Supplementary information

Lewis acid promoted fluorine-alkoxy group exchange reactions for the synthesis of 5-alkoxy-4,4-difluoroisoxazoline systems

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Table of Contents

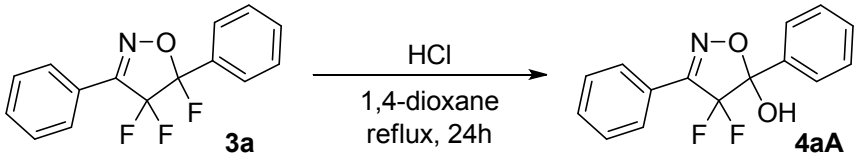
General Information:

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on JEOL JNM-ECZ400 spectrometers. Chemical shifts of ^{1}H NMR and ^{13}C NMR are reported in ppm from tetramethylsilane (TMS: 0 ppm) as an internal standard. Chemical shifts of ^{19}F NMR are reported in ppm from benzotrifluoride (BTF: 0 ppm) as an internal standard. All data are reported as follows: chemical shifts, relative integration value, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz). Mass spectra were obtained on JEOL JMS-700T spectrometers. IR spectra were recorded on JASCO FT/IR-410 spectrophotometer. Melting points were measured on Yanagimoto micro melting point apparatus MP-S3. Analytical gas-liquid chromatography (GLC) was carried out on Hitachi G-3500 gas chromatograph (column; TO-5 0.25 mm x 15 m, carrier; He at 2.2 mL/min). Peak areas were calculated on Hitachi D-2500 Chromato-integrator. Microwave reactions were performed in microwave tubes with clip lids using Biotage Initiator+ microwave reactor.

Materials:

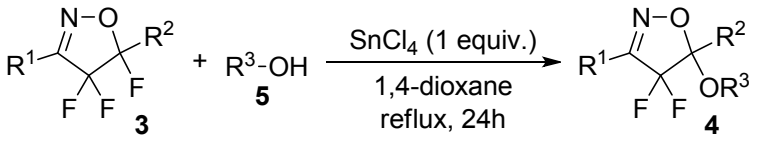
Sulfolane and 1,4-dioxane were distilled before use. All other commercially available reagents were used without further purification. All experiments were carried out under argon atmosphere unless otherwise noted. Syntheses of 4,4,5-trifluoroisoxazolines derivatives (**3**) were reported earlier.

Synthesis of 4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazol-5-ol (4aA).



4,4,5-Trifluoro-3,5-diphenyl-4,5-dihydroisoxazole (**3a**; 0.4 mmol) was disolved in HCl–1,4-dioxane solution (3 mL, HCl : 1,4-dioxane = 1:2), and the mixture was heated at reflux for 24 h. The resulting mixture was quenched with 10% HCl and extracted with AcOEt. The AcOEt layer was washed with sat. aq. NaCl and dried ($MgSO_4$). The solvent was evaporated and the residue was purified by column chromatography (AcOEt : hexane = 1:9) to give **4aA** (86 mg, 78%).

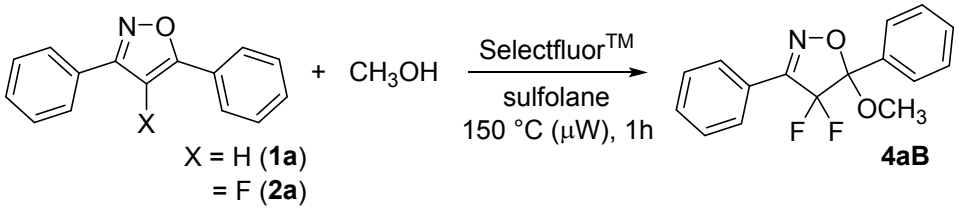
General procedure for Lewis acid promoted fluorine-alkoxy group exchange reaction.



To a solution of 4,4,5-trifluoroisoxazoline (**3**; 0.4 mmol) and alcohol (**5**, 0.6 mmol) in 1,4-

dioxane (3 mL) was added 1.0 M $SnCl_4$ in heptane (0.4 mL, 0.4 mmol) at ambient temperature and the mixture was refluxed for 24 h. The resulting mixture was quenched with 10% HCl and extracted with AcOEt. The AcOEt layer was washed with sat. aq. NaCl and dried ($MgSO_4$). The solvent was evaporated and the residue was purified by column chromatography on silica gel to give 5-alkoxy-4,4-difluoroisoxazoline (**4**).

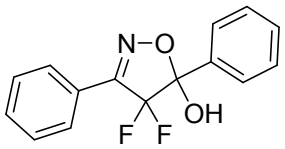
General procedure for alkoxy-fluorination of isoxazoles.



Isoxazole (**1** or **2**; 1 mmol), MeOH (1.5 mmol) and Selectfluor™ (3 mmol when using **1**, or 2 mmol when using **2**) were added to a microwave vial and suspended in sulfolane (4 mL). The vial was sealed and heated by microwave irradiation for 1h at 150 °C. The resulting mixture was quenched with $NaHCO_3$ and, extracted with AcOEt. The AcOEt layer was washed with sat. NaCl and dried over $MgSO_4$. The solvent was removed *in vacuo* and the residue was purified by column chromatography to give **4aB**.

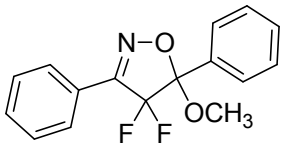
Spectroscopic Data:

4,4-Difluoro-3,5-diphenyl-4,5-dihydroisoxazol-5-ol (4aA)



Colorless solid; M.p. 109.0–111.0 °C (recrystallized from hexane–AcOEt); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.96 (1H, s), 7.41–7.53 (6H, m), 7.63–7.66 (2H, m), 7.83–7.85 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 103.0 (dd, J = 33.1, 19.4 Hz), 124.6 (dd, J = 267.8, 255.2 Hz), 124.9 (m), 126.8 (d, J = 1.5 Hz), 127.1 (d, J = 1.5 Hz), 128.5, 129.1, 130.3, 131.6, 132.7 (d, J = 1.4 Hz), 153.7 (dd, J = 25.9, 24.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -37.54 (1F, d, J = 266.3 Hz), -57.23 (1F, d, J = 266.3 Hz); MS *m/z*: 275 (M^+); HRMS Calcd for $C_{15}H_{11}F_2NO_2$: 275.076 (M^+), Found: 275.076; IR (KBr) cm^{-1}: 2982, 1450, 1365, 1242, 1127, 1098.

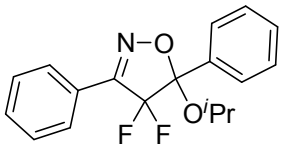
4,4-Difluoro-5-methoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aB)



Pale yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.35 (3H, s), 7.44–7.52 (6H, m), 7.63–7.65

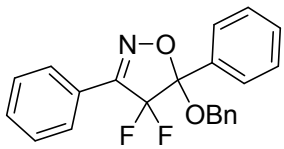
(2H, m), 7.85–7.88 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 51.71, 105.3 (dd, *J* = 33.2, 17.5 Hz), 125.0 (m), 125.1 (dd, *J* = 271.6, 252.7 Hz), 126.9 (m), 127.7 (m), 128.7, 129.0, 130.2, 131.5, 154.9 (dd, *J* = 26.1, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.8 (1F, d, *J* = 265.6 Hz), -62.61 (1F, d, *J* = 265.6 Hz); MS *m/z*: 289 (M^+); HRMS Calcd for $C_{16}H_{13}F_2NO_2$: 289.091 (M^+), Found: 289.092; IR (neat) cm^{-1}: 3064, 1247, 1130, 1098.

4,4-Difluoro-5-isopropoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aC)



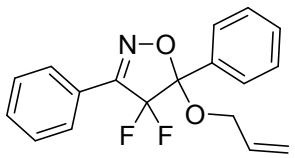
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.10 (3H, d, *J* = 6.2 Hz), 1.25 (3H, d, *J* = 6.2 Hz), 3.99 (1H, sep, *J* = 6.2 Hz), 7.45–7.53 (6H, m), 7.66–7.68 (2H, m), 7.86–7.87 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 23.66, 23.83, 69.19, 105.6 (dd, *J* = 32.1, 17.3 Hz), 125.1 (dd, *J* = 271.5, 252.7 Hz), 125.3 (m), 126.9 (m), 127.7 (m), 128.4, 129.0, 130.0, 131.4, 131.9 (m), 154.9 (dd, *J* = 26.1, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -35.4 (1F, d, *J* = 263.8 Hz), -62.3 (1F, d, *J* = 263.8 Hz); MS *m/z*: 317 (M^+); HRMS Calcd for $C_{18}H_{17}F_2NO_2$: 317.123 (M^+), Found: 317.123; IR (neat) cm^{-1}: 3063, 2977, 1247, 1129, 1091.

5-(Benzyloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aE)



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.47 (1H, m), 4.75 (1H, m), 7.24–7.53 (11H, m), 7.69–7.74 (2H, m), 7.86–7.88 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 66.31, 105.2 (dd, *J* = 33.4, 17.6 Hz), 125.0, 125.1 (dd, *J* = 272.2, 251.9 Hz), 126.9, 127.6, 127.7, 127.8, 128.4, 128.7, 129.0, 130.3, 130.6, 131.6, 136.9, 155.0 (dd, *J* = 25.4, 24.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.7 (1F, d, *J* = 265.1 Hz), -62.1 (1F, d, *J* = 265.1 Hz); MS *m/z*: 365 (M^+); HRMS Calcd for $C_{22}H_{17}F_2NO_2$: 365.123 (M^+), Found: 365.123; IR (neat) cm^{-1}: 3063, 2977, 1247, 1129, 1091.

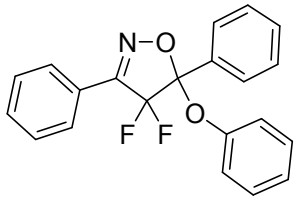
5-(Allyloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aF)



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.96 (1H, m), 4.20 (1H, m), 5.16 (1H, m), 5.28 (1H, m), 5.89 (1H, m), 7.45–7.53 (6H, m), 7.64–7.67 (2H, m), 7.86–7.88 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 65.53, 105.2 (dd, *J* = 33.3, 17.7 Hz), 117.2, 125.1 (dd, *J* = 272.0,

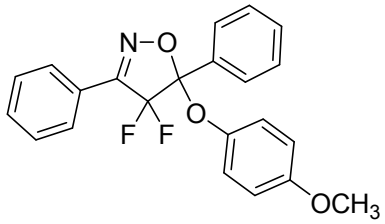
252.8 Hz), 125.0 (m), 126.9 (m), 127.6 (m), 128.7, 129.0, 130.2, 130.6 (m), 131.5, 133.4, 154.8 (dd, *J* = 26.0, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.8 (1F, d, *J* = 265.1 Hz), -62.3 (1F, d, *J* = 265.1 Hz); MS *m/z*: 315 (M^+); HRMS Calcd for $C_{18}H_{15}F_2NO_2$: 315.107 (M^+), Found: 315.107; IR (neat) cm^{-1}: 3065, 1247, 1130, 1091.

4,4-Difluoro-5-phenoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aG)



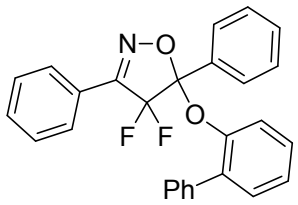
Pale yellow sticky oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.93–7.01 (3H, m), 7.12–7.16 (2H, m), 7.39–7.43 (3H, m), 7.45–7.54 (3H, m), 7.64–7.67 (2H, m), 7.88–7.90 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 105.1 (dd, *J* = 34.1, 17.4 Hz), 120.2, 123.3, 124.7 (m), 125.5 (dd, *J* = 274.2, 253.3 Hz), 127.0 (m), 127.7, 128.6, 129.1, 129.1, 130.2, 130.4, 131.8, 153.0, 154.9 (dd, *J* = 25.8, 24.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -35.1 (1F, d, *J* = 263.4 Hz), -61.1 (1F, d, *J* = 263.4 Hz); MS *m/z*: 351 (M^+); HRMS Calcd for $C_{21}H_{15}F_2NO_2$: 351.107 (M^+), Found: 351.106; IR (neat) cm^{-1}: 3064, 3042, 1591, 1494, 1450, 1247, 1214, 1132, 1061.

4,4-Difluoro-5-(4-methoxyphenoxy)-3,5-diphenyl-4,5-dihydroisoxazole (4aH)



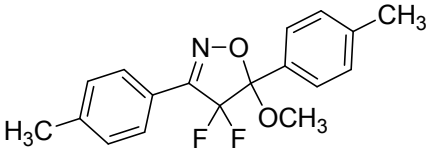
Colorless sticky oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.68 (3H, s), 6.64–6.69 (2H, m), 6.89–6.93 (2H, m), 7.40–7.43 (3H, m), 7.46–7.55 (3H, m), 7.64–7.67 (2H, m), 7.88–7.91 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 55.41, 105.2 (dd, *J* = 33.8, 17.5 Hz), 114.1, 121.9, 124.8 (m), 125.5 (dd, *J* = 273.8, 253.3 Hz), 127.0 (m), 127.8 (m), 128.5, 129.1, 130.2, 130.5 (m), 131.7, 146.5, 155.1 (dd, *J* = 26.0, 24.1 Hz), 155.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -35.0 (1F, d, *J* = 263.8 Hz), -61.3 (1F, d, *J* = 263.8 Hz); MS *m/z*: 381 (M^+); HRMS Calcd for $C_{22}H_{17}F_2NO_3$: 381.118 (M^+), Found: 381.117; IR (neat) cm^{-1}: 3063, 2953, 1247, 1206, 1130, 1063.

5-([1,1'-Biphenyl]-2-yloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aJ)



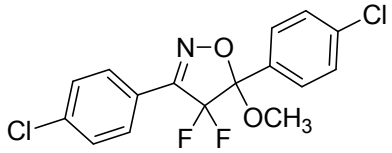
Colorless sticky oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.02–7.12 (3H, m), 7.19–7.53 (14H, m), 7.76–7.78 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 105.3 (dd, *J* = 34.2, 17.5 Hz), 120.4, 123.8, 124.6 (m), 125.5 (dd, *J* = 275.1, 253.4 Hz), 126.9, 127.0 (m), 127.6, 127.8, 127.9, 128.5, 129.0, 129.8, 130.1, 130.5, 130.9, 131.6, 134.2, 138.0, 149.8, 154.8 (dd, *J* = 25.7, 24.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.8 (1F, d, *J* = 262.5 Hz), -59.7 (1F, d, *J* = 262.5 Hz); MS *m/z*: 427 (M^+); HRMS Calcd for $C_{27}H_{19}F_2NO_2$: 427.138 (M^+), Found: 427.139; IR (neat) cm^{-1}: 3063, 1600, 1502, 1479, 1247, 1207, 1061.

4,4-Difluoro-5-methoxy-3,5-di-*p*-tolyl-4,5-dihydroisoxazole (4bB)



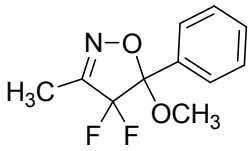
Colorless soid; M.p. 86.0–86.5 °C (recrystallized from MeOH); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.40 (3H, s), 2.41 (3H, s), 3.33 (3H, s), 7.26–7.30 (4H, m), 7.50–7.53 (2H, m), 7.74–7.76 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.36, 21.62, 51.58, 105.2 (dd, *J* = 33.2, 17.7 Hz), 122.2 (m), 125.1 (dd, *J* = 271.3, 252.4 Hz), 126.8 (m), 127.2 (m), 127.6 (m), 129.4, 129.7, 140.2, 142.0, 154.8 (dd, *J* = 26.1, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.9 (1F, d, *J* = 265.1 Hz), -62.8 (1F, d, *J* = 265.1 Hz); MS *m/z*: 317 (M^+); HRMS Calcd for $C_{18}H_{17}F_2NO_2$: 317.123 (M^+), Found: 317.123; IR (KBr) cm^{-1}: 3017, 2976, 2942, 1249, 1127, 1092.

