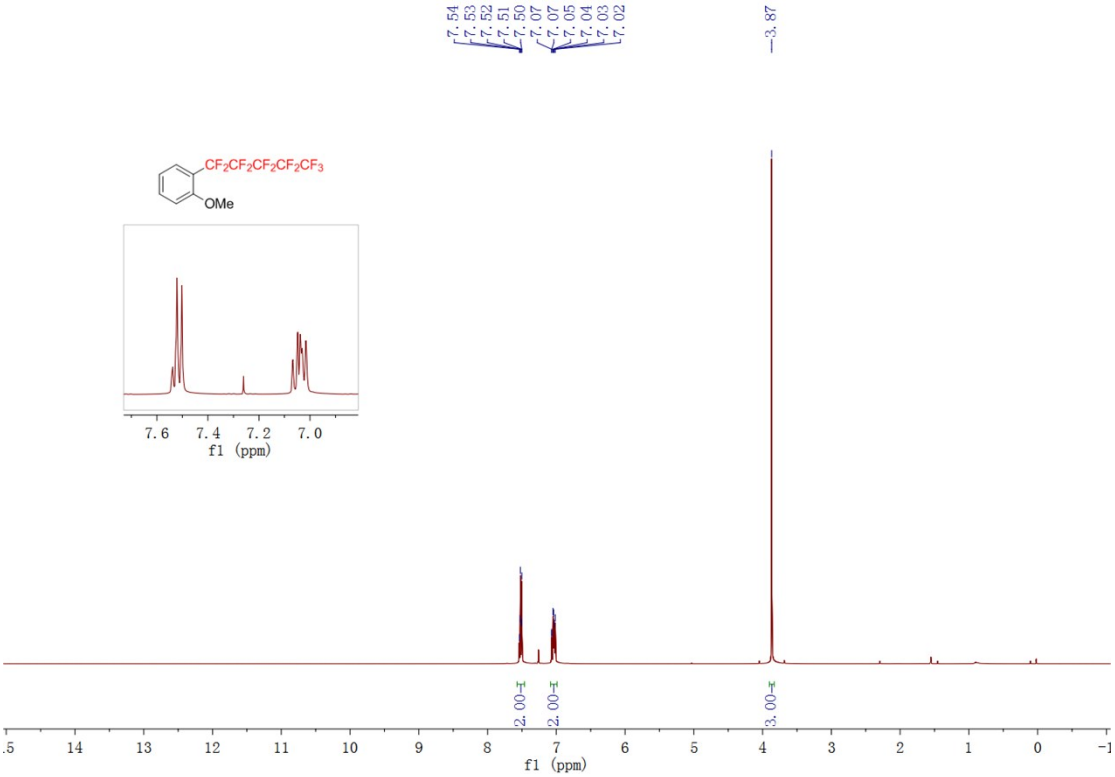
^{13}C NMR spectrum of **6k** in $CDCl_3$



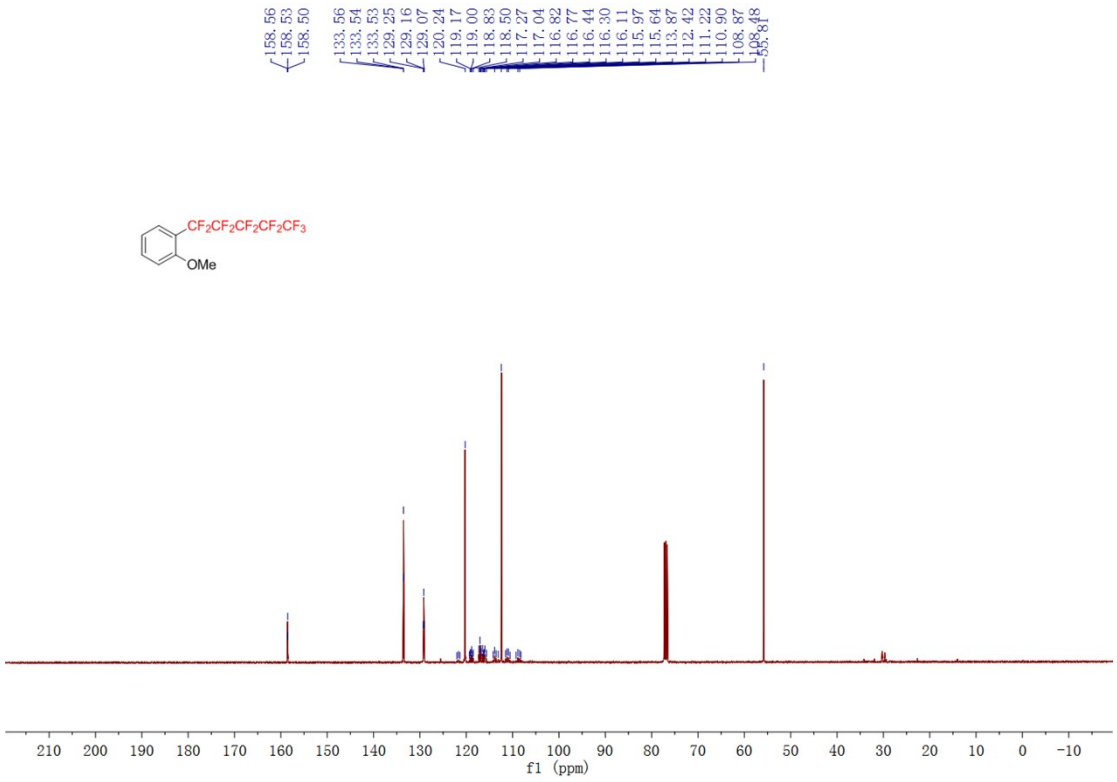
^{19}F NMR spectrum of **6l** in $CDCl_3$



