Controllable Double CF_2-Insertion into sp^2 C–Cu Bond Using $TMSCF_3$: A Facile Access to Tetrafluoroethylene-Bridged Structures

Qiqiang Xie, Ziyue Zhu, Lingchun Li, Chuanfa Ni, and Jinbo Hu*

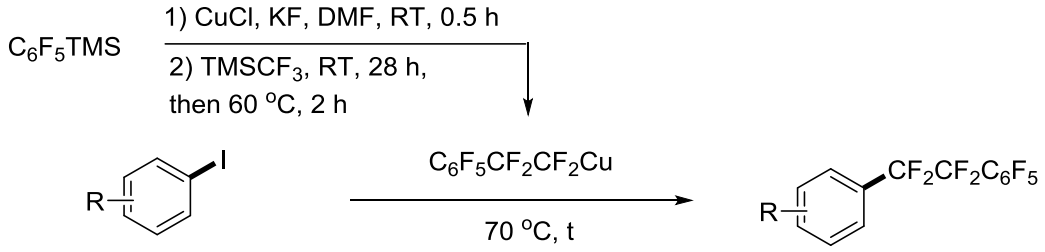
Key Laboratory of Organofluorine Chemistry
Center for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, University of Chinese Academy of Sciences,
Chinese Academy of Sciences
345 Ling-Ling Road, Shanghai, 200032 (China)
Fax: (+86) 21-64166128
E-mail: jinbohu@sioc.ac.cn

Table of Contents

1. General Information

Unless otherwise mentioned, all solvents and reagents were purchased from commercial sources and used as received. *N*,*N*-dimethylformamide (DMF) was dried by passing through a solvent purification system. All the melting points were uncorrected. ^{1}H NMR spectra were recorded at 400 MHz. ^{19}F NMR spectra were recorded at 376 MHz. ^{13}C NMR spectra were recorded at 100 MHz. ^{1}H NMR chemical shifts were determined relative to internal $(CH_3)_4Si$ (TMS) at δ 0.00 ppm or to the signal of the residual protonated solvent: $CDCl_3$ at δ 7.26 ppm. ^{19}F NMR chemical shifts were determined relative to internal or external $CFCl_3$ at δ 0.00 ppm. ^{13}C NMR chemical shifts were determined relative to the signal of the solvent: $CDCl_3$ at δ 77.16 ppm. Data for ^{1}H, ^{13}C, ^{19}F NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets, qt = quartet of triplets, tq = triplet of quartets, br = broad). Mass spectra were obtained on a mass spectrometer. High-resolution mass data were recorded on a high-resolution mass spectrometer.

2. Procedures for Perfluorophenylethylation of Aryl Iodides



General procedure A:

To an oven-dried sealed tube were added CuCl (3.0 mmol, 297 mg, 6.0 equiv) and KF (2.25 mmol, 130.5 mg, 4.5 equiv) in glove box. Then in fume hood, DMF (8 mL) and C_6F_5TMS (0.75 mmol, 142 μL, 1.5 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (1.425 mmol, 202 μL, 2.85 equiv) was added in two equal portions and the second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 °C and stirred at that temperature for 2 hours. After that, aryl iodide **1** (0.5 mmol, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 °C for time as indicated. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 20 mL ammonium hydroxide, extracted with CH_2Cl_2 (30 mL×3). The combined organic layer was washed with H_2O (30 mL×2) and brine (40 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel to afford **2**.

General procedure B:

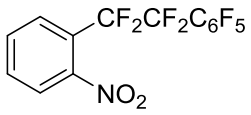
To an oven-dried sealed tube were added CuCl (3.2 mmol, 316.8 mg, 6.4 equiv) and KF (2.4 mmol, 139.2 mg, 4.8 equiv) in glove box. Then in fume hood, DMF (8 mL) and C_6F_5TMS (0.8 mmol, 151 μL, 1.6 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (1.52 mmol, 216 μL, 3.04 equiv) was added in two equal portions and the

second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 ^{o}C and stirred at that temperature for 2 hours. After that, aryl iodide **1** (0.5 mmol, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 ^{o}C for time as indicated. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 20 mL ammonium hydroxide, extracted with CH_2Cl_2 (20 mL×3). The combined organic layer was washed with H_2O (30 mL×2) and brine (40 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel to afford **2**.

General procedure C:

To an oven-dried sealed tube were added CuCl (3.6 mmol, 356.4 mg, 7.2 equiv) and KF (2.7 mmol, 156.6 mg, 5.4 equiv) in glove box. Then in fume hood, DMF (8 mL) and C_6F_5TMS (0.9 mmol, 170 μL, 1.8 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (1.71 mmol, 242 μL, 3.42 equiv) was added in two equal portions and the second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 ^{o}C and stirred at that temperature for 2 hours. After that, aryl iodide **1** (0.5 mmol, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 ^{o}C for time as indicated. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 20 mL ammonium hydroxide, extracted with CH_2Cl_2 (20 mL×3). The combined organic layer was washed with H_2O (30 mL×2) and brine (40 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to afford **2**.

1-Nitro-2-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzene (**2a**)



2a

Prepared from general procedure A; the reaction time was 6 hours; **2a** (132 mg, 68% yield) was obtained.

Yellow solid. Mp: 115–117 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.84–7.78 (m, 1H), 7.77–7.69 (m, 2H), 7.64–7.56 (m, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.0 (t, J = 30.8 Hz, 2F), –107.6 (m, 2F), –138.1 (m, 2F), –147.2 (tt, J = 21.1, 5.6 Hz, 1F), –160.2 (m, 2F);

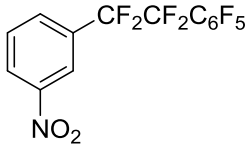
^{13}C NMR ($CDCl_3$, 150 MHz) δ 149.7, 145.9 (dm, J = 259.8 Hz), 143.7 (dm, J = 259.5 Hz), 138.1 (dm, J = 253.0 Hz), 133.4, 131.3, 130.4 (t, J = 7.4 Hz), 124.1, 121.2 (t, J = 25.0 Hz), 115.5 (tt, J = 255.1, 35.4 Hz), 114.9 (tt, J = 258.0, 39.8 Hz), 105.5-104.7 (m);

MS (**EI**, *m/z*, %): 389 (M^+, 18.59), 217 (100);

HRMS (**EI**): Calcd. For $C_{14}H_4F_9NO_2$: 389.0098; Found: 389.0093;

IR (film): 2923, 1655, 1548, 1526, 1507, 1443, 1370, 1334, 1303, 1265, 1197, 1174, 1094, 1058, 1041, 1002, 992, 937, 852, 800, 784, 738, 692, 679, 614 cm^{-1}.

1-Nitro-3-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^{8}-octa-3,5,7-triyn-1-yl)benzene (**2b**)



2b

Prepared from general procedure A; the reaction time was 20 hours; **2b** (170 mg, 87% yield) was obtained.

Yellow solid. Mp: 125–127 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.52 (s, 1H), 8.47 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.76 (t, J = 8.0 Hz, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.4 (t, J = 31.2 Hz, 2F), –112.0 (t, J = 9.8 Hz, 2F), –138.0 (m, 2F), –147.0 (tt, J = 21.4, 5.6 Hz, 1F), –159.9 (m, 2F);

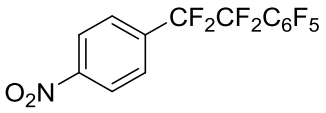
^{13}C NMR ($CDCl_3$, 150 MHz) δ 148.4, 145.9 (dm, J = 258.9 Hz), 143.7 (dm, J = 259.5 Hz), 138.2 (dm, J = 253.0 Hz), 133.1 (t, J = 6.0 Hz), 131.2 (t, J = 25.7 Hz), 130.2, 126.7, 122.7 (t, J = 6.8 Hz) , 115.6 (tt, J = 252.3, 36.1 Hz), 114.8 (tt, J = 256.2, 41.8 Hz), 105.3-104.6 (m);

MS (**EI**, *m/z*, %): 389 (M^+, 12.29), 172 (100);

HRMS (**EI**): Calcd. For $C_{14}H_4F_9NO_2$: 389.0098; Found: 389.0091;

IR (film): 3093, 1656, 1536, 1502, 1353, 1336, 1302, 1275, 1204, 1159, 1112, 1095, 1068, 1004, 992, 961, 910, 798, 750, 737, 713, 616 cm^{-1}.

1-Nitro-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^{8}-octa-3,5,7-triyn-1-yl)benzene (**2c**)



2c

Prepared from general procedure A; the reaction time was 20 hours; **2c** (157 mg, 81% yield) was obtained.

Yellow solid. Mp: 103–105 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.38 (d, J = 7.2 Hz, 2H), 7.85 (d, J = 7.2 Hz, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.4 (t, J = 32.0 Hz, 2F), –112.4 (m, 2F), –138.1 (m, 2F), –147.0 (tt, J = 21.1, 6.0 Hz, 1F), –159.9 (m, 2F);

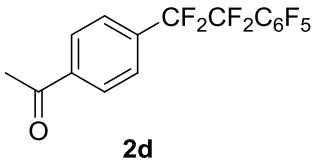
^{13}C NMR ($CDCl_3$, 125 MHz) δ 150.2, 145.9 (dm, J = 261.4 Hz), 143.7 (dm, J = 259.6 Hz), 138.1 (dm, J = 254.1 Hz), 135.2 (t, J = 24.8 Hz), 128.7 (t, J = 6.3 Hz), 123.8, 115.8 (tt, J = 252.2, 36.4 Hz), 114.8 (tt, J = 255.9, 41.5 Hz), 105.5-104.5 (m);

MS (**EI**, *m/z*, %): 389 (M^+, 64.56), 217 (100);

HRMS (**EI**): Calcd. For $C_{14}H_4F_9NO_2$: 389.0098; Found: 389.0105;

IR (film): 3121, 3085, 1654, 1613, 1532, 1505, 1429, 1413, 1348, 1335, 1286, 1197, 1160, 1139, 1096, 1070, 1016, 996, 939, 862, 798, 758, 712, 667, 467 cm^{-1}.

1-(4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)ethan-1-one (**2d**)



2d

Prepared from general procedure B; the reaction time was 20 hours; **2d** (172 mg, 89% yield) was obtained.

White solid. Mp: 105–107 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.08 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H), 2.66 (s, 3H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.7 (t, J = 31.2 Hz, 2F), –112.6 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.6 (tt, J = 21.1, 5.6 Hz, 1F), –160.3 (m, 2F);

^{13}C NMR ($CDCl_3$, 150 MHz) δ 197.2, 145.8 (dm, J = 262.8 Hz), 143.5 (dm, J = 258.9 Hz), 139.7, 138.1 (dm, J = 252.9 Hz), 133.3 (t, J = 24.4 Hz), 128.4, 127.6 (t, J = 6.4 Hz), 116.2 (tt, J = 251.3, 35.6 Hz), 114.9 (tt, J = 256.7, 41.4 Hz), 105.7-105.0 (m), 26.7;

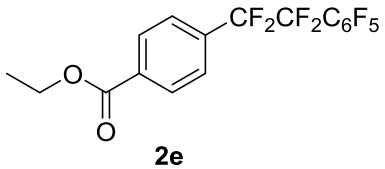
MS (**EI**, *m/z*, %): 386 (M^+, 20.71), 169 (100);

HRMS (**EI**): Calcd. For $C_{16}H_7F_9O$: 386.0353; Found: 386.0352;

IR (film): 2927, 1692, 1656, 1531, 1501, 1425, 1408, 1336, 1289, 1261, 1200, 1151, 1107, 1096, 1019, 938, 838, 858, 798, 756, 710, 604 cm^{-1}.

^{13}C NMR ($CDCl_3$, 100 MHz) δ133.5 (t, J = 25.5 Hz), 132.4, 128.0 (t, J = 6.5 Hz), 117.6, 116.1,;

Ethyl 4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzoate (**2e**)



2e

Prepared from general procedure B; the reaction time was 20 hours; **2e** (199 mg, 96% yield) was obtained.

White solid. Mp: 115–116 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.17 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H), 4.42 (q, J = 7.2 Hz, 2H), 1.42 (q, J = 7.2 Hz, 3H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.7 (t, J = 31.2 Hz, 2F), –112.6 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.7 (tt, J = 21.4, 5.3 Hz, 1F), –160.3 (m, 2F);

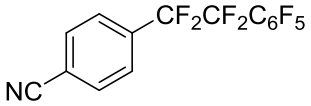
^{13}C NMR ($CDCl_3$, 125 MHz) δ 165.6, 145.9 (dm, J = 262.2 Hz), 143.5 (dm, J = 258.5 Hz), 138.1 (dm, J = 253.3 Hz), 133.8, 133.2 (t, J = 23.9 Hz), 129.7, 127.3 (t, J = 6.2 Hz), 116.2 (tt, J = 251.5, 35.9 Hz), 114.9 (tt, J = 256.5, 40.6 Hz), 105.9-105.0 (m), 61.6, 14.3;

MS (**EI**, *m/z*, %): 416 (M^+, 3.31), 199 (100);

HRMS (**EI**): Calcd. For $C_{17}H_9F_9O_2$: 416.0459; Found: 416.0463;

IR (film): 2980, 1722, 1655, 1532, 1501, 1412, 1370, 1278, 1201, 1151, 1138, 1097, 1022, 1009, 991, 939, 863, 800, 771, 714, 692 cm^{-1}.

4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzonitrile (**2f**)



2f

Prepared from general procedure A; the reaction time was 20 hours; **2f** (170 mg, 92% yield) was obtained.

White solid. Mp: 103–104 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.83 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.5 (t, J = 31.6 Hz, 2F), –112.9 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.1 (tt, J = 21.4, 5.3 Hz, 1F), –160.0 (m, 2F);

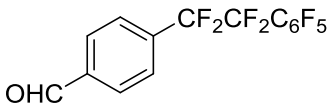
^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.8 (dm, J = 259.4 Hz), 143.6 (dm, J = 259.2 Hz), 138.1 (dm, J = 254.5 Hz), 133.5 (t, J = 25.5 Hz), 132.4, 128.0 (t, J = 6.5 Hz), 117.6, 116.1, 115.8 (tt, J = 252.2, 36.1 Hz), 114.8 (tt, J = 256.9, 40.7 Hz), 105.5-104.3 (m);

MS (**EI**, *m/z*, %): 369 (M^+, 6.7), 152 (100);

HRMS (**EI**): Calcd. For $C_{15}H_4F_9N$: 369.0200; Found: 369.0206;

IR (film): 3113, 3081, 3065, 2236, 1655, 1527, 1509, 1424, 1337, 1287, 1197, 1157, 1091, 1072, 1023, 998, 940, 854, 840, 809, 773, 712, 674, 594, 551, 525 cm^{-1}.

4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzaldehyde (**2g**)



2g

Prepared from general procedure A; the reaction time was 20 hours; **2g** (167 mg, 90% yield) was obtained.

White solid. Mp: 104–105 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 10.12 (s, 1H), 8.03 (d, J = 8.0 Hz, 2H), 7.82 (d, J = 8.0 Hz, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.6 (t, J = 31.2 Hz, 2F), –112.6 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.5 (tt, J = 21.1, 5.3 Hz, 1F), –160.2 (m, 2F);

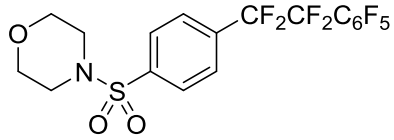
^{13}C NMR ($CDCl_3$, 125 MHz) δ 191.4, 145.9 (dm, J = 260.6 Hz), 143.6 (dm, J = 258.9 Hz), 138.7, 138.1 (dm, J = 253.6 Hz), 134.6 (t, J = 24.2 Hz), 129.7, 128.1 (t, J = 6.3 Hz) , 116.1 (tt, J = 252.2, 35.6 Hz), 114.9 (tt, J = 256.5, 43.2 Hz), 105.6-104.8 (m);

MS (**EI**, *m/z*, %): 372 (M^+, 31.89), 155 (100);

HRMS (**EI**): Calcd. For $C_{15}H_5F_9O$: 372.0197; Found: 372.0193;

IR (film): 2867, 1706, 1653, 1614, 1528, 1506, 1425, 1389, 1334, 1287, 1195, 1162, 1138, 1099, 1007, 995, 937, 850, 787, 722, 674 cm^{-1}.

4-((4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)sulfonyl)morpholine (**2h**)



2h

Prepared from general procedure A; the reaction time was 6 hours; **2h** (214 mg, 87% yield) was obtained.

White solid. Mp: 198–200 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.90 (d, J = 8.4 Hz, 2H), 7.84 (d, J = 8.0 Hz, 2H), 3.77 (t, J = 4.4 Hz, 4H), 3.05 (t, J = 4.8 Hz, 4H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.6 (t, J = 31.2 Hz, 2F), –112.6 (t, J = 9.4 Hz, 2F), –138.1 (m, 2F), –147.1 (tt, J = 21.1, 5.6 Hz, 1F), –160.0 (m, 2F);

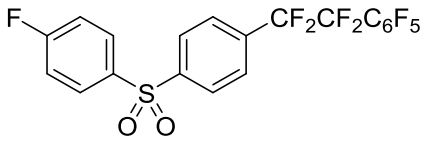
^{13}C NMR ($CDCl_3$, 100 MHz) δ145.8 (dm, J = 260.2 Hz), 143.6 (dm, J = 259.1 Hz), 138.1 (dm, J = 254.3 Hz), 139.0, 133.8 (t, J = 25.0 Hz), 128.2 (t, J = 6.3 Hz), 128.1, 115.9 (tt, J = 252.1, 36.1 Hz), 114.8 (tt, J = 257.4, 38.9 Hz), 105.7-104.5 (m), 66.2, 46.1;

MS (**EI**, *m/z*, %): 493 (M^+, 2.31), 91 (100);

HRMS (**EI**): Calcd. For $C_{18}H_{12}F_9NO_3S$: 493.0394; Found: 493.0397;

IR (film): 2984, 2891, 2859, 1657, 1529, 1502, 1405, 1351, 1329, 1287, 1258, 1191, 1171, 1140, 1109, 1099, 1071, 1019, 991, 948, 939, 839, 757, 613, 598 cm^{-1}.

1-Fluoro-4-((4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)sulfonyl)benzene (**2i**)



2i

Prepared from general procedure A; the reaction time was 20 hours; **2i** (230 mg, 91% yield) was obtained.

White solid. Mp: 164–165 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.07 (d, J = 8.4 Hz, 2H), 8.03–7.96 (m, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.22 (t, J = 8.8 Hz, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –103.5 (m, 1F), –106.4 (t, J = 31.2 Hz, 2F), –112.4 (t, J = 10.2 Hz, 2F), –138.1 (m, 2F), –147.2 (tt, J = 21.4, 5.6 Hz, 1F), –160.1 (m, 2F);

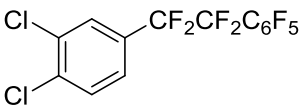
^{13}C NMR ($CDCl_3$, 125 MHz) δ 165.9 (d, J = 255.5 Hz), 145.9 (dm, J = 258.9 Hz), 145.1, 143.6 (dm, J = 259.2 Hz), 138.1 (dm, J = 253.8 Hz), 136.9 (d, J = 3.2 Hz), 134.0 (t, J = 24.9 Hz), 131.0 (d, J = 9.7 Hz), 128.5 (t, J = 6.2 Hz), 127.9, 117.0 (d, J = 22.6 Hz), 115.8 (tt, J = 252.0, 36.4 Hz), 114.8 (tt, J = 257.4, 40.5 Hz), 105.5-104.6 (m);

MS (**EI**, *m/z*, %): 502 (M^+, 4.36), 143 (100);

HRMS (**EI**): Calcd. For $C_{20}H_8F_{10}O_2S$: 502.0085; Found: 502.0079;

IR (film): 3109, 3085, 1657, 1594, 1531, 1504, 1404, 1326, 1290, 1242, 1196, 1165, 1154, 1136, 1104, 1092, 1073, 994, 836, 804, 752, 629, 551 cm^{-1}.

1,2-Dichloro-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzene (**2j**)



2j

Prepared from general procedure A; the reaction time was 20 hours; **2j** (189 mg, 92% yield) was obtained.

White solid. Mp: 93–95 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.73 (s, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.4 Hz, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.5 (t, J = 31.2 Hz, 2F), –112.1 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.4 (tt, J = 21.4, 5.6 Hz, 1F), –160.1 (m, 2F);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 145.9 (dm, J = 260.2 Hz), 143.6 (dm, J = 258.9 Hz), 138.2 (dm, J = 254.6 Hz), 136.9, 133.6, 130.9, 129.4 (t, J = 6.8 Hz), 129.1 (t, J = 25.3 Hz), 126.5 (t, J = 6.3 Hz) , 115.7 (tt, J = 252.0, 36.3 Hz), 114.8 (tt, J = 258.1, 41.6 Hz), 105.6-104.8 (m);

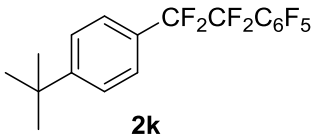
MS (**EI**, *m/z*, %): 412 (M^+, 3.1), 195 (100);

HRMS (**EI**): Calcd. For $C_{14}H_3Cl_2F_9$: 411.9468; Found: 411.9466;

IR (film): 3097, 1656, 1527, 1505, 1474, 1424, 1387, 1333, 1294, 1252, 1201, 1162, 1092, 1077, 995, 951, 891, 823, 770, 728, 677 cm^{-1}.

^{13}C NMR ($CDCl_3$, 100 MHz) δ133.5 (t, J = 25.5 Hz), 132.4, 128.0 (t, J = 6.5 Hz), 117.6, 116.1;

1-(*tert*-Butyl)-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzene (**2k**)



2k

Prepared from general procedure A; the reaction time was 27 hours; **2k** (162 mg, 81% yield) was obtained.

White solid. Mp: 102–103 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.55 (d, J = 8.8 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 1.36 (s, 9H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.9 (t, J = 31.2 Hz, 2F), –118.6 (m, 2F), –138.2 (m, 2F), –148.5 (m, 1F), –160.8 (m, 2F);

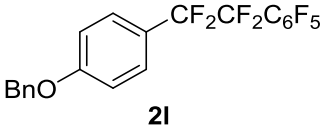
^{13}C NMR ($CDCl_3$, 150 MHz) δ 155.3, 145.9 (dm, J = 258.5 Hz), 143.3 (dm, J = 258.2 Hz), 138.1 (dm, J = 252.9 Hz), 126.9 (t, J = 6.1 Hz), 126.2 (t, J = 24.4 Hz), 125.6, 116.8 (tt, J = 250.6, 35.3 Hz), 115.1 (tt, J = 256.2, 43.1 Hz), 106.4-105.8 (m), 35.1, 31.3;

MS (**EI**, *m/z*, %): 400 (M^+, 7.68), 183 (100);

HRMS (**EI**): Calcd. For $C_{18}H_{13}F_9$: 400.0874; Found: 400.0872;

IR (film): 2968, 2879, 1927, 1654, 1613, 1527, 1501, 1408, 1366, 1333, 1294, 1195, 1160, 1140, 1105, 1093, 1071, 1017, 835, 800, 709, 596 cm^{-1}.

1-(Benzyloxy)-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzene (**2l**)



2l

Prepared from general procedure A; the reaction time was 26 hours; **2l** (185 mg, 82% yield) was obtained.

White solid. Mp: 136–138 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.53 (d, J = 8.8 Hz, 2H), 7.48–7.32 (m, 5H), 7.07 (d, J = 8.8 Hz, 2H), 5.13 (s, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.0 (t, J = 31.6 Hz, 2F), –111.4 (t, J = 9.8 Hz, 2F), –138.2 (m, 2F), –148.4 (tt, J = 21.1, 5.3 Hz, 1F), –160.7 (m, 2F);

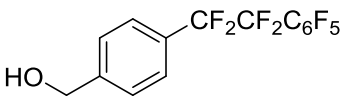
^{13}C NMR ($CDCl_3$, 150 MHz) δ 161.4, 145.8 (dm, J = 258.6 Hz), 143.3 (dm, J = 258.5 Hz), 138.0 (dm, J = 252.5 Hz), 136.4, 128.8, 128.77 (t, J = 6.4 Hz), 128.4, 127.6, 121.3 (t, J = 24.9 Hz), 116.7 (tt, J = 250.8, 35.3 Hz), 115.0 (tt, J = 258.2, 39.8 Hz), 114.9, 106.4-105.6 (m), 70.3;

MS (**EI**, *m/z*, %): 450 (M^+), 91 (100);

HRMS (**EI**): Calcd. For $C_{21}H_{11}F_9O$: 450.0666; Found: 450.0671;

IR (film): 3085, 3040, 2944, 2883, 1654, 1613, 1530, 1504, 1455, 1423, 1384, 1331, 1255, 1197, 1155, 1138, 1106, 1092, 1007, 992, 929, 842, 815, 789, 754, 698 cm^{-1}.

(4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)methanol (**2m**)



2m

Prepared from general procedure C; the reaction time was 50 hours; **2m** (148 mg, 79% yield) was obtained.

White solid. Mp: 114–115 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.61 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 4.80 (d, J = 4.8 Hz, 2H), 1.79 (t, J = 5.6 Hz, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.9 (t, J = 31.6 Hz, 2F), –112.1 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –148.2 (tt, J = 21.1, 5.3 Hz, 1F), –160.6 (m, 2F);

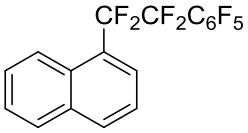
^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.8 (dm, J = 260.1 Hz), 144.8, 143.3 (dm, J = 258.6 Hz), 138.0 (dm, J = 252.6 Hz), 128.3 (t, J = 24.6 Hz), 127.4 (t, J = 6.3 Hz), 126.8, 116.5 (tt, J = 251.0, 35.4 Hz), 114.8 (tt, J = 256.8, 41.0 Hz), 105.5-104.3 (m), 64.6;

MS (**EI**, *m/z*, %): 374 (M^+, 4.41), 157 (100);

HRMS (**EI**): Calcd. For $C_{15}H_7F_9O$: 374.0353; Found: 374.0348;

IR (film): 3327, 2960, 2879, 1653, 1613, 1527, 1506, 1424, 1332, 1290, 1195, 1158, 1139, 1093, 1071, 1018, 999, 934, 819, 779 cm^{-1}.

1-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)naphthalene (**2n**)



2n

Prepared from general procedure A; the reaction time was 27 hours; **2n** (154 mg, 78% yield) was obtained.

White solid. Mp: 208–209 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.30 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 7.6 Hz, 1H), 7.64–7.52 (m, 3H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –105.5 (t, J = 9.0 Hz, 2F), –105.9 (t, J = 30.8 Hz, 2F), –138.2 (m, 2F), –148.2 (tt, J = 21.4, 5.6 Hz, 1F), –160.6 (m, 2F);

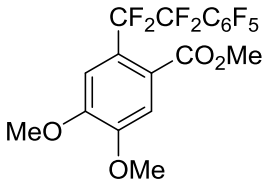
^{13}C NMR ($CDCl_3$, 150 MHz) δ 146.9-142.1 (m), 138.1 (dm, J = 252.3 Hz), 134.2, 133.2, 130.6, 129.1, 128.1 (t, J = 9.6 Hz), 127.6, 126.4, 125.3, 124.8 (t, J = 21.7 Hz), 124.4;

MS (**EI**, *m/z*, %): 394 (M^+, 18.61), 177 (100);

HRMS (**EI**): Calcd. For $C_{18}H_7F_9$: 394.0404; Found: 394.0415;

IR (film): 1655, 1527, 1501, 1423, 1328, 1255, 1184, 1120, 1089, 1004, 989, 806, 783, 769, 719, 614, 539 cm^{-1}.

Methyl
4,5-dimethoxy-2-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)benzoate (**2o**)



2o

Prepared from general procedure A; the reaction time was 33 hours; **2o** (191 mg, 83% yield) was obtained.

White solid. Mp: 102–103 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.09 (s, 1H), 7.00 (s, 1H), 3.97 (s, 3H), 3.94 (s, 3H), 3.84 (s, 3H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –105.7 (m, 2F), –106.0 (t, J = 31.2 Hz, 2F), –138.5 (m, 2F), –148.4 (tt, J = 21.48, 5.3 Hz, 1F), –160.9 (m, 2F);

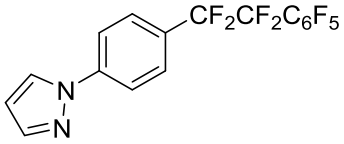
^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.4, 151.1, 150.0, 147.5-141.7 (m), 138.0 (dm, J = 253.4 Hz), 126.5 (t, J = 3.5 Hz), 118.9 (t, J = 24.1 Hz), 116.5 (tt, J = 254.0, 35.5 Hz), 115.2 (tt, J = 258.0, 39.7 Hz), 111.6, 111.3 (t, J = 7.9 Hz) , 106.5-105.5 (m), 56.4, 56.3, 52.8;

MS (**ESI**, *m/z*): 463 ($M+H^+$);

HRMS (**DART**): Calcd. For $C_{18}H_{12}F_9O_4$: 463.0586 ($M+H^+$); Found: 463.0585;

IR (film): 3012, 2954, 2855, 1736, 1657, 1607, 1529, 1507, 1466, 1436, 1361, 1331, 1283, 1216, 1195, 1173, 1130, 995, 961, 871, 826, 783, cm^{-1}.

1-(4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)-1H-pyrazole (**2p**)



2p

Prepared from general procedure A; the reaction time was 41 hours; **2p** (175 mg, 85% yield) was obtained.

White solid. Mp: 143–144 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.01 (d, J = 2.4 Hz, 1H), 7.86 (d, J = 8.8 Hz, 2H), 7.77 (d, J = 1.6 Hz, 1H), 7.71 (d, J = 8.8 Hz, 2H), 6.52 (t, J = 2.4 Hz, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.8 (t, J = 31.2 Hz, 2F), –112.1 (t, J = 9.4 Hz, 2F), –138.1 (m, 2F), –147.9 (tt, J = 21.4, 5.6 Hz, 1F), –160.4 (m, 2F);

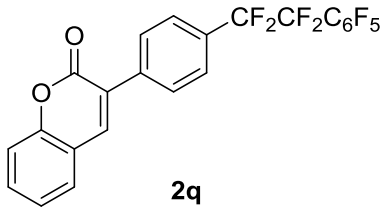
^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.8 (dm, J = 256.4 Hz), 143.4 (dm, J = 258.6 Hz), 142.7, 142.1, 138.1 (dm, J = 252.8 Hz), 128.6 (t, J = 6.3 Hz), 126.9, 126.7 (t, J = 25.2 Hz), 118.7, 116.4 (tt, J = 252.0, 35.2 Hz), 114.9 (tt, J = 254.9, 42.2 Hz), 108.6, 106.0-105.3 (m) ;

MS (**ESI**, *m/z*): 411 ($M+H^+$);

HRMS (**DART**): Calcd. For $C_{17}H_8F_9N_2$: 411.0538 ($M+H^+$); Found: 411.0540;

IR (film): 3129, 1654, 1618, 1529, 1499, 1438, 1395, 1412, 1337, 1293, 1193, 1156, 1136, 1121, 1100, 1073, 990, 931, 846, 798, 756, 699 cm^{-1}.

3-(4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl)-2H-chromen-2-one (**2q**)



2q

Prepared from general procedure A; the reaction time was 20 hours; **2q** (215 mg, 88% yield) was obtained.

White solid. Mp: 228–230 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.91 (s, 1H), 7.87 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H), 7.58 (t, J = 7.6 Hz, 2H), 7.40 (d, J = 8.4 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.6 (t, J = 31.6 Hz, 2F), –112.1 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –148.0 (tt, J = 21.1, 5.6 Hz, 1F), –160.5 (m, 2F);

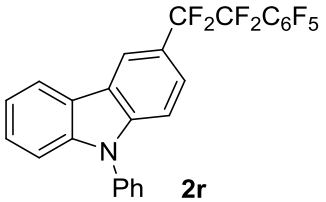
^{13}C NMR ($CDCl_3$, 150 MHz) δ 160.3, 153.9, 145.9 (dm, J = 259.4 Hz), 143.4 (dm, J = 258.2 Hz), 141.1, 138.2, 138.1 (dm, J = 253.2 Hz), 132.2, 129.4 (t, J = 24.6 Hz), 128.8, 128.3, 127.4 (t, J = 6.3 Hz), 127.2, 124.9, 119.5, 116.8, 116.4 (tt, J = 251.0, 35.6 Hz), 114.8 (tt, J = 258.0, 42.0 Hz), 105.5-104.3 (m);

MS (**EI**, *m/z*, %): 488 (M^+, 10.48), 271 (100);

HRMS (**EI**): Calcd. For $C_{23}H_9F_9O_2$: 488.0459; Found: 488.0462;

IR (film): 1725, 1658, 1608, 1537, 1499, 1455, 1356, 1292, 1195, 1153, 1136, 1103, 1093, 990, 938, 830, 757, 641 cm^{-1}.

3-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)-9-phenyl-9H-carbazole (**2r**)



2r

Prepared from general procedure A; the reaction time was 41 hours; **2r** (190 mg, 75% yield) was obtained.

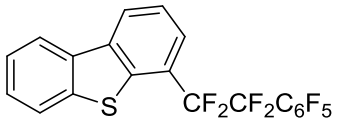
White solid. Mp: 209–212 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.41 (s, 1H), 8.22 (d, J = 8.0 Hz, 1H), 7.68–7.49 (m, 9H), 7.39–7.33 (m, 1H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.4 (t, J = 31.2 Hz, 2F), –109.8 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –148.6 (tt, J = 21.4, 5.3 Hz, 1F), –160.7 (m, 2F);

^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.9 (dm, J = 258.9 Hz), 143.2 (dm, J = 258.6 Hz), 142.6, 141.7, 138.1 (dm, J = 253.2 Hz), 137.2, 130.2, 128.2, 127.3, 127.0, 124.5 (t, J = 5.8 Hz), 123.3, 123.0, 120.9, 120.8, 120.2 (t, J = 25.2 Hz), 119.9 (t, J = 6.8 Hz), 117.4 (tt, J = 251.2, 35.3 Hz), 115.2 (tt, J = 256.5, 41.3 Hz), 105.5-104.3 (m), 110.3,

109.8;
MS (**ESI**, *m/z*): 510.1 ($M+H^+$);
HRMS (**EI**): Calcd. For $C_{26}H_{13}F_9N$: 510.0899 ($M+H^+$); Found: 510.0898;
IR (film): 1654, 1599, 1526, 1504, 1456, 1423, 1330, 1262, 1238, 1191, 1139, 1089, 992, 893, 815, 773, 752, 697 cm^{-1}.

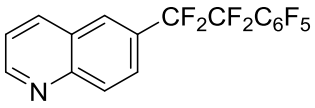
4-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)dibenzo*[b,d]*thiophene (**2s**)



2s

Prepared from general procedure B; the reaction time was 41 hours; **2s** (188 mg, 83% yield) was obtained.
White solid. Mp: 173–175 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.38 (d, J = 8.0 Hz, 1H), 8.22 –8.16 (m, 1H), 7.90–7.85 (m, 1H), 7.71 (d, J = 7.6 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.55–7.46 (m, 2H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.9 (t, J = 31.2 Hz, 2F), –111.5 (t, J = 9.4 Hz, 2F), –138.0 (m, 2F), –147.8 (tt, J = 21.4, 5.6 Hz, 1F), –160.5 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.9 (dm, J = 256.5 Hz), 143.5 (dm, J = 258.7 Hz), 139.7 (t, J = 3.2 Hz), 138.2, 138.1 (dm, J = 252.5 Hz), 137.5, 134.2, 127.7, 126.9 (t, J = 7.3 Hz), 124.9, 124.8, 124.4, 123.8 (t, J = 25.6 Hz), 122.5, 121.8, 117.4 (tt, J = 253.6, 35.7 Hz), 115.6 (tt, J = 256.6, 42.3 Hz), 106.0-105.3 (m);
MS (**EI**, *m/z*, %): 450 (M^+, 27.55), 233 (100);
HRMS (**EI**): Calcd. For $C_{20}H_7F_9S$: 450.0125; Found: 450.0140;
IR (film): 2908, 1658, 1531, 1503, 1403, 1331, 1277, 1187, 1129, 1090, 1038, 990, 946, 822, 774, 756, 743, 704, 612 cm^{-1}.

6-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)quinoline (**2t**)

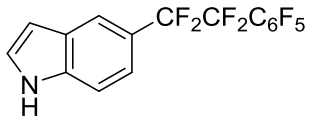


2t

Prepared from general procedure A; the reaction time was 33 hours; **2t** (164 mg, 83% yield) was obtained.
White solid. Mp: 162–164 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 9.05 (dd, J = 4.4, 1.6 Hz, 1H), 8.29 (d, J = 8.4 Hz, 1H), 8.24 (d, J = 8.8 Hz, 1H), 7.16 (s, 1H), 7.91 (d, J = 8.8 Hz, 1H), 7.53 (dd, J = 8.4, 4.0 Hz, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.4 (t, J = 31.6 Hz, 2F), –111.5 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.8 (tt, J = 21.4, 5.3 Hz, 1F), –160.4 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 152.6, 149.3, 145.8 (dm, J = 258.4 Hz), 143.4 (dm, J = 258.7 Hz), 138.1 (dm, J = 252.9 Hz), 137.0, 130.4, 128.1 (t, J = 6.9 Hz), 127.4,

127.2 (t, *J* = 24.2 Hz), 126.8 (t, *J* = 5.7 Hz), 122.3, 116.5 (tt, *J* = 251.7, 35.7 Hz), 114.8 (tt, *J* = 258.3, 44.0 Hz), 106.0-105.3 (m);
MS (**ESI**, *m/z*): 396 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{17}H_7F_9N$: 396.0429 ($M+H^+$); Found: 396.0430;
IR (film): 1659, 1594, 1570, 1532, 1501, 1425, 1362, 1329, 1202, 1184, 1154, 1128, 1094, 1070, 991, 900, 846, 802, 616 cm^{-1}.

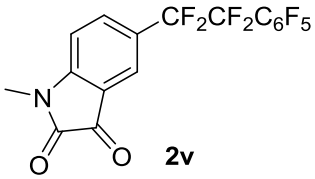
5-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)-1H-indole (**2u**)



2u

Prepared from general procedure C; the reaction time was 41 hours; **2u** (159 mg, 83% yield) was obtained.
Pale yellow solid. Mp: 191–192 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.34 (s, 1H), 7.93 (s, 1H), 7.48 (d, *J* = 8.7 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 1H), 7.32 (t, *J* = 2.8 Hz, 1H), 6.68–6.40 (m, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.7 (t, *J* = 31.2Hz, 2F), –110.0 (t, *J* = 10.2 Hz, 2F), –138.2 (m, 2F), –148.8 (tt, *J* = 21.1, 5.3 Hz, 1F), –160.9 (m, 2F);
^{13}C NMR ($CDCl_3$, 125 MHz) δ 145.8 (dm, *J* = 260.9 Hz), 143.2 (dm, *J* = 257.6 Hz), 138.0 (dm, *J* = 252.4 Hz), 137.3, 127.5, 125.8, 120.8–120.4 (m), 120.0–112.5 (m), 111.1, 103.7;
MS (**ESI**, *m/z*): 384 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{16}H_7F_9N$: 384.0429 ($M+H^+$); Found: 384.0430;
IR (film): 3484, 1657, 1619, 1527, 1506, 1420, 1332, 1304, 1198, 1174, 1090, 1059, 991, 962, 793, 735, 696, 481 cm^{-1}.

1-Methyl-5-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)indoline-2,3-dione (**2v**)

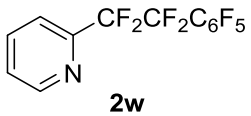


2v

Prepared from general procedure A; the reaction time was 26 hours; **2v** (198 mg, 84% yield) was obtained.
Red solid. Mp: 195–197 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.93–7.81 (m, 2H), 7.06 (d, *J* = 8.4 Hz, 1H), 3.33 (s, 3H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.6 (t, *J* = 31.2Hz, 2F), –111.9 (m, 2F), –138.1 (m, 2F), –147.3 (tt, *J* = 21.4, 5.6 Hz, 1F), –160.1 (m, 2F);
^{13}C NMR ($CDCl_3$, 125 MHz) δ 182.3, 158.0, 153.9, 145.8 (dm, *J* = 259.3 Hz), 143.5 (dm, *J* = 259.0 Hz), 138.1 (dm, *J* = 253.4 Hz), 137.2 (t, *J* = 6.3 Hz), 124.8 (t, *J* = 25.3

Hz), 124.3 (t, *J* = 6.4 Hz), 117.4, 115.9 (tt, *J* = 251.2, 36.3 Hz), 114.8 (tt, *J* = 255.5, 42.4 Hz), 105.5-104.6 (m), 110.3, 26.6;
MS (**ESI**, *m/z*): 428 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{17}H_7F_9N\ O_2$: 428.0328 ($M+H^+$); Found: 428.0327;
IR (film): 3077, 2952, 1748, 1626, 1601, 1529, 1503, 1425, 1359, 1332, 1301, 1276, 1122, 1092, 996, 794, 739, 705, 477 cm^{-1}.

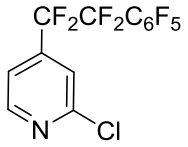
2-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)pyridine (**2w**)



2w

Prepared from general procedure A; the reaction time was 20 hours; **2w** (125 mg, 72% yield) was obtained.
White solid. Mp: 92–93 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.68 (d, *J* = 4.8 Hz, 1H), 7.90 (t, *J* = 4.8 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.49 (dd, *J* = 7.2, 4.8 Hz, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.7 (t, *J* = 31.2Hz, 2F), –116.9 (m, 2F), –138.2 (m, 2F), –148.2 (tt, *J* = 21.4, 5.6 Hz, 1F), –160.8 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 149.8, 148.5 (t, *J* = 25.7 Hz), 145.8 (dm, *J* = 255.6Hz), 143.4 (dm, *J* = 258.5 Hz), 138.0 (dm, *J* = 252.9 Hz), 137.3, 126.2, 122.9 (t, *J* = 4.1 Hz), 115.0 (tt, *J* = 258.9, 37.6 Hz), 114.1 (tt, *J* = 253.1, 34.2 Hz), 106.2-105.5 (m);
MS (**EI**, *m/z*, %): 345 (M^+, 44.05), 128 (100);
HRMS (**EI**): Calcd. For $C_{13}H_4F_9N$: 345.0200; Found: 345.0206;
IR (film): 1656, 1587, 1501, 1437, 1427, 1336, 1301, 1204, 1155, 1136, 1108, 1081, 1048, 990, 943, 809, 782, 693, 615 cm^{-1}.

2-Chloro-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)pyridine (**2x**)

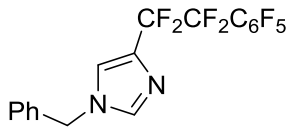


2x

Prepared from general procedure A; the reaction time was 20 hours; **2x** (132 mg, 70% yield) was obtained.
White solid. Mp: 86–88 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 8.61 (d, *J* = 5.2 Hz, 1H), 7.60 (s, 1H), 7.49 (d, *J* = 5.2 Hz, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –106.4 (t, *J* = 31.6Hz, 2F), –113.9 (m, 2F), –138.0 (m, 2F), –146.7 (tt, *J* = 21.4, 5.6 Hz, 1F), –159.8 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 152.6, 150.6, 145.9 (dm, *J* = 259.6 Hz), 143.8 (dm, *J* = 260.0 Hz), 140.4 (t, *J* = 26.0 Hz), 138.2 (dm, *J* = 253.3 Hz), 122.5 (t, *J* = 6.5 Hz), 120.1 (t, *J* = 6.0 Hz), 114.8 (tt, *J* = 252.3, 36.8 Hz), 114.6 (tt, *J* = 256.4, 40.4 Hz),

105.5-104.3 (m);
MS (**ESI**, *m/z*): 380 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{13}H_4ClF_9N$: 379.9883 ($M+H^+$); Found: 379.9884;
IR (film): 1658, 1590, 1552, 1529, 1512, 1427, 1373, 1335, 1300, 1272, 1202, 1129, 1099, 1080, 990, 956, 890, 845, 815, 763, 718, 696 cm^{-1}.

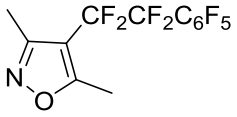
1-Benzyl-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)-1H-imidazole (**2y**)



2y

Prepared from general procedure C; the reaction time was 41 hours; **2y** (128 mg, 60% yield) was obtained.
White solid. Mp: 90–91 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.56 (s, 1H), 7.44–7.34 (m, 3H), 7.29 (s, 1H), 7.18 (dd, J = 8.0, 1.6 Hz, 2H), 5.16 (s, 2H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –108.3 (tt, J = 31.2, 4.5 Hz, 2F), –112.3 (m, 2F), –138.1 (m, 2F), –148.6 (tt, J = 21.4, 5.3 Hz, 1F), –161.0 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.8 (dm, J = 258.6 Hz), 143.2 (dm, J = 257.4 Hz), 138.4, 137.9 (dm, J = 252.1 Hz), 135.0, 131.7 (t, J = 30.7 Hz), 129.4, 128.9, 127.5, 121.2 (t, J = 4.0 Hz), 114.8 (tt, J = 257.8, 39.7 Hz), 113.9 (tt, J = 248.3 34.4 Hz), 106.2-105.3 (m), 51.4;
MS (**EI**, *m/z*, %): 424 (M^+, 24.86), 91 (100);
HRMS (**EI**): Calcd. For $C_{18}H_9F_9N_2$: 424.0622; Found: 424.0626;
IR (film): 3101, 3032, 2944, 1656, 1562, 1528, 1505, 1456, 1331, 1230, 1179, 1120, 1100, 1045, 995, 912, 842, 806, 718 cm^{-1}.

3,5-Dimethyl-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)isoxazole (**2z**)

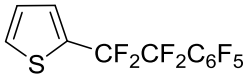


2z

Prepared from general procedure C; the reaction time was 41 hours; **2z** (153 mg, 84% yield) was obtained.
White solid. Mp: 95–97 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 2.51 (s, 3H), 2.33 (s, 3H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.3 (tt, J = 31.6, 10.9 Hz, 2F), –109.1 (t, J = 10.2 Hz, 2F), –138.4 (m, 2F), –147.3 (tt, J = 21.1, 5.6 Hz, 1F), –160.1 (m, 2F);
^{13}C NMR ($CDCl_3$, 100 MHz) δ 171.7 (t, J = 4.3 Hz), 158.5, 145.8 (dm, J = 255.4 Hz), 143.6 (dm, J = 259.0 Hz), 138.2 (dm, J = 254.2 Hz), 115.4 (tt, J = 254.5, 39.7 Hz), 115.2 (tt, J = 248.2, 37.9 Hz), 105.7 (t, J = 29.0 Hz), 105.2-104.5 (m), 12.3, 10.9 (t, J = 2.0 Hz);

MS (**ESI**, *m/z*): 364 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{13}H_7F_9NO$: 364.0378 ($M+H^+$); Found: 364.0382;
IR (film): 2996, 1662, 1633, 1531, 1505, 1425, 1332, 1303, 1257, 1197, 1127, 1091, 1070, 992, 928, 791, 731, 658 cm^{-1}.

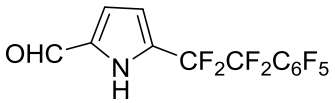
2-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)thiophene (**2aa**)



2aa

Prepared from general procedure C; the reaction time was 41 hours; **2aa** (123 mg, 70% yield) was obtained.
White solid. Mp: 89–91 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.58 (d, J = 5.2 Hz, 1H), 7.46 (d, J = 3.6 Hz, 1H), 7.17–7.12 (m, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –102.4 (t, J = 9.8Hz, 2F), –106.7 (tt, J = 31.6, 14.3 Hz, 2F), –137.9 (m, 2F), –147.9 (tt, J = 21.1, 5.3 Hz, 1F), –160.5 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 145.9 (dm, J = 258.4 Hz), 143.5 (dm, J = 258.6 Hz), 138.1 (dm, J = 253.4 Hz), 130.4 (t, J = 5.4 Hz), 130.0, 129.8 (t, J = 29.2 Hz), 127.5, 115.7 (tt, J = 250.5, 35.8 Hz), 114.7 (tt, J = 256.9, 41.8 Hz), 105.8-105.2 (m) ;
MS (**EI**, *m/z*, %): 350 (M^+, 4.14), 133 (100);
HRMS (**EI**): Calcd. For $C_{12}H_3F_9S$: 349.9812; Found: 349.9819;
IR (film): 1654, 1533, 1503, 1427, 1359, 1332, 1278, 1203, 1153, 1121, 1093, 1031, 1002, 990, 910, 785, 725 cm^{-1}.

5-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)-1*H*-pyrrole-2-carbaldehyde (**2ab**)

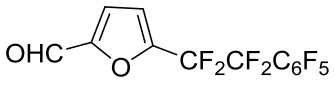


2ab

Prepared from general procedure C; the reaction time was 41 hours; **2ab** (97 mg, 54% yield) was obtained.
White solid. Mp: 154–156 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 10.3 (br, 1H), 9.60 (s, 1H), 7.46 (s, 1H), 7.21 (s, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.1 (m, 4F), –138.1 (m, 2F), –148.0 (tt, J = 21.1, 5.3 Hz, 1F), –160.5 (m, 2F);
^{13}C NMR ($CDCl_3$, 150 MHz) δ 179.9, 145.8 (dm, J = 255.2 Hz), 143.4 (dm, J = 258.5 Hz), 138.1 (dm, J = 252.5 Hz), 133.4, 125.9 (t, J = 6.6 Hz), 119.2 (t, J = 4.4 Hz), 115.7 (t, J = 28.4 Hz), 115.2 (tt, J = 247.6, 36.9 Hz), 114.8 (tt, J = 255.2, 44.1 Hz), 106.0-105.4 (m);
MS (**ESI**, *m/z*): 361.9 ($M+H^+$);
HRMS (**DART**): Calcd. For $C_{13}H_5F_9NO$: 362.0222 ($M+H^+$); Found: 362.0223;
IR (film): 3143, 3065, 3012, 2964, 1663, 1578, 1527, 1503, 1456, 1400, 1358, 1330,

1289, 1179, 1143, 1110, 1089, 992, 899, 844, 758, 765, 725, 692 cm^{-1}.

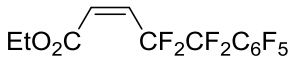
5-(1,1,2,2,8,8,8,8,8-Nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)furan-2-carbaldehyde (**2ac**)



2ac

Prepared from general procedure C; the reaction time was 41 hours; **2ac** (135 mg, 75% yield) was obtained.
White solid. Mp: 53–54 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 9.78 (s, 1H), 7.32 (d, J = 3.6 Hz, 1H), 7.05 (d, J = 3.6 Hz, 1H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.1 (t, J = 31.2 Hz, 2F), –113.3 (m, 2F), –138.1 (m, 2F), –146.8 (tt, J = 21.1, 5.6 Hz, 1F), –159.9 (m, 2F);
^{13}C NMR ($CDCl_3$, 125 MHz) δ 178.2, 154.5, 147.2–142.2 (m), 145.9 (t, J = 33.8 Hz), 138.1 (dm, J = 253.9 Hz), 119.2, 115.6 (t, J = 3.6 Hz), 114.5 (tt, J = 258.5, 38.4 Hz), 113.7 (tt, J = 251.1, 37.0 Hz);
MS (**EI**, *m/z*, %): 362 (M^+, 21.2), 145 (100);
HRMS (**EI**): Calcd. For $C_{13}H_3F_9O_2$: 361.9989; Found: 361.9980;
IR (film): 3137, 2843, 1696, 1655, 1589, 1529, 1506, 1426, 1286, 1233, 1142, 1109, 1090, 1022, 997, 963, 804, 790, 753, 730 cm^{-1}.