3,5-Bis(4-chlorophenyl)-4,4-difluoro-5-methoxy-4,5-dihydroisoxazole (4cB)



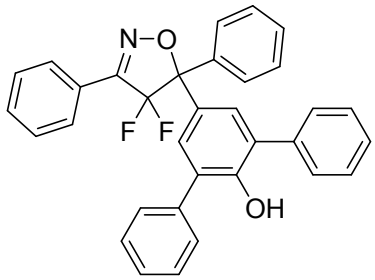
Colorless soid; M.p. 95.5–96.5 °C (recrystallized from MeOH); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.34 (3H, s), 7.44–7.49 (4H, m), 7.54–7.58 (2H, m), 7.78–7.80 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 51.80, 105.0 (dd, *J* = 33.1, 17.6 Hz), 123.2 (m), 124.8 (dd, *J* = 271.9, 252.9 Hz), 128.1 (m), 128.5 (m), 129.1, 129.1 (m), 129.5, 136.6, 138.0, 154.1 (dd, *J* = 26.1, 24.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.9 (1F, d, *J* = 265.5 Hz), -62.6 (1F, d, *J* = 265.5 Hz); MS *m/z*: 357 (M^+); HRMS Calcd for $C_{16}H_{11}Cl_2F_2NO_2$: 357.014 (M^+), Found: 357.014; IR (KBr) cm^{-1}: 2977, 1246, 1123, 1091.

4,4-Difluoro-5-methoxy-3-methyl-5-phenyl-4,5-dihydroisoxazole (4dB)



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.16 (3H, d, *J* = 2.4 Hz), 3.28 (3H, s), 7.44–7.47 (3H, m), 7.55–7.59 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 8.78, 51.49, 104.0 (dd, *J* = 33.2, 16.9 Hz), 124.6 (dd, *J* = 269.4, 251.5 Hz), 127.6, 128.6, 130.1, 130.4, 154.6 (dd, *J* = 29.2, 25.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -40.3 (1F, dq, *J* = 266.4, 2.4 Hz), -68.0 (1F, d, *J* = 266.4 Hz); MS *m/z*: 227 (M^+); HRMS Calcd for $C_{11}H_{11}F_2NO_2$: 227.076 (M^+), Found: 227.075; IR (neat) cm^{-1}: 3065, 2946, 1243, 1119.

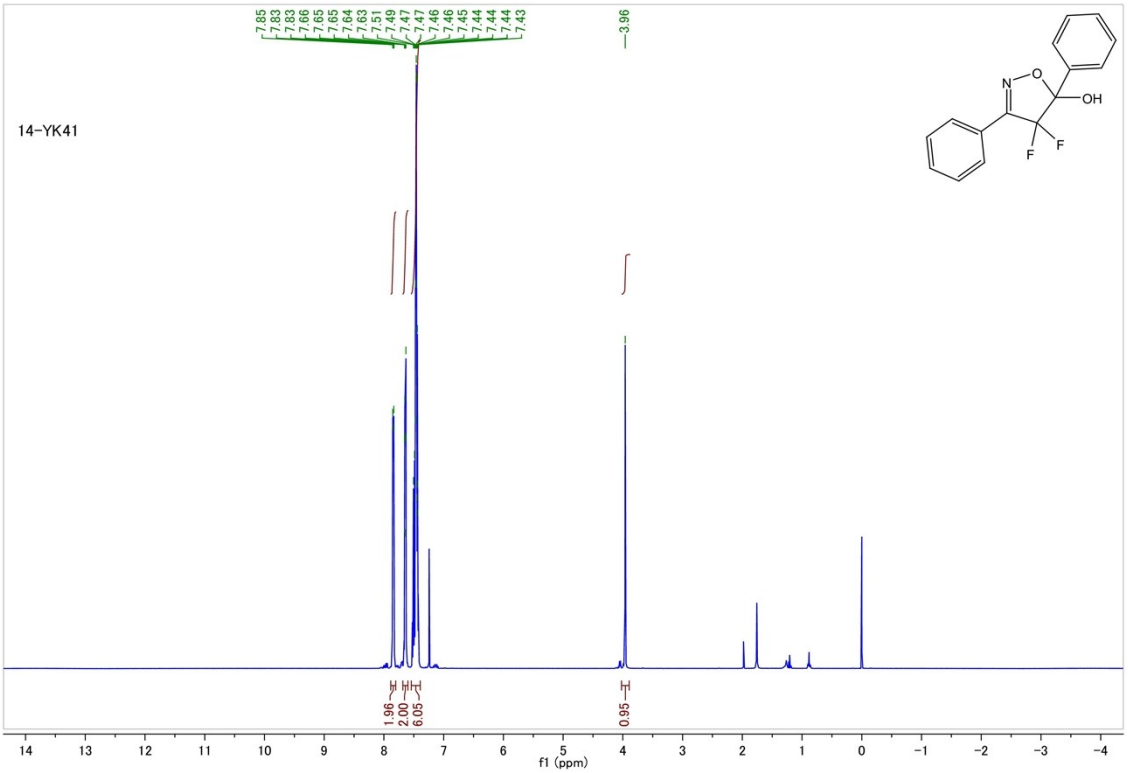
5'-(4,4-Difluoro-3,5-diphenyl-4,5-dihydroisoxazol-5-yl)-[1,1':3',1''-terphenyl]-2'-ol (6aK)

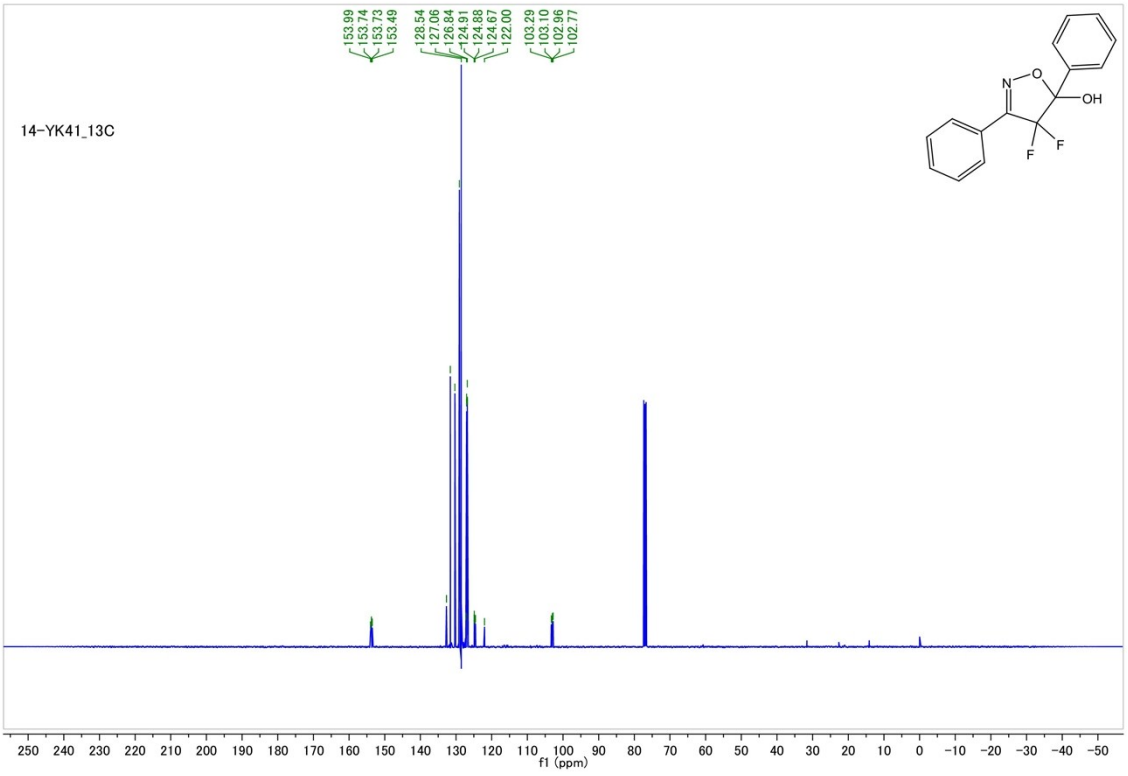


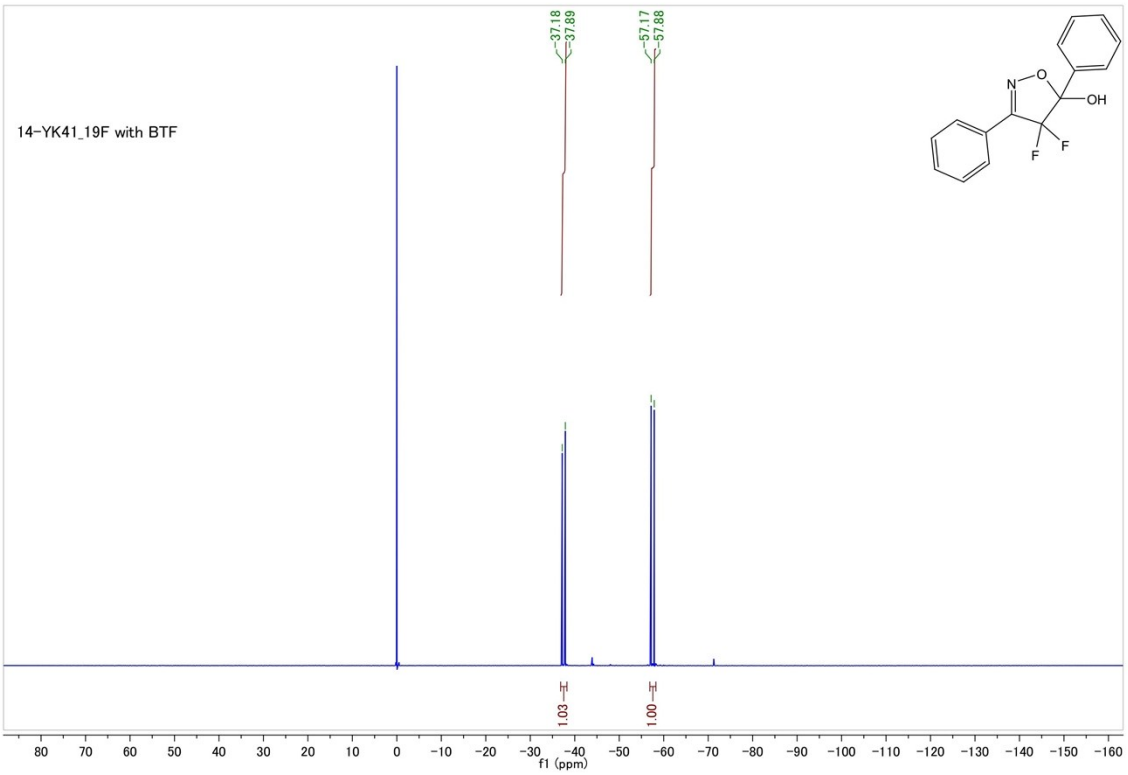
Colorless solid; M.p. 65.5–71.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.50 (1H, s), 7.31–7.54 (18H, m), 7.60–7.62 (2H, m), 7.86–7.88 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 90.51 (t, *J* = 23.3 Hz), 128.2 (t, *J* = 260.2 Hz), 125.2 (m), 126.8, 127.2, 127.7 (m), 127.9, 128.4, 128.6, 128.6, 128.9, 128.9, ,129.0, 129.4, 131.2, 135.7 (m), 137.1, 149.6, 153.6 (t, *J* = 25.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -34.7 (1F, d, *J* = 257.8 Hz), -35.5 (1F, d, *J* = 257.8 Hz); MS *m/z*: 503 (M^+); HRMS Calcd for $C_{33}H_{23}F_2NO_2$: 503.170 (M^+), Found: 503.170; IR (KBr) cm^{-1}: 3533, 3060, 1496, 1469, 1233, 1106.

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

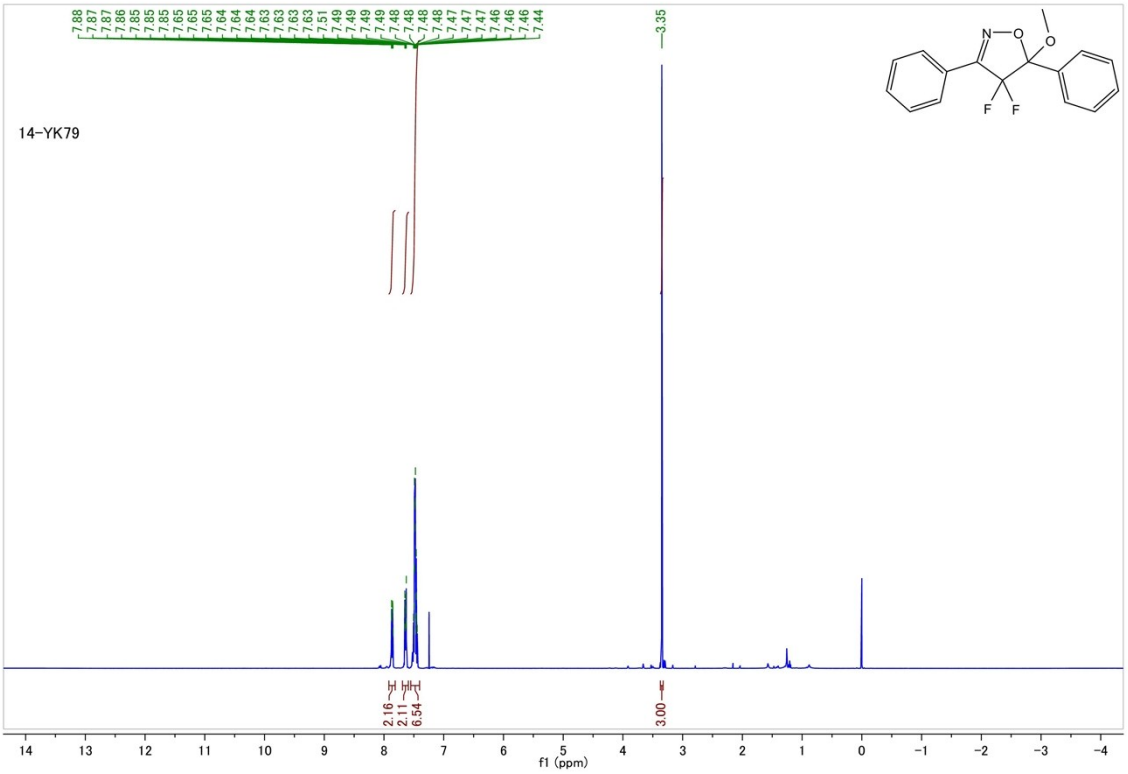
4,4-Difluoro-3,5-diphenyl-4,5-dihydroisoxazol-5-ol (4aA)