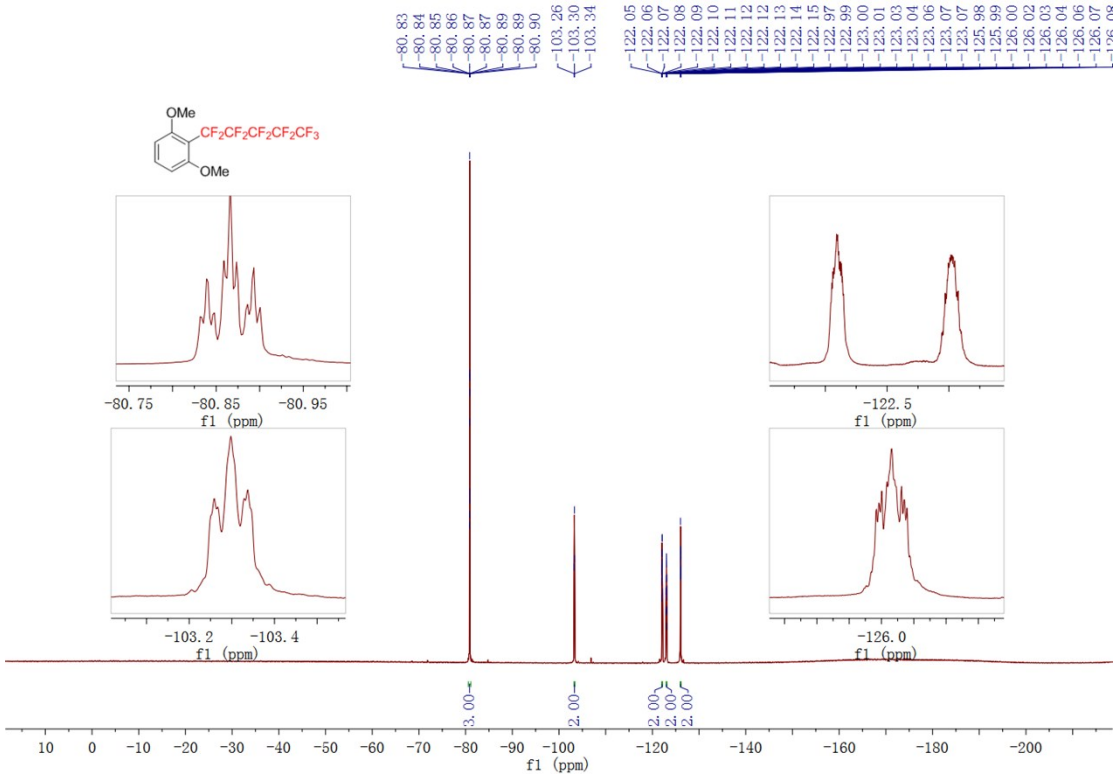
^{1}H NMR spectrum of **6l** in $CDCl_3$



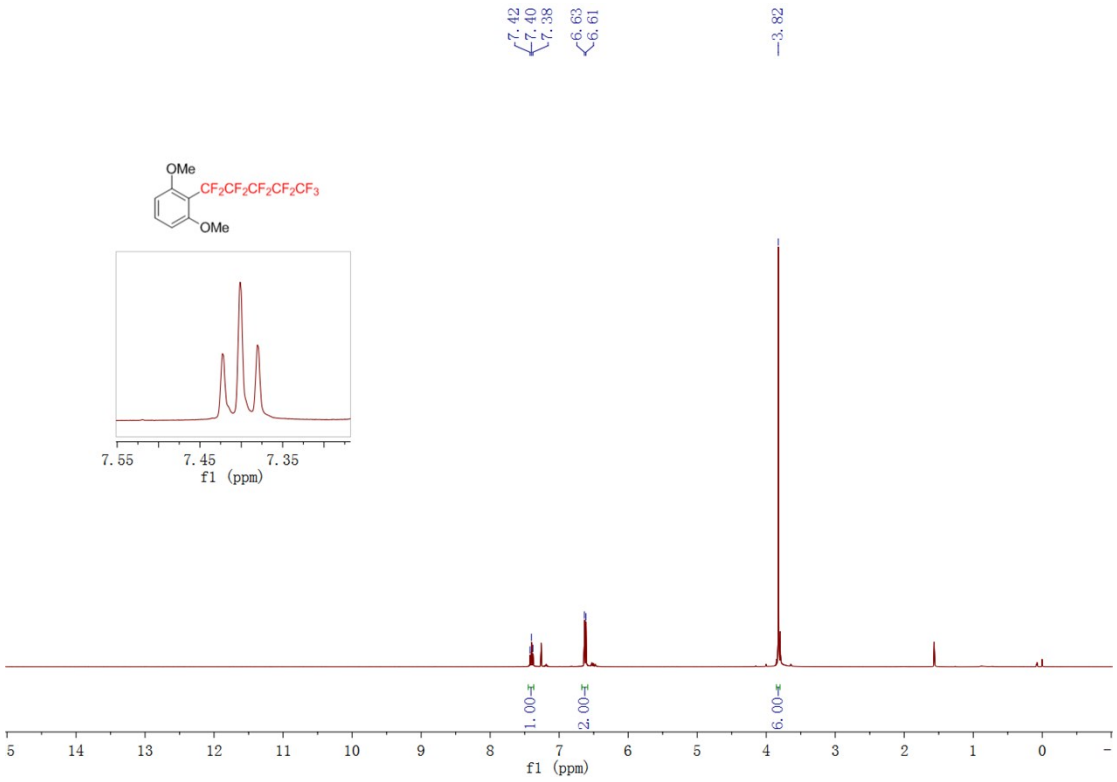
^{13}C NMR spectrum of **6l** in $CDCl_3$



