Supporting Information

Preparation of Potassium Azidoaryltrifluoroborates
and
Their Cross-Coupling with Aryl Halides

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Contents

General Considerations…....……………………………………………….………...….S2

Preparation of Potassium Haloaryltrifluoroborates……….....…..…..…… ……….S2

Preparation of Potassium Azidoaryltrifluoroborates…...……….....…..…………....S9

Suzuki-Miyaura Cross-Coupling Reactions………………………………….…….…..S17

A One-Pot Cross-Coupling and 1,3-Dipolar Cycloaddition Reaction..…………..S20

A One-Pot Cross-Coupling and Reduction Reaction……………………………….….S20

References…………………………………....…………………………………S21

^{1}H, ^{13}C, ^{19}F, and ^{11}B NMR Spectra……………………………...…..……...S22

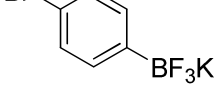
General Considerations

^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded at 500, 126, and 376 MHz, respectively. ^{19}F NMR chemical shifts were referenced to external $CFCl_3$ (0.0 ppm). ^{11}B NMR spectra at 128 MHz were obtained on a spectrometer equipped with the appropriate decoupling accessories. All ^{11}B NMR chemical shifts were referenced to external $BF_3{\cdot}OEt_2$ (0.0 ppm) with a negative sign indicating an upfield shift. Mass spectra of potassium organotrifluoroborates were performed using negative FAB at the mass spectrometry facilities at the Seoul National University.

Preparation of Potassium Haloaryltrifluoroborates

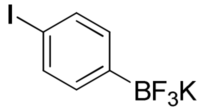
General Procedure I

To a soln of aryl dihalide (2.0 mmol) and triisopropyl borate (384 mg, 2.0 mmol) in THF (15 mL) was slowly added *n*-BuLi (2.0 M soln in hexane, 1.0 mL, 2.0 mmol) at -78 °C for 20 min under N_2. The reaction mixture was vigorously stirred for 1 h at -78 °C and then warmed to rt for 40 min. After the reaction was complete, 1 N KHF_2 (6.0 mL, 6.0 mmol) was added at rt. After stirring for 30 min, the suspension was concentrated and dried in vacuo for 3 h. The residual white solid was dissolved in dry acetone (10 mL), and the insoluble salts were filtered off through Celite. The solvent was concentrated on a rotary evaporator, and then redissolved in a minimal amount of acetone. The addition of ether led to the precipitation of the product (**7a**, **8a**, **14a**, and **15a** were precipitated from heptane). The product was filtered, collected, and dried in vacuo to afford the desired pure product.



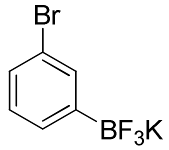
Potassium 4-bromophenyltrifluoroborate[1] (1a-Br)

General procedure I was used employing 1,4-dibromobenzene (472 mg, 2.0 mmol), to give the desired product in 86% yield (452 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.39 (d, 2H, J = 8.0 Hz), 7.24 (d, 2H, J = 8.0 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 133.7, 129.0, 118.7. ^{19}F NMR (376 MHz, Acetone-d_6) δ -143.1. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.31. FT-IR (KBr): 3068, 1580, 1382, 1210, 1064, 949, 933, 807 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_4BF_3Br$ $[M-K^+]^-$ 222.9542, found 222.9545.



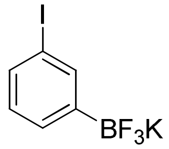
Potassium 4-iodophenyltrifluoroborate[2] (1a-I)

General procedure I was used employing 1,4-diiodobenzene (660 mg, 2.0 mmol), to give the desired product in 90% yield (558 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.48 (d, 2H, *J* = 8.0 Hz), 7.28 (d, 2H, *J* = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 135.2, 134.1, 90.6. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -143.0. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.44. FT-IR (KBr): 3024, 1578, 1373, 1221, 956, 811 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_6H_4BF_3I$ [M-K$^+$]$^-$ 270.9403, found 270.9400.



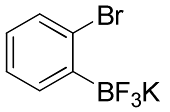
Potassium 3-bromophenyltrifluoroborate[2] (2a-Br)

General procedure I was used employing 1,3-dibromobenzene (472 mg, 2.0 mmol), to give the desired product in 56% yield (295 mg, a white solid). mp = 185 °C. ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.61 (s, 1H), 7.44 (d, 1H, *J* = 7.0 Hz), 7.22 (m, 1H), 7.07 (t, 1H, *J* = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 134.3, 130.2, 128.5, 127.8, 121.2. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -143.3. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.01. FT-IR (KBr): 3071, 1552, 1394, 1263, 1073, 907, 875, 779, 734 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_6H_4BF_3Br$ [M-K$^+$]$^-$ 222.9542, found 222.9542.



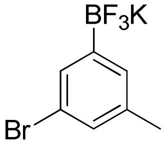
Potassium 3-iodophenyltrifluoroborate (2a-I)

General procedure I was used employing 1,3-diiodobenzene (660 mg, 2.0 mmol), to give the desired product in 85% yield (527 mg, a white solid). mp = 190 °C. ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.84 (s, 1H), 7.48 (d, 1H, *J* = 7.5 Hz), 7.43 (d, 1H, *J* = 8.0 Hz), 6.95 (t, 1H, *J* = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 140.6, 134.0, 130.7, 128.8, 94.1. ^{19}F NMR (376 MHz, Acetone-d_6) δ -143.2. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.83. FT-IR (KBr): 3065, 1693, 1548, 1388, 1201, 1168, 1066, 969, 881, 778, 723 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_4BF_3I$ [M-K+]$^-$ 270.9403, found 270.9398.



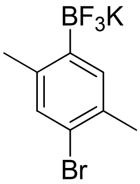
Potassium 2-bromophenyltrifluoroborate[3] (3a)

General procedure I was used employing 1,2-dibromobenzene (472 mg, 2.0 mmol), to give the desired product in 52% yield (273 mg, a white solid). mp = 227 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.57 (d, 1H, J = 7.0 Hz), 7.35 (d, 1H, J = 8.5 Hz), 7.10 (t, 1H, J = 7.5 Hz), 6.97 (td, 1H, J = 7.5, 2.0 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 134.4, 131.4, 127.9, 127.3, 125.2. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.2. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.80. FT-IR (KBr): 3057, 1698, 1424, 1254, 1203, 1053, 944, 743 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_4BF_3Br$ [M-K$^+$]$^-$ 222.9542, found 222.9546.



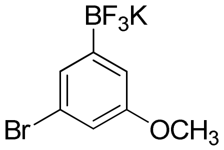
Potassium 3-bromo-5-methylphenyltrifluoroborate (4a)

General procedure I was used employing 3,5-dibromotoluene (500 mg, 2.0 mmol), to give the desired product in 81% yield (449 mg, a white solid). mp = 212−216 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.41 (s, 1H), 7.28 (s, 1H), 7.08 (s, 1H), 2.24 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 138.0, 131.4, 131.1, 128.6, 121.1, 20.3. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.9. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.18. FT-IR (KBr): 3045, 1560, 1410, 1243, 1172, 1026, 928, 842, 747 cm^{-1}. HRFABMS: *m/z* calcd for $C_7H_6BF_3Br$ [M-K$^+$]$^-$ 236.9698, found 236.9697.



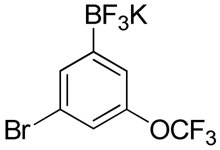
Potassium 4-bromo-2,5-dimethylphenyltrifluoroborate (5a)

General procedure I was used employing 1,4-dibromo-2,5-dimethylbenzene (528 mg, 2.0 mmol), to give the desired product in 47% yield (274 mg, a white solid). mp = 237 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.37 (s, 1H), 7.09 (s, 1H), 2.34 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 141.2, 134.9, 131.4, 131.1, 121.0, 21.4, 20.3. ^{19}F NMR (376 MHz, Acetone- d_6) δ -140.8. ^{11}B NMR (128 MHz, Acetone- d_6) δ 3.46. FT-IR (KBr): 3039, 1603, 1589, 1438, 1236, 1151, 1010, 969, 945, 883, 752 cm^{-1}. HRFABMS: *m/z* calcd for $C_8H_8BF_3Br$ $[M-K^+]^-$ 250.9855, found 250.9855.



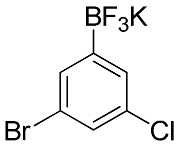
Potassium 3-bromo-5-methoxyphenyltrifluoroborate (6a)

General procedure I was used employing 3,5-dibromoanisole (532 mg, 2.0 mmol), to give the desired product in 82% yield (480 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.20 (d, 1H, J = 1.5 Hz), 7.01 (d, 1H, J = 2.0 Hz), 6.79 (t, 1H, J = 2.5 Hz), 3.74 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 159.6, 126.8, 121.1, 115.6, 113.7, 54.5. ^{19}F NMR (376 MHz, Acetone-d_6) δ -143.4. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.91. FT-IR (KBr): 3057, 2989, 1557, 1411, 1259, 1240, 986, 845, 749 cm^{-1}. HRFABMS: *m/z* calcd for $C_7H_6BF_3BrO$ $[M-K^+]^-$ 252.9647, found 252.9648.



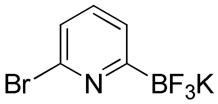
Potassium 3-bromo-5-(trifluoromethoxy)phenyltrifluoroborate (7a)

General procedure I was used employing 1,3-dibromo-5-(trifluoromethoxy)benzene (640 mg, 2.0 mmol), to give the desired product in 82% yield (569 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.60 (s, 1H), 7.33 (s, 1H), 7.19 (s, 1H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 148.6, 133.2, 122.2, 120.8, 120.6 (q, J = 255.0 Hz), 120.5. ^{19}F NMR (376 MHz, Acetone-d_6) δ -58.3, -144.1. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.49. FT-IR (KBr): 3083, 1564, 1403, 1289, 1240, 1198, 1160, 1027, 915, 868, 834, 752 cm^{-1}. HRFABMS: *m/z* calcd for $C_7H_3BF_6BrO$ $[M-K^+]^-$ 306.9365, found 306.9360.



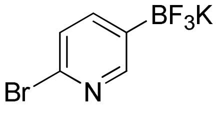
Potassium 3-bromo 5-chlorophenyltrifluoroborate (8a)

General procedure I was used employing 1-chloro-3,5-dibromobenzene (569 mg, 2.0 mmol), to give the desired product in 72% yield (428 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.52 (d, 1H, J = 1.5 Hz), 7.40 (d, 1H, J = 2.0 Hz), 7.27 (t, 1H, J = 2.0 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 133.1, 132.8, 130.2, 127.4, 121.3. ^{19}F NMR (376 MHz, Acetone-d_6) δ -143.8. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.56. FT-IR (KBr): 3059, 1547, 1392, 1206, 1013, 926, 857, 773, 746 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_3BF_3BrCl$ [M-K$^+$]$^-$ 256.9152, found 256.9151.



Potassium 6-bromopyridin-2-yltrifluoroborate (9a)

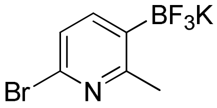
General procedure I was used employing 2,6-dibromopyridine (474 mg, 2.0 mmol), to give the desired product in 90% yield (475 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.41 (td, 1H, J = 7.5, 0.5 Hz), 7.31 (dd, 1H, J = 7.5, 1.5 Hz), 7.23 (dd, 1H, J = 7.5, 0.5 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 142.1, 137.3, 125.2, 124.6. ^{19}F NMR (376 MHz, DMSO-d_6) δ -141.6. ^{11}B NMR (128 MHz, DMSO-d_6) δ 1.45. FT-IR (KBr): 2959, 1538, 1379, 1241, 11545, 1106, 991, 958, 783, 748 cm^{-1}. HRFABMS: *m/z* calcd for $C_5H_3BF_3BrN$ [M-K$^+$]$^-$ 223.9494, found 223.9493.



Potassium 6-bromopyridin-3-yltrifluoroborate (10a)

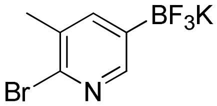
General procedure I was used employing 2,5-dibromopyridine (474 mg, 2.0 mmol), to give the desired product in 87% yield (459 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 8.35 (s, 1H), 7.66 (dd, 1H, J = 7.5, 1.5 Hz), 7.29 (d, 1H, J = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 153.6, 142.3, 139.2, 126.1. ^{19}F NMR (376 MHz, Acetone-d_6) δ -143.1. ^{11}B NMR (128 MHz, Acetone- d_6) δ 2.89. FT-IR (KBr):

2915, 1570, 1448, 1343, 1214, 1077, 946, 821 cm^{-1}. $C_5H_3BF_3BrN$ [M-K$^+$]$^-$ 223.9494, found 223.9492.



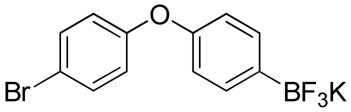
Potassium 6-bromo-2-methylpyridin-3-yltrifluoroborate (11a)

General procedure I was used employing 3,6-dibromo-2-methylpyridine (502 mg, 2.0 mmol), to give the desired product in 90% yield (500 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.62 (d, 1H, J = 8.0 Hz), 7.07 (d, 1H, J = 8.0 Hz), 2.51 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 163.3, 142.7, 137.8, 123.0, 23.6. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.1. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.08. FT-IR (KBr): 2932, 1563, 1416, 1382, 1357, 1213, 1113, 943, 815 cm^{-1}. HRFABMS: m/z calcd for $C_6H_5BF_3BrN$ [M-K$^+$]$^-$ 237.9651, found 237.9651.



Potassium 6-bromo-5-methylpyridin-3-yltrifluoroborate (12a)

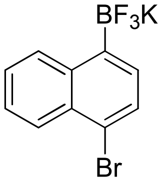
General procedure I was used employing 2,5-dibromo-3-methylpyridine (502 mg, 2.0 mmol), to give the desired product in 85% yield (473 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 8.16 (s, 1H), 7.62 (s, 1H), 2.27 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 150.9, 142.8, 141.5, 131.9, 21.0. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.8. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.90. FT-IR (KBr): 2930, 1578, 1556, 1371, 1296, 1207, 1022, 954, 893, 852, 728 cm^{-1}. HRFABMS: m/z calcd for $C_6H_5BF_3BrN$ [M-K$^+$]$^-$ 237.9651, found 237.9647.



Potassium 4-(4-bromophenoxy)phenyltrifluoroborate (13a)

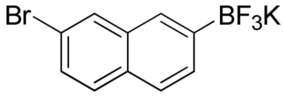
General procedure I was used employing bis(4-bromophenyl)ether (656 mg, 2.0 mmol), to give the desired product in 93% yield (660 mg, a white solid). mp > 250 °C. ^{1}H NMR

(500 MHz, DMSO-d_6) δ 7.46 (d, 2H, *J* = 9.0 Hz), 7.34 (d, 2H, *J* = 8.5 Hz), 6.86 (d, 2H, *J* = 9.0 Hz), 6.78 (d, 2H, *J* = 8.5 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.9, 153.7, 133.3, 132.9, 119.9, 118.0, 114.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ -138.9. ^{11}B NMR (128 MHz, DMSO-d_6) δ 3.30. FT-IR (KBr): 3021, 1601, 1579, 1481, 1221, 970, 918, 847, 823 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{12}H_8BF_3BrO$ [M-K$^+$]$^-$ 314.9804, found 314.9800.



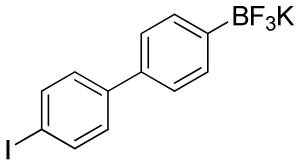
Potassium 4-bromonaphthalen-1-yltrifluoroborate (14a)

General procedure I was used employing 1,4-dibromonaphthalene (572 mg, 2.0 mmol), to give the desired product in 94% yield (588 mg, a white solid). mp = 194 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 8.63 (d, 1H, *J* = 8.0 Hz), 8.14 (ddd, 1H, J = 8.5, 1.5, 0.5 Hz), 7.64 (d, 1H, *J* = 7.5 Hz), 7.61 (d, 1H, *J* = 7.5 Hz), 7.50 (m, 1H), 7.42 (m, 1H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 138.7, 131.4, 131.1, 129.7, 129.1, 126.0, 125.6, 124.5, 119.9. ^{19}F NMR (376 MHz, Acetone-d_6) δ -138.3. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.76. FT-IR (KBr): 2955, 1562, 1502, 1227, 1158, 1109, 1062, 933, 832, 761 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{10}H_6BF_3Br$ [M-K$^+$]$^-$ 272.9698, found 272.9703.



Potassium 7-bromonaphthalen-2-yltrifluoroborate (15a)

General procedure I was used employing 2,7-dibromonaphthalene (572 mg, 2.0 mmol), to give the desired product in 90% yield (563 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.96 (d, 1H, *J* = 2.0 Hz), 7.95 (s, 1H), 7.77 (d, 1H, *J* = 8.0 Hz), 7.73 (d, 1H, *J* = 9.0 Hz), 7.68 (d, 1H, *J* = 8.0 Hz), 7.44 (dd, 1H, *J* = 8.5, 2.0 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 134.6, 131.6, 131.1, 129.5, 129.4, 129.1, 126.9, 125.0, 117.6. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.5. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.75. FT-IR (KBr): 3048, 1588, 1447, 1269, 1195, 963, 933, 832 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{10}H_6BF_3Br$ [M-K$^+$]$^-$ 272.9698, found 272.9707.



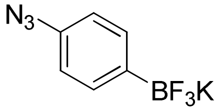
Potassium 4’-iodobiphenyl-4-yltrifluoroborate (16a)

General procedure I was used employing 4,4’-diiodobiphenyl (812 mg, 2.0 mmol), to give the desired product in 80% yield (618 mg, a white solid). mp > 250 °C. ^{1}H NMR (500 MHz, Acetone-d_6 + DMSO-d_6) δ 7.76 (d, 2H, J = 8.0 Hz), 7.56 (d, 2H, J = 8.0 Hz), 7.43 (d, 2H, J = 9.0 Hz), 7.38 (d, 2H, J = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-d_6 + DMSO-d_6) δ 142.6, 138.0, 136.2, 132.9, 129.2, 124.9, 91.6. ^{19}F NMR (376 MHz, Acetone-d_6 + DMSO-d_6) δ -142.0. ^{11}B NMR (128 MHz, DMSO-d_6) δ 3.12. FT-IR (KBr): 3018, 1607, 1480, 1382, 1226, 972, 924, 809 cm^{-1}. HRFABMS: m/z calcd for $C_{12}H_8BF_3I$ [M-K$^+$]$^-$ 346.9716, found 346.9712.

Preparation of Potassium Azidoaryltrifluoroborates

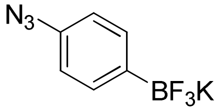
General Procedure II

Potassium haloaryltrifluoroborate (**1a**−**16a**, 1.0 mmol), NaN_3 (65 mg, 1.0 mmol), CuBr (14.4 mg, 10 mol %), Cs_2CO_3 (326 mg, 1.0 mmol), and N,N’-dimethyl ethylenediamine (17.6 mg, 20 mol %) were dissolved in DMSO (4 mL) under atmospheric conditions (except for **7b**, **8b**, and **13b**−**16b**, which were carried out under N_2). The reaction mixture was heated in an oil bath at 90 °C until the ^{1}H NMR (in D_2O) indicated completion of the reaction (see Table 3). After the completion of the reaction, the solvent was removed in vacuo at 60−70 °C (the reactions of **13b**−**16b** were quenched with 3 mL of 1 N KHF_2 before the removal of the solvent). The residual product was dissolved in dry acetone (6 mL), and the insoluble salts were removed by filtration through Celite. The solvent was concentrated on a rotary evaporator and redissolved in a minimal amount of dry acetone. The addition of Et_2O led to the precipitation of the product. The product was filtered, concentrated and, dried in vacuo to afford the desired pure product.



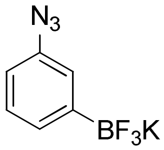
Potassium 4-azidophenyltrifluoroborate (1b)

General procedure II was used employing potassium 4-bromophenyltrifluoroborate (**1a-Br**, 263 mg, 1.0 mmol), to give the desired product in 95% yield (214 mg, a yellow solid). mp = 169 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.51 (d, 2H, J = 8.0 Hz), 6.84 (d, 2H, J = 7.5 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 136.2, 133.1, 116.8. ^{19}F NMR (376 MHz, Acetone-d_6) δ -141.4. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.36. FT-IR (KBr): 3031, 2122, 2084, 1710, 1599, 1361, 1287, 1222, 963, 927, 820 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_4BF_3N_3$ [M-K$^+$]$^-$ 186.0450, found 186.0450.



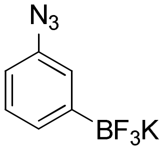
Potassium 4-azidophenyltrifluoroborate (1b, 3.0 mmole scale reaction of 1a-I)

General procedure II was used employing potassium 4-iodophenyltrifluoroborate (**1a-I**, 930 mg, 3.0 mmol), to give the desired product in 95% yield (641 mg, a yellow solid).



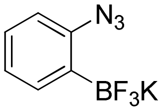
Potassium 3-azidophenyltrifluoroborate (2b)

General procedure II was used employing potassium 3-bromophenyltrifluoroborate (**2a-Br**, 263 mg, 1.0 mmol), to give the desired product in 90% yield (203 mg, a yellow solid). mp = 168 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.31 (d, 1H, J = 7.5 Hz), 7.22 (s, 1H), 7.14 (t, 1H, J = 7.5 Hz), 6.73 (m, 1H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 137.3, 128.7, 127.6, 121.7, 115.6. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.8. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.20. FT-IR (KBr): 3046, 2127, 2099, 1571, 1414, 1284, 1205, 967, 868, 775, 694 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_4BF_3N_3$ [M-K$^+$]$^-$ 186.0450, found 186.0455.



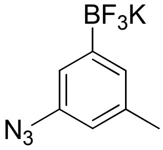
Potassium 3-azidophenyltrifluoroborate (2b)

General procedure II was used employing potassium 3-iodophenyltrifluoroborate (**2a-I**, 310 mg, 1.0 mmol), to give the desired product in 93% yield (209 mg, a yellow solid).



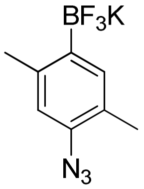
Potassium 2-azidophenyltrifluoroborate (3b)

General procedure II was used employing potassium 2-bromophenyltrifluoroborate (**3a**, 263 mg, 1.0 mmol), to give the desired product in 73% yield (164 mg, a yellow solid). mp 182 °C (dec.). ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.57 (d, 1H, J = 7.0 Hz), 7.17 (td, 1H, J = 8.0, 2.0 Hz), 6.97 (t, 1H, J = 7.5 Hz), 6.97 (d, 1H, J = 8.5 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 142.0, 134.1, 127.0, 123.4, 117.3. ^{19}F NMR (376 MHz, Acetone-d_6) δ -138.8. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.91. FT-IR (KBr): 3055, 2119, 1711, 1968, 1438, 1268, 1199, 960, 753 cm^{-1}. HRFABMS: m/z calcd for $C_6H_4BF_3N_3$ $[M-K^+]^-$ 186.0450, found 186.0446.



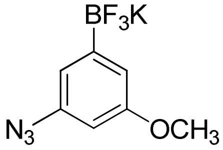
Potassium 3-azido-5-methylphenyltrifluoroborate (4b)

General procedure II was used employing potassium 3-bromo-5-methylphenyltrifluoroborate (**4a**, 277 mg, 1.0 mmol), to give the desired product in 93% yield (222 mg, a yellow solid). mp = 150−152 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.98 (s, 1H), 6.83 (s, 1H), 6.56 (s, 1H), 2.22 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 137.4, 137.2, 129.9, 118.9, 116.8, 21.4. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.5. ^{11}B NMR (128 MHz, Acetone-d_6) δ 3.09. FT-IR (KBr): 2917, 2102, 1594, 1415, 1301, 1168, 1043, 988, 943, 872, 813, 709 cm^{-1}. HRFABMS: m/z calcd for $C_7H_6BF_3N_3$ $[M-K^+]^-$ 200.0607, found 200.0612.



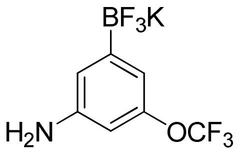
Potassium 4-azido-2,5-dimethylphenyltrifluoroborate (5b)

General procedure II was used employing potassium 4-bromo-2,5-dimethylphenyltrifluoroborate (**5a**, 291 mg, 1.0 mmol), to give the desired product in 90% yield (228 mg, a yellow solid). mp = 175−179 °C. ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.33 (s, 1H), 6.72 (s, 1H), 2.42 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 140.7, 135.2, 133.9, 123.1, 117.4, 20.8, 15.9. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -138.3. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.07. FT-IR (KBr): 2928, 2112, 2093, 1562, 1384, 1291, 1161, 1063, 948, 901, 849 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_8H_8BF_3N_3$ [M-K$^+$]$^-$ 214.0763, found 214.0762.



Potassium 3-azido-5-methoxyphenyltrifluoroborate (6b)

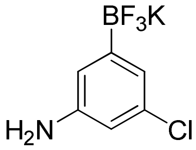
General procedure II was used employing potassium 3-bromo-5-methoxyphenyltrifluoroborate (293 mg, 1.0 mmol), to give the desired product in 92% yield (235 mg, a brown amorphous solid). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 6.89 (d, 1H, *J* = 2.5 Hz), 6.84 (d, 1H, *J* = 2.0 Hz), 6.28 (t, 1H, *J* = 2.5 Hz), 3.74 (s, 3H). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 159.8, 138.4, 114.1, 113.8, 101.9, 54.3. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -142.4. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.09. FT-IR (KBr): 2950, 2103, 1585, 1412, 1298, 1237, 1168, 1027, 820, 762 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_7H_6BF_3N_3O$ [M-K$^+$]$^-$ 216.0556 , found 216.0563.



Potassium 3-amino-5-(trifluoromethoxy)phenyltrifluoroborate (7b)

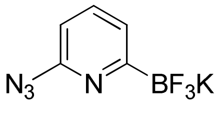
General procedure II under N_2 was used employing potassium 3-bromo-5-

(trifluoromethoxy)phenyltrifluoroborate (**7a**, 347 mg, 1.0 mmol), to give the aminoaryltrifluoroborate **7b** product in 83% yield (235 mg, a brown amorphous solid). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 6.78 (s, 1H), 6.63 (s, 1H), 6.28 (s, 1H), 4.39 (br s, 2H). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 149.3, 148.3, 120.1 (q, J = 254 Hz), 116.8, 111.8, 103.9. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -57.7, -142.1. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.09. FT-IR (KBr): 3365, 2919, 1615, 1585, 1259, 1216, 1154, 1035, 981 cm^{-1}. HRFABMS: *m/z* calcd for $C_7H_5BF_6NO$ [M-K$^+$]$^-$ 244.0368, found 244.0368.



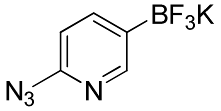
Potassium 3-amino-5-chlorophenyltrifluoroborate (8b)

General procedure II under N_2 was used employing potassium 3-bromo-5-chlorophenyltrifluoroborate (**8a**, 297 mg, 1.0 mmol), to give the aminoaryltrifluoroborate 8b product in 91% yield (213 mg, a dark brown amorphous solid). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 6.75 (s, 1H), 6.74 (s, 1H), 6.40 (s, 1H), 4.31 (br s, 2H). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 148.0, 132.3, 120.4, 116.7, 111.0. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -140.8. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.07. FT-IR (KBr): 3363, 2918, 1623, 1568, 1423, 1285, 1177, 1030, 1004, 903, 851, 770 cm^{-1}. HRFABMS: *m/z* calcd for $C_6H_5BF_3ClN$ [M-K$^+$]$^-$ 194.0156, found 194.0146.



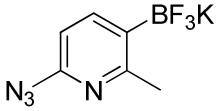
Potassium 6-azidopyridin-2-yltrifluoroborate (9b)

General procedure II was used employing potassium 6-bromopyridin-2-yltrifluoroborate (**9a**, 264 mg, 1.0 mmol), to give the desired product in 98% yield (222 mg, an ivory solid). mp = 256 °C (dec.). ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 7.90 (dd, 1H, J = 9.0, 1.0 Hz), 7.64 (dd, 1H, J = 9.0, 6.5 Hz), 7.16 (d, 1H, J = 6.0 Hz). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 148.2, 132.4, 118.6, 112.3. ^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -142.4. ^{11}B NMR (128 MHz, DMSO-*d*$_6$) δ 1.17. FT-IR (KBr): 3088, 1623, 1505, 1261, 1176, 1087, 1019, 995, 977, 919, 797 cm^{-1}. HRFABMS: *m/z* calcd for $C_5H_3BF_3N_4$ [M-K$^+$]$^-$ 187.0403, found 187.0399.



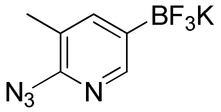
Potassium 6-azidopyridin-3-yltrifluoroborate (10b)

General procedure II was used employing potassium 6-bromopyridin-3-yltrifluoroborate (**10a**, 264 mg, 1.0 mmol), to give the desired product in 98% yield (222 mg, an ivory solid). mp = 271 °C (dec.). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 8.65 (s, 1H), 7.85 (d, 1H, *J* = 8.5 Hz), 7.82 (d, 1H, *J* = 9.0 Hz). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 148.2, 137.7, 124.8, 112.5. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -142.3. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 2.51. FT-IR (KBr): 3084, 1621, 1499, 1243, 1201, 1098, 1021, 975, 915, 815, 800, 718 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_5H_3BF_3N_4$ [M-K$^+$]$^-$ 187.0403, found 187.0404.



Potassium 6-azido-2-methylpyridin-3-yltrifluoroborate (11b)

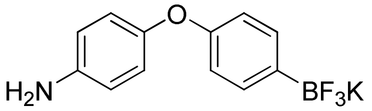
General procedure II was used employing potassium 6-bromo-2-methylpyridin-3-yltrifluoroborate (**11a**, 278 mg, 1.0 mmol), to give the desired product in 95% yield (228 mg, a yellow solid). mp = 246 °C (dec.). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 7.92 (d, 1H, *J* = 8.5 Hz), 7.68 (d, 1H, *J* = 9.0 Hz), 2.93 (s, 3H). ^{13}C NMR (126 MHz, Acetone-*d*$_6$) δ 148.2, 138.0, 136.8, 109.2, 15.6. ^{19}F NMR (376 MHz, Acetone-*d*$_6$) δ -138.7. ^{11}B NMR (128 MHz, Acetone-*d*$_6$) δ 3.16. FT-IR (KBr): 2921, 2101, 1583, 1433, 1297, 1171, 960, 836, 710 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_6H_5BF_3N_4$ [M-K$^+$]$^-$ 201.0559, found 201.0557.



Potassium 6-azido-5-methylpyridin-3-yltrifluoroborate (12b)

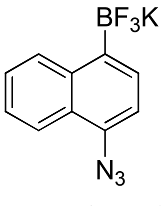
General procedure II was used employing potassium 6-bromo-5-methylpyridin-3-yltrifluoroborate (**12a**, 278 mg, 1.0 mmol), to give the desired product in 95% yield (228 mg, a yellow solid). mp = 250 °C (dec.). ^{1}H NMR (500 MHz, Acetone-*d*$_6$) δ 8.50

(s, 1H), 7.57 (s, 1H), 2.62 (s, 3H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 148.7, 136.0, 123.0, 122.4, 15.7. ^{19}F NMR (376 MHz, Acetone-d_6) δ -142.9. ^{11}B NMR (128 MHz, Acetone-d_6) δ 2.57. FT-IR (KBr): 3073, 2058, 1613, 1380, 1234, 1204, 1137, 1023, 1004, 973, 889, 871, 771 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_6H_5BF_3N_4$ [M-K$^+$]$^-$ 201.0559, found 201.0563.