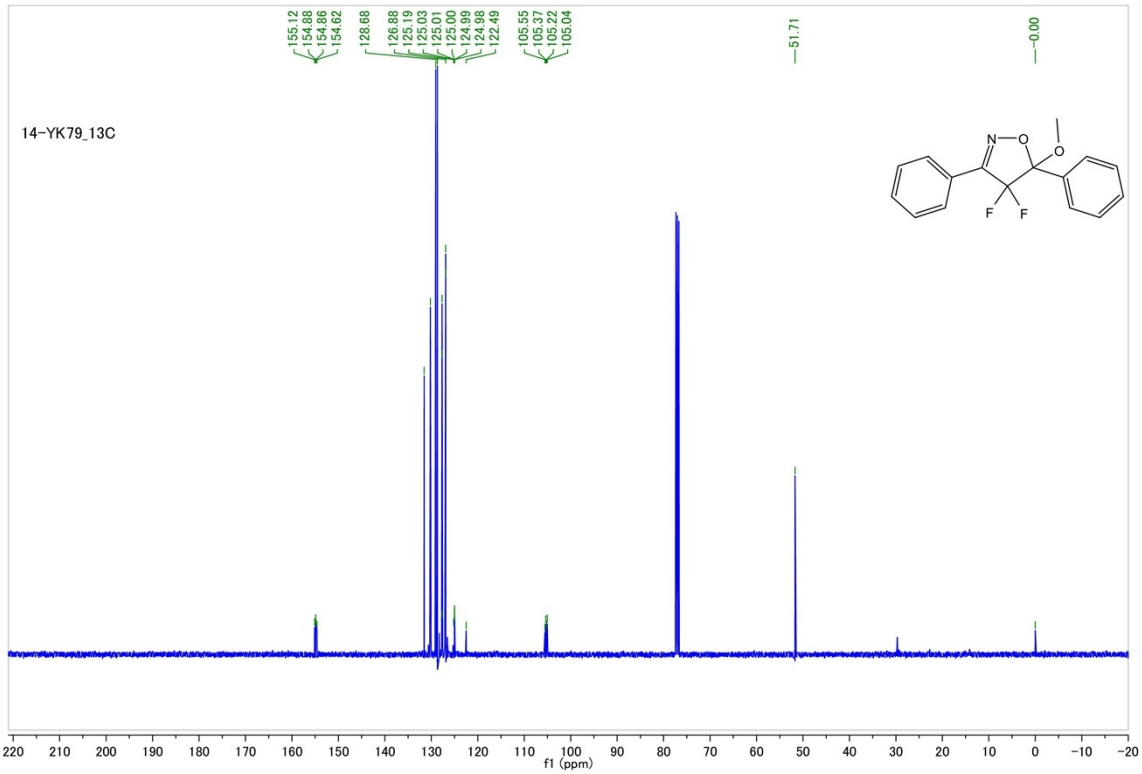


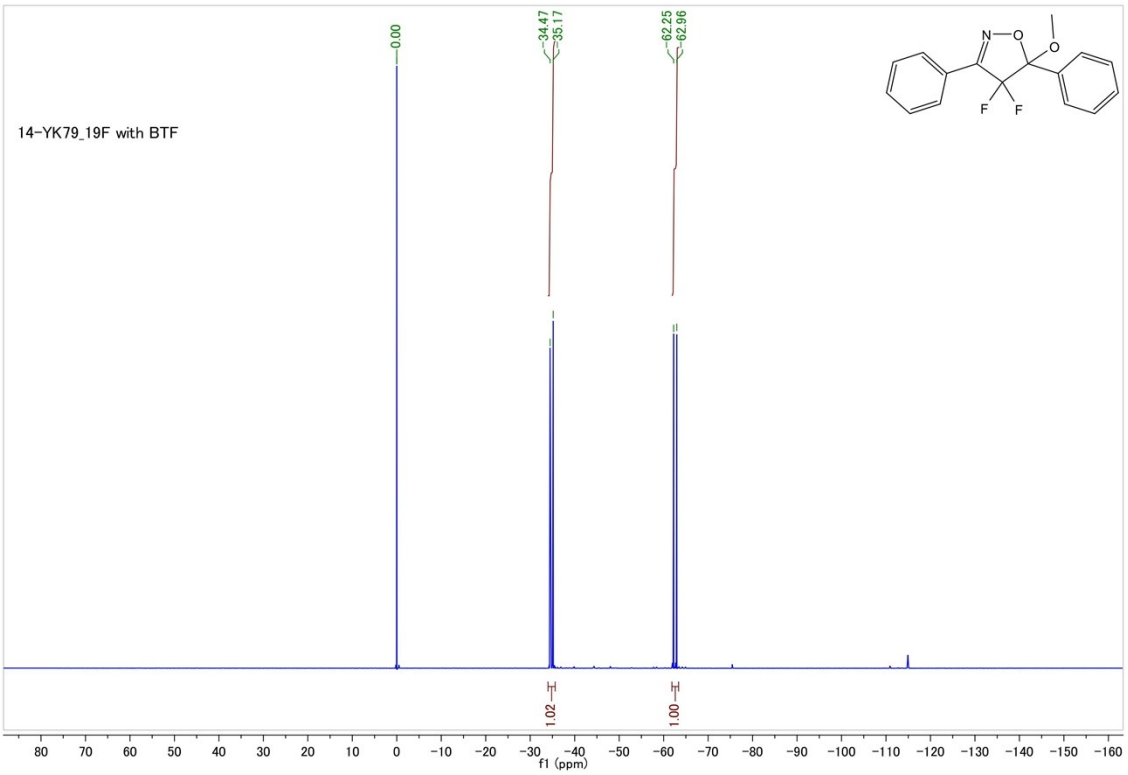



14-YK41_19F with BTF
-37.18
-37.89
-57.17
-57.88
N
O
OH
F
F
1.03
1.00
80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

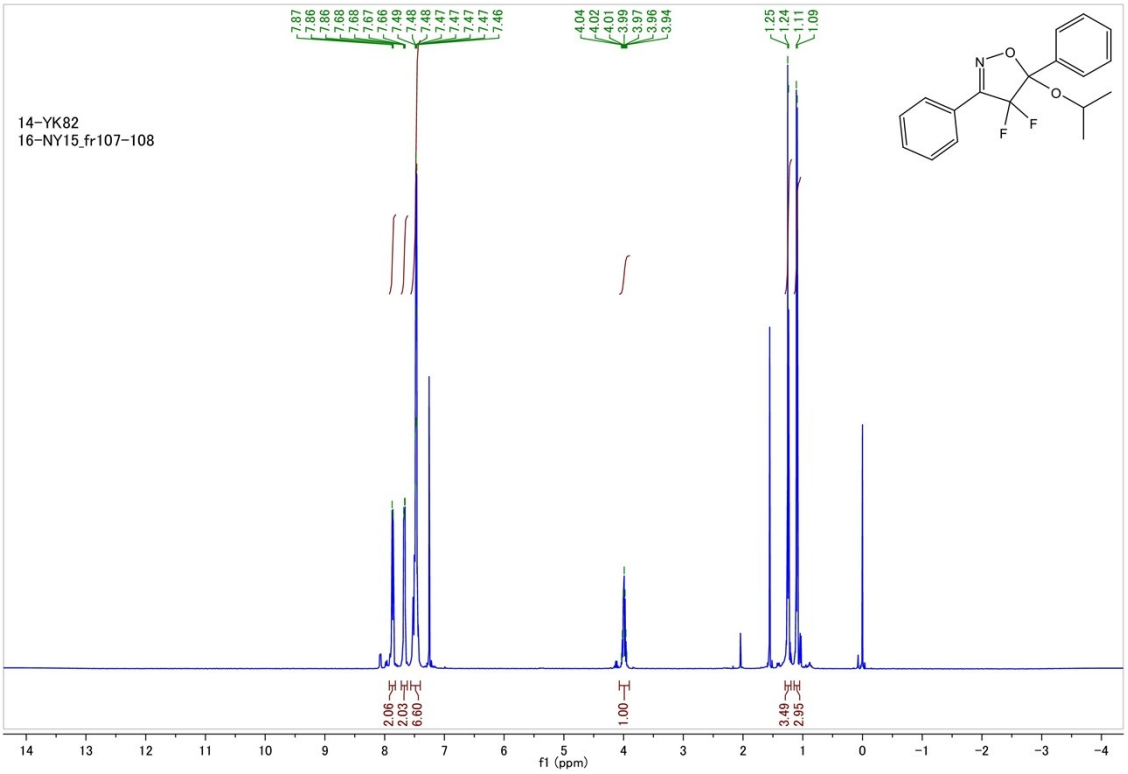
4,4-Difluoro-5-methoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aB)

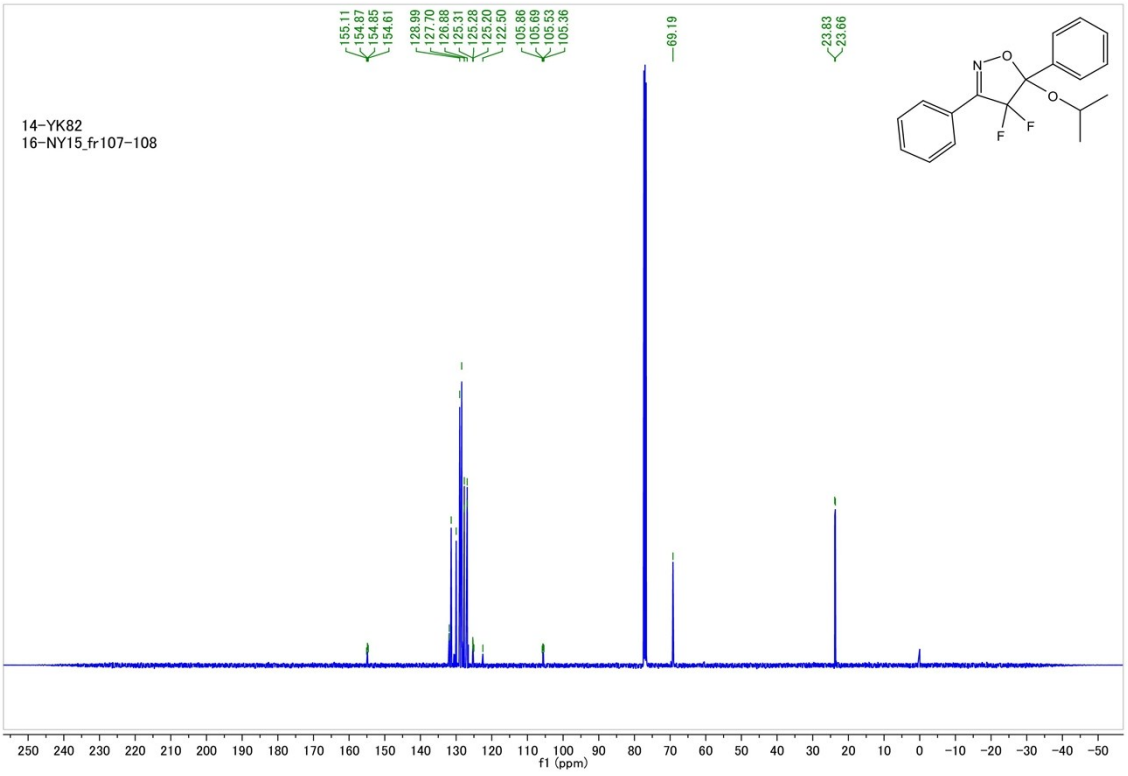


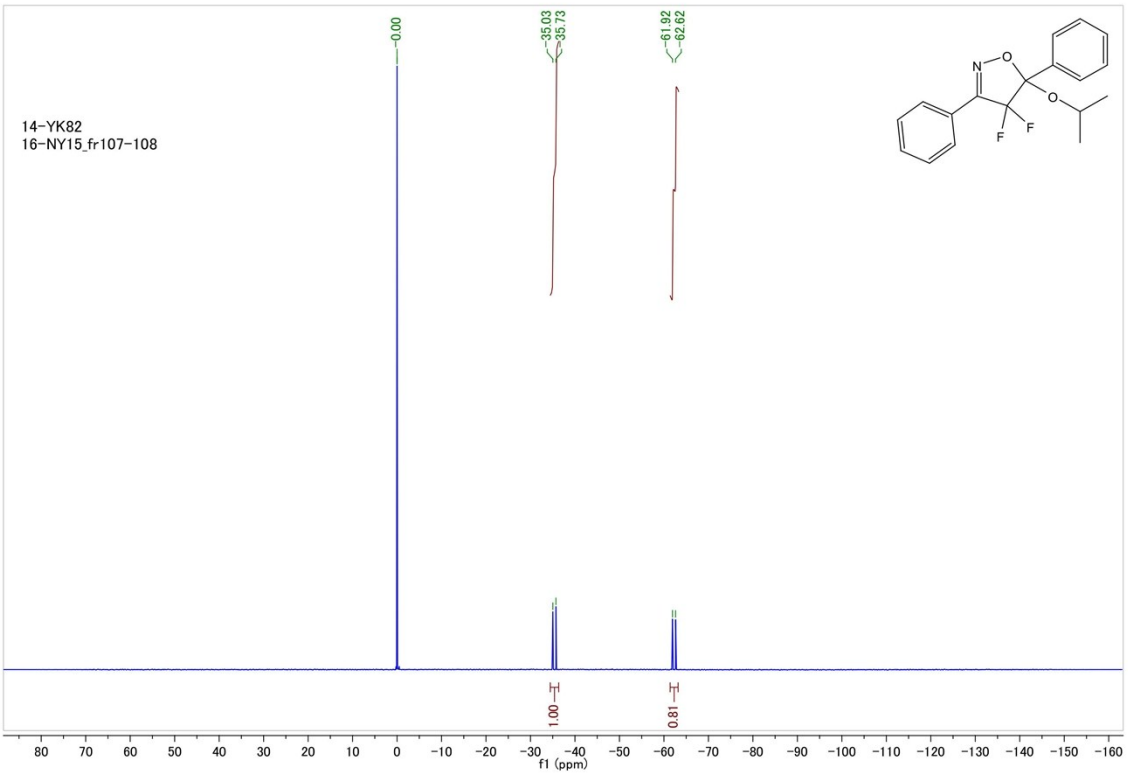



14-YK79_19F with BTF
0.00
-34.47
-35.17
-62.25
-62.96
N
O
O
F
F
1.02
1.00
80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

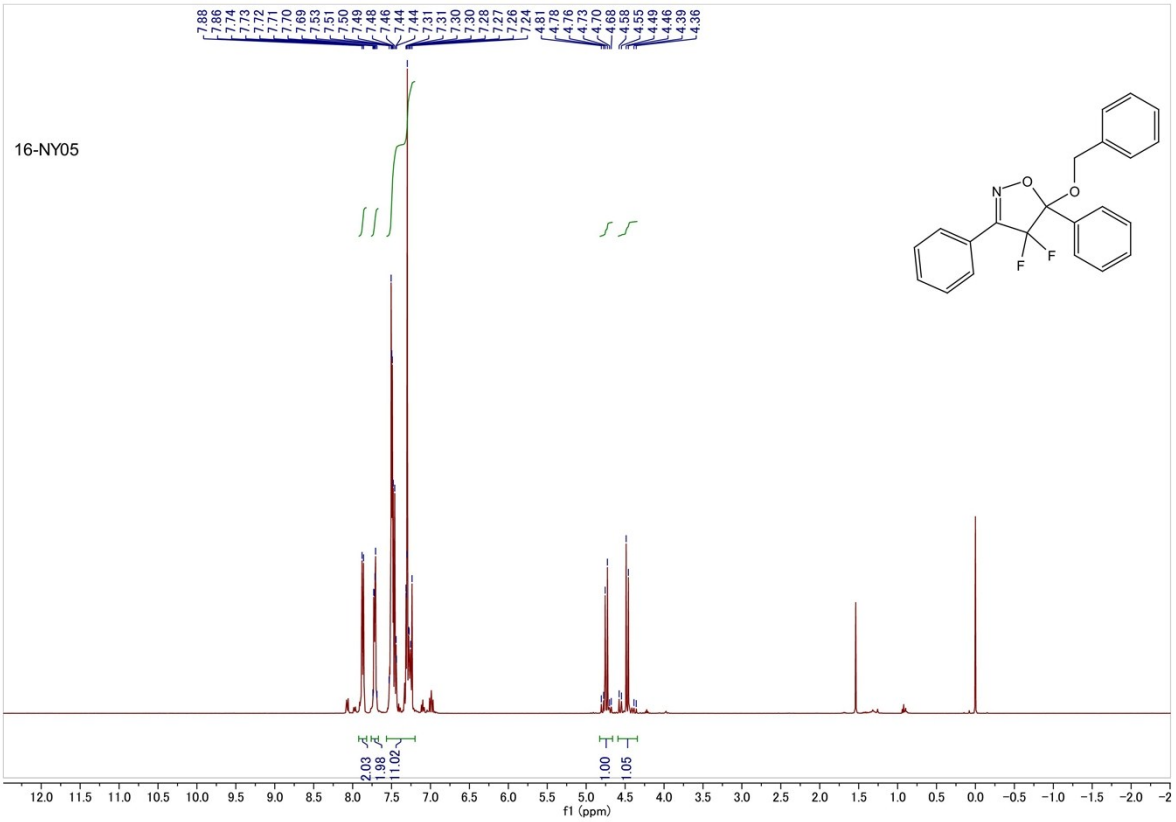
4,4-Difluoro-5-isopropoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aC)