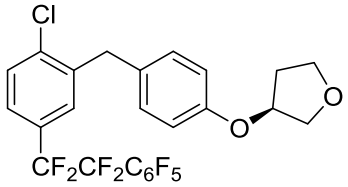
Ethyl (*Z*)-4,4,5,5,11,11,11,11,11-nonafluoro-11λ^8-undeca-2-en-6,8,10-triynoate (**2ad**)



2ad

Prepared from general procedure B; the reaction time was 41 hours; **2ad** (161 mg, 88% yield) was obtained.
Yellow oil. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 6.43 (d, J = 12.4 Hz, 1H), 6.03 (q, J = 12.8 Hz, 1H), 4.21 (q, J = 7.2 Hz, 2H), 1.28 (t, J = 7.2 Hz, 3H);
^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.8 (t, J = 31.2 Hz, 2F), –111.7 (m, 2F), –138.0 (m, 2F), –147.8 (tt, J = 21.4, 5.3 Hz, 1F), –160.6 (m, 2F);
^{13}C NMR ($CDCl_3$, 100 MHz) δ 164.3, 131.8 (t, J = 5.9 Hz), 123.2 (t, J = 24.5 Hz), 61.8, 13.9;
MS (**EI**, *m/z*, %): 366 (M^+, 11.51), 217 (100);
HRMS (**EI**): Calcd. For $C_{13}H_7F_9O_2$: 366.0302; Found: 366.0294;
IR (film): 2996, 2952, 1742, 1658, 1529, 1507, 1426, 1389, 1333, 1230, 1166, 1110, 997, 807 cm^{-1}.

(*S*)-3-(4-((2-Chloro-5-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)phenyl) methyl)phenoxy)tetrahydrofuran (**2ae**)



2ae

Prepared from general procedure A; the reaction time was 33 hours; **2ae** (265 mg, 96% yield) was obtained.

White solid. Mp: 81−83 °C. $[\alpha]_D$ = 5.23 ($CHCl_3$, c= 1.1050 w/v%). **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.51 (d, J = 8.4 Hz, 1H), 7.46–7.39 (m, 1H), 7.35 (s, 1H), 7.07 (d, J = 8.8 Hz, 2H), 6.80 (d, J = 8.8 Hz, 2H), 4.93–4.87 (m, 1H), 4.09 (s, 2H), 4.03–3.94 (m, 3H), 3.93–3.86 (m, 1H), 2.25–2.08 (m, 2H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –107.1 (t, J = 31.2 Hz, 2F), –112.5 (t, J = 9.8 Hz, 2F), –138.1 (m, 2F), –147.8 (tt, J = 21.1, 5.3 Hz, 1F), –160.4 (m, 2F);

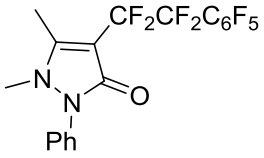
^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.2, 147.2-141.8 (m), 139.8, 138.2, 137.9 (dm, J = 253.7 Hz), 130.9, 130.0, 129.9, 129.4 (t, J = 6.3 Hz), 127.8 (t, J = 24.5 Hz), 126.4 (t, J = 6.3 Hz), 116.1 (tt, J = 251.9, 34.9 Hz), 115.5, 114.8 (tt, J = 256.9, 41.0 Hz), 77.4, 73.2, 67.3, 38.5, 33.1;

MS (**ESI**, *m/z*): 572 ($M+NH_4^+$);

HRMS (**DART**): Calcd. For $C_{25}H_{20}O_2ClF_9N$: 572.1033 ($M+NH_4^+$); Found: 572.1033;

IR (film): 2988, 2944, 2859, 1655, 1610, 1333, 1302, 1242, 1179, 1123, 1080, 1046, 996, 913, 801 cm^{-1}.

1,5-Dimethyl-4-(1,1,2,2,8,8,8,8,8-nonafluoro-8λ^8-octa-3,5,7-triyn-1-yl)-2-phenyl-1,2-dihydro-3*H*-pyrazol-3-one (**2af**)



2af

Prepared from general procedure C; the reaction time was 41 hours; **2af** (201 mg, 88% yield) was obtained.

White solid. Mp: 208–210 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ 7.46 (t, J = 7.2 Hz, 2H), 7.36 (t, J = 8.0 Hz, 1H), 7.25 (d, J = 8.8 Hz, 2H), 3.24 (s, 3H), 2.42 (s, 3H);

^{19}F NMR ($CDCl_3$, 376 MHz) δ –109.5 (tt, J = 31.2, 8.3 Hz, 2F), –111.2 (m, 2F), –139.1 (m, 2F), –148.0 (tt, J = 21.4, 5.3 Hz, 1F), –161.1 (m, 2F);

^{13}C NMR ($CDCl_3$, 125 MHz) δ 161.9 (t, J = 3.6 Hz), 154.6 (t, J = 2.9 Hz), 145.9 (dm, J = 257.1 Hz), 143.3 (dm, J = 257.9 Hz), 138.0 (dm, J = 252.1 Hz), 134.1, 129.6, 128.3, 125.9, 115.4 (tt, J = 252.8, 34.0 Hz), 115.37 (tt, J = 230.2, 14.5 Hz), 106.4-105.6 (m), 96.3 (t, J = 27.1 Hz), 34.6, 12.0;

MS (**ESI**, *m/z*): 455 ($M+H^+$);

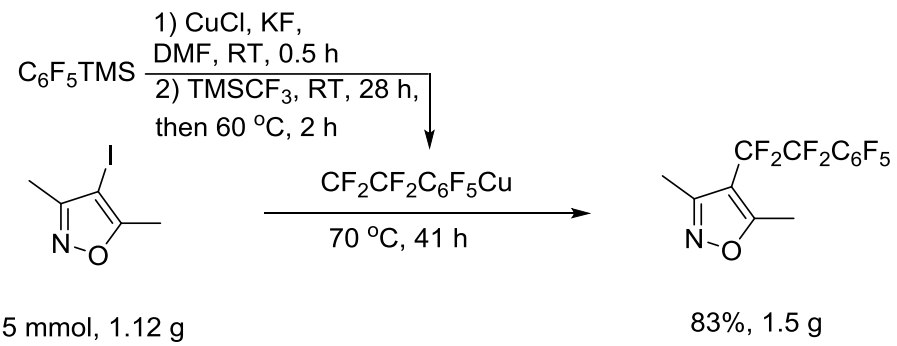
HRMS (**DART**): Calcd. For $C_{19}H_{12}F_9N_2O$: 455.0800 ($M+H^+$); Found: 455.0800;

IR (film): 3044, 1671, 1565, 1532, 1499, 1457, 1419, 1333, 1306, 1127, 1088, 989,

949, 811, 776, 763, 748, 719, 598 cm^{-1}.

^{13}C NMR ($CDCl_3$, 100 MHz) δ133.5 (t, J = 25.5 Hz), 132.4, 128.0 (t, J = 6.5 Hz), 117.6, 116.1;

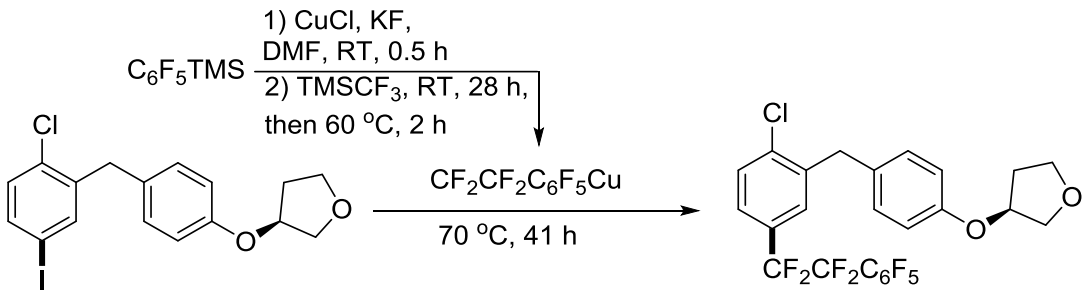
3. Procedures for Gram-Scale Synthesis



5 mmol, 1.12 g

83%, 1.5 g

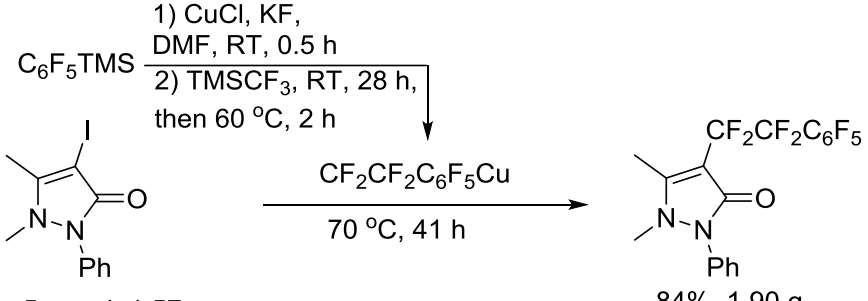
To an oven-dried sealed tube were added CuCl (36 mmol, 3.56 g, 7.2 equiv) and KF (27 mmol, 1.57 g, 5.4 equiv) in glove box. Then in fume hood, DMF (80 mL) and C_6F_5TMS (9 mmol, 1.70 mL, 1.8 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (17.1 mmol, 2.42 mL, 3.42 equiv) was added in two equal portions and the second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 °C and stirred at that temperature for 2 hours. After that, aryl iodide **1z** (5 mmol, 1.12 g, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 °C for 41 hours. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 200 mL ammonium hydroxide, extracted with CH_2Cl_2 (100 mL × 3). The combined organic layer was washed with H_2O (50 mL × 2) and brine (80 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to afford **2z** (83%, 1.5 g).



5 mmol, 2.07 g

98%, 2.71 g

To an oven-dried sealed tube were added CuCl (30 mmol, 2.97 g, 6.0 equiv) and KF (22.5 mmol, 1.305 g, 4.5 equiv) in glove box. Then in fume hood, DMF (80 mL) and C_6F_5TMS (7.5 mmol, 1.42 mL, 1.5 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (14.25 mmol, 2.02 mL, 2.85 equiv) was added in two equal portions and the second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 °C and stirred at that temperature for 2 hours. After that, aryl iodide **1ae** (5 mmol, 2.07 g, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 °C for 41 hours. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 200 mL ammonium hydroxide, extracted with CH_2Cl_2 (100 mL × 3). The combined organic layer was washed with H_2O (50 mL × 2) and brine (80 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to afford **2ae** (98%, 2.71 g).



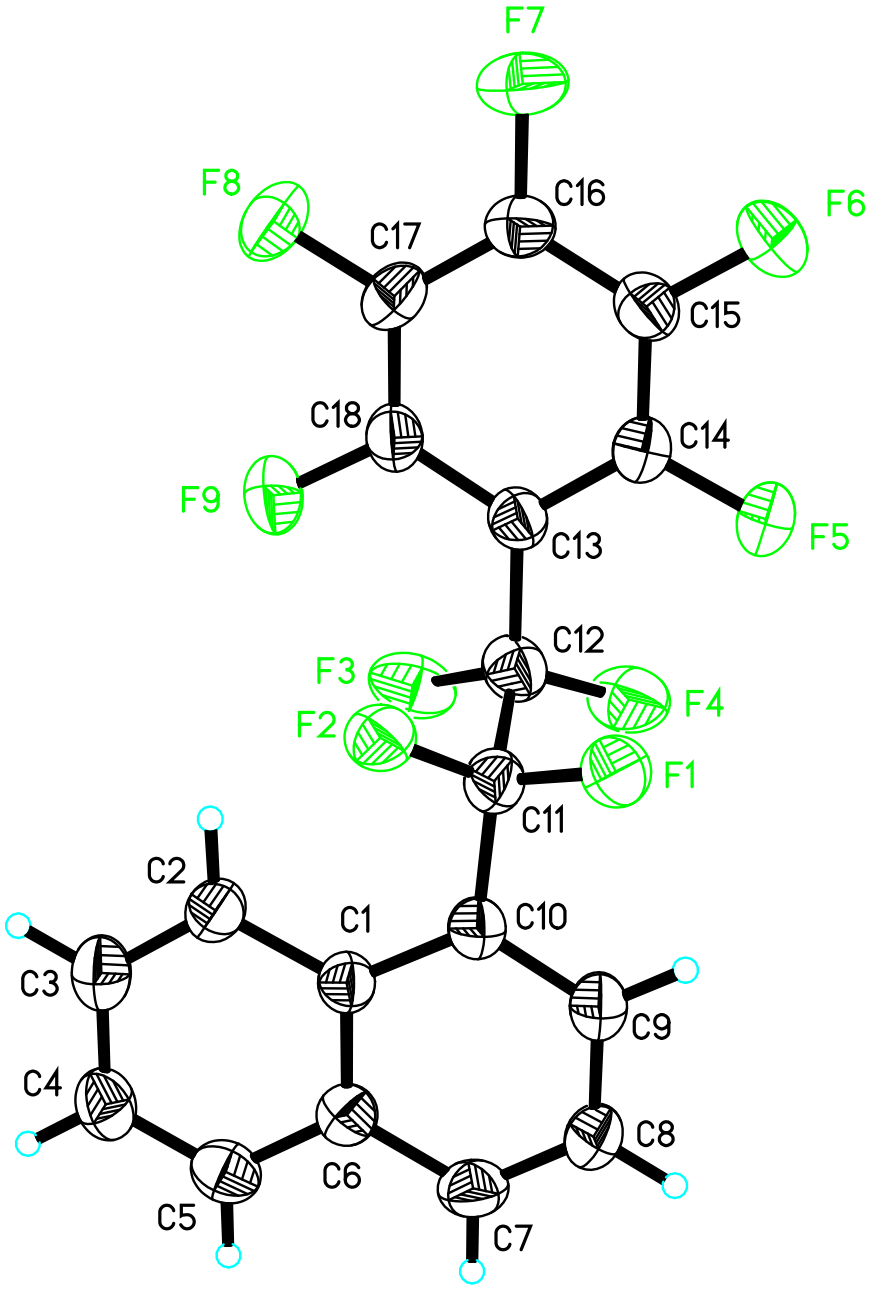
5 mmol, 1.57 g

84%, 1.90 g

To an oven-dried sealed tube were added CuCl (36 mmol, 3.56 g, 7.2 equiv) and KF (27 mmol, 1.57 g, 5.4 equiv) in glove box. Then in fume hood, DMF (80 mL) and

C_6F_5TMS (9 mmol, 1.70 mL, 1.8 equiv) were successively added under N_2 atmosphere. The mixture was stirred at room temperature for 30 minutes, then $TMSCF_3$ (17.1 mmol, 2.42 mL, 3.42 equiv) was added in two equal portions and the second portion was added 6 hours later. The mixture was stirred at room temperature for another 22 hours and then heated to 60 ^oC and stirred at that temperature for 2 hours. After that, aryl iodide **1af** (5 mmol, 1.57 g, 1.0 equiv) was added under N_2 atmosphere. The reaction mixture was stirred at 70 ^oC for 41 hours. After the reaction was completed, the reaction mixture was cooled to room temperature and quenched with 200 mL ammonium hydroxide, extracted with CH_2Cl_2 (100 mL × 3). The combined organic layer was washed with H_2O (50 mL × 2) and brine (80 mL), dried over Na_2SO_4, then concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to afford **2af** (84%, 1.9 g).

4. X-ray Crystal Structure of 2n



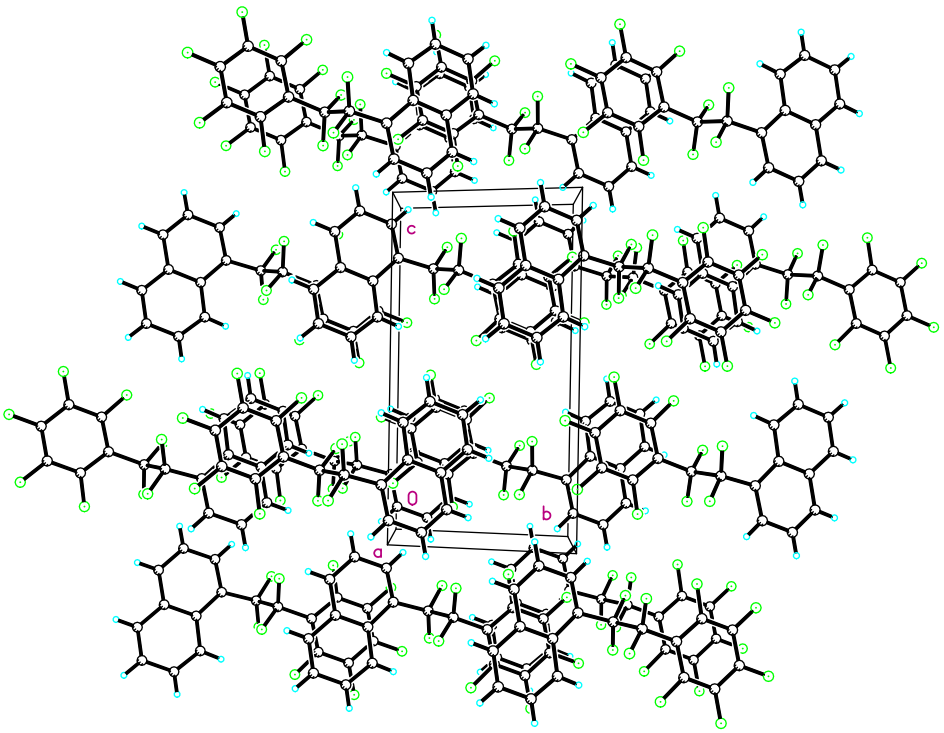

c
0
b
a

Table 1. Crystal data and structure refinement for mo_d8v18839_0m.

Identification code	mo_d8v18839_0m	
Empirical formula	C18 H7 F9	
Formula weight	394.24	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.427(2) Å	α= 89.382(10) °.
	b = 7.782(3) Å	β= 89.146(10) °.
	c = 13.740(5) Å	γ = 68.679(10) °.
Volume	739.7(4) $Å^3$	
Z	2	
Density (calculated)	1.770 Mg/m^3	
Absorption coefficient	0.182 mm^{-1}	
F(000)	392	
Crystal size	0.190 x 0.160 x 0.120 mm^3	
Theta range for data collection	2.810 to 24.998 °.	
Index ranges	-8<=h<=8, -9<=k<=9, -16<=l<=16	
Reflections collected	8138	
Independent reflections	2575 [R(int) = 0.0651]	
Completeness to theta = 25.242 °	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5257	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2575 / 0 / 246	
Goodness-of-fit on F^2	1.231	
Final R indices [I>2sigma(I)]	R1 = 0.0956, wR2 = 0.2657	
R indices (all data)	R1 = 0.1222, wR2 = 0.3183	
Extinction coefficient	0.24(5)	
Largest diff. peak and hole	0.306 and -0.318 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_d8v18839_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	4753(5)	2892(5)	8604(3)	80(1)
F(2)	5315(5)	2234(4)	7070(3)	72(1)
F(3)	8817(5)	2839(5)	7271(4)	92(1)
F(4)	7889(6)	3718(5)	8742(3)	96(1)
F(5)	4799(7)	6582(5)	9041(3)	90(1)
F(6)	2671(6)	9877(5)	8331(3)	95(1)
F(7)	2613(6)	10581(5)	6406(3)	94(1)
F(8)	4777(8)	7931(7)	5171(3)	105(2)
F(9)	6902(7)	4612(6)	5837(3)	94(1)
C(1)	8618(8)	-1096(8)	7531(4)	58(1)
C(2)	8645(9)	-813(8)	6493(4)	67(1)
C(3)	9708(10)	-2206(9)	5904(5)	78(2)
C(4)	10825(10)	-3944(9)	6271(5)	76(2)
C(5)	10876(9)	-4241(8)	7252(5)	73(2)
C(6)	9784(8)	-2842(8)	7894(4)	62(1)
C(7)	9881(10)	-3189(8)	8925(5)	75(2)
C(8)	8822(11)	-1882(9)	9550(4)	79(2)
C(9)	7603(10)	-159(9)	9202(4)	74(2)
C(10)	7478(8)	251(7)	8215(4)	61(1)
C(11)	6218(8)	2171(8)	7931(4)	65(1)
C(12)	7214(9)	3587(8)	7857(5)	70(2)
C(13)	6004(8)	5461(7)	7477(4)	61(1)
C(14)	4858(9)	6855(8)	8080(4)	65(1)
C(15)	3730(9)	8561(8)	7732(5)	70(2)
C(16)	3702(9)	8944(8)	6743(5)	66(1)
C(17)	4787(9)	7577(9)	6121(4)	70(2)
C(18)	5906(9)	5880(8)	6477(4)	66(2)

Table 3. Bond lengths [Å] and angles [°] for mo_d8v18839_0m.

F(1)-C(11)	1.375(7)
F(2)-C(11)	1.361(7)
F(3)-C(12)	1.372(8)
F(4)-C(12)	1.340(8)
F(5)-C(14)	1.339(7)
F(6)-C(15)	1.326(7)
F(7)-C(16)	1.319(7)
F(8)-C(17)	1.331(7)
F(9)-C(18)	1.328(7)
C(1)-C(6)	1.410(8)
C(1)-C(10)	1.432(8)
C(1)-C(2)	1.442(8)
C(2)-C(3)	1.353(9)
C(2)-H(2)	0.9300
C(3)-C(4)	1.398(10)
C(3)-H(3)	0.9300
C(4)-C(5)	1.363(10)
C(4)-H(4)	0.9300
C(5)-C(6)	1.407(9)
C(5)-H(5)	0.9300
C(6)-C(7)	1.437(9)
C(7)-C(8)	1.344(10)
C(7)-H(7)	0.9300
C(8)-C(9)	1.401(10)
C(8)-H(8)	0.9300
C(9)-C(10)	1.386(9)
C(9)-H(9)	0.9300
C(10)-C(11)	1.497(8)
C(11)-C(12)	1.537(9)
C(12)-C(13)	1.500(9)
C(13)-C(14)	1.383(8)
C(13)-C(18)	1.405(9)
C(14)-C(15)	1.372(9)
C(15)-C(16)	1.388(9)
C(16)-C(17)	1.373(9)
C(17)-C(18)	1.369(9)

C(6)-C(1)-C(10)	117.8(5)
C(6)-C(1)-C(2)	117.3(5)
C(10)-C(1)-C(2)	124.9(5)
C(3)-C(2)-C(1)	120.3(6)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	121.9(6)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	119.3(5)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.0(6)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	120.2(6)
C(5)-C(6)-C(7)	119.8(5)
C(1)-C(6)-C(7)	120.0(5)
C(8)-C(7)-C(6)	120.7(5)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	120.2(6)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9
C(10)-C(9)-C(8)	121.3(6)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(9)-C(10)-C(1)	120.0(5)
C(9)-C(10)-C(11)	116.6(5)
C(1)-C(10)-C(11)	123.3(5)
F(2)-C(11)-F(1)	105.2(4)
F(2)-C(11)-C(10)	112.6(4)
F(1)-C(11)-C(10)	110.5(5)
F(2)-C(11)-C(12)	106.7(5)
F(1)-C(11)-C(12)	104.9(5)
C(10)-C(11)-C(12)	116.1(5)
F(4)-C(12)-F(3)	105.7(5)

F(4)-C(12)-C(13)	110.5(5)
F(3)-C(12)-C(13)	109.5(6)
F(4)-C(12)-C(11)	107.3(6)
F(3)-C(12)-C(11)	107.2(5)
C(13)-C(12)-C(11)	116.1(5)
C(14)-C(13)-C(18)	115.9(5)
C(14)-C(13)-C(12)	122.4(5)
C(18)-C(13)-C(12)	121.7(5)
F(5)-C(14)-C(15)	116.8(5)
F(5)-C(14)-C(13)	120.7(5)
C(15)-C(14)-C(13)	122.5(6)
F(6)-C(15)-C(14)	121.0(6)
F(6)-C(15)-C(16)	118.8(5)
C(14)-C(15)-C(16)	120.2(5)
F(7)-C(16)-C(17)	120.8(6)
F(7)-C(16)-C(15)	120.3(6)
C(17)-C(16)-C(15)	118.8(5)
F(8)-C(17)-C(18)	120.2(6)
F(8)-C(17)-C(16)	119.4(6)
C(18)-C(17)-C(16)	120.4(6)
F(9)-C(18)-C(17)	117.4(5)
F(9)-C(18)-C(13)	120.4(5)
C(17)-C(18)-C(13)	122.2(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_d8v18839_0m. The anisotropic

displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	77(2)	73(2)	78(2)	-1(2)	13(2)	-13(2)
F(2)	74(2)	65(2)	72(2)	4(2)	-19(2)	-18(2)
F(3)	63(2)	67(2)	140(4)	3(2)	6(2)	-18(2)
F(4)	107(3)	76(2)	103(3)	10(2)	-49(2)	-29(2)
F(5)	120(3)	88(2)	51(2)	-2(2)	9(2)	-26(2)
F(6)	101(3)	73(2)	92(3)	-19(2)	13(2)	-8(2)
F(7)	96(3)	70(2)	111(3)	24(2)	-26(2)	-23(2)
F(8)	151(4)	111(3)	57(2)	15(2)	-9(2)	-54(3)
F(9)	119(3)	91(3)	66(2)	-20(2)	22(2)	-32(2)
C(1)	61(3)	60(3)	54(3)	-3(2)	-2(2)	-21(2)
C(2)	71(3)	68(3)	56(3)	3(2)	0(3)	-19(3)
C(3)	82(4)	91(4)	63(4)	-13(3)	8(3)	-35(4)
C(4)	74(4)	79(4)	73(4)	-18(3)	16(3)	-24(3)
C(5)	65(3)	64(3)	88(5)	-1(3)	-5(3)	-21(3)
C(6)	60(3)	65(3)	62(3)	0(3)	-3(3)	-25(3)
C(7)	86(4)	60(3)	77(4)	13(3)	-16(3)	-23(3)
C(8)	106(5)	73(4)	50(3)	3(3)	-6(3)	-23(3)
C(9)	90(4)	72(4)	54(3)	-7(3)	2(3)	-22(3)
C(10)	68(3)	60(3)	54(3)	-3(2)	-3(2)	-21(2)
C(11)	67(3)	65(3)	56(3)	-1(2)	-4(3)	-16(3)
C(12)	62(3)	67(3)	73(4)	-6(3)	-7(3)	-15(3)
C(13)	64(3)	59(3)	60(3)	-6(2)	-1(2)	-22(3)
C(14)	74(4)	68(3)	53(3)	-3(2)	-1(3)	-24(3)
C(15)	67(4)	64(3)	71(4)	-10(3)	-1(3)	-16(3)
C(16)	68(3)	60(3)	73(4)	5(3)	-8(3)	-25(3)
C(17)	77(4)	82(4)	54(3)	11(3)	-12(3)	-32(3)
C(18)	77(4)	69(3)	55(3)	-10(3)	9(3)	-32(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_d8v18839_0m.

	x	y	z	U(eq)
H(2)	7929	332	6227	80
H(3)	9696	-2001	5236	93
H(4)	11525	-4888	5852	91
H(5)	11644	-5386	7500	87
H(7)	10685	-4330	9163	90
H(8)	8898	-2122	10216	95
H(9)	6864	727	9641	89

Table 6. Torsion angles [°] for mo_d8v18839_0m.

C(6)-C(1)-C(2)-C(3)	2.1(9)
C(10)-C(1)-C(2)-C(3)	-177.0(6)
C(1)-C(2)-C(3)-C(4)	-0.7(10)
C(2)-C(3)-C(4)-C(5)	-1.2(10)
C(3)-C(4)-C(5)-C(6)	1.7(10)
C(4)-C(5)-C(6)-C(1)	-0.3(9)
C(4)-C(5)-C(6)-C(7)	-179.4(6)
C(10)-C(1)-C(6)-C(5)	177.5(5)
C(2)-C(1)-C(6)-C(5)	-1.6(8)
C(10)-C(1)-C(6)-C(7)	-3.4(8)
C(2)-C(1)-C(6)-C(7)	177.5(6)
C(5)-C(6)-C(7)-C(8)	-178.8(6)
C(1)-C(6)-C(7)-C(8)	2.1(9)
C(6)-C(7)-C(8)-C(9)	0.1(11)
C(7)-C(8)-C(9)-C(10)	-0.9(11)
C(8)-C(9)-C(10)-C(1)	-0.4(10)
C(8)-C(9)-C(10)-C(11)	-176.5(6)
C(6)-C(1)-C(10)-C(9)	2.6(8)
C(2)-C(1)-C(10)-C(9)	-178.4(6)
C(6)-C(1)-C(10)-C(11)	178.4(5)
C(2)-C(1)-C(10)-C(11)	-2.6(9)
C(9)-C(10)-C(11)-F(2)	-145.9(5)
C(1)-C(10)-C(11)-F(2)	38.1(7)
C(9)-C(10)-C(11)-F(1)	-28.6(7)
C(1)-C(10)-C(11)-F(1)	155.4(5)
C(9)-C(10)-C(11)-C(12)	90.6(7)
C(1)-C(10)-C(11)-C(12)	-85.3(7)
F(2)-C(11)-C(12)-F(4)	171.9(4)
F(1)-C(11)-C(12)-F(4)	60.6(5)
C(10)-C(11)-C(12)-F(4)	-61.7(6)
F(2)-C(11)-C(12)-F(3)	-75.0(6)
F(1)-C(11)-C(12)-F(3)	173.7(5)
C(10)-C(11)-C(12)-F(3)	51.4(7)
F(2)-C(11)-C(12)-C(13)	47.7(7)
F(1)-C(11)-C(12)-C(13)	-63.6(6)
C(10)-C(11)-C(12)-C(13)	174.1(5)

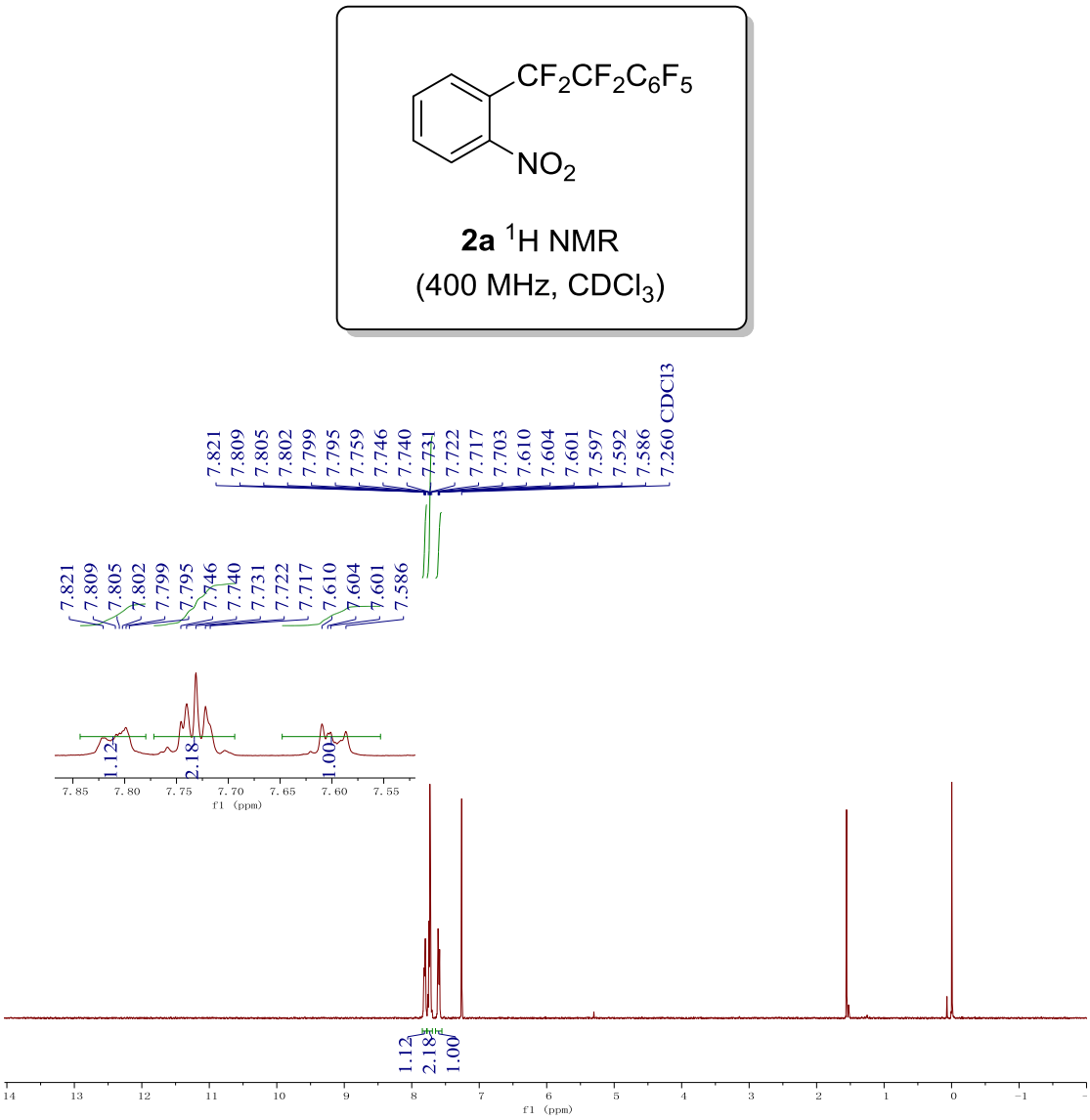
F(4)-C(12)-C(13)-C(14)	-34.3(8)
F(3)-C(12)-C(13)-C(14)	-150.3(6)
C(11)-C(12)-C(13)-C(14)	88.2(7)
F(4)-C(12)-C(13)-C(18)	148.3(6)
F(3)-C(12)-C(13)-C(18)	32.4(8)
C(11)-C(12)-C(13)-C(18)	-89.1(7)
C(18)-C(13)-C(14)-F(5)	178.0(5)
C(12)-C(13)-C(14)-F(5)	0.5(9)
C(18)-C(13)-C(14)-C(15)	-1.6(9)
C(12)-C(13)-C(14)-C(15)	-179.1(5)
F(5)-C(14)-C(15)-F(6)	1.4(9)
C(13)-C(14)-C(15)-F(6)	-178.9(6)
F(5)-C(14)-C(15)-C(16)	-179.5(6)
C(13)-C(14)-C(15)-C(16)	0.1(10)
F(6)-C(15)-C(16)-F(7)	-1.2(9)
C(14)-C(15)-C(16)-F(7)	179.7(5)
F(6)-C(15)-C(16)-C(17)	-179.5(5)
C(14)-C(15)-C(16)-C(17)	1.4(9)
F(7)-C(16)-C(17)-F(8)	1.9(9)
C(15)-C(16)-C(17)-F(8)	-179.8(6)
F(7)-C(16)-C(17)-C(18)	-179.7(6)
C(15)-C(16)-C(17)-C(18)	-1.4(9)
F(8)-C(17)-C(18)-F(9)	-2.4(9)
C(16)-C(17)-C(18)-F(9)	179.2(5)
F(8)-C(17)-C(18)-C(13)	178.2(5)
C(16)-C(17)-C(18)-C(13)	-0.2(9)
C(14)-C(13)-C(18)-F(9)	-177.7(5)
C(12)-C(13)-C(18)-F(9)	-0.2(9)
C(14)-C(13)-C(18)-C(17)	1.6(9)
C(12)-C(13)-C(18)-C(17)	179.1(6)

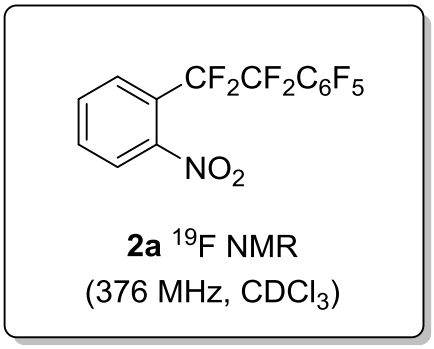
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_d8v18839_0m [Å and °].

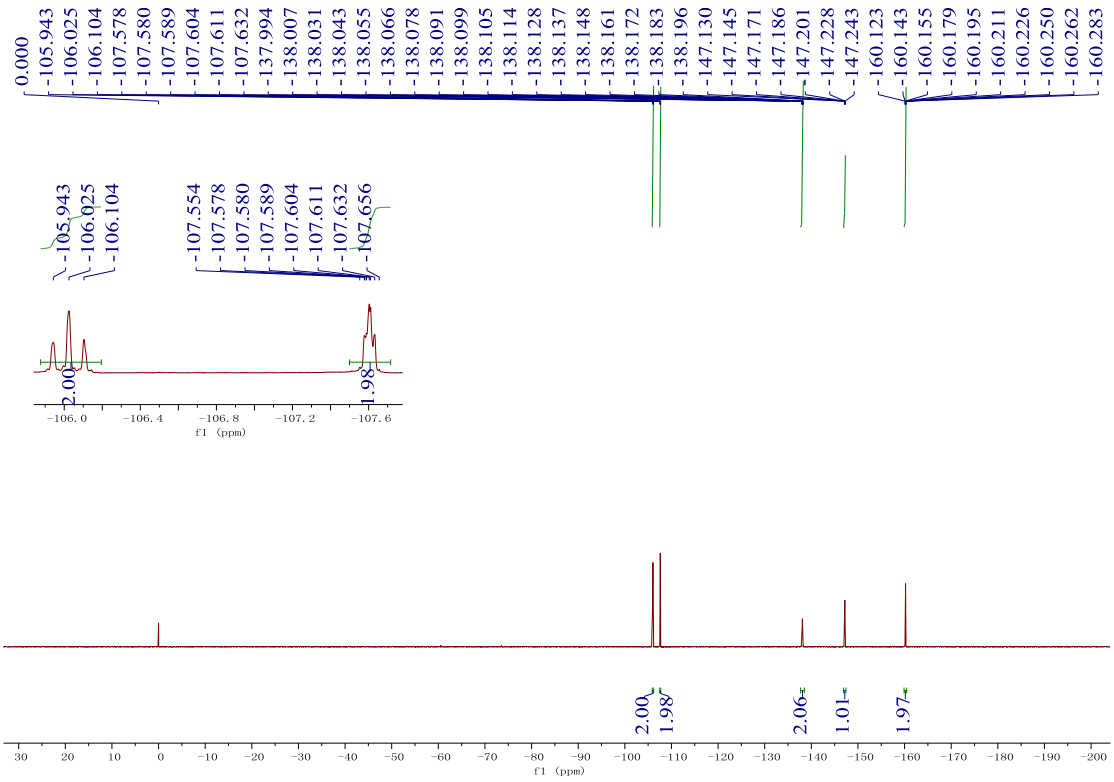
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

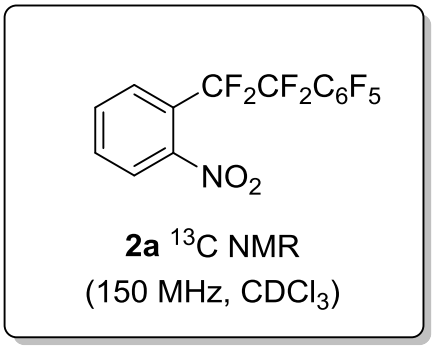
5. ^{1}H, ^{19}F, ^{13}C Spectroscopy of the New Compounds



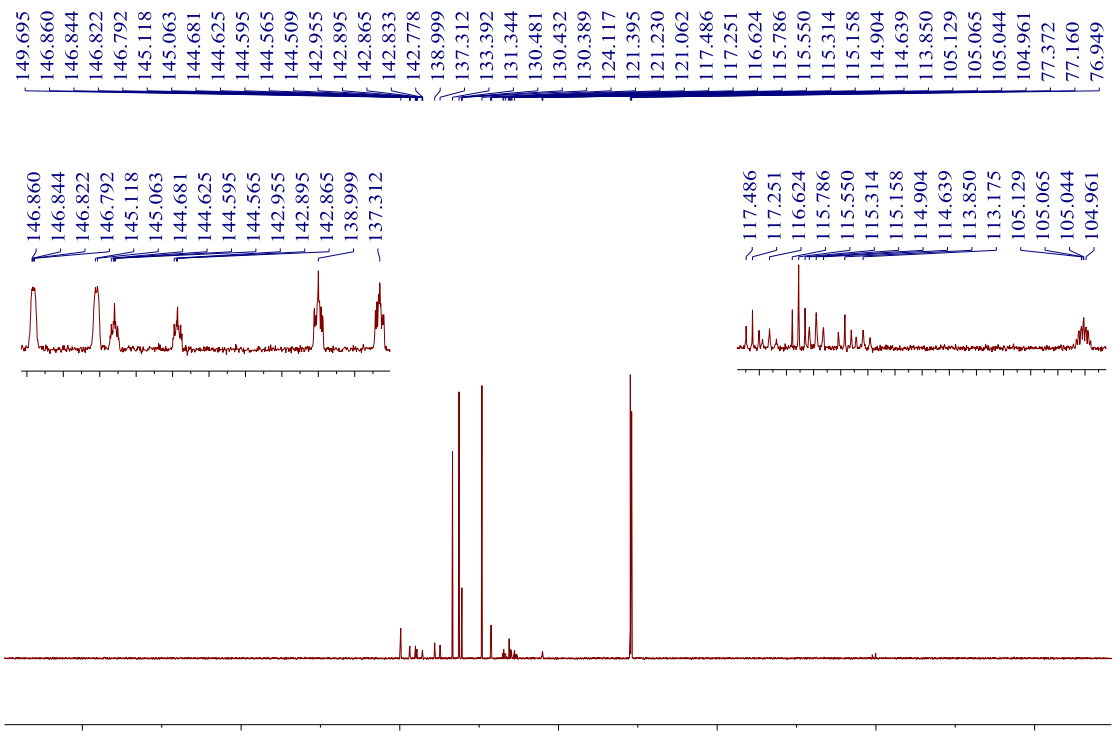


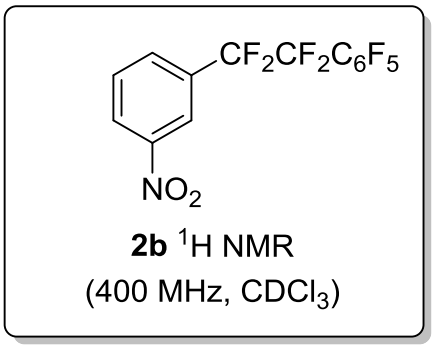
2a ^{19}F NMR
(376 MHz, $CDCl_3$)

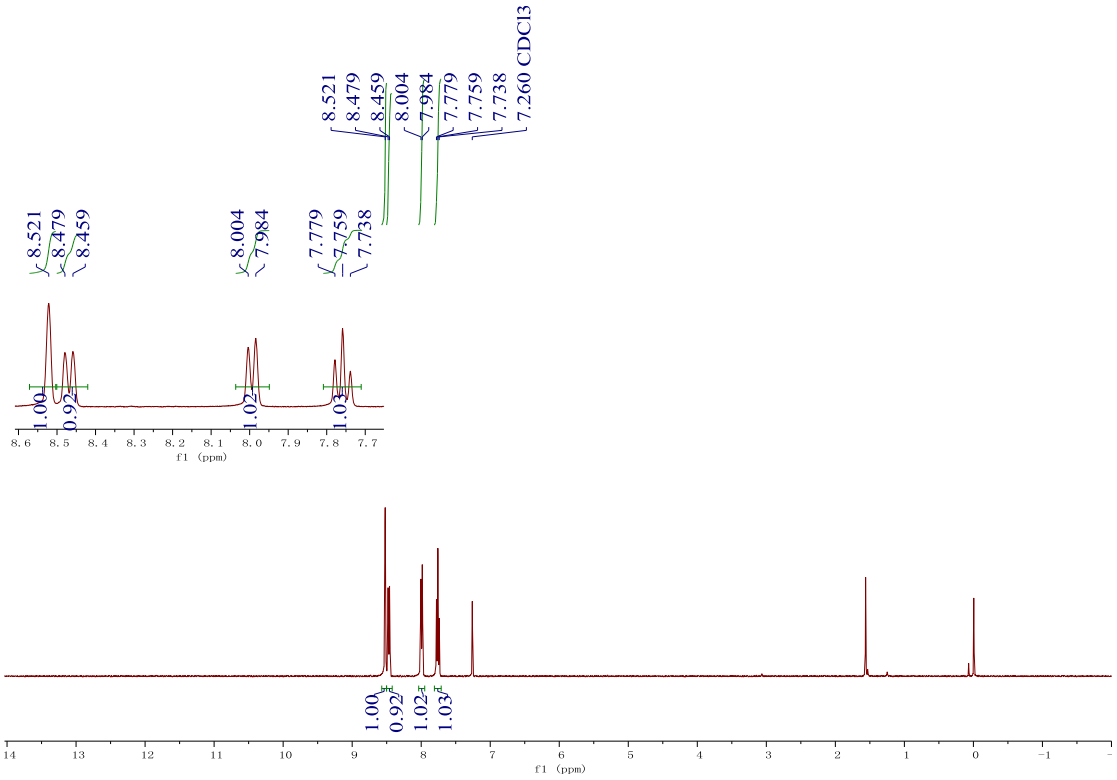


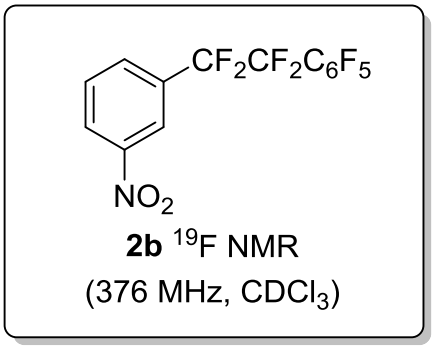


2a ^{13}C NMR
(150 MHz, $CDCl_3$)



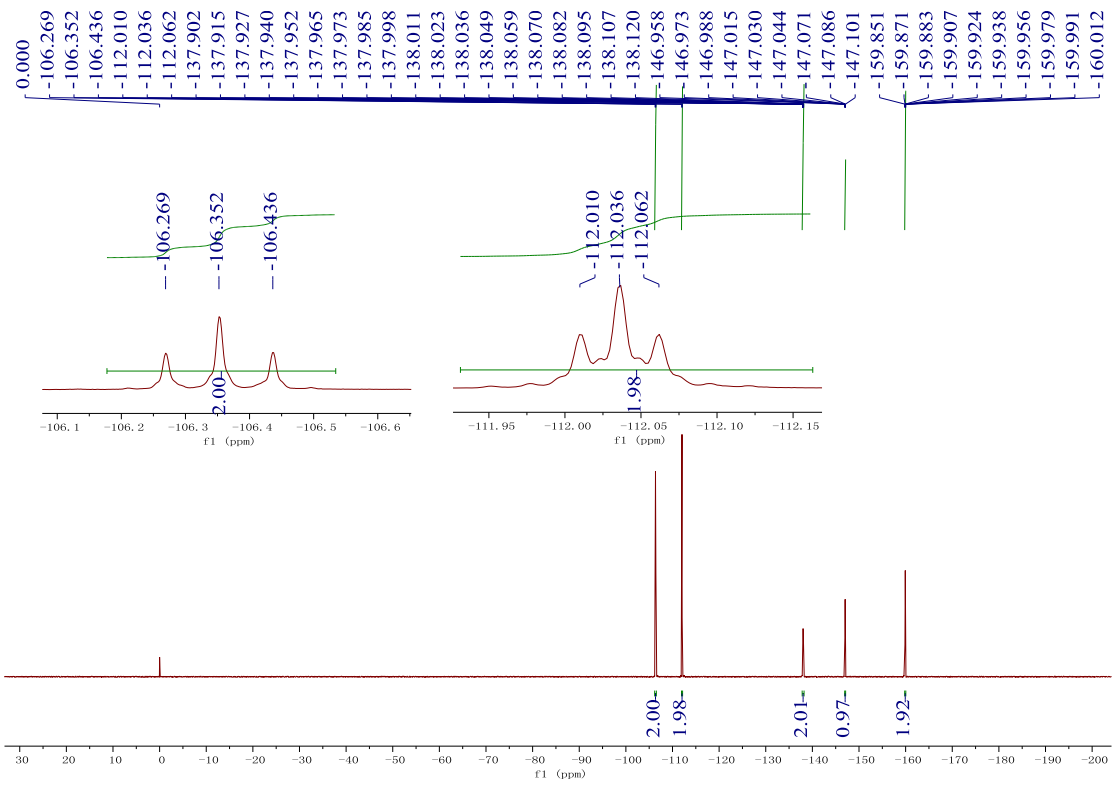

CF2CF2C6F5
NO2
2b 1H NMR
(400 MHz, CDCl3)

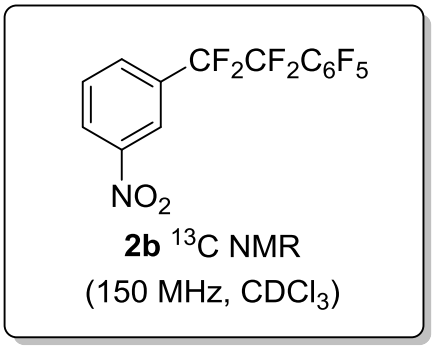

8.521
8.479
8.459
8.004
7.984
7.779
7.759
7.738
7.260 CDCl3
1.00
0.92
1.02
1.03
f1 (ppm)



2b ^{19}F NMR

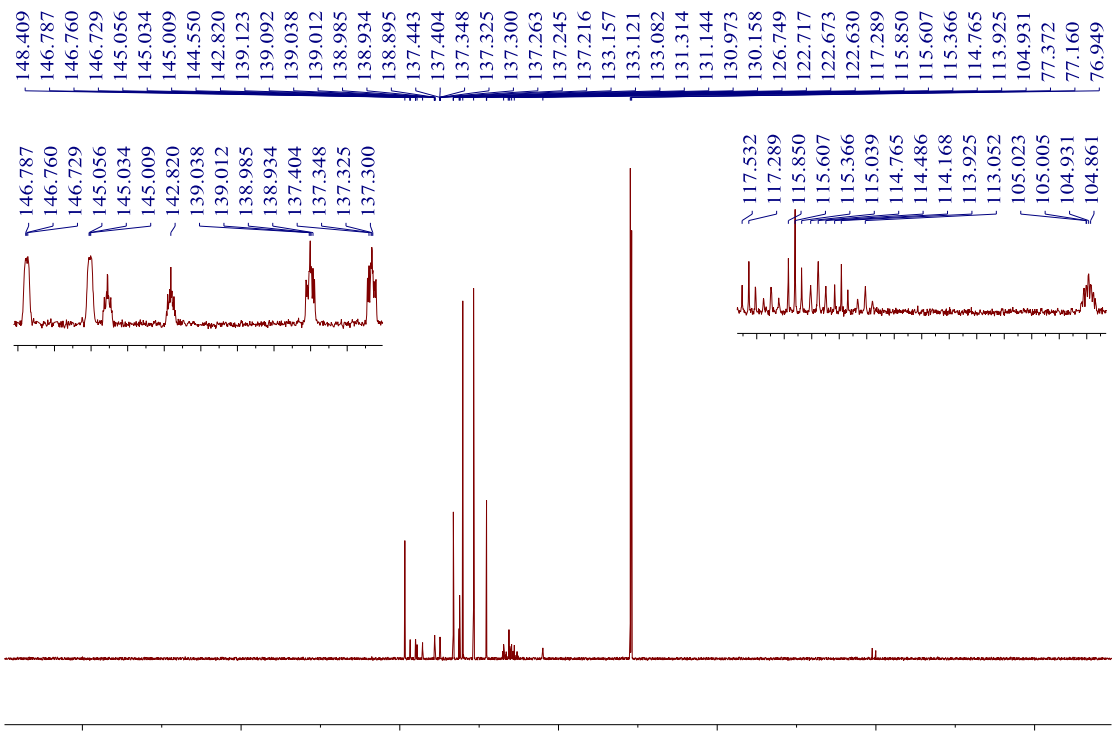
(376 MHz, $CDCl_3$)