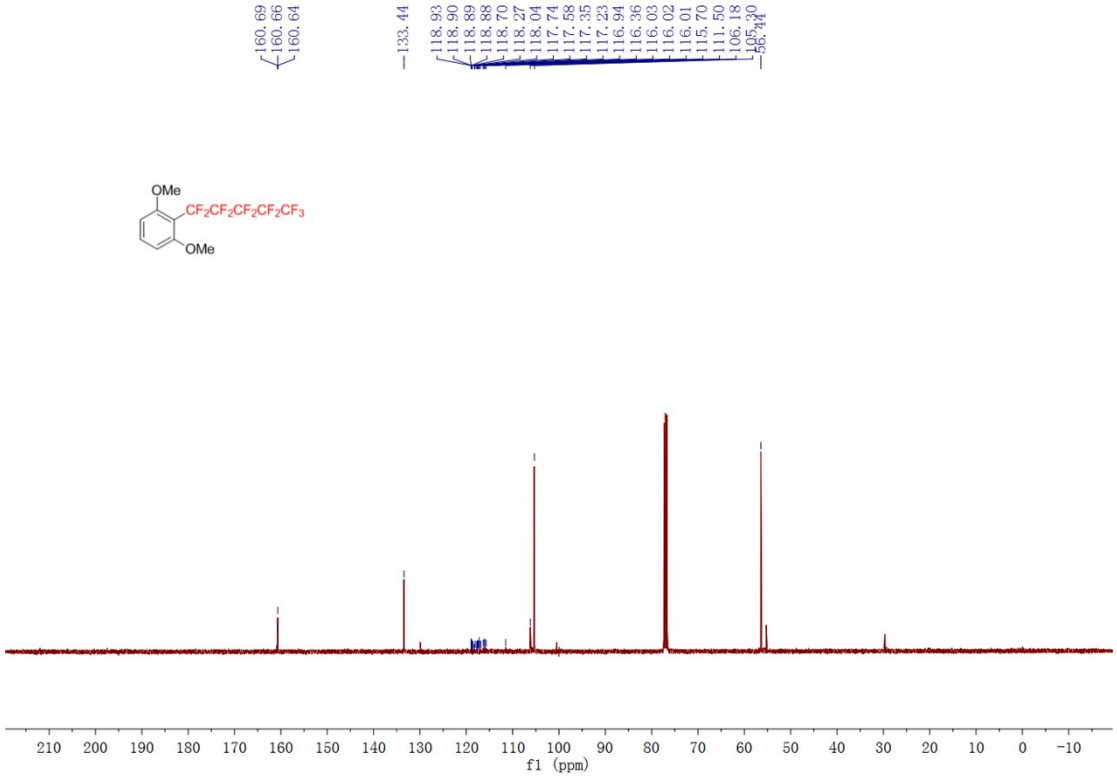
^{19}F NMR spectrum of **6m** in $CDCl_3$



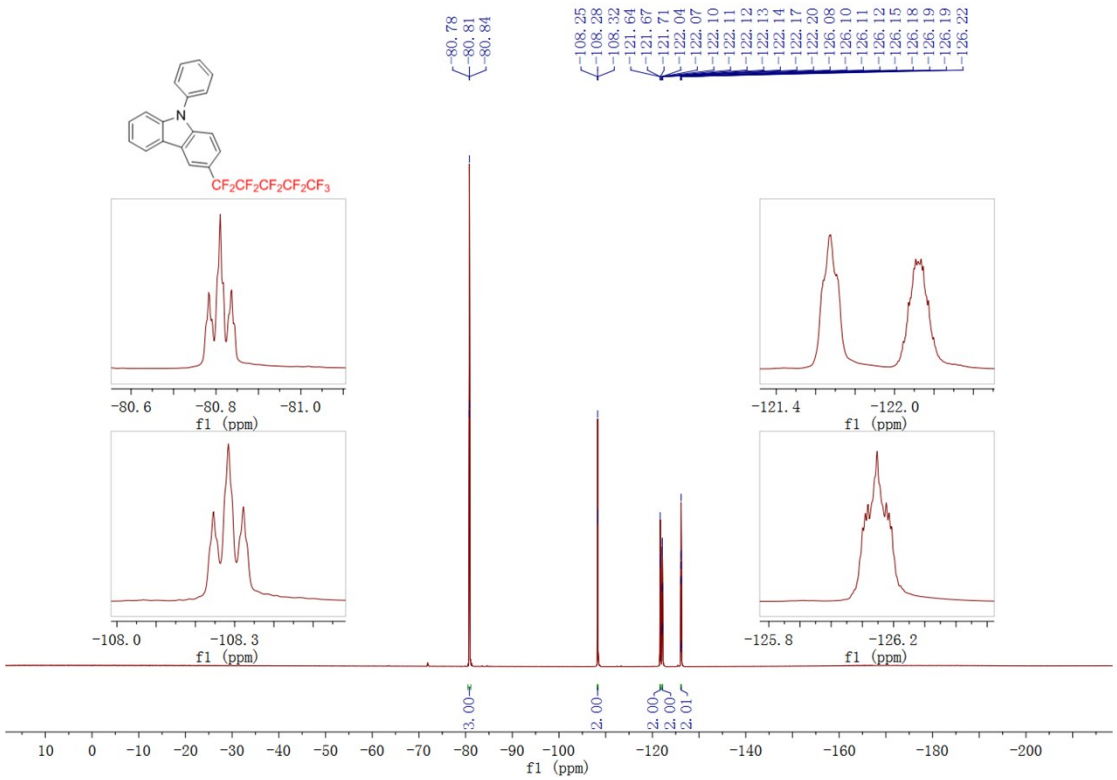
^{1}H NMR spectrum of **6m** in $CDCl_3$