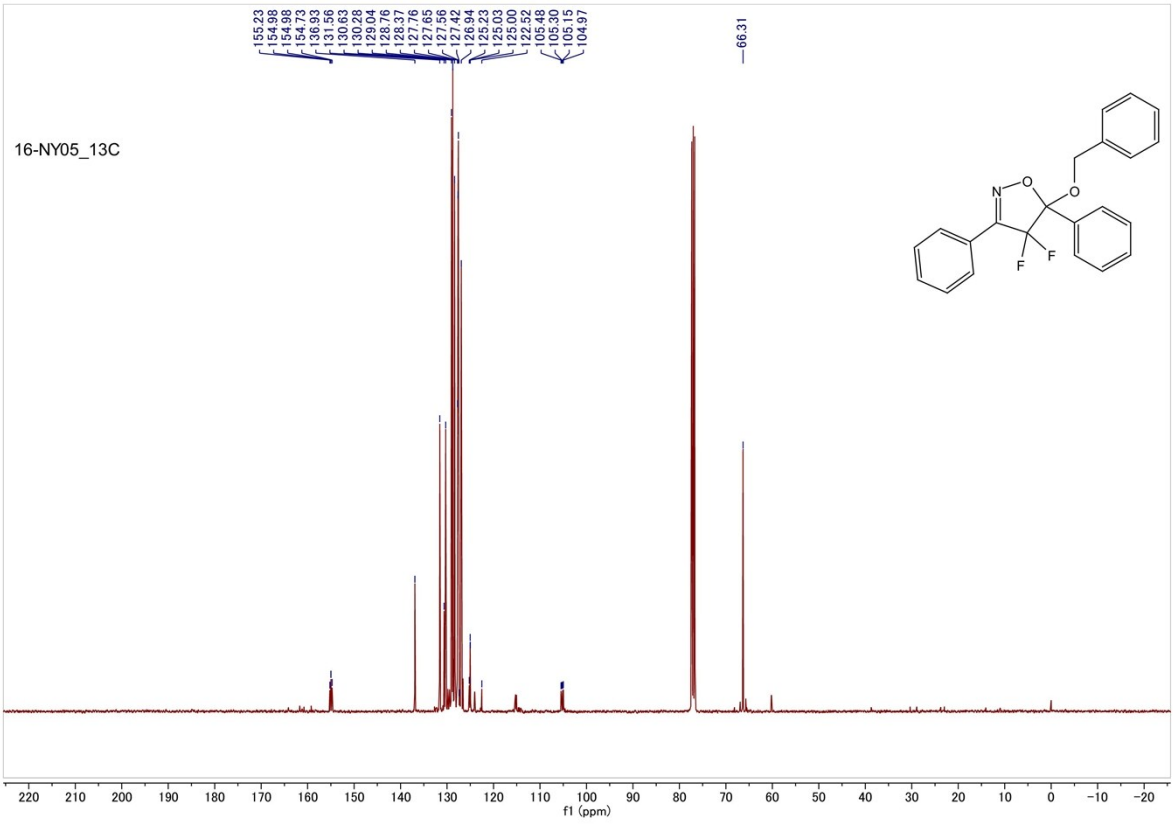


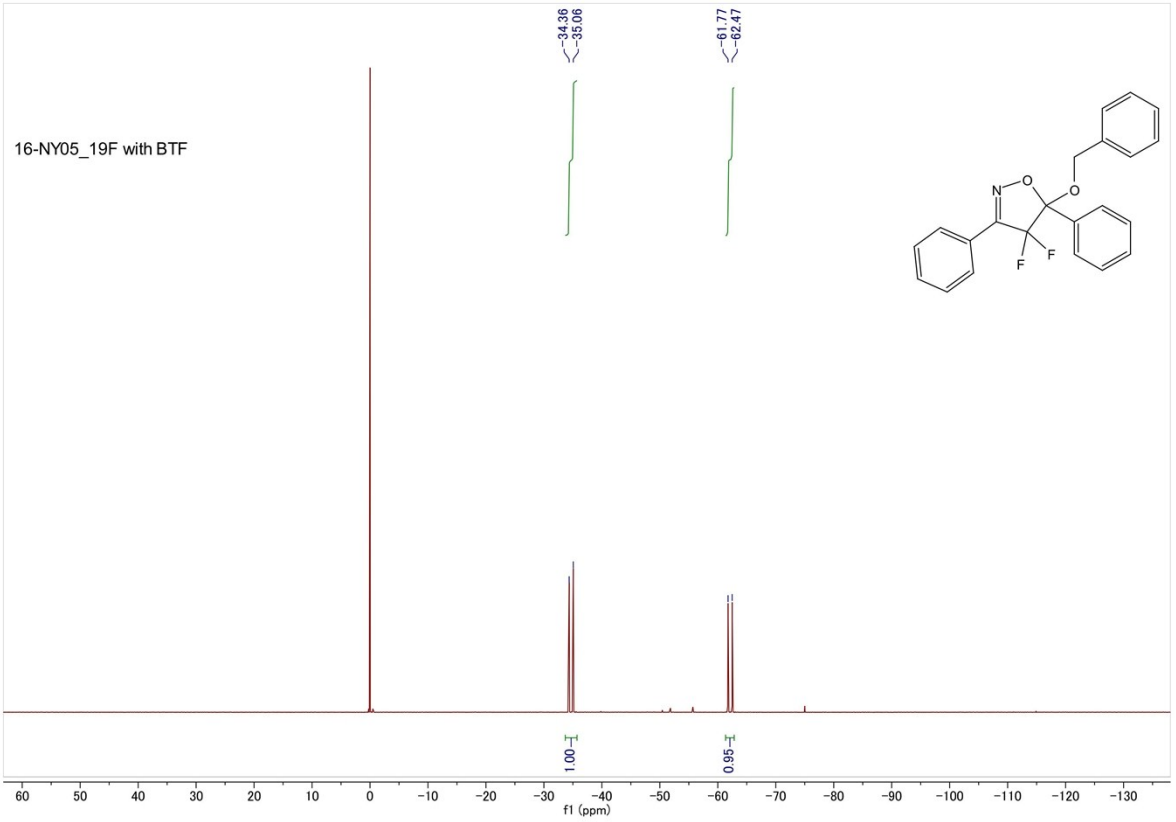



14-YK82
16-NY15_fr107-108
0.00
35.03
35.73
61.92
62.62
1.00
0.81
N
O
O
F
F
f1 (ppm)

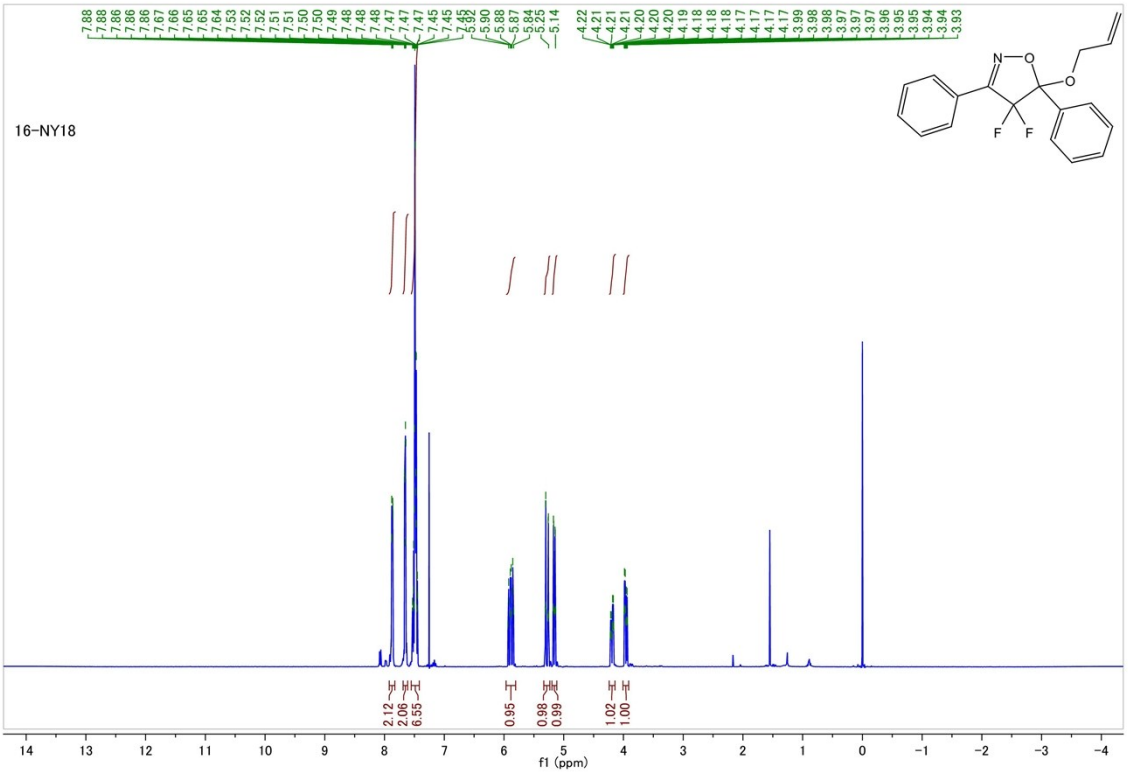
5-(Benzyloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aE)

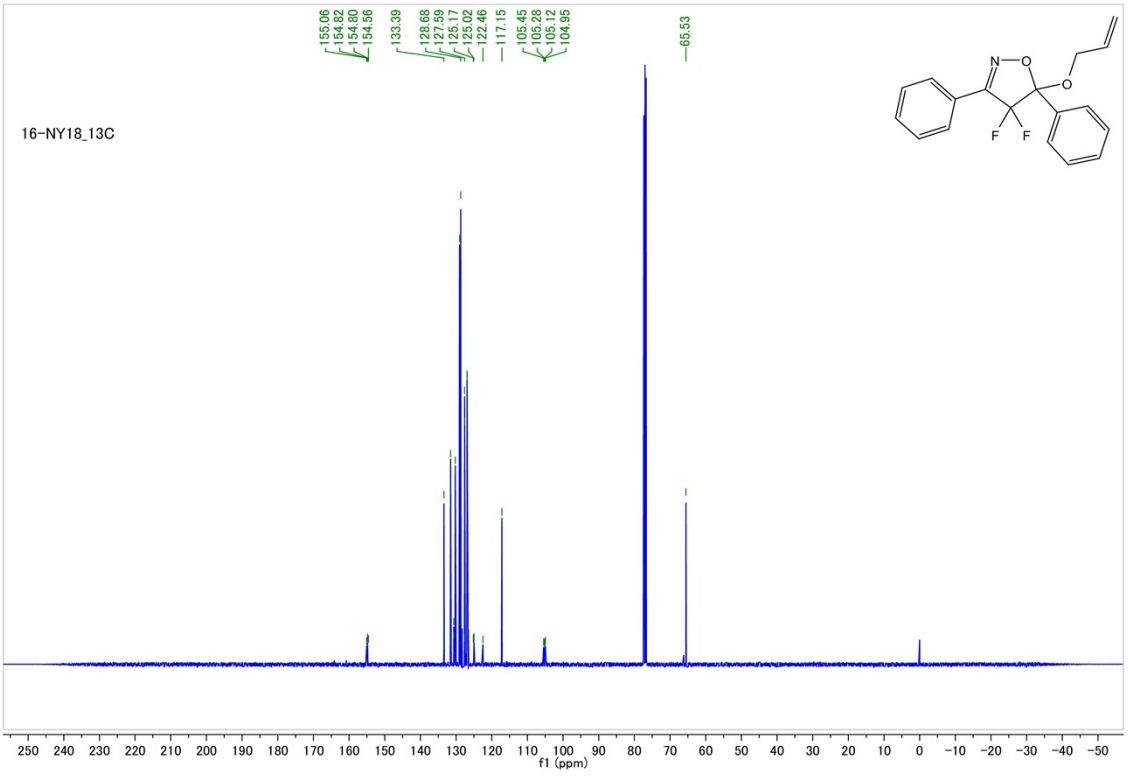


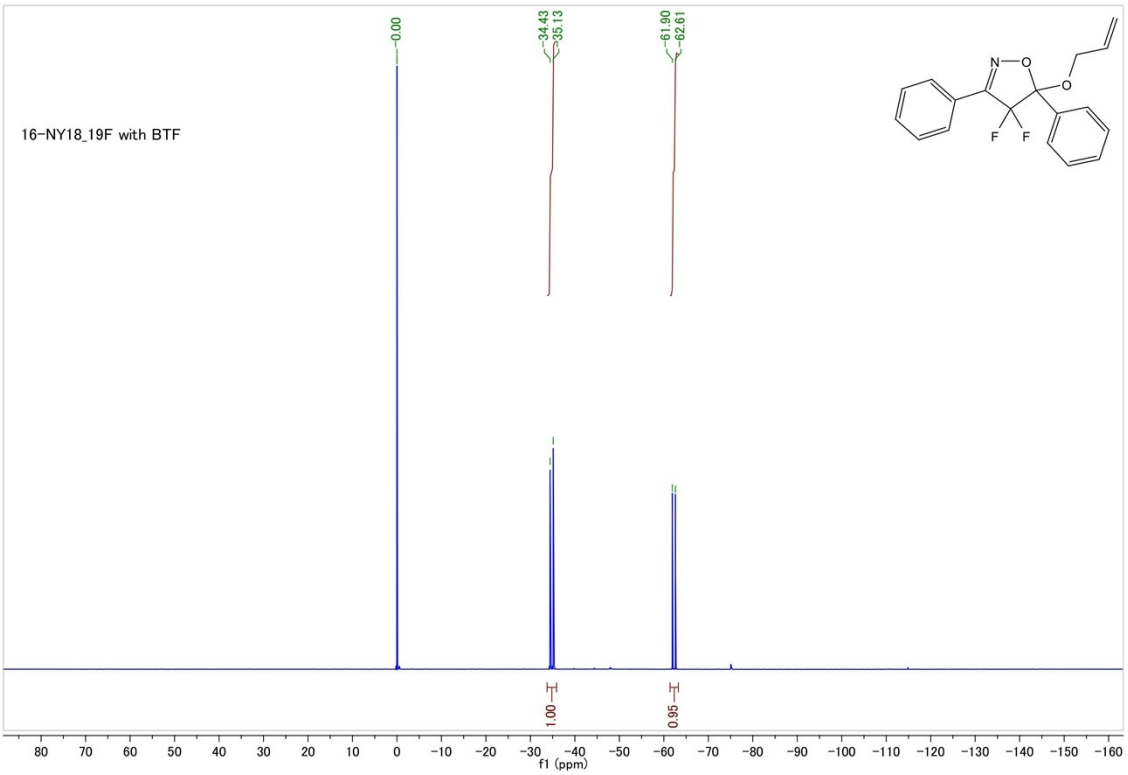



16-NY05_19F with BTF
-34.36
-35.06
-61.77
-62.47
1.00
0.95
60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130
f1 (ppm)
N
O
O
F
F