Potassium 4-(4-aminophenoxy)phenyltrifluoroborate (13b)

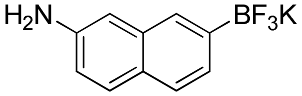
General procedure II under N_2 was used employing potassium 4-(4-bromophenoxy)phenyltrifluoroborate (**13a**, 355 mg, 1.0 mmol), to give the desired product in 90% yield (262 mg, a brown solid). mp = 197 °C. ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.42 (d, 2H, *J* = 8.0 Hz), 6.73 (d, 2H, *J* = 9.0 Hz), 6.69 (d, 2H, *J* = 8.0 Hz), 6.65 (d, 2H, *J* = 9.0 Hz), 4.39 (br s, 2H). ^{13}C NMR (126 MHz, Acetone-d_6) δ 156.6, 148.7, 138.9, 132.6, 119.9, 115.5, 115.1. ^{19}F NMR (376 MHz, Acetone-d_6) δ -140.4. ^{11}B NMR (128 MHz, Acetone- d_6) δ 3.63. FT-IR (KBr): 3418, 3021, 2924, 1595, 1497, 1208, 955, 826 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{12}H_{10}BF_3NO$ [M-K$^+$]$^-$ 252.0808, found 252.0799.



Potassium 4-azidonaphthalen-1-yltrifluoroborate (14b)

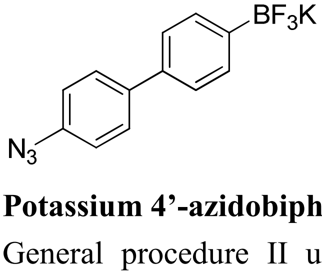
General procedure II under N_2 was used employing potassium 4-bromonaphthalen-1-yltrifluoroborate (**14a**, 313 mg, 1.0 mmol), to give the desired product in 82% yield (226 mg, a brown amorphous solid, and mixed with 10% of starting material **14a**). **14b:** ^{1}H NMR (500 MHz, Acetone-d_6) δ 8.61 (m, 1H), 7.94 (m, 1H), 7.73 (d, 1H, *J* = 7.0 Hz), 7.34 (m, 2H), 7.16 (d, 1H, *J* = 7.0 Hz). **14a:** ^{1}H NMR (500 MHz, Acetone-d_6) δ 8.66 (d, 1H, *J* = 8.5 Hz), 8.08 (d, 1H, *J* = 8.5 Hz), 7.59 (d, 1H, *J* = 7.5 Hz), 7.57 (d, 1H, *J* = 7.5 Hz), 7.44 (t, 1H, *J* = 8.0 Hz), 7.37 (t, 1H, *J* = 8.5 Hz). **14b+14a mixture:** ^{13}C NMR (126 MHz, Acetone-d_6) δ 138.2, 132.8, 131.6, 130.9, 129.1, 128.7, 126.1, 125.8, 125.4, 124.2, 124.1, 121.3, 119.5, 113.2. **14b+14a mixture:** ^{19}F NMR (376 MHz, Acetone-d_6)

δ -136.9. **14b+14a mixture:** ^{11}B NMR (128 MHz, Acetone- d_6) δ 3.71. **14b+14a mixture:** FT-IR (KBr): 3062, 2923, 2116, 1616, 1575, 1421, 1310, 1226, 1157, 1057, 995, 885, 826, 765 cm^{-1}. **14b:** HRFABMS: *m/z* calcd for $C_{10}H_6BF_3N_3$ [M-K$^+$]$^-$ 236.0607, found 236.0619.



Potassium 7-aminonaphthalen-2-yltrifluoroborate (15b)

General procedure II under N_2 was used employing potassium 7-bromonaphthalen-2-yltrifluoroborate (**15a**, 313 mg, 1.0 mmol), to give the aminoaryltrifluoroborate product 15b in 82% yield (204 mg, a brown solid, and mixed with 15% of potassium 7-azidonaphthalen-2-yltrifluoroborate). **15b (amine):** ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.67 (s, 1H), 7.47 (d, 1H, J = 8.5 Hz), 7.41 (d, 1H, J = 8.0 Hz), 7.37 (d, 1H, J = 8.0 Hz), 6.87 (d, 1H, J = 2.0 Hz), 6.84 (dd, 1H, J = 8.5, 2.5 Hz), 4.56 (br s, 2H). **15b (azide):** 7.96 (s, 1H), 7.72 (m, 2H), 7.62 (d, 1H, J = 8.0 Hz), 7.31 (m, 2H). **15b (amine+azide) mixture:** ^{13}C NMR (126 MHz, Acetone-d_6) δ 144.7, 135.1, 132.6, 131.2, 128, 127.6, 127.2, 127.9, 127.1, 126.6, 124.8, 124.7, 124.1, 123.6, 116.4, 107.6. **15b (amine+azide) mixture:** ^{19}F NMR (376 MHz, Acetone-d_6) δ -139.2, -139.9. **15b (amine+azide) mixture:** ^{11}B NMR (128 MHz, Acetone- d_6) δ 3.84. **15b (amine+azide) mixture:** FT-IR (KBr): 3374, 3042, 1703, 1627, 1513, 1462, 1362, 1224, 1177, 997, 902, 841 cm^{-1}. **15b (amine):** HRFABMS: *m/z* calcd for $C_{10}H_8BF_3N$ [M-K$^+$]$^-$ 210.0702, found 210.0704.



Potassium 4’-azidobiphenyl-4-yltrifluoroborate (16b)

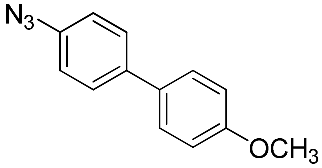
General procedure II under N_2 was used employing potassium 4’-iodobiphenyl-4-yltrifluoroborate (**16a**, 386 mg, 1.0 mmol), to give the aminoaryltrifluoroborate product **16b** in 96% yield (288 mg, an ivory solid). mp = 125 °C (dec.). ^{1}H NMR (500 MHz, Acetone-d_6) δ 7.67 (d, 2H, J = 8.5 Hz), 7.57 (d, 2H, J = 8.0 Hz), 7.40 (d, 2H, J = 7.5 Hz), 7.15 (d, 2H, J = 8.5 Hz). ^{13}C NMR (126 MHz, Acetone-d_6) δ 139.5, 137.9, 136.3, 132.3, 128.0, 124.5, 119.2. ^{19}F NMR (376 MHz, Acetone-d_6) δ -141.4. ^{11}B NMR (128 MHz, Acetone- d_6) δ 3.40. FT-IR (KBr): 3059, 3021, 2127, 2093, 1603, 1493, 1390, 1290, 1225, 970, 814 cm^{-1}. HRFABMS: *m/z* calcd for $C_{12}H_8BF_3N_3$ $[M-K^+]^-$ 262.0763, found 262.0768.

Suzuki-Miyaura Cross-Coupling Reactions

General Procedure III

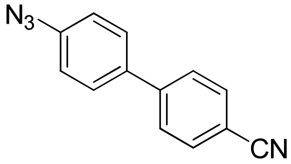
A. Aryl bromide: To a 16×90 mm glass vessel containing a stirring bar was added potassium 4-azidophenyltrifluoroborate (45 mg, 0.2 mmol), Cs_2CO_3 (196 mg, 0.6 mmol), $PdCl_2(dppf)\cdot CH_2Cl_2$ (16.3 mg, 2×10^{-2} mmol, 10 mol %), and aryl bromide (0.2 mmol)). The vessel was sealed with a septum, and methanol (1.5 mL) was added via syringe. The reaction was heated in an oil bath at 80 °C. After the aryl bromide was totally consumed (the reaction was monitored by TLC), the reaction mixture was cooled to rt. The solvent was removed in vacuo. The residual compound was dissolved in ethyl acetate (2.0 mL), and the insoluble salts were filtered through a thin pad of silica gel. The solvent was concentrated on a rotary evaporator, and the crude product was purified by preparative TLC (0.5 mm).

B. Aryl chloride : To a 16×90 mm glass vessel containing a stirring bar was added the potassium 4-azidophenyltrifluoroborate (0.2 mmol), Cs_2CO_3 (196 mg, 0.6 mmol), $Pd(OAc)_2$ (1.4 mg, 6×10^{-3} mmol, 3 mol %), XPhos (2-dicyclohexylphosphino-2',4',6'-triisopropylbiphenyl, 5.7 mg, 1.2×10^{-2} mmol, 6 mol %), and aryl chloride (0.2 mmol). The vessel was sealed with a septum, and 1,4-dioxane/H_2O (v/v = 10:1, 1.5 mL) was added via syringe. The reaction was heated in an oil bath at 80 °C. After the aryl chloride was totally consumed (the reaction was monitored by TLC), the reaction mixture was cooled to rt. The solvent was removed in vacuo. The residual compound was dissolved in ethyl acetate (2.0 mL), and the insoluble salts were filtered through a thin pad of silica gel. The solvent was concentrated on a rotary evaporator and the crude product was purified by preparative TLC (0.5 mm).



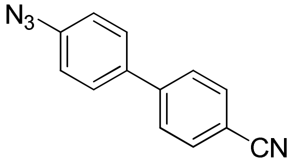
4-Azido-4'-methoxybiphenyl[4,5] (17)

General procedure III-A was used employing 4-bromoanisole (38 mg, 0.2 mmol), to give the desired product in 85% yield (38.4 mg, a yellow solid). mp = 131−133 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, 2H, *J* = 8.5 Hz), 7.49 (d, 2H, *J* = 9.5 Hz), 7.07 (d, 2H, *J* = 8.5 Hz), 6.97 (d, 2H, *J* = 9.0 Hz), 3.85 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2, 138.4, 137.6, 132.7, 127.9, 127.8, 119.3, 114.2, 55.3. FT-IR (KBr): 2930, 2109, 1605, 1498, 1287, 1035, 825, 807 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{13}H_{11}N_3O$ $[M]^+$ 225.0902, found 225.0895.



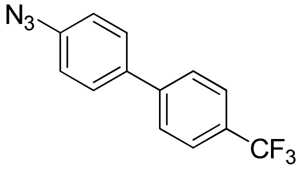
4-Azido-4'-cyanobiphenyl (18)

General procedure III-A was used employing 4-bromobenzonitrile (37 mg, 0.2 mmol), to give the desired product in 83% yield (36.6 mg, a yellow solid). mp = 88 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, 2H, *J* = 8.0 Hz), 7.66 (d, 2H, *J* = 8.5 Hz), 7.59 (d, 2H, *J* = 8.5 Hz), 7.14 (d, 2H, *J* = 8.5 Hz) ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.5, 140.7, 135.7, 132.7, 128.6, 127.3, 119.7, 118.8, 110.9. FT-IR (KBr): 3065, 2929, 2262, 2106, 1599, 1498, 2307, 1131, 817 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{13}H_9N_4$ $[M+H]^+$ 221.0827, found 221.0823.



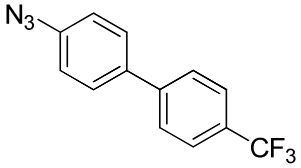
4-Azido-4'-cyanobiphenyl (18)

General procedure III-B was used employing 4-chlorobenzonitrile (28 mg, 0.2 mmol), to give the desired product in 48% yield (21.2 mg, a yellow solid).



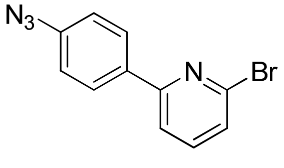
4-Azido-4’-(trifluoromethyl)biphenyl[5] (19)

General procedure III-A was used employing 4-bromobenzotrifluoride (45 mg, 0.2 mmol), to give the desired product in 58% yield (30.7 mg, a yellow solid). mp = 51 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, 2H, *J* = 8.5 Hz), 7.66 (d, 2H, *J* = 8.5 Hz), 7.59 (d, 2H, *J* = 8.5 Hz), 7.13 (d, 2H, *J* = 8.5 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.6, 140.1, 136.4, 129.4 (q, *J* = 32.6 Hz), 128.6, 127.1, 125.8 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 272.8 Hz), 119.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4. FT-IR (KBr): 3221, 3036, 2932, 2131, 2099, 1605, 1499, 1328, 1298, 1166, 1125, 1071, 823 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{13}H_8F_3N_3$ [M]$^+$ 263.0670, found 263.0671.



4-Azido-4’-(trifluoromethyl)biphenyl[5] (19)

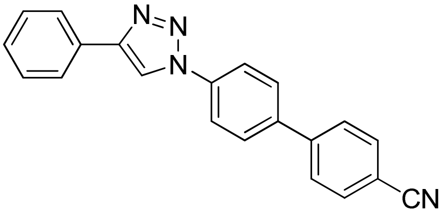
General procedure III-B was used employing 4-chlorobenzotrifluoride (36 mg, 0.2 mmol), to give the desired product in 45% yield (23.5 mg, a yellow solid).



2-Bromo-6-(4-Azidophenyl)-pyridine (20)

General procedure III-A was used employing 2,6-dibromopyridine (47.4 mg, 0.2 mmol), to give the desired product in 81% yield (44.6 mg, a yellow solid). mp = 95 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, 2H, *J* = 8.5 Hz), 7.65 (dd, 1H, *J* = 7.5, 0.5 Hz), 7.58 (t, 1H, *J* = 7.5 Hz), 7.40 (dd, 1H, *J* = 8.0, 0.5 Hz), 7.11 (d, 2H, *J* = 8.5 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 142.2, 141.4, 139.0, 134.3, 128.4, 126.3, 119.3, 118.5. FT-IR (KBr): 3043, 2920, 2847, 2107, 1601, 1578, 1507, 1312, 1124, 1045, 843, 791, 678 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{11}H_8BrN_4$ [M+H]$^+$ 274.9932, found 274.9930.

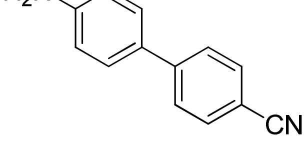
A One-Pot Cross-Coupling and 1,3-Dipolar Cycloaddition Reaction



4’-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)biphenyl-4-carbonitrile (21)

To a 25 mL round-bottom flask containing a stirring bar was added the potassium 4-azidophenyltrifluoroborate (113 mg, 0.5 mmol), Cs_2CO_3 (490 mg, 1.5 mmol), $PdCl_2(dppf)\cdot CH_2Cl_2$ (41 mg, 5×10^{-2} mmol, 10 mol %), and 4-bromobenzonitrile (91 mg, 0.5 mmol). The vessel was sealed with a septum, and methanol (6 mL) was added via syringe. The reaction was heated in an oil bath at 80 °C for 1 h. After 4-bromobenzonitrile was totally consumed (the reaction was monitored by TLC), CuI (9.5 mg, 5×10^{-2} mmol, 10 mol %) and phenylacetylene (51 mg, 0.5 mmol) were added. The reaction mixture was heated at 80 ^{o}C for an additional 30 min. After the reaction was complete (the reaction was monitored by TLC), the reaction mixture was cooled to rt. The solvent was removed in vacuo. The residual compound was dissolved in ethyl acetate, and the insoluble salts were filtered through a thin pad of silica gel. The solvent was concentrated on a rotary evaporator, and the crude product was purified by silica gel column chromatography (hexane/EtOAc 3:1) to give the pure product **21** (a white solid, 114 mg, 71% overall yield). mp = 215−219 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.90 (m, 4H), 7.74 (m, 4H), 7.70 (d, 2H, J = 8.5 Hz), 7.44 (t, 2H, J = 7.5 Hz), 7.31 (t, 1H, J = 7.5 Hz). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.6, 144.0, 139.5, 137.1, 132.8, 130.0, 128.9, 128.6, 128.5, 127.7, 125.8, 120.9, 118.6, 117.3, 111.6. FT-IR (KBr): 3096, 2221, 1604, 1499, 1455, 1396, 1226, 1074, 1043, 819, 772, 693, 539 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{21}H_{15}N_4$ $[M+H]^+$ 323.1297, found 323.1308.

A One-Pot Cross-Coupling and Reduction Reaction



4’-Aminobiphenyl-4-carbonitrile[6] (22)

To a 25 mL round-bottom flask containing a stirring bar was added the potassium 4-azidophenyltrifluoroborate (113 mg, 0.5 mmol), Cs_2CO_3 (490 mg, 1.5 mmol), $PdCl_2(dppf)\cdot CH_2Cl_2$ (41 mg, 5×10^{-2} mmol, 10 mol %), and 4-bromobenzonitrile (91 mg, 0.5 mmol). The vessel was sealed with a septum and methanol (6 mL) was added via syringe. The reaction was heated in an oil bath at 80 °C for 1 h. After 4-bromobenzonitrile was totally consumed (the reaction was monitored by TLC), the reaction mixture was cooled to 0 ^{o}C and then $NaBH_4$ (28 mg, 0.75 mmol, 1.5 equiv) was added. The reaction mixture was slowly warmed to rt and stirred for 1 h at rt. After the reaction was complete (the reaction was monitored by TLC), the solvent was removed in vacuo. The residual compound was dissolved in ethyl acetate, and the insoluble salts were filtered through a thin pad of silica gel. The solvent was concentrated on a rotary evaporator, and the crude product was purified by silica gel column chromatography (hexane/EtOAc 3:1) to give the pure product **22** (a yellow solid, 74 mg, 76% overall yield). mp = 182−184 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, 2H, J = 8.5 Hz), 7.61 (d, 2H, J = 8.5 Hz), 7.43 (d, 2H, J = 8.5 Hz), 6.77 (d, 2H, J = 8.5 Hz), 3.84 (br s, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 147.1, 145.5, 132.5, 129.0, 128.2, 126.6, 119.3, 115.3, 109.4. FT-IR (KBr): 3469, 3373, 2925, 2224, 1709, 1599, 1495, 1362, 1292, 1222, 1182, 818, 528 cm^{-1}. HRFABMS: *m*/*z* calcd for $C_{13}H_{10}N_2$ $[M]^+$ 194.0844, found 194.0852.

References

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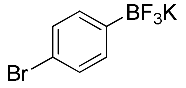


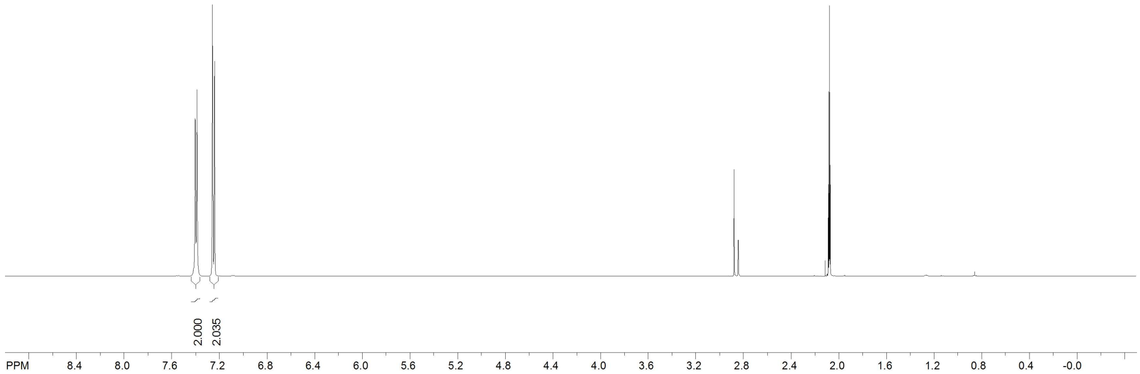


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **1a-Br** in Acetone-d_6

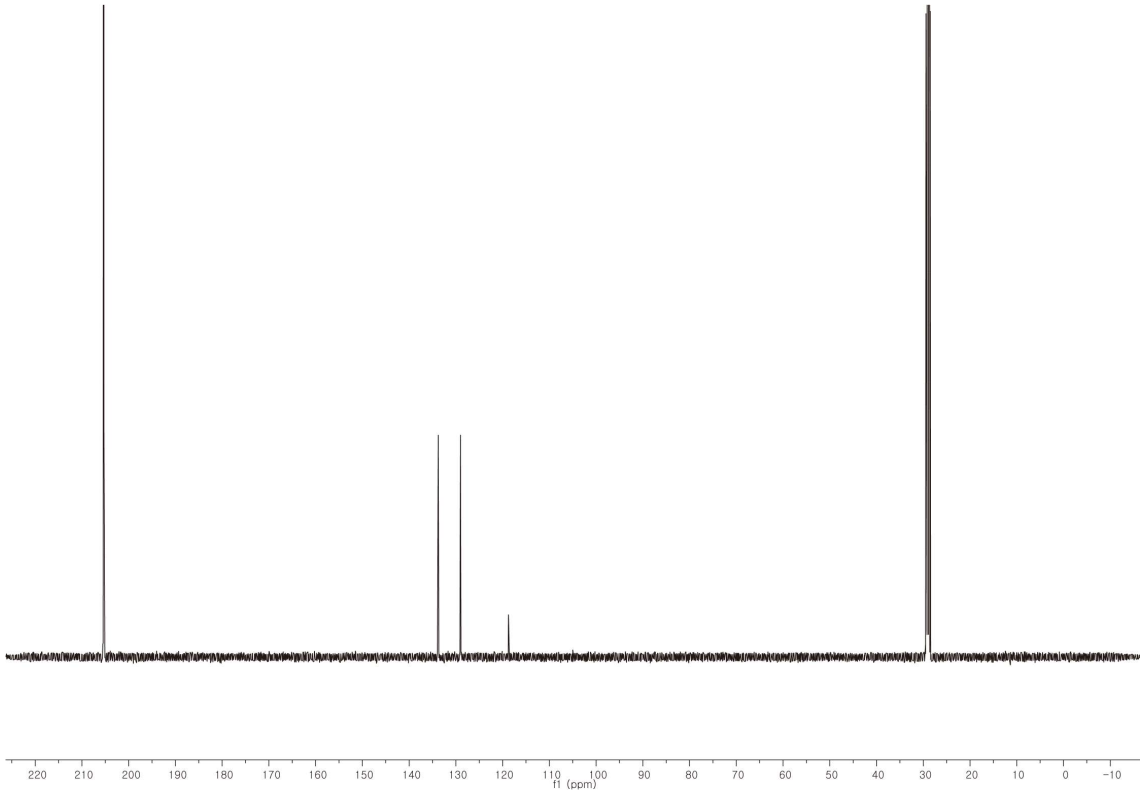
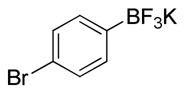


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **1a-Br** in Acetone-d_6



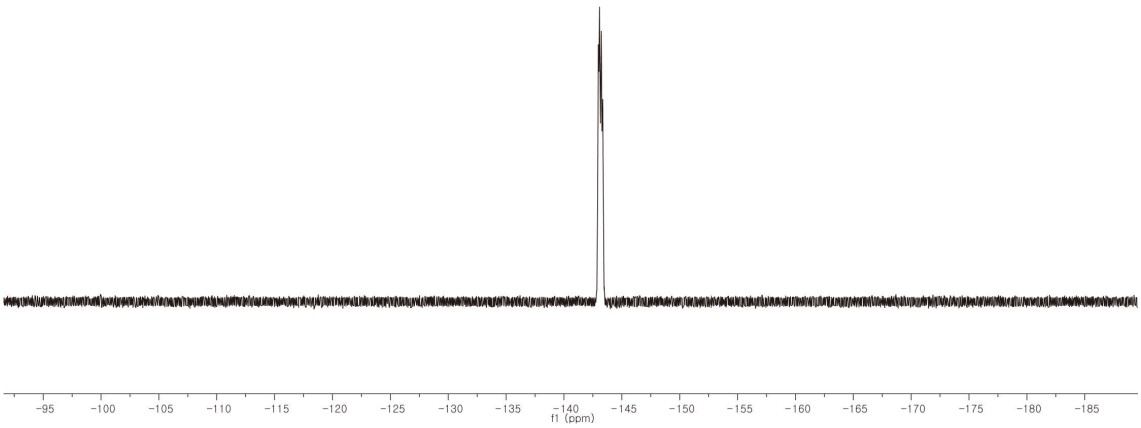


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **1a-Br** in Acetone-d_6

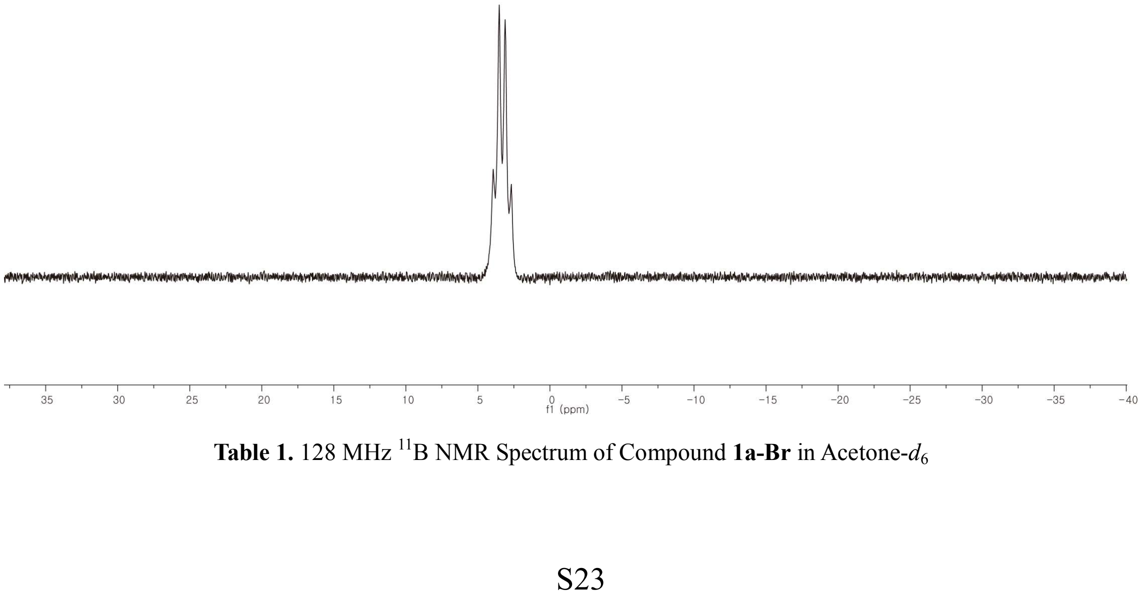
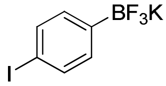


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **1a-Br** in Acetone-d_6



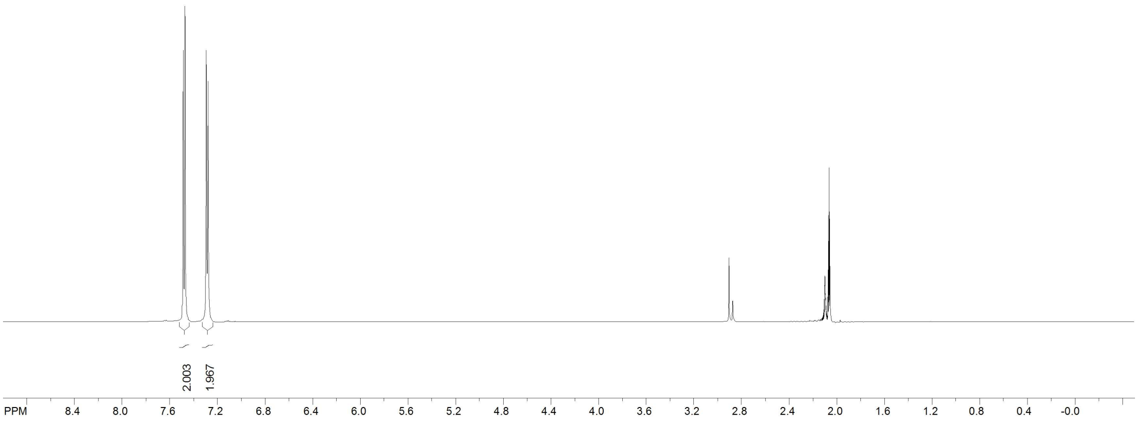


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **1a-I** in Acetone-d_6

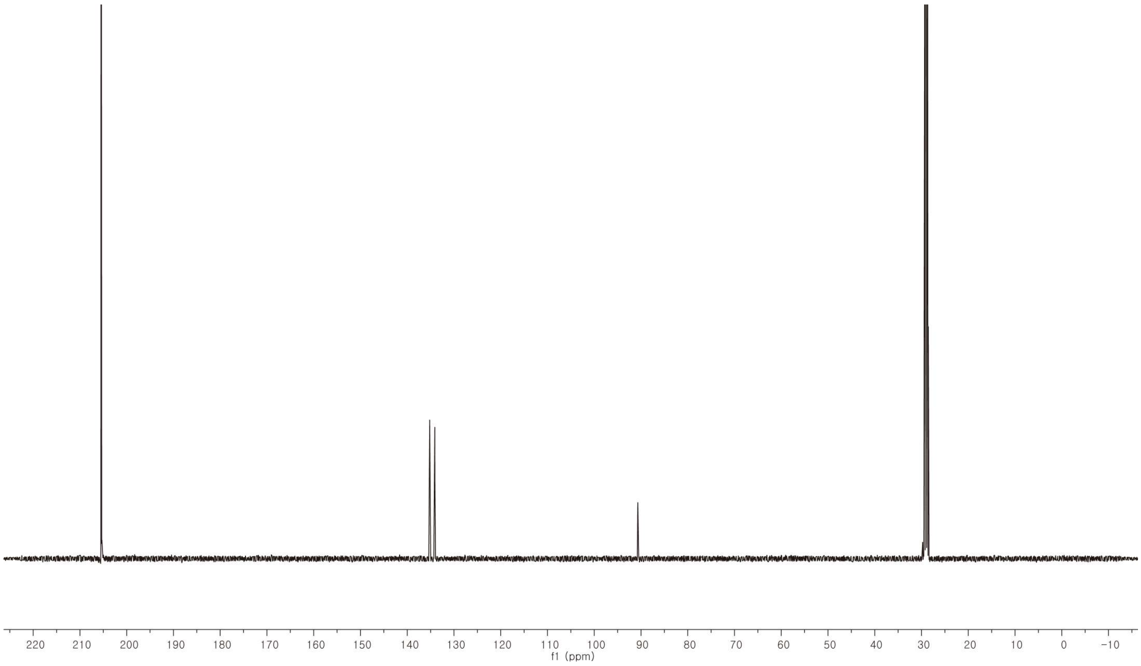
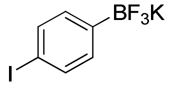


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **1a-I** in Acetone-d_6



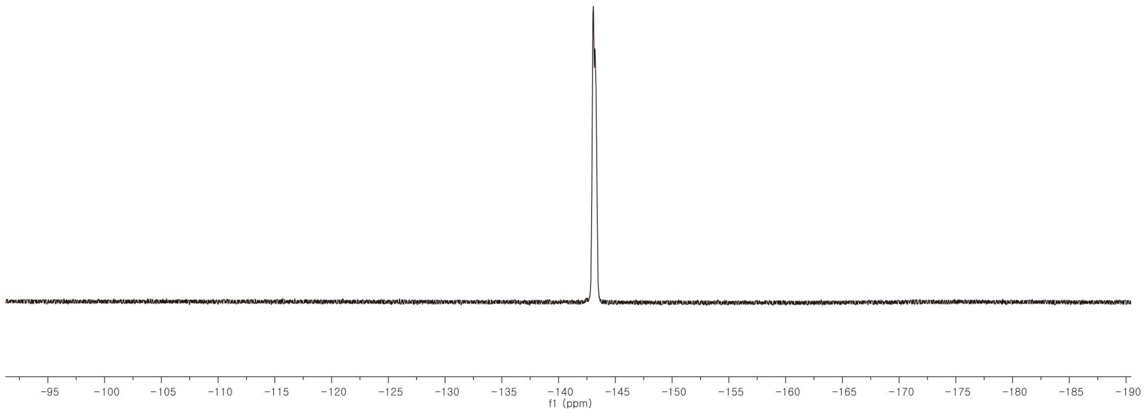


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **1a-I** in Acetone-d_6

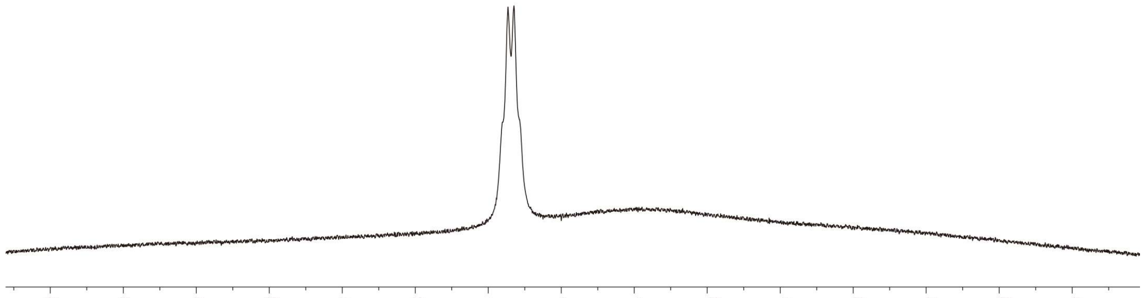
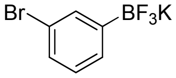