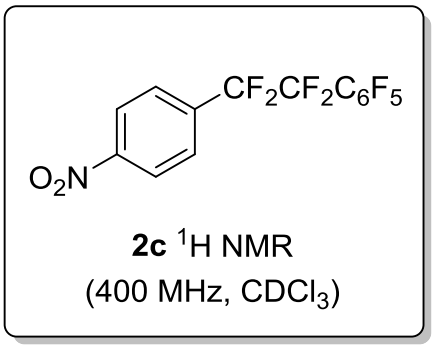


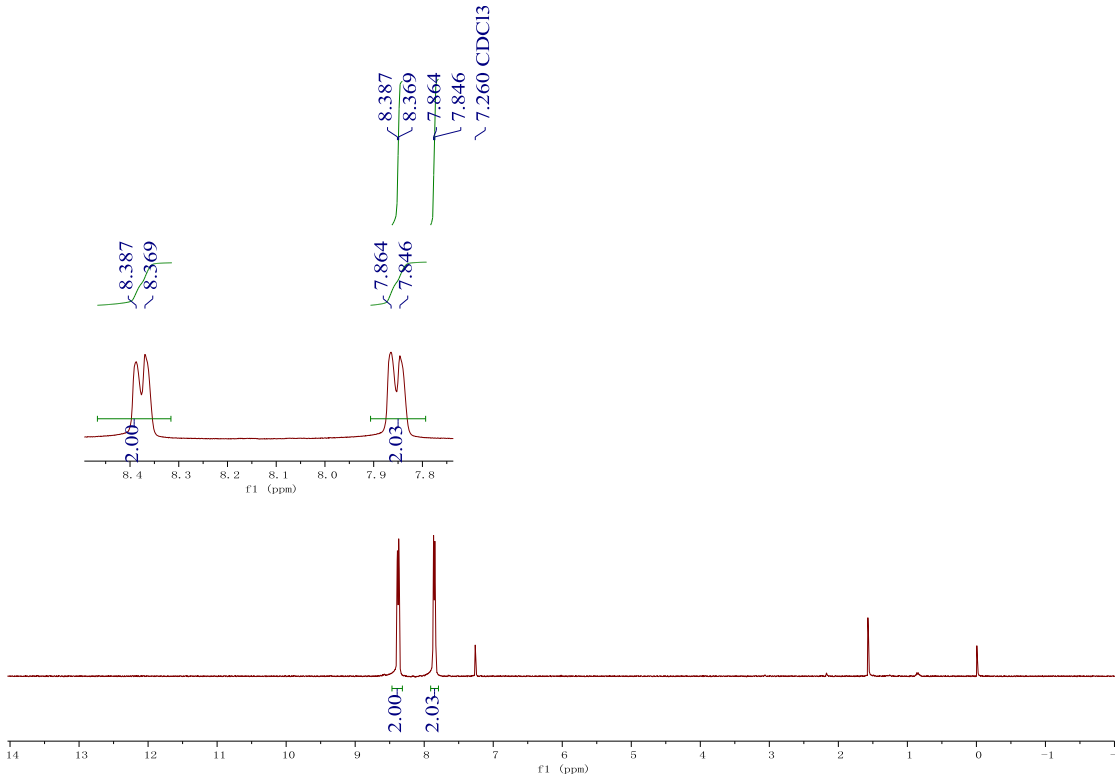


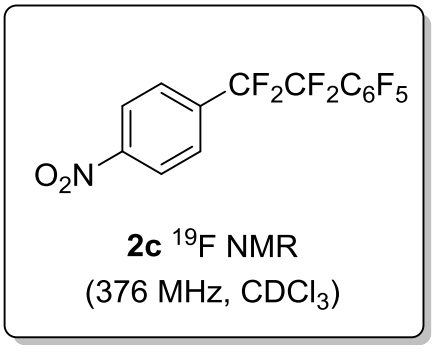
2b ^{13}C NMR

(150 MHz, $CDCl_3$)

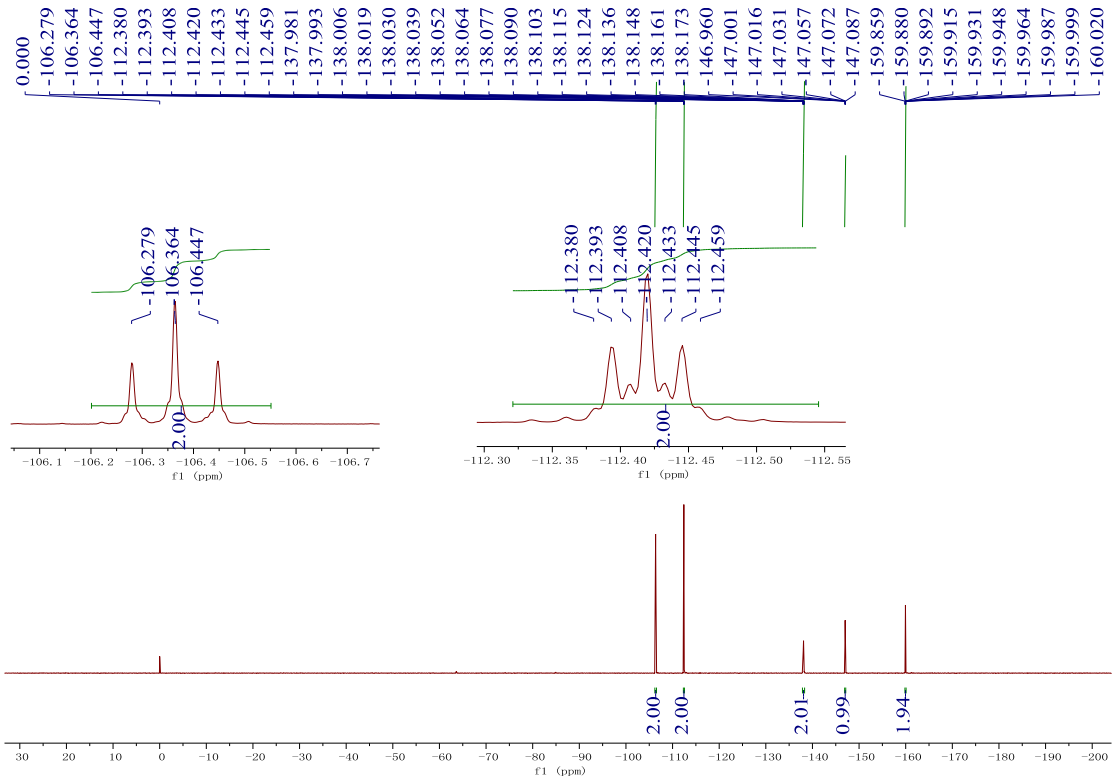


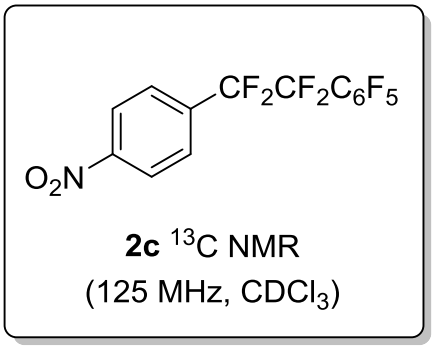

$CF_2CF_2C_6F_5$
O_2N
2c ^{1}H NMR
(400 MHz, $CDCl_3$)


8.387
8.369
7.864
7.846
7.260 CDCl3
2.00
2.03
f1 (ppm)
2.00
2.03
f1 (ppm)

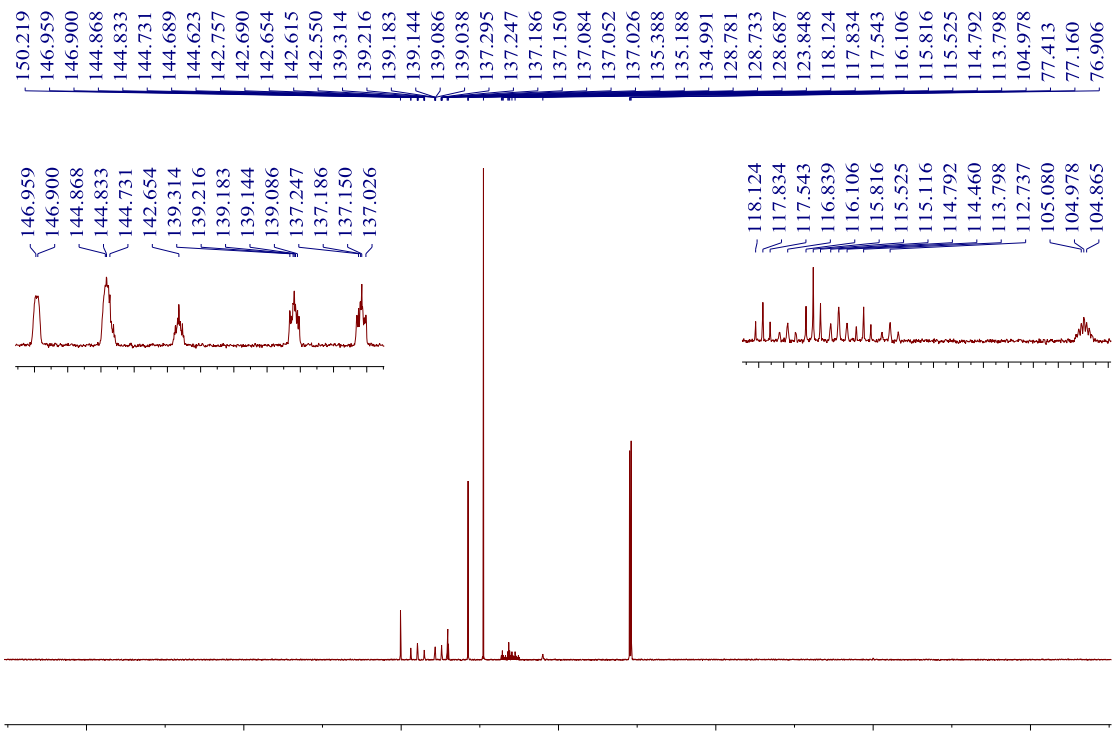


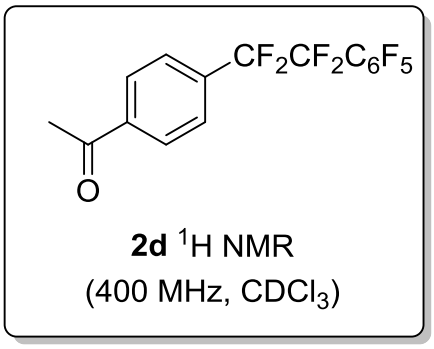
2c ^{19}F NMR
(376 MHz, $CDCl_3$)



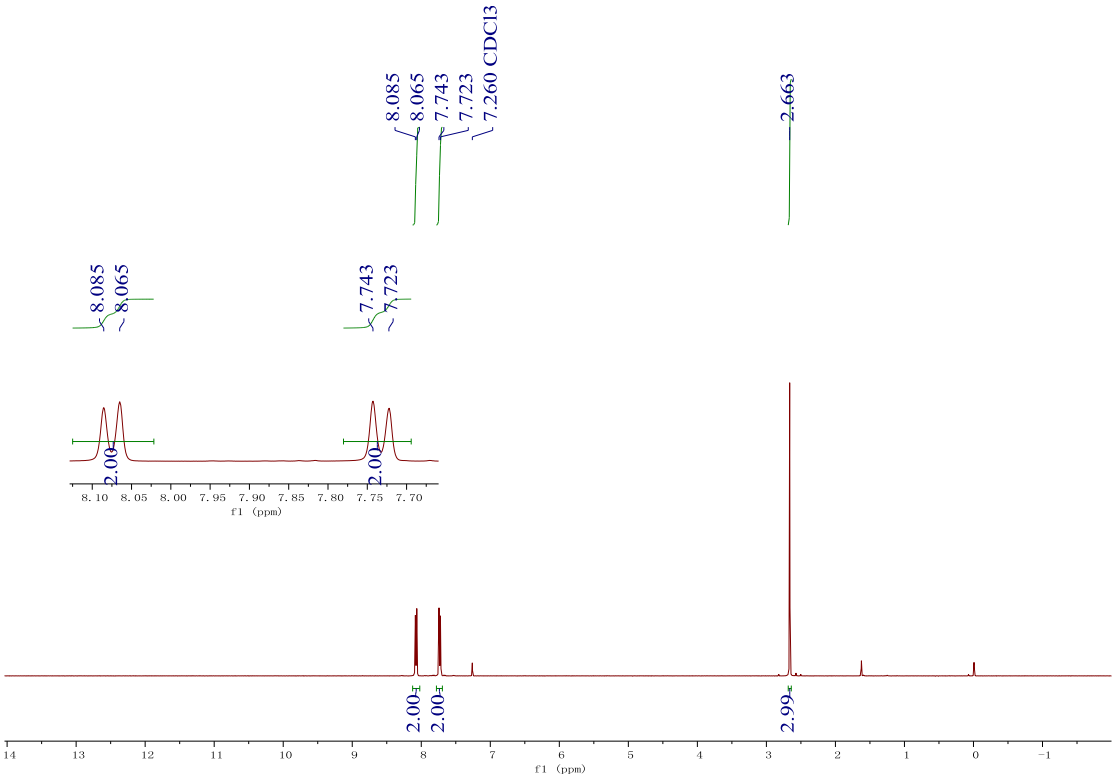


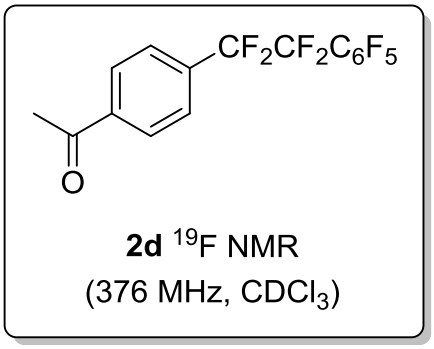
2c ^{13}C NMR
(125 MHz, $CDCl_3$)



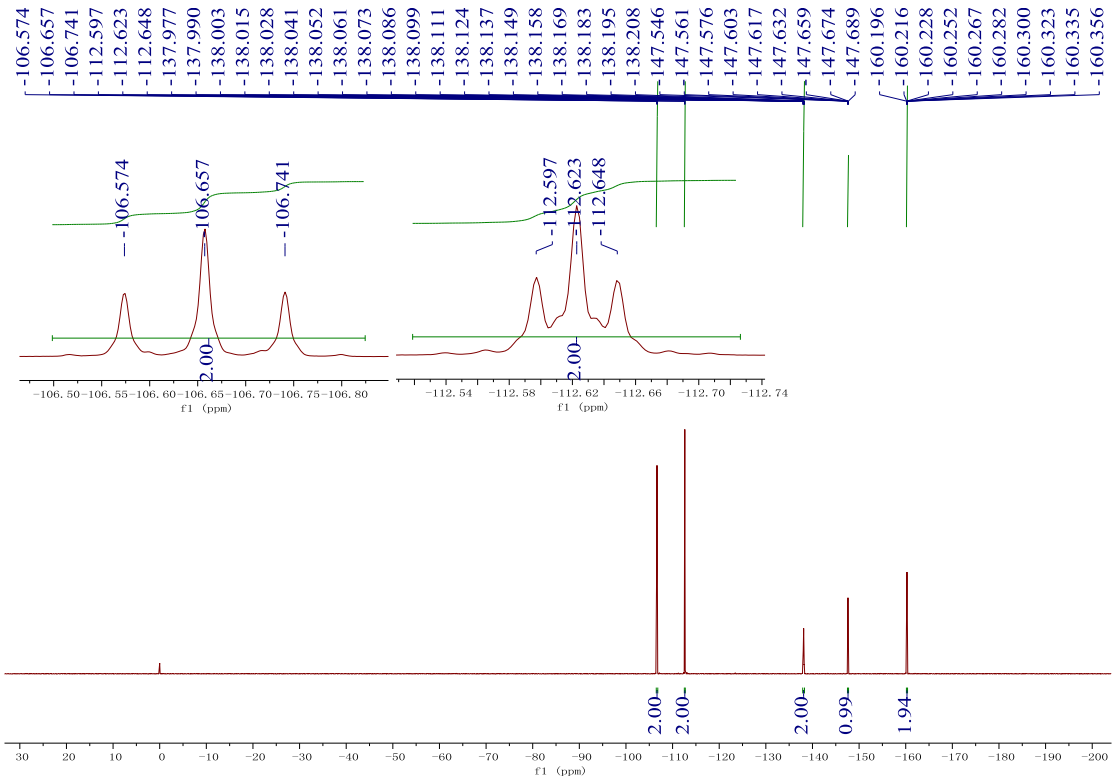


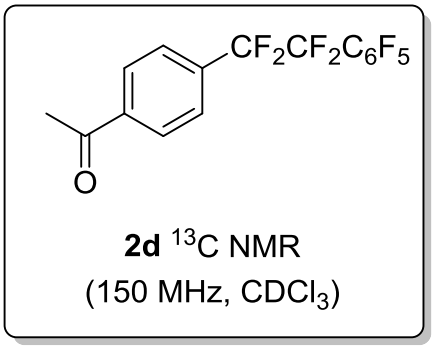
2d ^{1}H NMR
(400 MHz, $CDCl_3$)



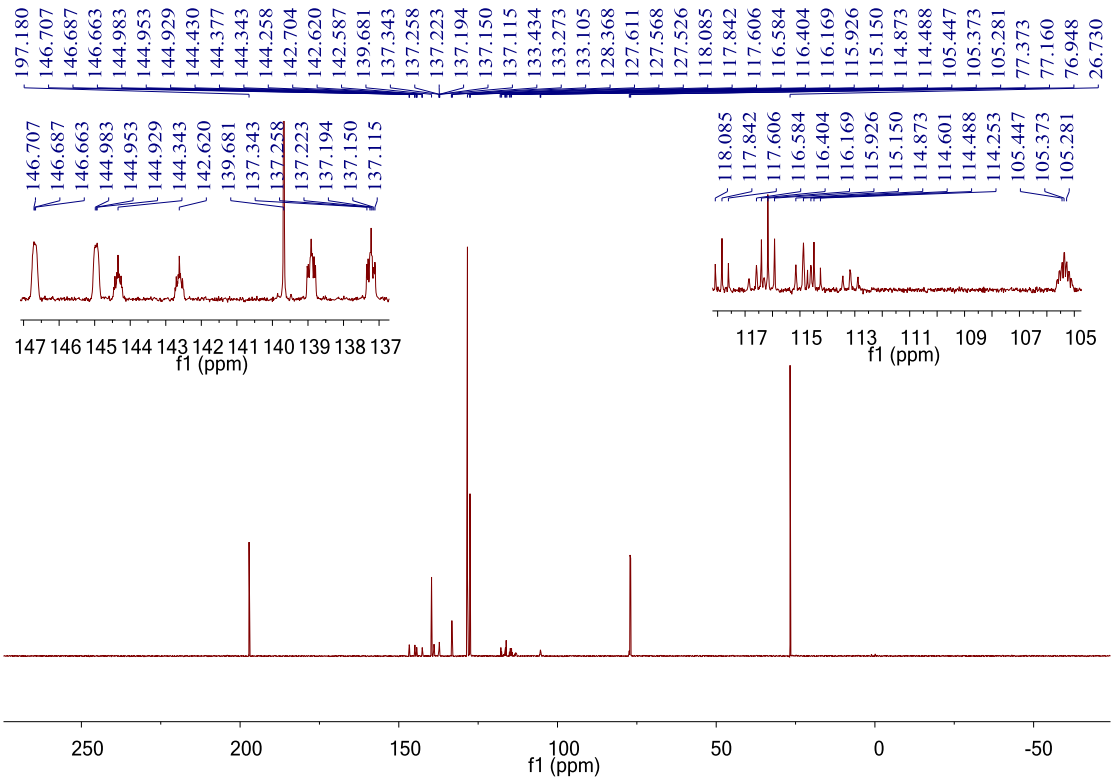


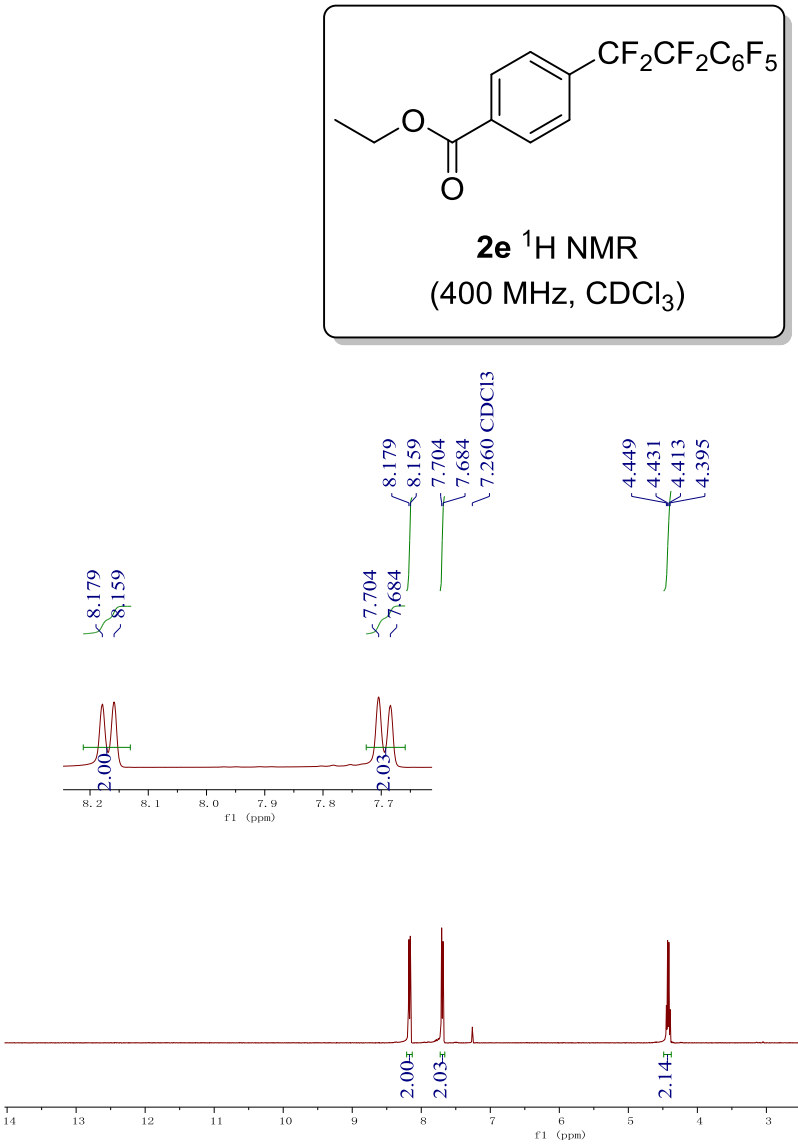
2d ^{19}F NMR
(376 MHz, $CDCl_3$)

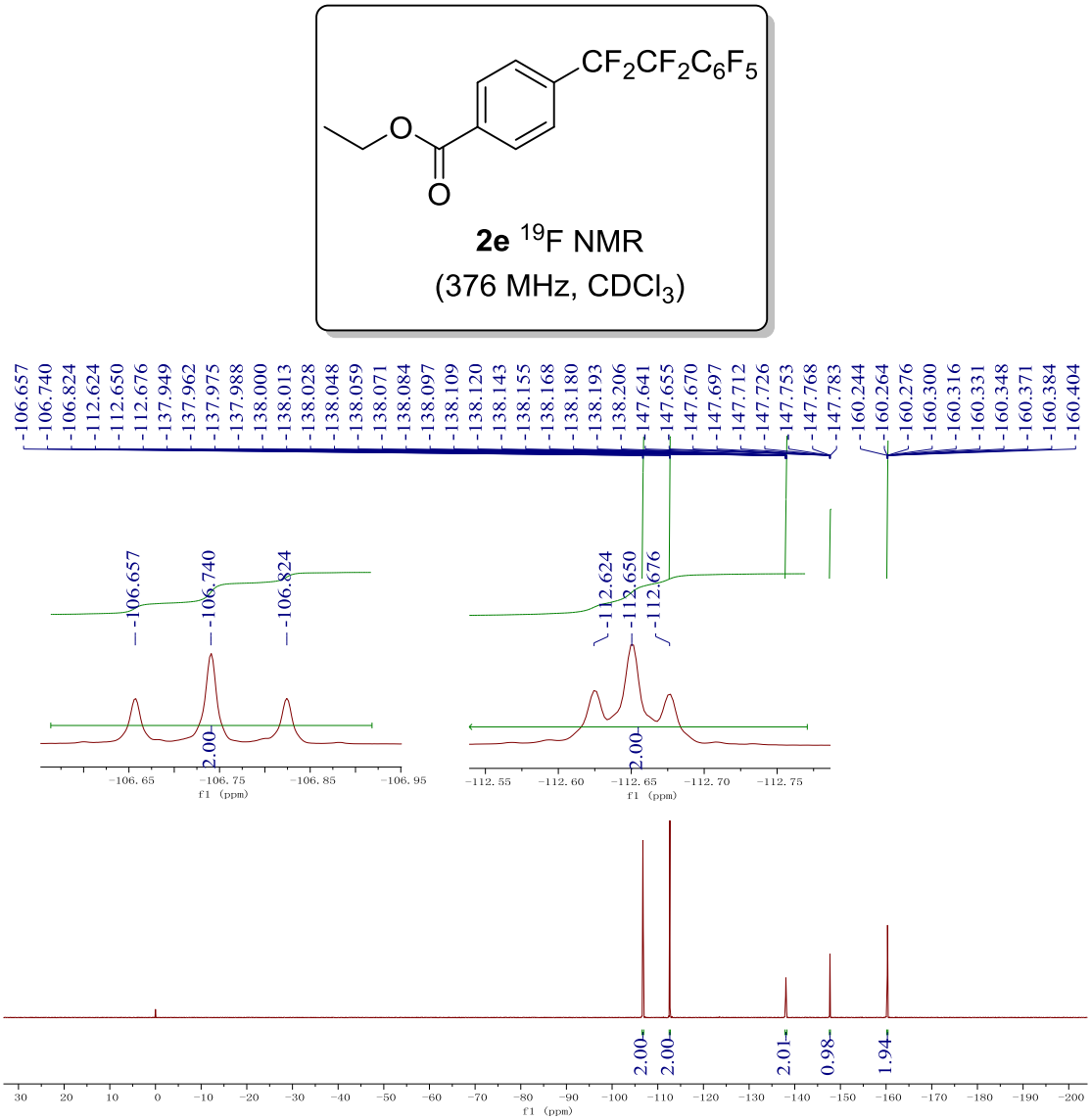


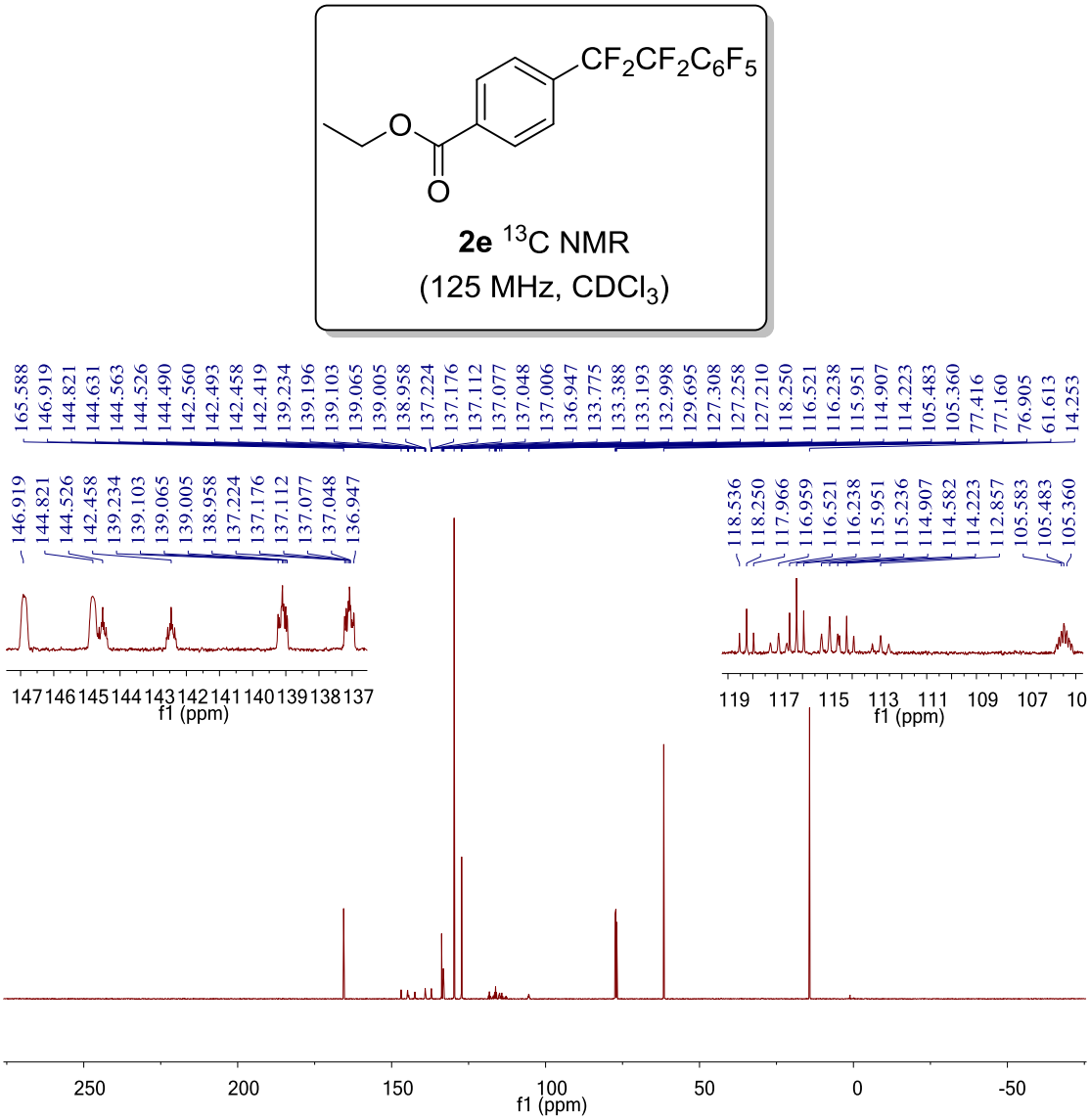


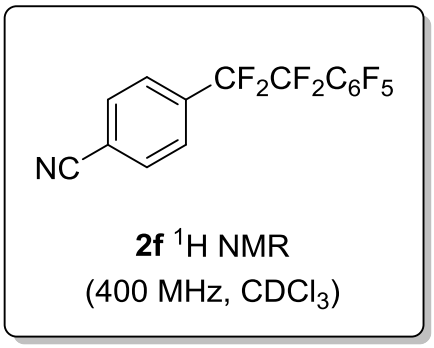
2d ^{13}C NMR
(150 MHz, $CDCl_3$)

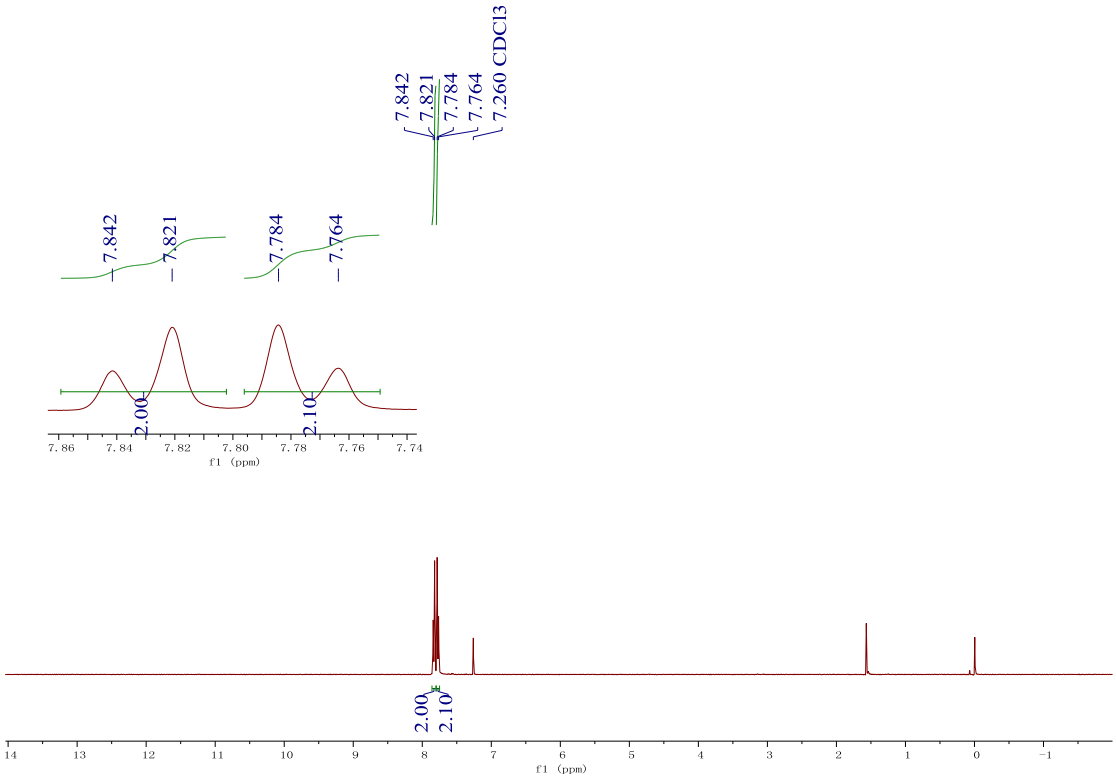


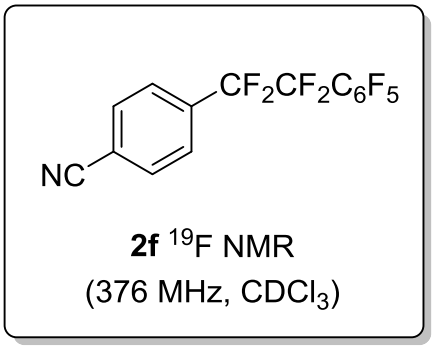

CF2CF2C6F5
O
O
2e 1H NMR
(400 MHz, CDCl3)
8.179
8.159
7.704
7.684
7.260 CDCl3
4.449
4.431
4.413
4.395
1.438
1.420
1.402
2.00
2.03
f1 (ppm)
2.00
2.03
2.14
3.12
f1 (ppm)


CF2CF2C6F5
O
O
2e 19F NMR
(376 MHz, CDCl3)
-106.657
-106.740
-106.824
-112.624
-112.650
-112.676
-137.949
-137.962
-137.975
-137.988
-138.000
-138.013
-138.028
-138.048
-138.059
-138.071
-138.084
-138.097
-138.109
-138.120
-138.143
-138.155
-138.168
-138.180
-138.193
-138.206
-147.641
-147.655
-147.670
-147.697
-147.712
-147.726
-147.753
-147.768
-147.783
-160.244
-160.264
-160.276
-160.300
-160.316
-160.331
-160.348
-160.371
-160.384
-160.404
2.00
2.00
f1 (ppm)
2.00
2.00
2.01
0.98
1.94
f1 (ppm)

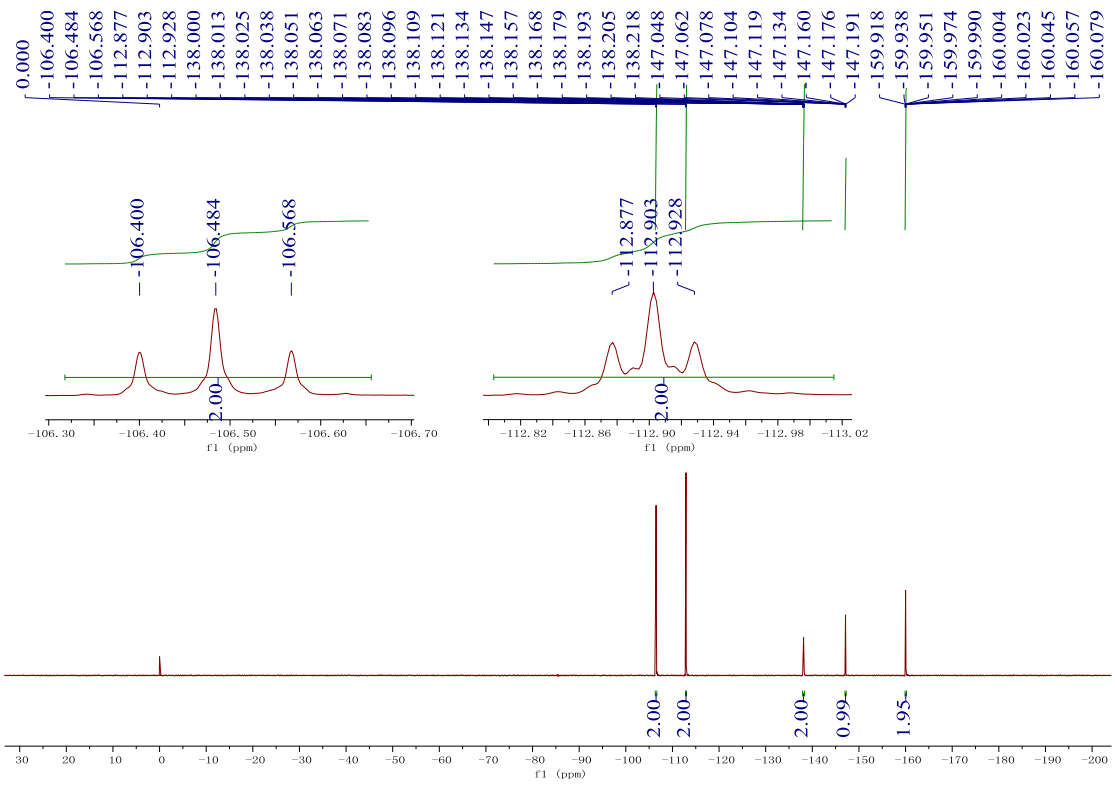

CF2CF2C6F5
O
O
2e 13C NMR
(125 MHz, CDCl3)
165.588
146.919
144.821
144.631
144.563
144.526
144.490
142.560
142.493
142.458
142.419
139.234
139.196
139.103
139.065
139.005
138.958
137.224
137.176
137.112
137.077
137.048
137.006
136.947
133.775
133.388
133.193
132.998
129.695
127.308
127.258
127.210
118.250
116.521
116.238
115.951
114.907
114.223
105.483
105.360
77.416
77.160
76.905
61.613
14.253
146.919
144.821
144.526
142.458
139.234
139.103
139.065
139.005
138.958
137.224
137.176
137.112
137.077
137.048
136.947
147 146 145 144 143 142 141 140 139 138 137
f1 (ppm)
118.536
118.250
117.966
116.959
116.521
116.238
115.951
115.236
114.907
114.582
114.223
112.857
105.583
105.483
105.360
119 117 115 113 111 109 107 10
f1 (ppm)
250 200 150 100 50 0 -50
f1 (ppm)

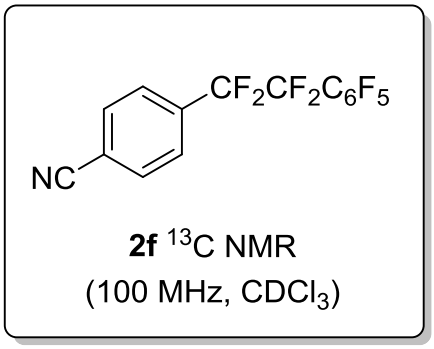

CF2CF2C6F5
NC
2f 1H NMR
(400 MHz, CDCl3)


7.842
7.821
7.784
7.764
7.260 CDCl3
2.00
2.10
f1 (ppm)

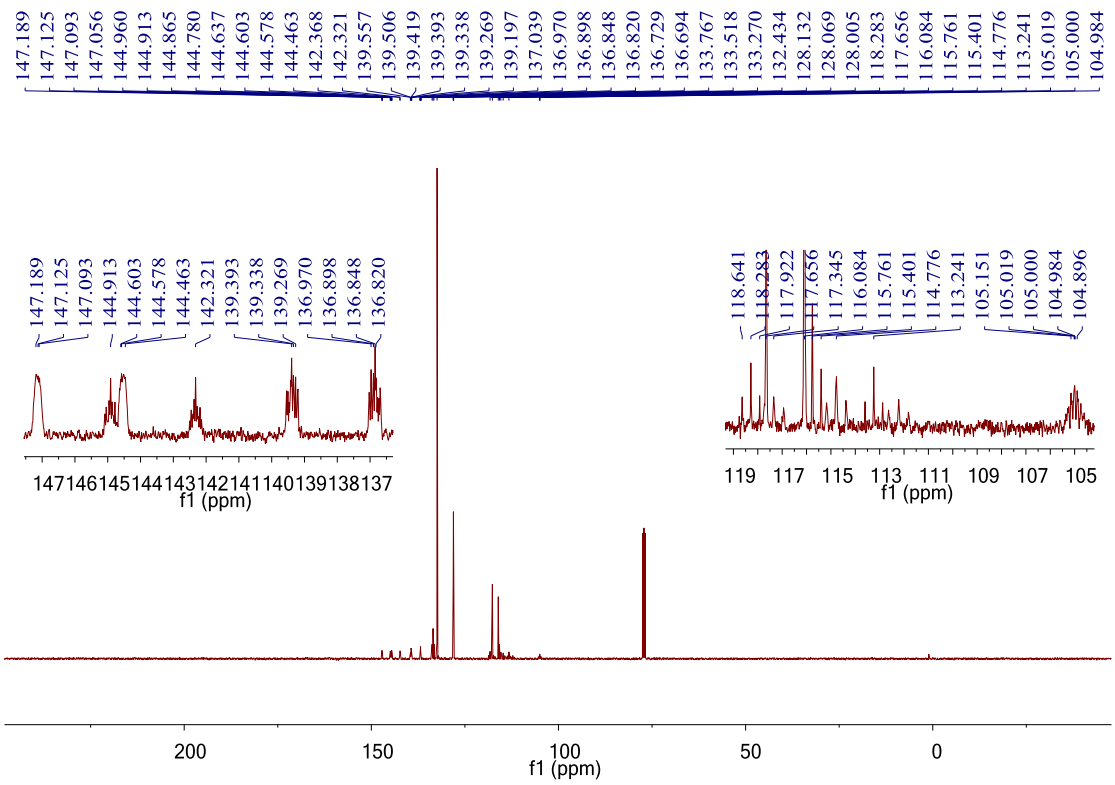


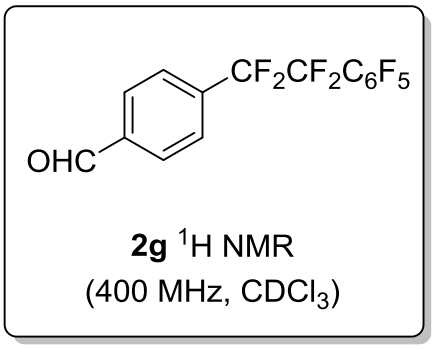
2f ^{19}F NMR
(376 MHz, $CDCl_3$)

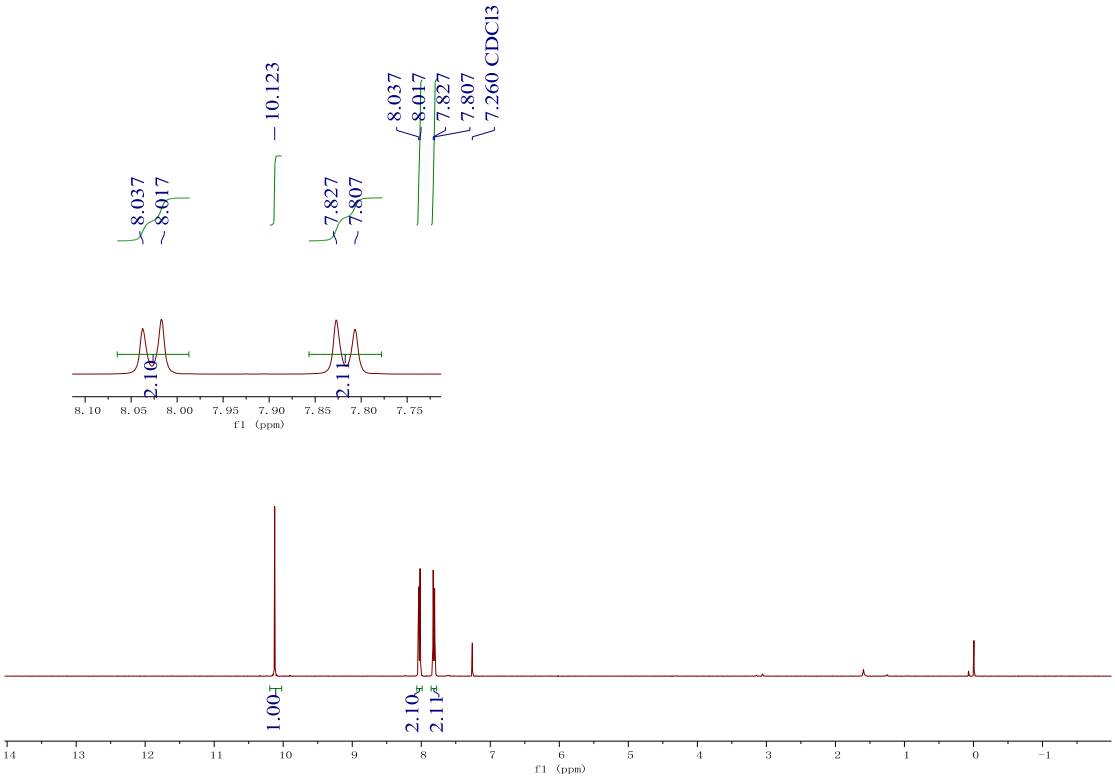


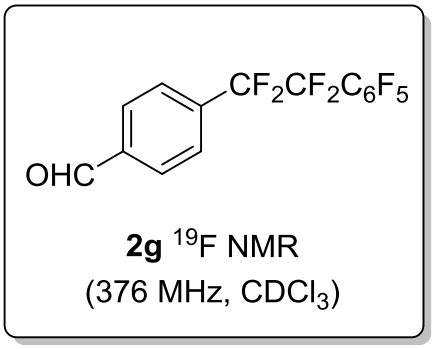


2f ^{13}C NMR
(100 MHz, $CDCl_3$)

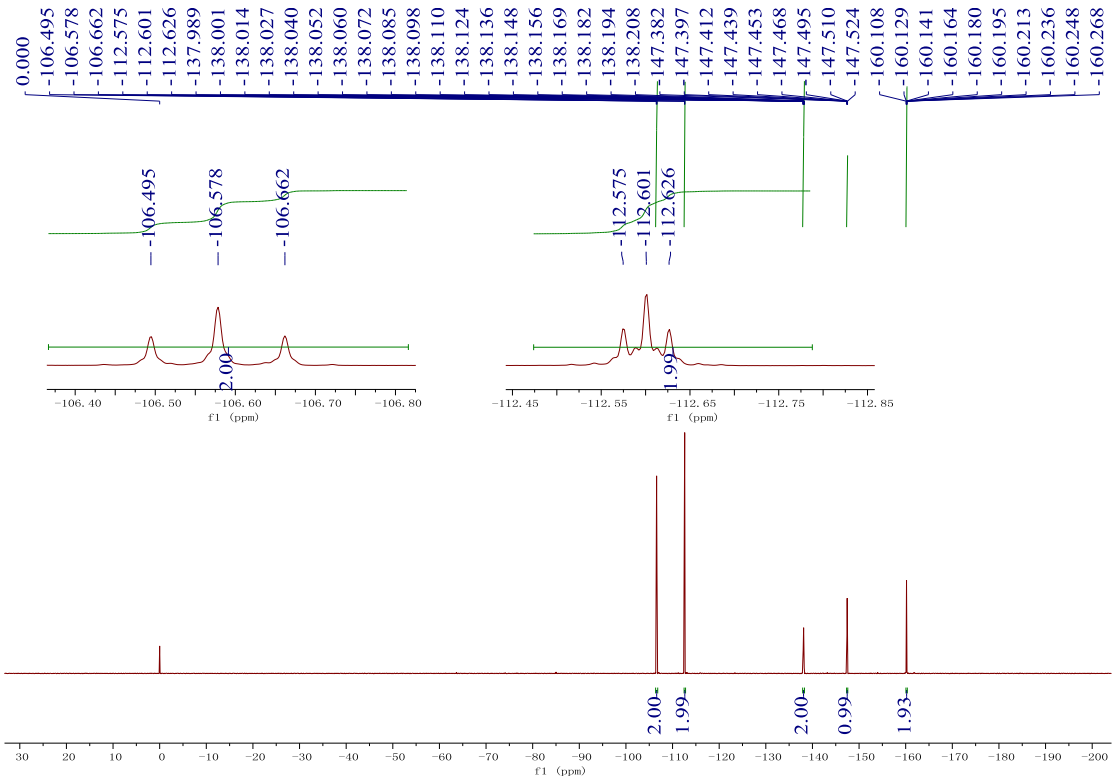


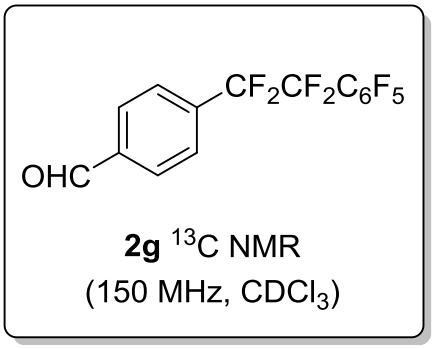

CF2CF2C6F5
OHC
2g 1H NMR
(400 MHz, CDCl3)


8.037
8.017
10.123
7.827
7.807
8.037
8.017
7.827
7.807
7.260 CDCl3
2.10
2.11
8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75
f1 (ppm)
1.00
2.10
2.11
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
f1 (ppm)