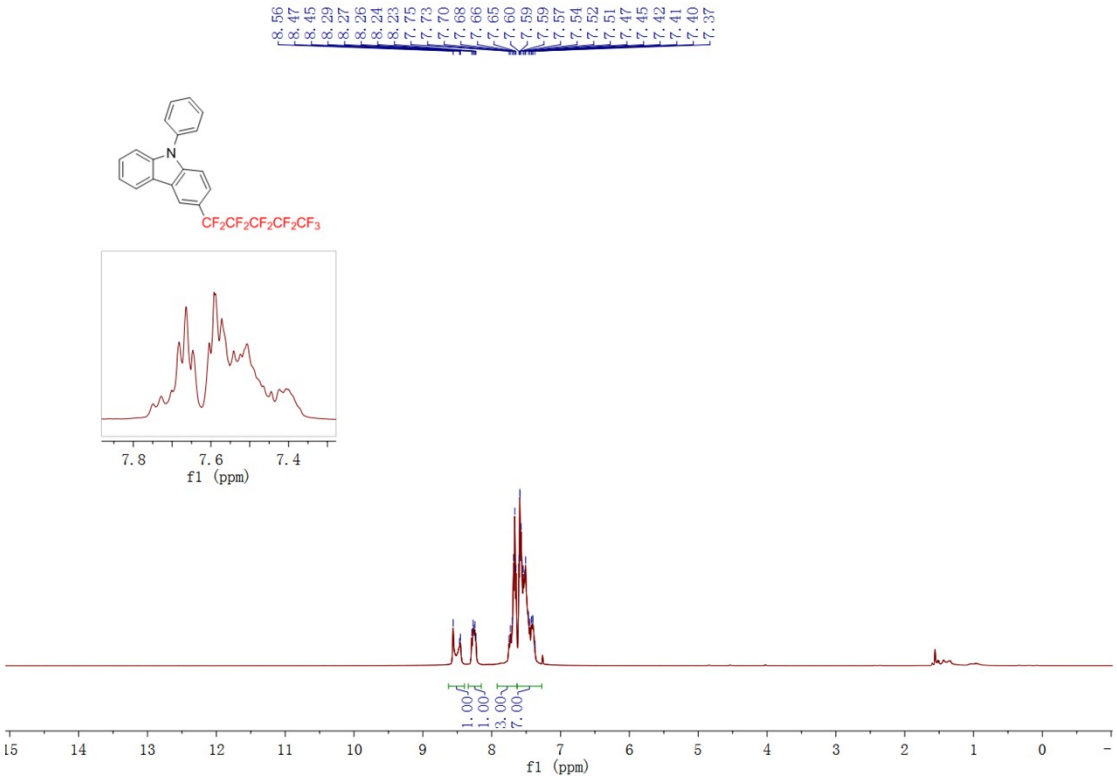
^{13}C NMR spectrum of **6m** in $CDCl_3$



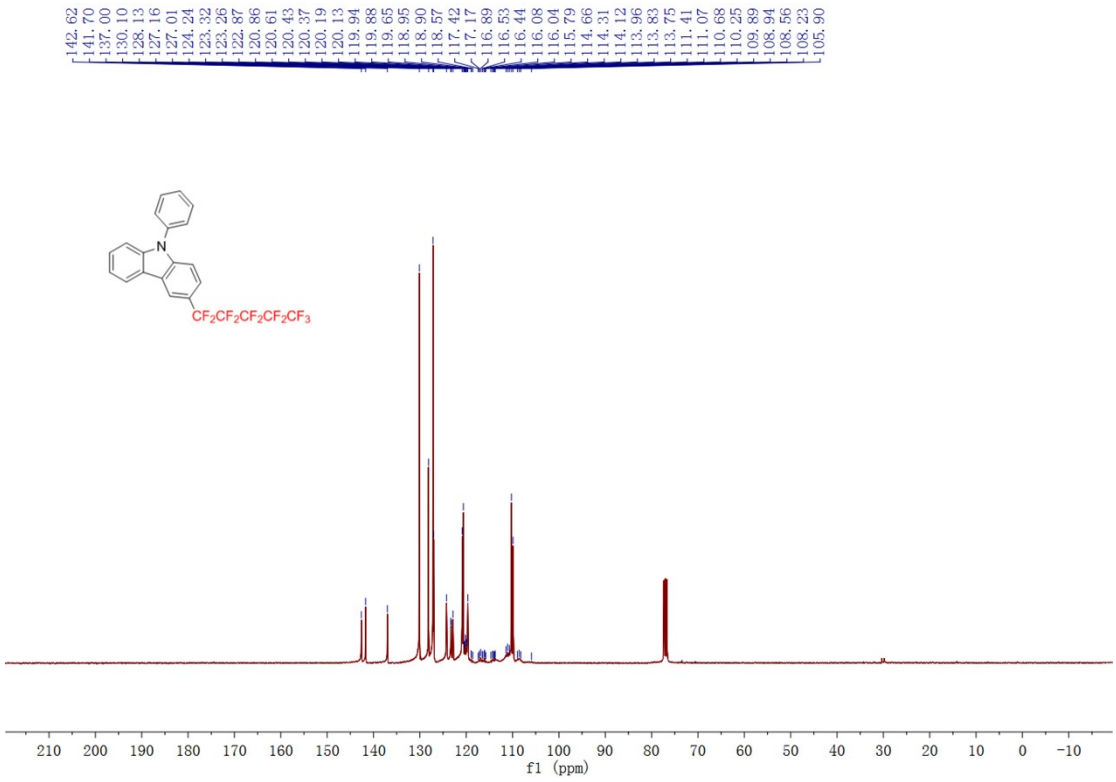
^{19}F NMR spectrum of **6o** in $CDCl_3$