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **1a-I** in Acetone-d_6



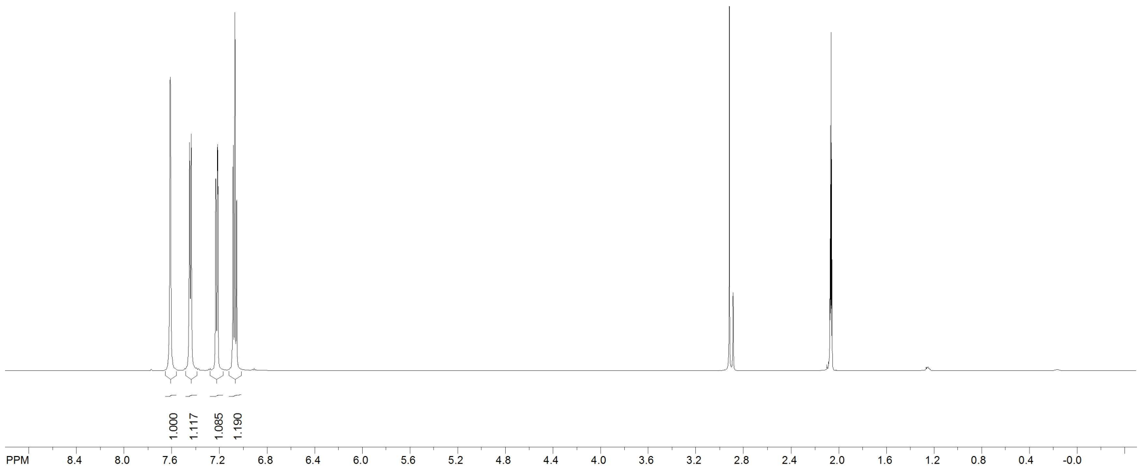


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **2a-Br** in Acetone-d_6

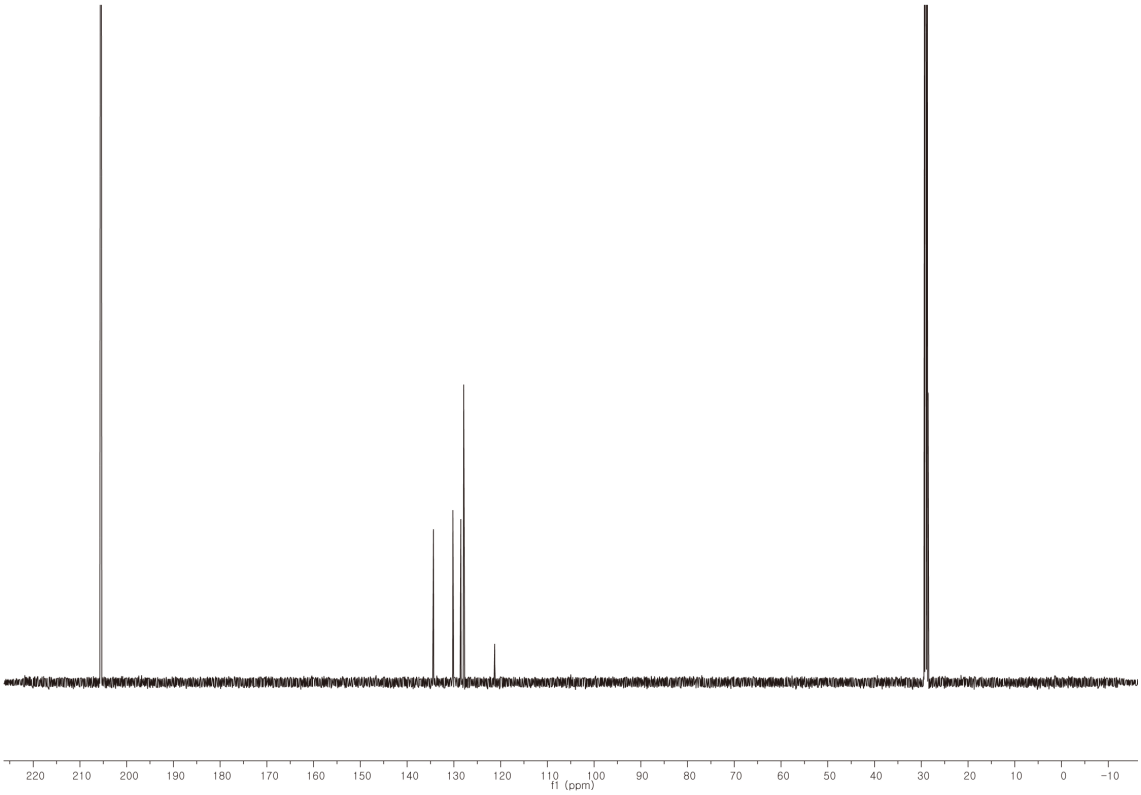
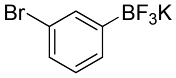


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **2a-Br** in Acetone-d_6



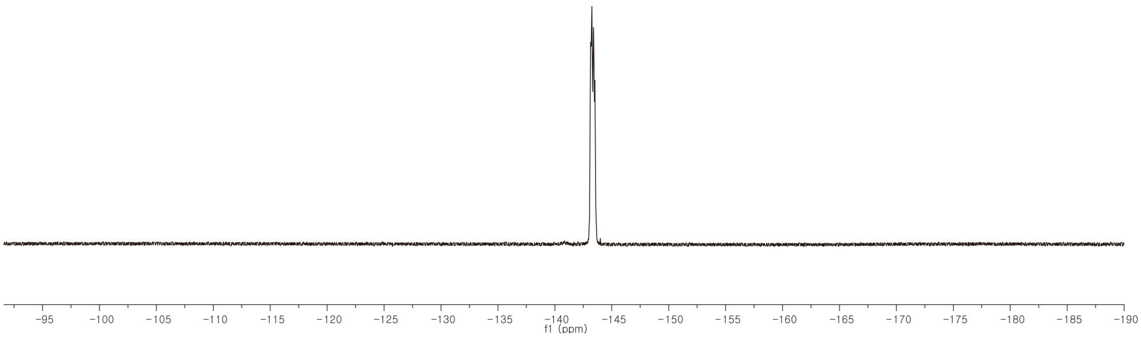


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **2a-Br** in Acetone-d_6

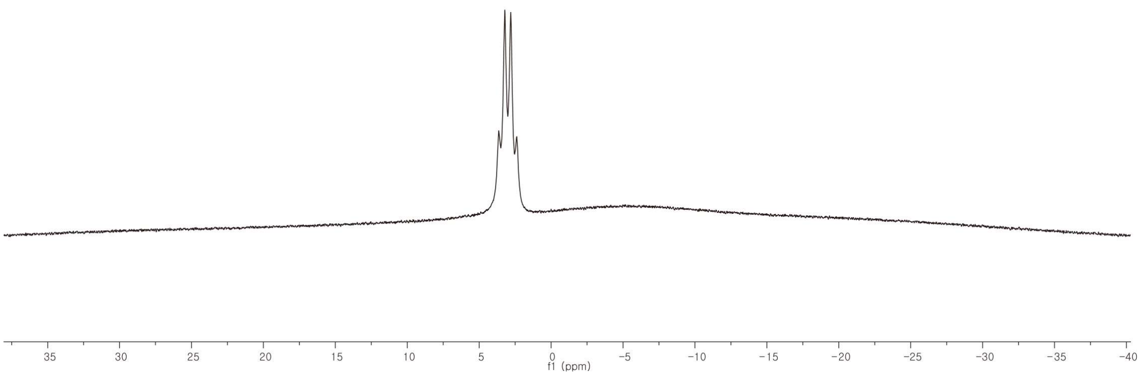
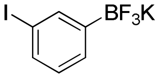


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **2a-Br** in Acetone-d_6



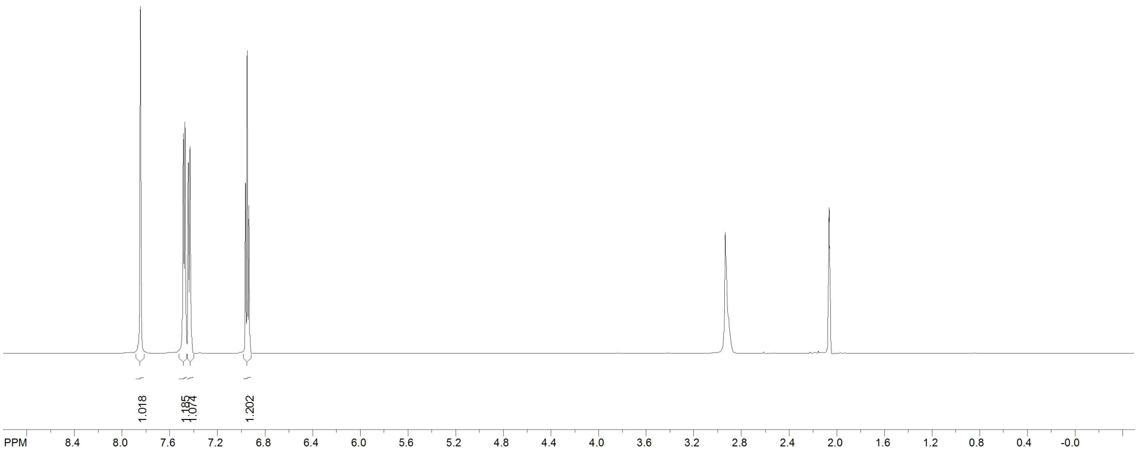


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **2a-I** in Acetone-d_6

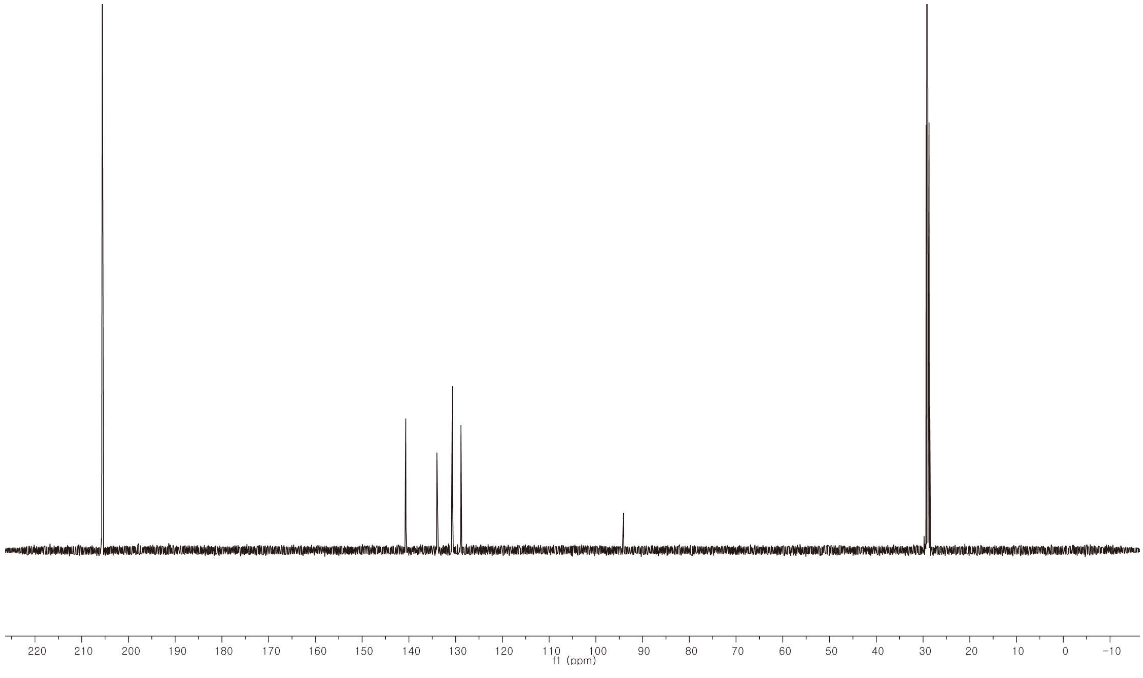
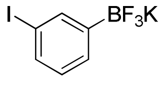


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **2a-I** in Acetone-d_6



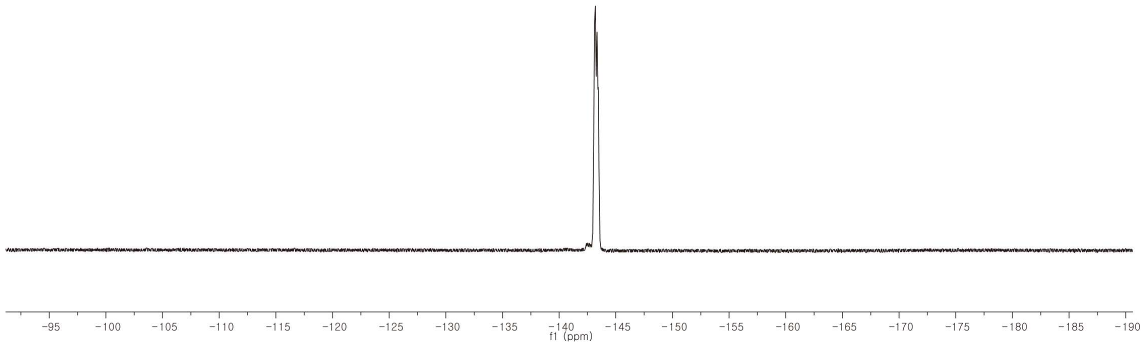


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **2a-I** in Acetone-d_6

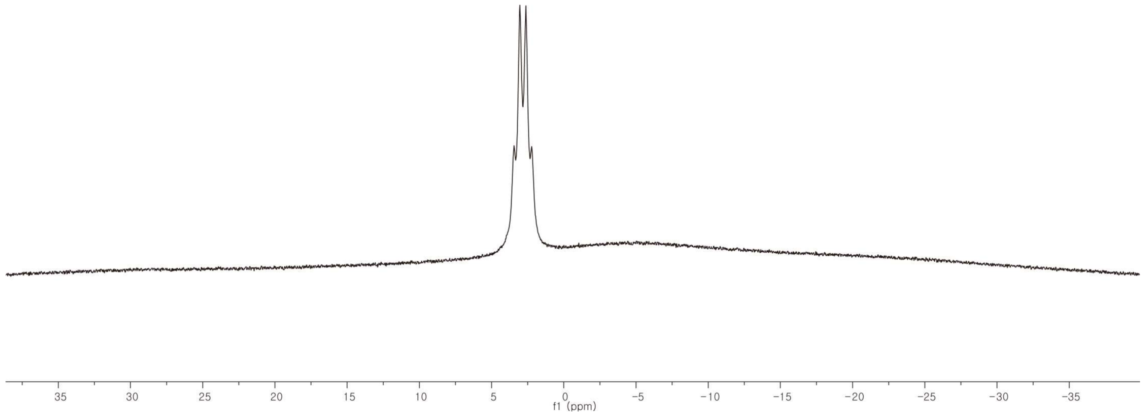
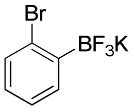


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **2a-I** in Acetone-d_6



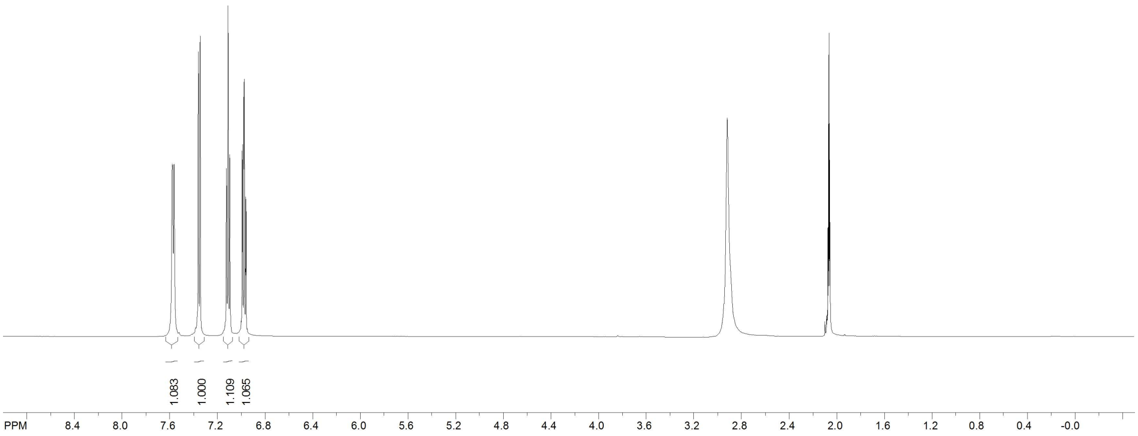


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **3a** in Acetone-d_6

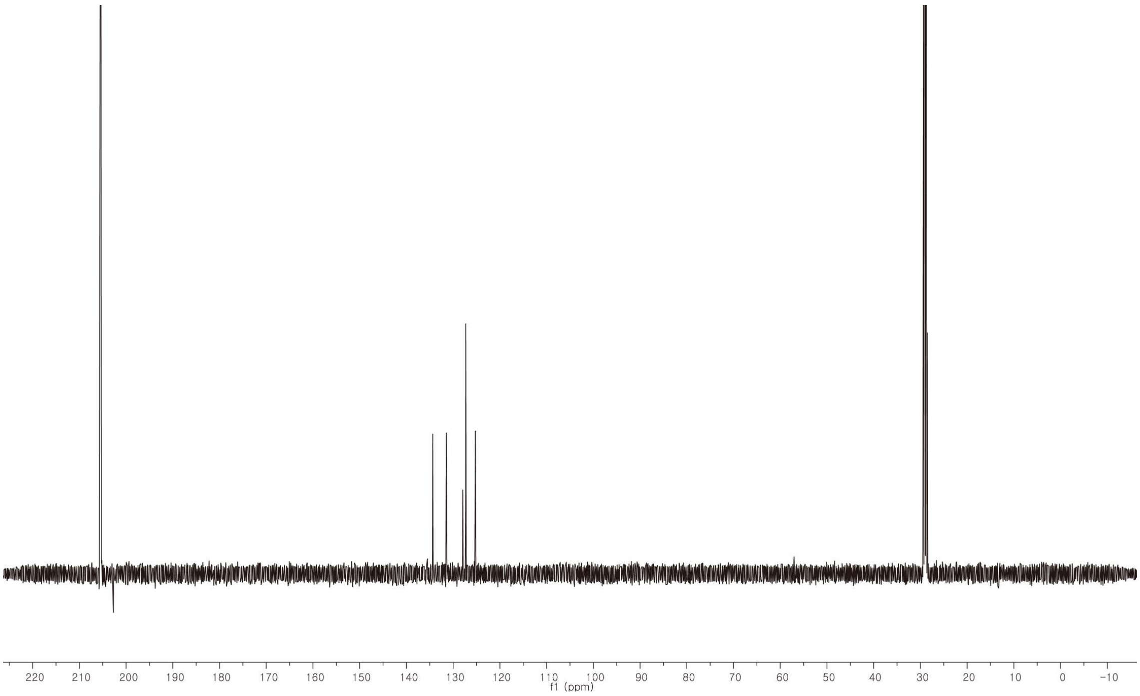
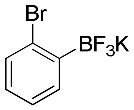


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **3a** in Acetone-d_6



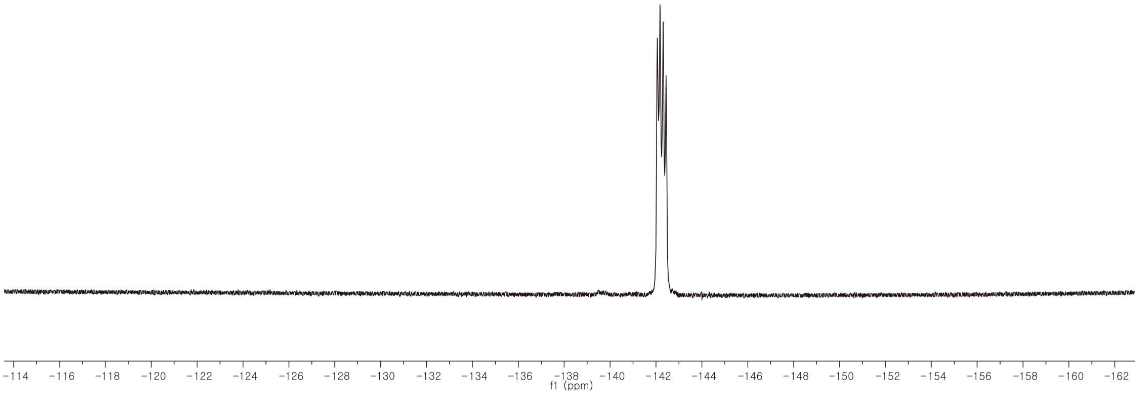


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **3a** in Acetone-d_6

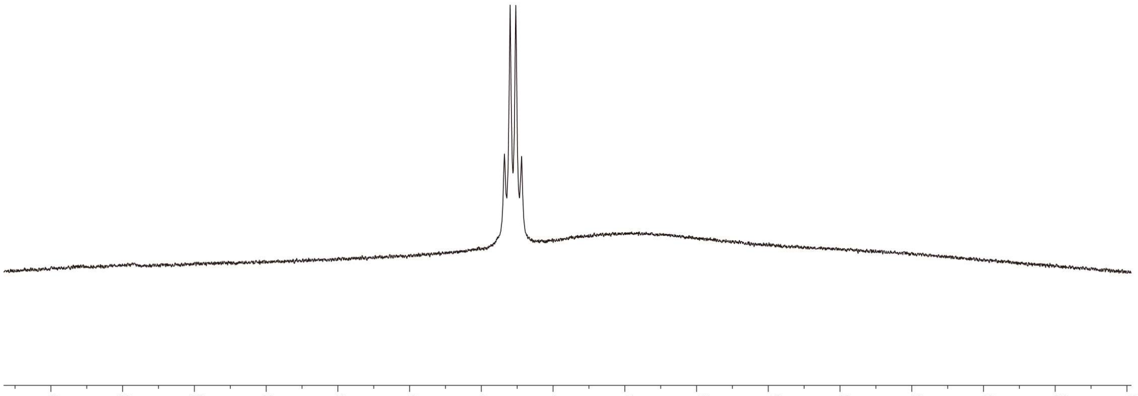
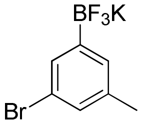


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **3a** in Acetone-d_6



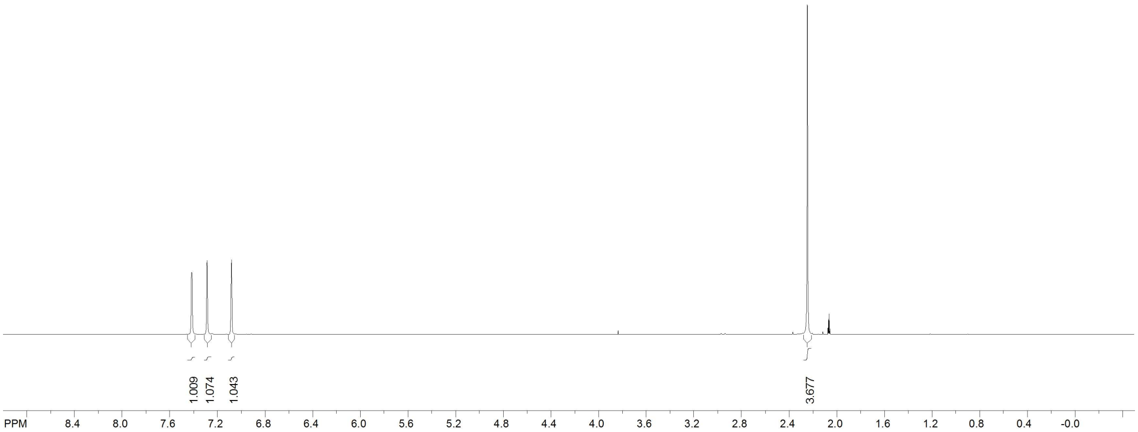


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **4a** in Acetone-d_6

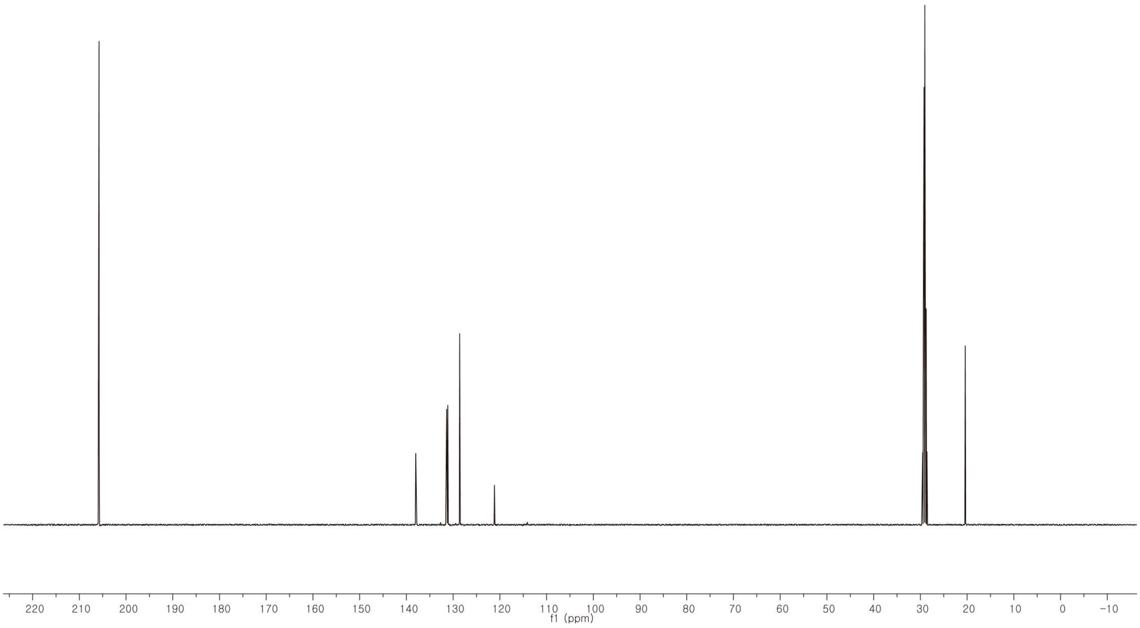
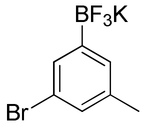


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **4a** in Acetone-d_6



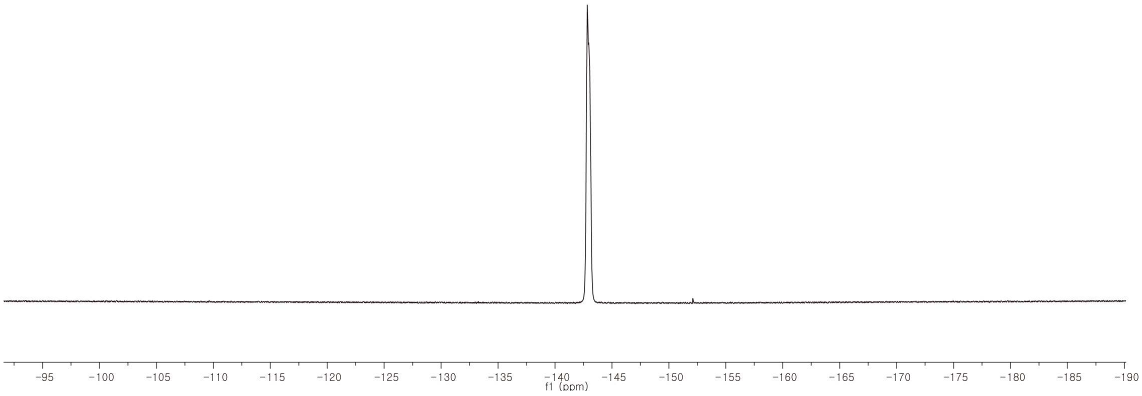


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **4a** in Acetone-d_6

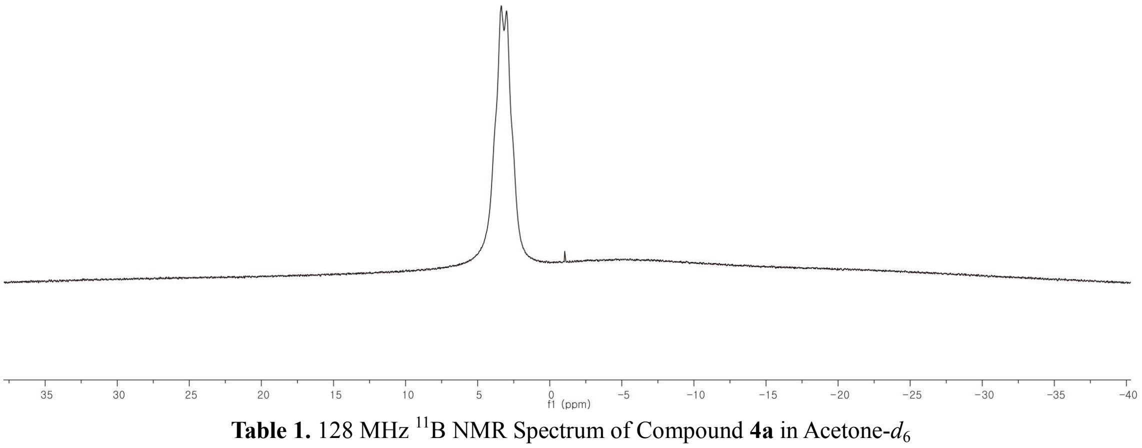
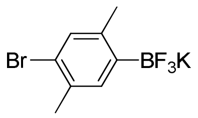