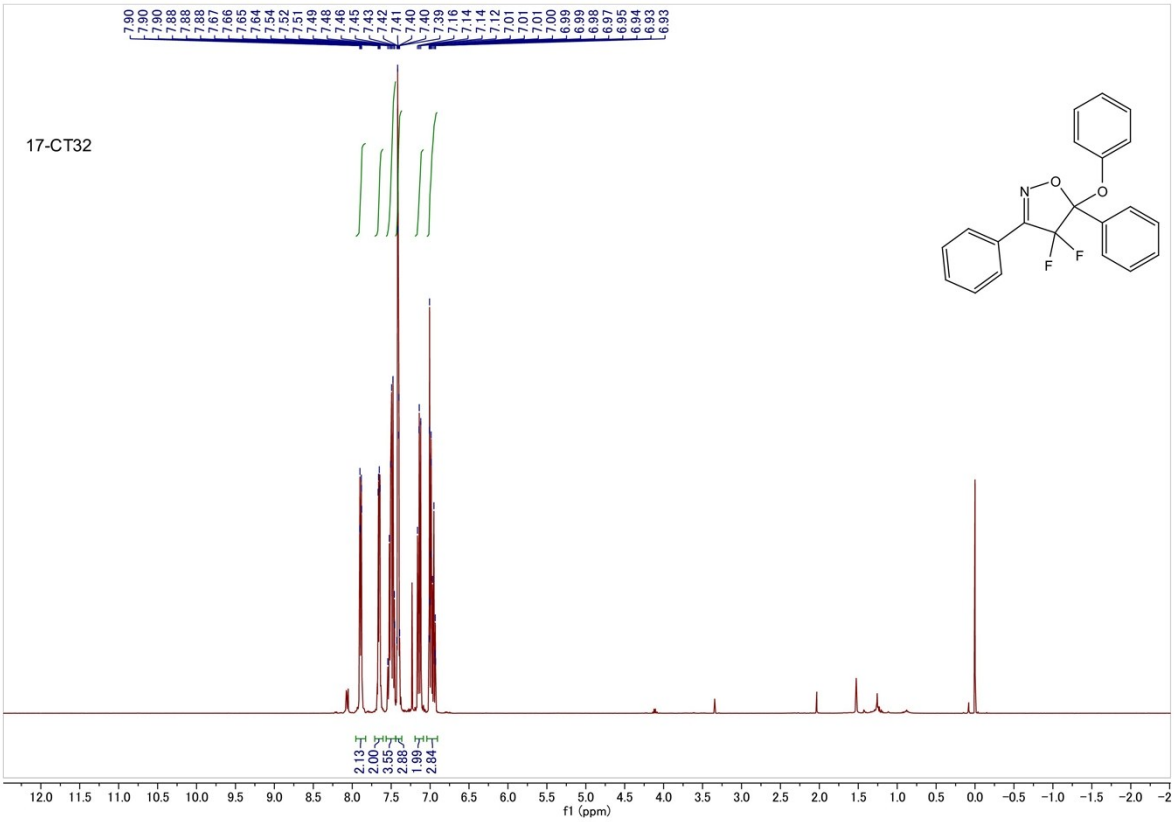
5-(Allyloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aF)

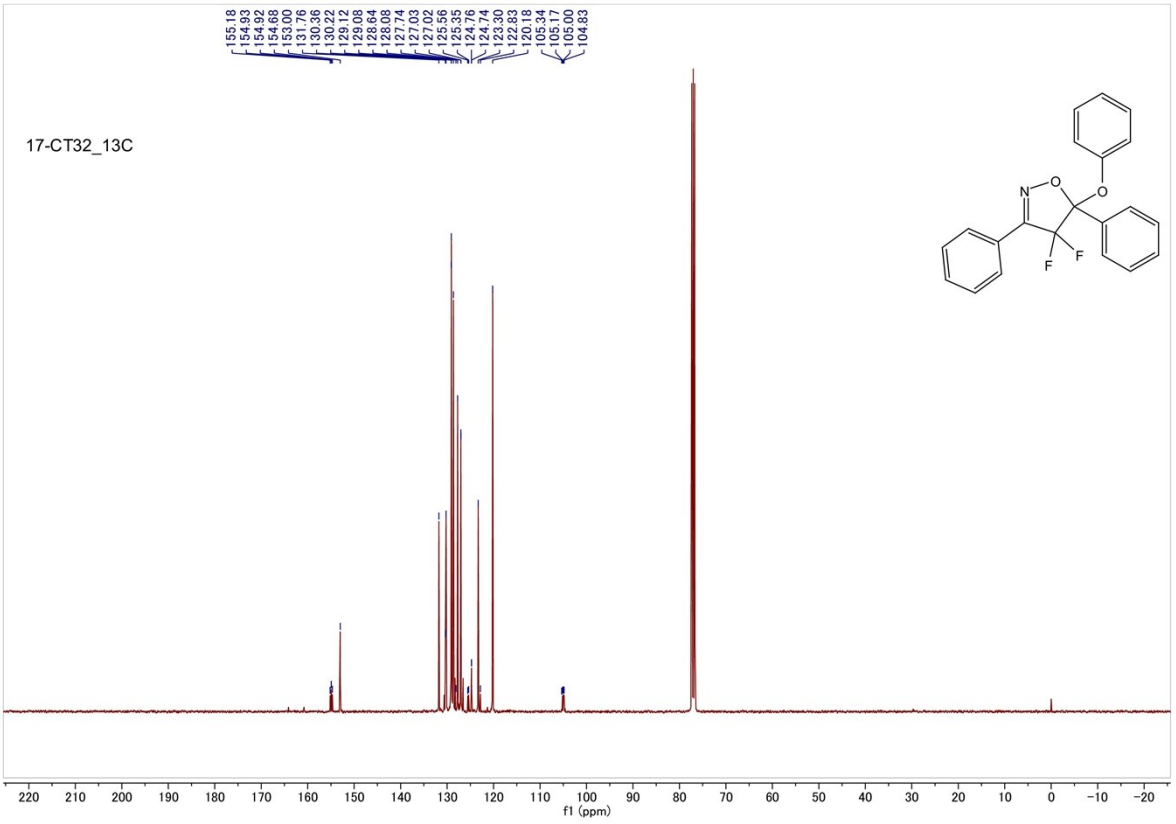


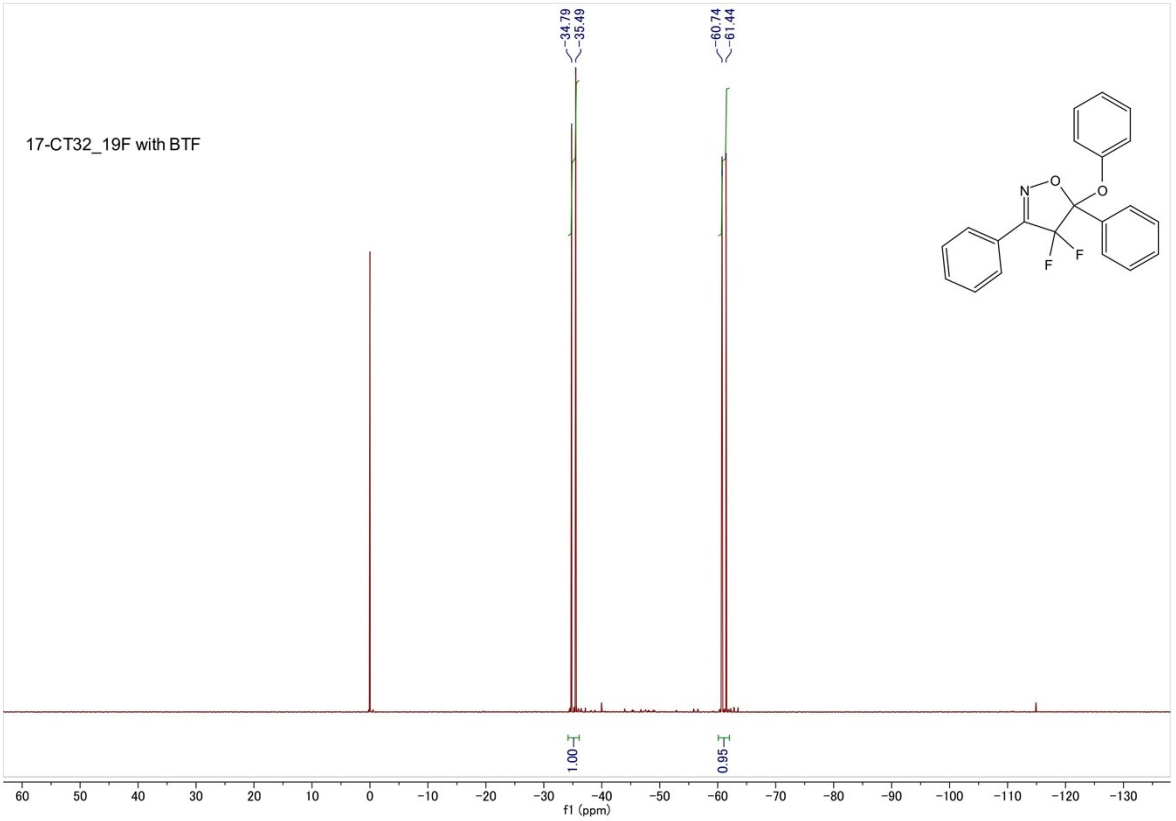



16-NY18_19F with BTF
0.00
-34.43
-35.13
-61.90
-62.61
N
O
O
F
F
1.00
0.95
80 70 60 50 40 30 20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160
f1 (ppm)

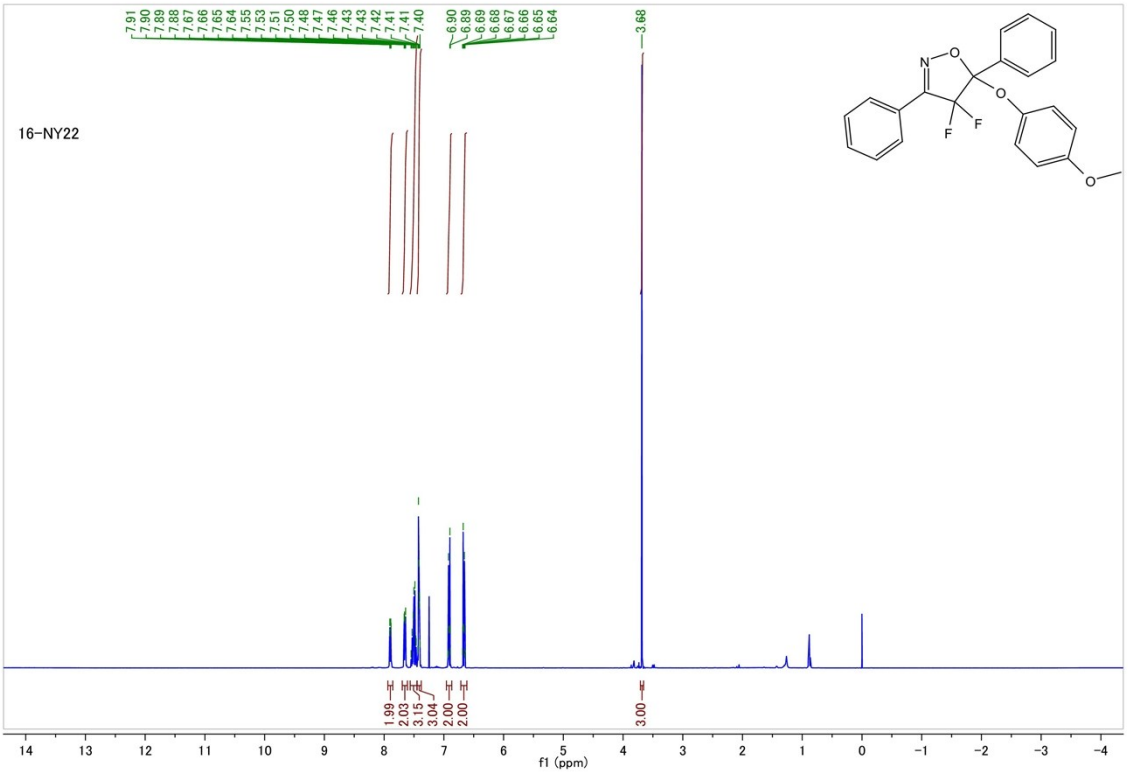
4,4-Difluoro-5-phenoxy-3,5-diphenyl-4,5-dihydroisoxazole (4aG)

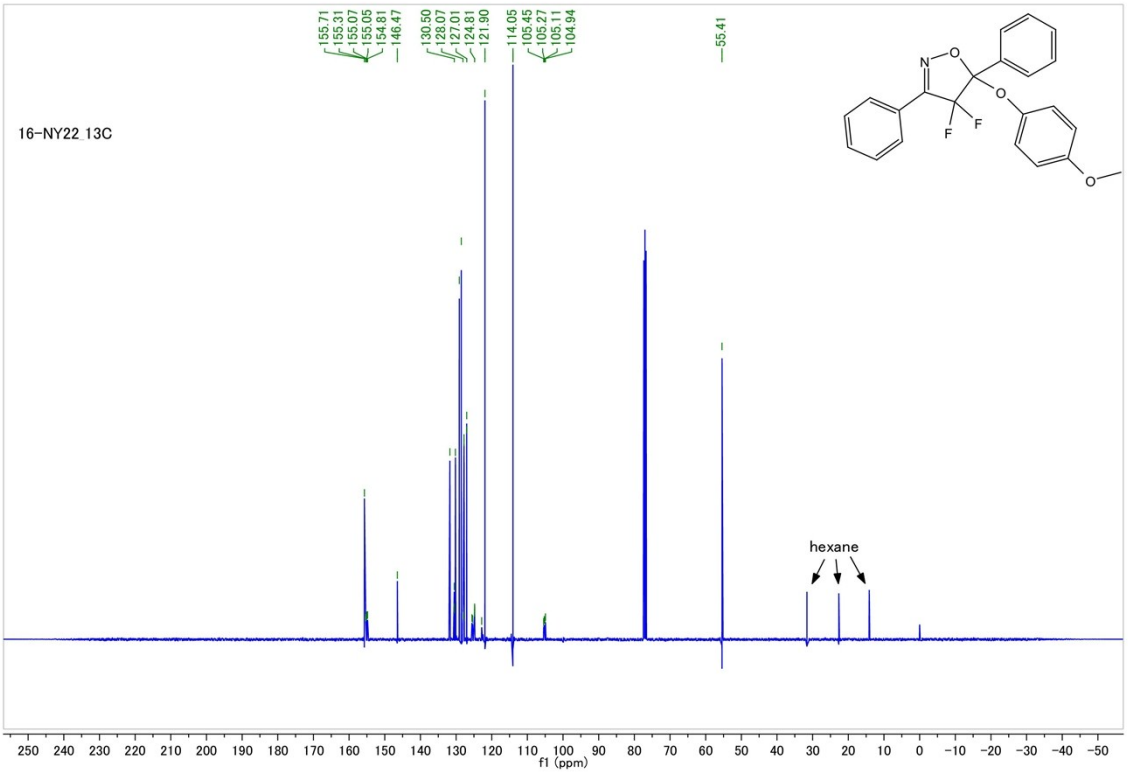


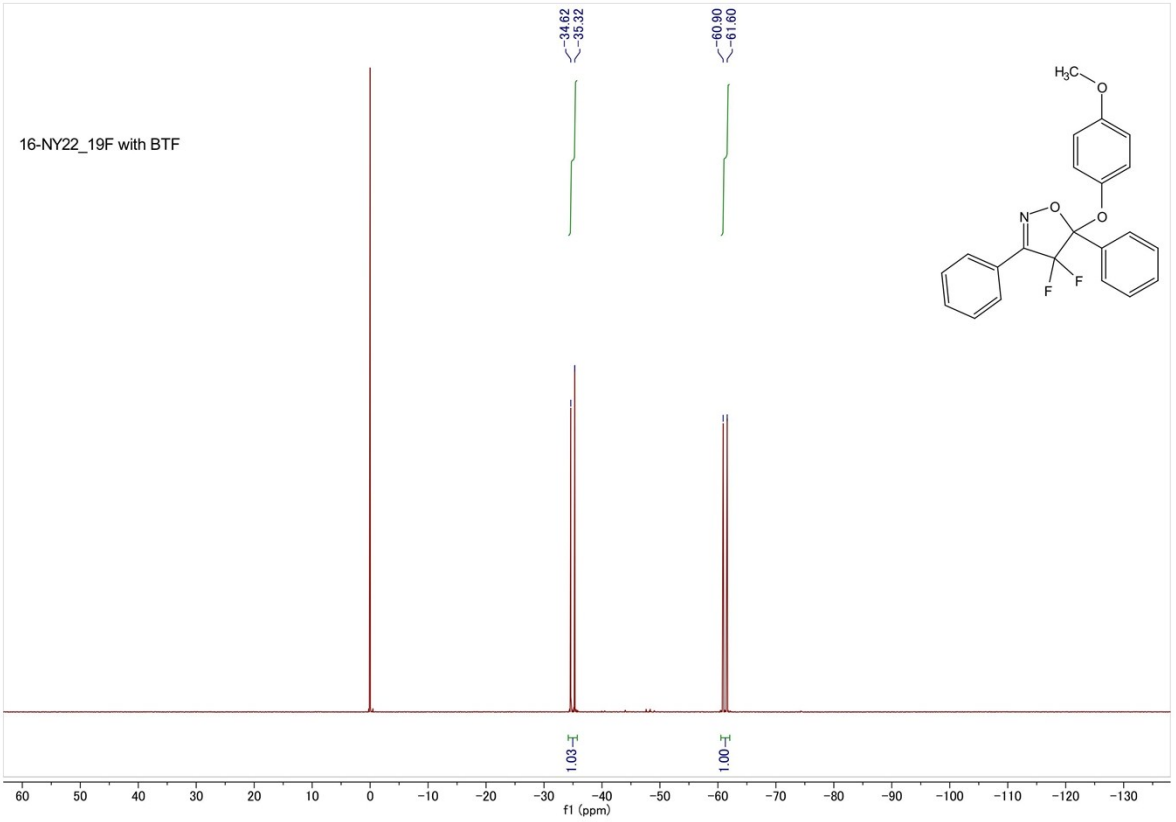



17-CT32_19F with BTF
-34.79
-35.49
-60.74
-61.44
1.00
0.95
N
O
O
F
F
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
f1 (ppm)