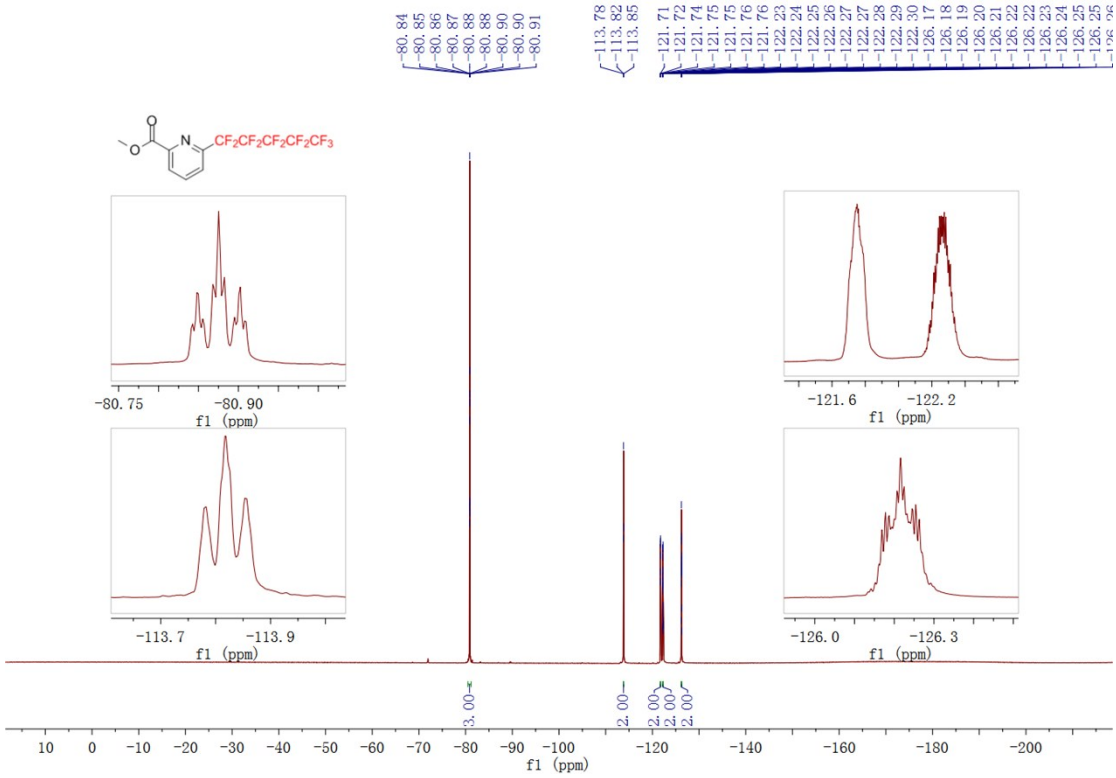
^{1}H NMR spectrum of **6o** in $CDCl_3$



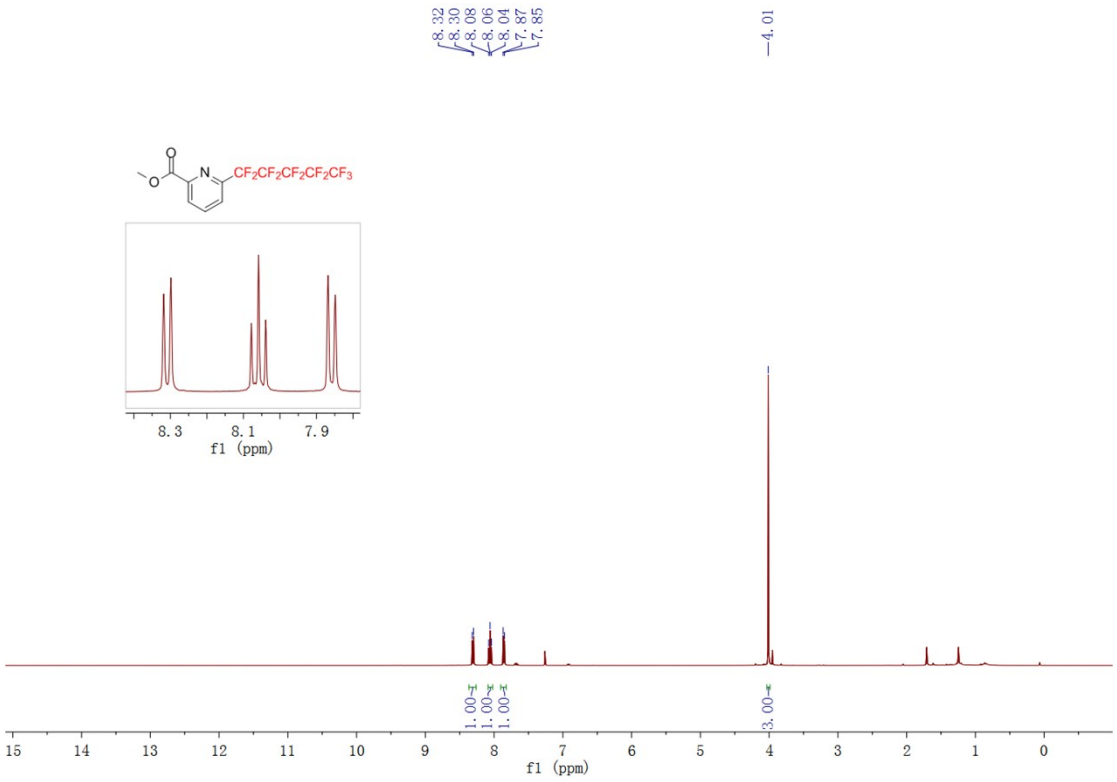
^{13}C NMR spectrum of **6o** in $CDCl_3$