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **4a** in Acetone-d_6



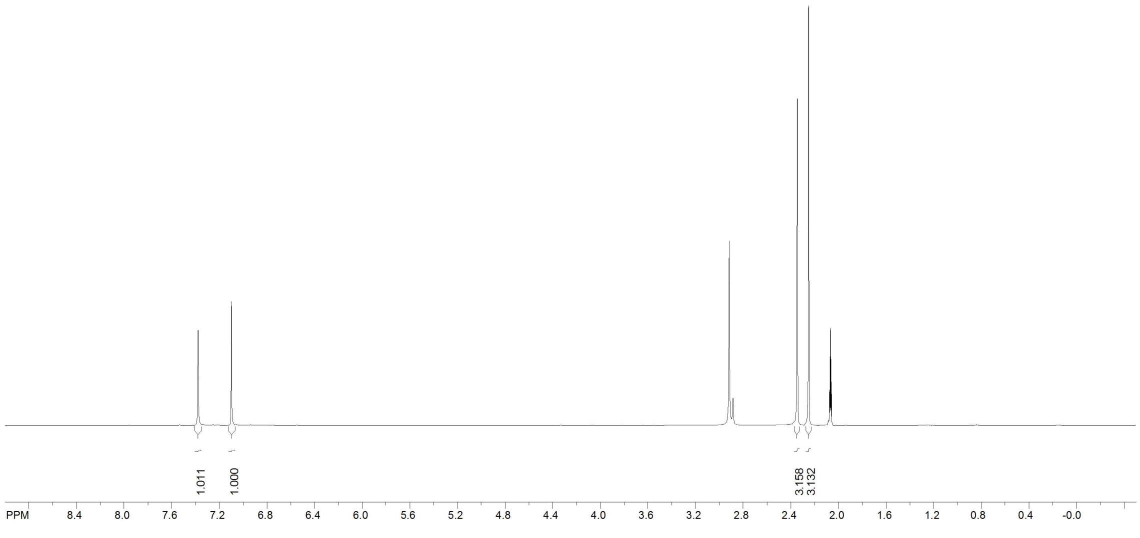


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **5a** in Acetone-d_6

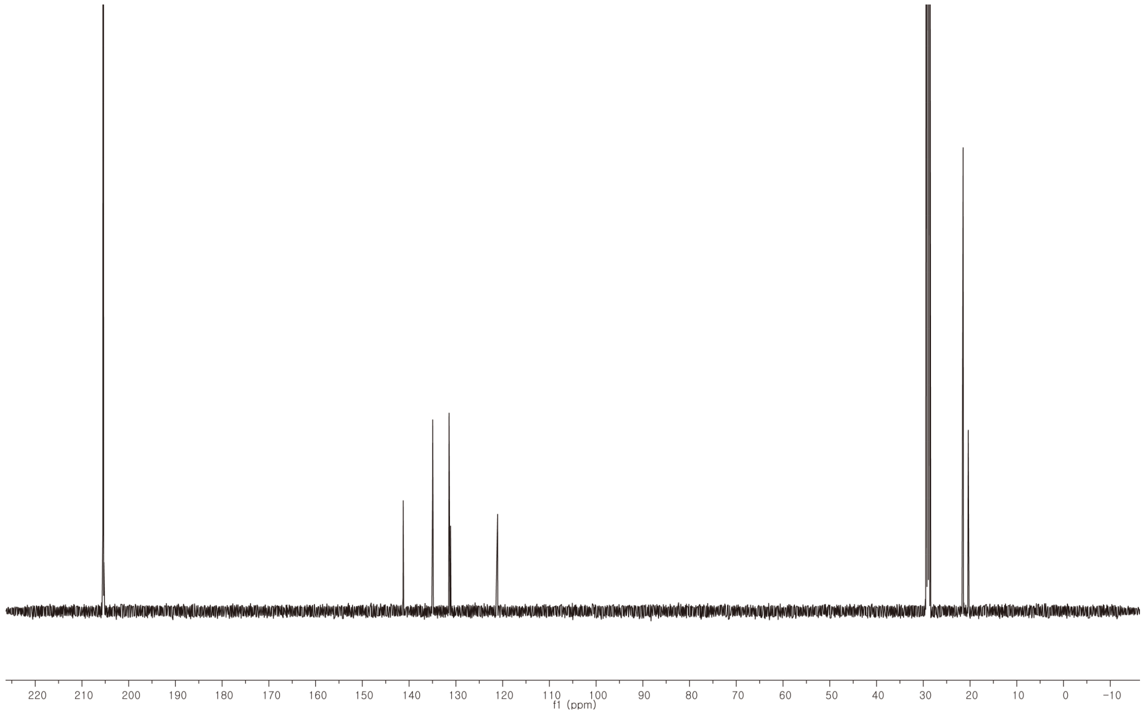
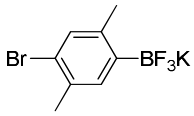


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **5a** in Acetone-d_6



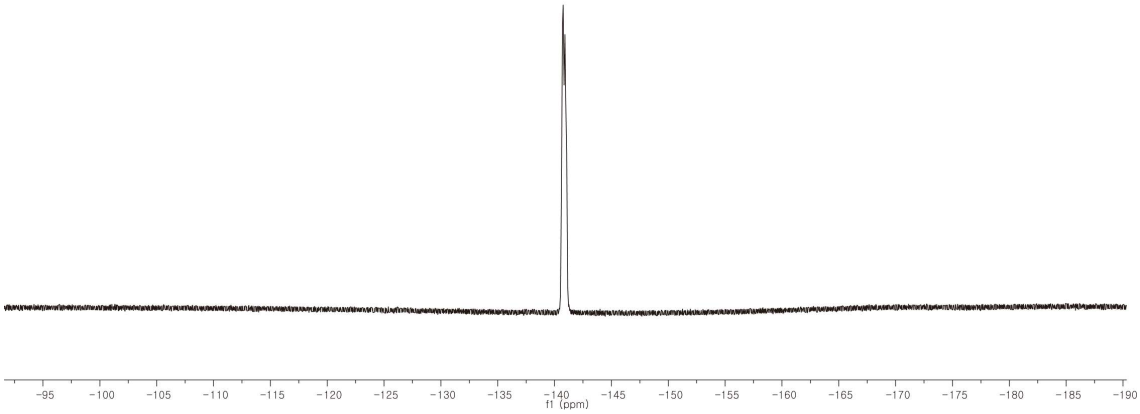


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **5a** in Acetone-d_6

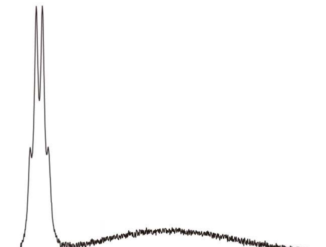
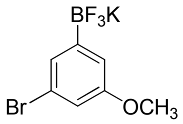


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **5a** in Acetone-d_6



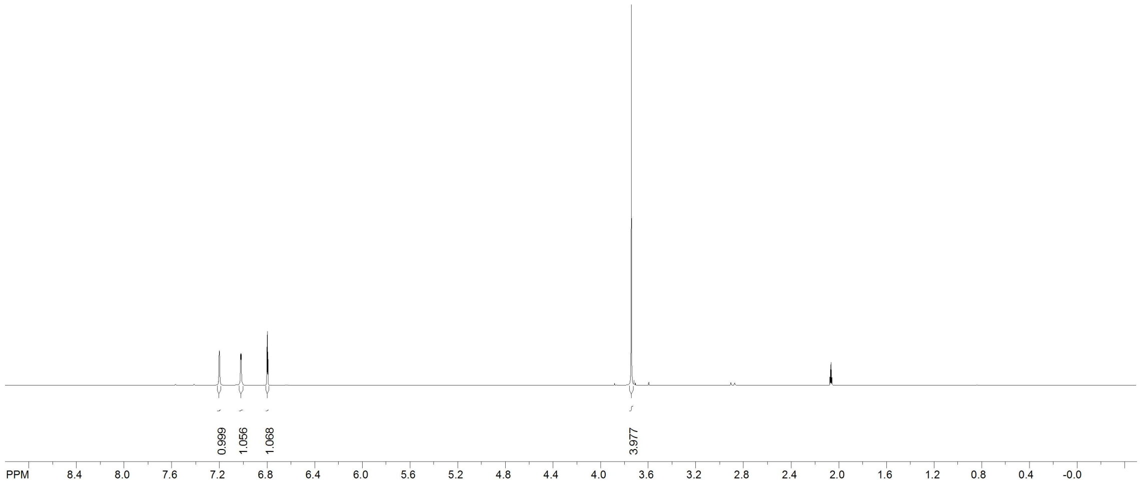


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **6a** in Acetone-d_6

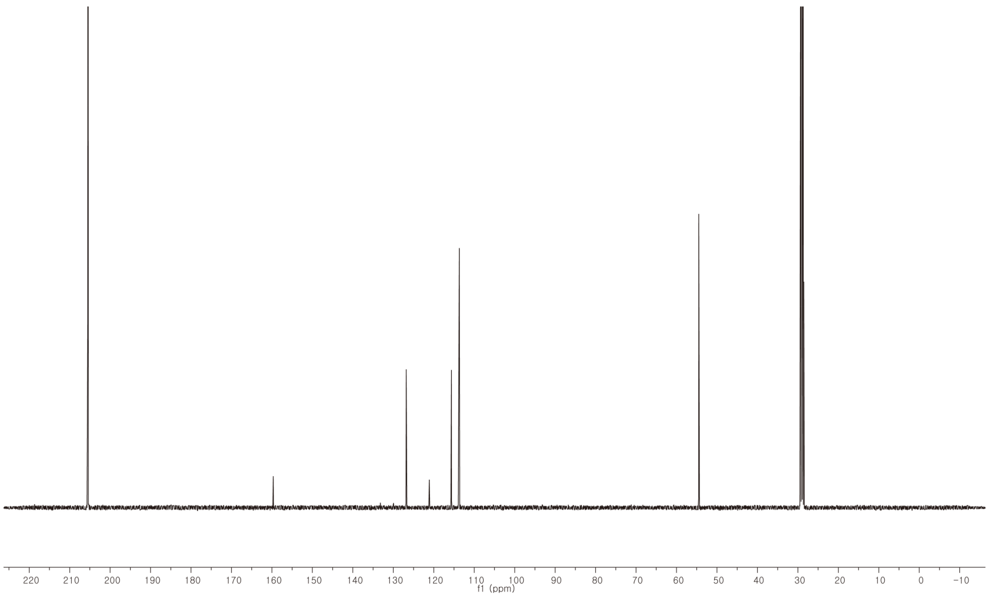
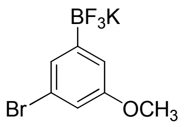


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **6a** in Acetone-d_6



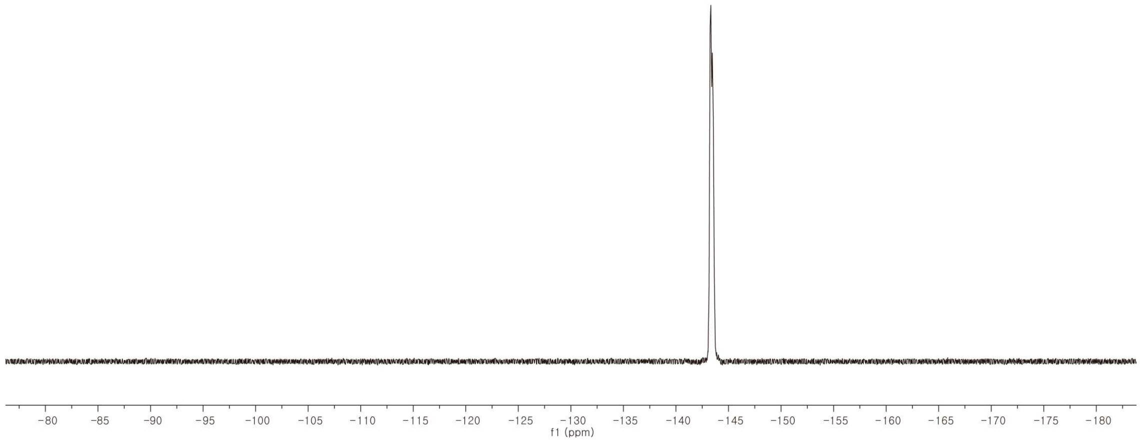


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **6a** in Acetone-d_6

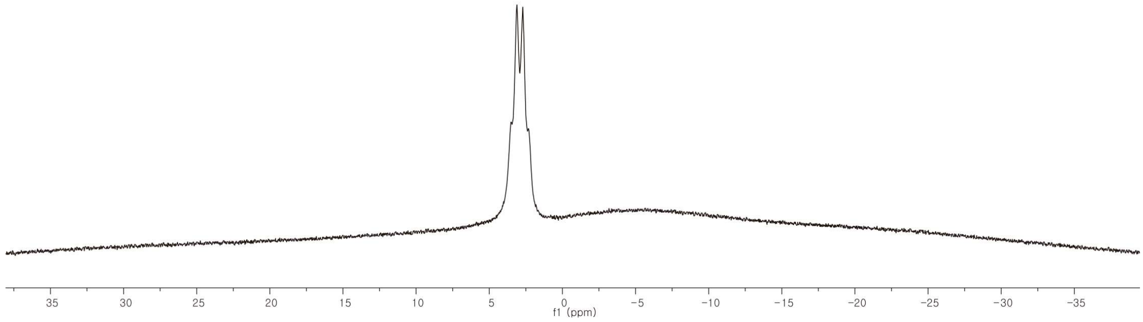
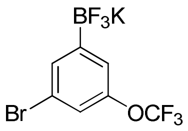


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **6a** in Acetone-d_6



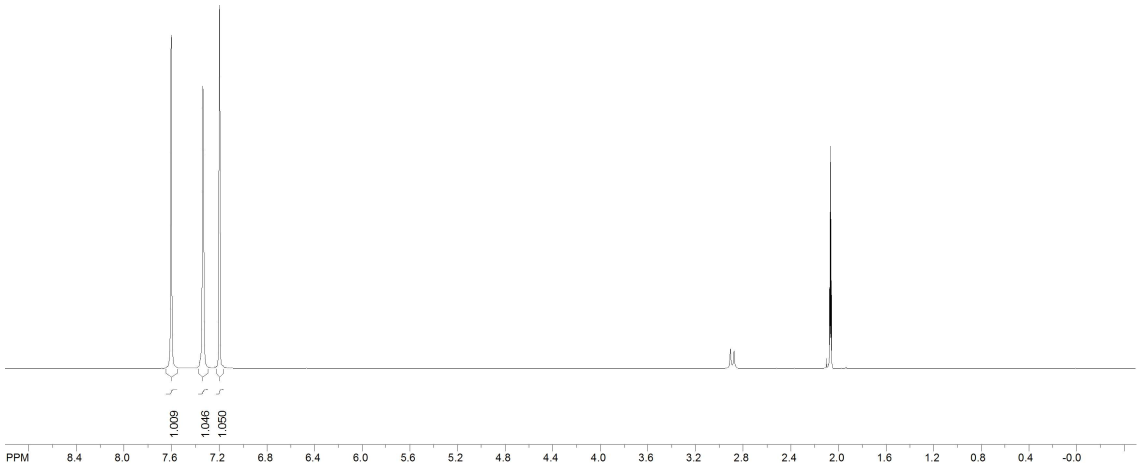


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **7a** in Acetone-d_6

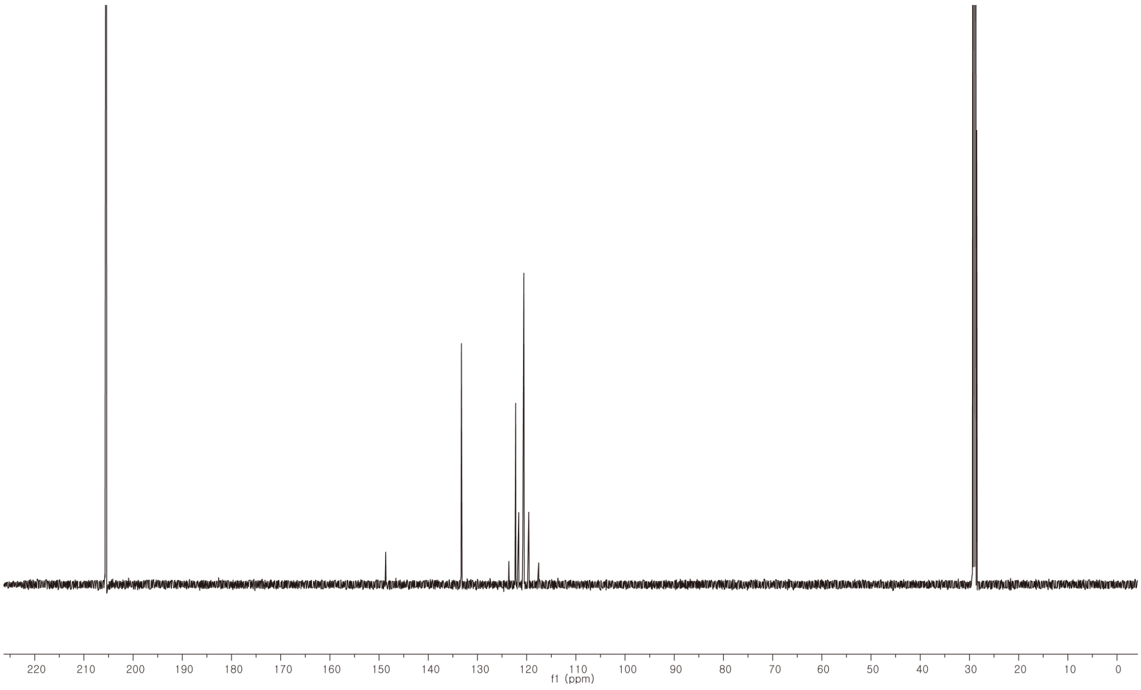
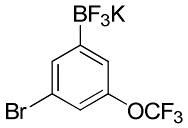


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **7a** in Acetone-d_6



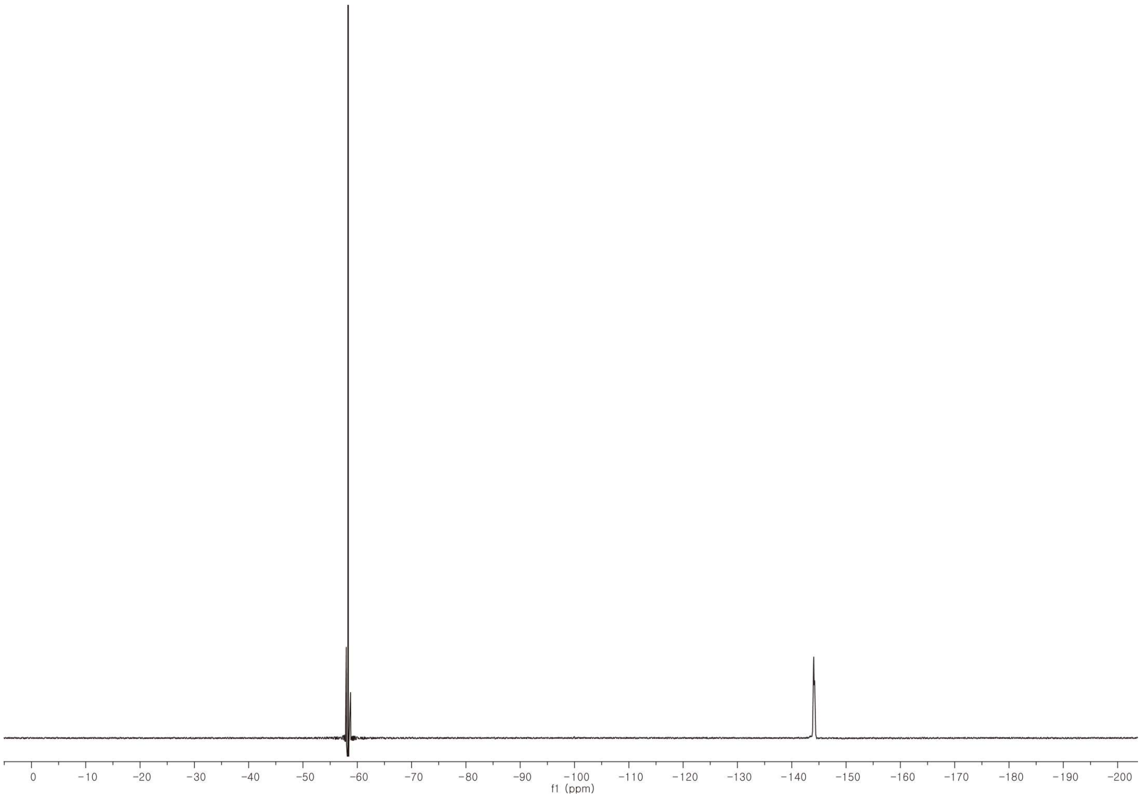


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **7a** in Acetone-d_6

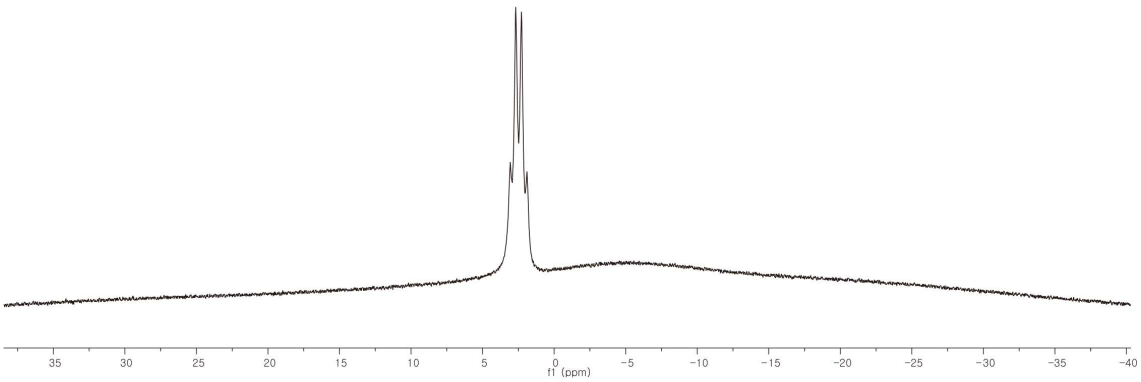
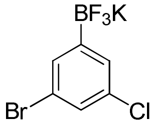


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **7a** in Acetone-d_6



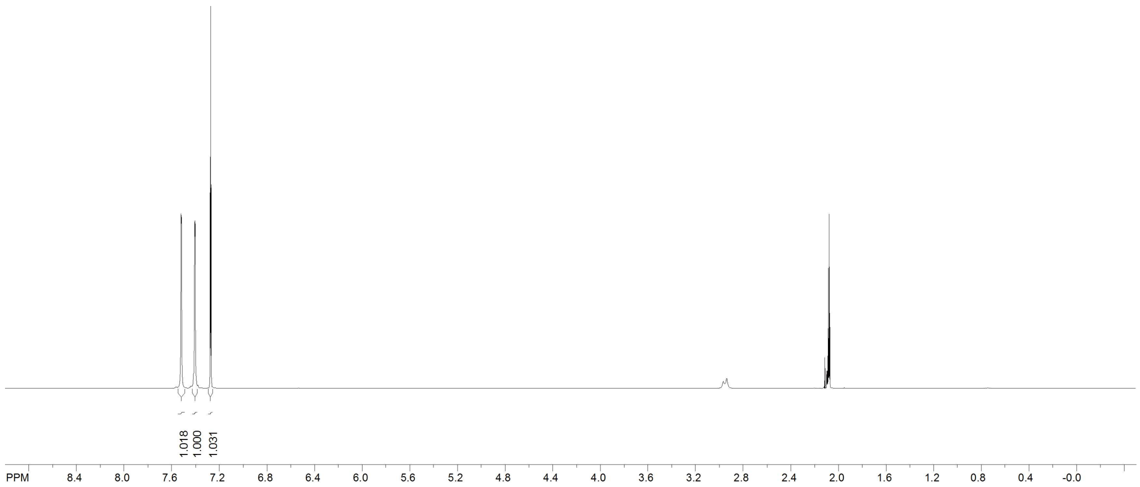


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **8a** in Acetone-d_6

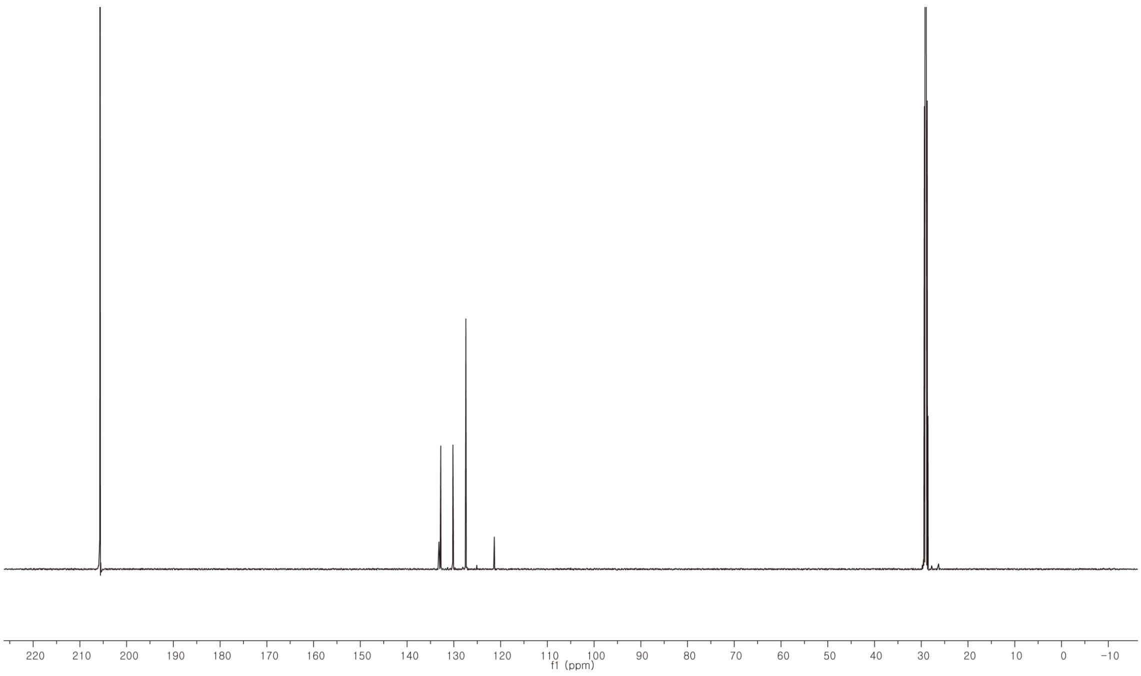
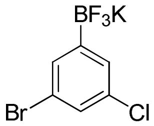


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **8a** in Acetone-d_6



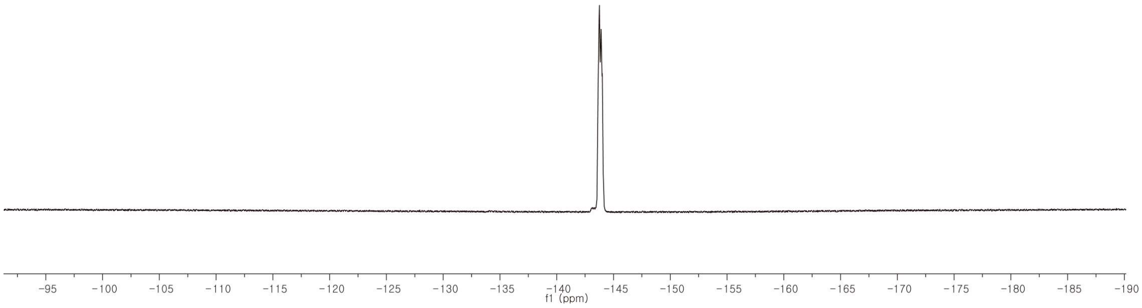


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **8a** in Acetone-d_6

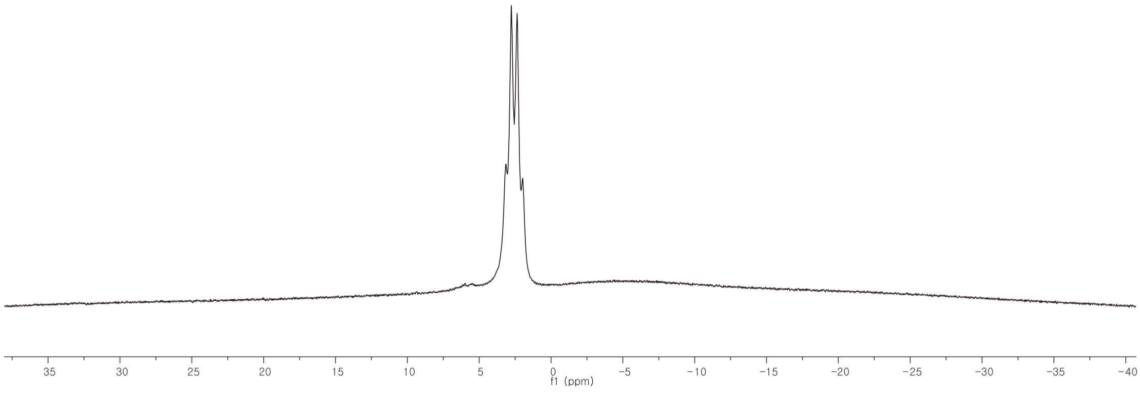
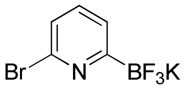


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **8a** in Acetone-d_6



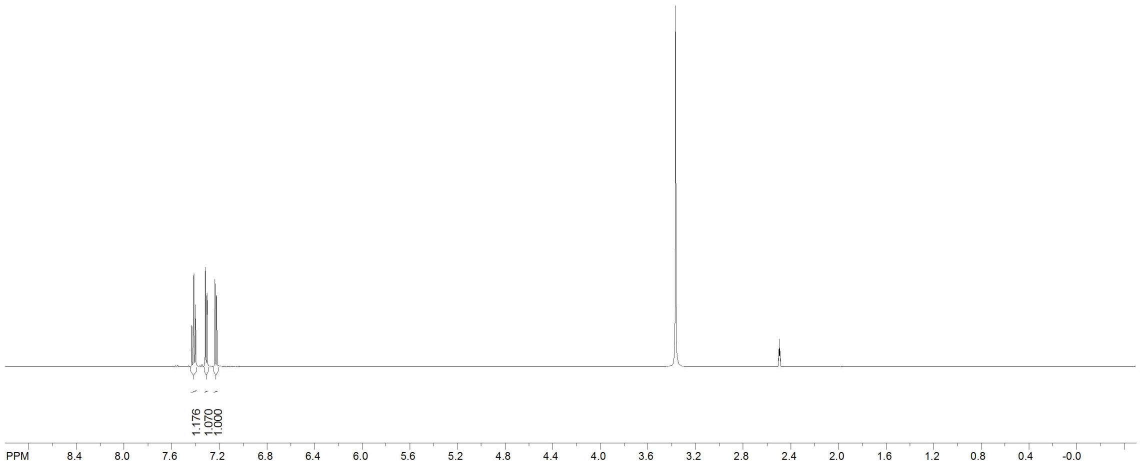


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **9a** in DMSO-d_6

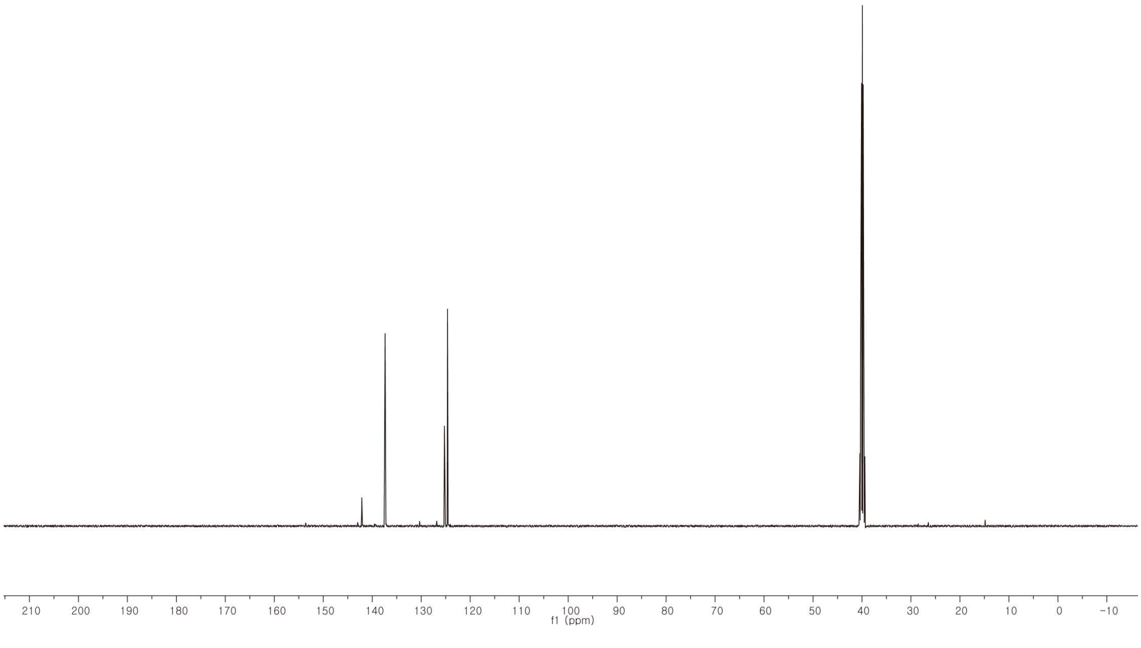
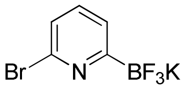