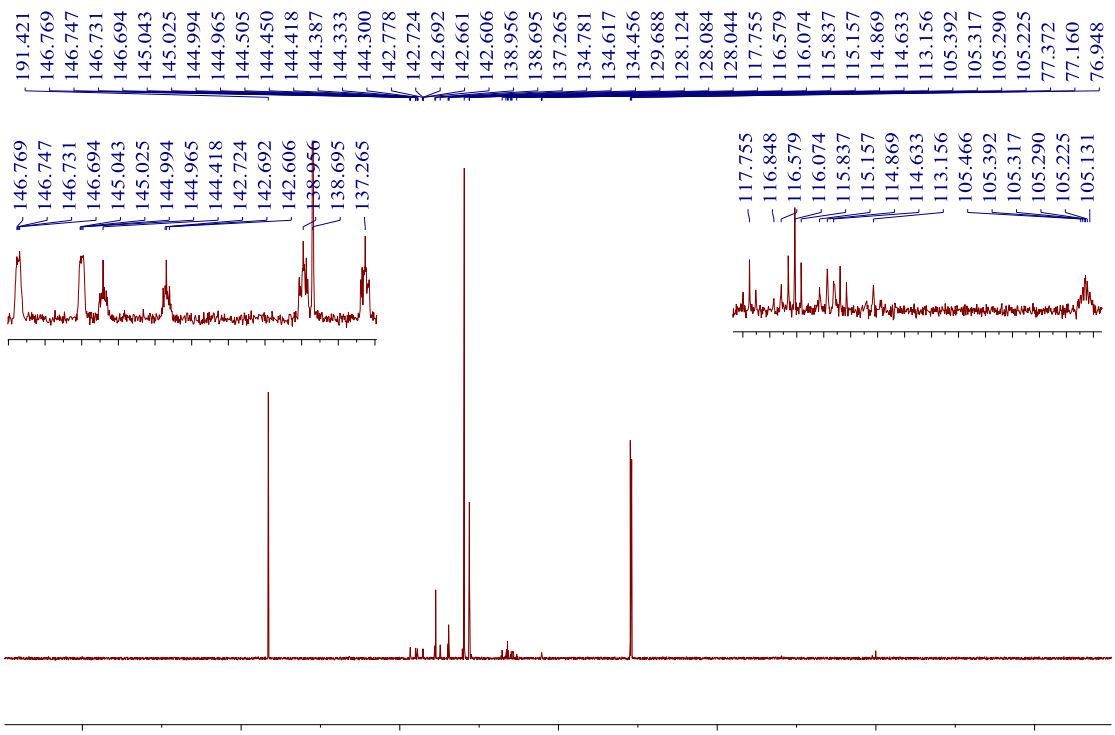


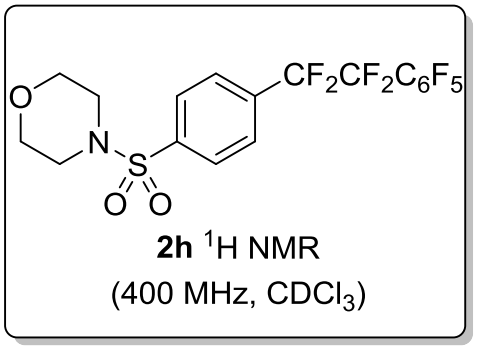
2g ^{19}F NMR
(376 MHz, $CDCl_3$)





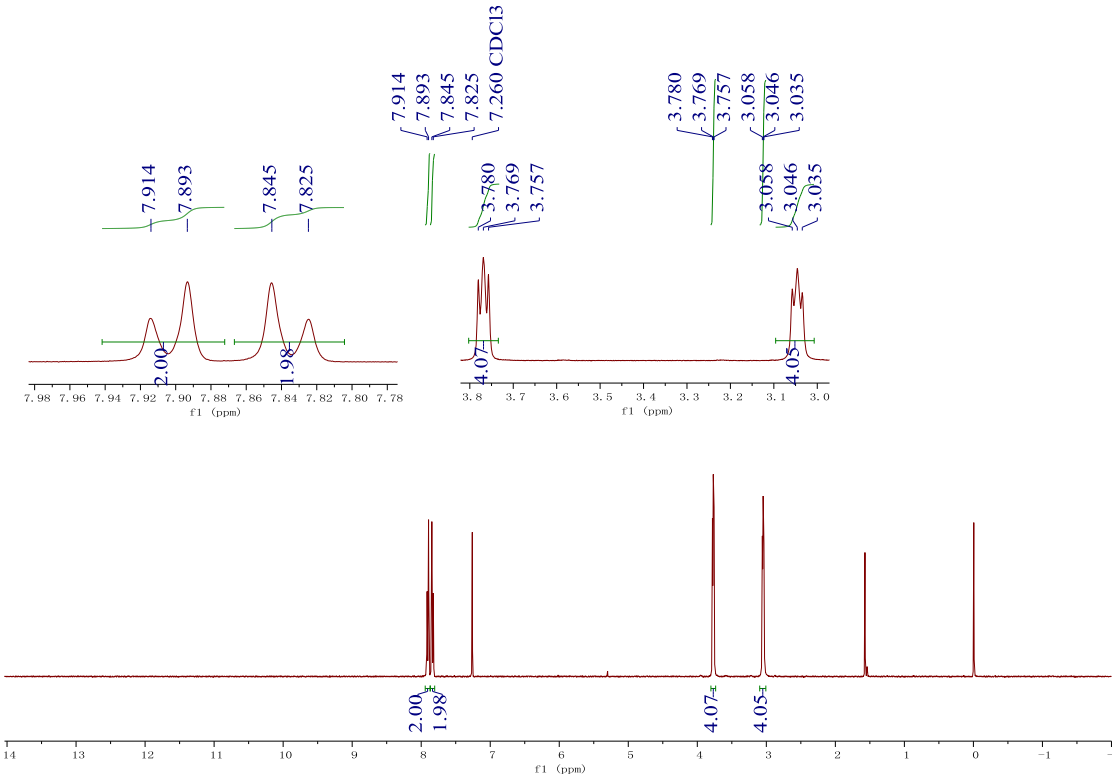
2g ^{13}C NMR
(150 MHz, $CDCl_3$)

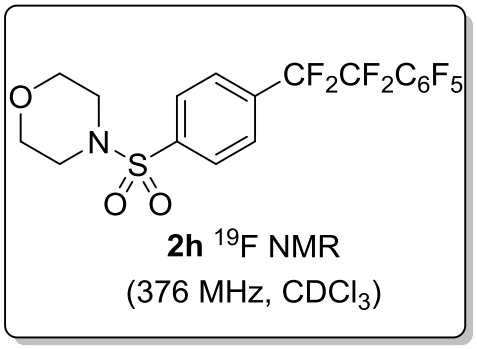




2h ^{1}H NMR

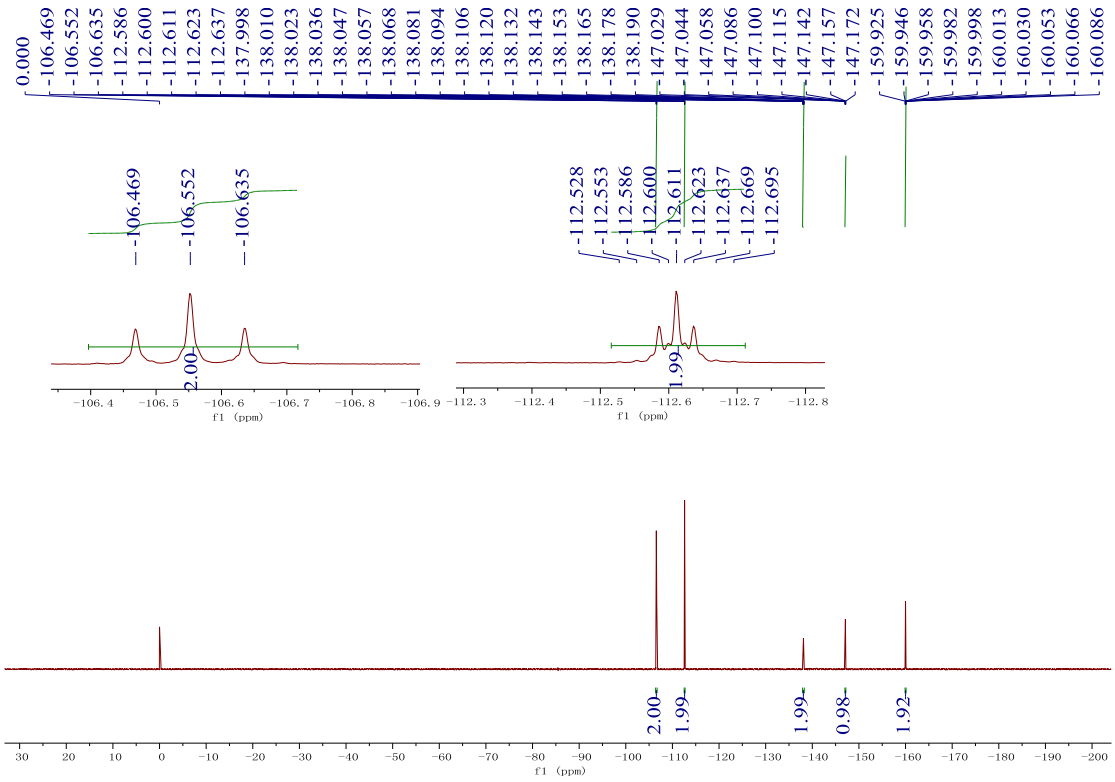
(400 MHz, $CDCl_3$)

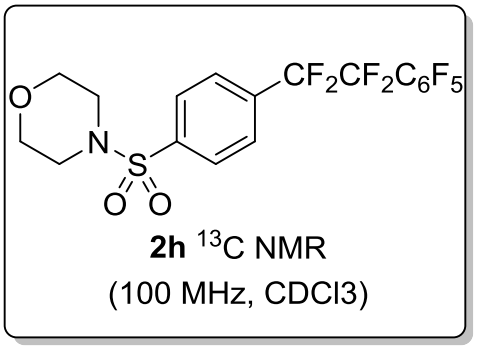




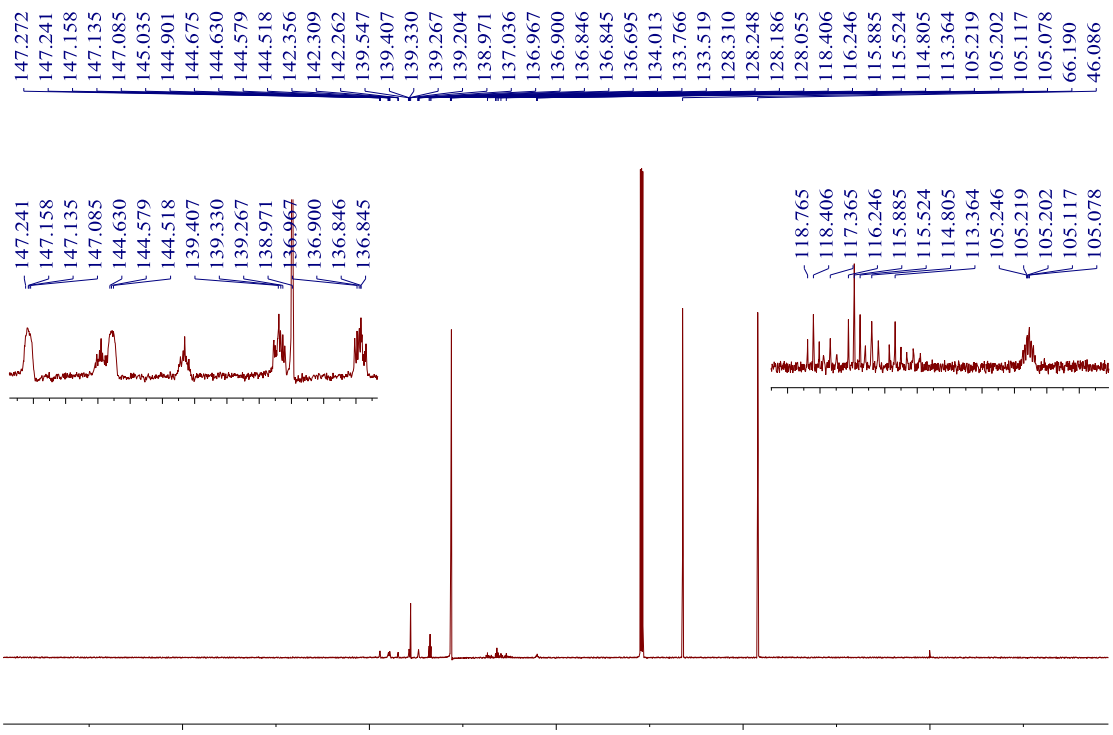
2h ^{19}F NMR

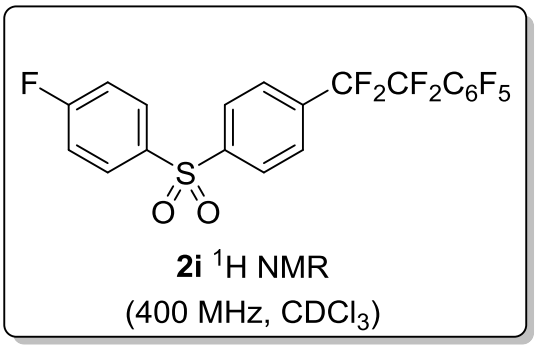
(376 MHz, $CDCl_3$)

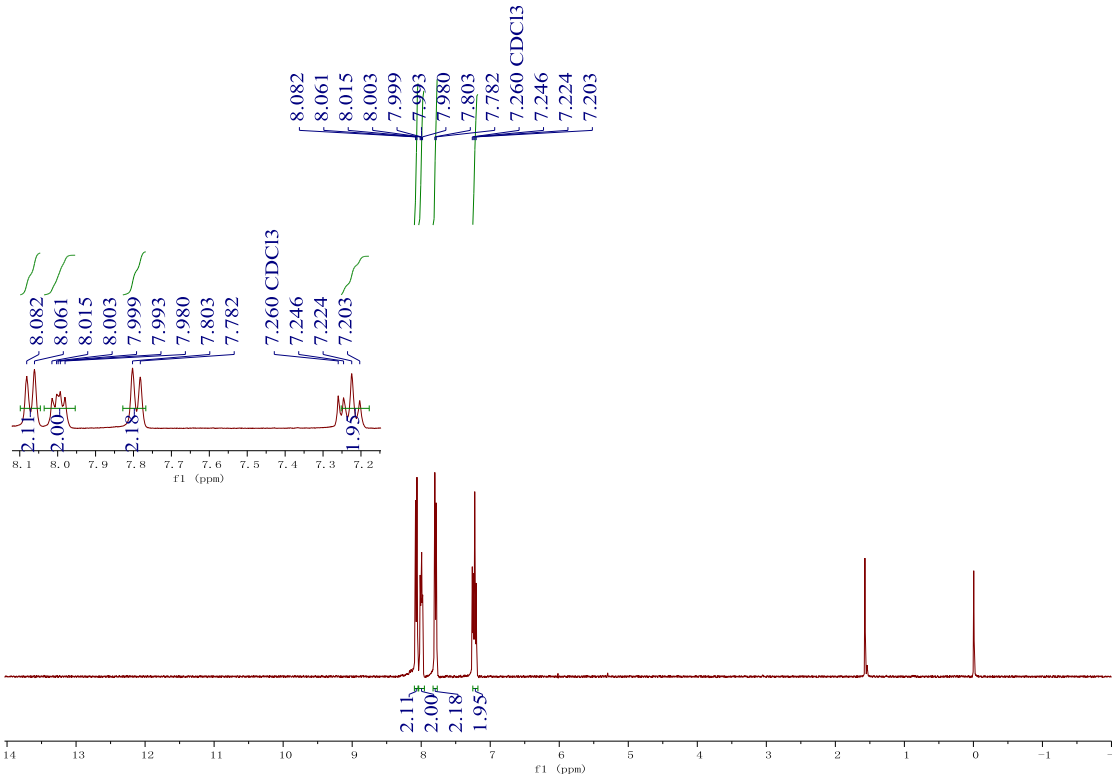


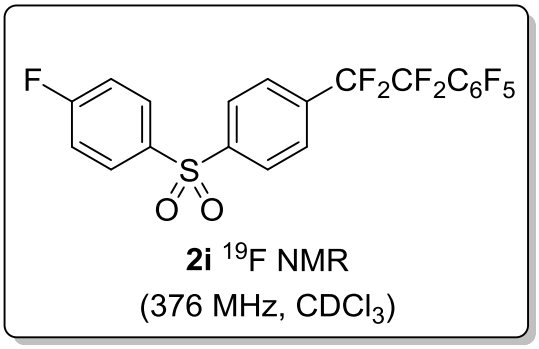


2h ^{13}C NMR
(100 MHz, CDCl3)



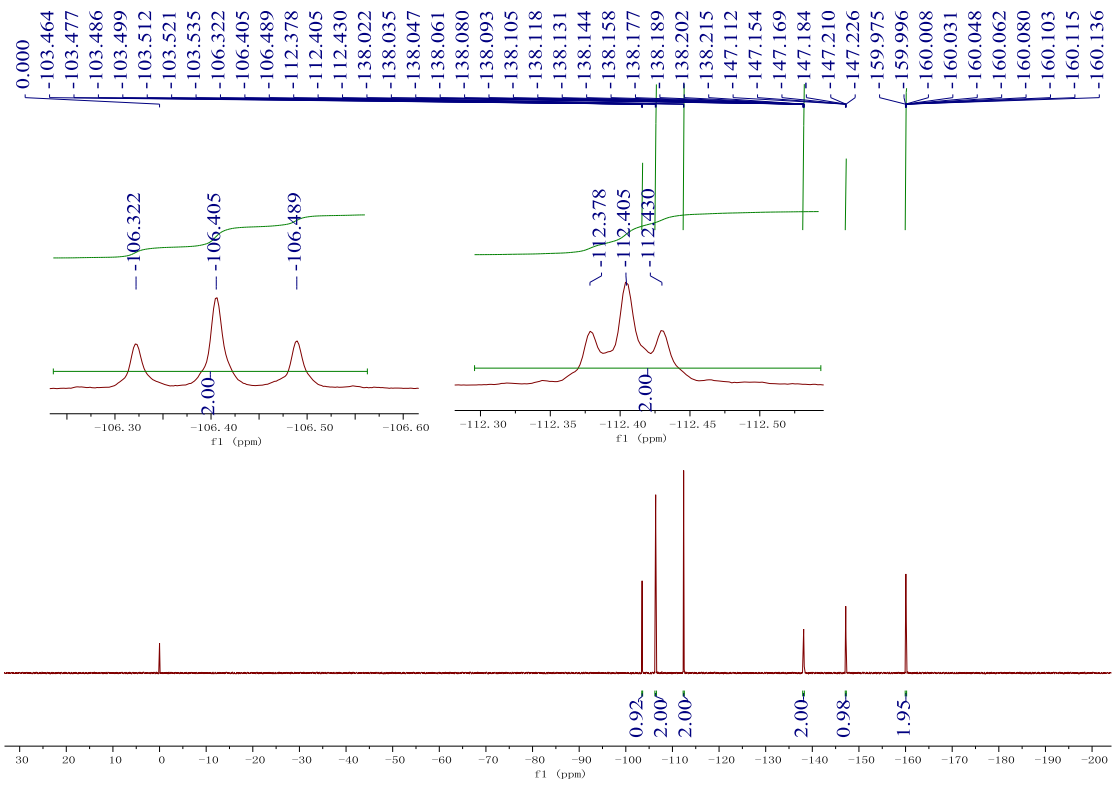

F
CF2CF2C6F5
S
O
O
2i 1H NMR
(400 MHz, CDCl3)

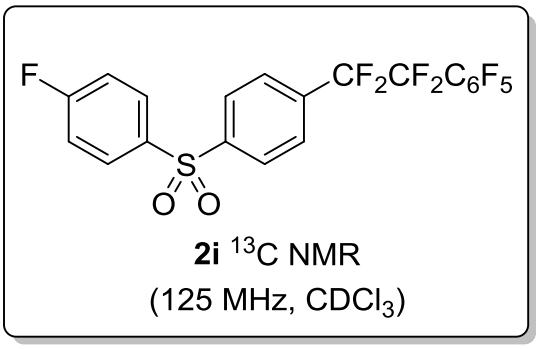

8.082
8.061
8.015
8.003
7.999
7.993
7.980
7.803
7.782
7.260 CDCl3
7.246
7.224
7.203
2.11
2.00
2.18
1.95
f1 (ppm)



2i ^{19}F NMR

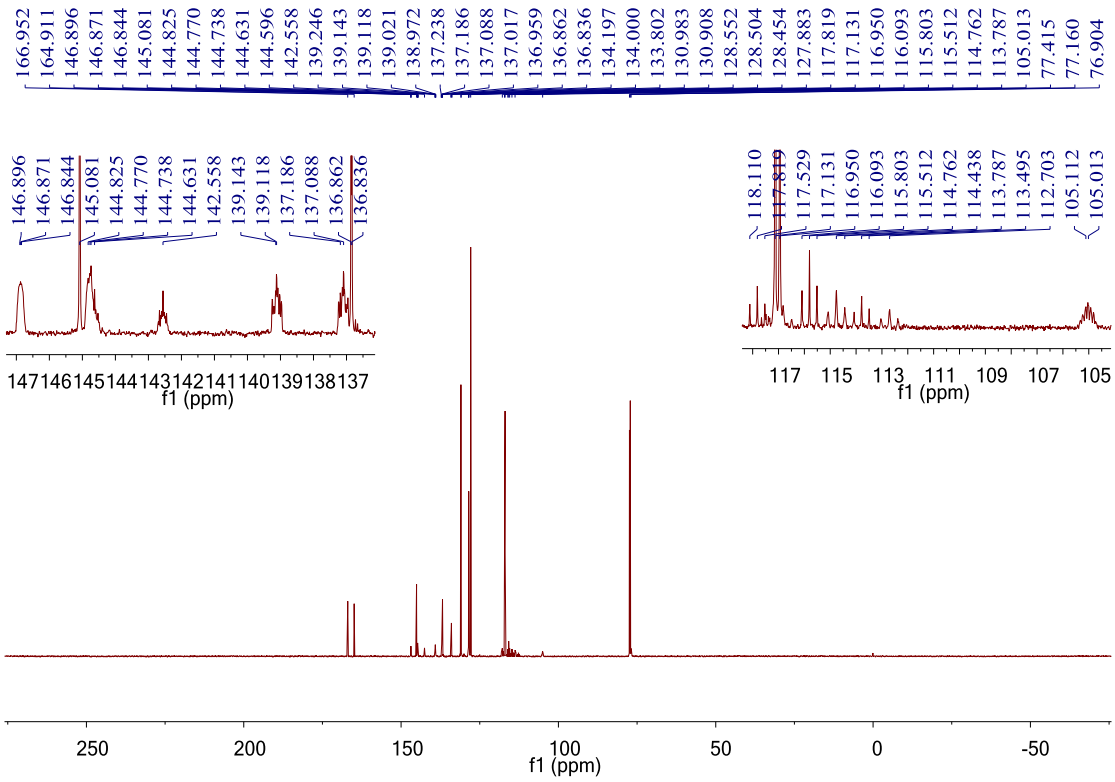
(376 MHz, $CDCl_3$)

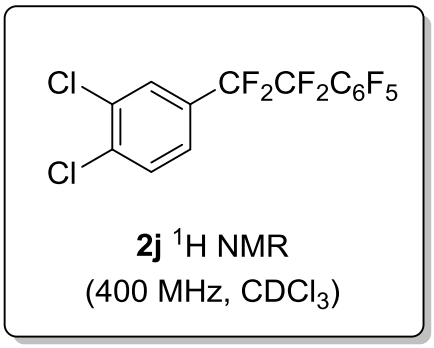


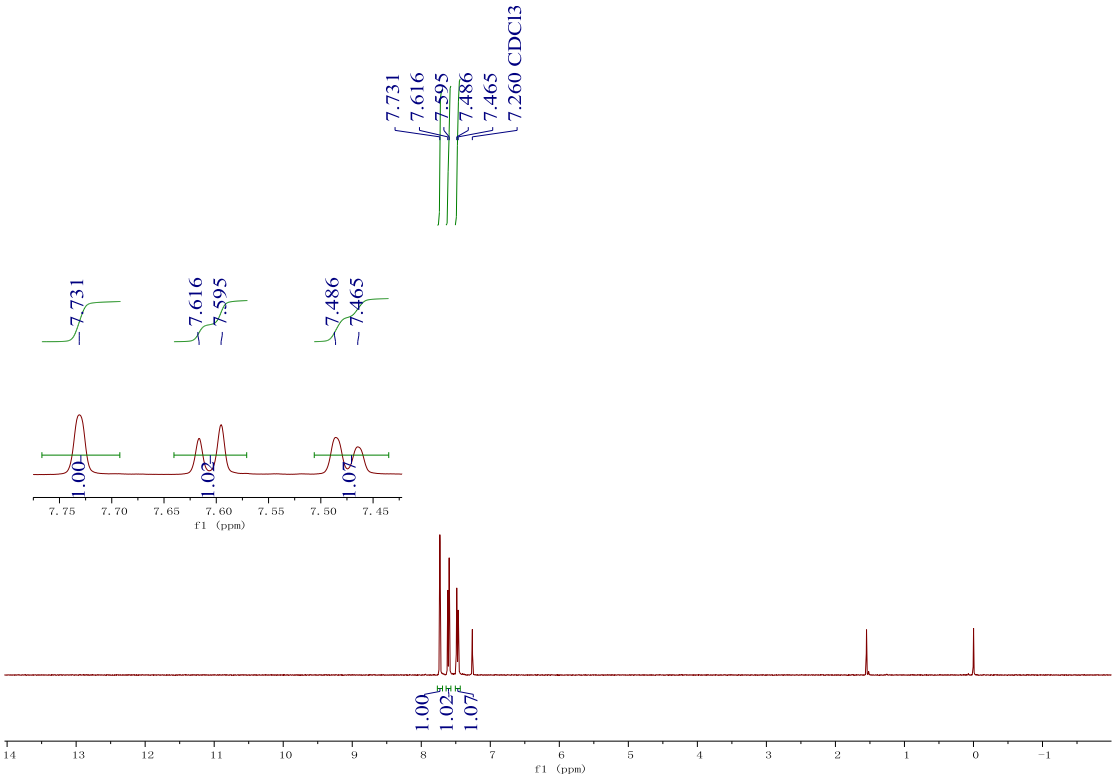


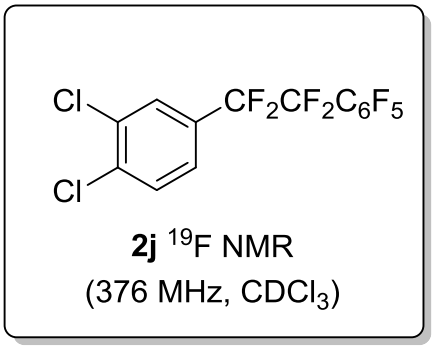
2i ^{13}C NMR

(125 MHz, $CDCl_3$)

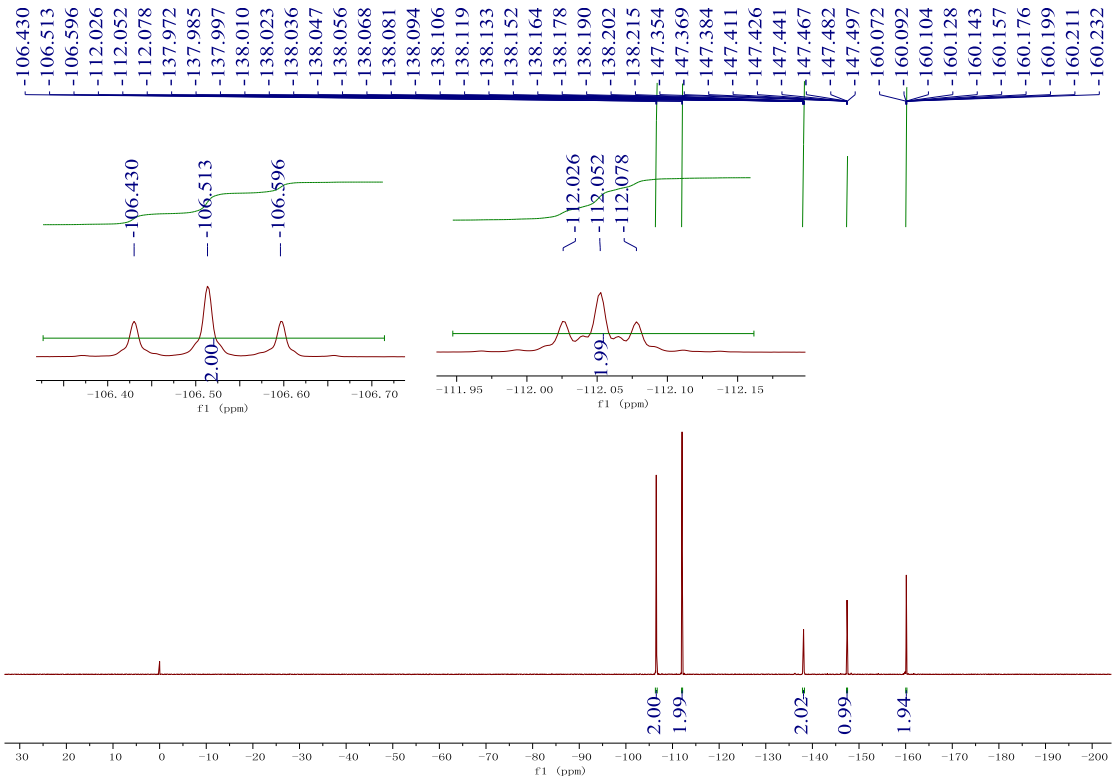


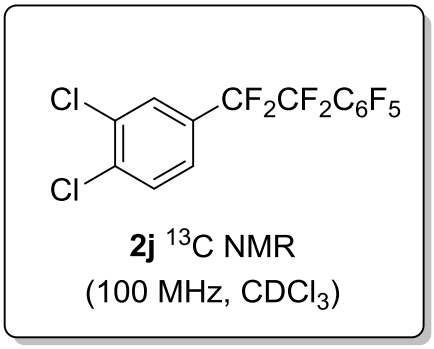

Cl
Cl
$CF_2CF_2C_6F_5$
2j ^{1}H NMR
(400 MHz, $CDCl_3$)


7.731
7.616
7.595
7.486
7.465
7.260 CDCl3
1.00
1.02
1.07
f1 (ppm)

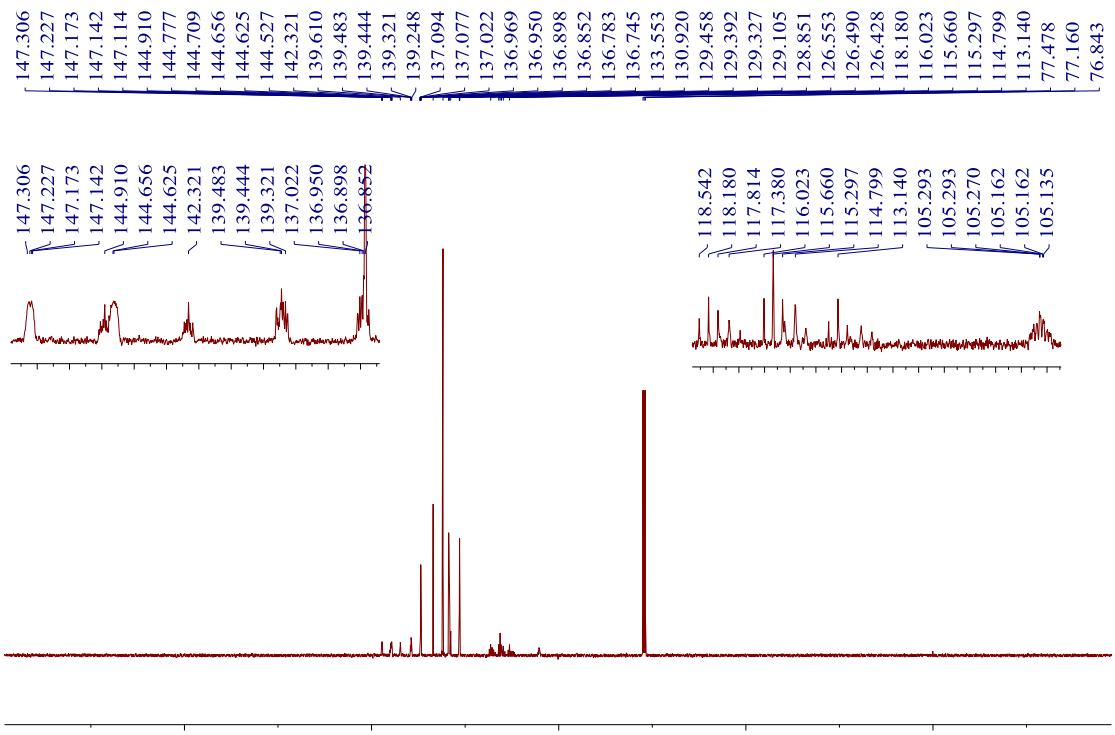


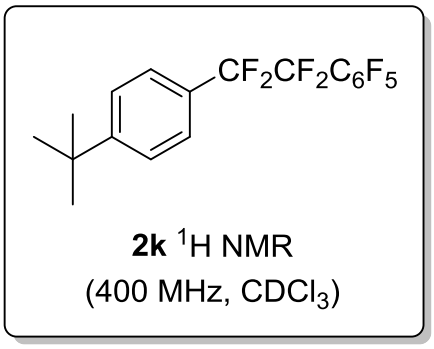
2j ^{19}F NMR
(376 MHz, $CDCl_3$)

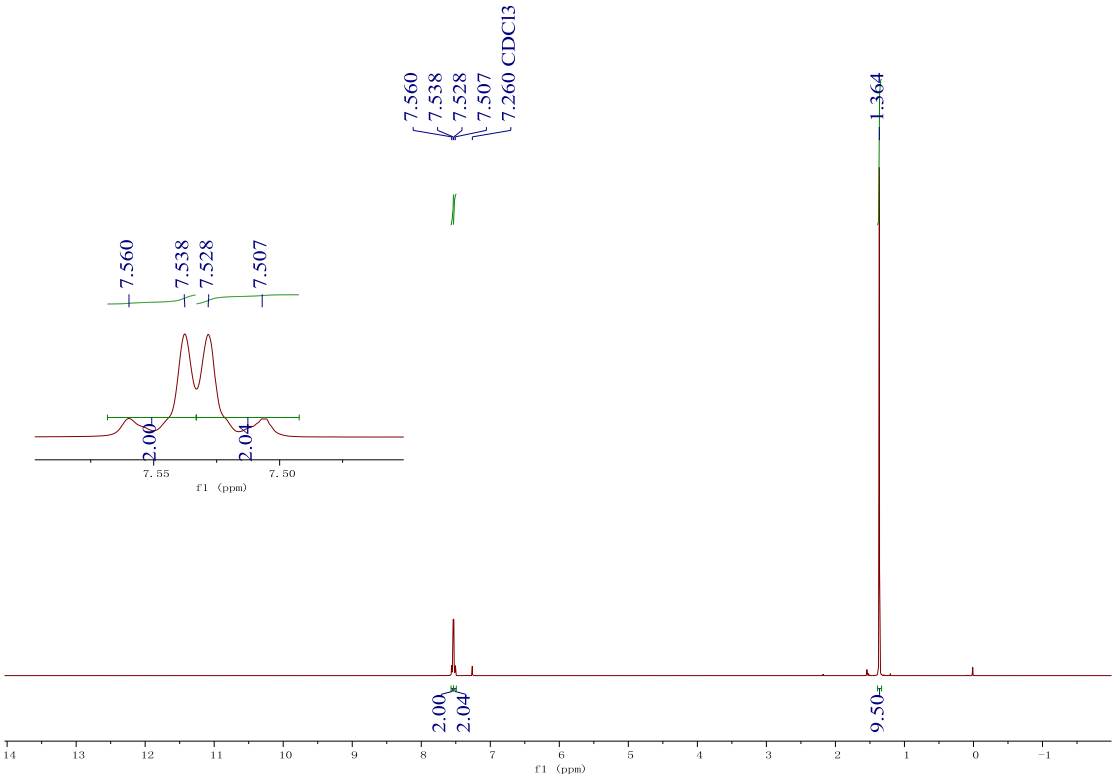


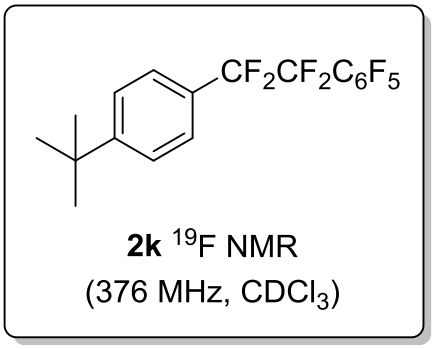


2j ^{13}C NMR
(100 MHz, $CDCl_3$)

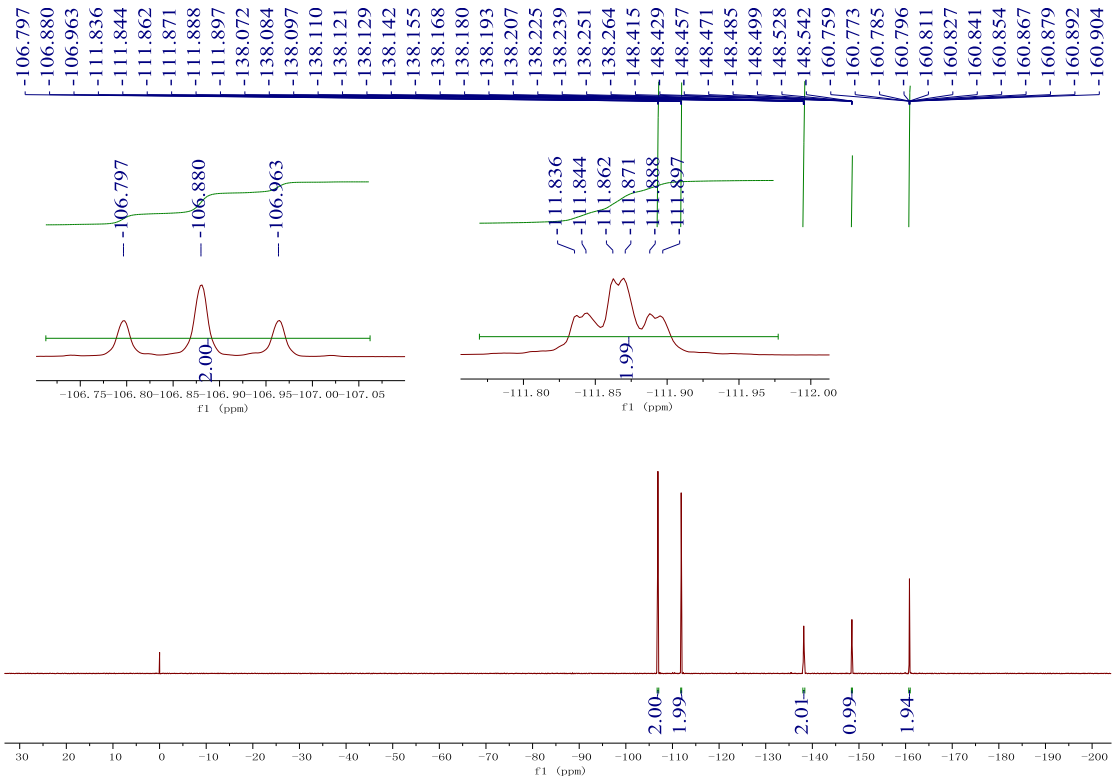


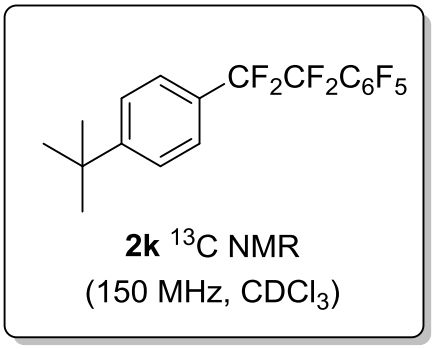

CF2CF2C6F5
2k 1H NMR
(400 MHz, CDCl3)


7.560
7.538
7.528
7.507
7.260 CDCl3
1.364
2.00
2.04
9.50
f1 (ppm)

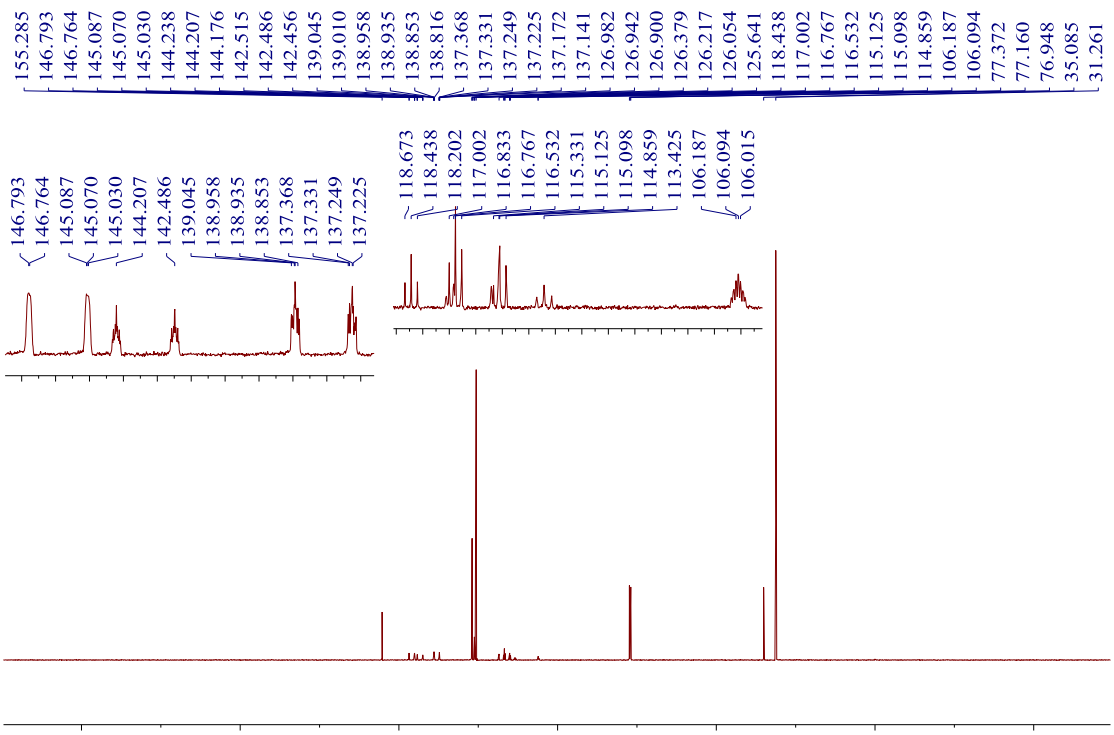


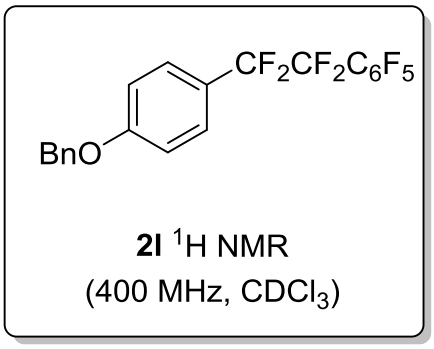
2k ^{19}F NMR
(376 MHz, $CDCl_3$)



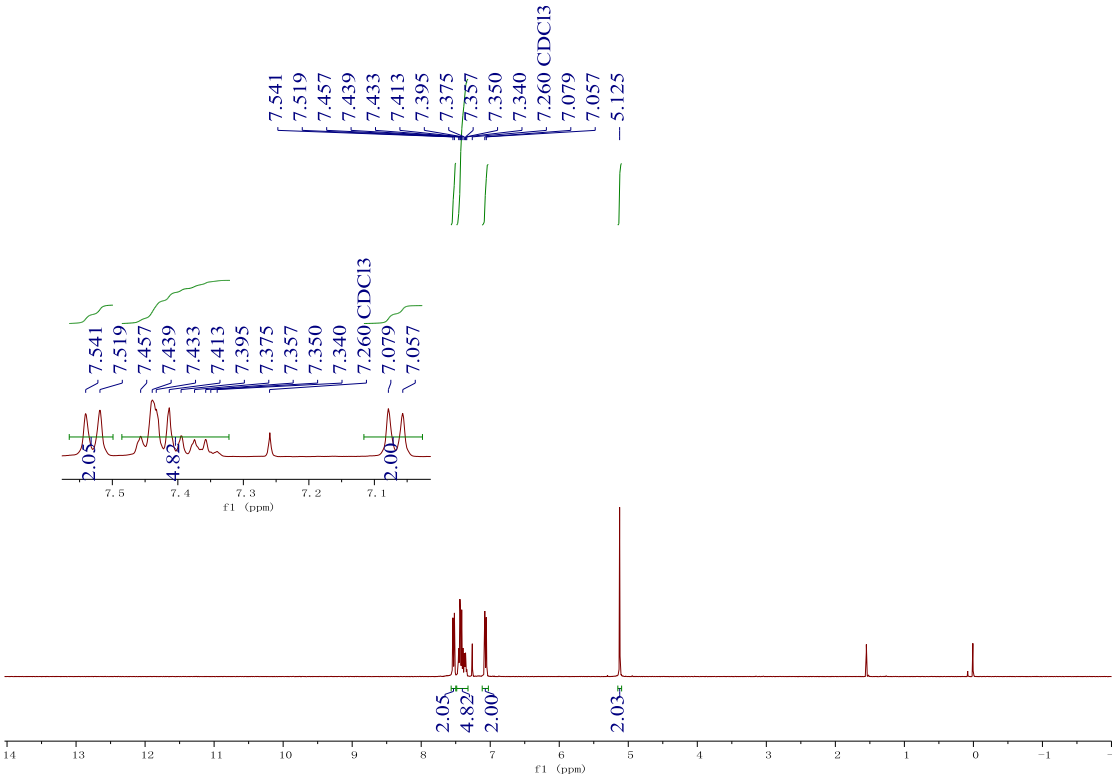


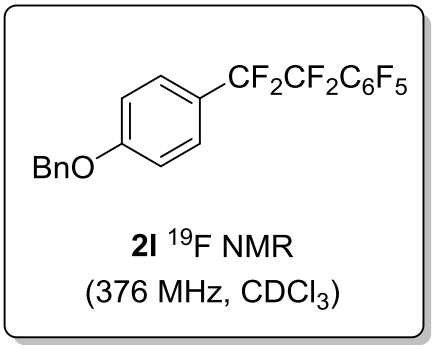
2k ^{13}C NMR
(150 MHz, $CDCl_3$)



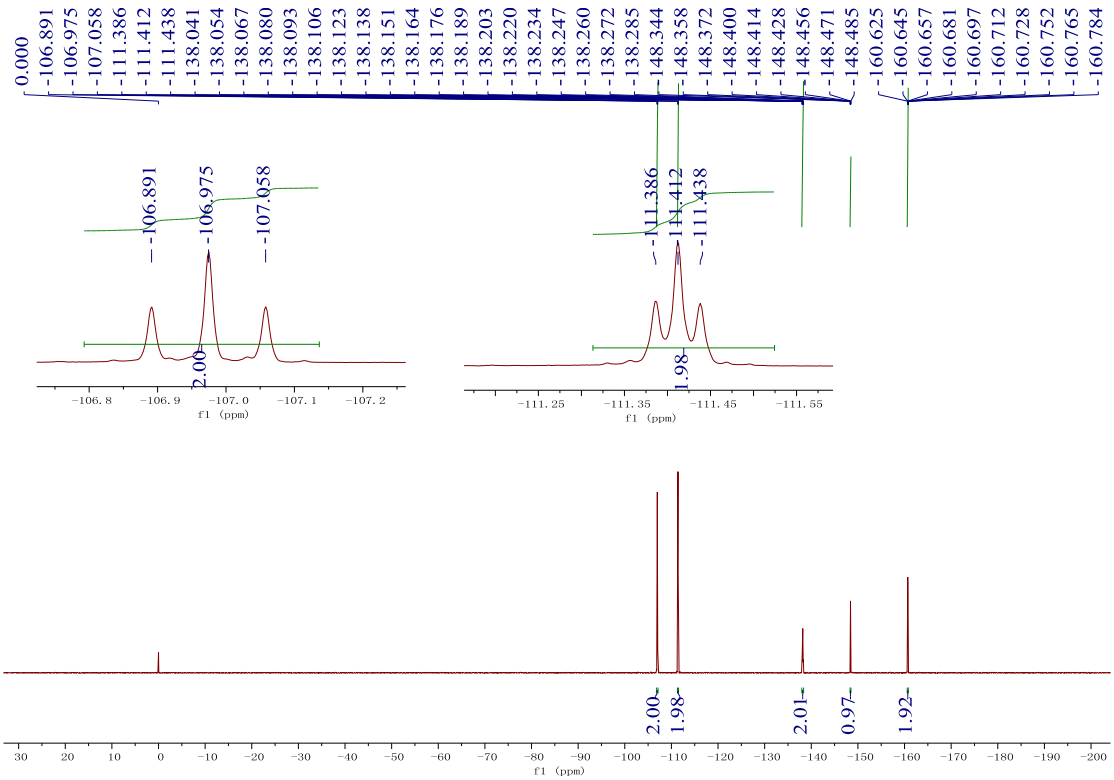


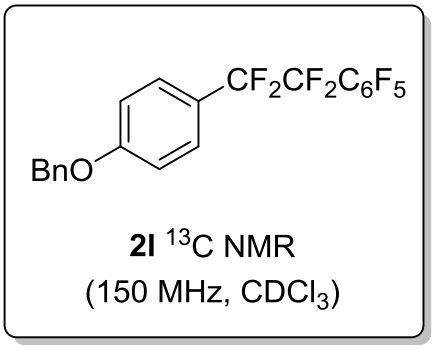
2l ^{1}H NMR
(400 MHz, $CDCl_3$)



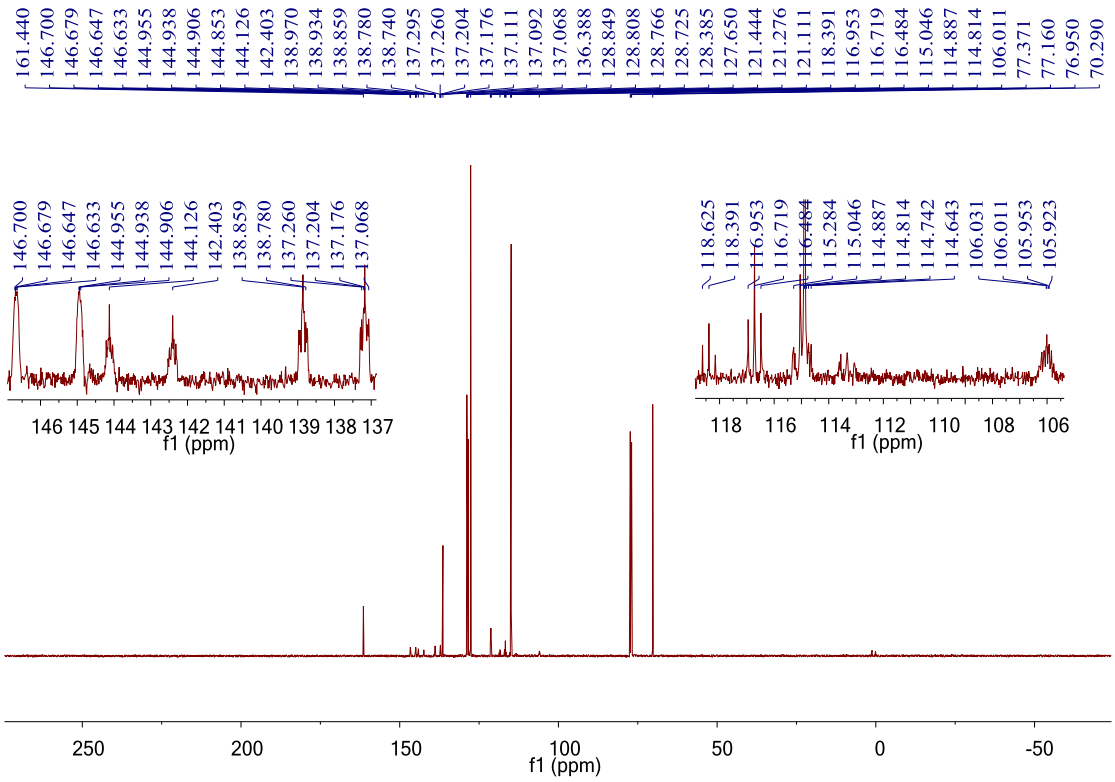


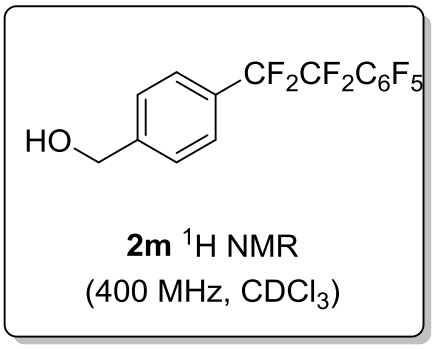
2l ^{19}F NMR
(376 MHz, $CDCl_3$)