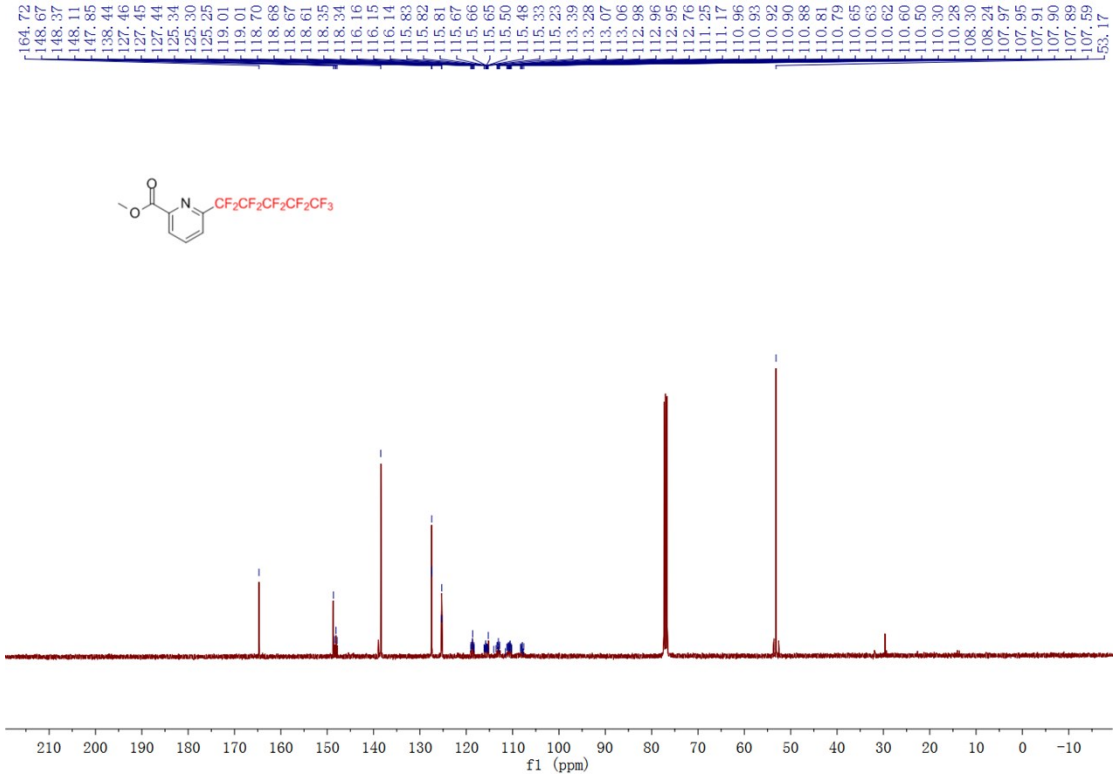
^{19}F NMR spectrum of **6p** in $CDCl_3$



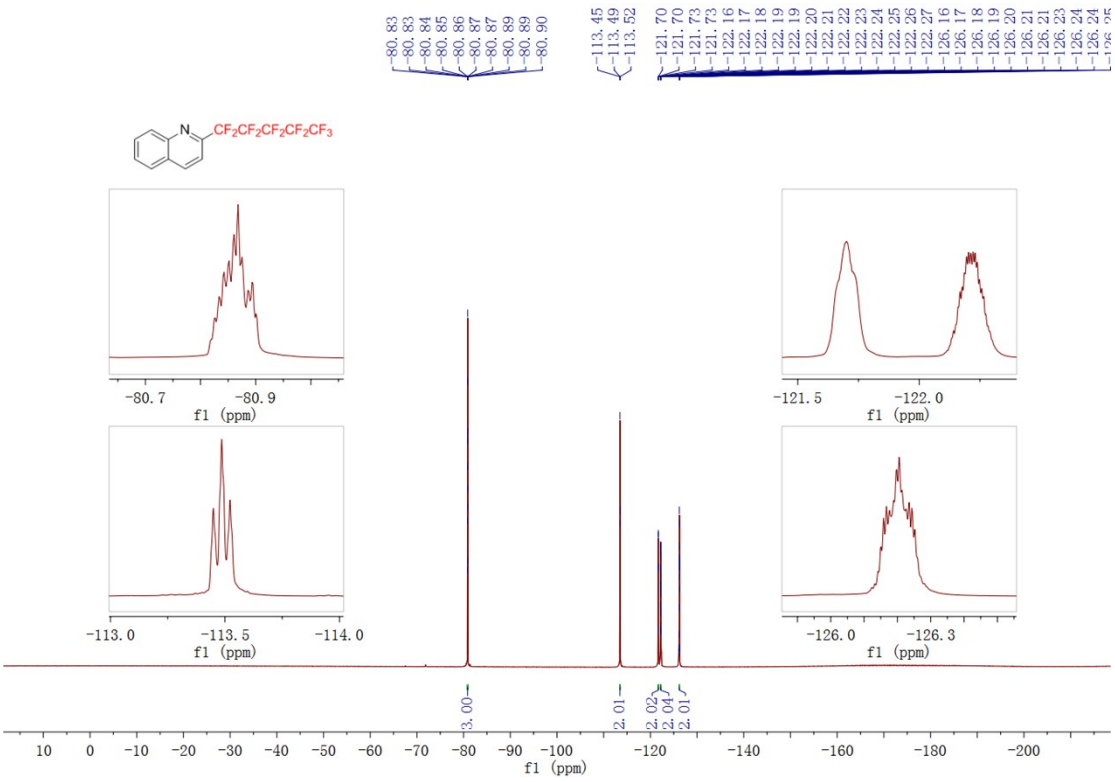
^{1}H NMR spectrum of **6p** in $CDCl_3$