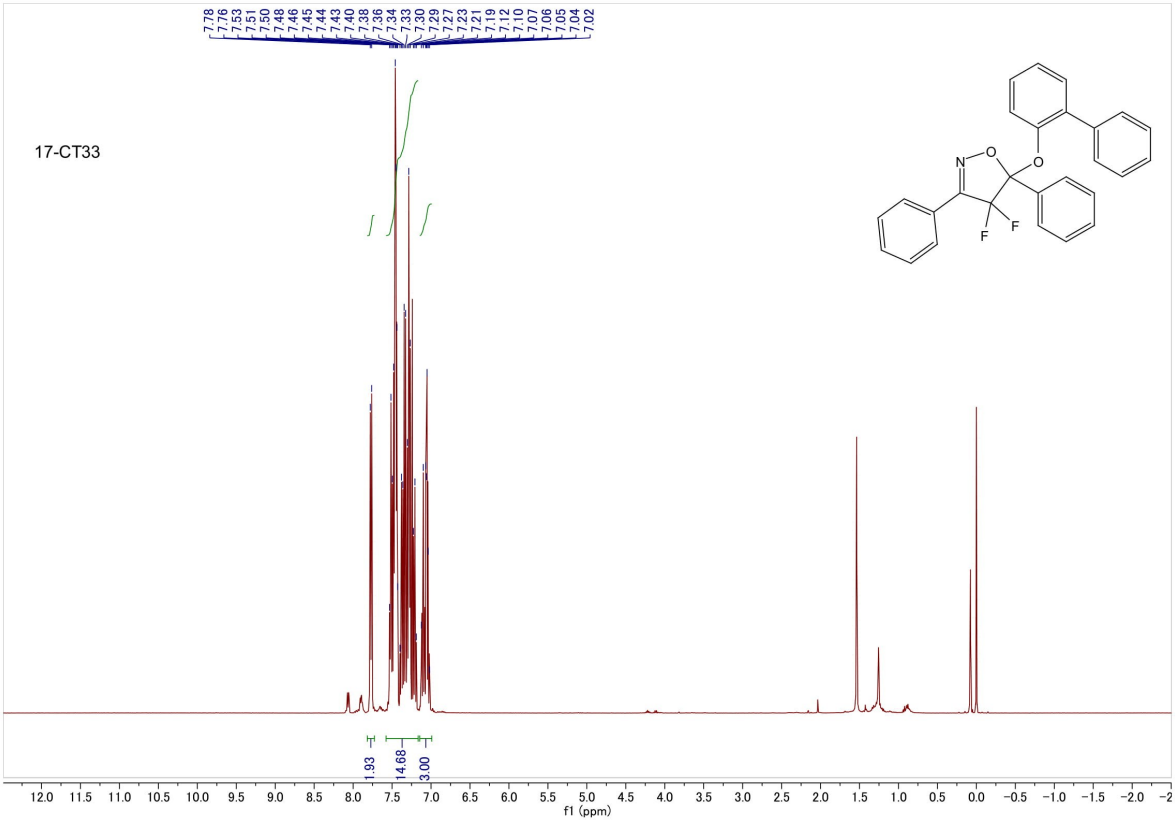
4,4-Difluoro-5-(4-methoxyphenoxy)-3,5-diphenyl-4,5-dihydroisoxazole (4aH)

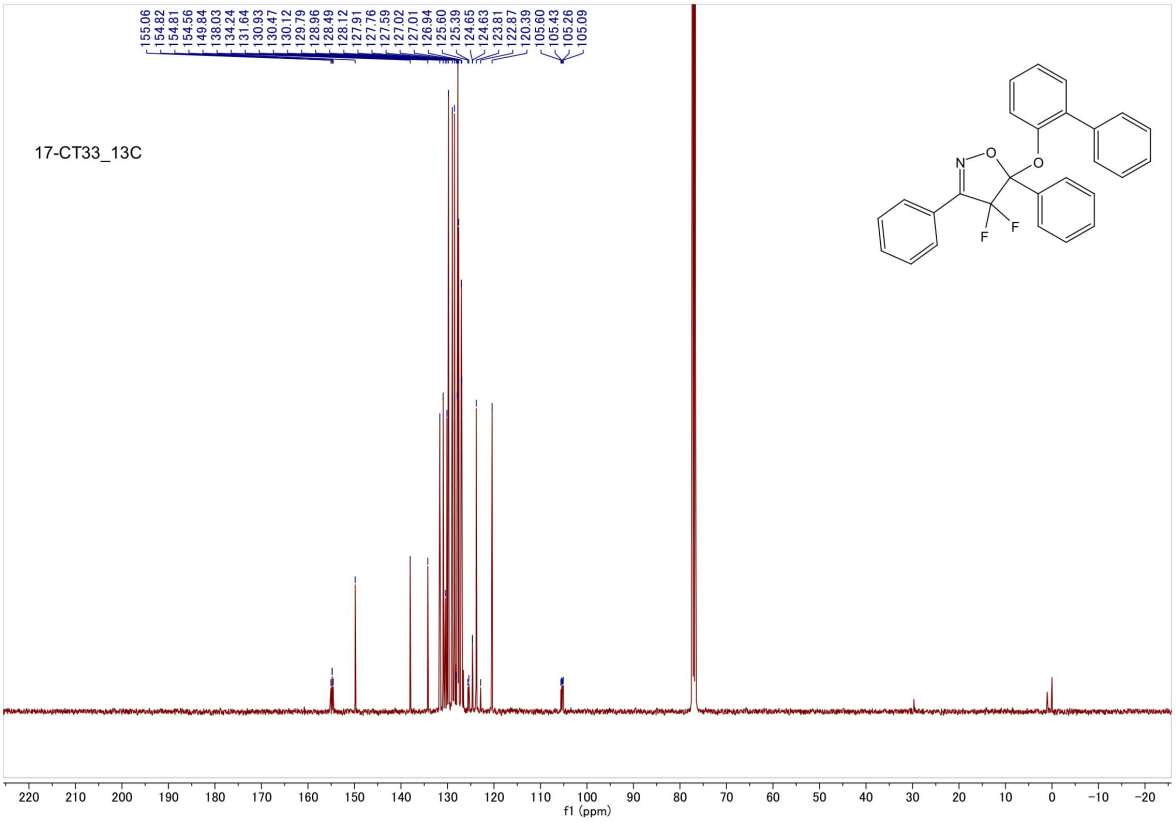


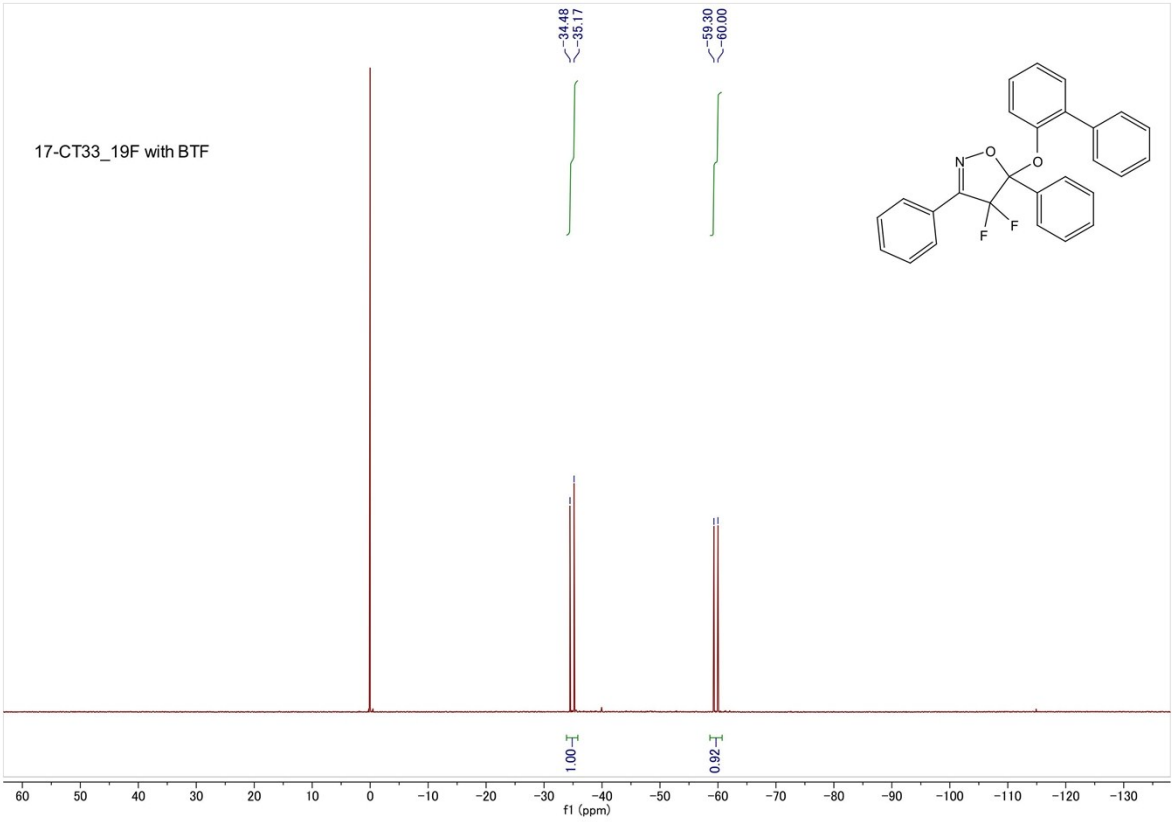



16-NY22_19F with BTF
-34.62
-35.32
-60.90
-61.60
1.03
1.00
f1 (ppm)

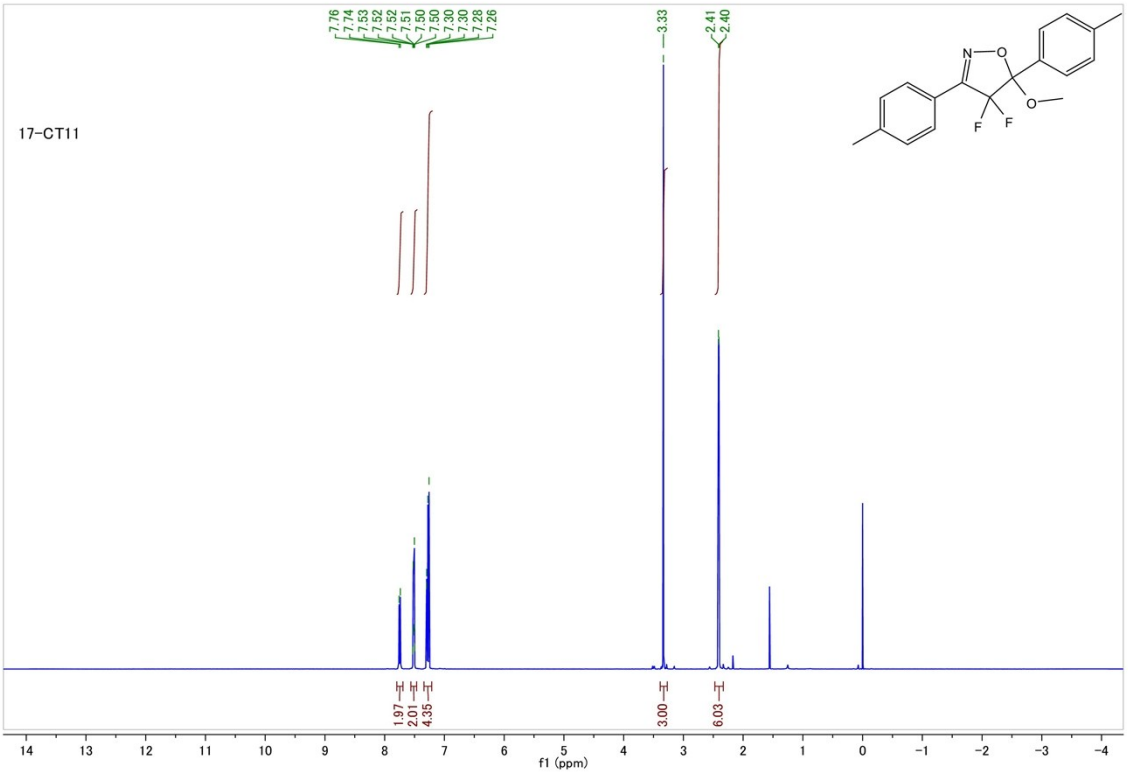
5-([1,1'-Biphenyl]-2-yloxy)-4,4-difluoro-3,5-diphenyl-4,5-dihydroisoxazole (4aJ)