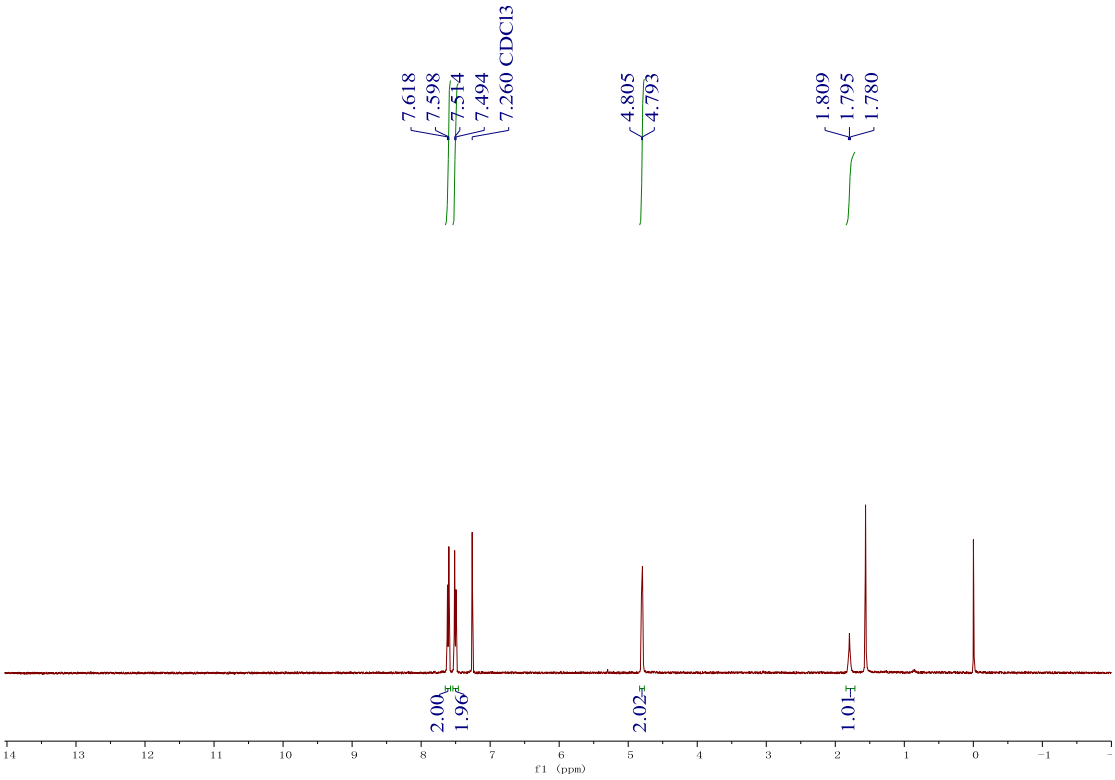


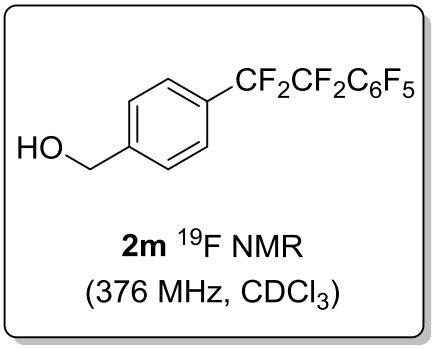


2l ^{13}C NMR
(150 MHz, $CDCl_3$)

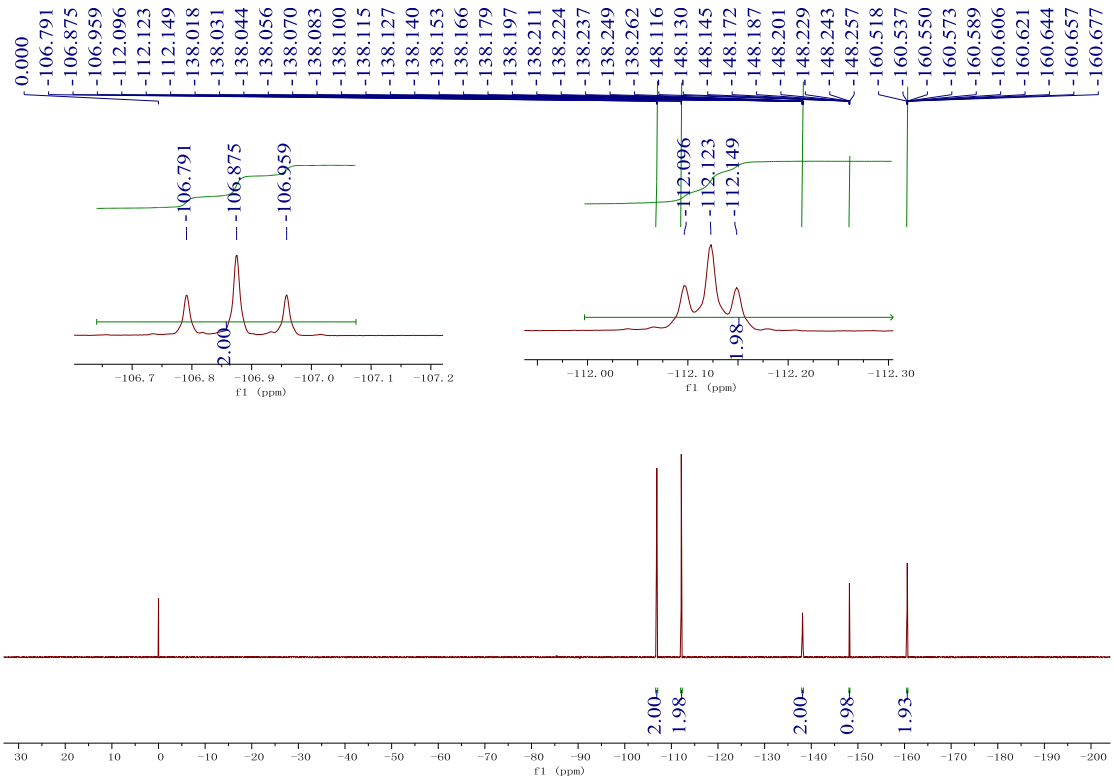


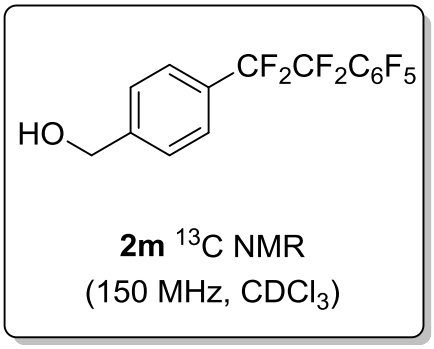

CF2CF2C6F5
HO
2m 1H NMR
(400 MHz, CDCl3)


7.618
7.598
7.514
7.494
7.260 CDCl3
4.805
4.793
1.809
1.795
1.780
2.00
1.96
2.02
1.01
f1 (ppm)

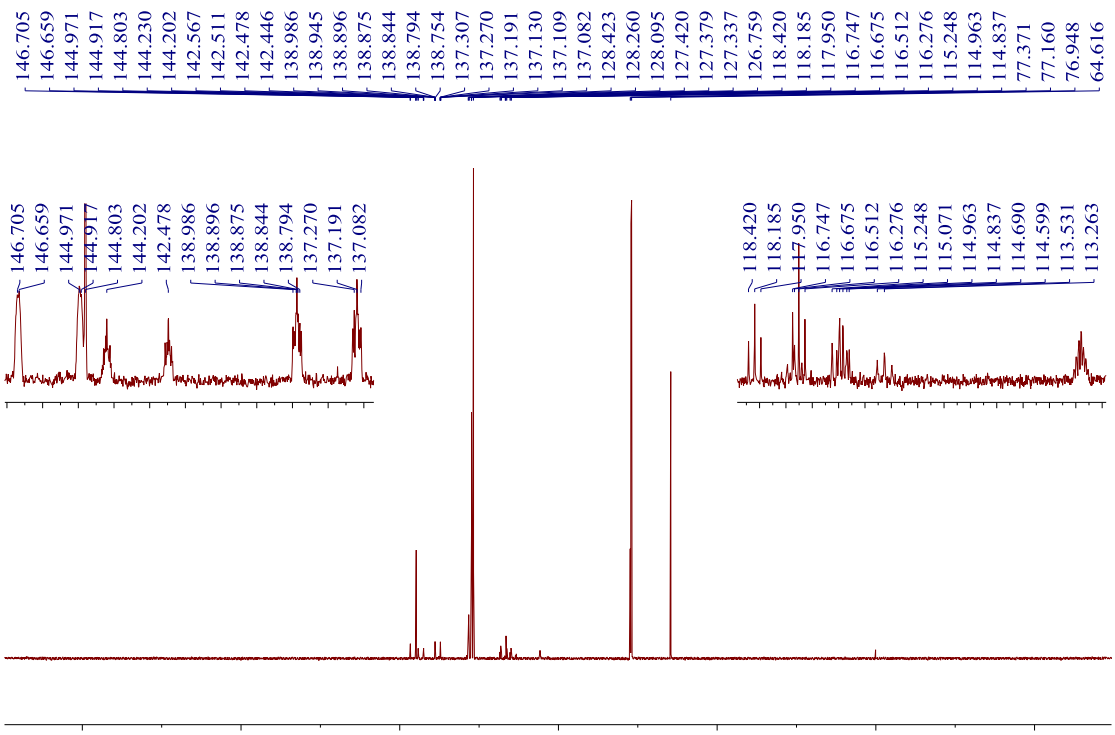


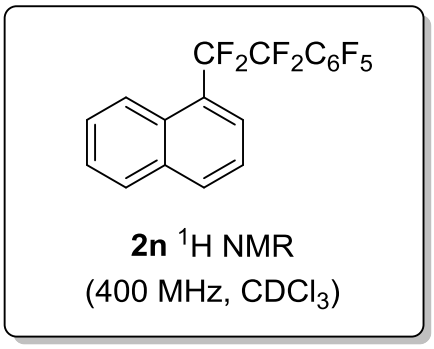
2m ^{19}F NMR
(376 MHz, $CDCl_3$)

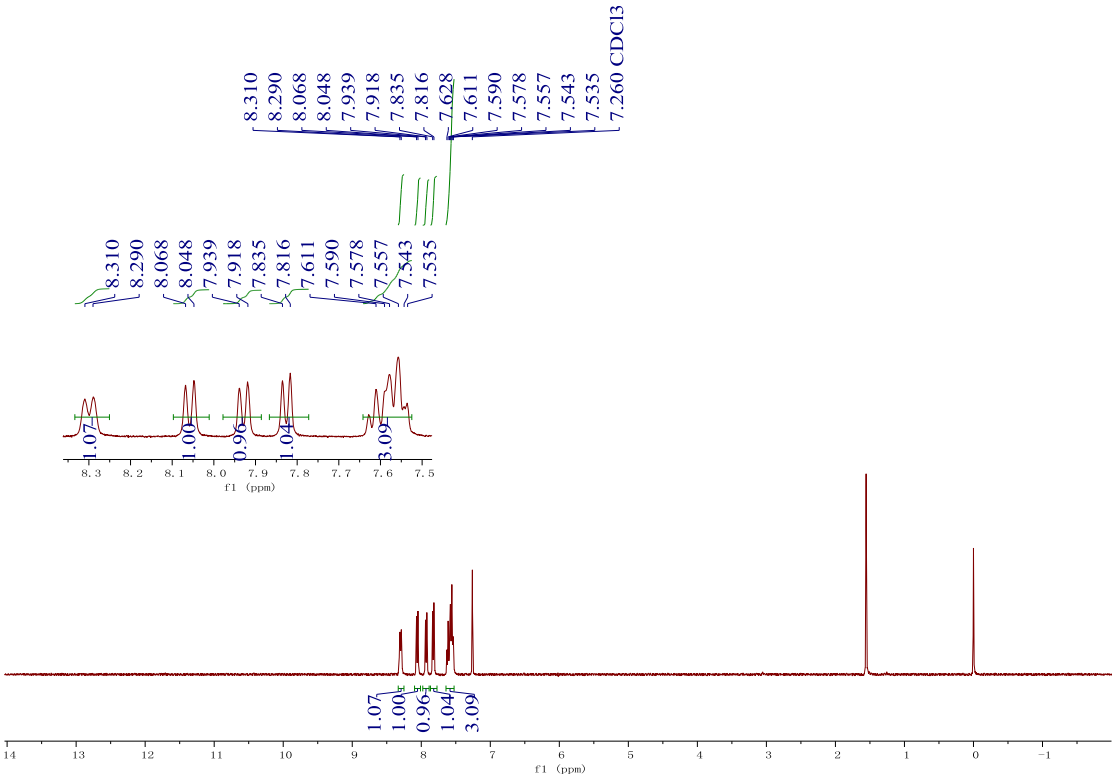


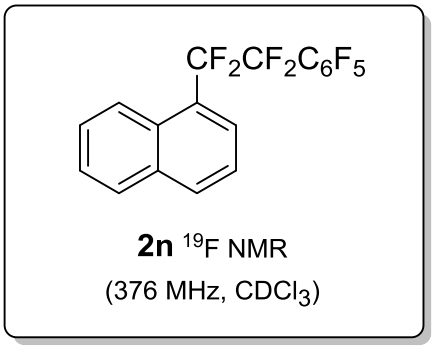


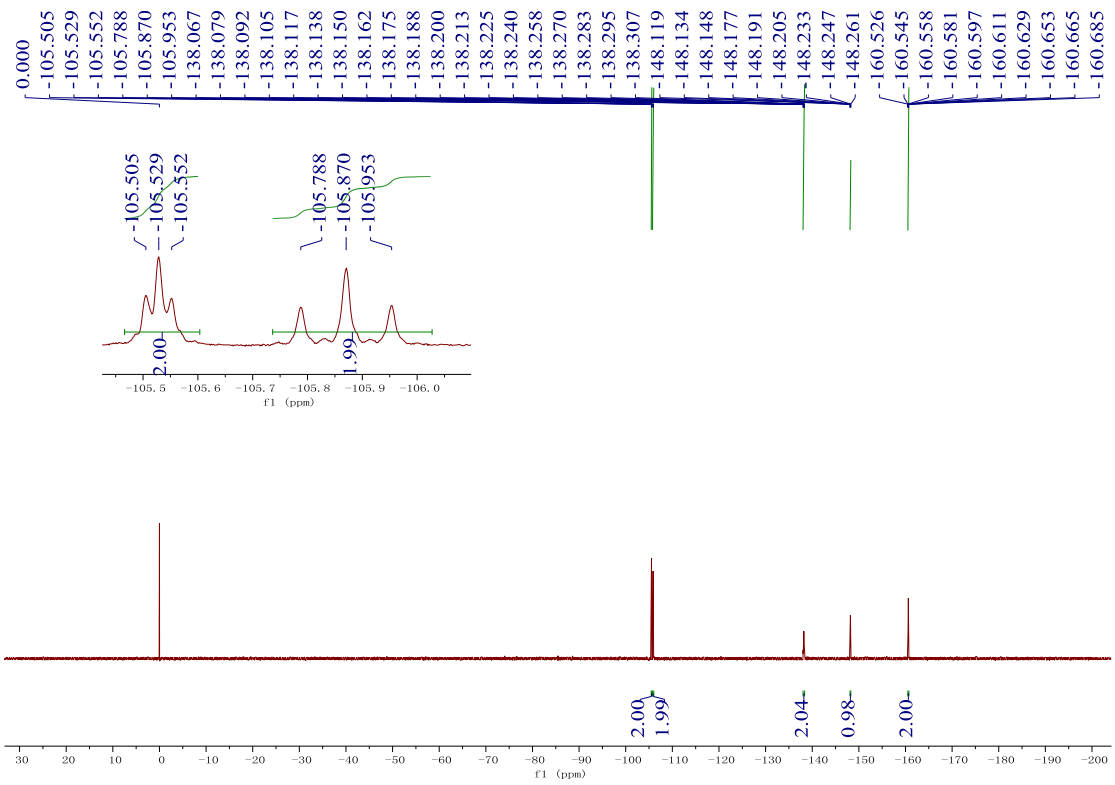
2m ^{13}C NMR
(150 MHz, $CDCl_3$)

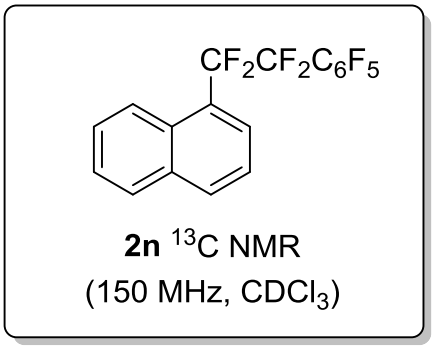


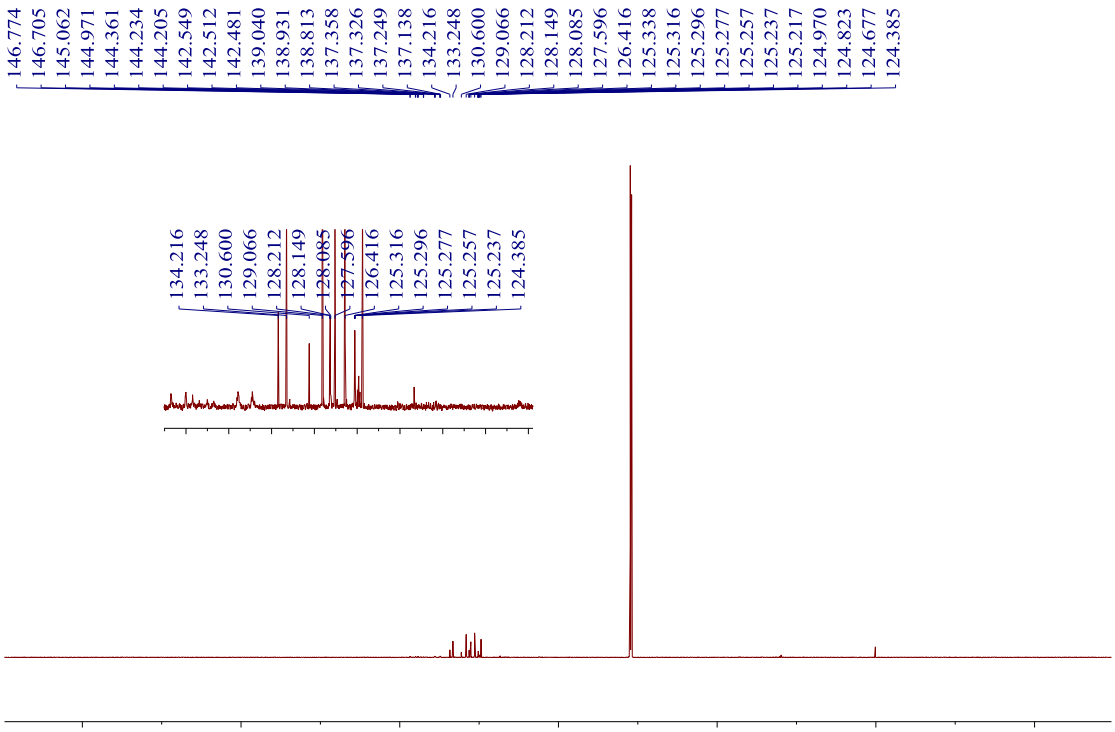

$CF_2CF_2C_6F_5$
2n ^{1}H NMR
(400 MHz, $CDCl_3$)

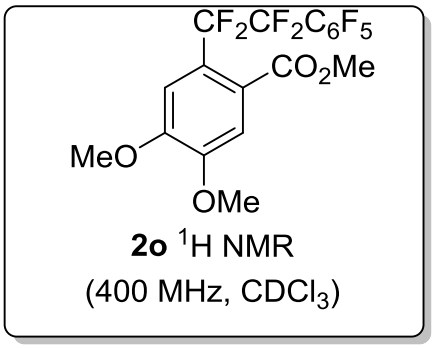

8.310
8.290
8.068
8.048
7.939
7.918
7.835
7.816
7.628
7.611
7.590
7.578
7.557
7.543
7.535
7.260 CDCl3
1.07
1.00
0.96
1.04
3.09
f1 (ppm)


$CF_2CF_2C_6F_5$
2n ^{19}F NMR
(376 MHz, $CDCl_3$)


0.000
-105.505
-105.529
-105.552
-105.788
-105.870
-105.953
-138.067
-138.079
-138.092
-138.105
-138.117
-138.138
-138.150
-138.162
-138.175
-138.188
-138.200
-138.213
-138.225
-138.240
-138.258
-138.270
-138.283
-138.295
-138.307
-148.119
-148.134
-148.148
-148.177
-148.191
-148.205
-148.233
-148.247
-148.261
-160.526
-160.545
-160.558
-160.581
-160.597
-160.611
-160.629
-160.653
-160.665
-160.685
2.00
1.99
f1 (ppm)
2.00
1.99
2.04
0.98
2.00
f1 (ppm)

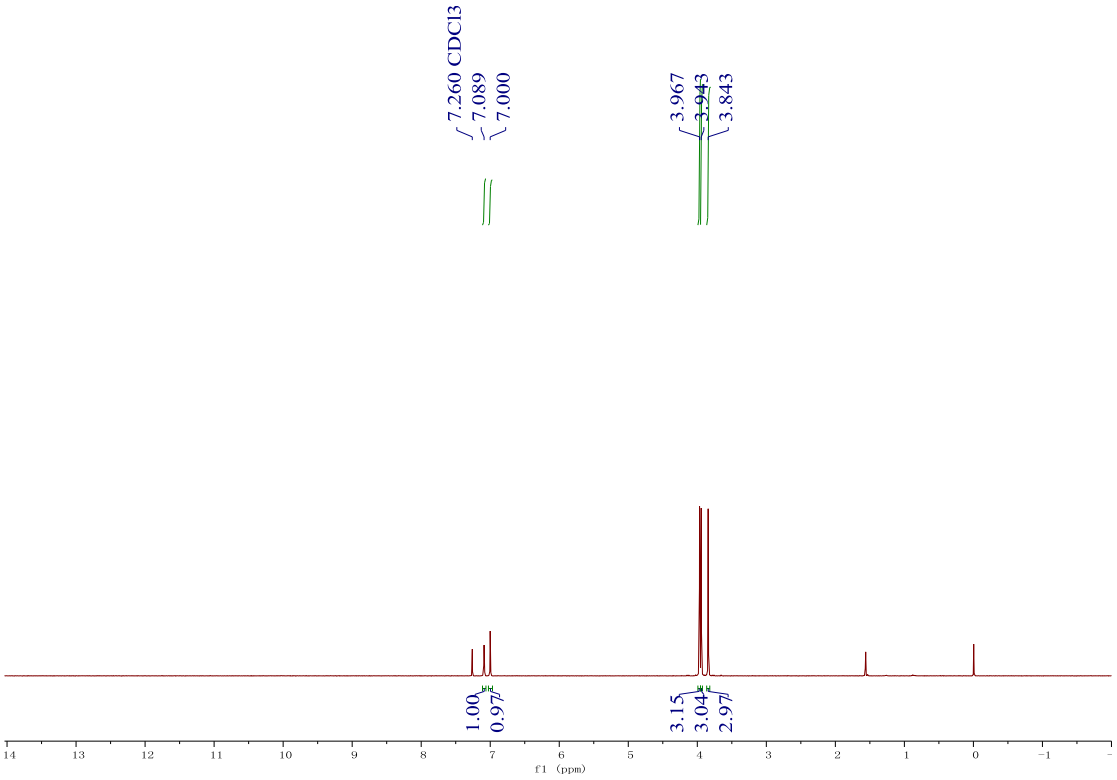

$CF_2CF_2C_6F_5$
2n ^{13}C NMR
(150 MHz, $CDCl_3$)

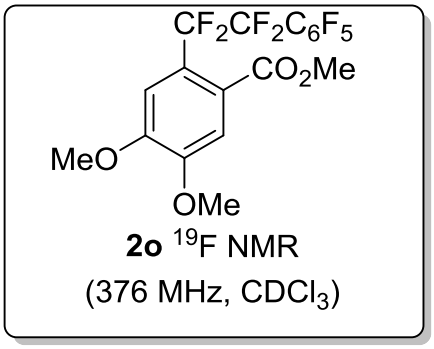

146.774
146.705
145.062
144.971
144.361
144.234
144.205
142.549
142.512
142.481
139.040
138.931
138.813
137.358
137.326
137.249
137.138
134.216
133.248
130.600
129.066
128.212
128.149
128.085
127.596
126.416
125.338
125.316
125.296
125.277
125.257
125.237
125.217
124.970
124.823
124.677
124.385
134.216
133.248
130.600
129.066
128.212
128.149
128.085
127.596
126.416
125.316
125.296
125.277
125.257
125.237
124.385



2o ^{1}H NMR

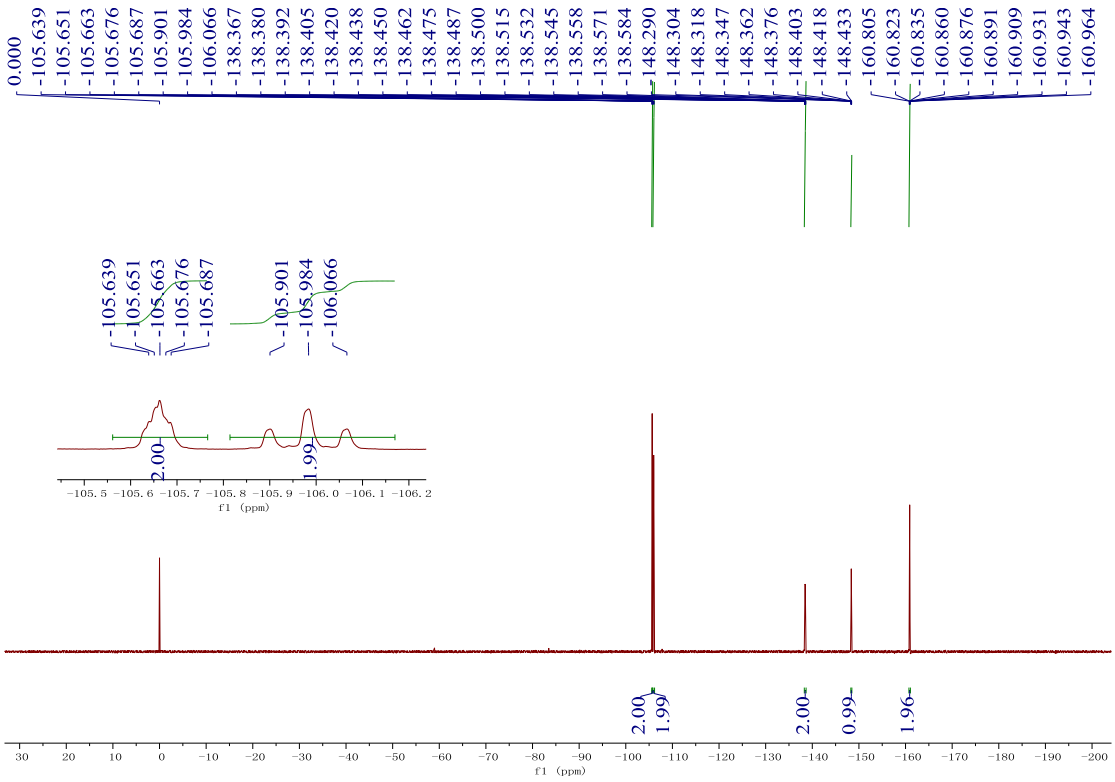
(400 MHz, $CDCl_3$)

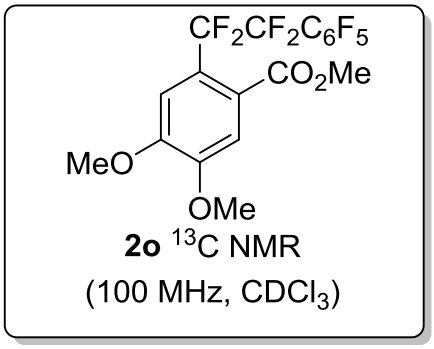




2o ^{19}F NMR

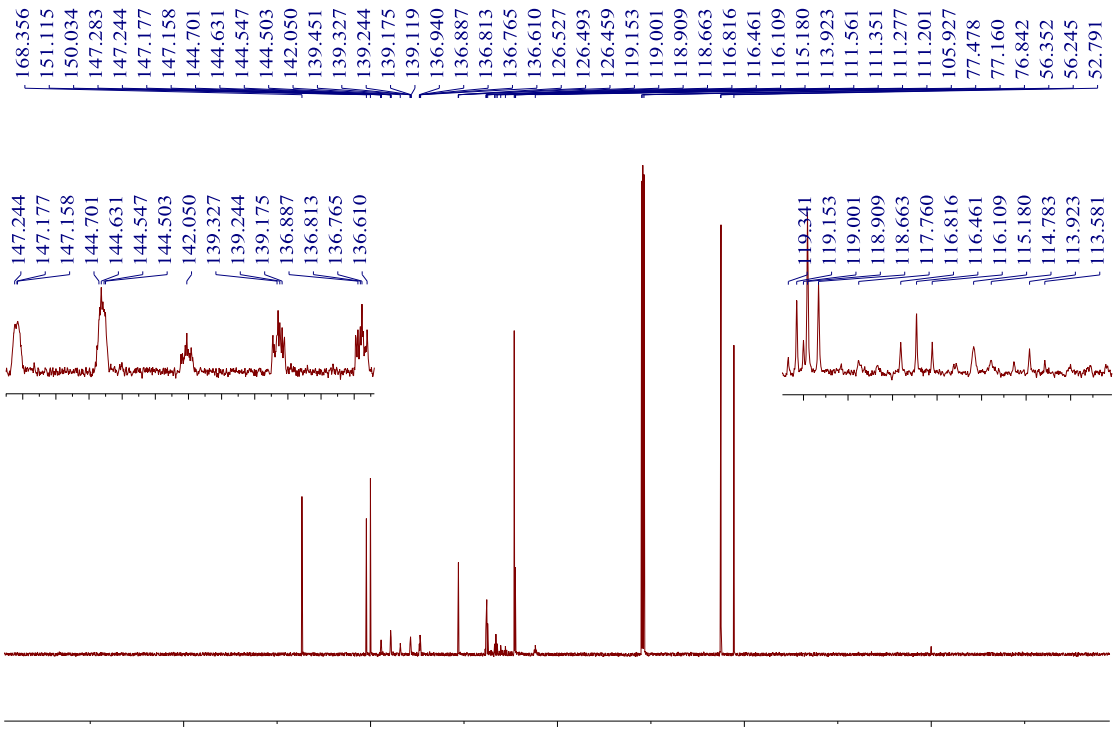
(376 MHz, $CDCl_3$)

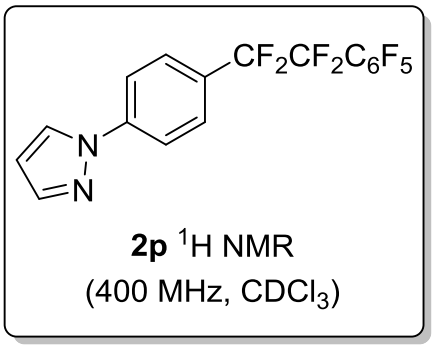


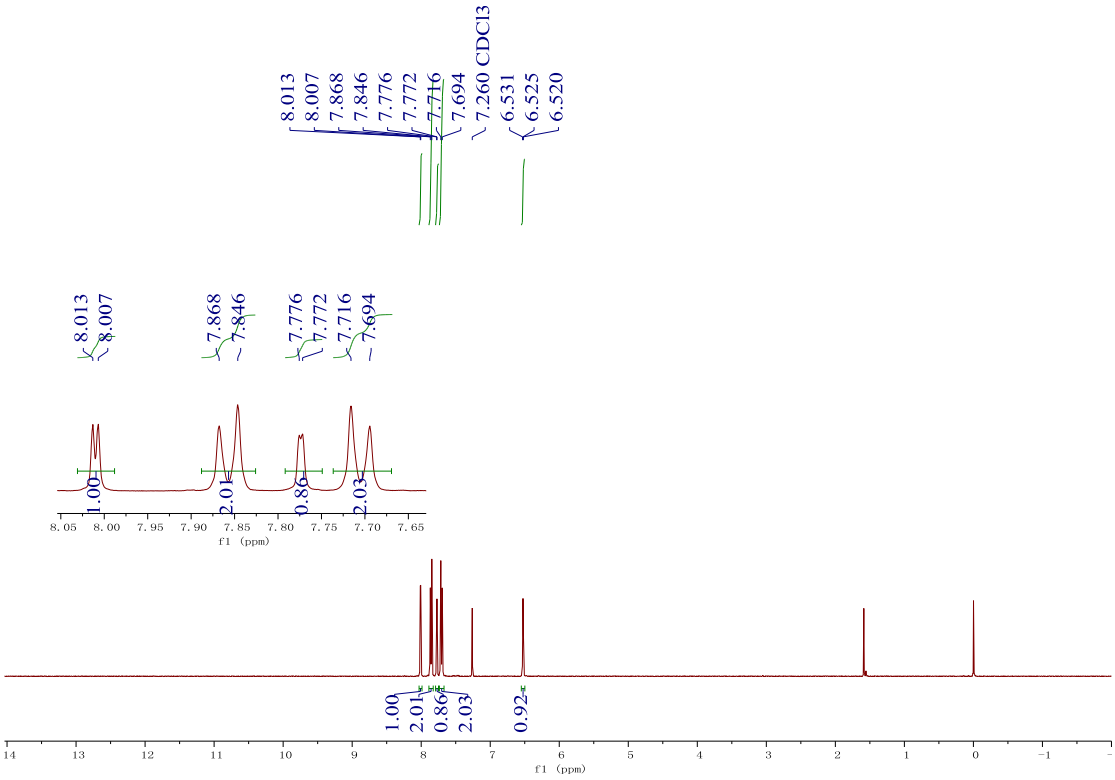


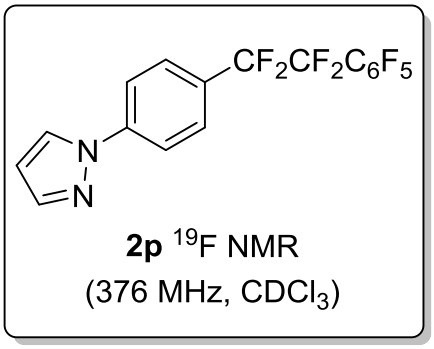
2o ^{13}C NMR

(100 MHz, $CDCl_3$)



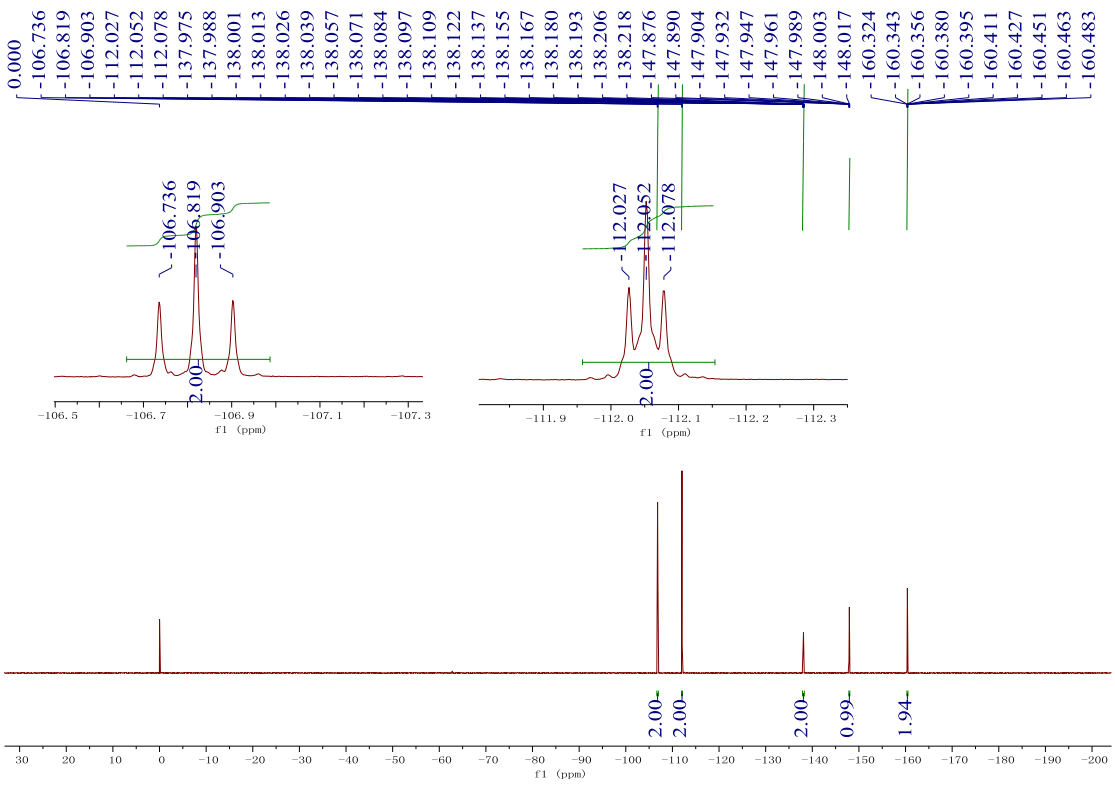

CF2CF2C6F5
N
N
2p 1H NMR
(400 MHz, CDCl3)

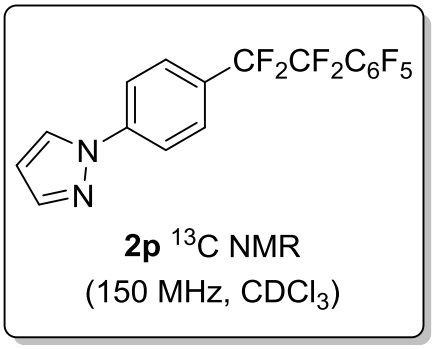

8.013
8.007
7.868
7.846
7.776
7.772
7.716
7.694
7.260 CDCl3
6.531
6.525
6.520
1.00
2.01
0.86
2.03
0.92
f1 (ppm)



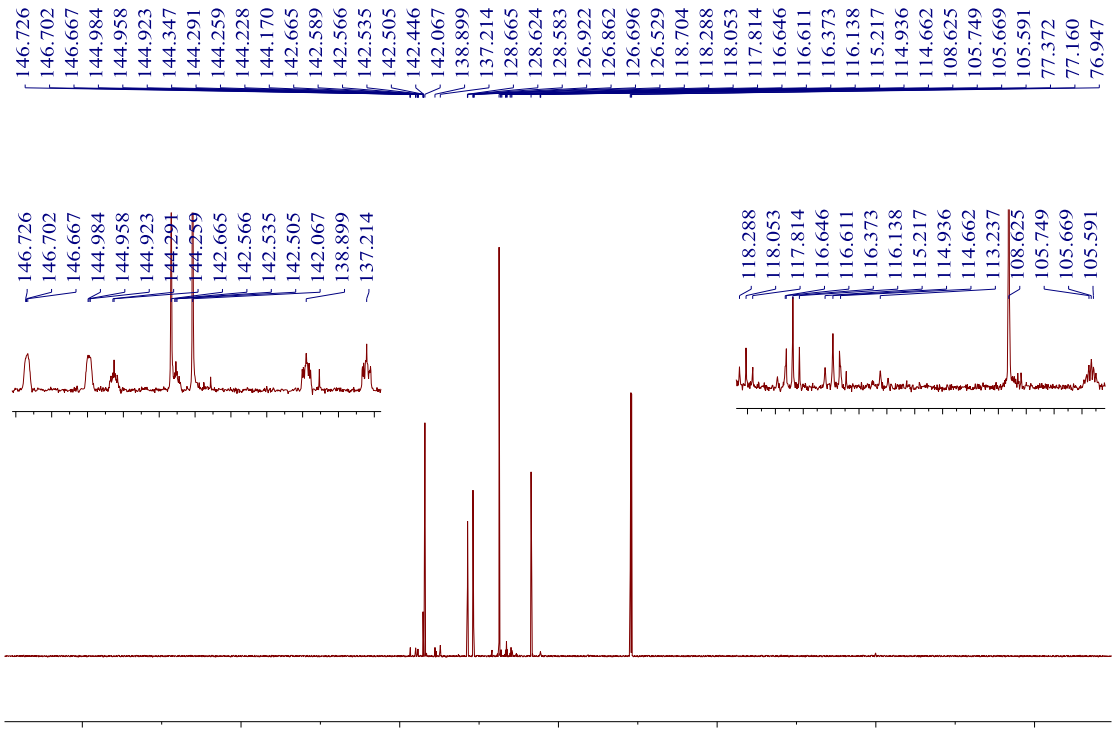
2p ^{19}F NMR

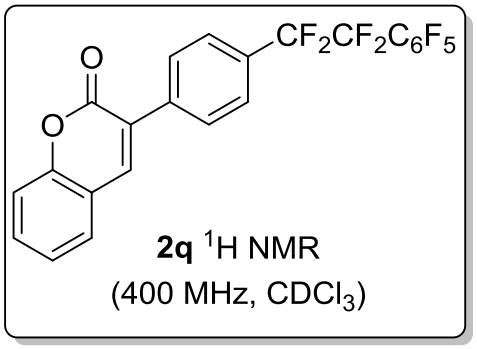
(376 MHz, $CDCl_3$)

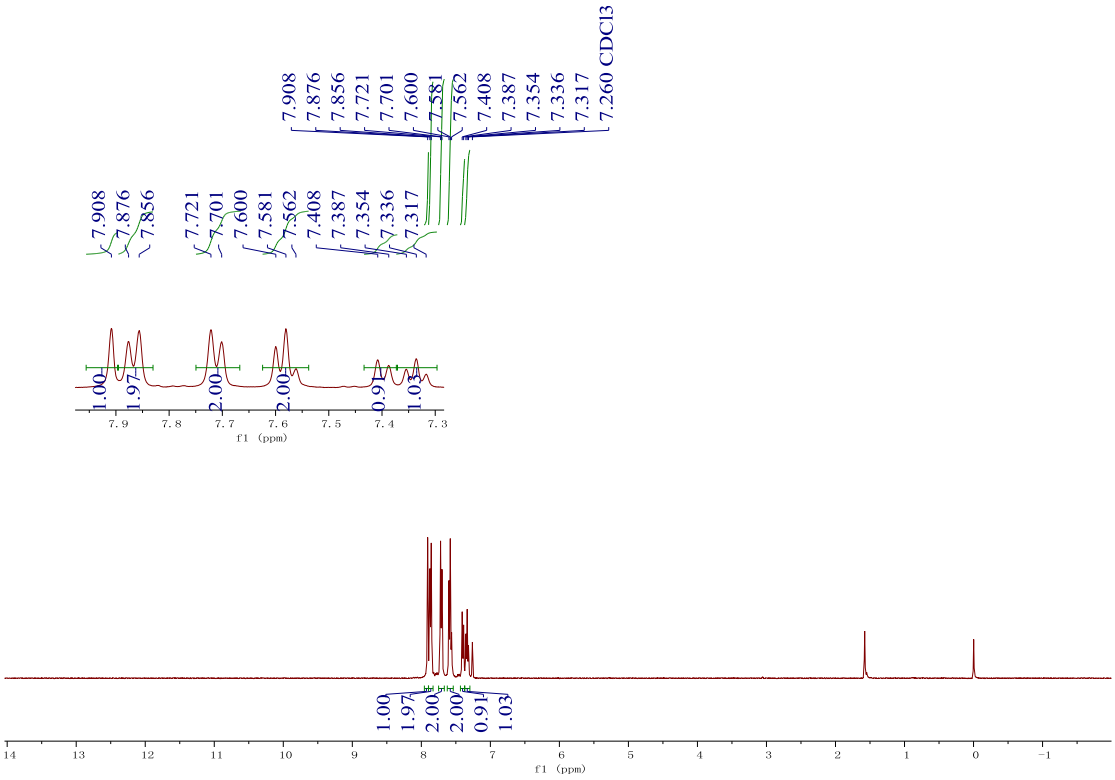


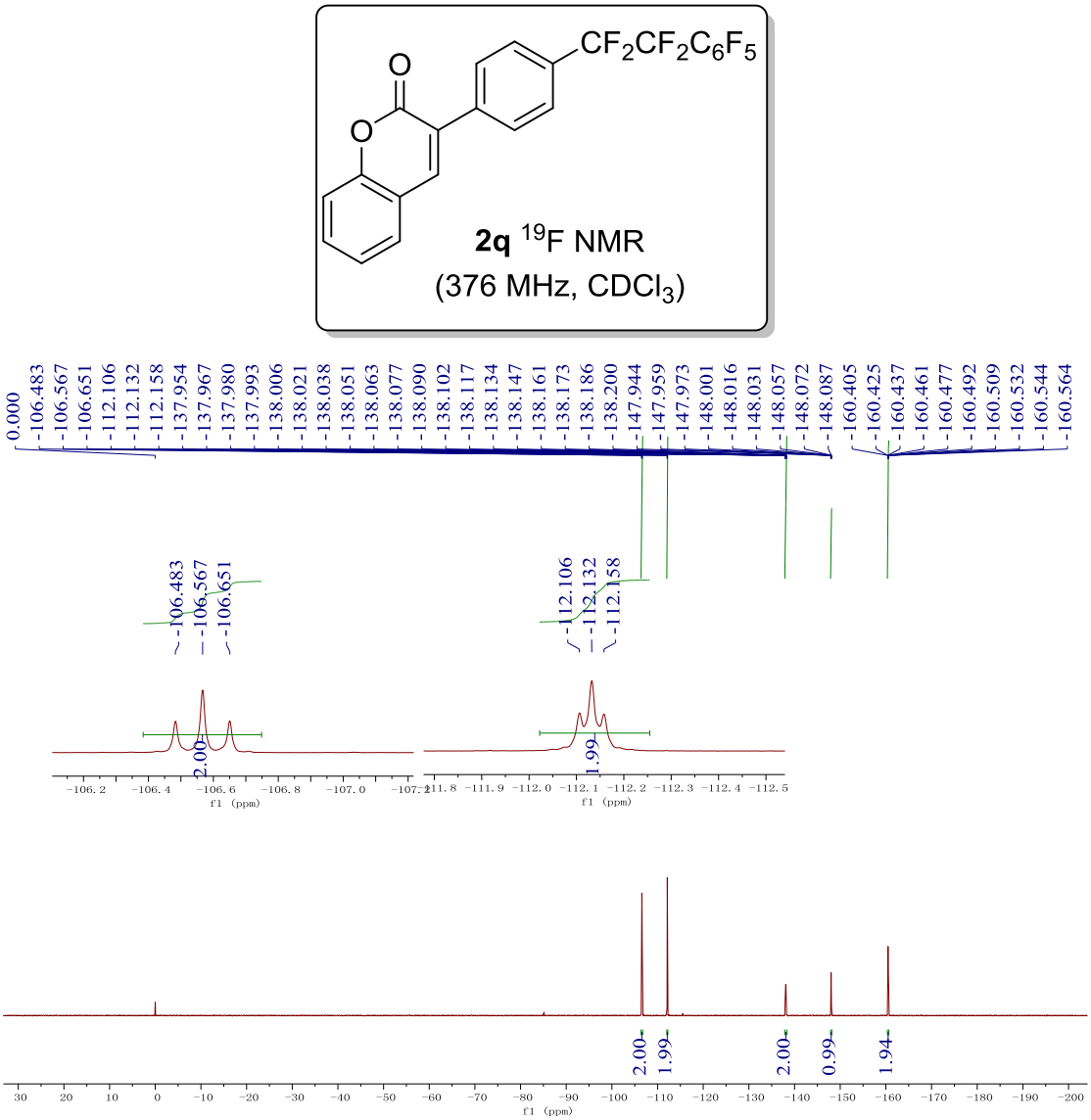


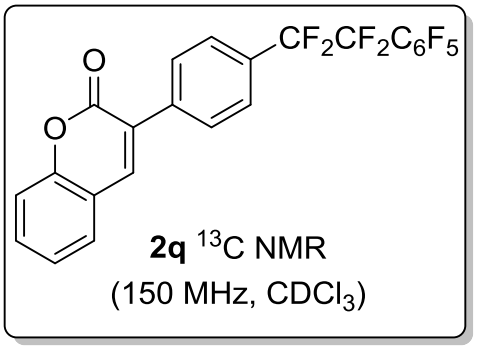
2p ^{13}C NMR
(150 MHz, $CDCl_3$)

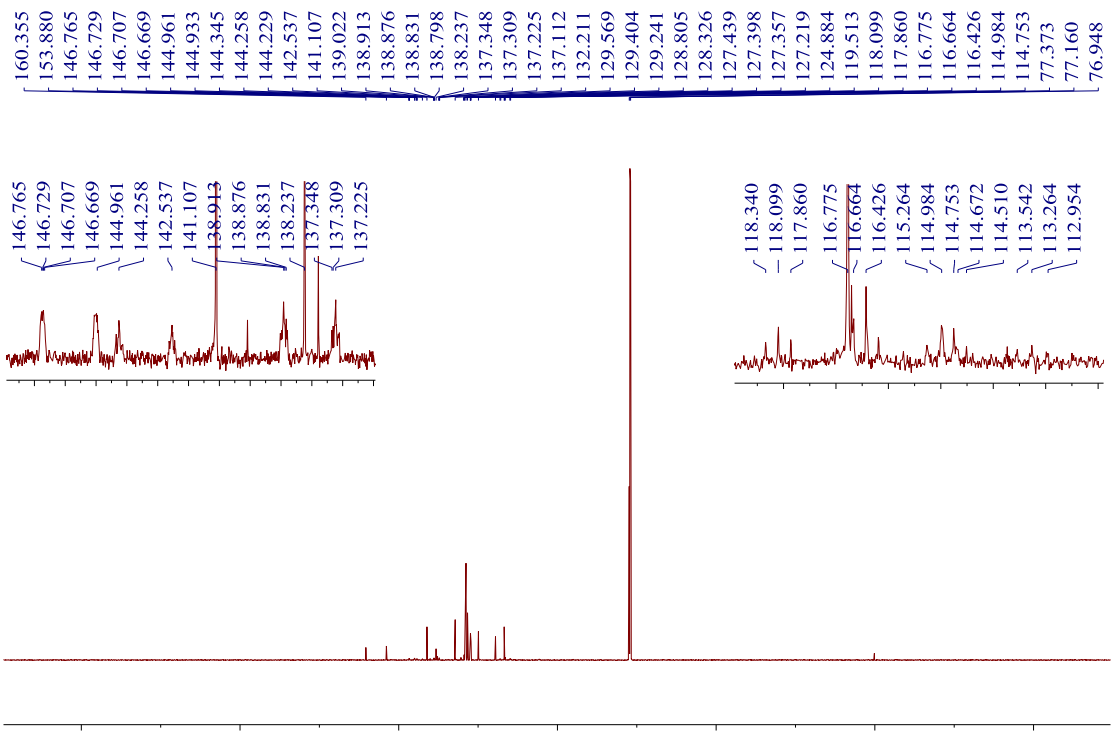


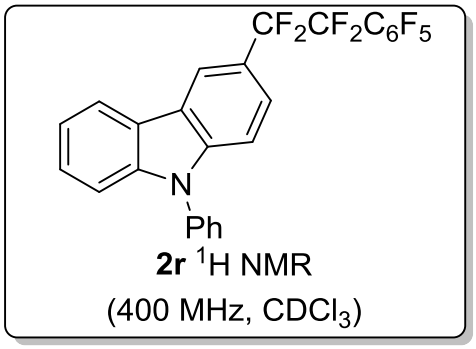

$CF_2CF_2C_6F_5$
O
O
2q ^{1}H NMR
(400 MHz, $CDCl_3$)