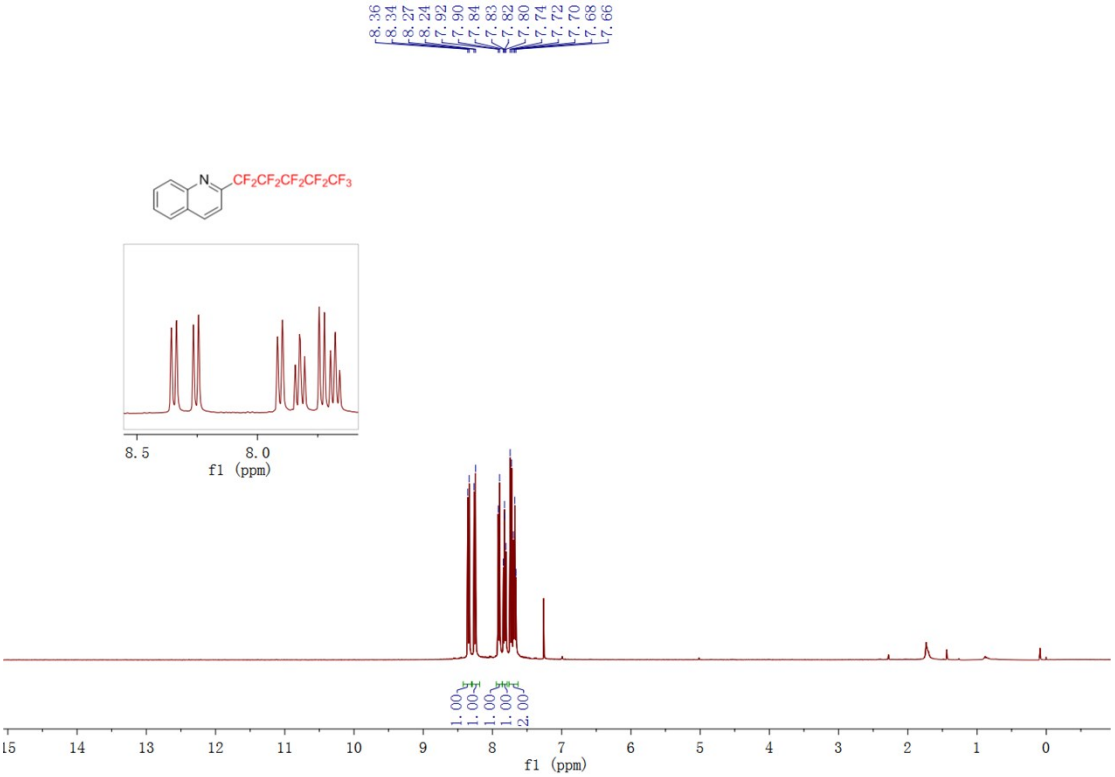
^{13}C NMR spectrum of **6p** in $CDCl_3$



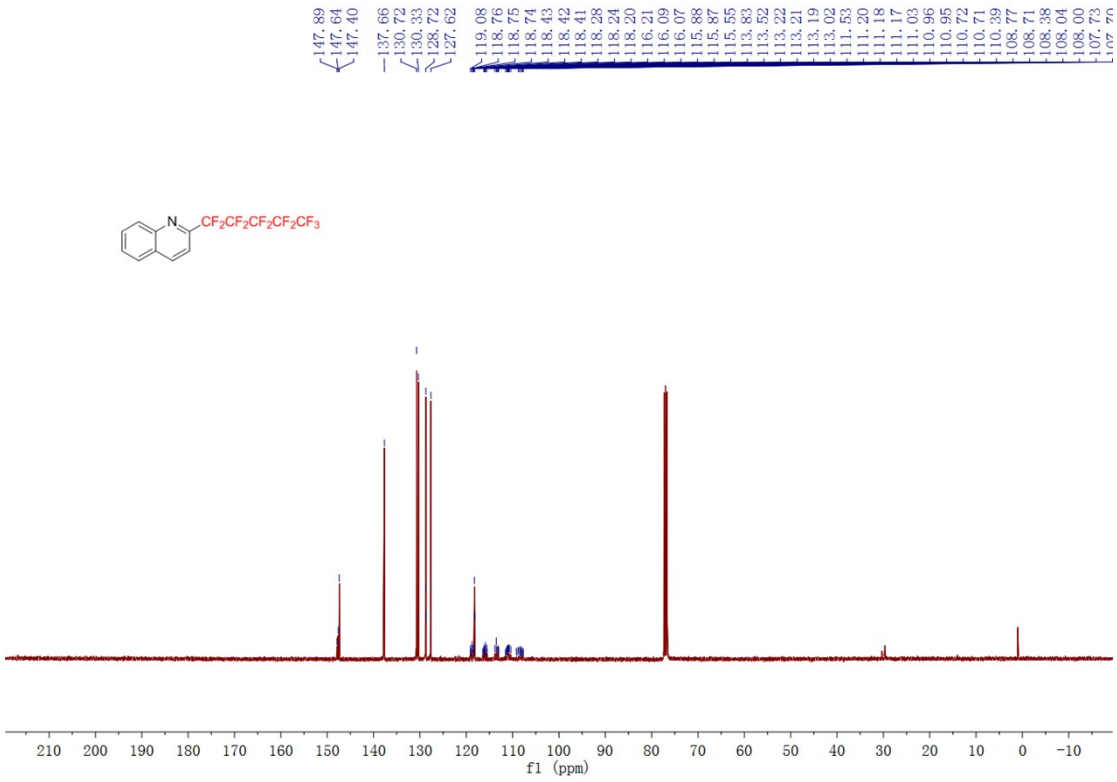
^{19}F NMR spectrum of **6s** in $CDCl_3$