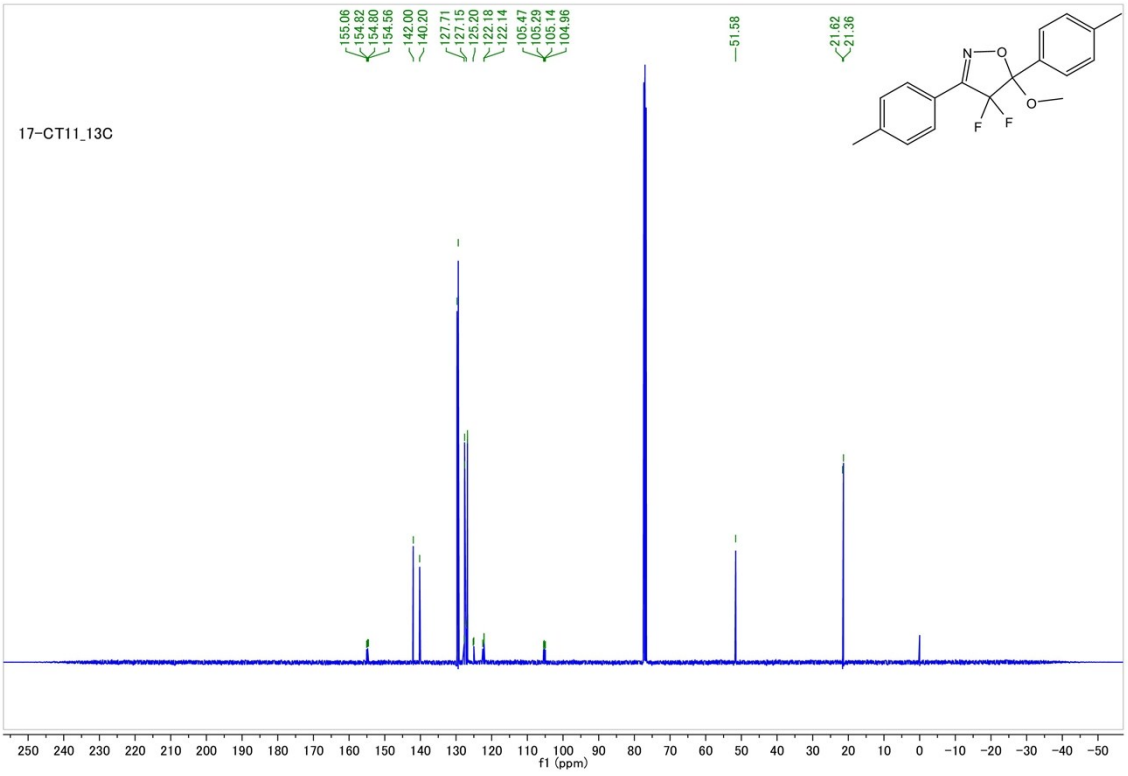


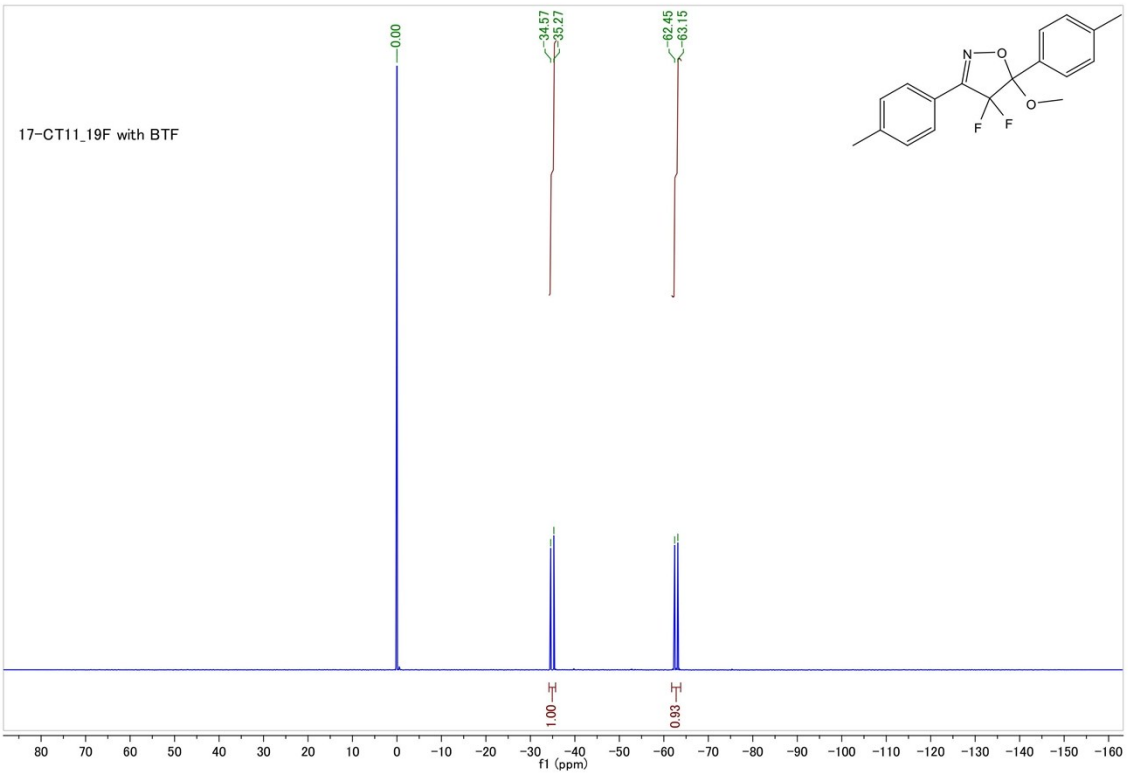



17-CT33_19F with BTF
-34.48
-35.17
-59.30
-60.00
N
O
O
F
F
1.00
0.92
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
f1 (ppm)

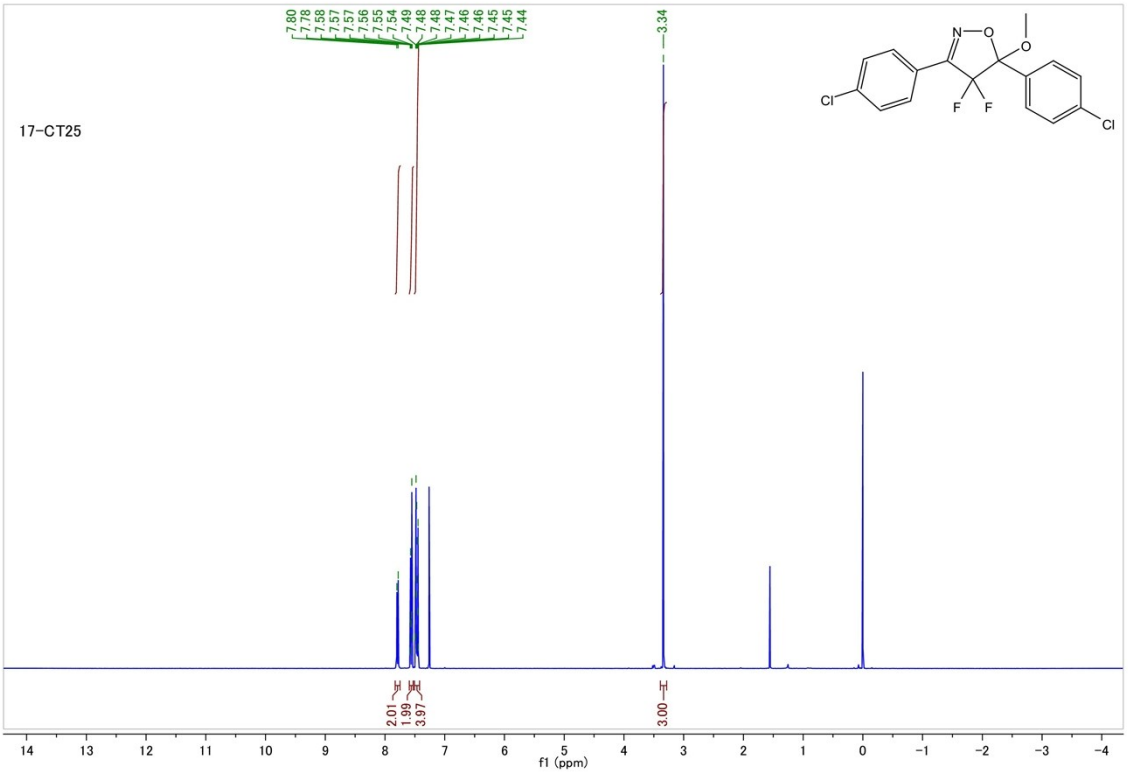
4,4-Difluoro-5-methoxy-3,5-di-*p*-tolyl-4,5-dihydroisoxazole (4bB)

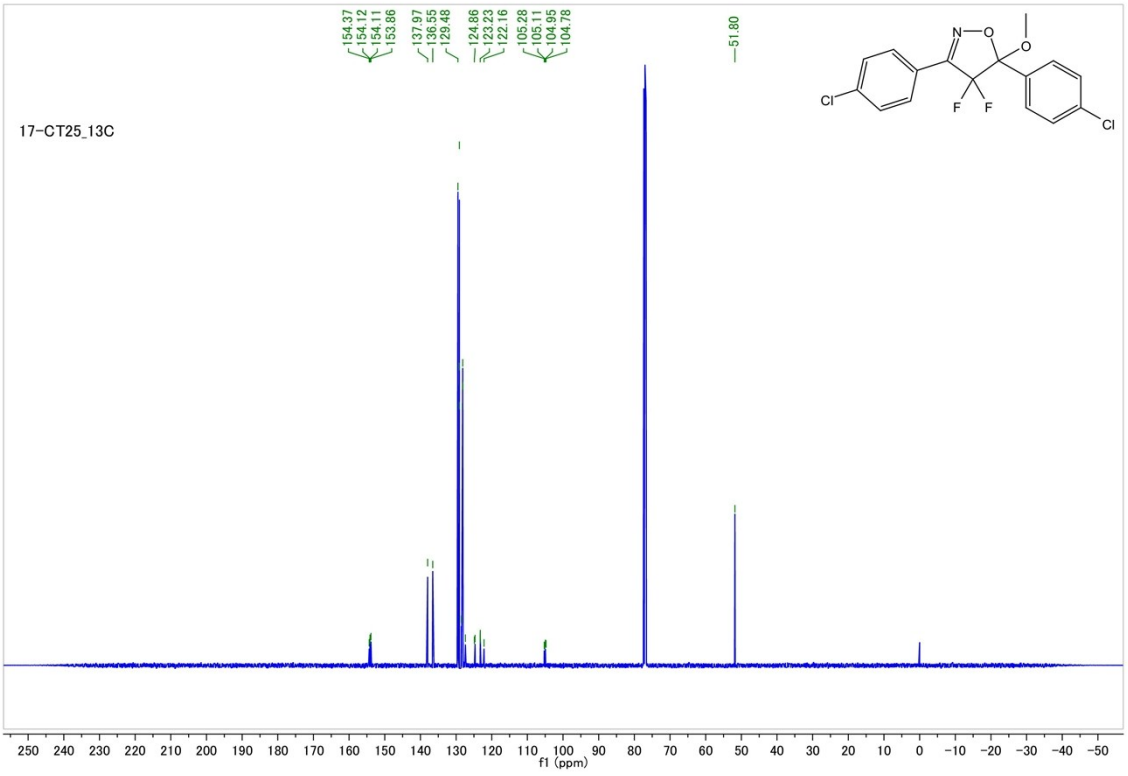


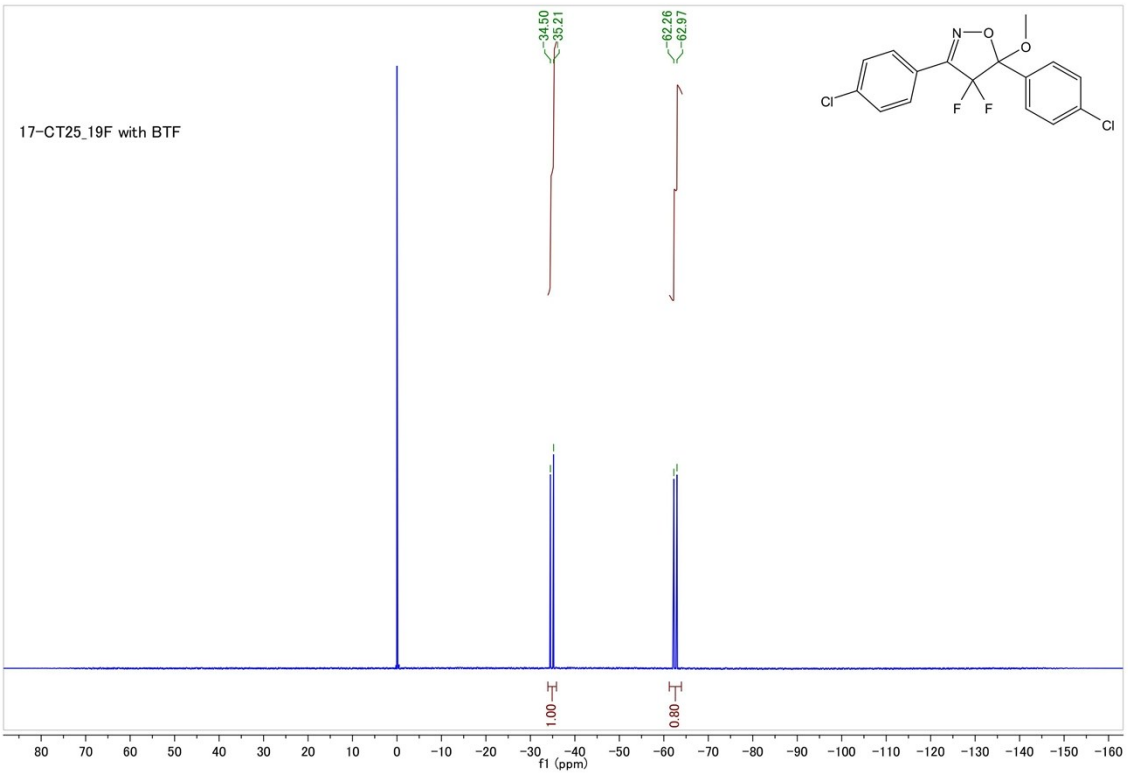



17-CT11_19F with BTF
0.00
-34.57
-35.27
-62.45
-63.15
N
O
O
F
F
1.00
0.93
80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

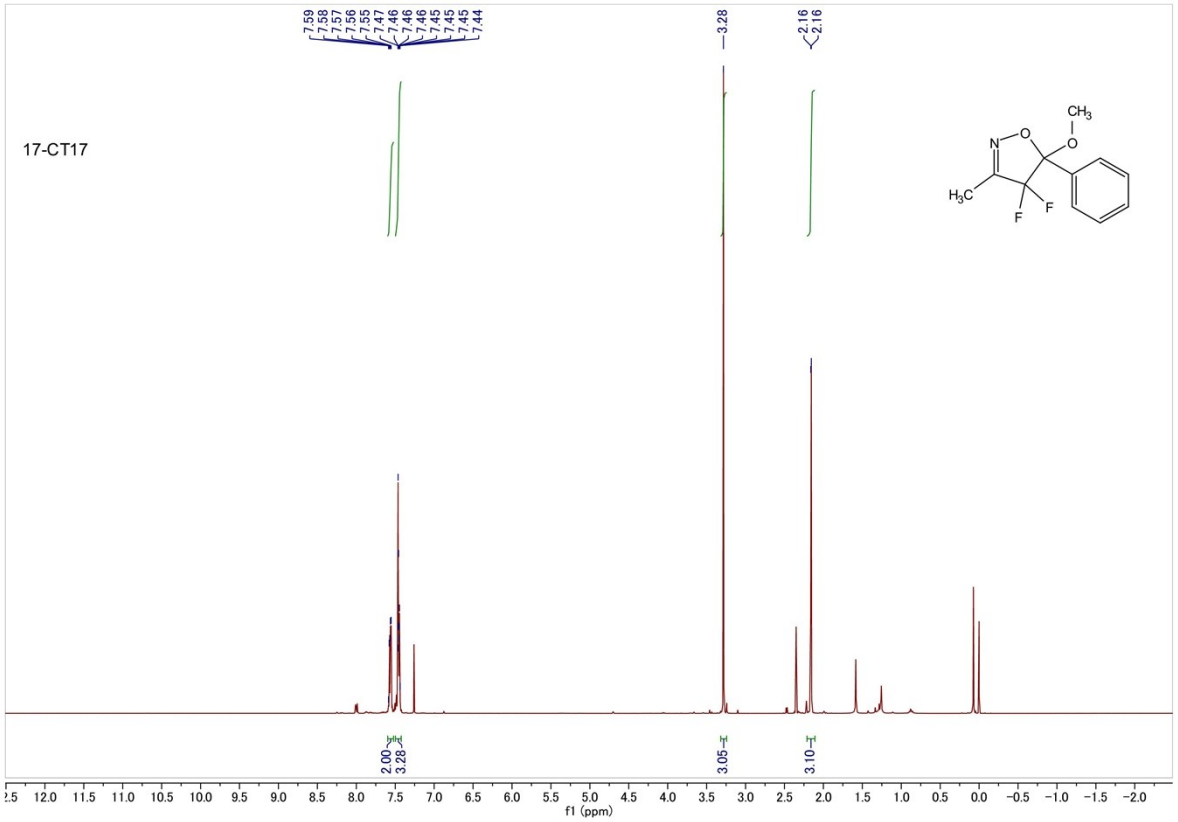
3,5-Bis(4-chlorophenyl)-4,4-difluoro-5-methoxy-4,5-dihydroisoxazole (4cB)