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **9a** in DMSO-d_6



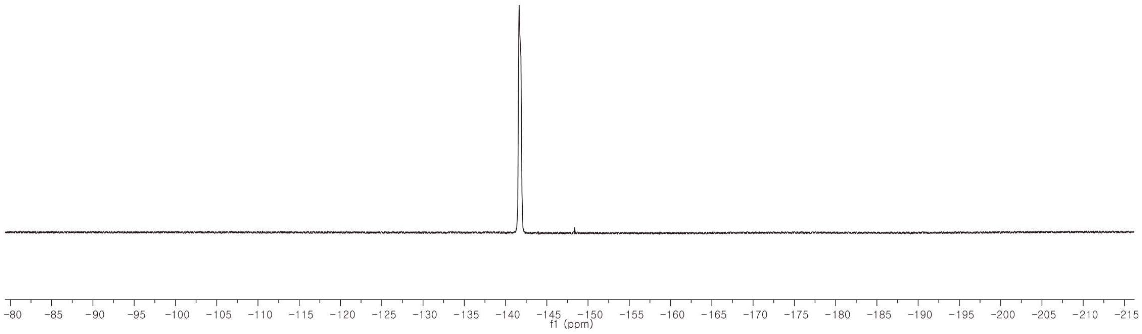


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **9a** in DMSO -d_6

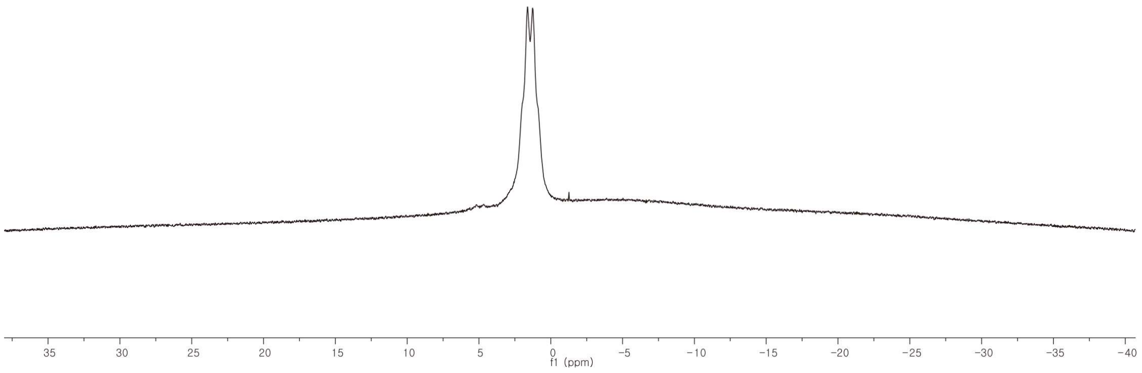
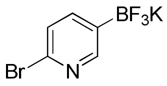


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **9a** in DMSO -d_6



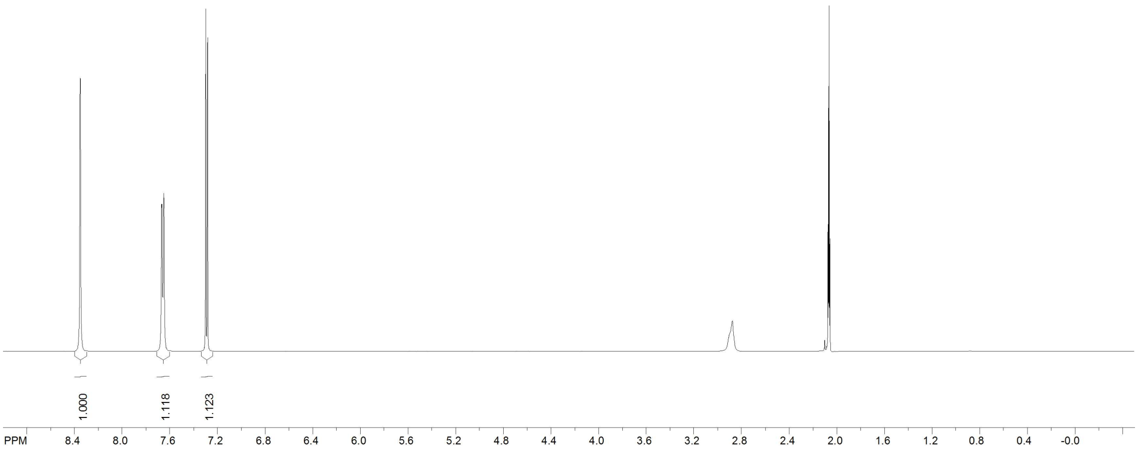


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **10a** in Acetone-d_6

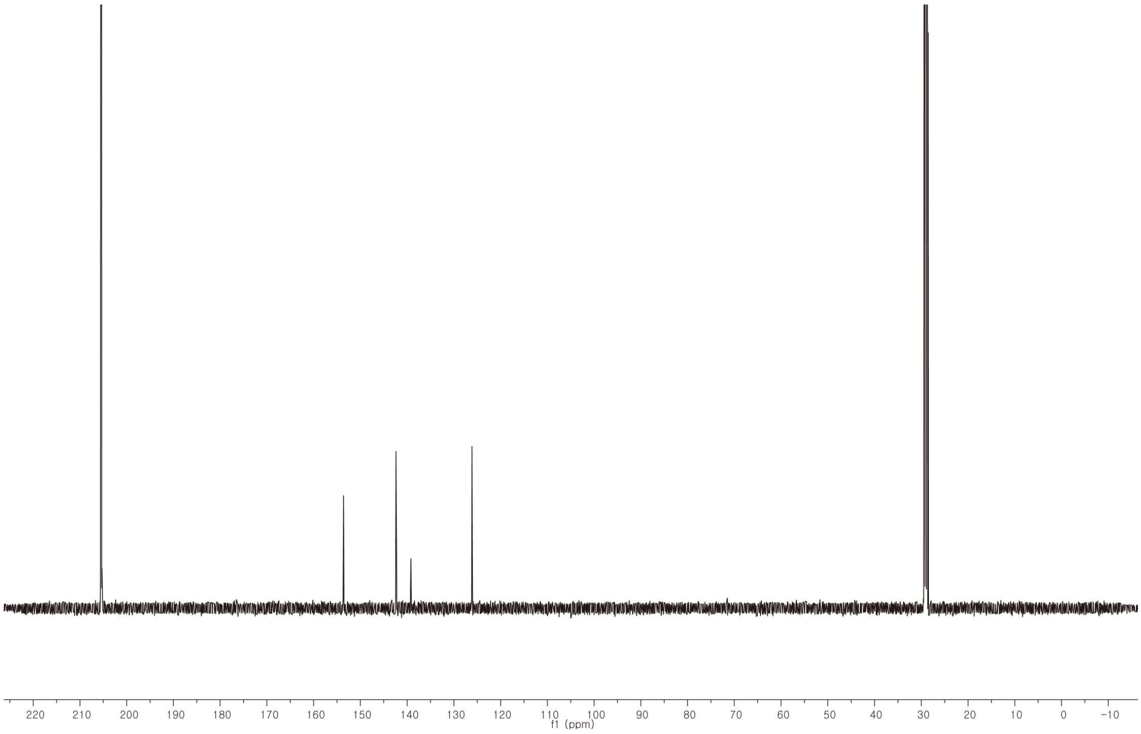
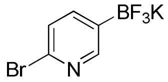


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **10a** in Acetone-d_6



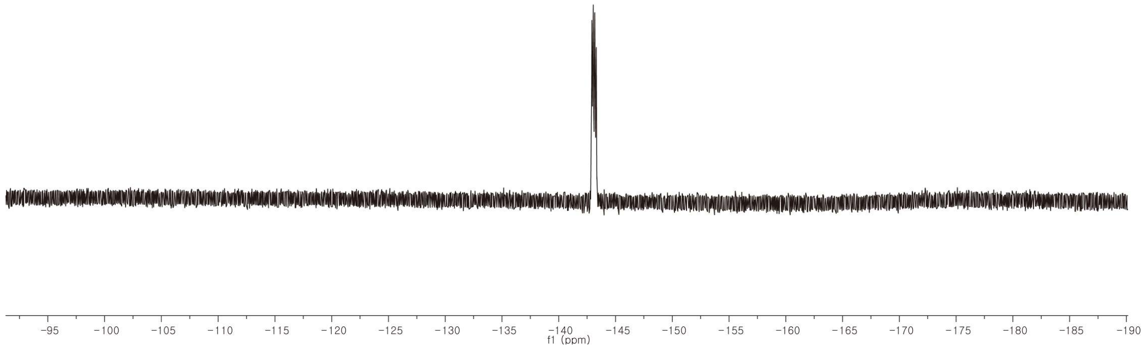


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **10a** in Acetone-d_6

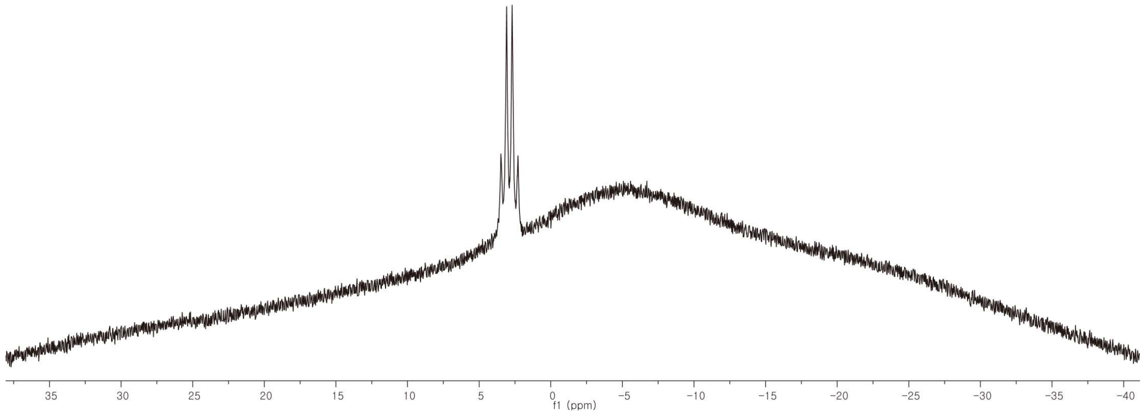
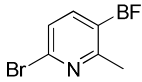


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **10a** in Acetone-d_6



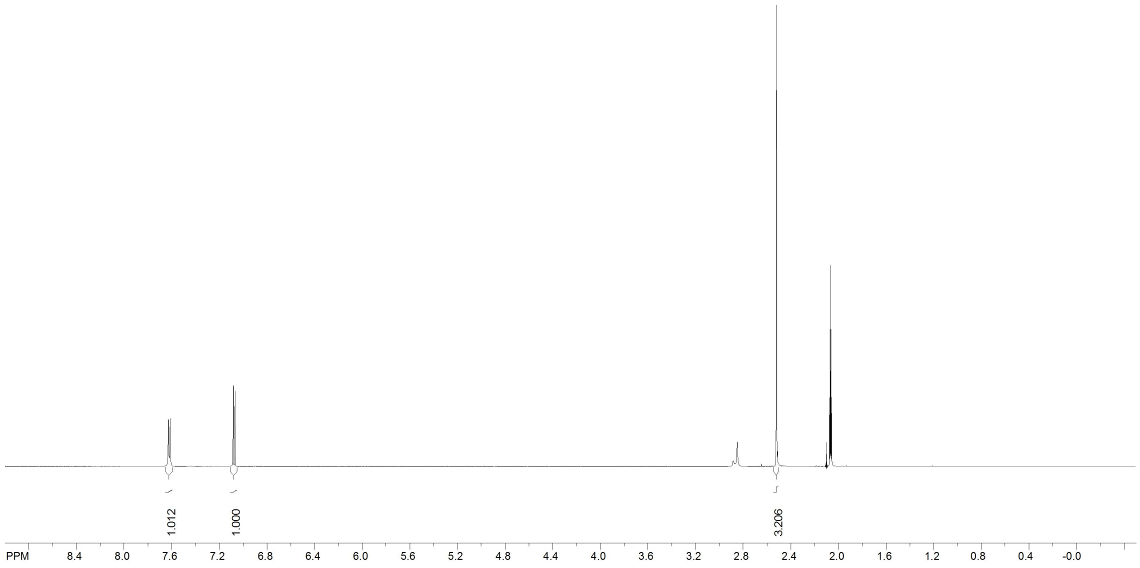


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **11a** in Acetone-d_6

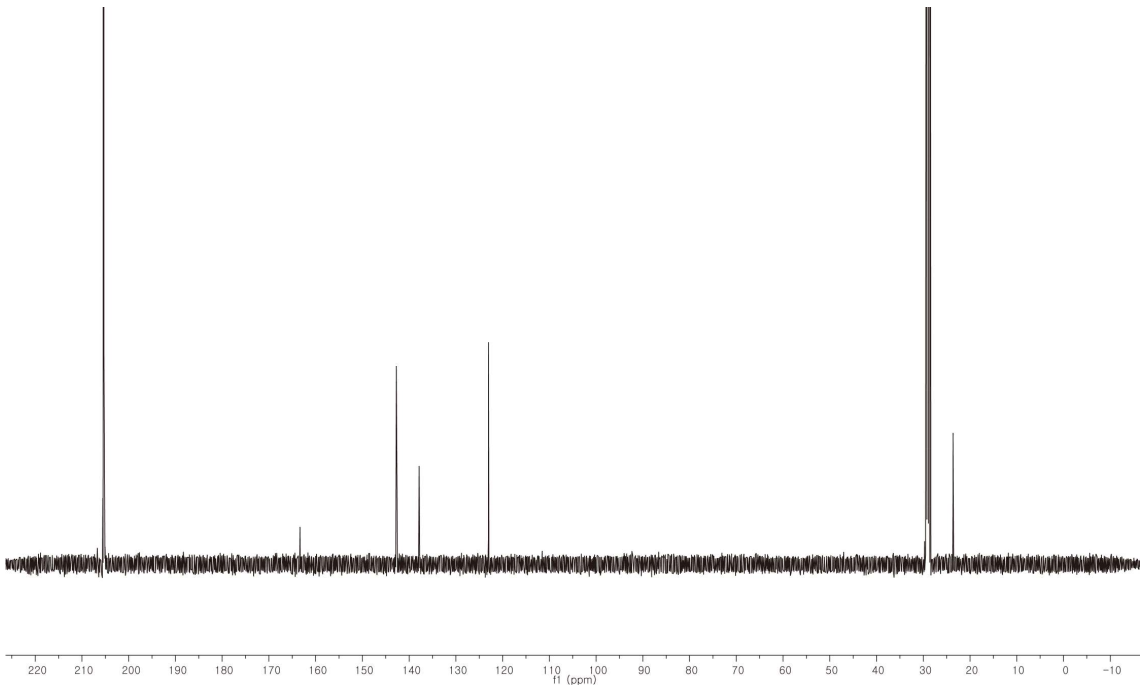
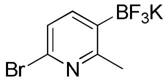


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **11a** in Acetone-d_6



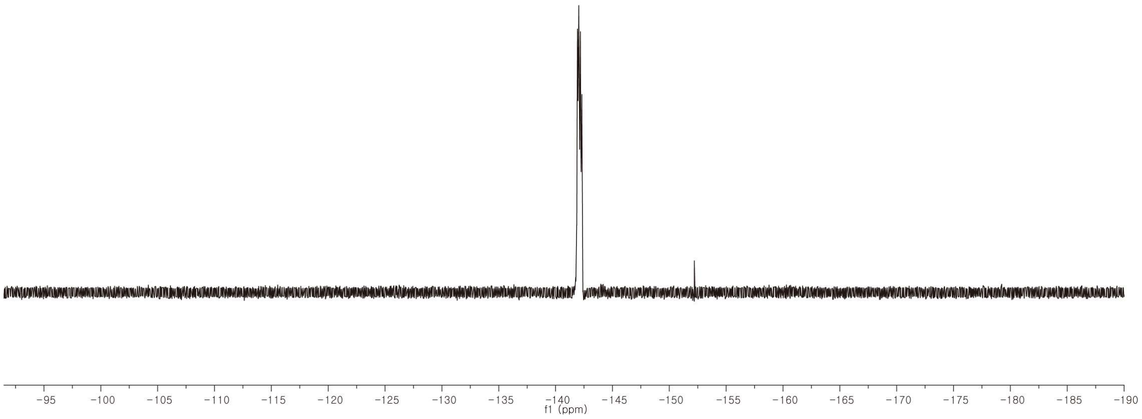


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **11a** in Acetone-d_6

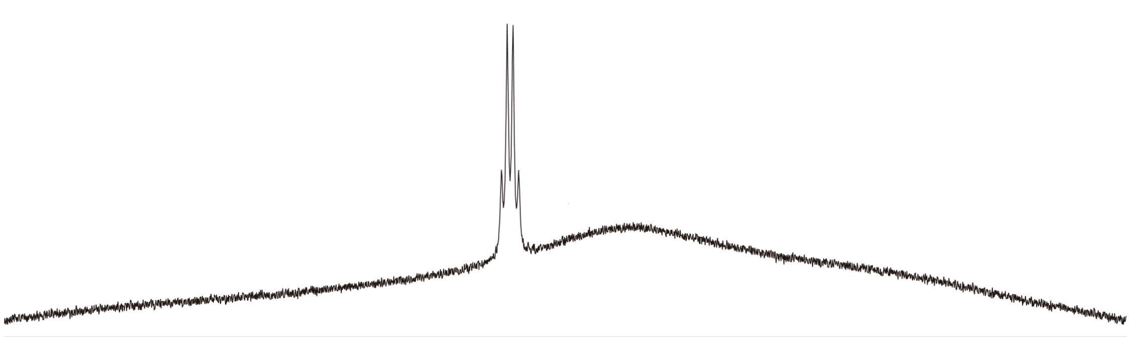
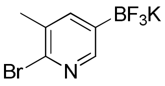


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **11a** in Acetone-d_6



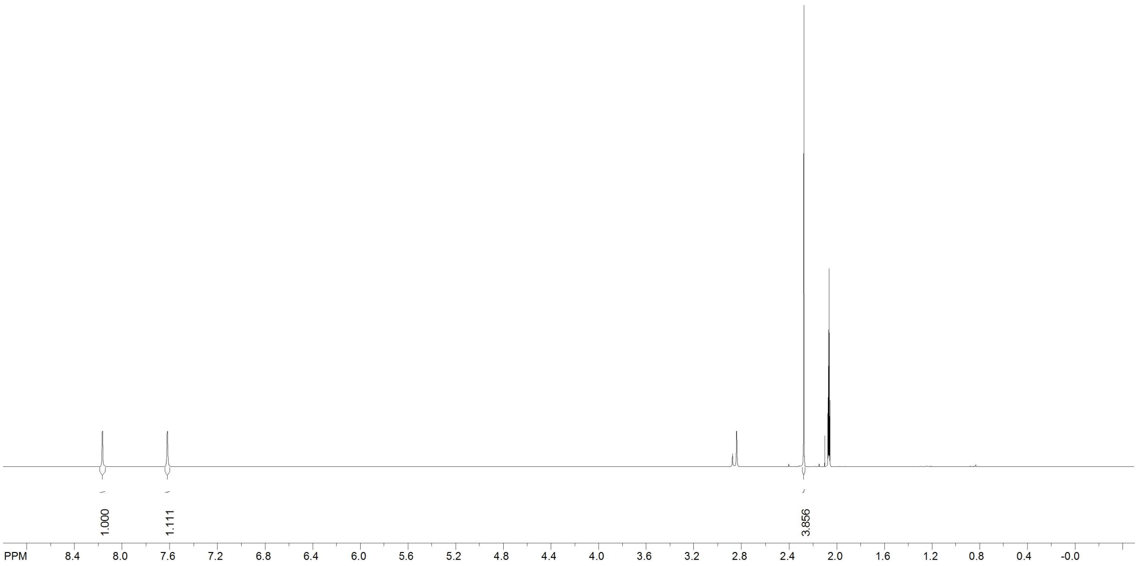


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **12a** in Acetone-d_6

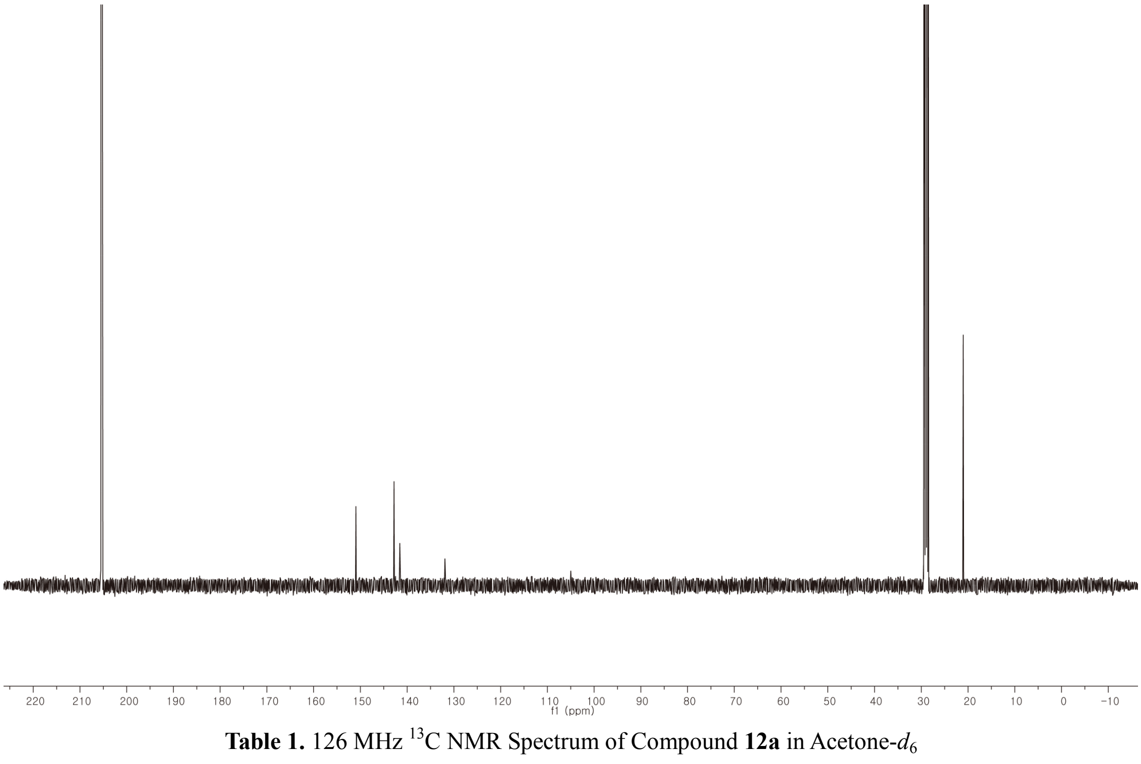
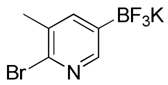


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **12a** in Acetone-d_6



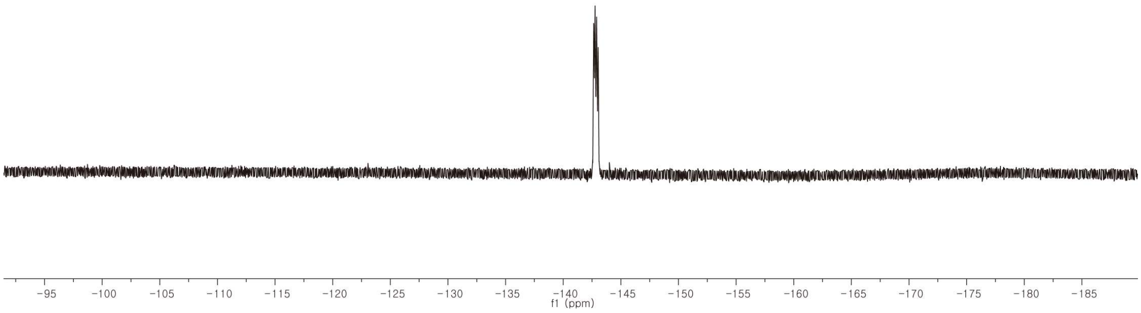


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **12a** in Acetone-d_6

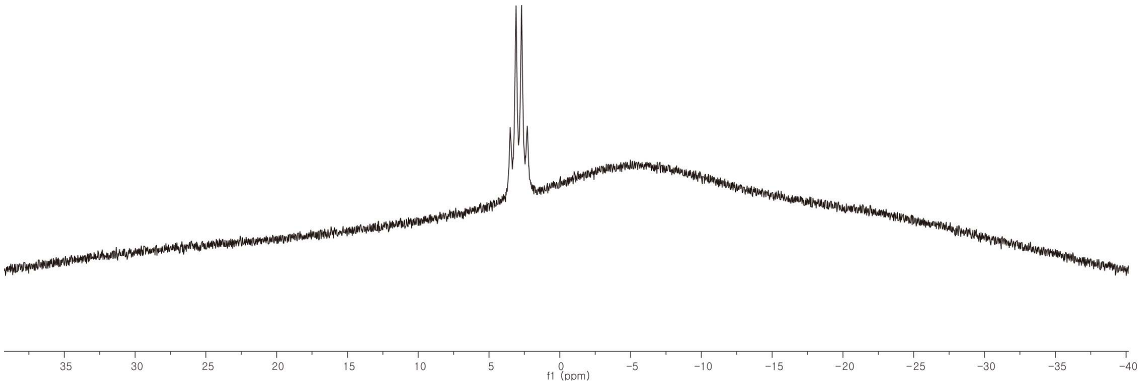
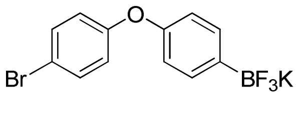


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **12a** in Acetone-d_6



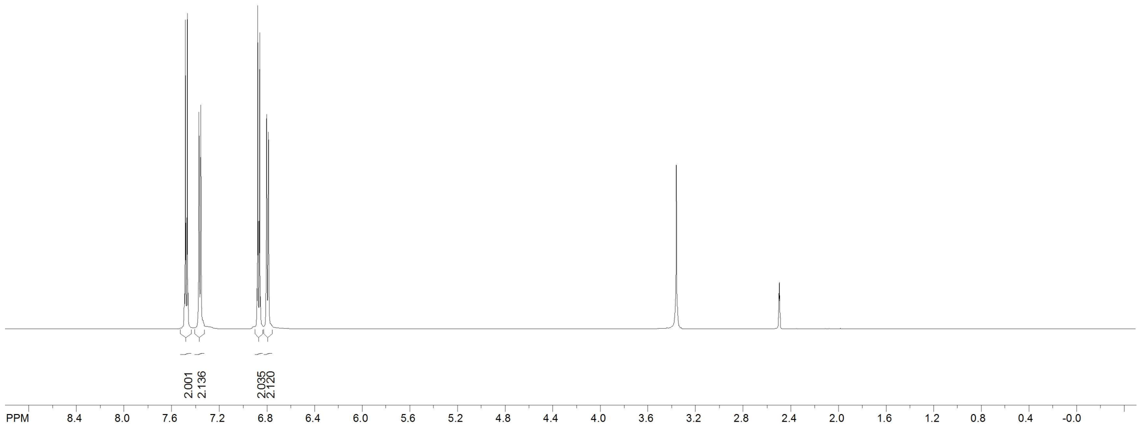


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **13a** in DMSO-d_6

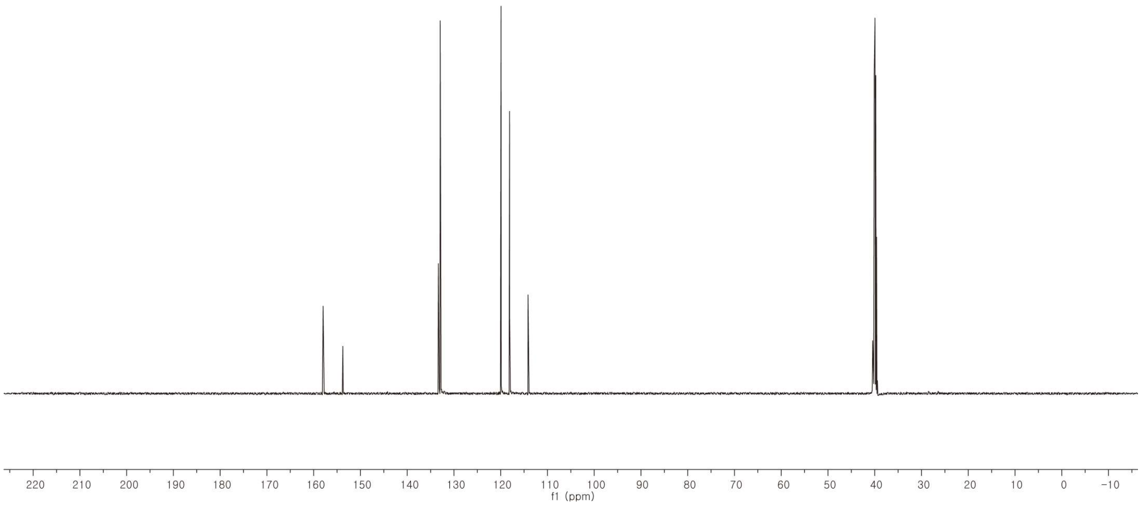
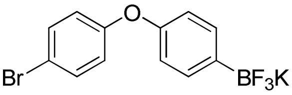


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **13a** in DMSO-d_6



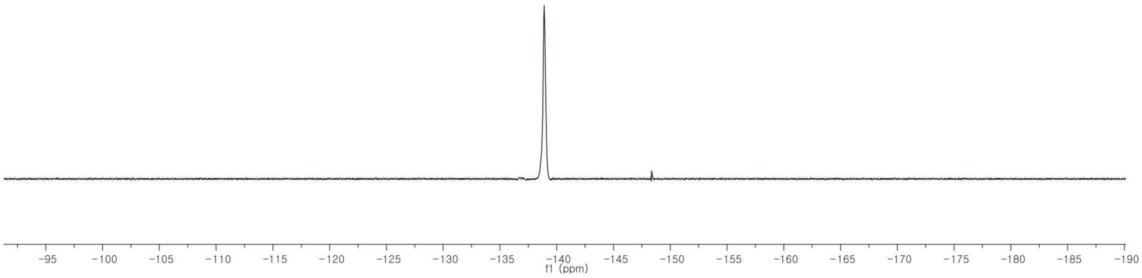


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **13a** in DMSO-d_6

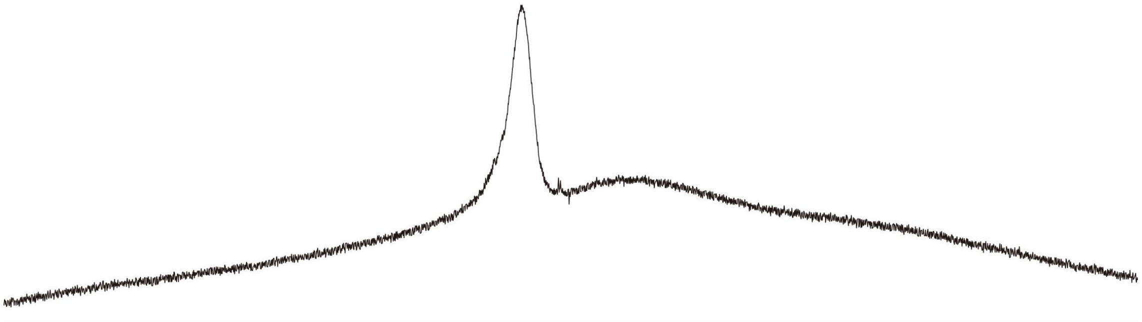
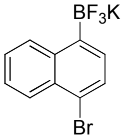