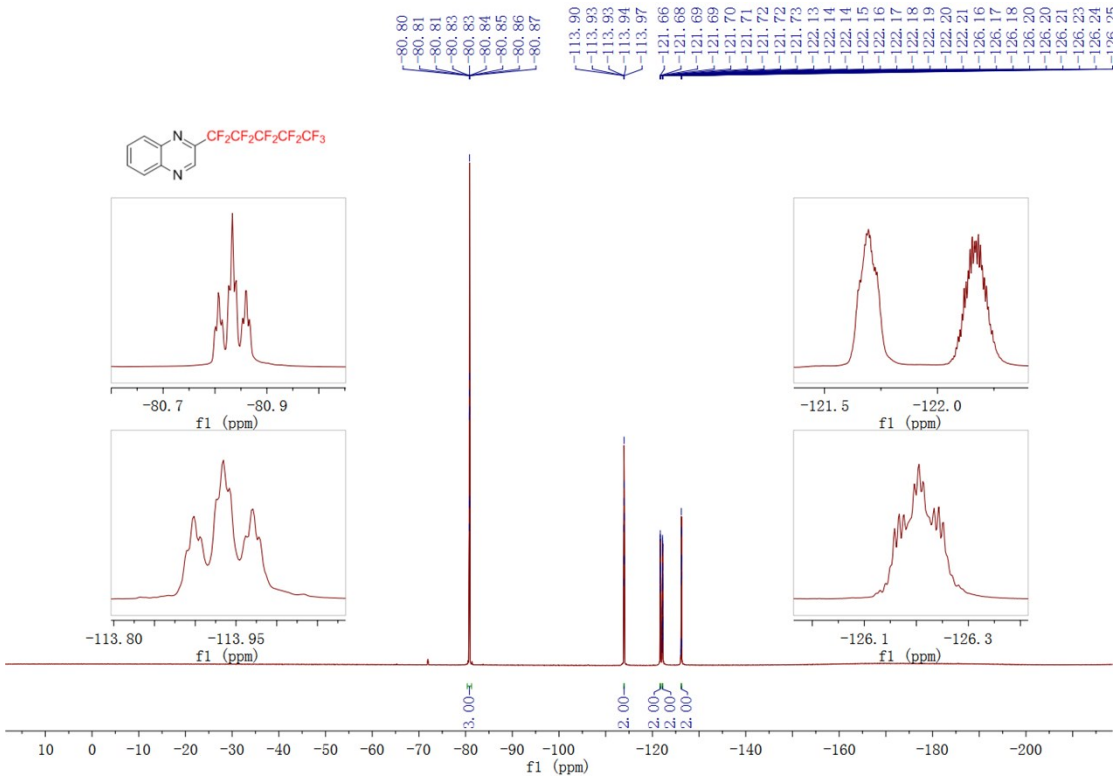
^{1}H NMR spectrum of **6s** in $CDCl_3$



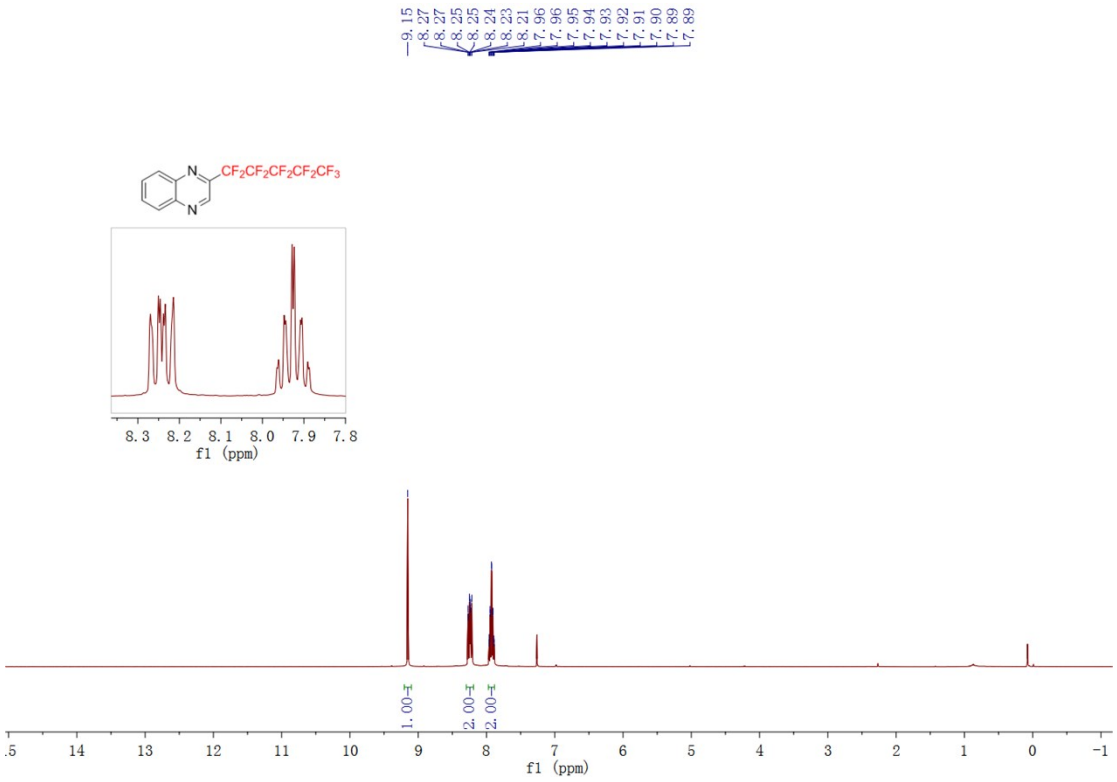
^{13}C NMR spectrum of **6s** in $CDCl_3$



^{19}F NMR spectrum of **6t** in $CDCl_3$



^{1}H NMR spectrum of **6t** in $CDCl_3$



^{13}C NMR spectrum of **6t** in $CDCl_3$