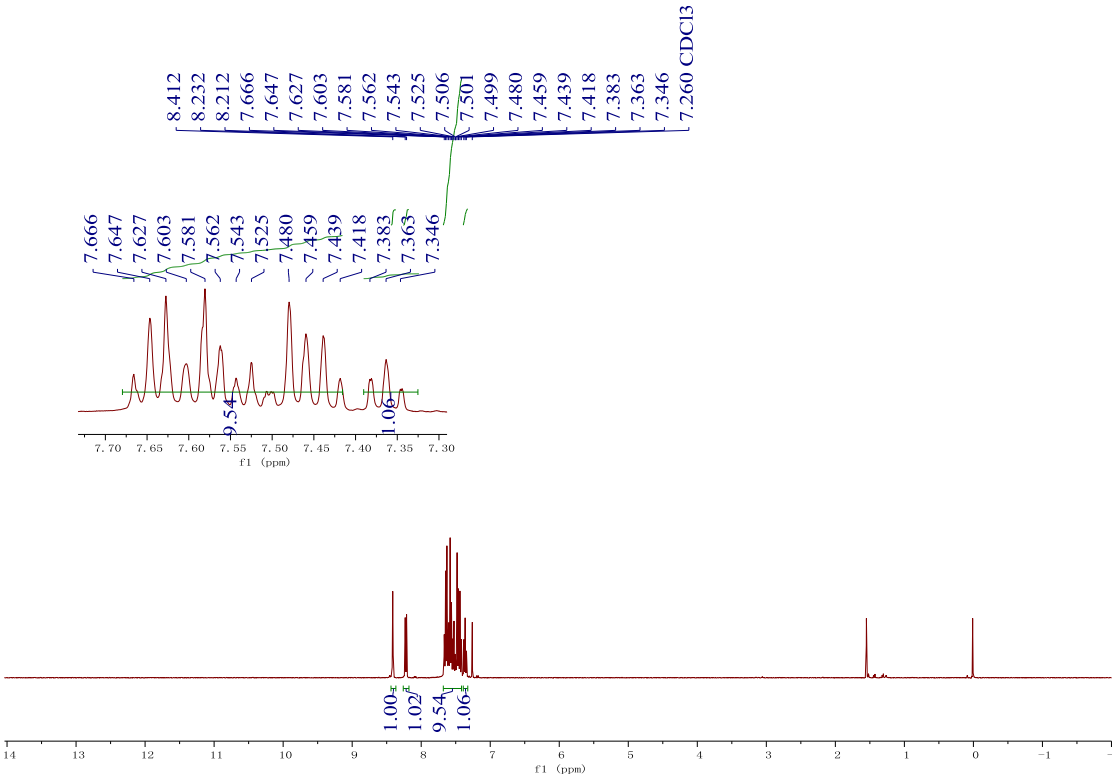

7.908
7.876
7.856
7.721
7.701
7.600
7.581
7.562
7.408
7.387
7.354
7.336
7.317
7.260 CDCl3
1.00
1.97
2.00
2.00
0.91
1.03
f1 (ppm)

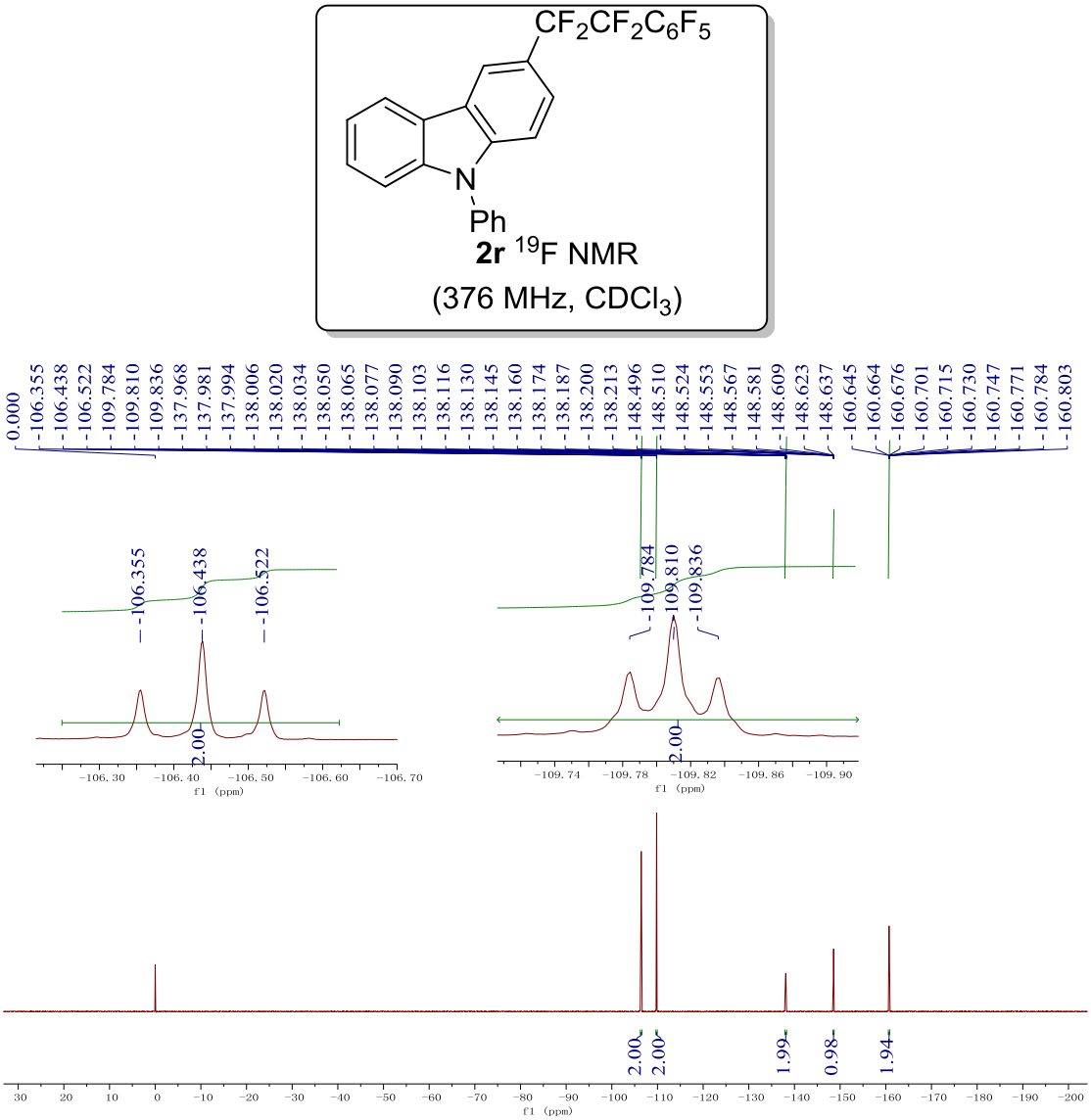

CF2CF2C6F5
O
O
2q 19F NMR
(376 MHz, CDCl3)
0.000
-106.483
-106.567
-106.651
-112.106
-112.132
-112.158
-137.954
-137.967
-137.980
-137.993
-138.006
-138.021
-138.038
-138.051
-138.063
-138.077
-138.090
-138.102
-138.117
-138.134
-138.147
-138.161
-138.173
-138.186
-138.200
-147.944
-147.959
-147.973
-148.001
-148.016
-148.031
-148.057
-148.072
-148.087
-160.405
-160.425
-160.437
-160.461
-160.477
-160.492
-160.509
-160.532
-160.544
-160.564
2.00
1.99
f1 (ppm)
2.00
1.99
2.00
0.99
1.94
f1 (ppm)

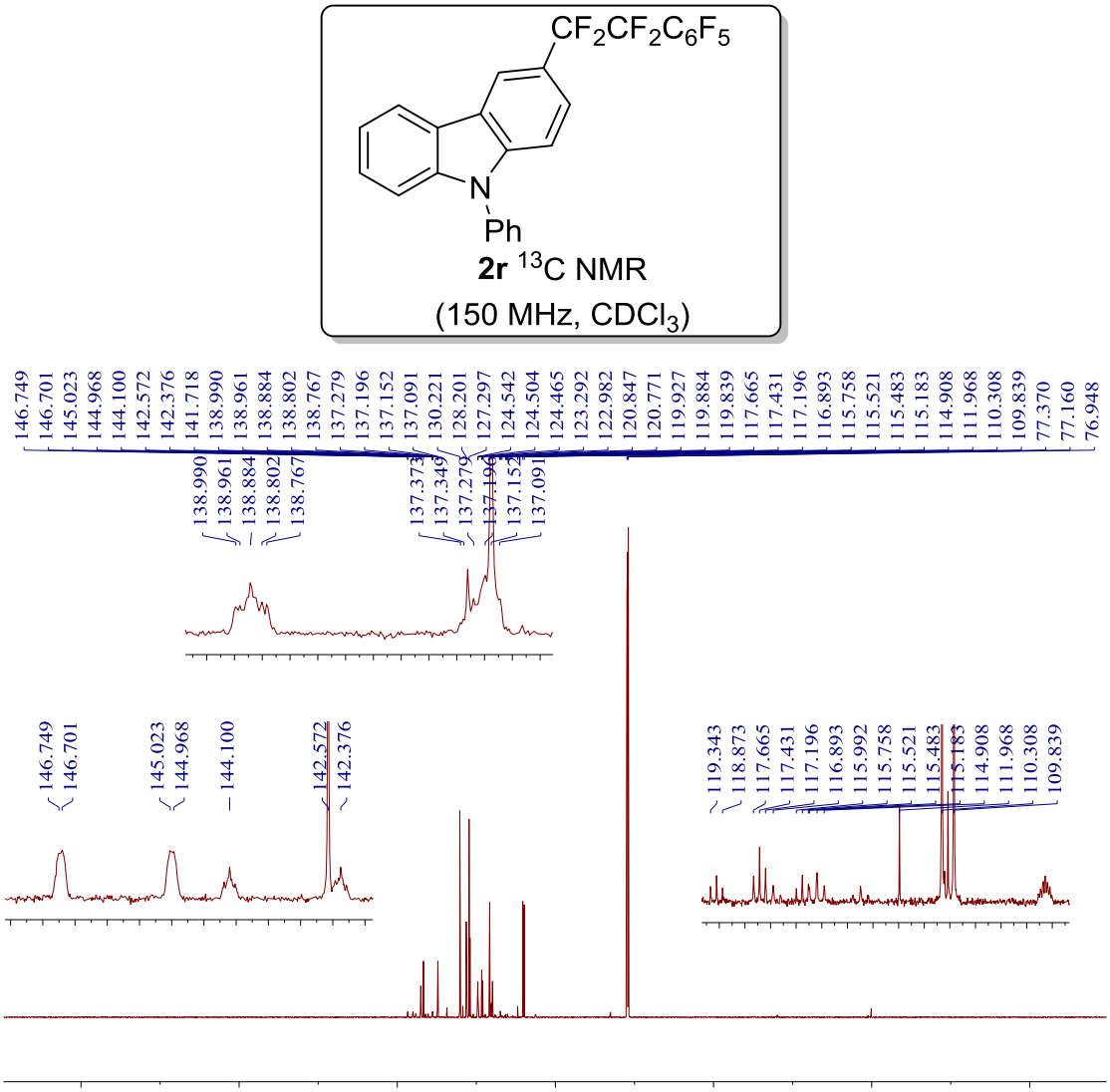

CF2CF2C6F5
O
O
2q 13C NMR
(150 MHz, CDCl3)

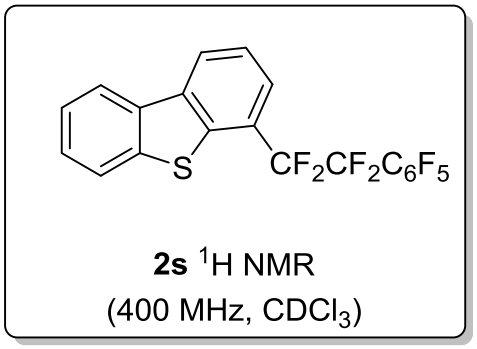

160.355
153.880
146.765
146.729
146.707
146.669
144.961
144.933
144.345
144.258
144.229
142.537
141.107
139.022
138.913
138.876
138.831
138.798
138.237
137.348
137.309
137.225
137.112
132.211
129.569
129.404
129.241
128.805
128.326
127.439
127.398
127.357
127.219
124.884
119.513
118.099
117.860
116.775
116.664
116.426
115.264
114.984
114.753
114.672
114.510
113.542
113.264
112.954
77.373
77.160
76.948

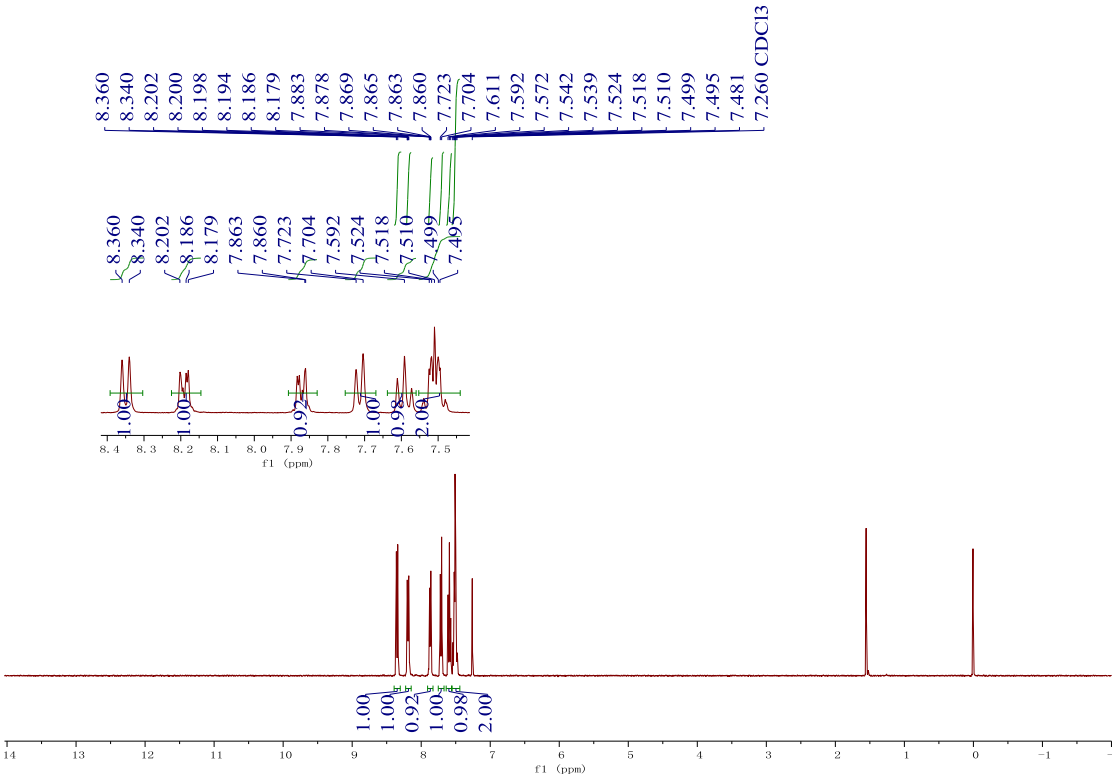

$CF_2CF_2C_6F_5$
N
Ph
2r ^{1}H NMR
(400 MHz, $CDCl_3$)

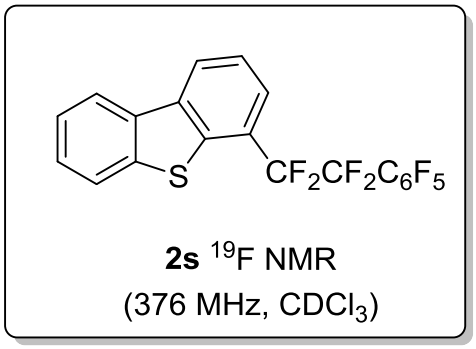

8.412
8.232
8.212
7.666
7.647
7.627
7.603
7.581
7.562
7.543
7.525
7.506
7.501
7.499
7.480
7.459
7.439
7.418
7.383
7.363
7.346
7.260 CDCl3
9.54
1.06
f1 (ppm)
1.00
1.02
9.54
1.06
f1 (ppm)


CF2CF2C6F5
N
Ph
2r 19F NMR
(376 MHz, CDCl3)
f1 (ppm)


CF2CF2C6F5
N
Ph
2r 13C NMR
(150 MHz, CDCl3)

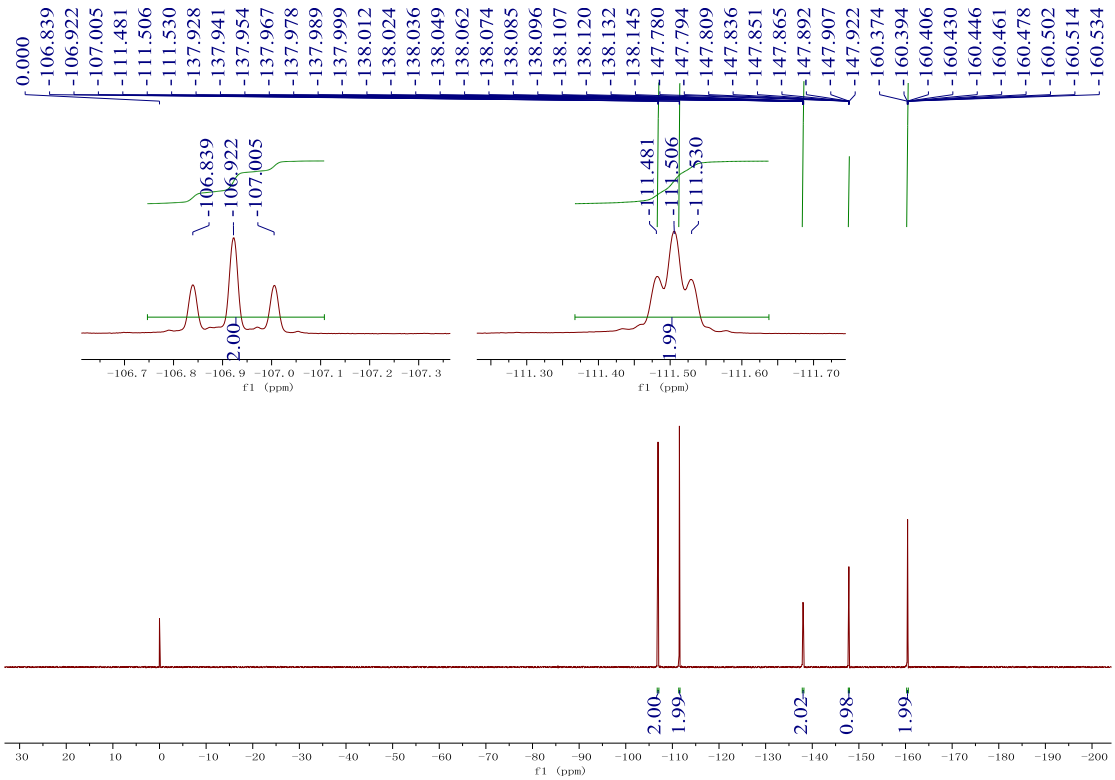

S
$CF_2CF_2C_6F_5$
2s ^{1}H NMR
(400 MHz, $CDCl_3$)

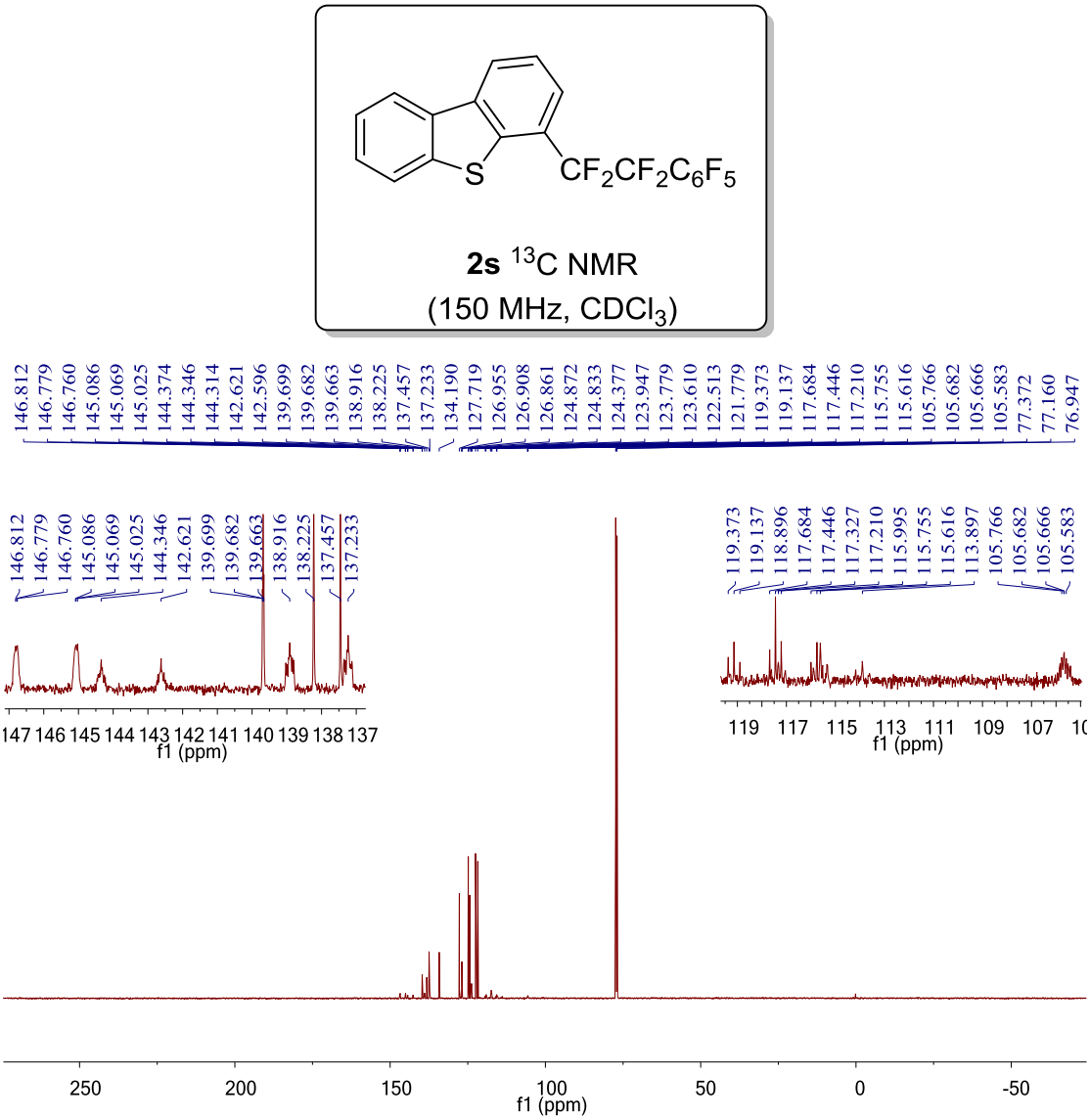

8.360
8.340
8.202
8.200
8.198
8.194
8.186
8.179
7.883
7.878
7.869
7.865
7.863
7.860
7.723
7.704
7.611
7.592
7.572
7.542
7.539
7.524
7.518
7.510
7.499
7.495
7.481
7.260 CDCl3
1.00
1.00
0.92
1.00
0.98
2.00
f1 (ppm)

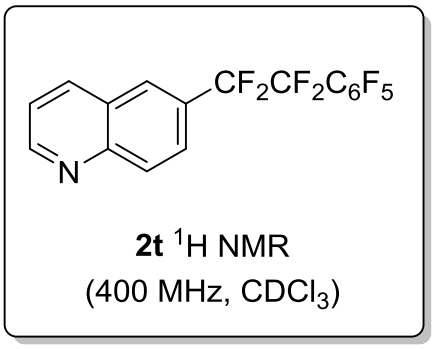


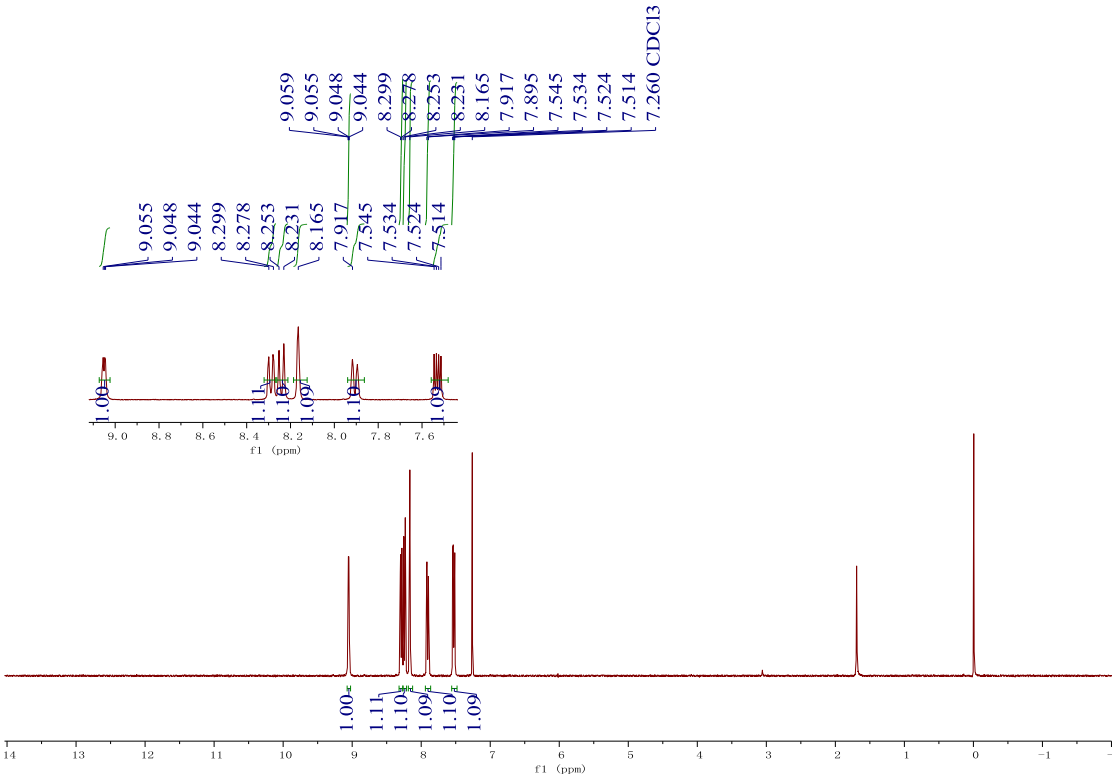
2s ^{19}F NMR

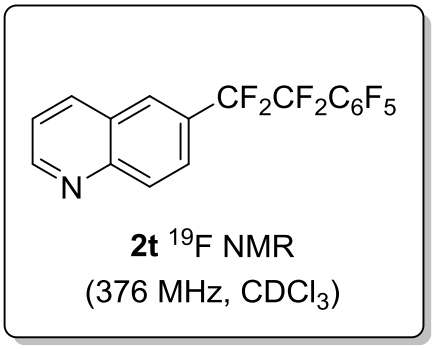
(376 MHz, $CDCl_3$)




S
CF2CF2C6F5
2s 13C NMR
(150 MHz, CDCl3)
146.812
146.779
146.760
145.086
145.069
145.025
144.374
144.346
144.314
142.621
142.596
139.699
139.682
139.663
138.916
138.225
137.457
137.233
134.190
127.719
126.955
126.908
126.861
124.872
124.833
124.377
123.947
123.779
123.610
122.513
121.779
119.373
119.137
117.684
117.446
117.210
115.755
115.616
105.766
105.682
105.666
105.583
77.372
77.160
76.947
147 146 145 144 143 142 141 140 139 138 137
f1 (ppm)
119 117 115 113 111 109 107
f1 (ppm)
250 200 150 100 50 0 -50
f1 (ppm)

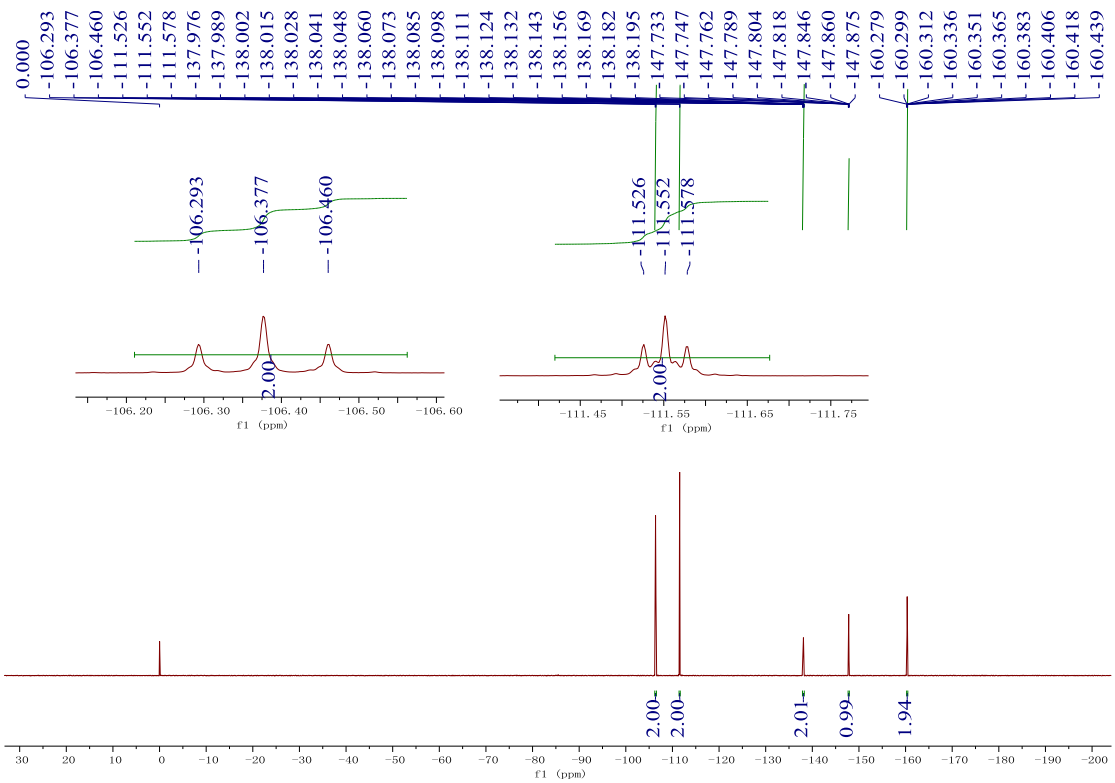

CF2CF2C6F5
N
2t 1H NMR
(400 MHz, CDCl3)

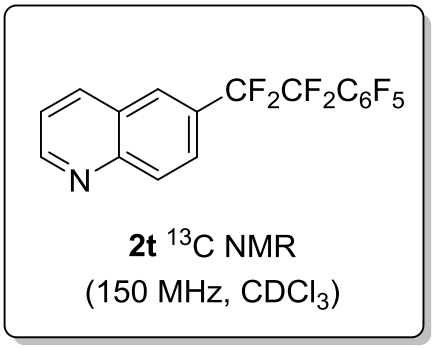

9.059
9.055
9.048
9.044
8.299
8.278
8.253
8.231
8.165
7.917
7.895
7.545
7.534
7.524
7.514
7.260 CDCl3
f1 (ppm)



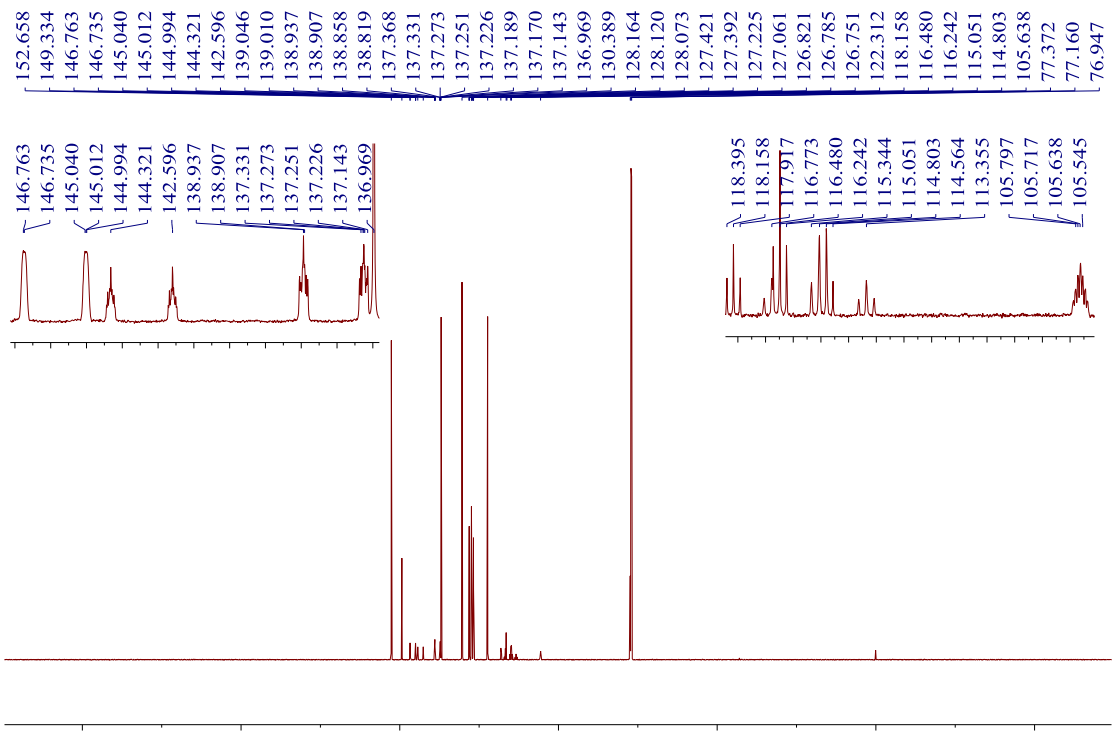
2t ^{19}F NMR

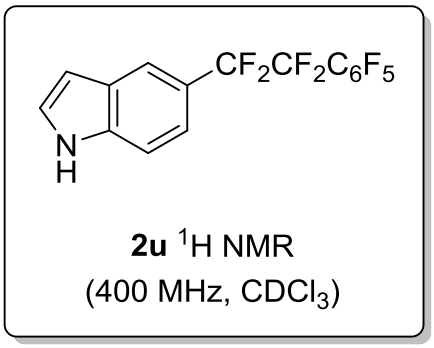
(376 MHz, $CDCl_3$)

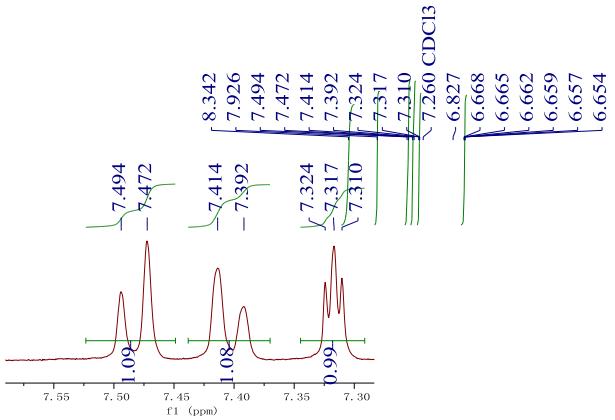


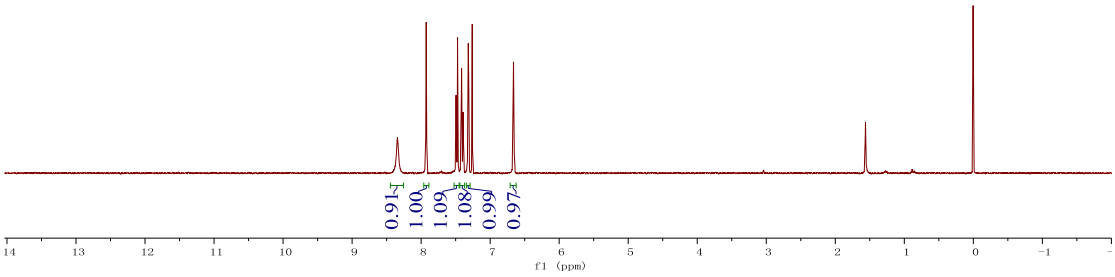


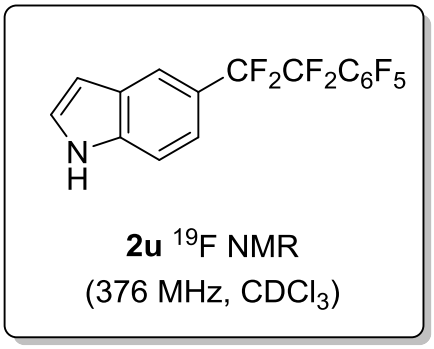
2t ^{13}C NMR
(150 MHz, $CDCl_3$)



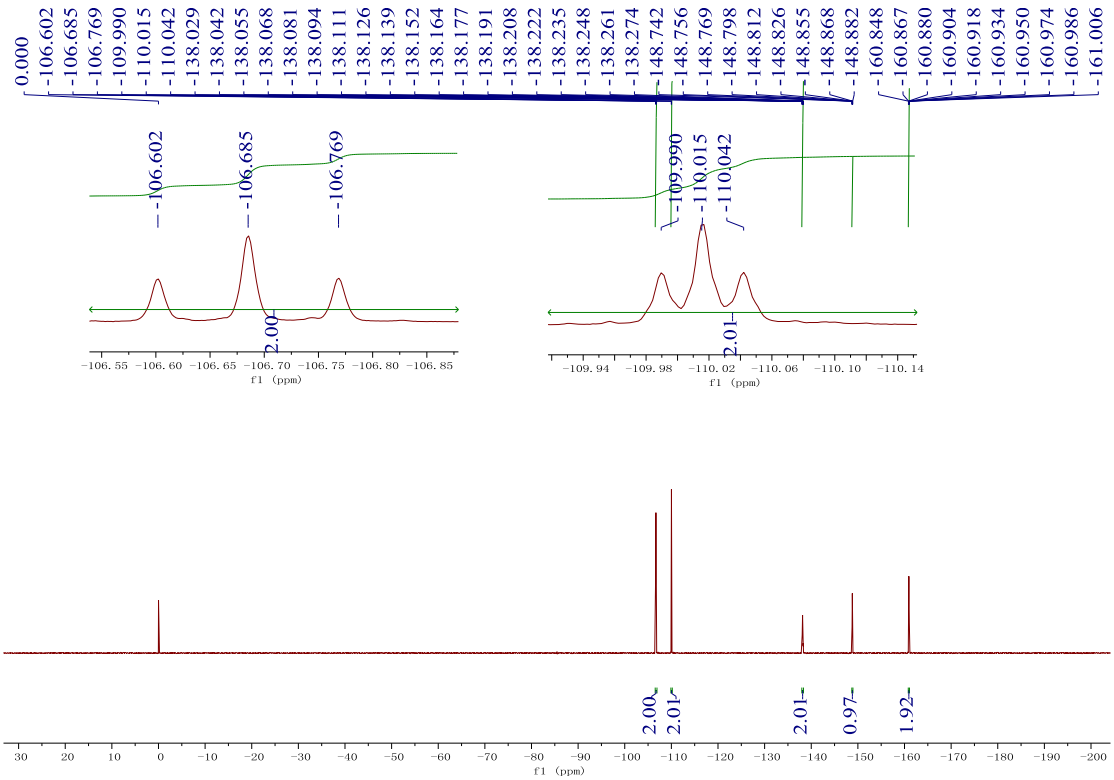

CF2CF2C6F5
N
H
2u 1H NMR
(400 MHz, CDCl3)

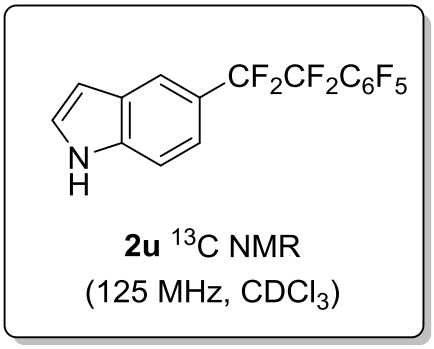

8.342
7.926
7.494
7.472
7.414
7.392
7.324
7.317
7.310
7.260 CDCl3
6.827
6.668
6.665
6.662
6.659
6.657
6.654
1.09
1.08
0.99
f1 (ppm)


0.91
1.00
1.09
1.08
0.99
0.97
f1 (ppm)

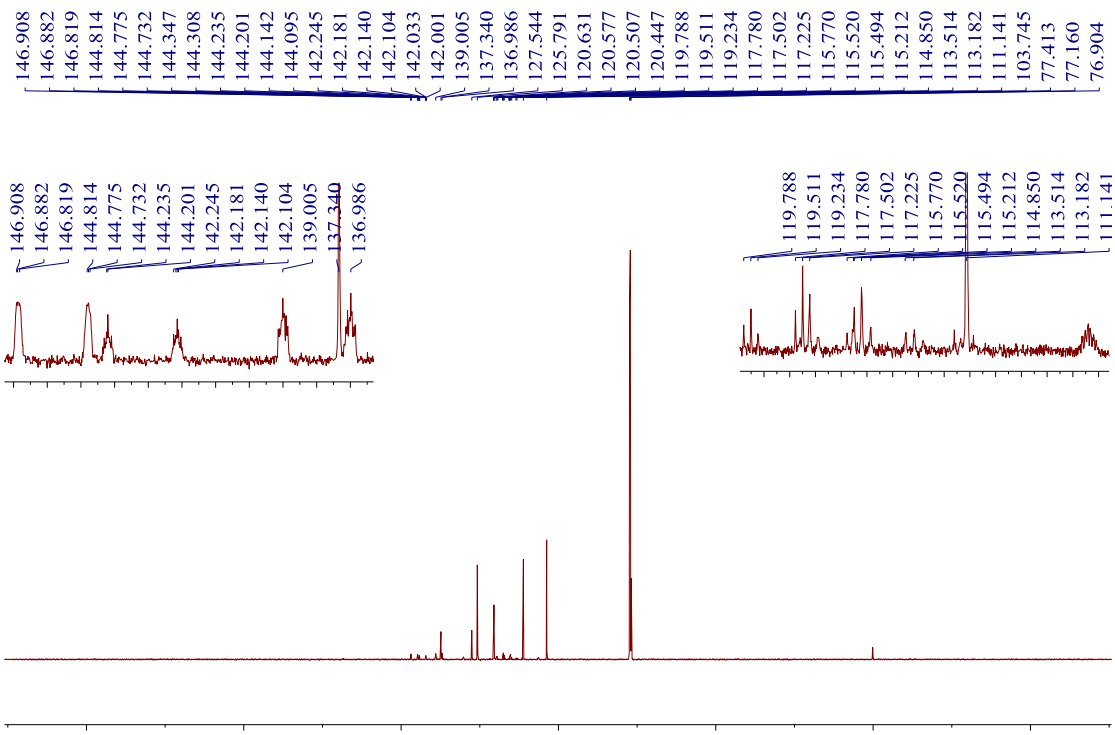


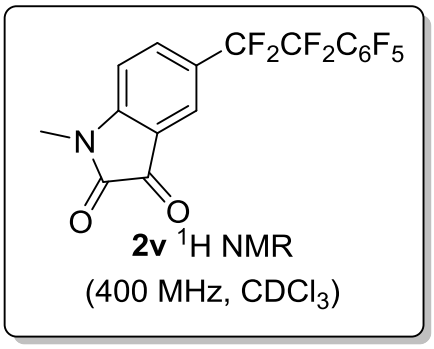
2u ^{19}F NMR
(376 MHz, $CDCl_3$)

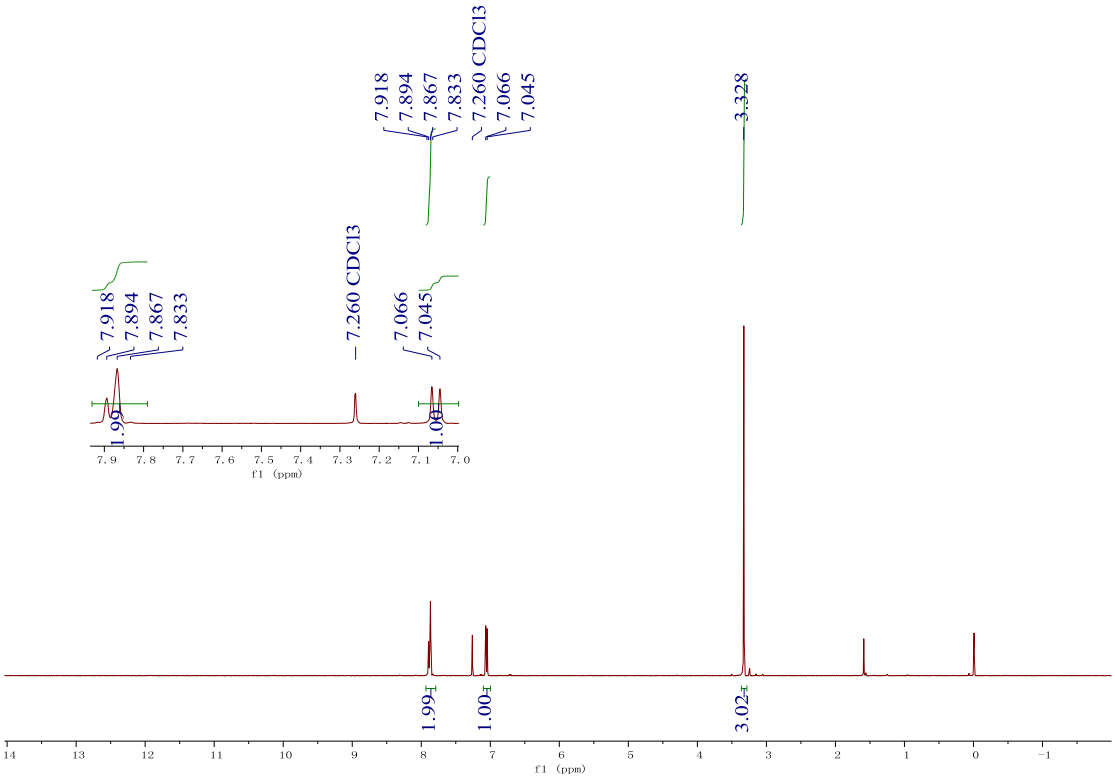


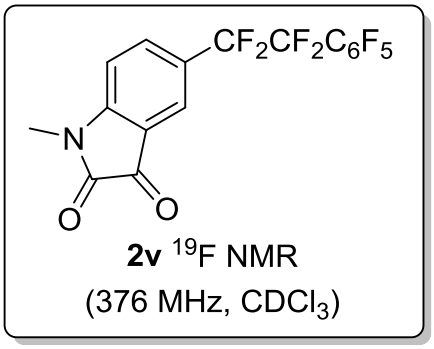


2u ^{13}C NMR
(125 MHz, $CDCl_3$)



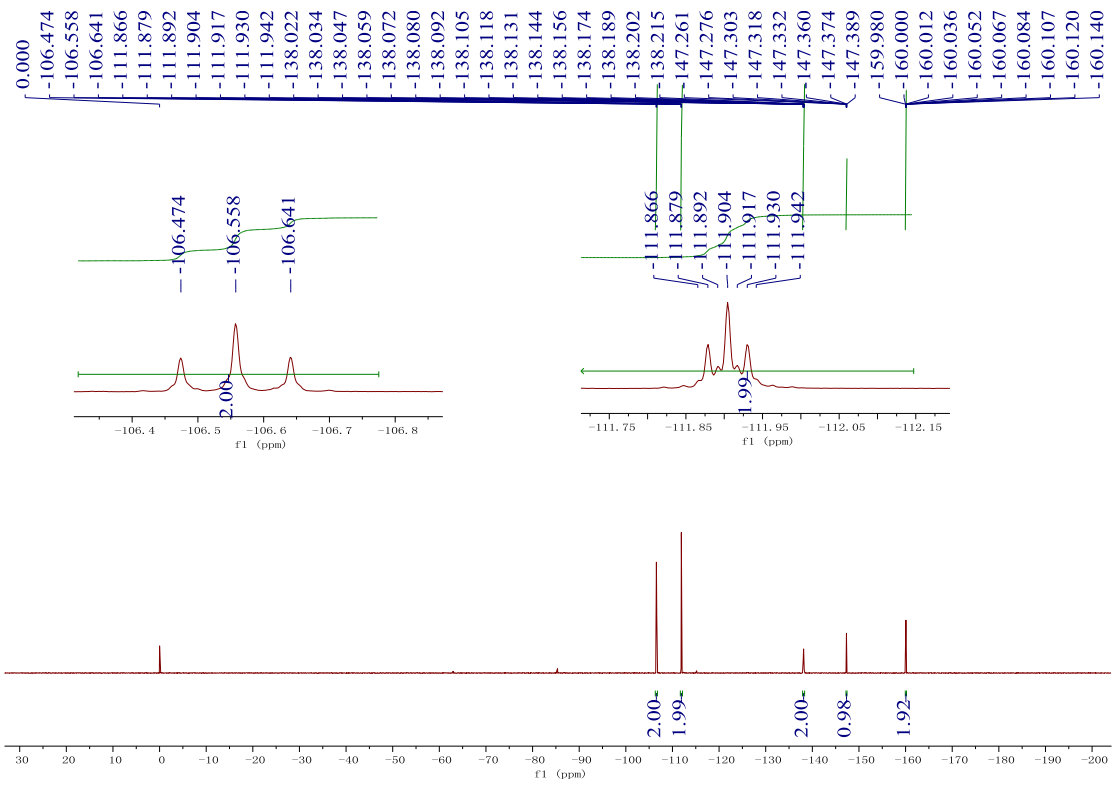

CF2CF2C6F5
N
O
O
2v 1H NMR
(400 MHz, CDCl3)

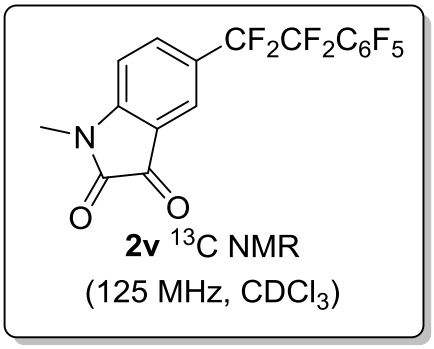

7.918
7.894
7.867
7.833
7.260 CDCl3
7.066
7.045
3.328
1.99
1.00
3.02
f1 (ppm)