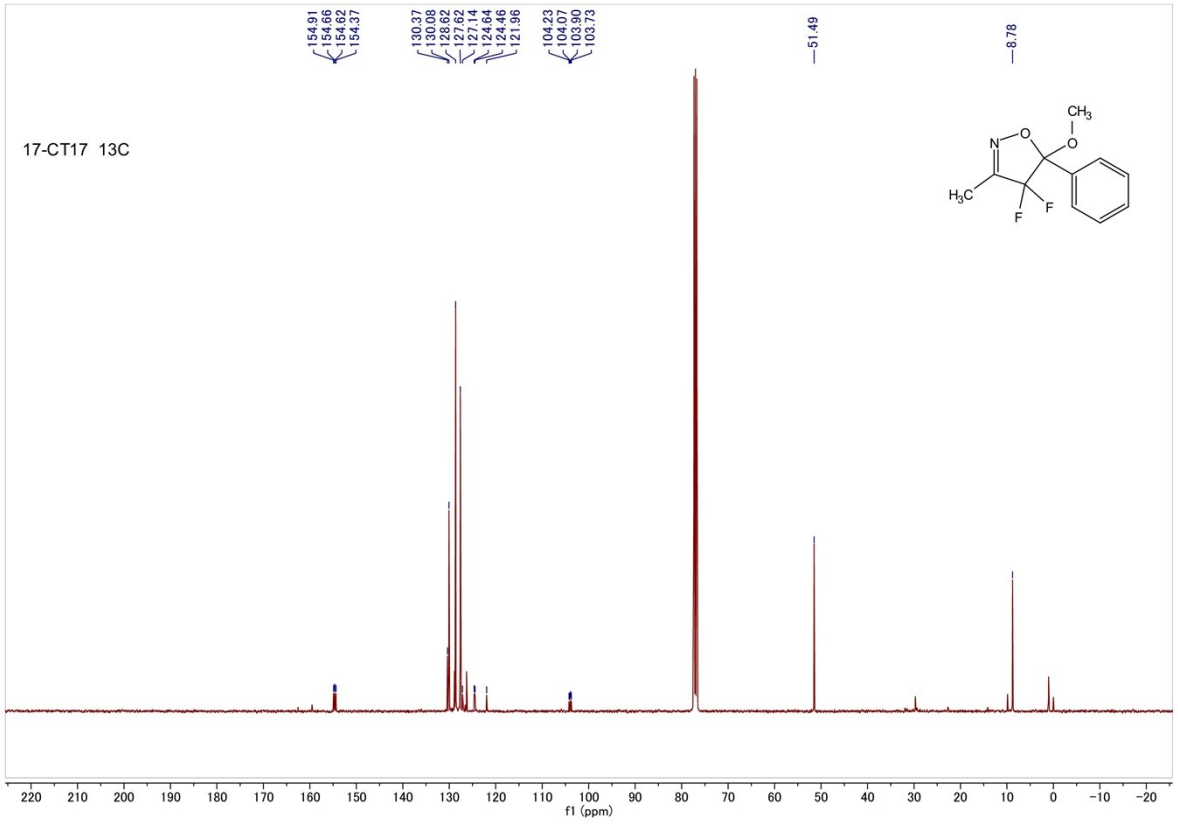


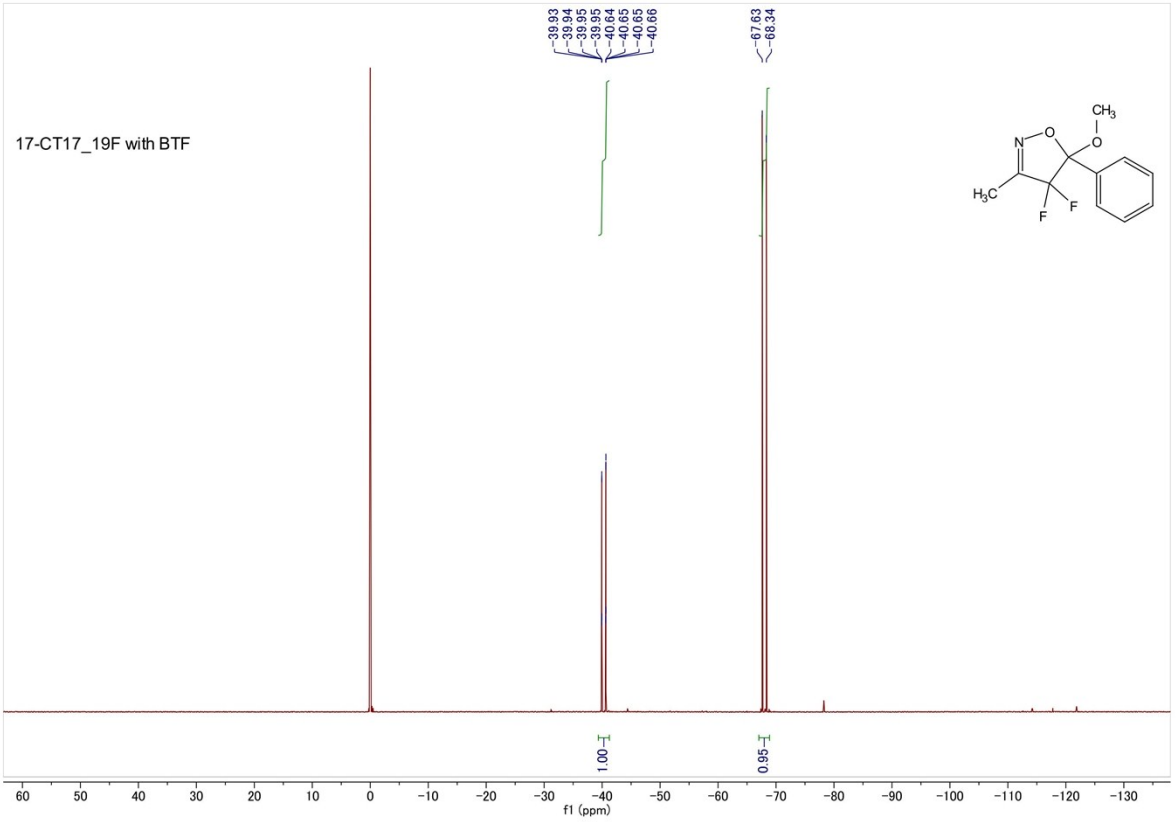



17-CT25_19F with BTF
-34.50
-35.21
-62.26
-62.97
N
O
O
Cl
F
F
Cl
1.00
0.80
80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160
f1 (ppm)

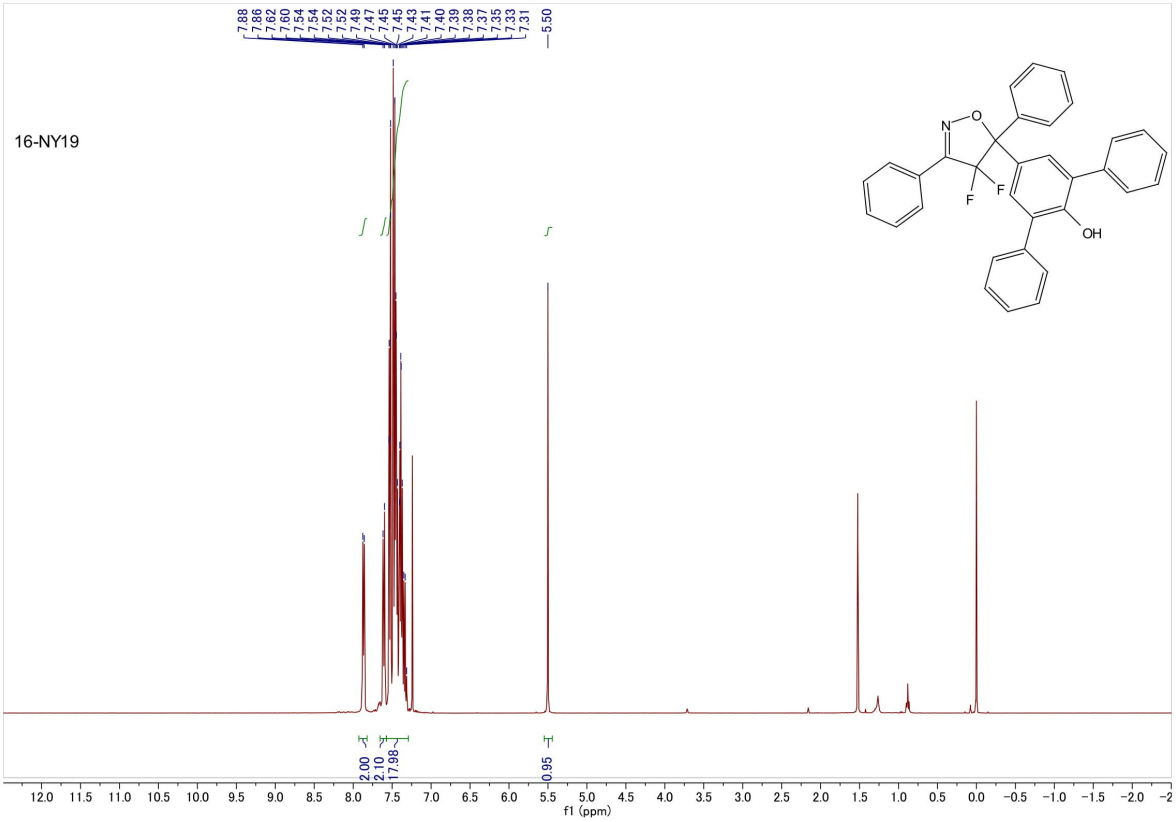
4,4-Difluoro-5-methoxy-3-methyl-5-phenyl-4,5-dihydroisoxazole (4dB)

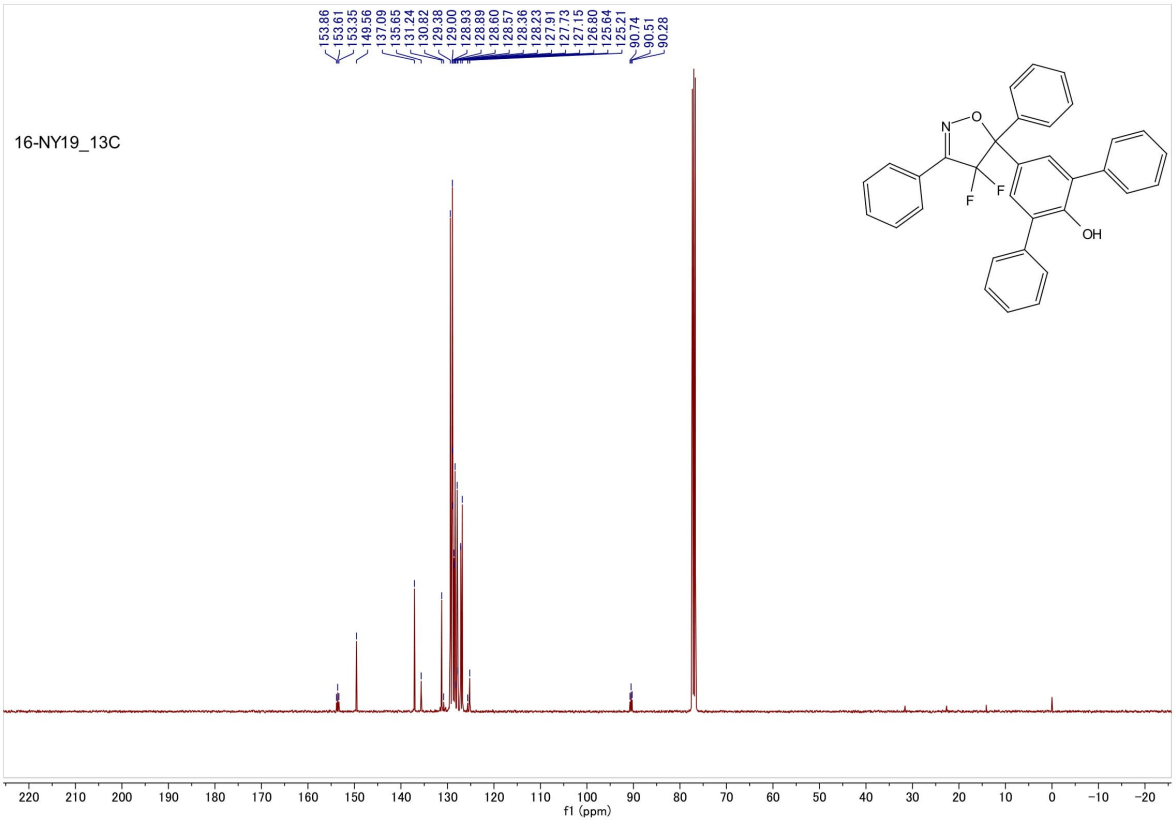


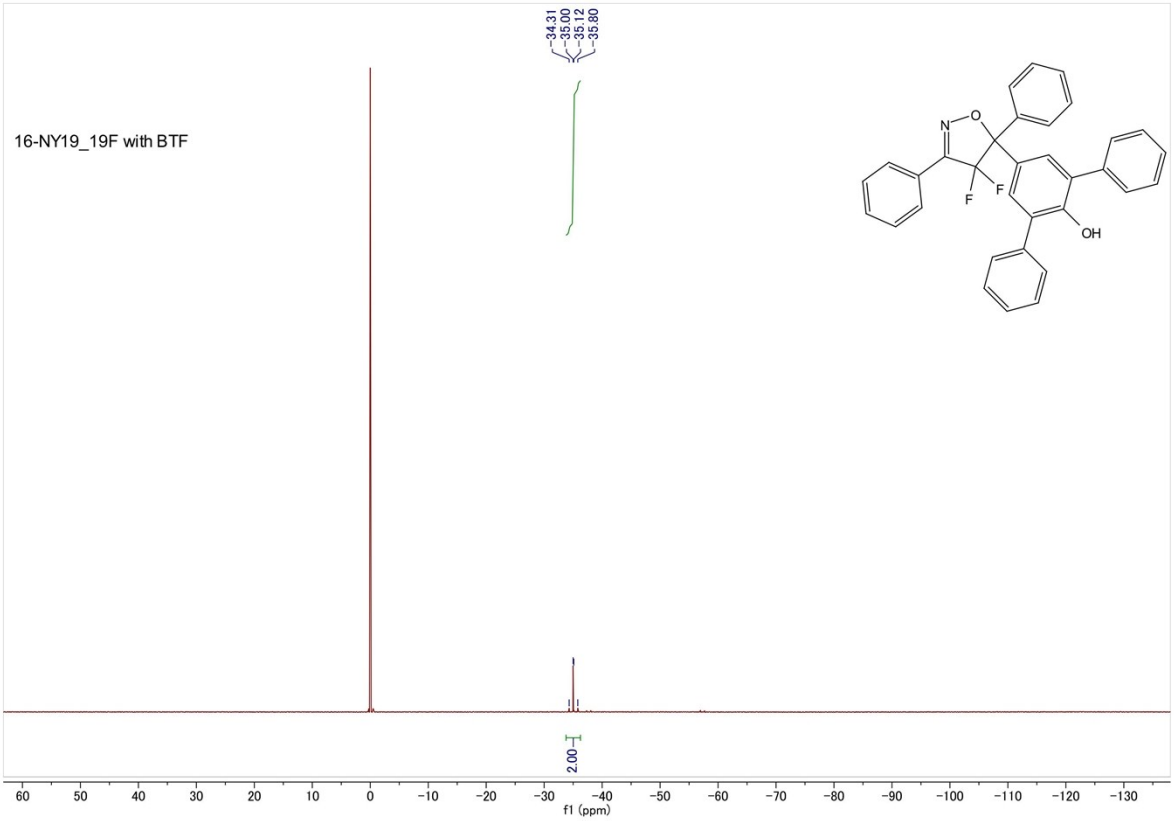



17-CT17_19F with BTF
-39.93
-39.94
-39.95
-39.95
-40.64
-40.65
-40.65
-40.66
-67.63
-68.34
1.00
0.95
f1 (ppm)

5'-(4,4-Difluoro-3,5-diphenyl-4,5-dihydroisoxazol-5-yl)-[1,1':3',1''-terphenyl]-2'-ol (6aK)






16-NY19_19F with BTF
-34.31
-35.00
-35.12
-35.80
N
O
F
F
OH
2.00
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
f1 (ppm)