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **13a** in DMSO-d_6



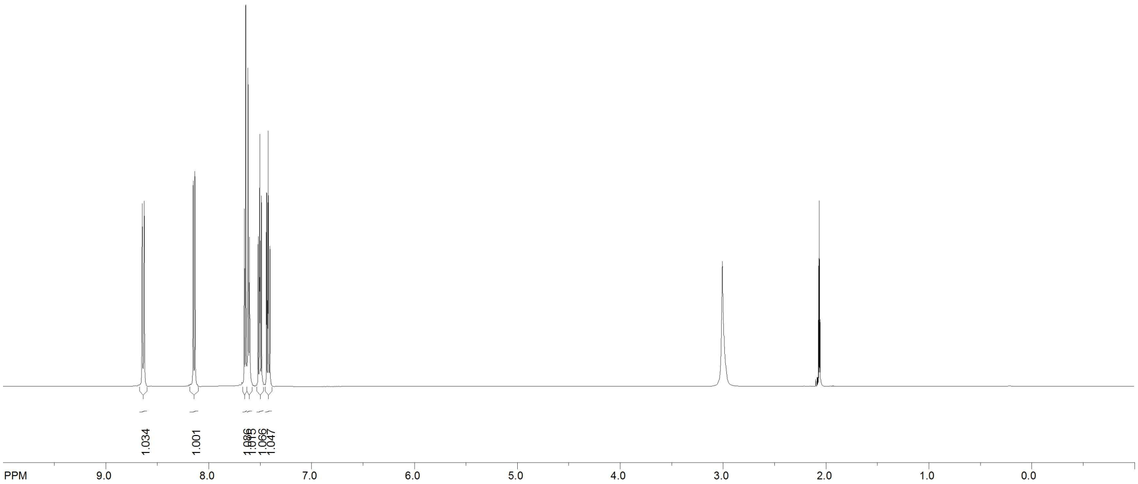


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **14a** in Acetone-d_6

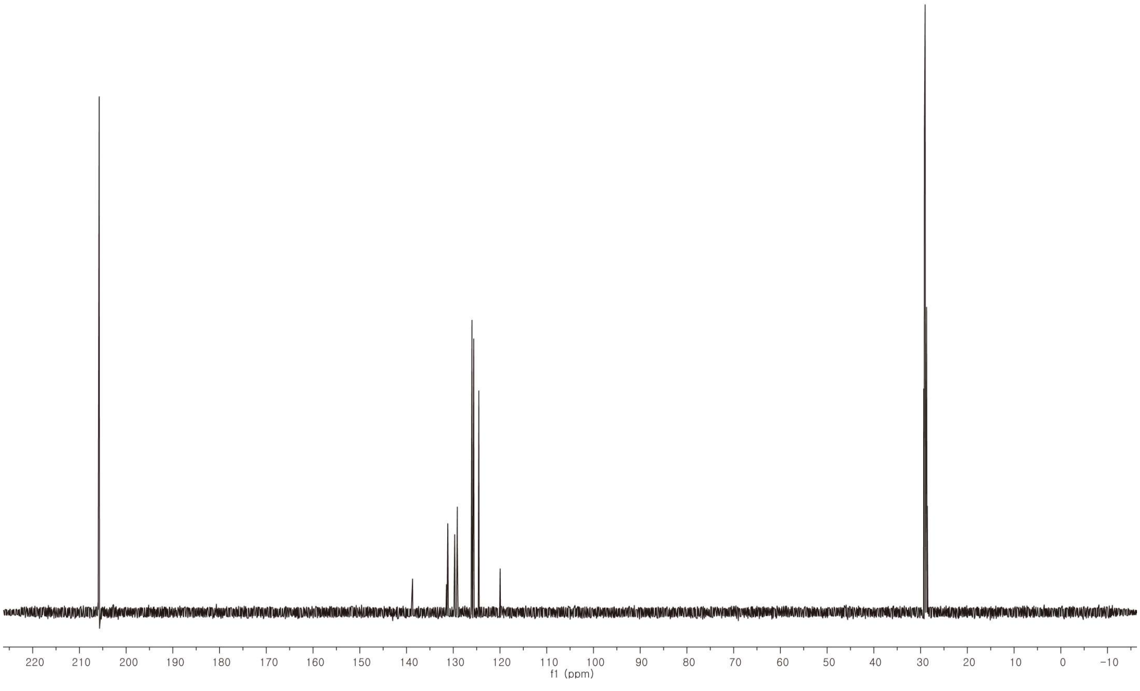
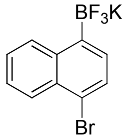


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **14a** in Acetone-d_6



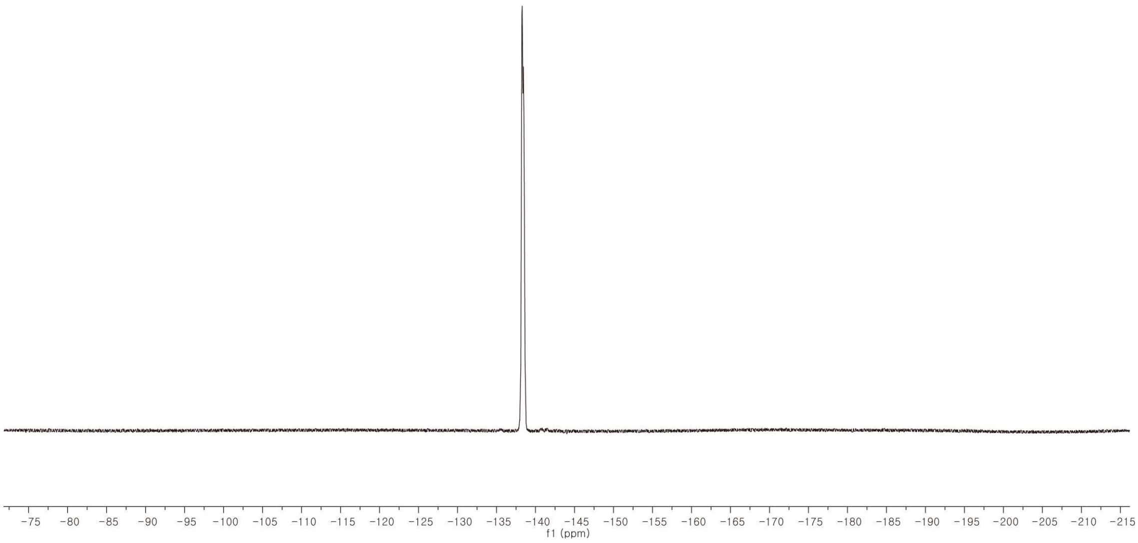


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **14a** in Acetone-d_6

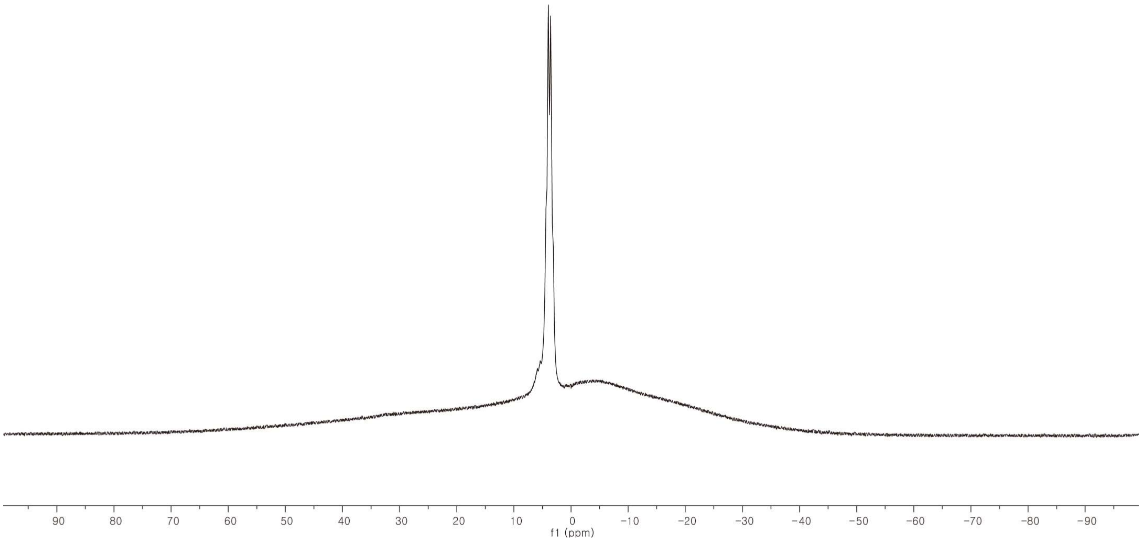
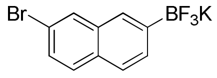


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **14a** in Acetone-d_6



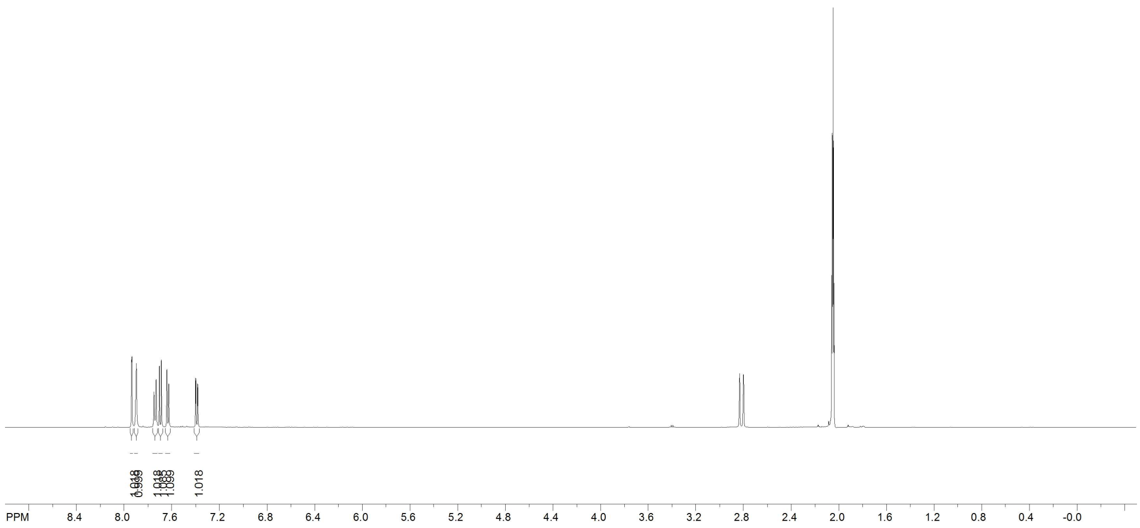


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **15a** in Acetone-d_6

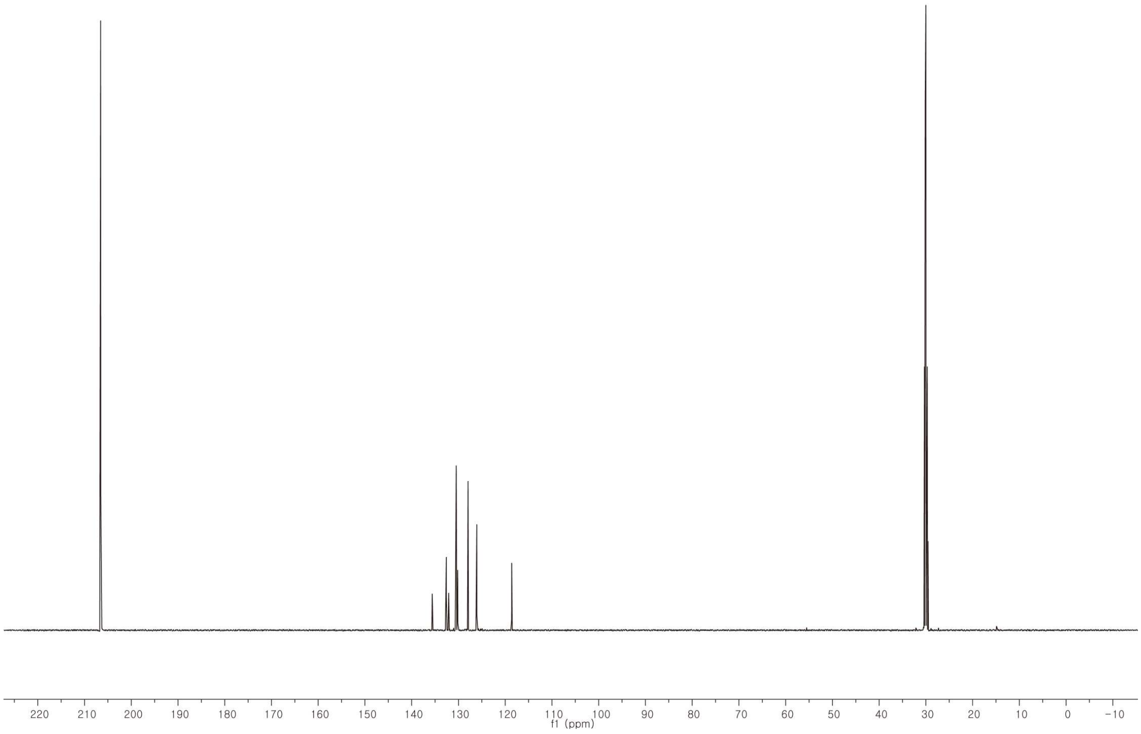
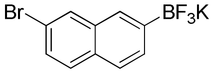


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **15a** in Acetone-d_6



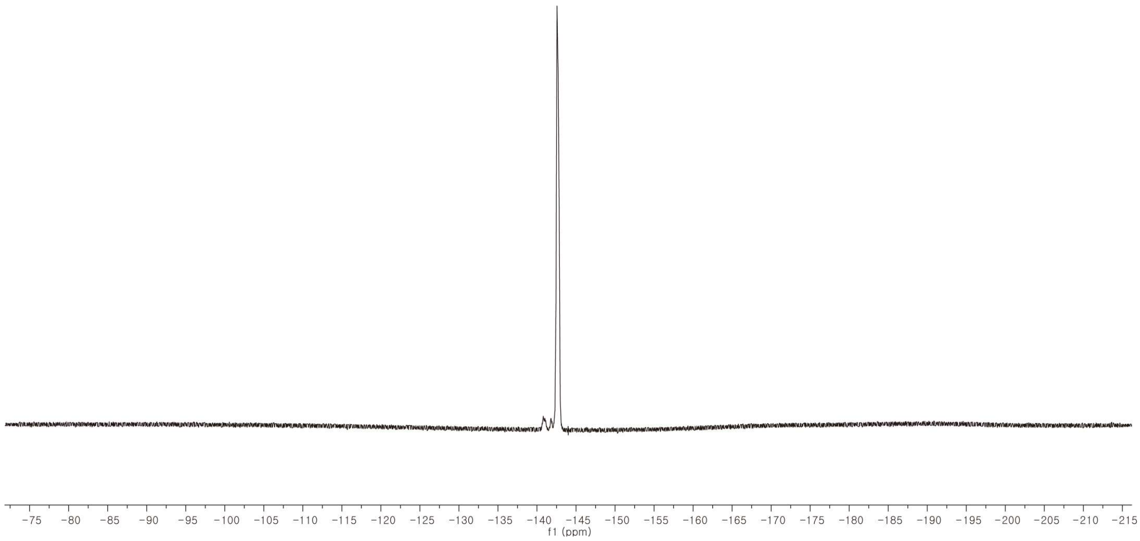


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **15a** in Acetone-d_6

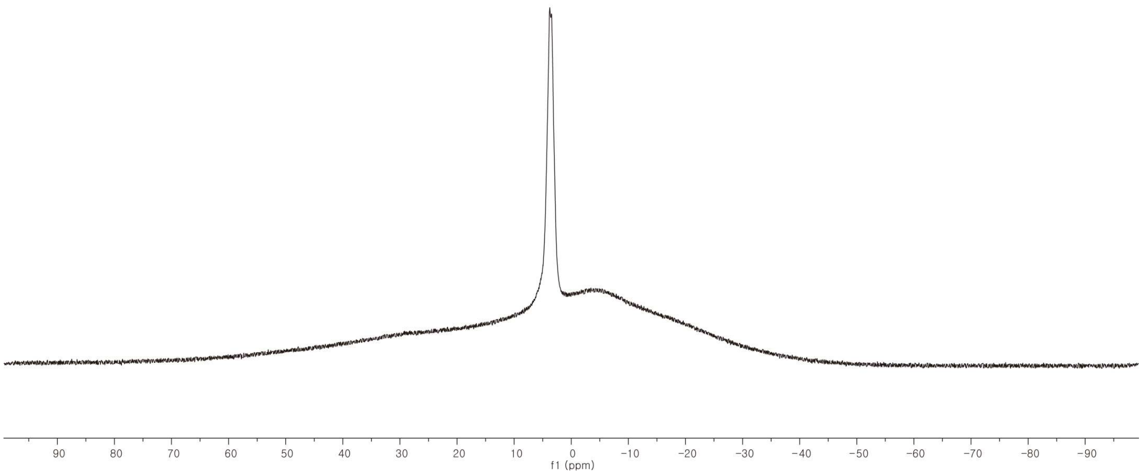
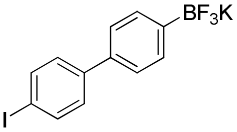


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **15a** in Acetone-d_6



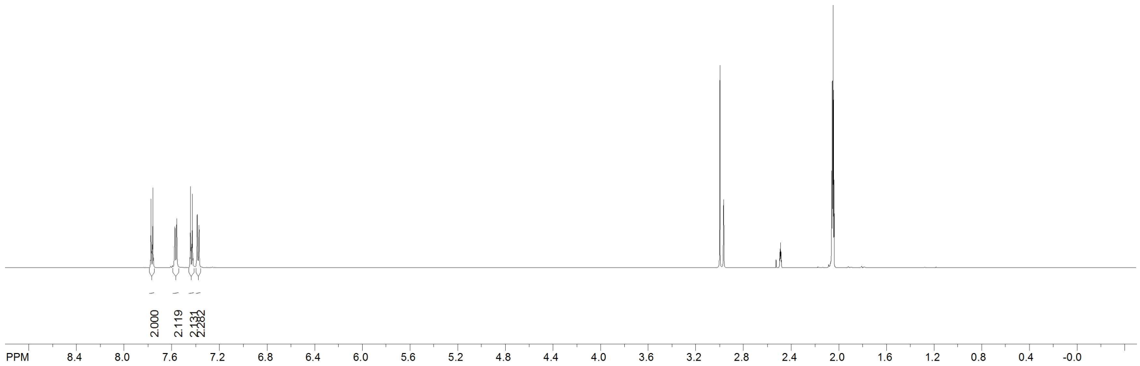


Table 1. 500 MHz ^{1}H NMR Spectrum of Compound **16a** in Acetone-d_6 + DMSO-d_6

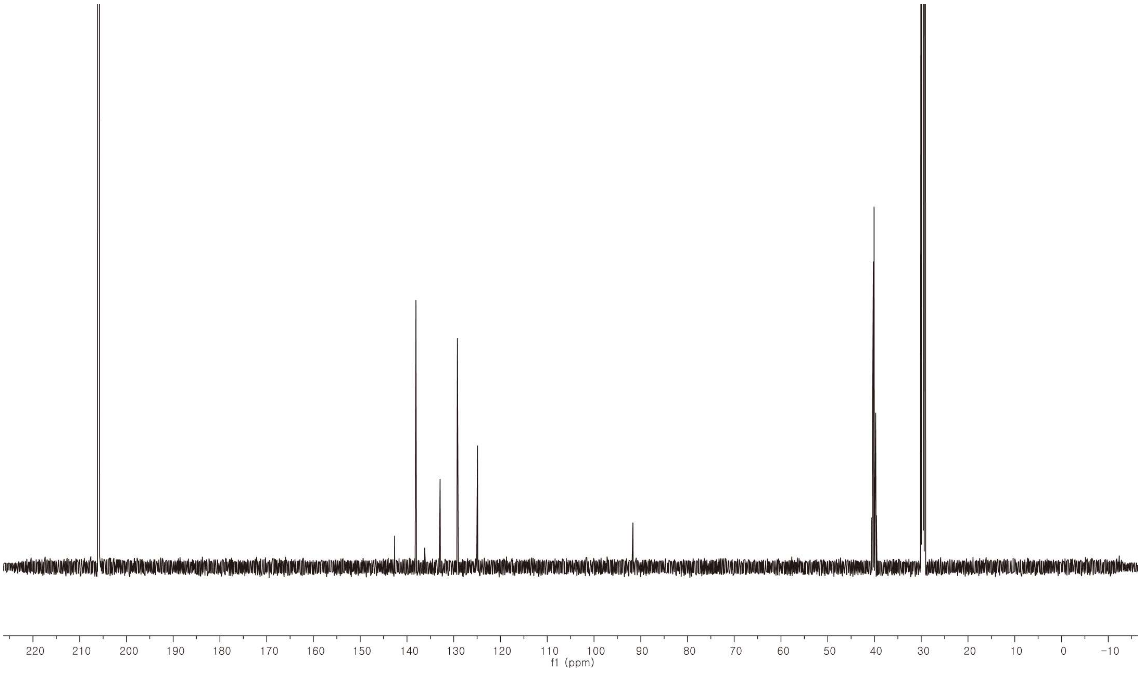
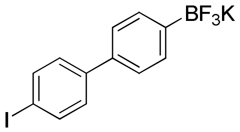


Table 1. 126 MHz ^{13}C NMR Spectrum of Compound **16a** in Acetone-d_6 + DMSO-d_6



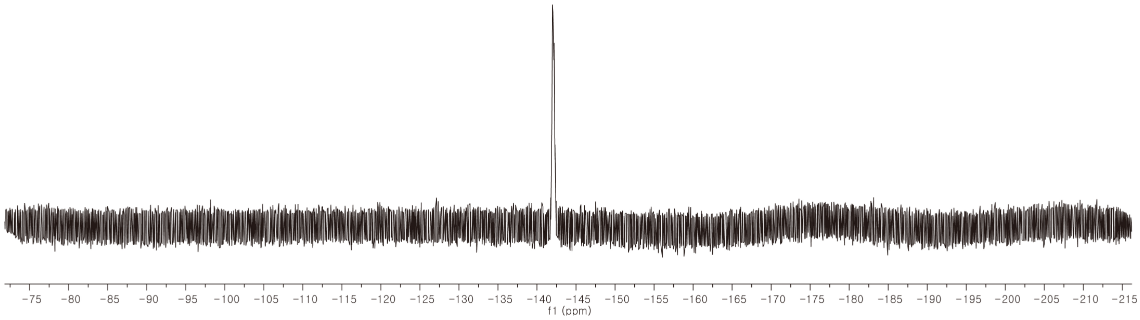


Table 1. 376 MHz ^{19}F NMR Spectrum of Compound **16a** in Acetone-d_6 + DMSO-d_6

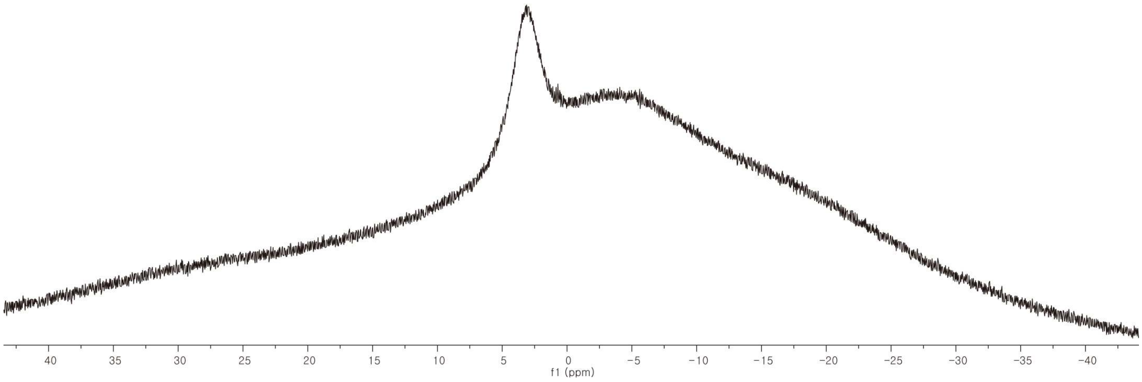
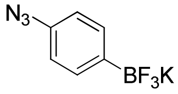


Table 1. 128 MHz ^{11}B NMR Spectrum of Compound **16a** in DMSO-d_6



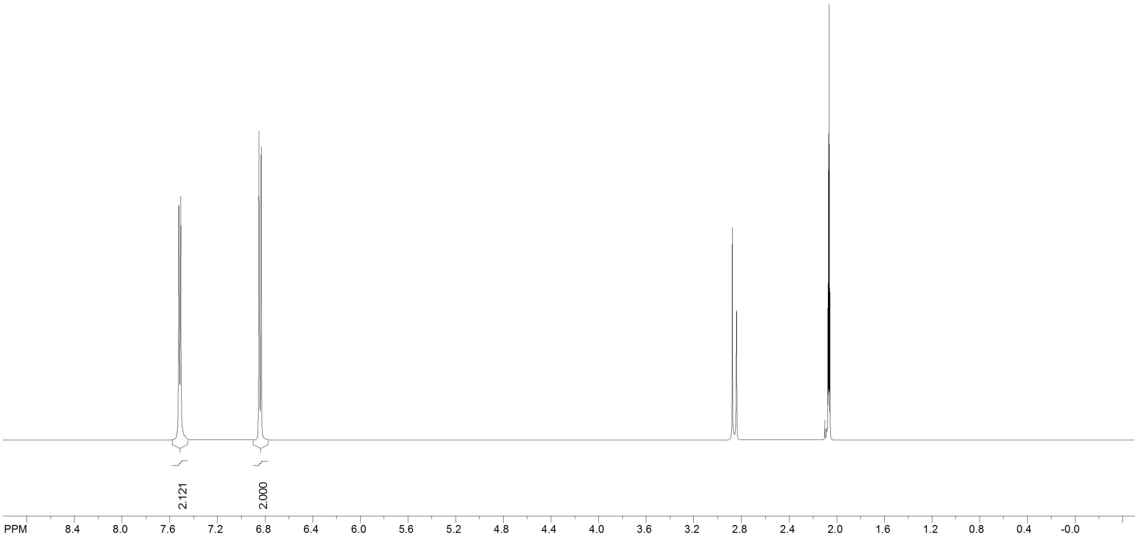


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **1b** in Acetone-d_6

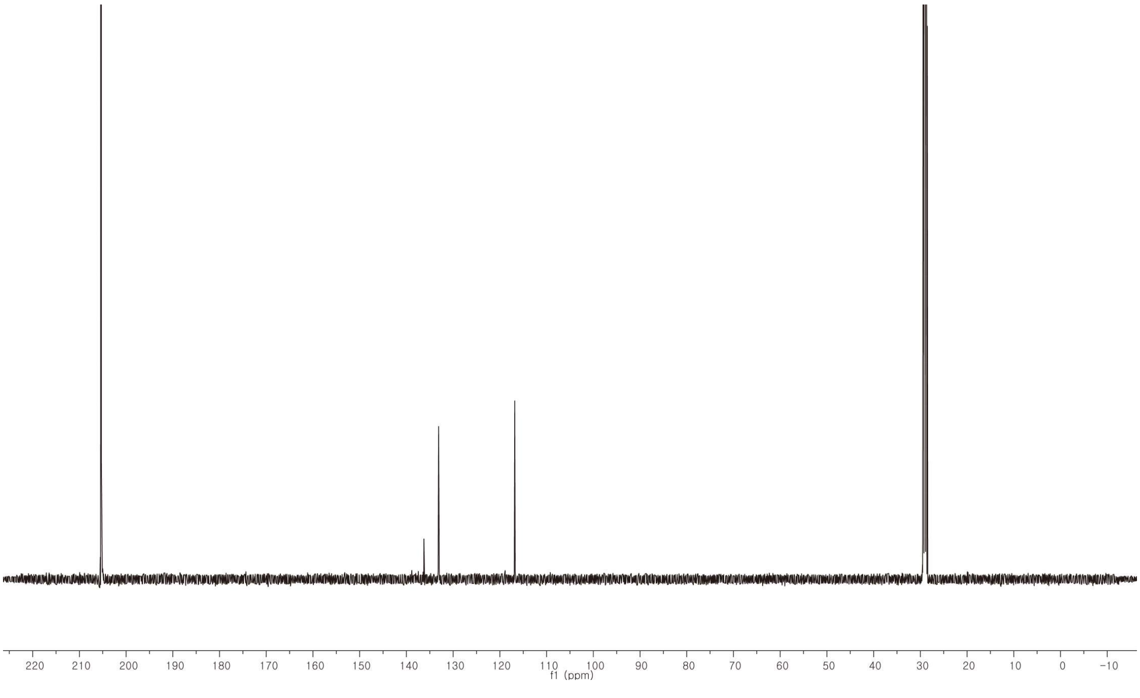
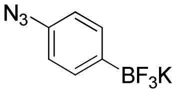


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **1b** in Acetone-d_6



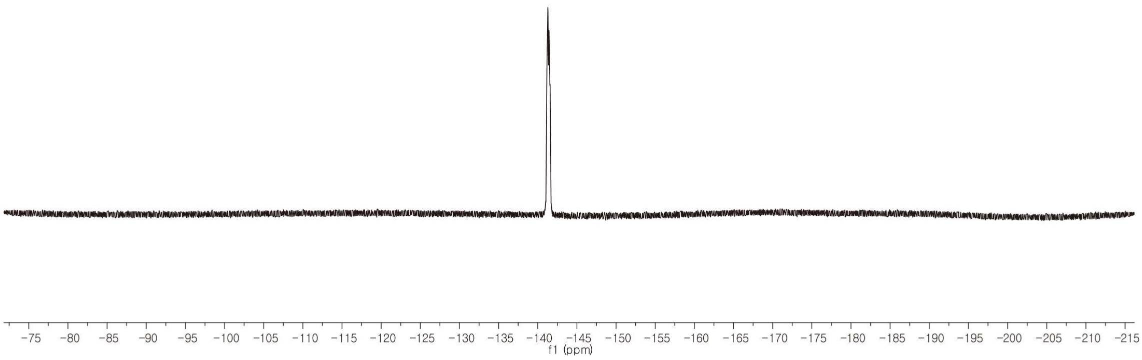


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **1b** in Acetone-d_6

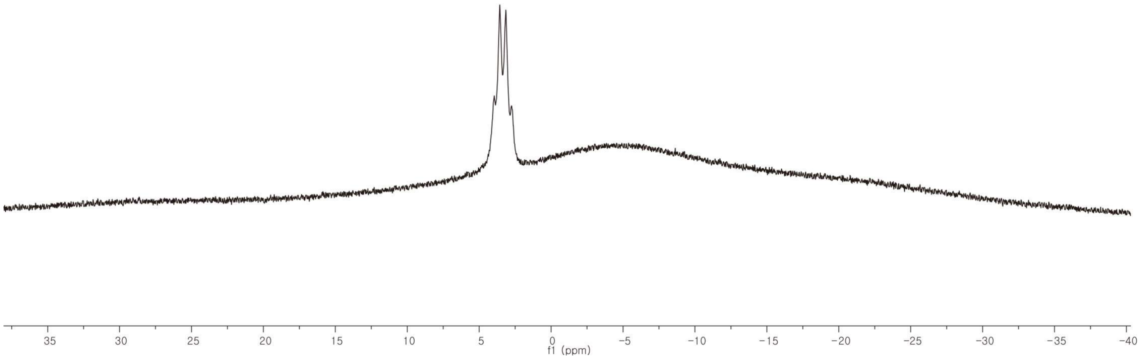
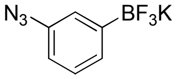