2v ^{19}F NMR

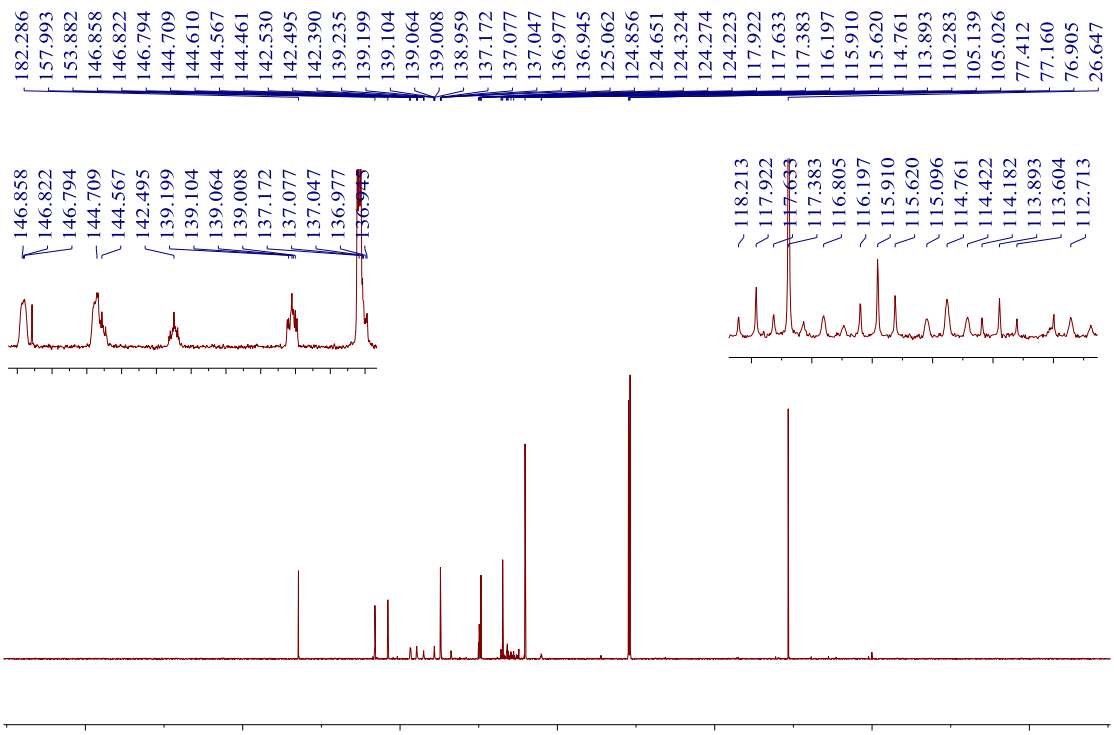
(376 MHz, $CDCl_3$)

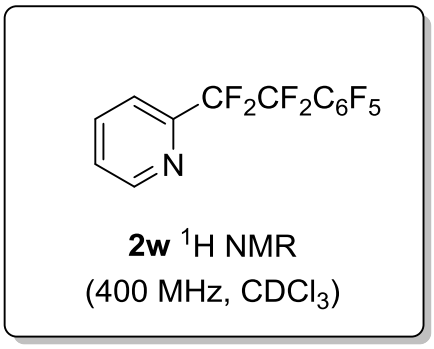


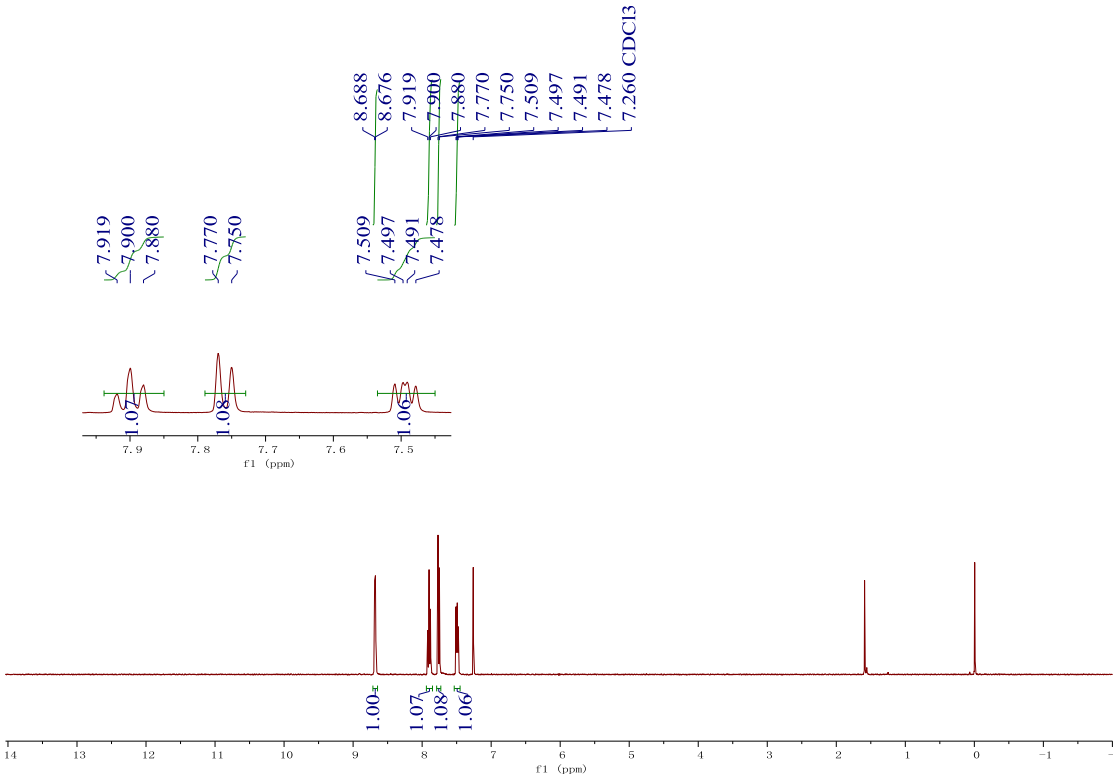


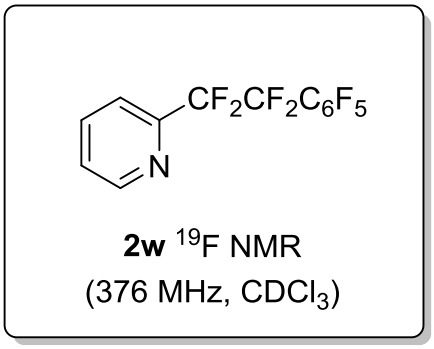
2v ^{13}C NMR

(125 MHz, $CDCl_3$)

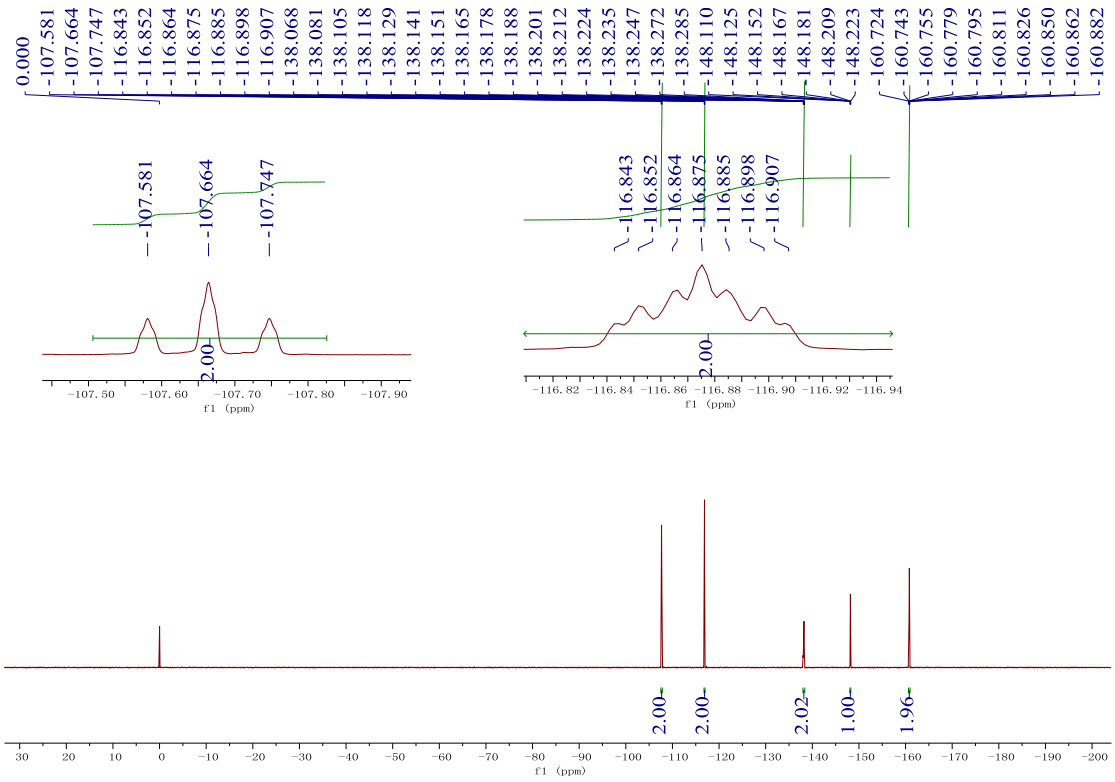


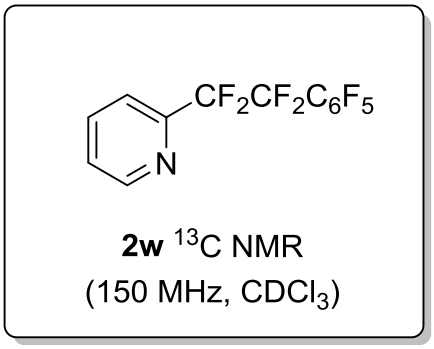

CF2CF2C6F5
N
2w 1H NMR
(400 MHz, CDCl3)

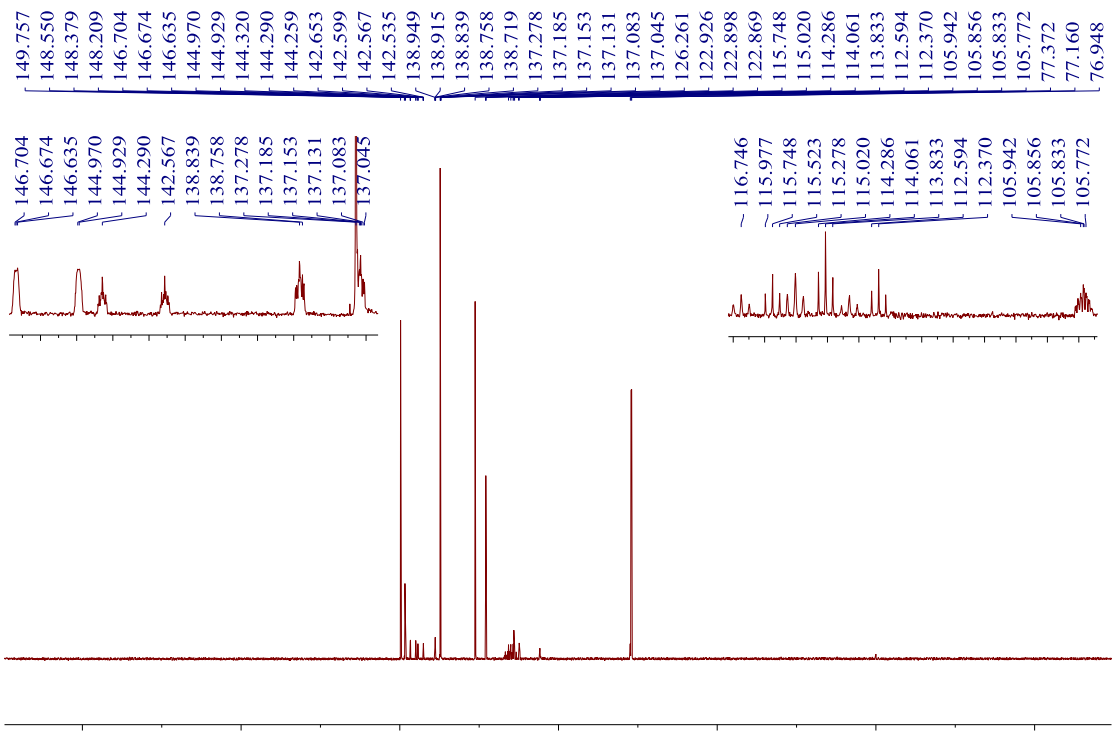

8.688
8.676
7.919
7.900
7.880
7.770
7.750
7.509
7.497
7.491
7.478
7.260 CDCl3
1.07
1.08
1.06
1.00
1.07
1.08
1.06
f1 (ppm)

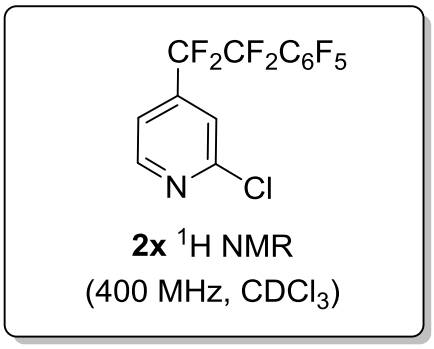


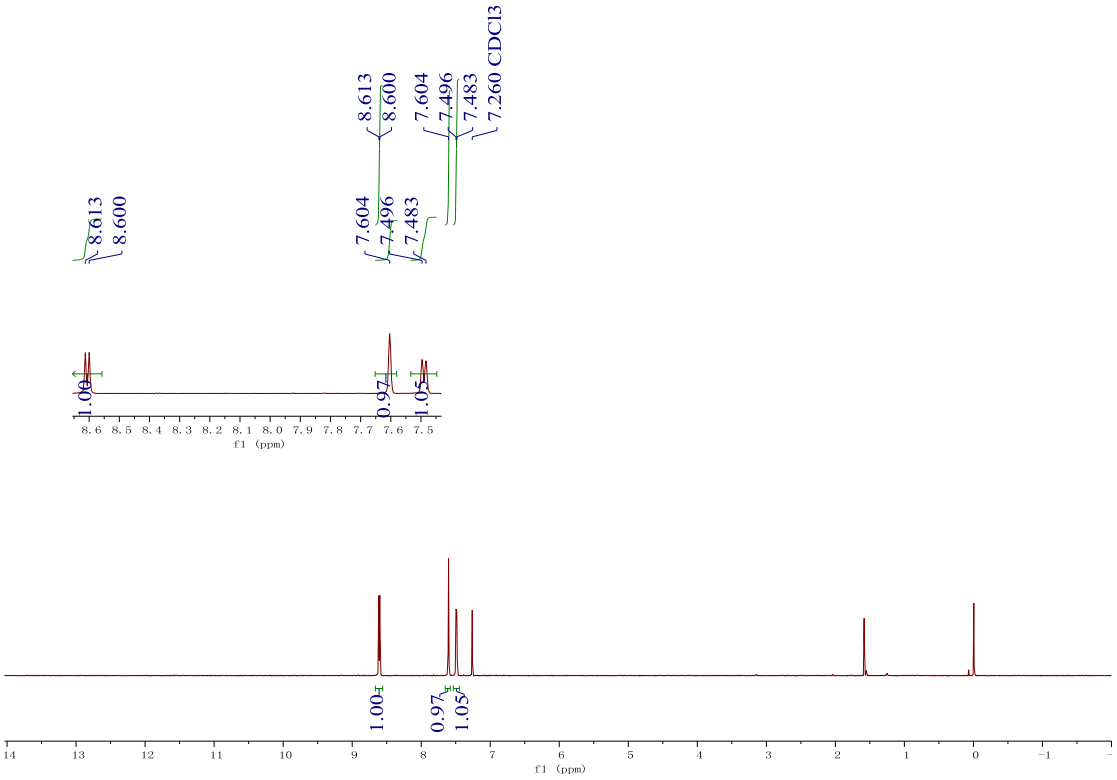
2w ^{19}F NMR
(376 MHz, $CDCl_3$)

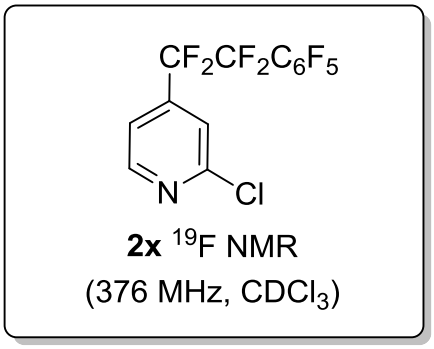


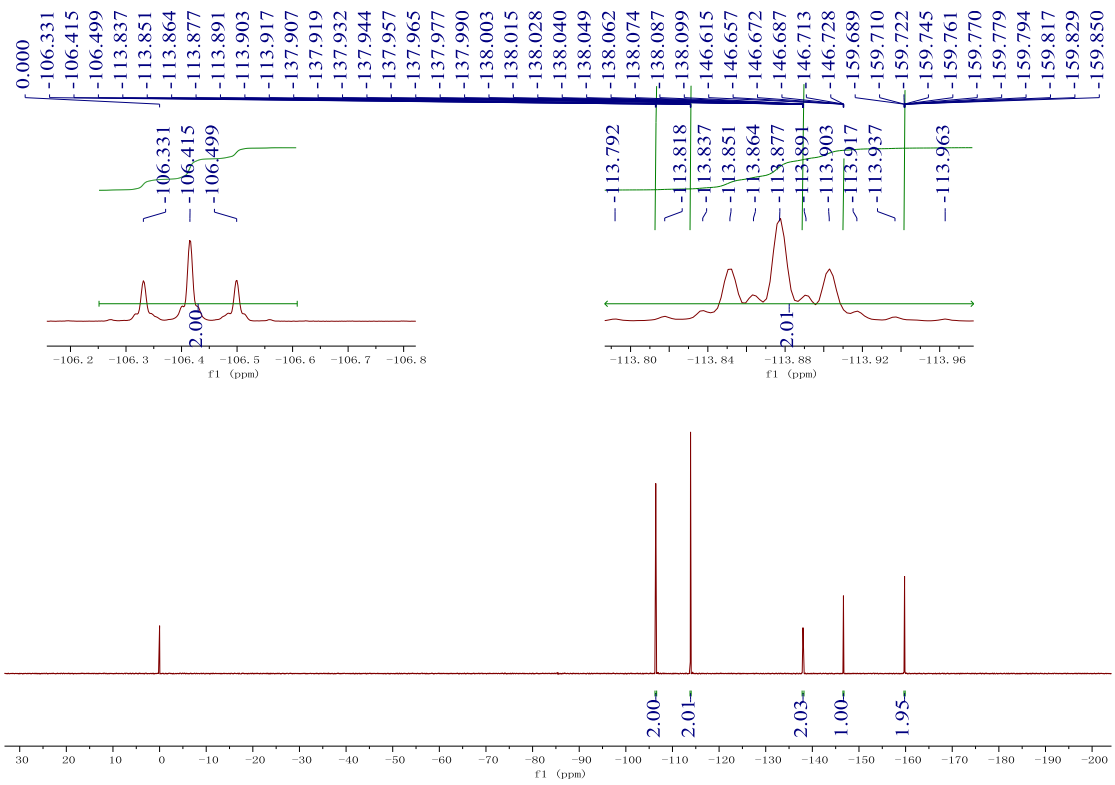

CF2CF2C6F5
N
2w 13C NMR
(150 MHz, CDCl3)

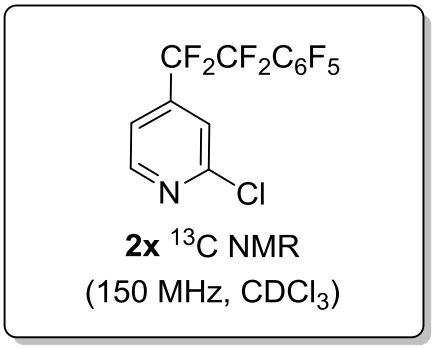

149.757
148.550
148.379
148.209
146.704
146.674
146.635
144.970
144.929
144.320
144.290
144.259
142.653
142.599
142.567
142.535
138.949
138.915
138.839
138.758
138.719
137.278
137.185
137.153
137.131
137.083
137.045
126.261
122.926
122.898
122.869
115.748
115.020
114.286
114.061
113.833
112.594
112.370
105.942
105.856
105.833
105.772
77.372
77.160
76.948

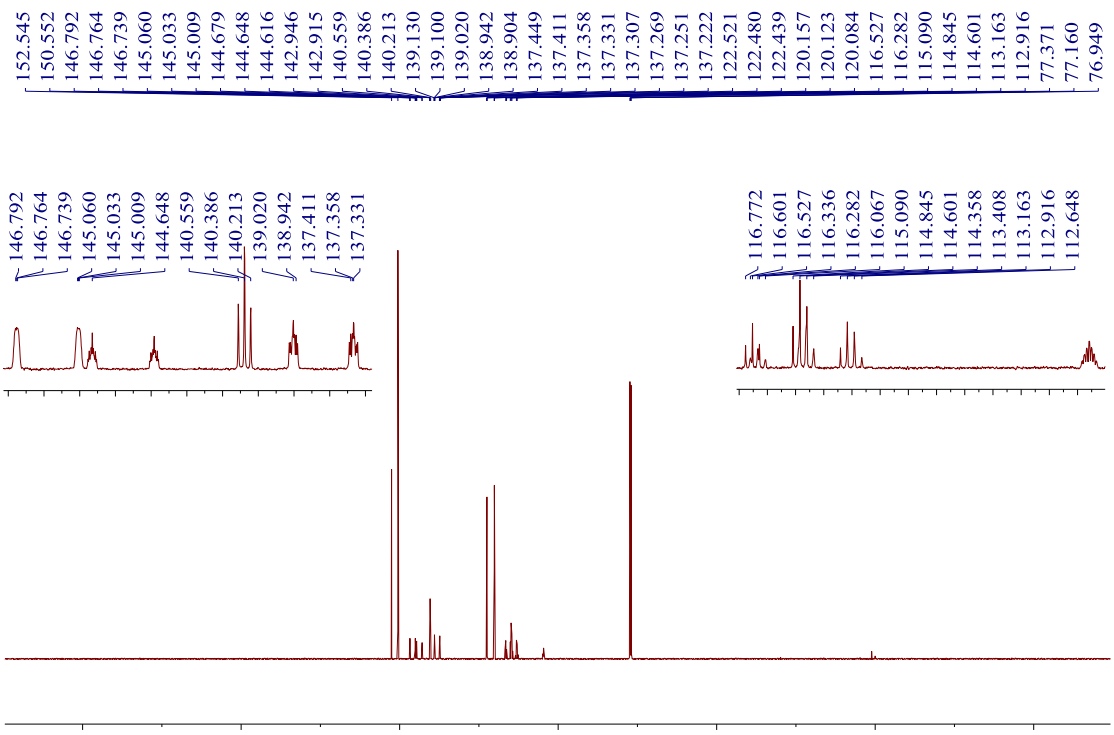

CF2CF2C6F5
N
Cl
2x 1H NMR
(400 MHz, CDCl3)

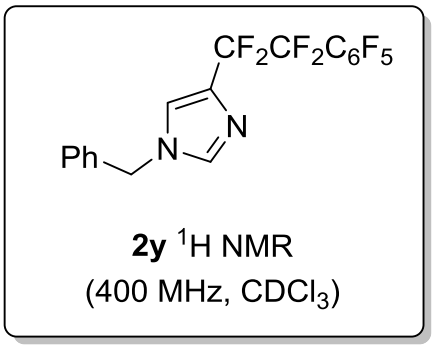

8.613
8.600
7.604
7.496
7.483
7.260 CDCl3
1.00
0.97
1.05
f1 (ppm)

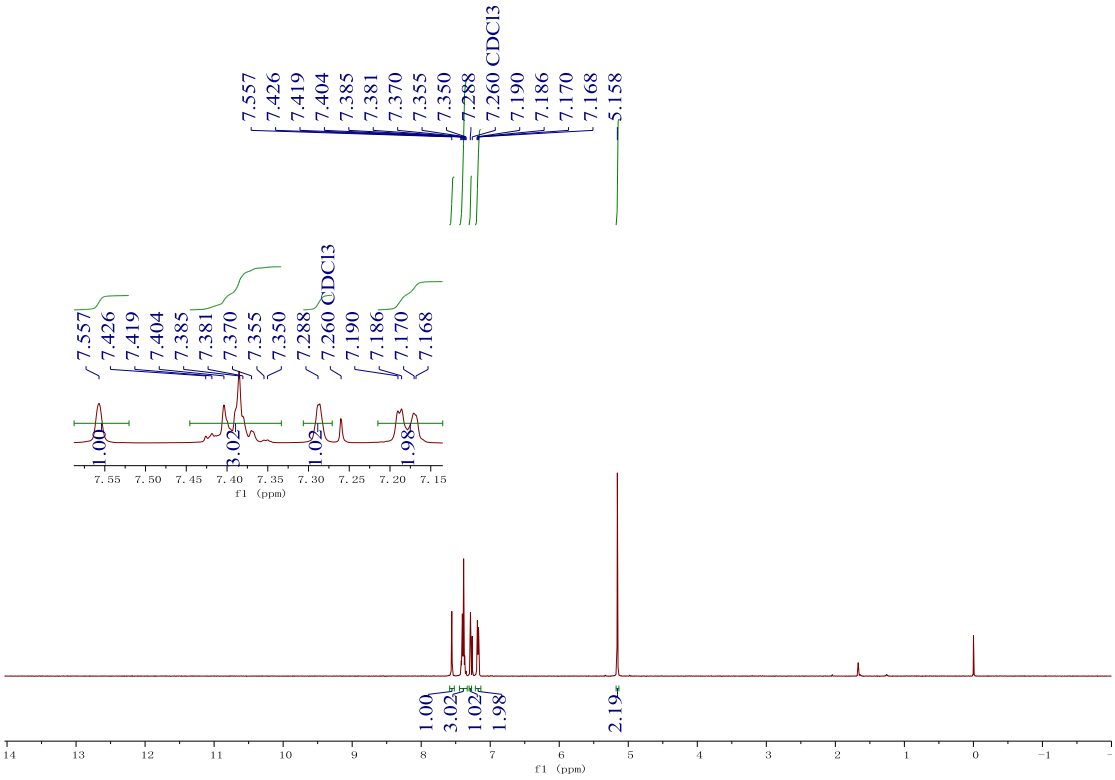

CF2CF2C6F5
N
Cl
2x 19F NMR
(376 MHz, CDCl3)

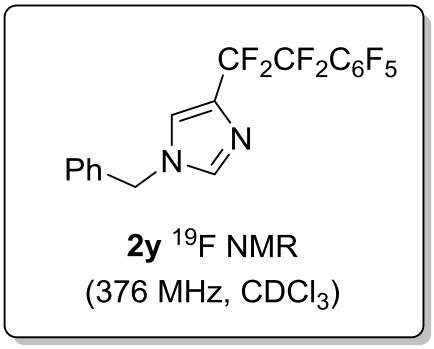

0.000
-106.331
-106.415
-106.499
-113.837
-113.851
-113.864
-113.877
-113.891
-113.903
-113.917
-137.907
-137.919
-137.932
-137.944
-137.957
-137.965
-137.977
-137.990
-138.003
-138.015
-138.028
-138.040
-138.049
-138.062
-138.074
-138.087
-138.099
-146.615
-146.657
-146.672
-146.687
-146.713
-146.728
-159.689
-159.710
-159.722
-159.745
-159.761
-159.770
-159.779
-159.794
-159.817
-159.829
-159.850
-113.792
-113.818
-113.837
-113.851
-113.864
-113.877
-113.891
-113.903
-113.917
-113.937
-113.963
2.00
2.01
f1 (ppm)
2.00
2.01
2.03
1.00
1.95
f1 (ppm)


CF2CF2C6F5
N
Cl
2x 13C NMR
(150 MHz, CDCl3)

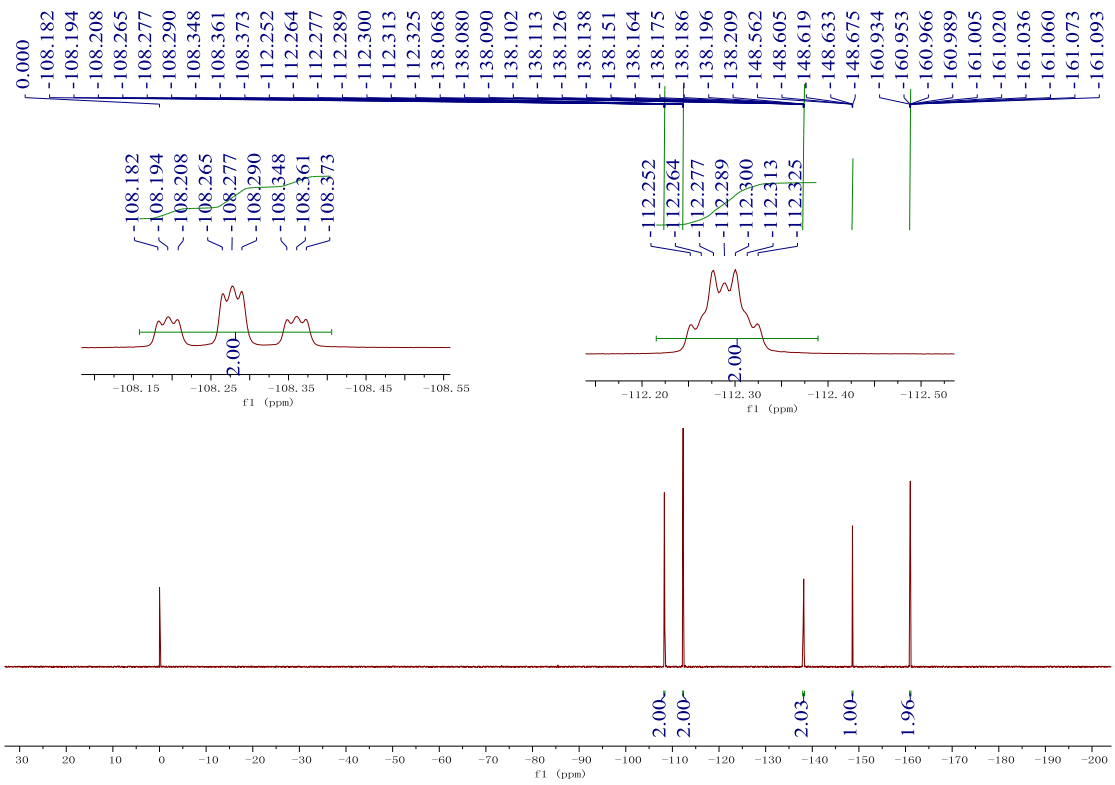

152.545
150.552
146.792
146.764
146.739
145.060
145.033
145.009
144.679
144.648
144.616
142.946
142.915
140.559
140.386
140.213
139.130
139.100
139.020
138.942
138.904
137.449
137.411
137.358
137.331
137.307
137.269
137.251
137.222
122.521
122.480
122.439
120.157
120.123
120.084
116.527
116.282
115.090
114.845
114.601
114.358
113.163
112.916
77.371
77.160
76.949
146.792
146.764
146.739
145.060
145.033
145.009
144.648
140.559
140.386
140.213
139.020
138.942
137.411
137.358
137.331
116.772
116.601
116.527
116.336
116.282
116.067
115.090
114.845
114.601
114.358
113.408
113.163
112.916
112.648

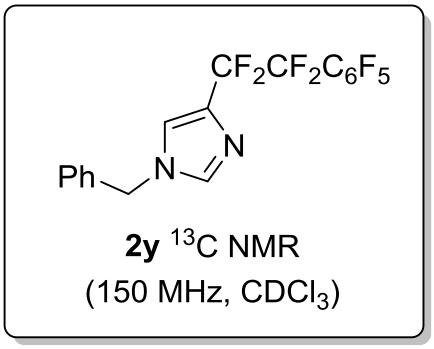

CF2CF2C6F5
N
N
Ph
2y 1H NMR
(400 MHz, CDCl3)


7.557
7.426
7.419
7.404
7.385
7.381
7.370
7.355
7.350
7.288
7.260 CDCl3
7.190
7.186
7.170
7.168
5.158
1.00
3.02
1.02
1.98
2.19
f1 (ppm)

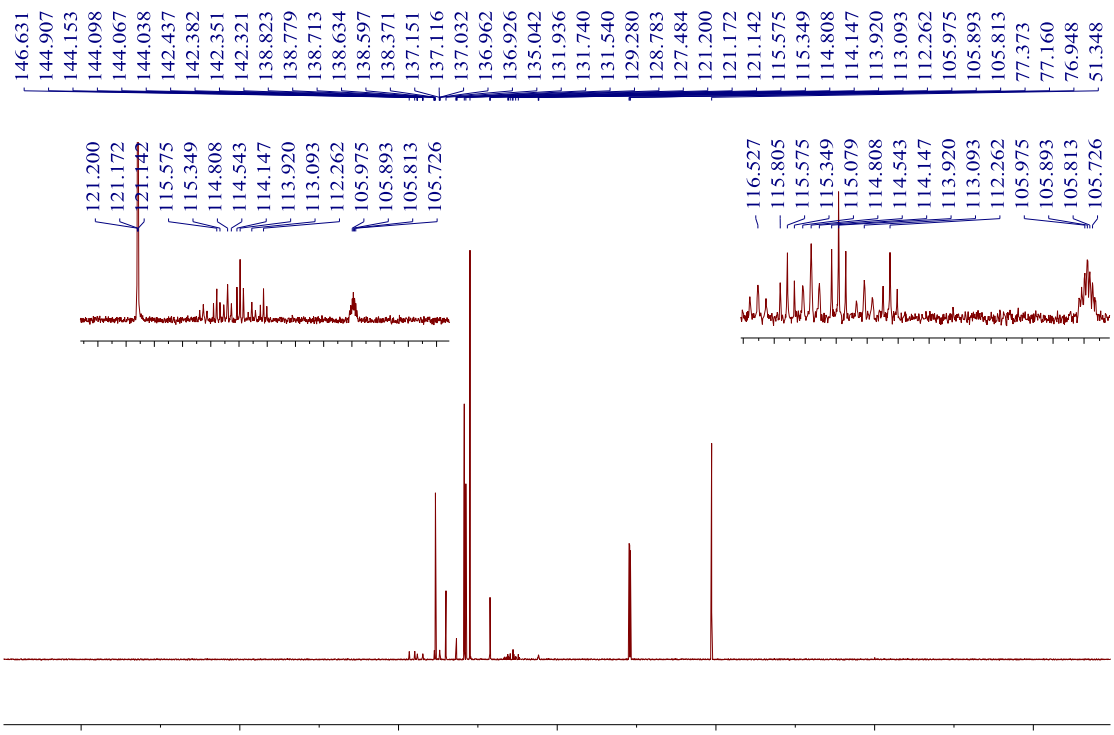


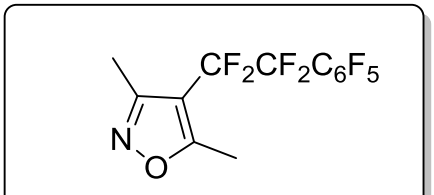
2y ^{19}F NMR
(376 MHz, $CDCl_3$)



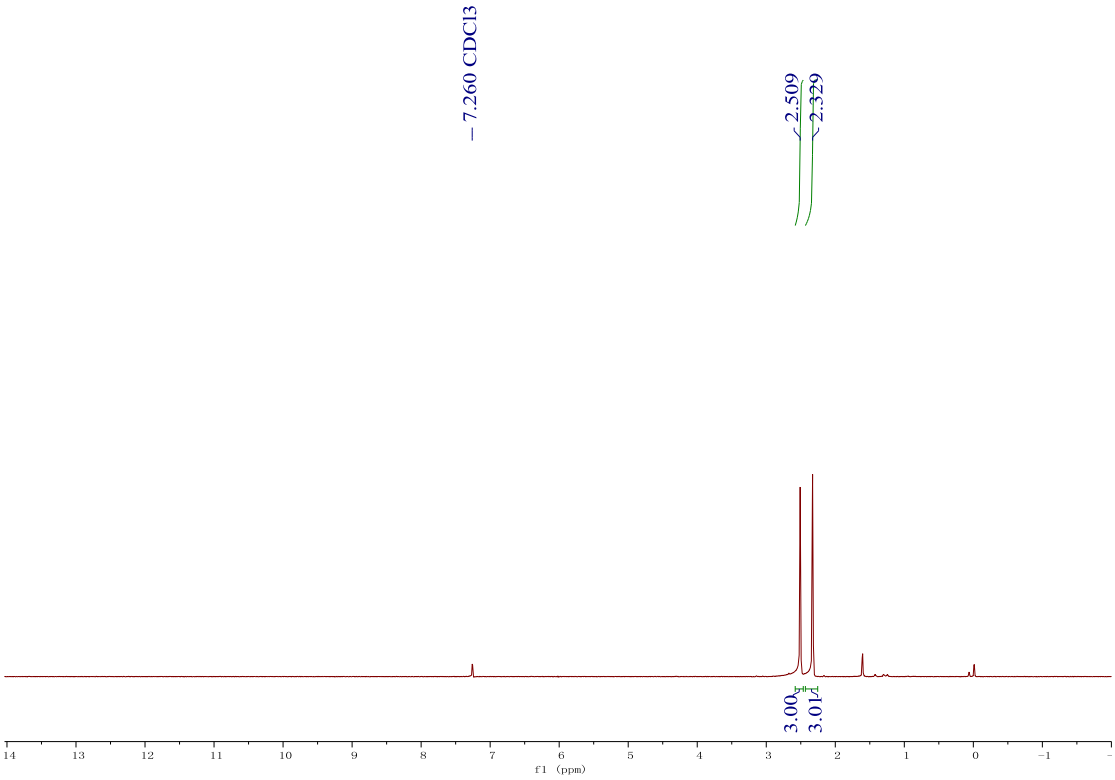


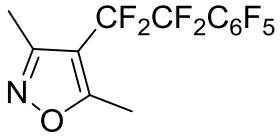
2y ^{13}C NMR
(150 MHz, $CDCl_3$)



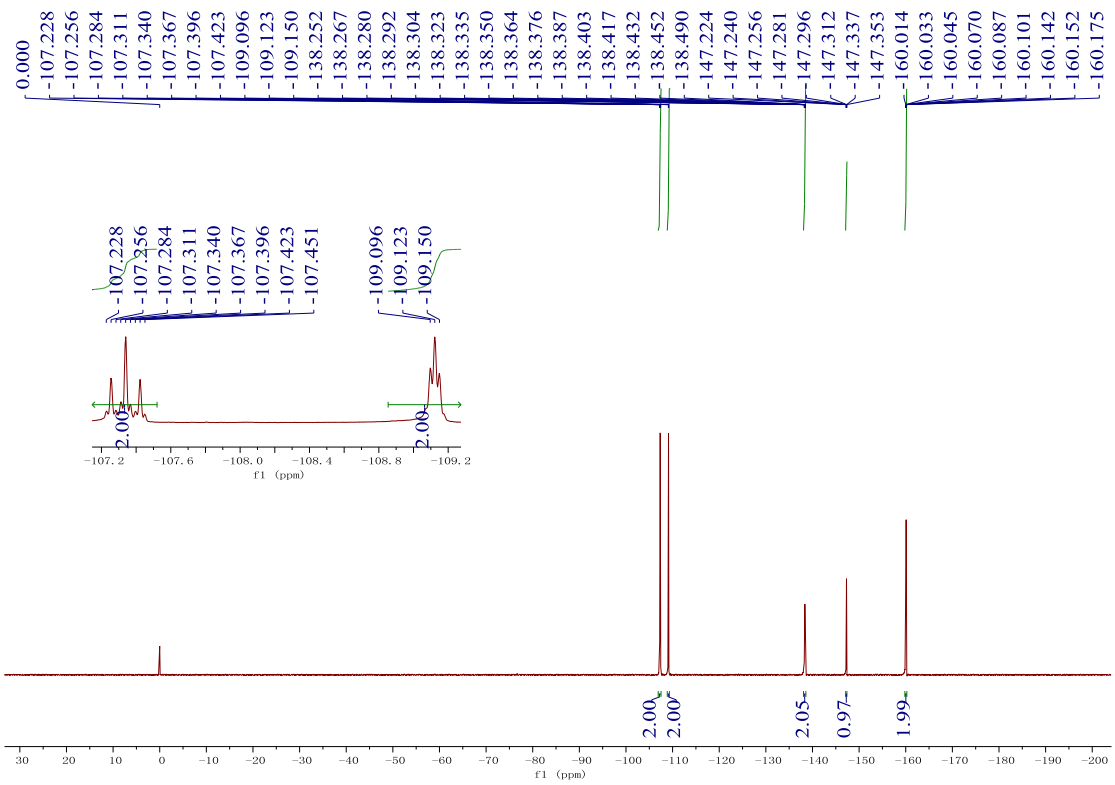


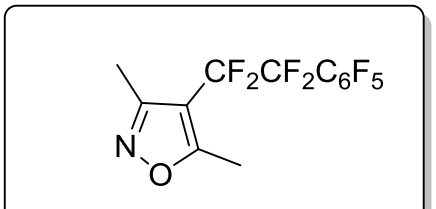
2z ^{1}H NMR
(400 MHz, $CDCl_3$)





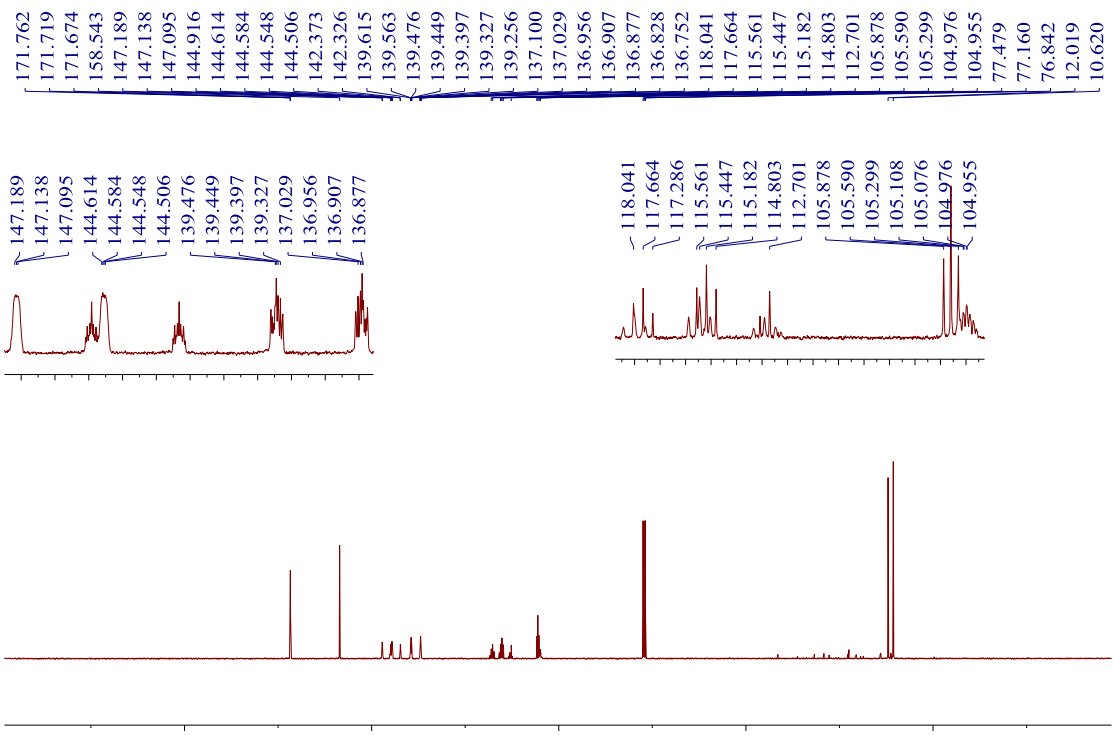
2z ^{19}F NMR
(376 MHz, $CDCl_3$)

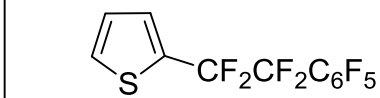




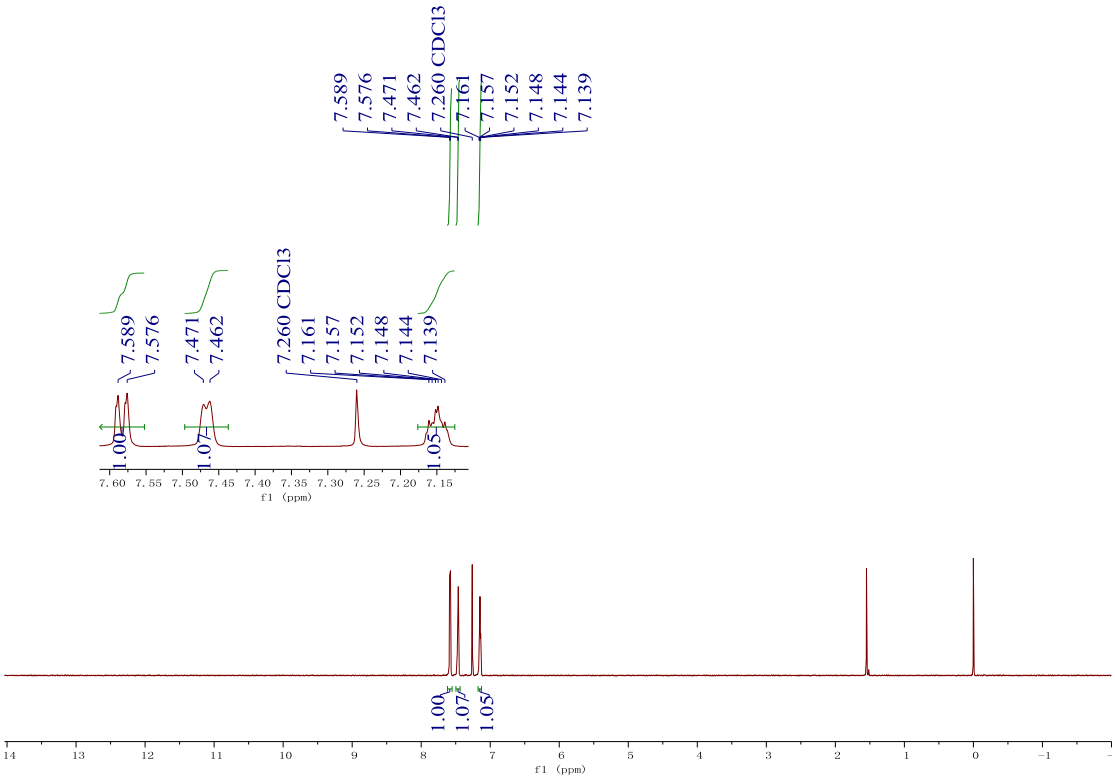
2z ^{13}C NMR

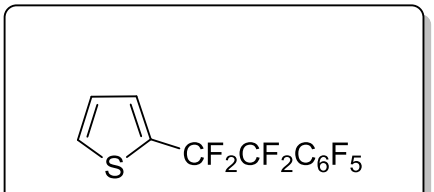
(100 MHz, $CDCl_3$)



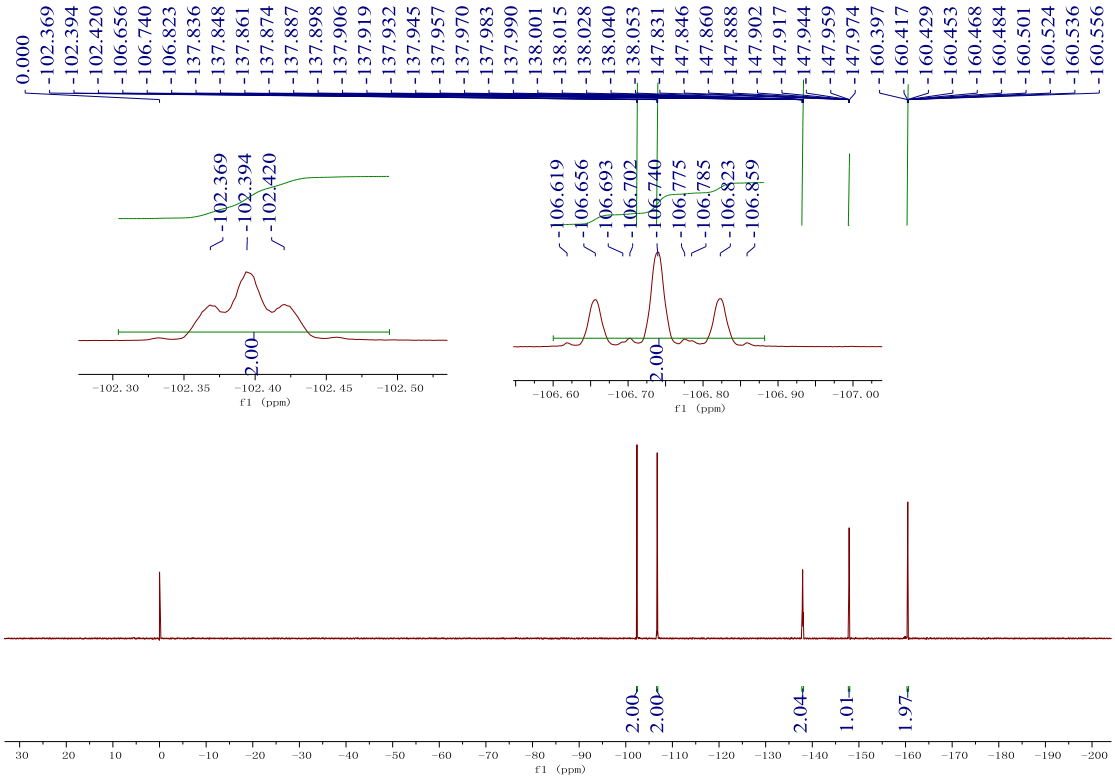


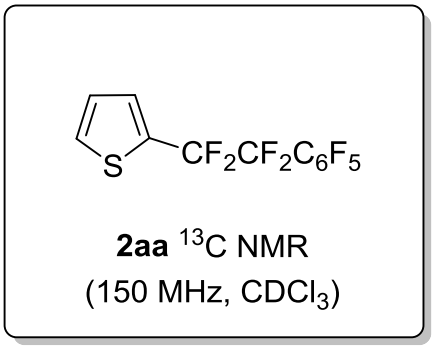
2aa ^{1}H NMR
(400 MHz, $CDCl_3$)



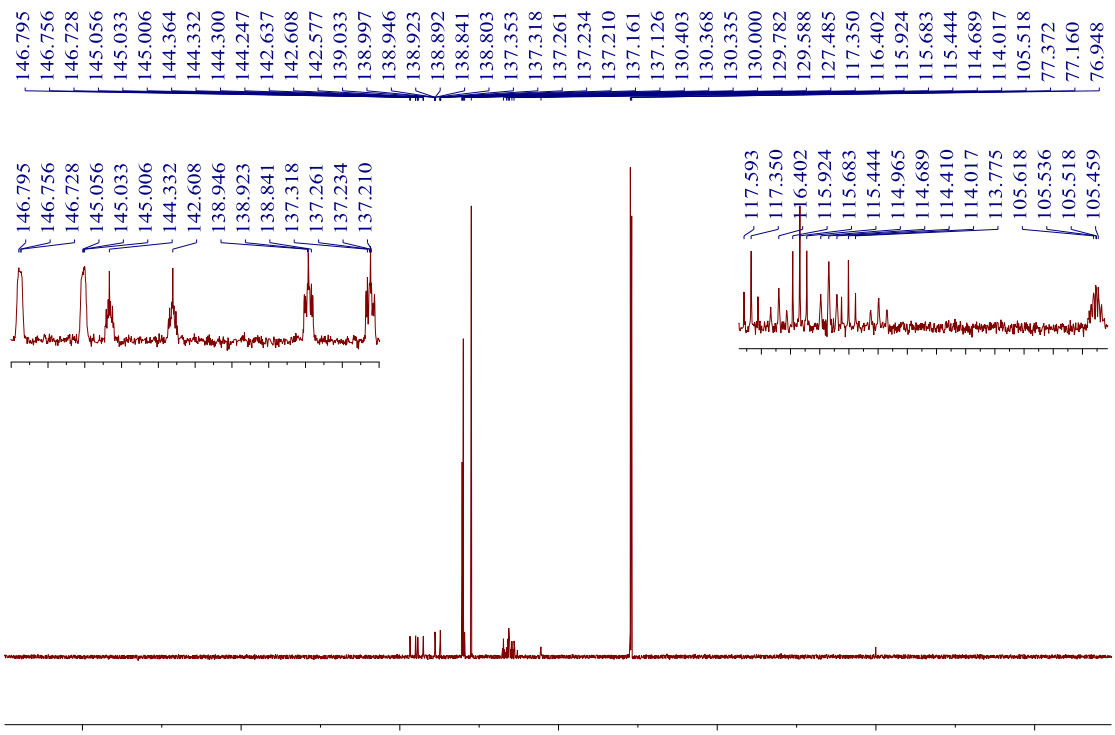


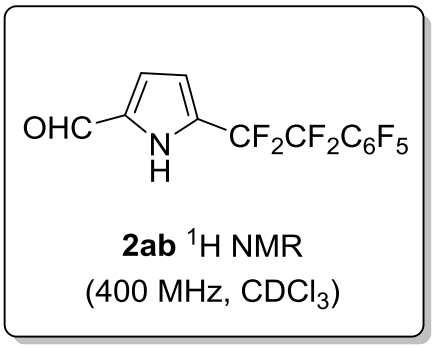
2aa ^{19}F NMR
(376 MHz, $CDCl_3$)


0.000
-102.369
-102.394
-102.420
-106.656
-106.740
-106.823
-137.836
-137.848
-137.861
-137.874
-137.887
-137.898
-137.906
-137.919
-137.932
-137.945
-137.957
-137.970
-137.983
-137.990
-138.001
-138.015
-138.028
-138.040
-138.053
-147.831
-147.846
-147.860
-147.888
-147.902
-147.917
-147.944
-147.959
-147.974
-160.397
-160.417
-160.429
-160.453
-160.468
-160.484
-160.501
-160.524
-160.536
-160.556
-102.369
-102.394
-102.420
2.00
-102.30
-102.35
-102.40
-102.45
-102.50
f1 (ppm)
-106.619
-106.656
-106.693
-106.702
-106.740
-106.775
-106.785
-106.823
-106.859
2.00
-106.60
-106.70
-106.80
-106.90
-107.00
f1 (ppm)
2.00
2.00
2.04
1.01
1.97
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

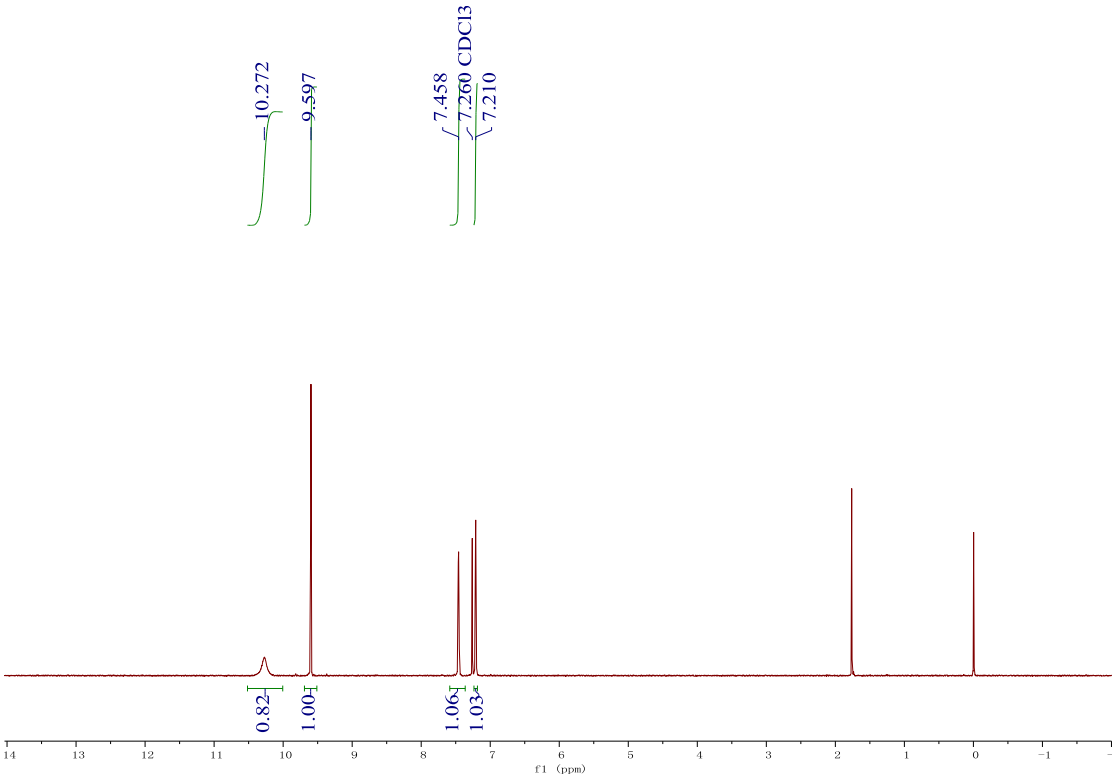


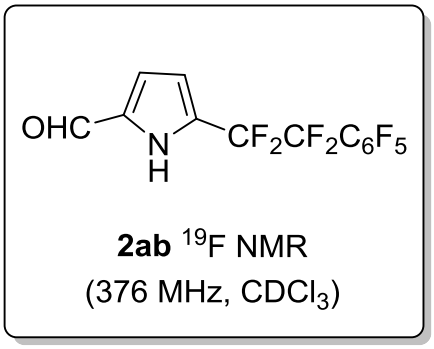
2aa ^{13}C NMR
(150 MHz, $CDCl_3$)



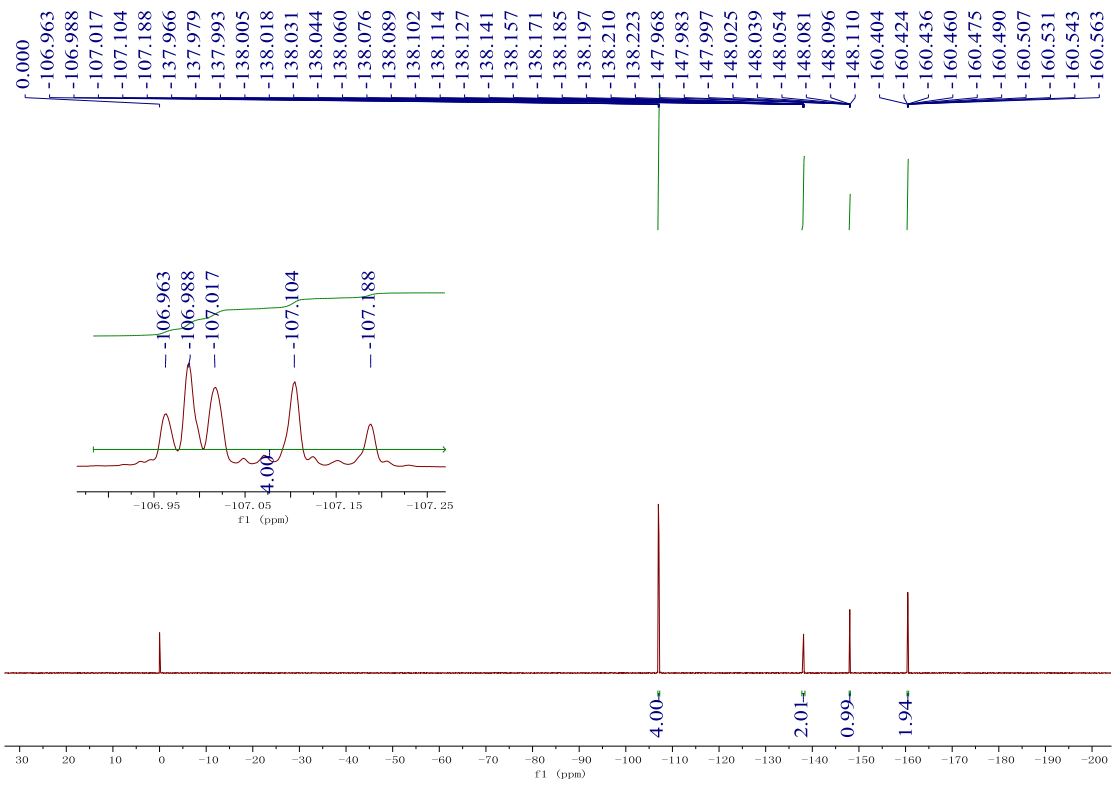


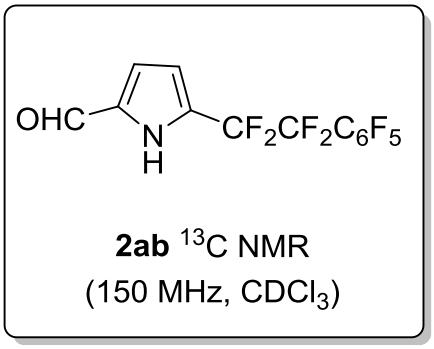
2ab ^{1}H NMR
(400 MHz, $CDCl_3$)



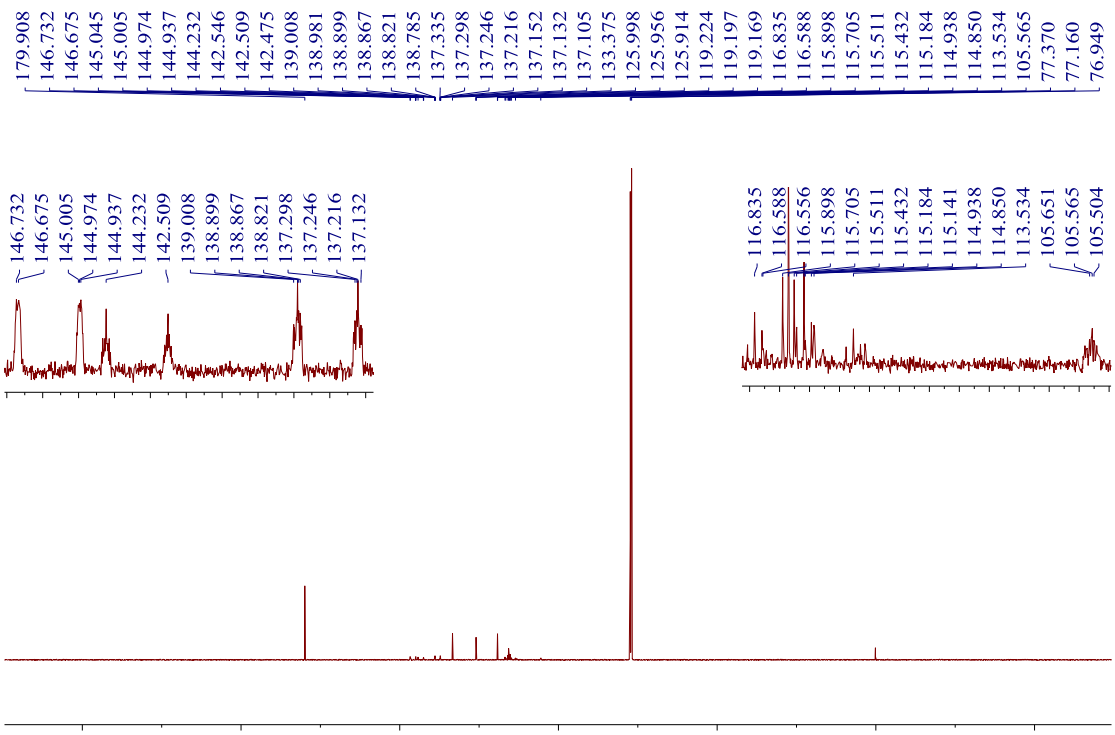


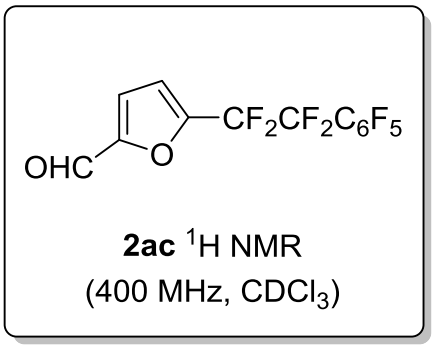
2ab ^{19}F NMR
(376 MHz, $CDCl_3$)



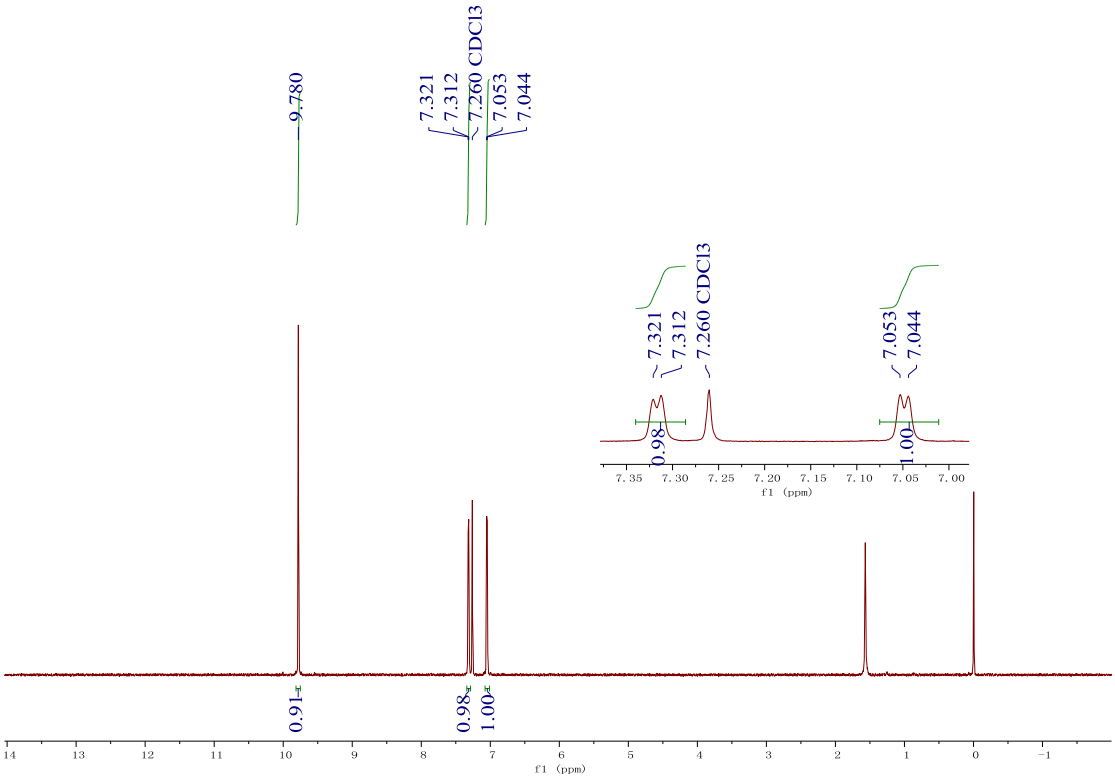


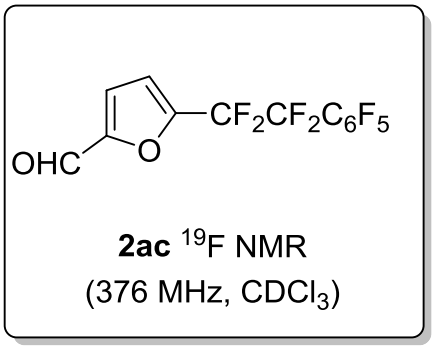
2ab ^{13}C NMR
(150 MHz, $CDCl_3$)



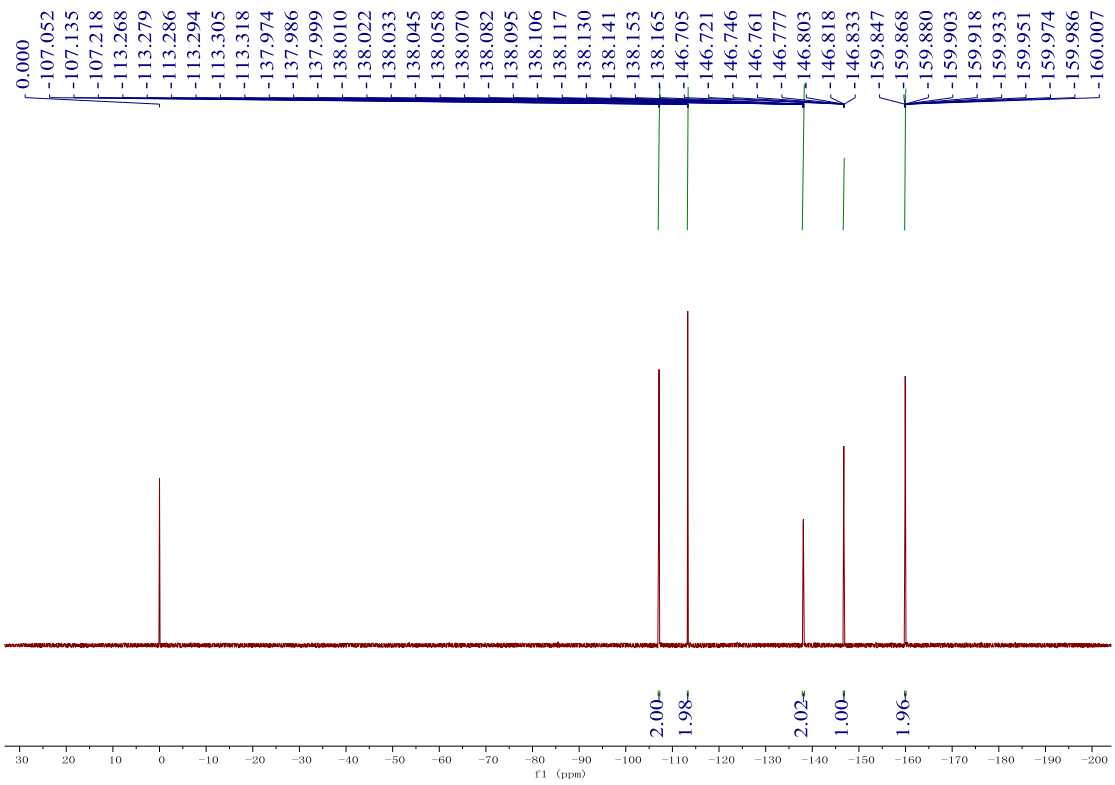


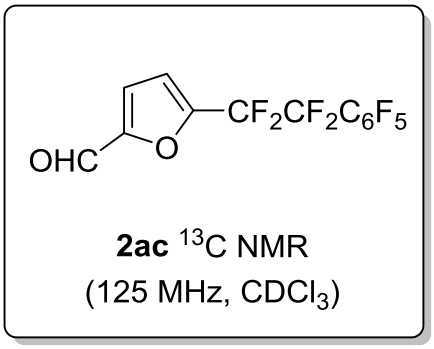
2ac ^{1}H NMR
(400 MHz, $CDCl_3$)



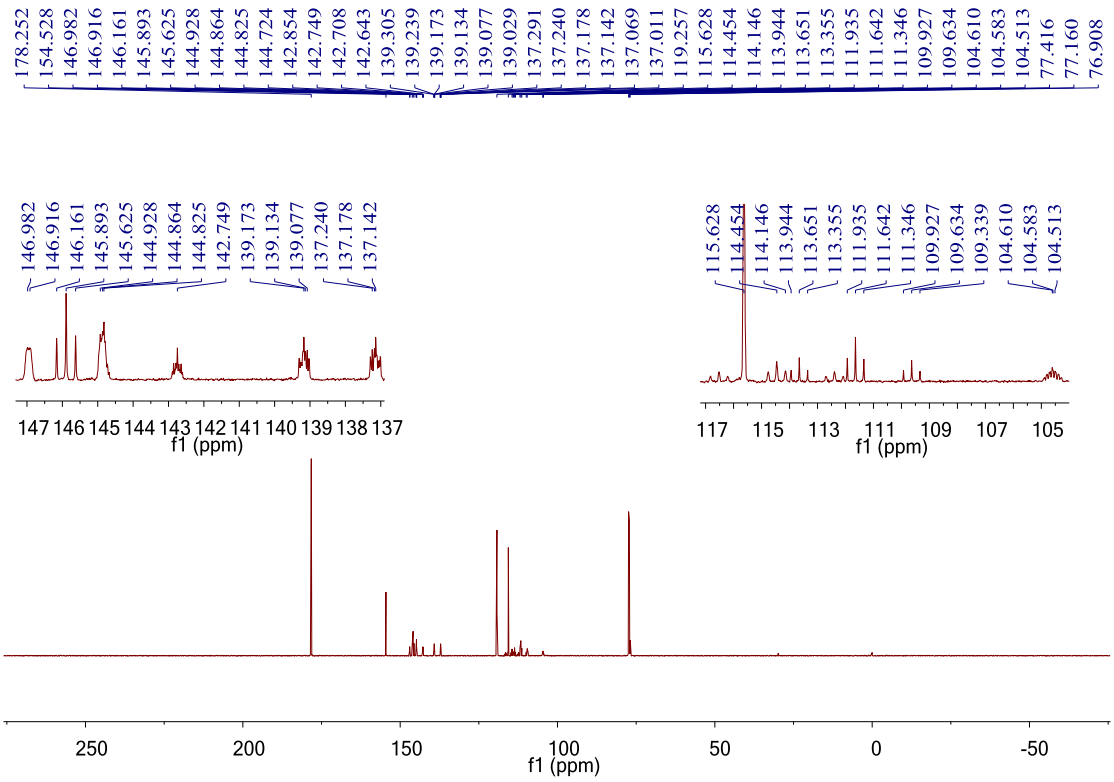


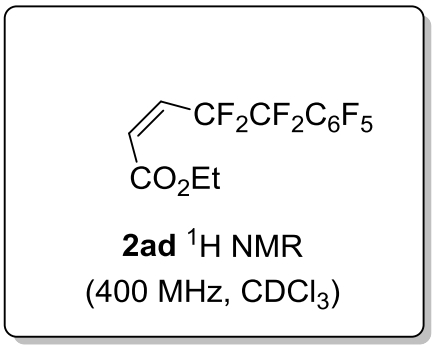
2ac ^{19}F NMR
(376 MHz, $CDCl_3$)

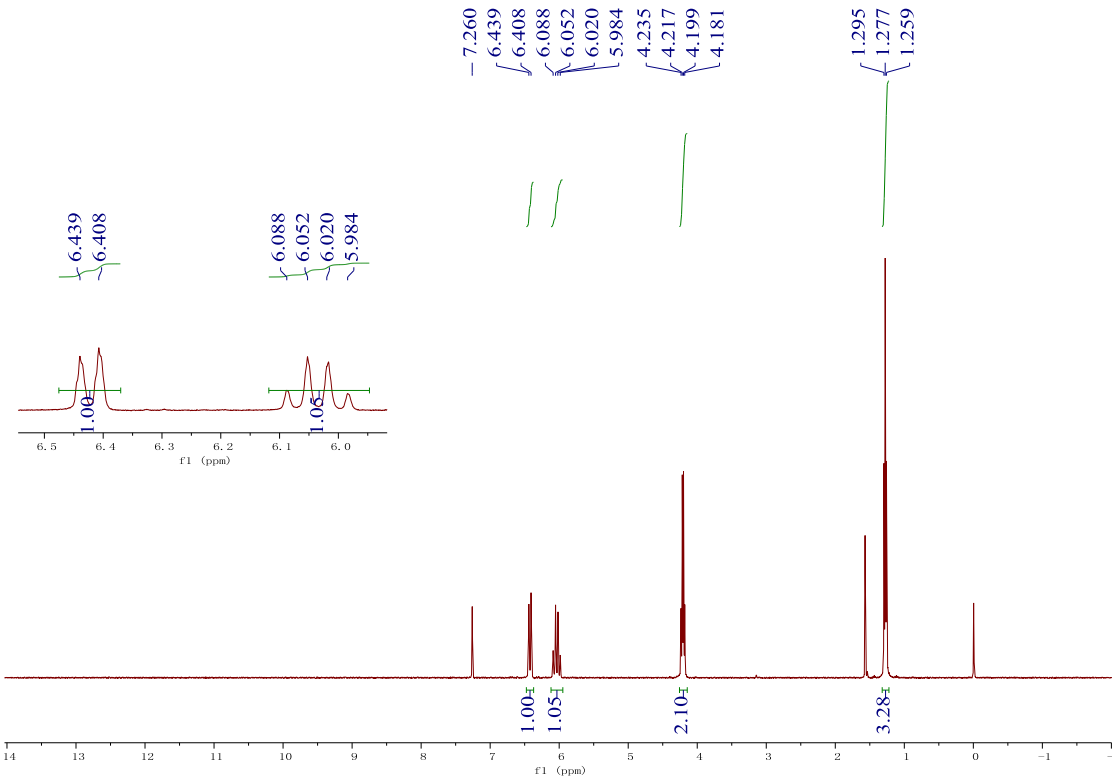


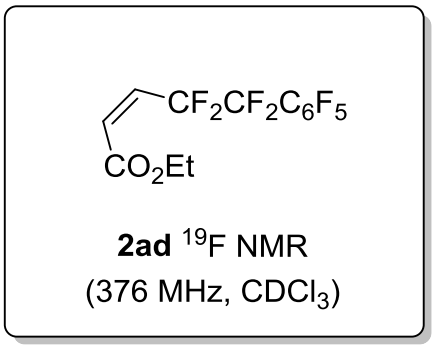


2ac ^{13}C NMR
(125 MHz, $CDCl_3$)

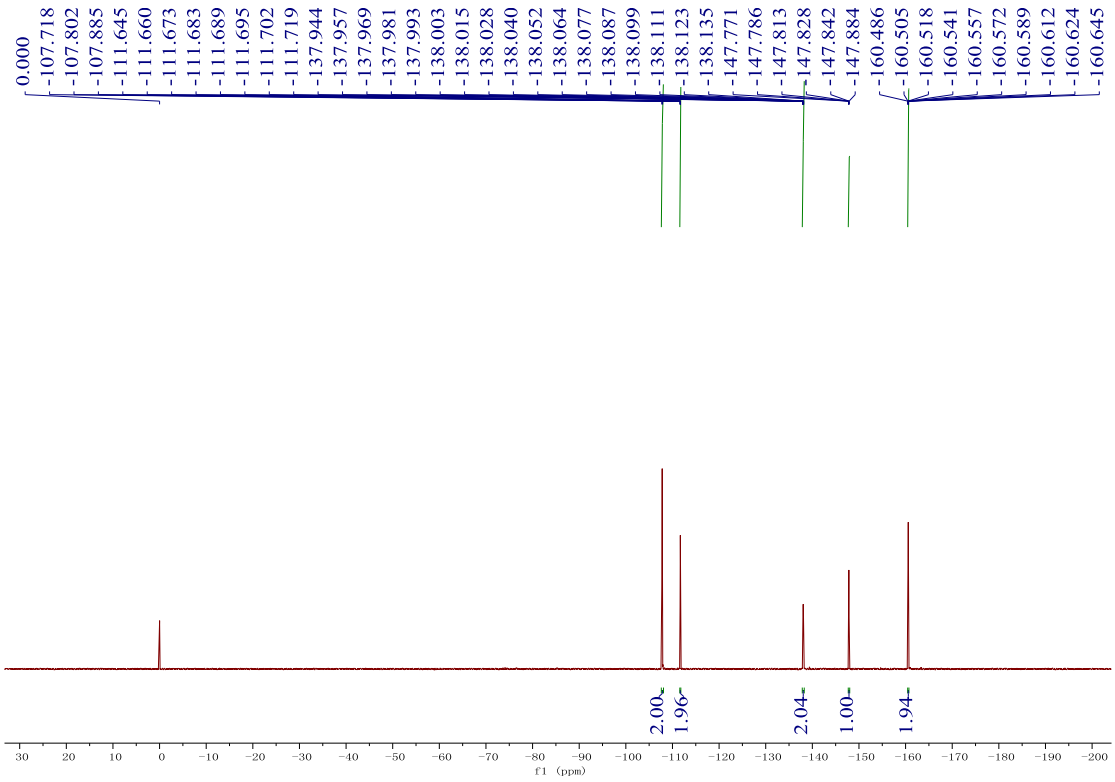


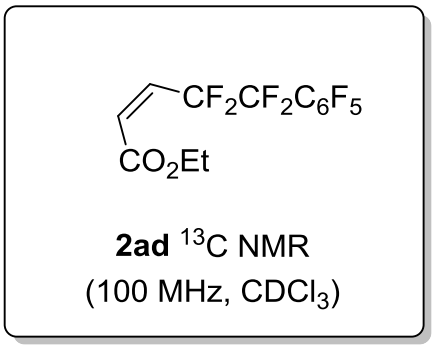

$CF_2CF_2C_6F_5$
CO_2Et
2ad ^{1}H NMR
(400 MHz, $CDCl_3$)

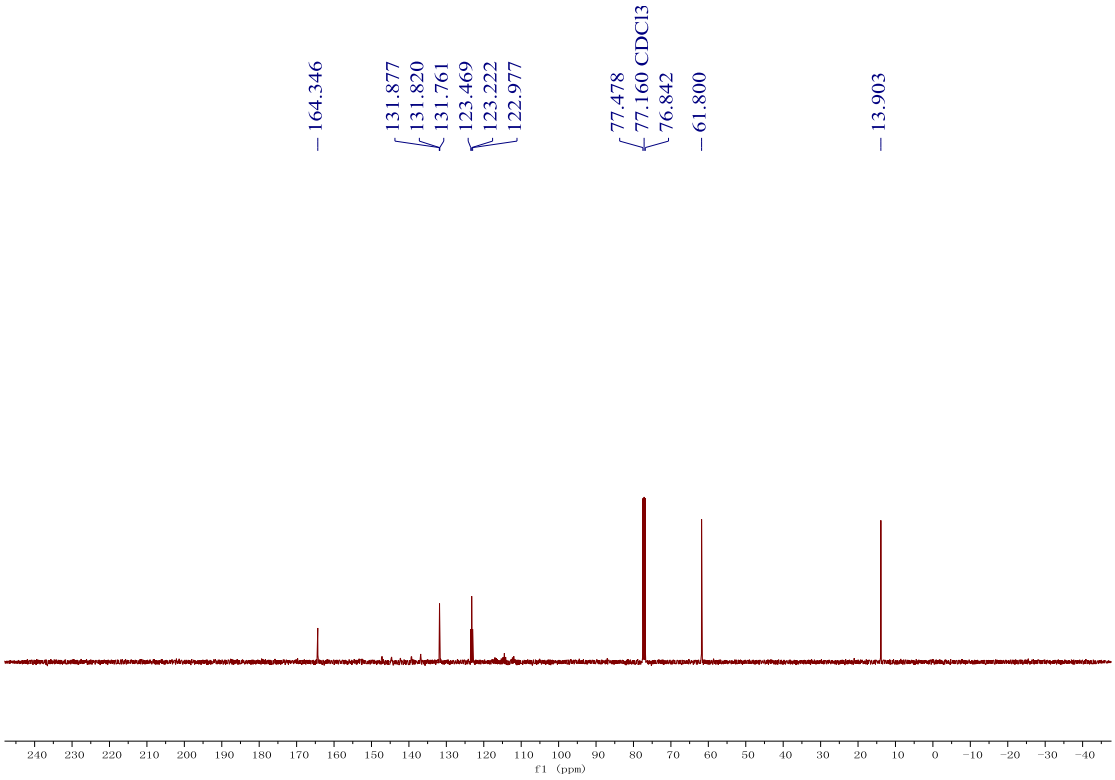

7.260
6.439
6.408
6.088
6.052
6.020
5.984
4.235
4.217
4.199
4.181
1.295
1.277
1.259
1.00
1.05
2.10
3.28
f1 (ppm)

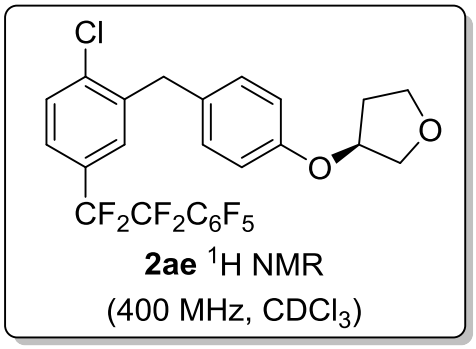


2ad ^{19}F NMR
(376 MHz, $CDCl_3$)



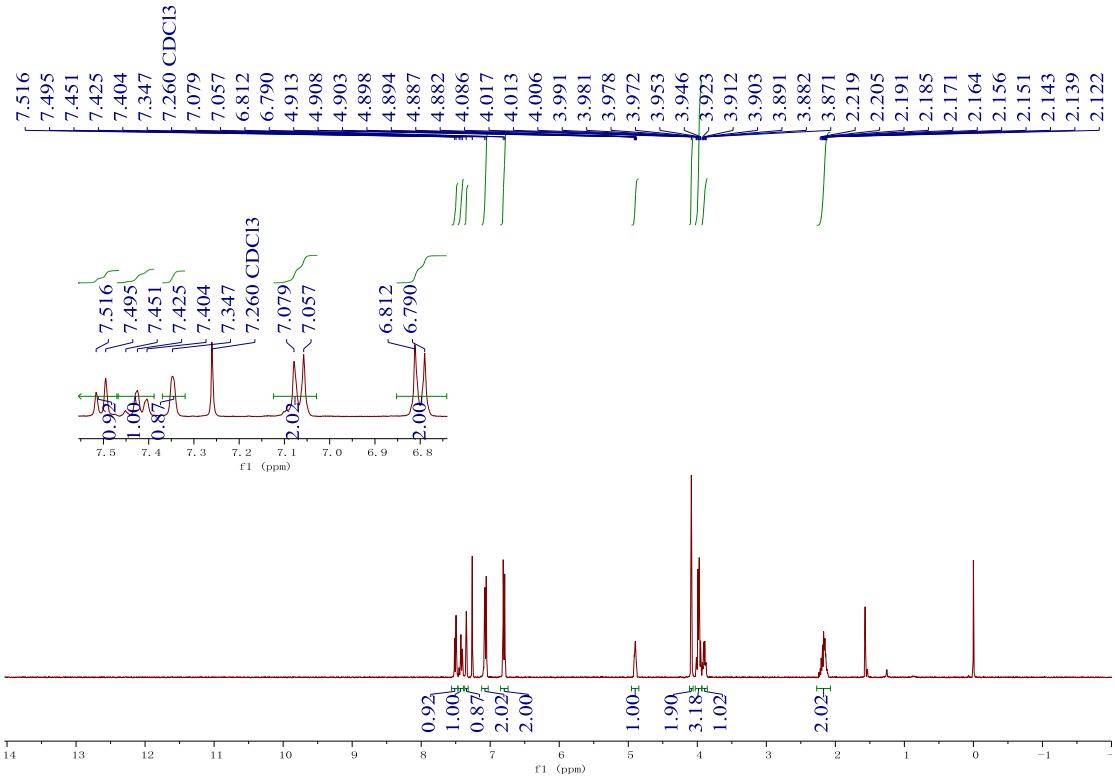

CF2CF2C6F5
CO2Et
2ad 13C NMR
(100 MHz, CDCl3)

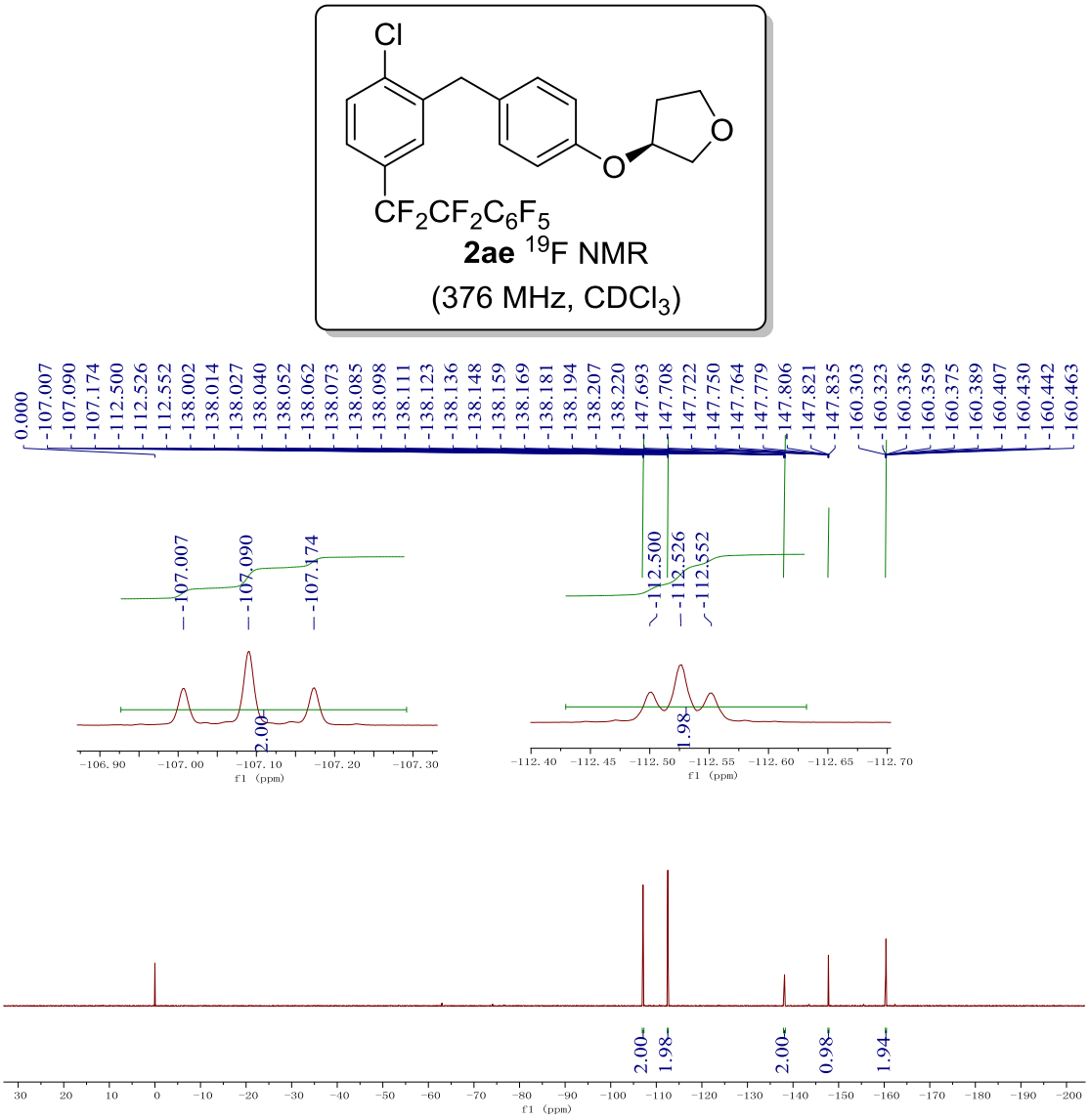

164.346
131.877
131.820
131.761
123.469
123.222
122.977
77.478
77.160 CDCl3
76.842
61.800
13.903
f1 (ppm)

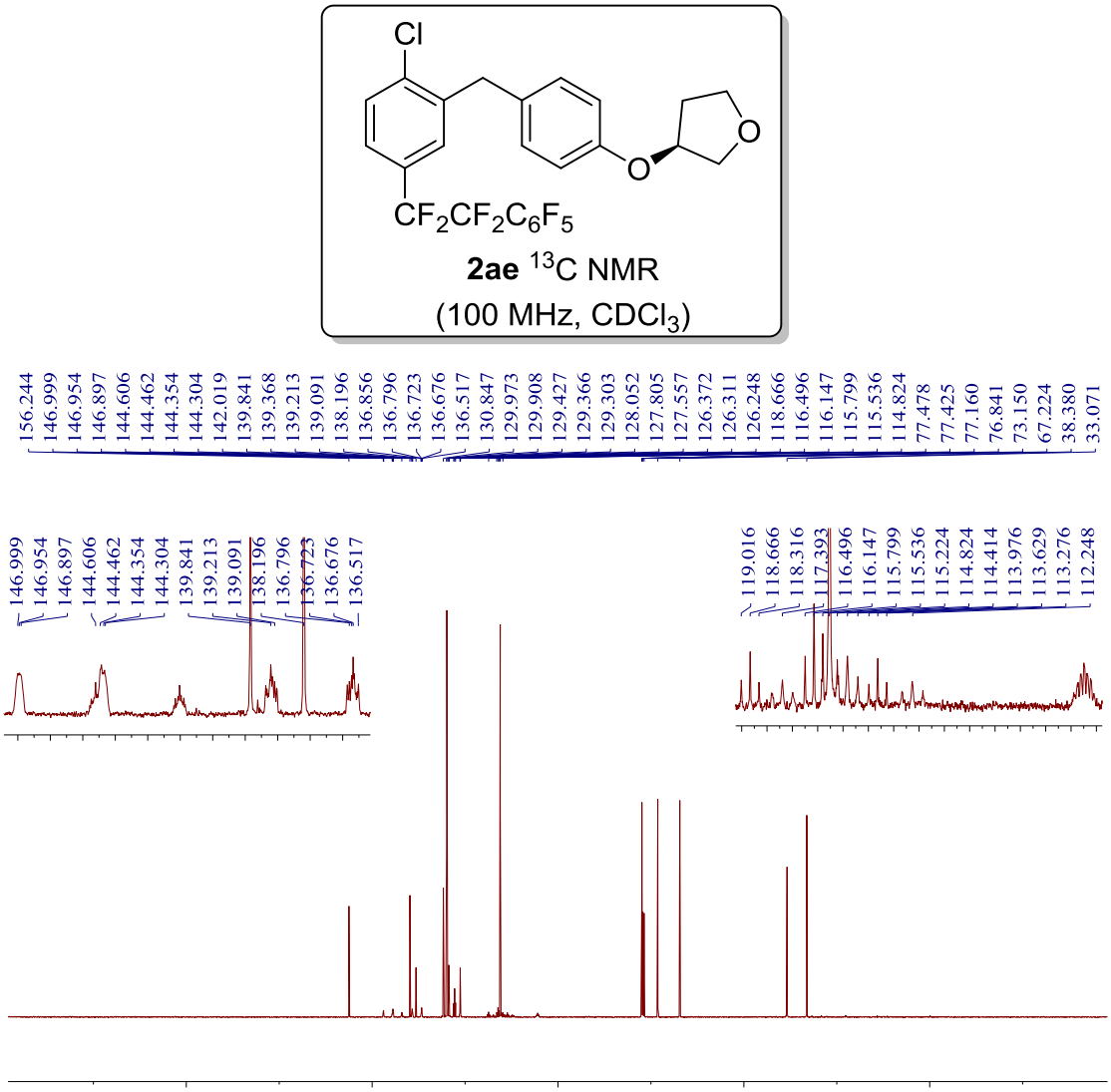


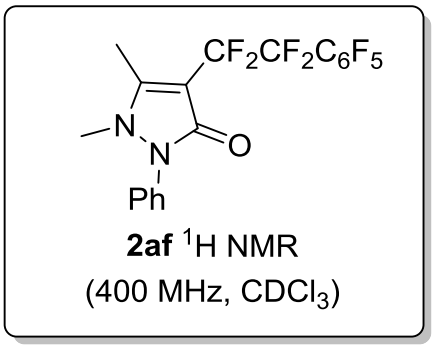
2ae ^{1}H NMR

(400 MHz, $CDCl_3$)

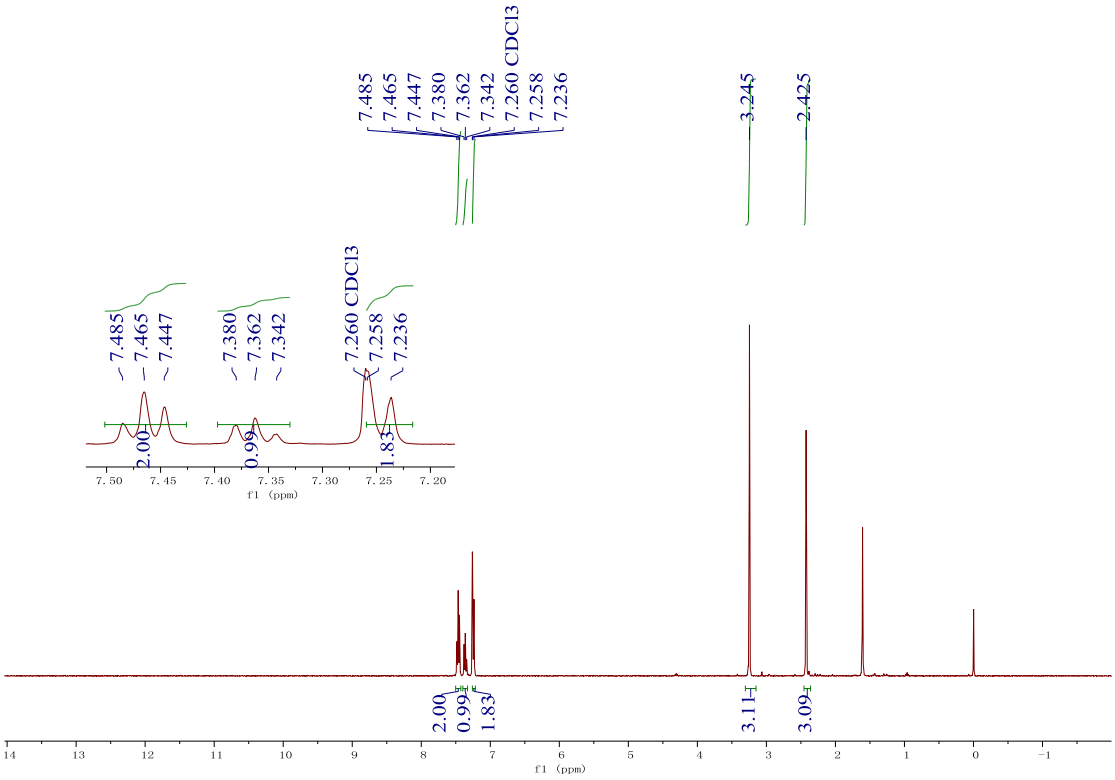


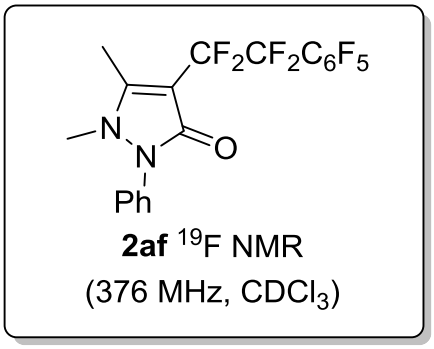

Cl
O
O
$CF_2CF_2C_6F_5$
2ae ^{19}F NMR
(376 MHz, $CDCl_3$)
f1 (ppm)
f1 (ppm)
f1 (ppm)


Cl
O
O
CF2CF2C6F5
2ae 13C NMR
(100 MHz, CDCl3)
156.244
146.999
146.954
146.897
144.606
144.462
144.354
144.304
142.019
139.841
139.368
139.213
139.091
138.196
136.856
136.796
136.723
136.676
136.517
130.847
129.973
129.908
129.427
129.366
129.303
128.052
127.805
127.557
126.372
126.311
126.248
118.666
116.496
116.147
115.799
115.536
114.824
77.478
77.425
77.160
76.841
73.150
67.224
38.380
33.071
146.999
146.954
146.897
144.606
144.462
144.354
144.304
139.841
139.213
139.091
138.196
136.796
136.723
136.676
136.517
119.016
118.666
118.316
117.393
116.496
116.147
115.799
115.536
115.224
114.824
114.414
113.976
113.629
113.276
112.248



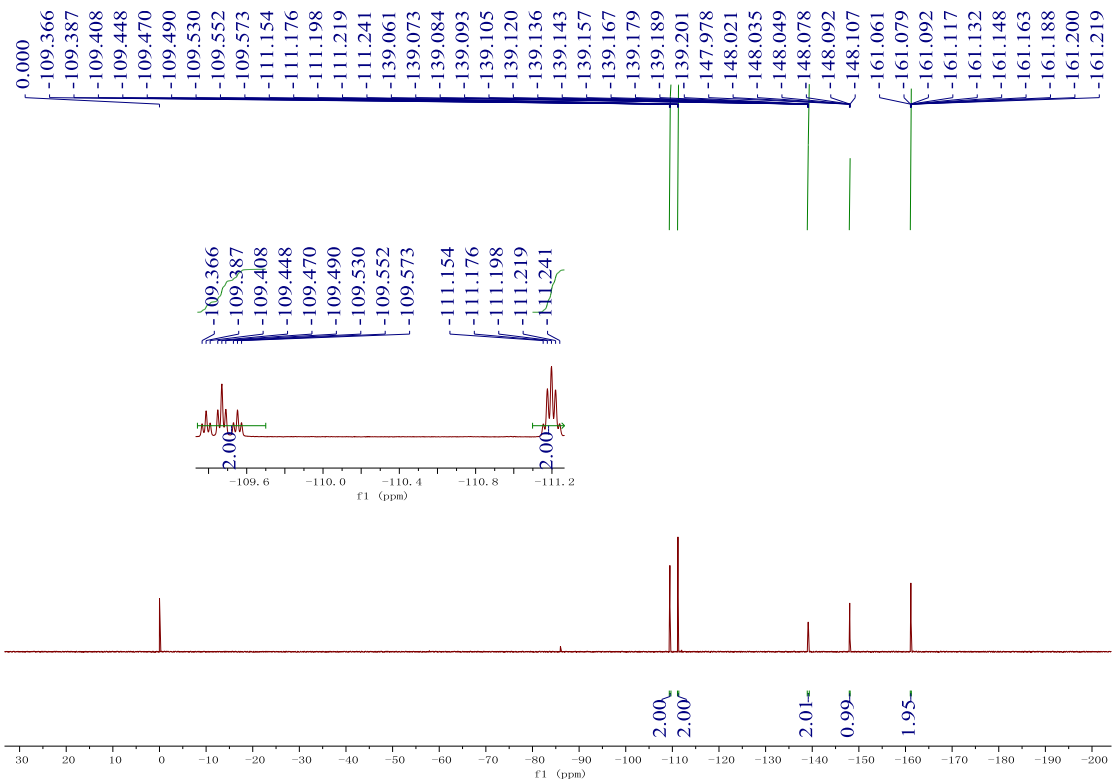
2af ^{1}H NMR
(400 MHz, $CDCl_3$)

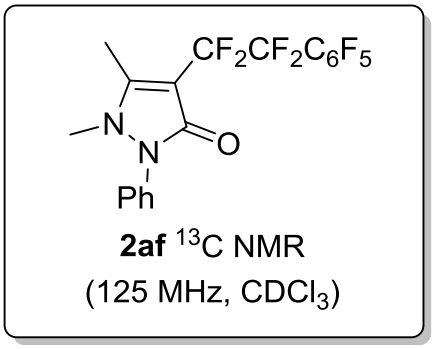




2af ^{19}F NMR

(376 MHz, $CDCl_3$)





2af ^{13}C NMR
(125 MHz, $CDCl_3$)