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **1b** in Acetone-d_6



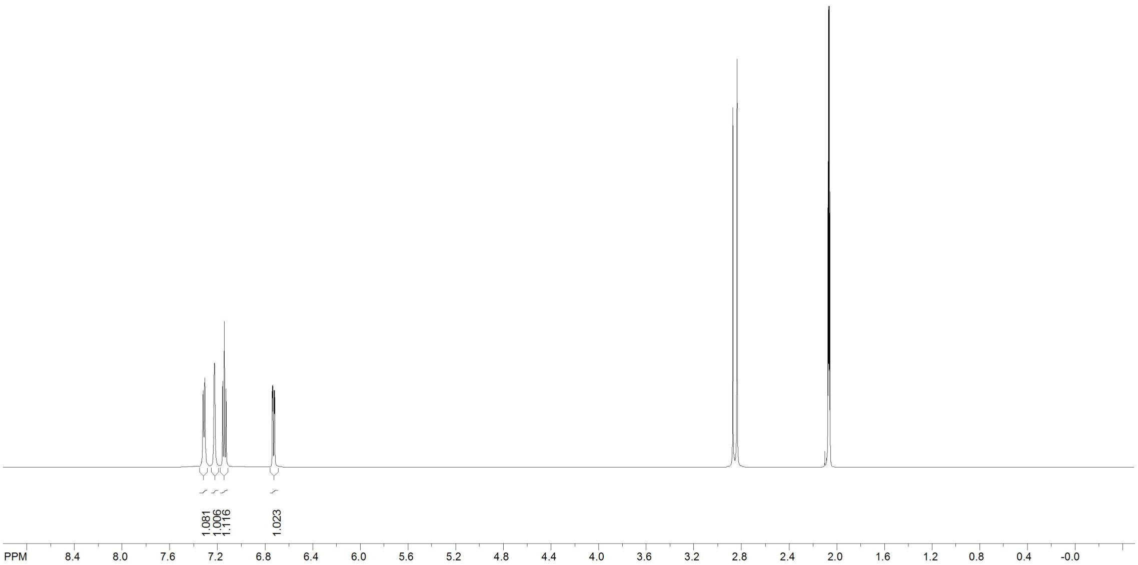


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **2b** in Acetone-d_6

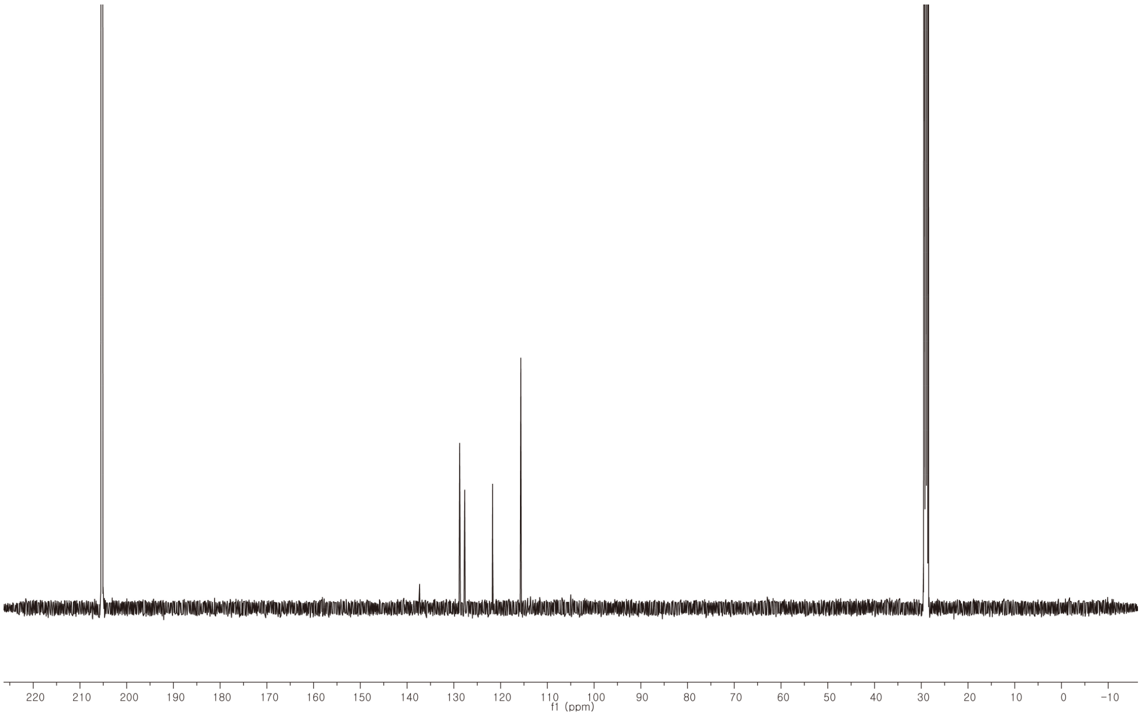
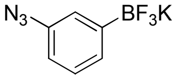


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **2b** in Acetone-d_6



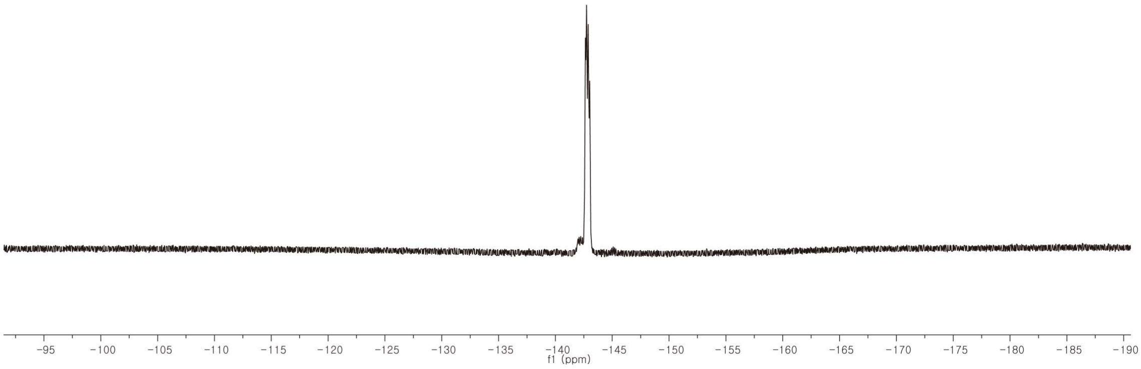


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **2b** in Acetone-d_6

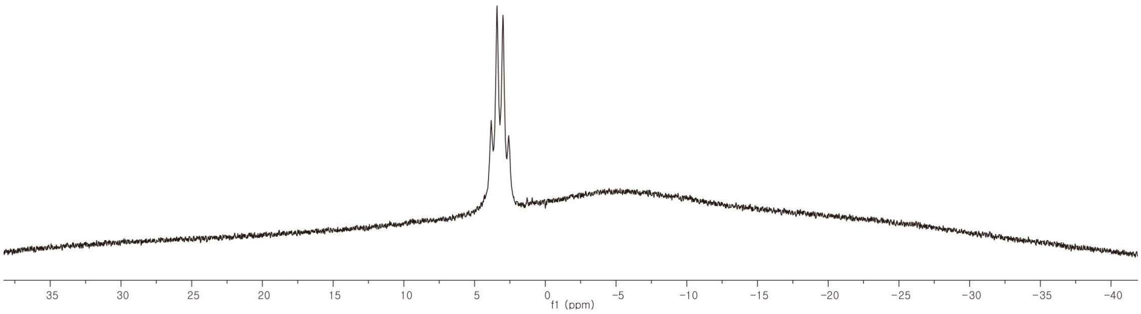
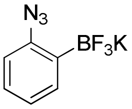


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **2b** in Acetone-d_6



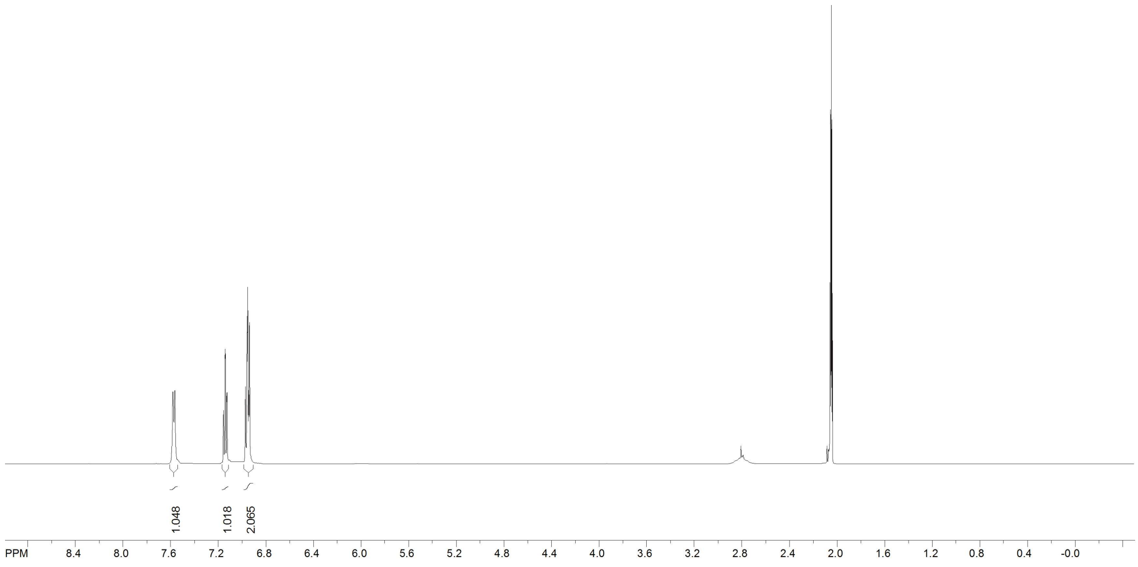


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **3b** in Acetone-d_6

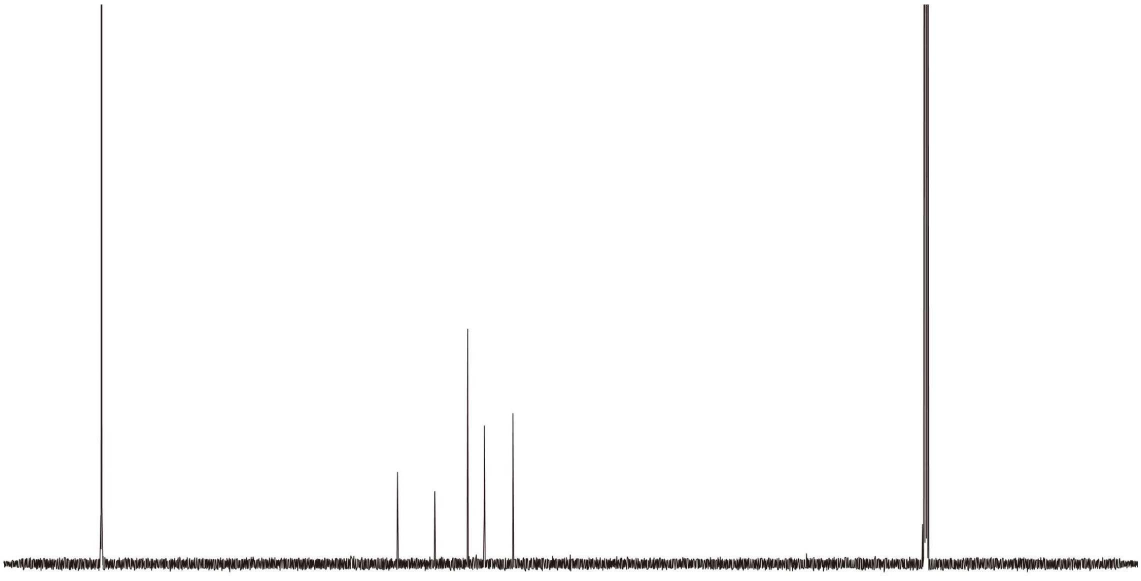
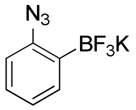


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **3b** in Acetone-d_6



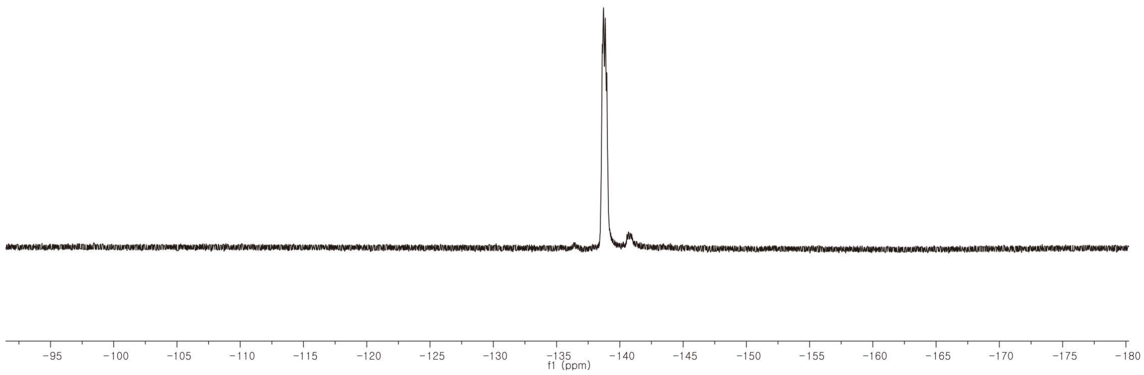


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **3b** in Acetone-d_6

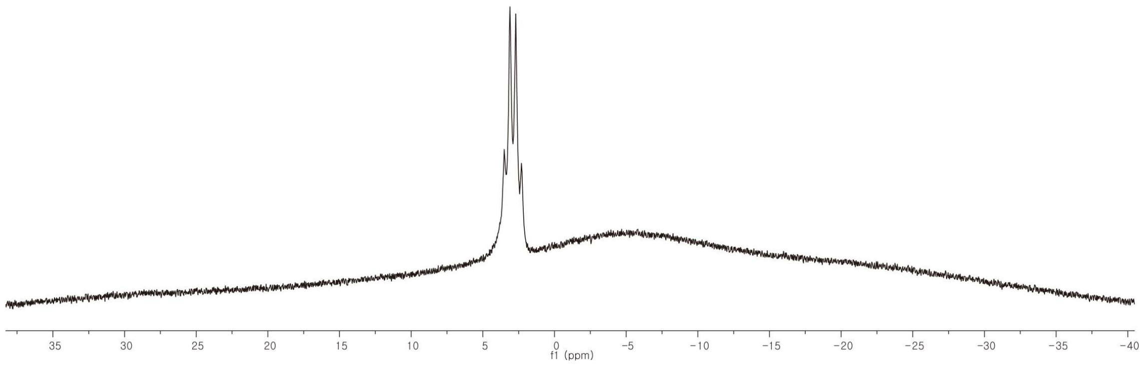
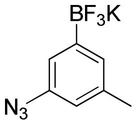


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **3b** in Acetone-d_6



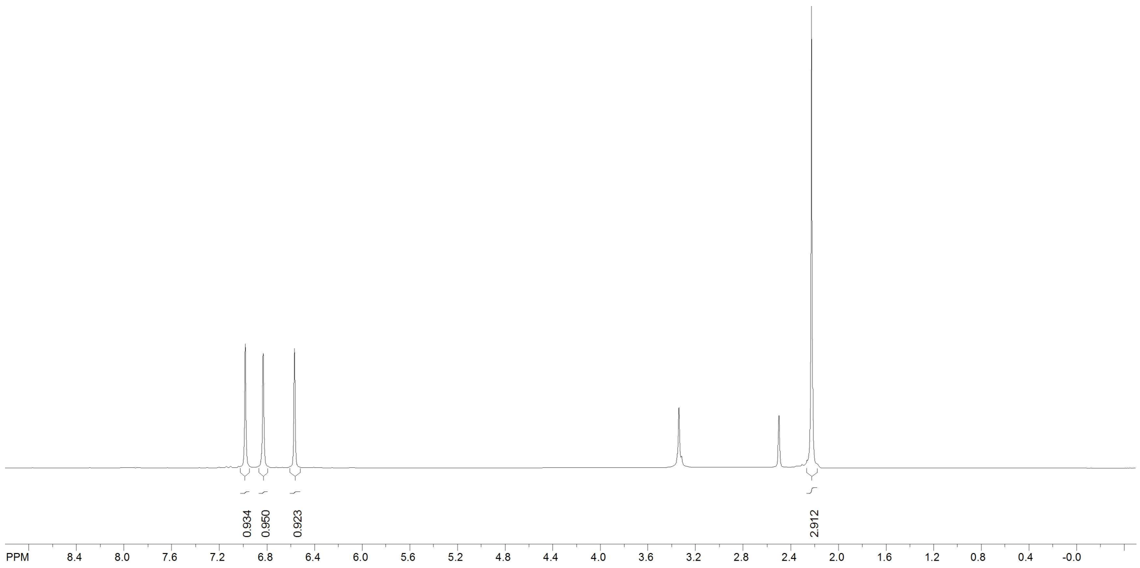


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **4b** in DMSO-d_6

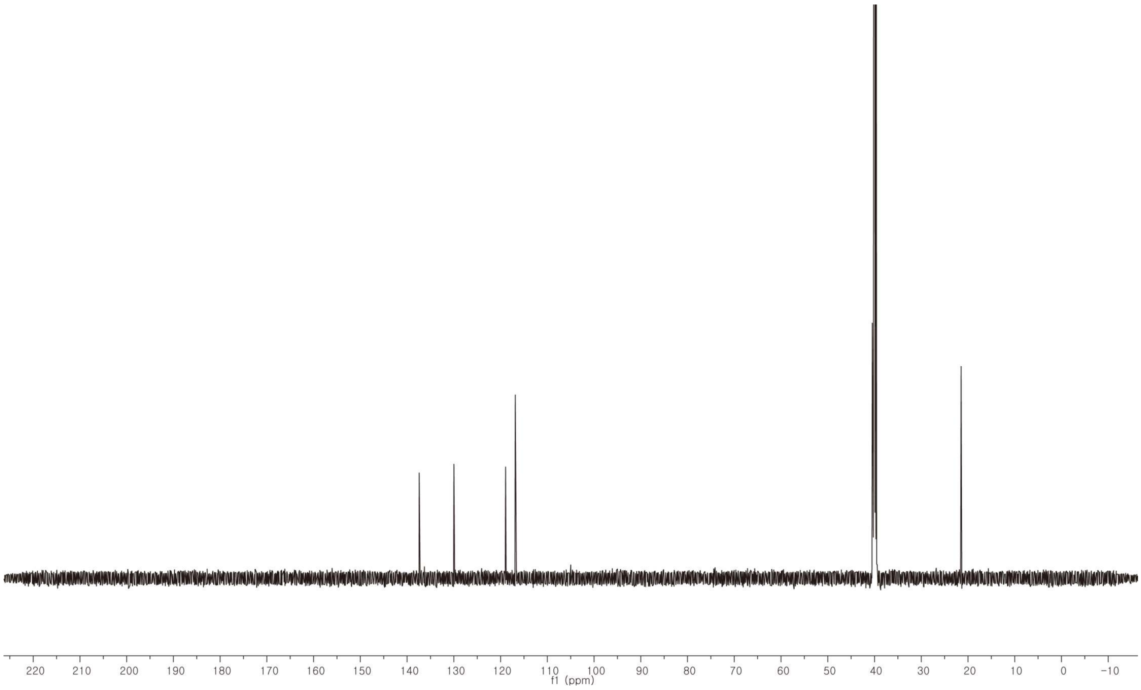
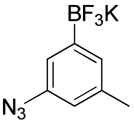


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **4b** in DMSO-d_6



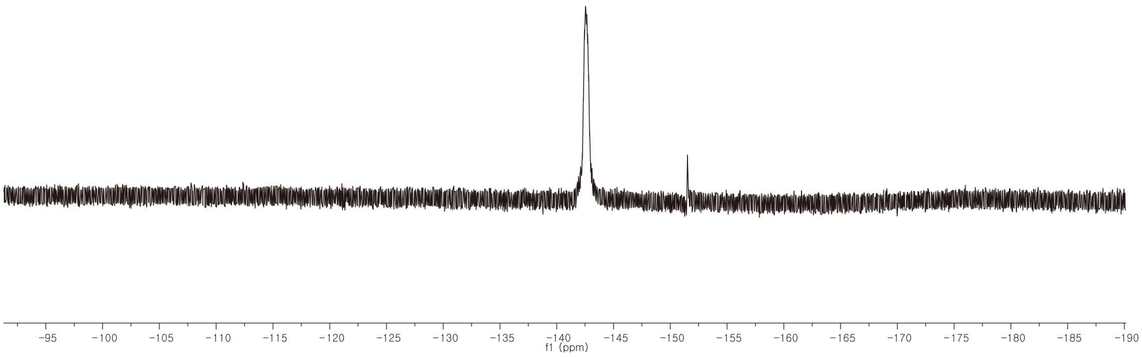


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **4b** in Acetone-d_6

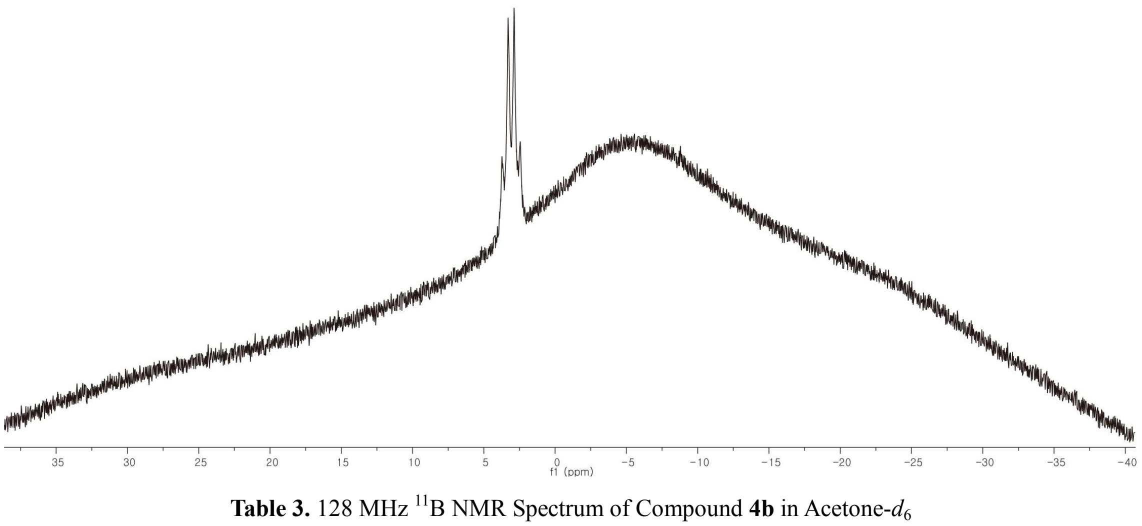
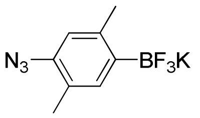


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **4b** in Acetone-d_6



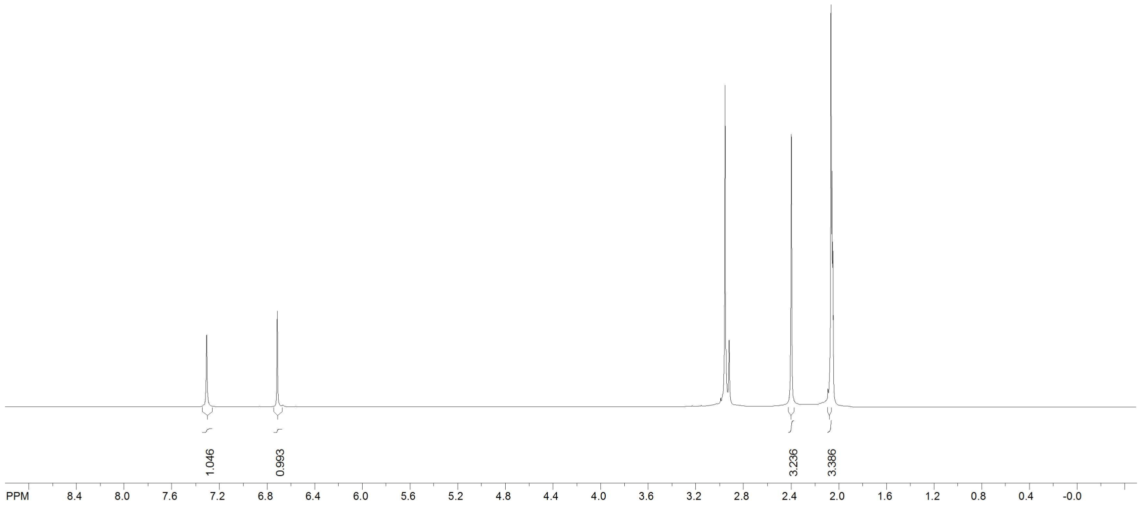


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **5b** in Acetone-d_6

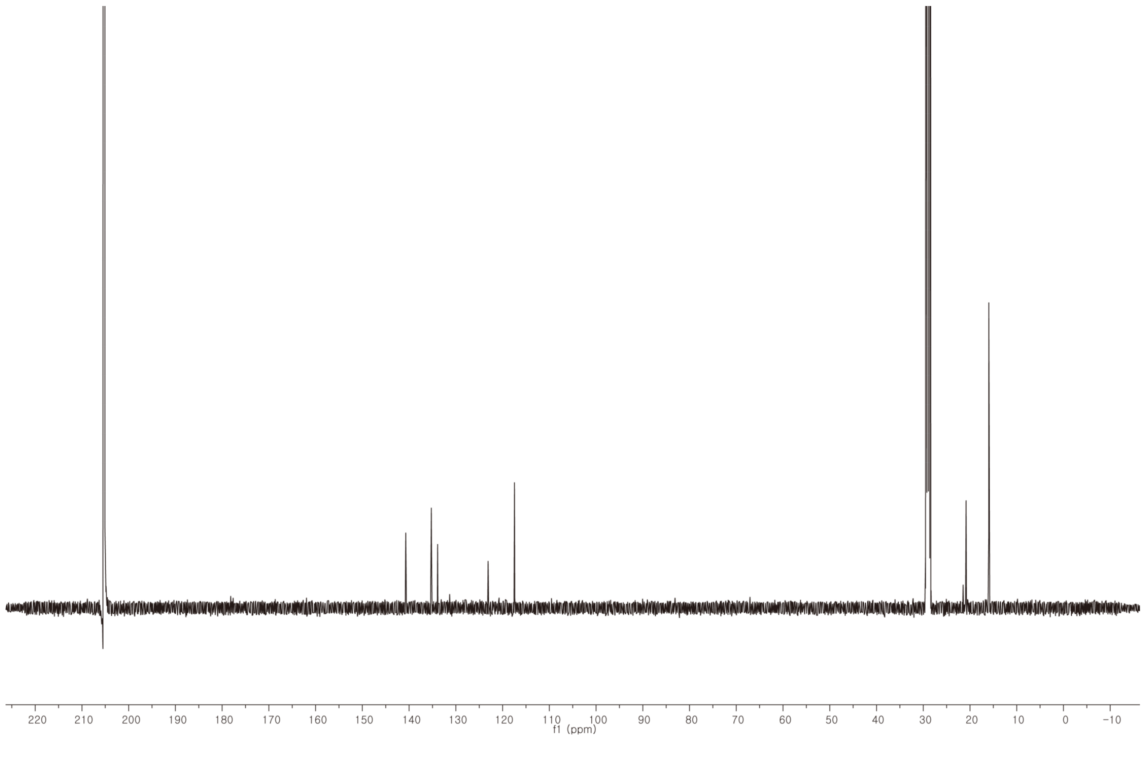
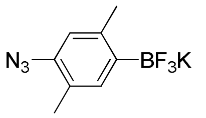


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **5b** in Acetone-d_6



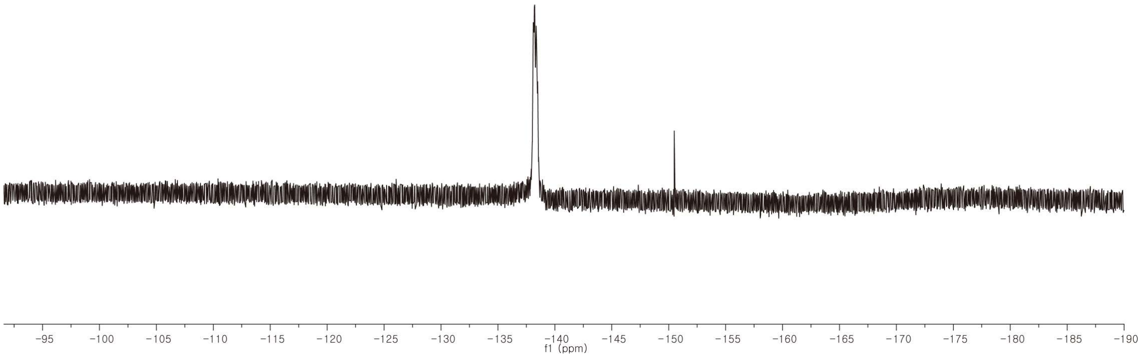


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **5b** in Acetone-d_6

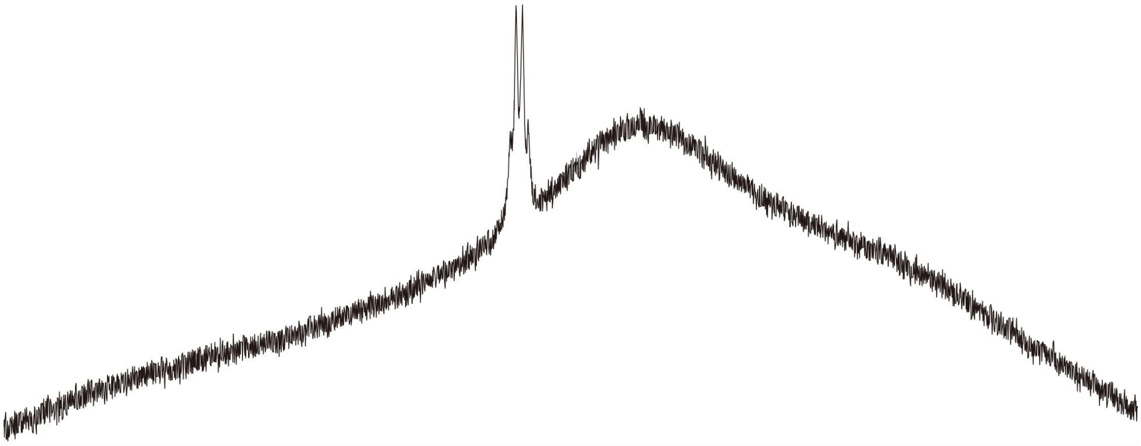
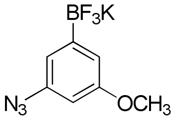


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **5b** in Acetone-d_6



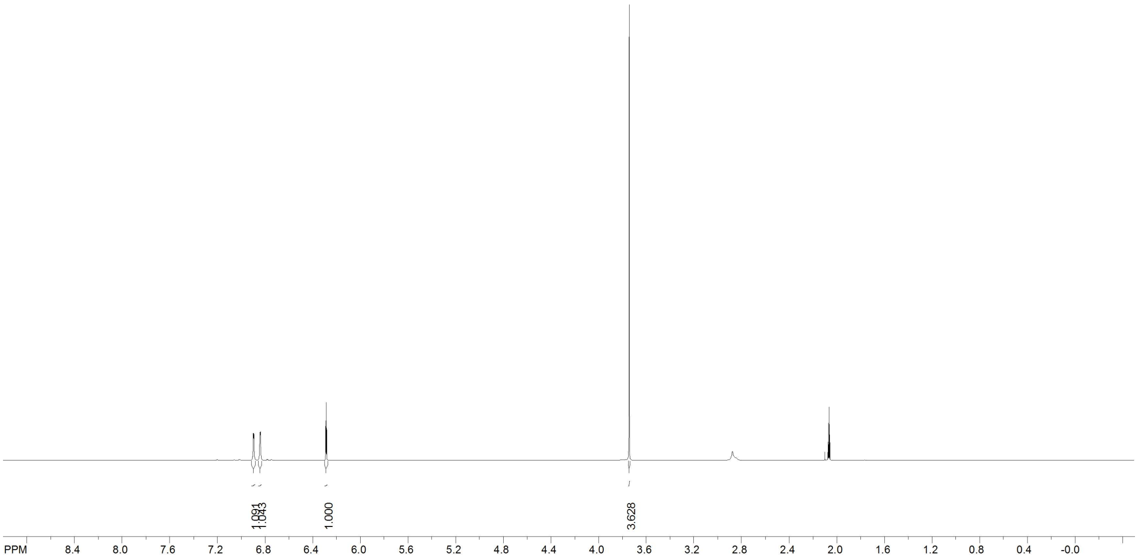


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **6b** in Acetone-d_6

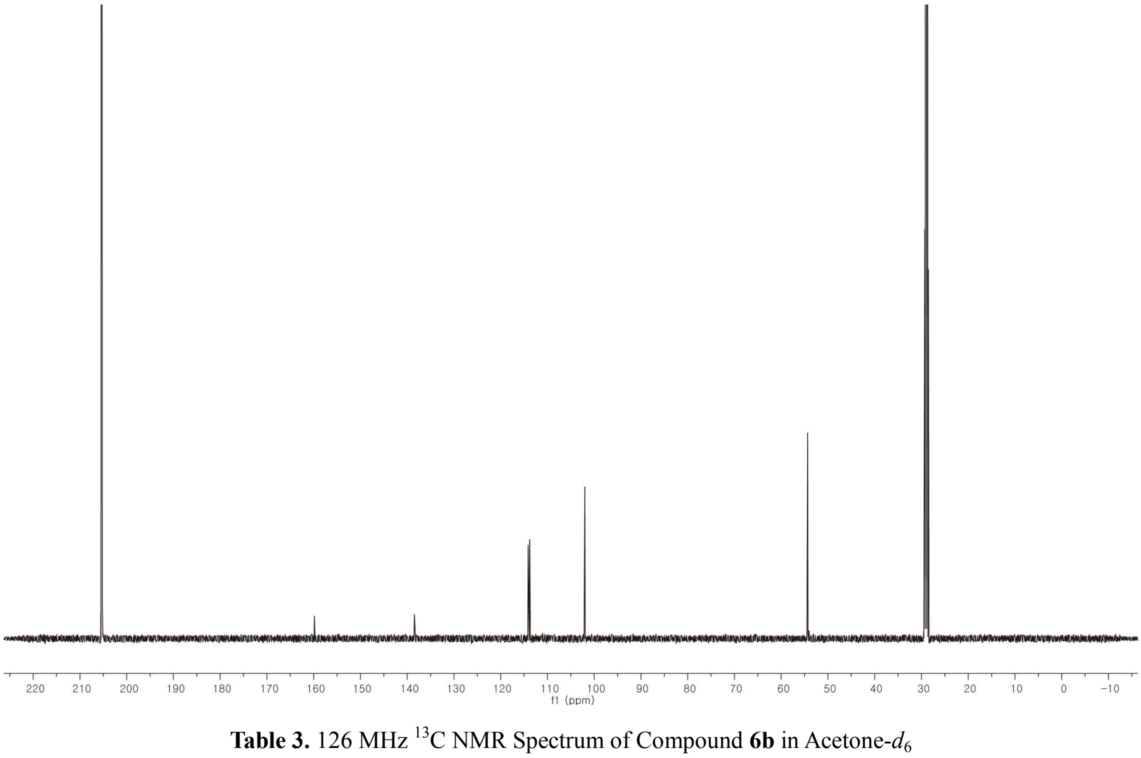
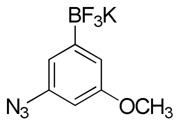


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **6b** in Acetone-d_6



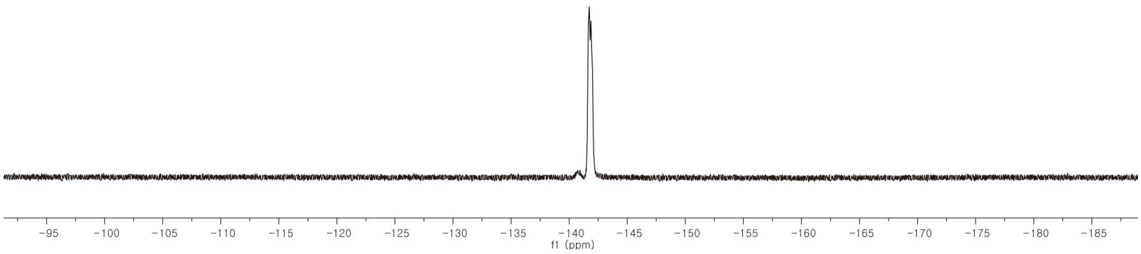


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **6b** in Acetone-d_6

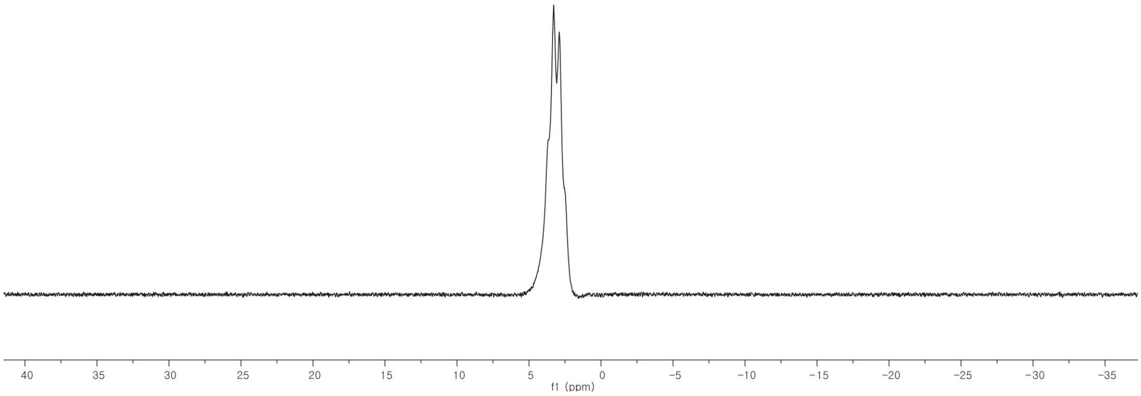
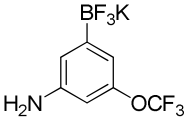


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **6b** in Acetone-d_6



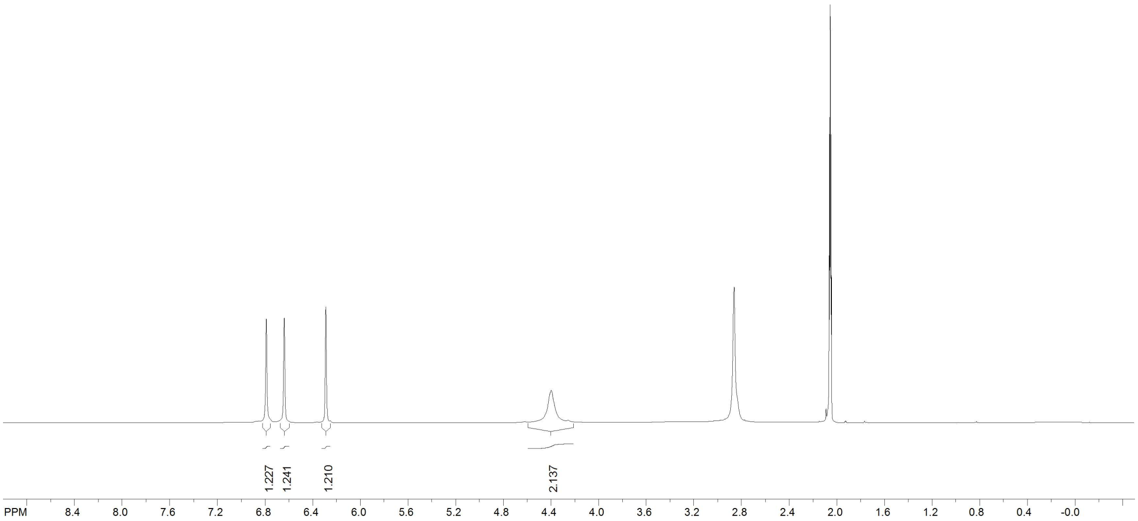


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **7b** in Acetone-d_6

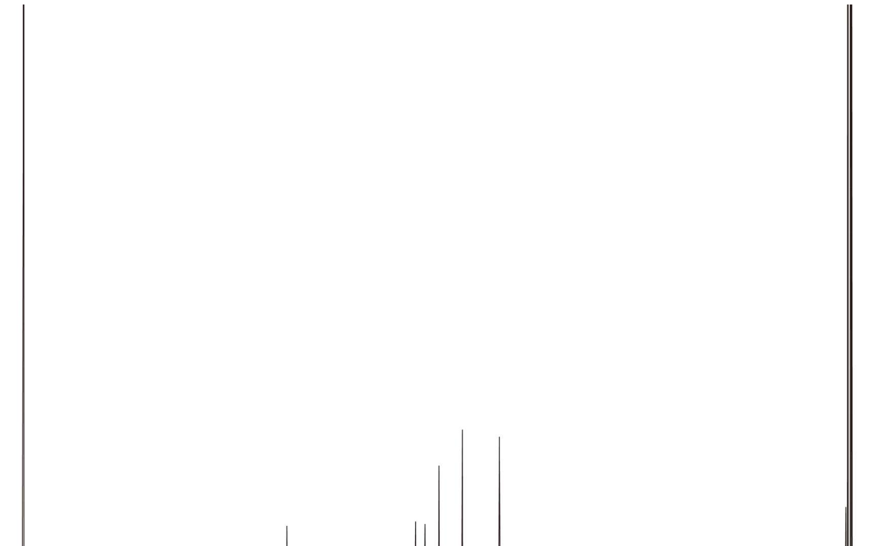


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **7b** in Acetone-d_6

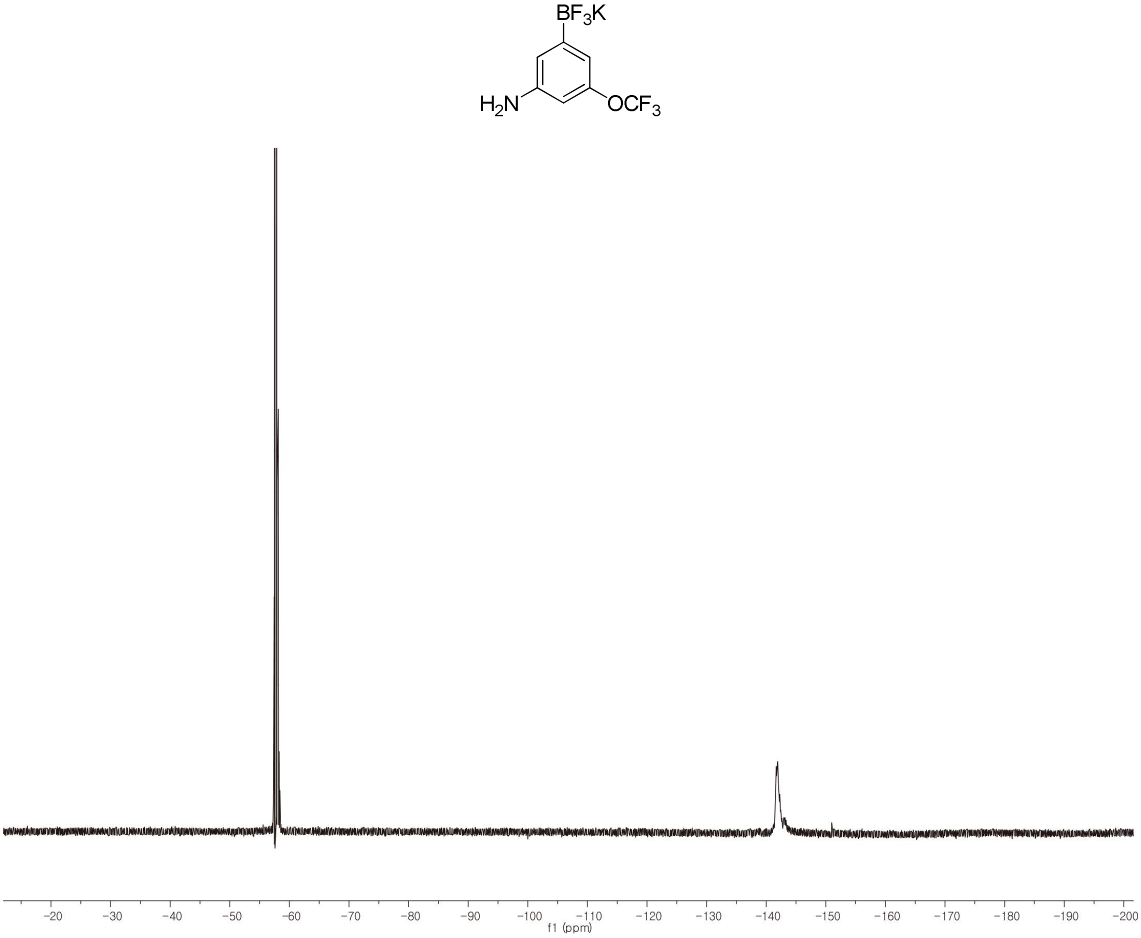


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **7b** in Acetone-d_6

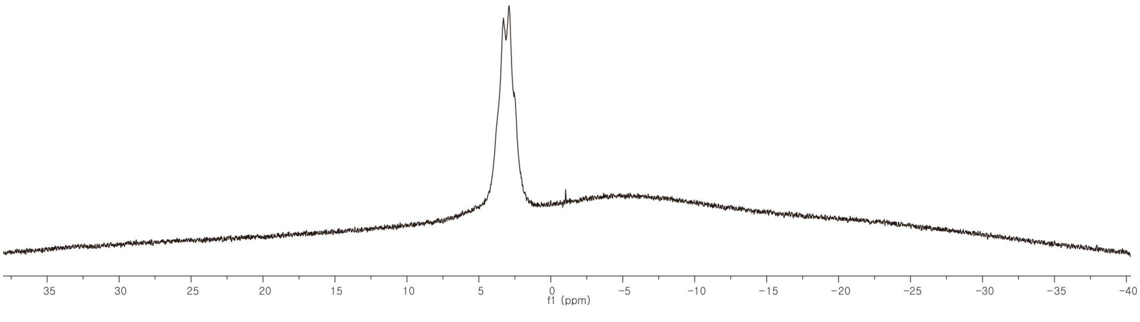
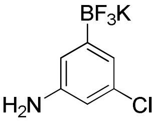


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **7b** in Acetone-d_6



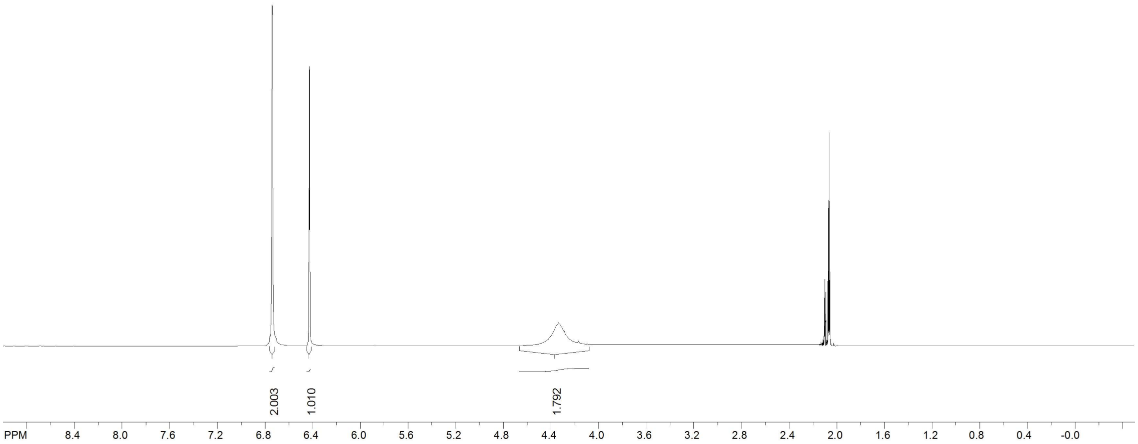


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **8b** in Acetone-d_6

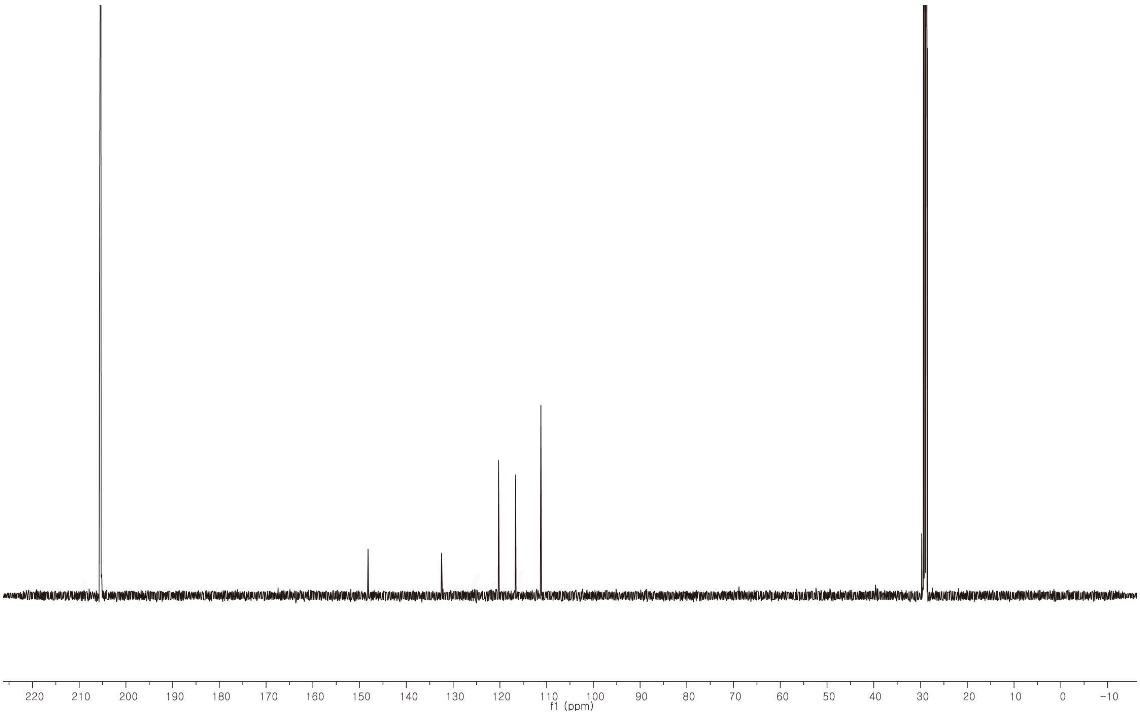
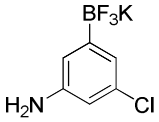


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **8b** in Acetone-d_6



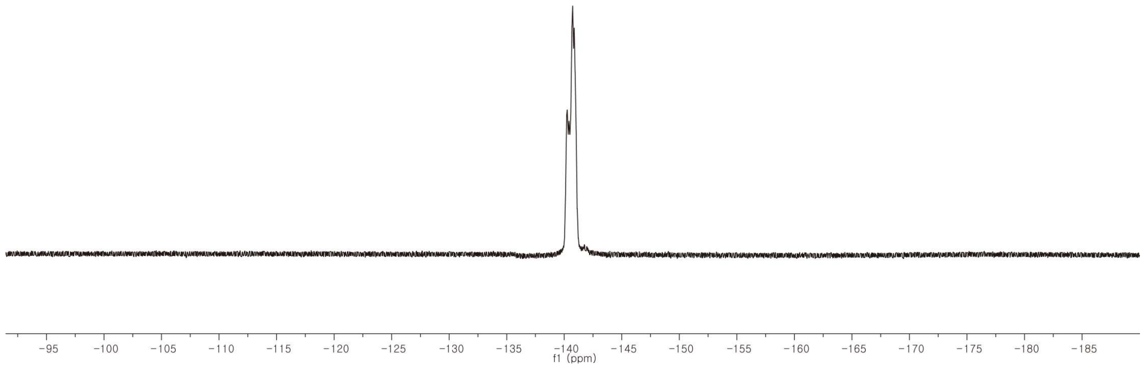


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **8b** in Acetone-d_6

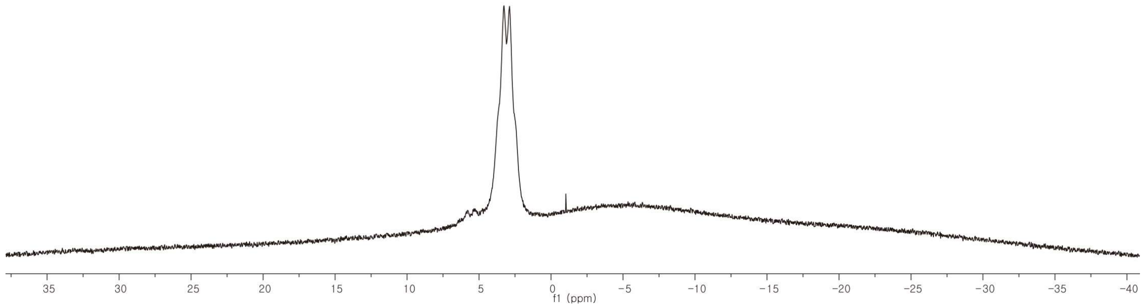
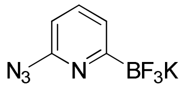


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **8b** in Acetone-d_6



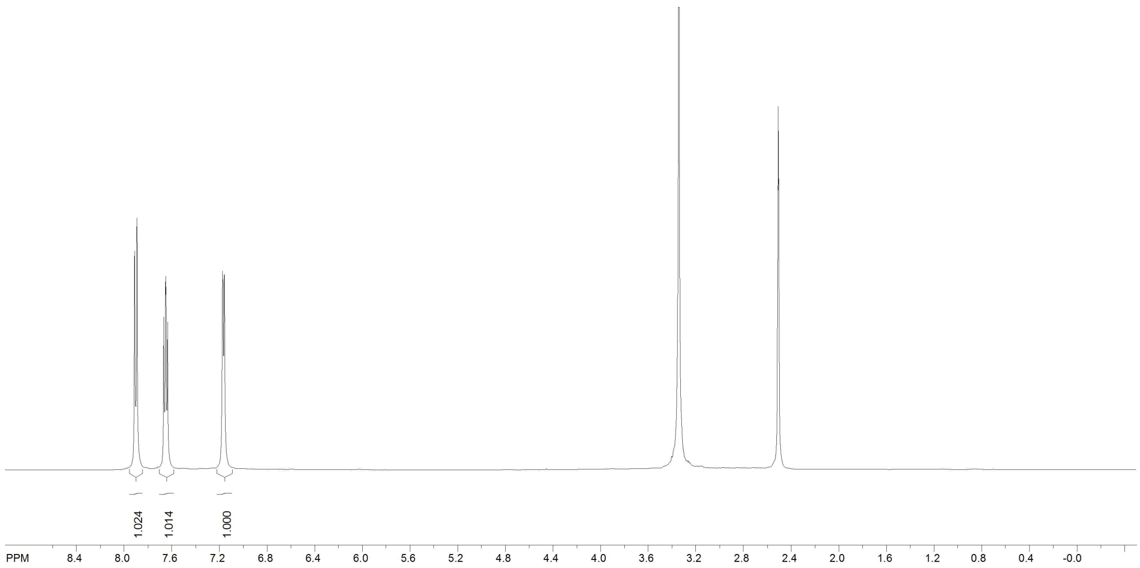


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **9b** in DMSO-d_6

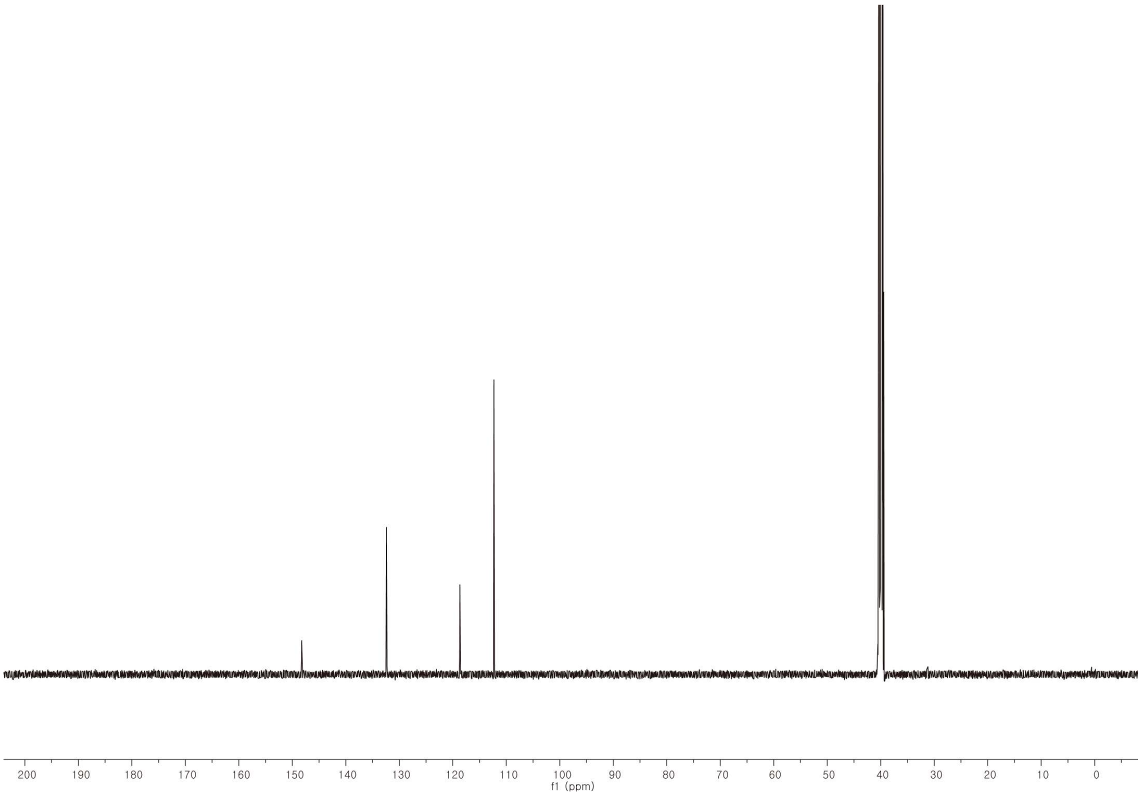
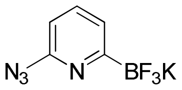


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **9b** in DMSO-d_6



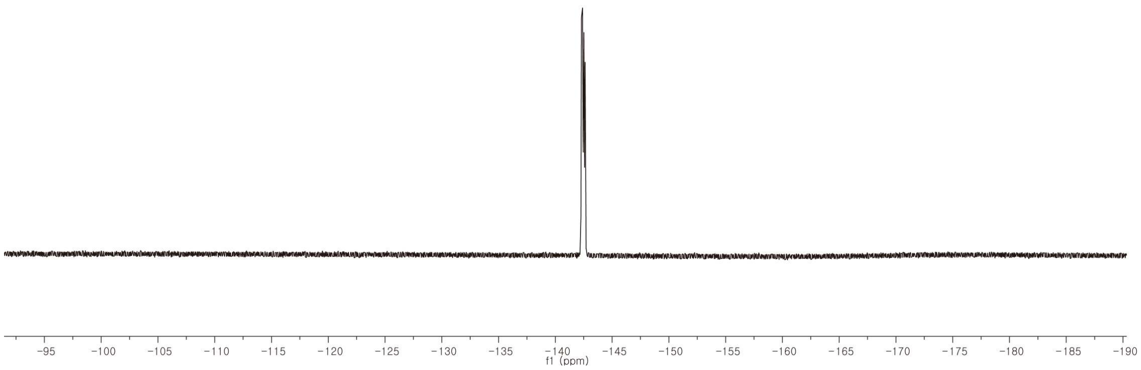


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **9b** in DMSO-d_6

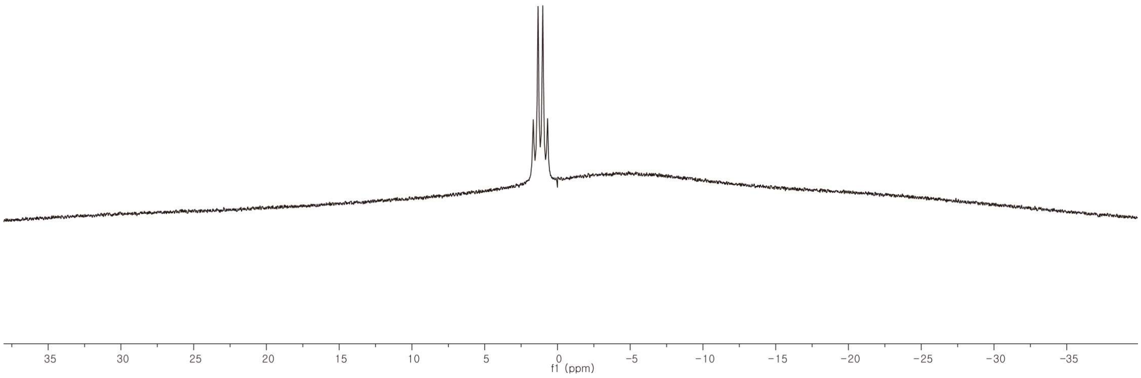
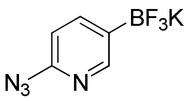


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **9b** in DMSO-d_6



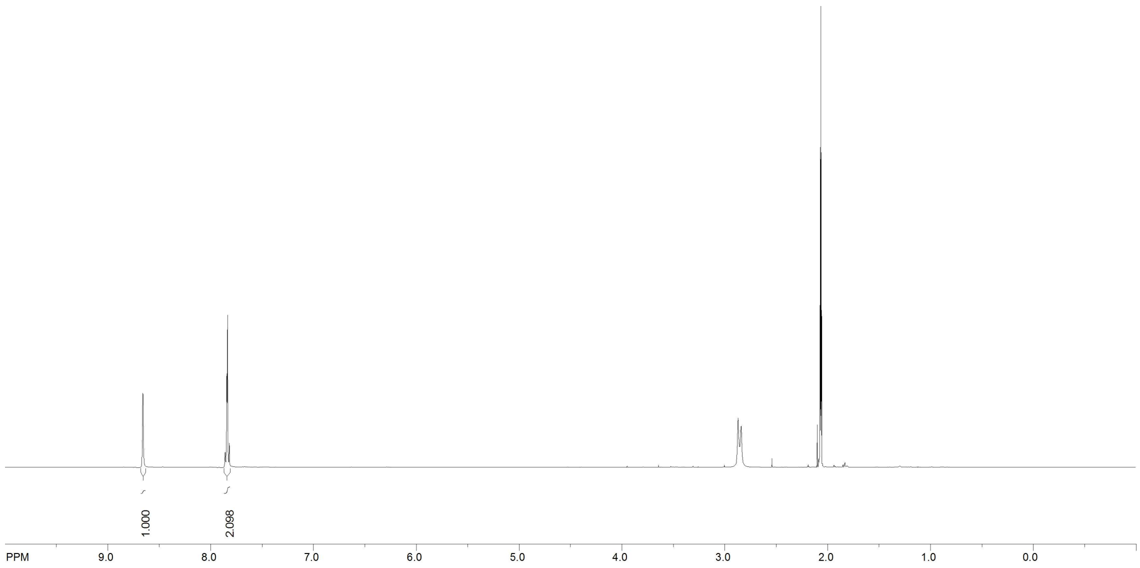


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **10b** in Acetone-d_6

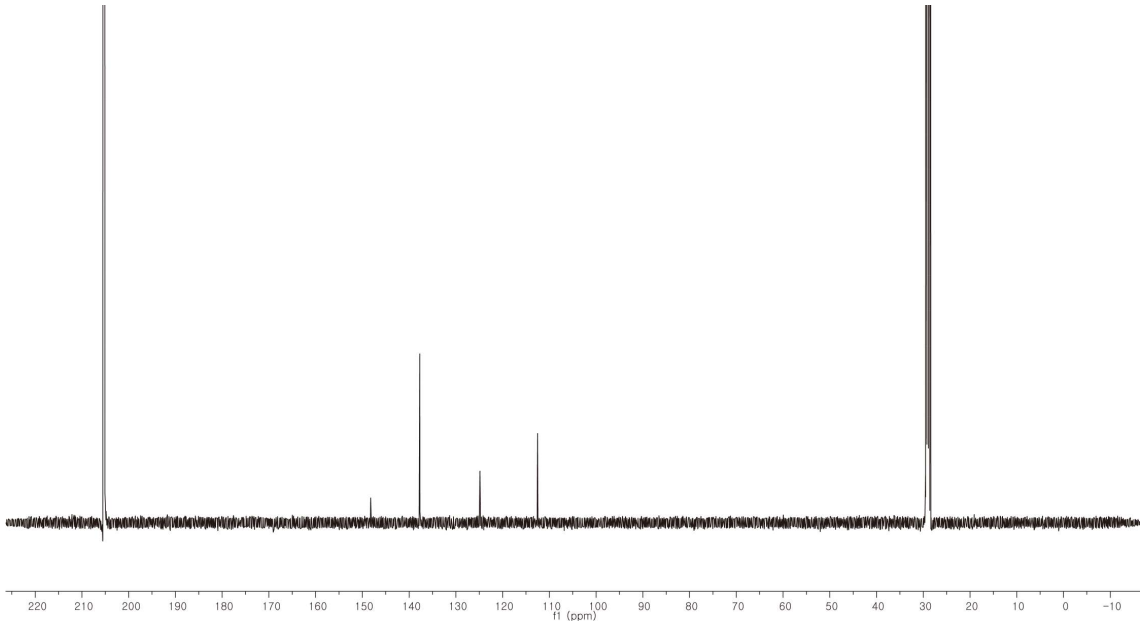
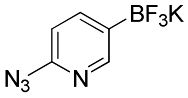


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **10b** in Acetone-d_6



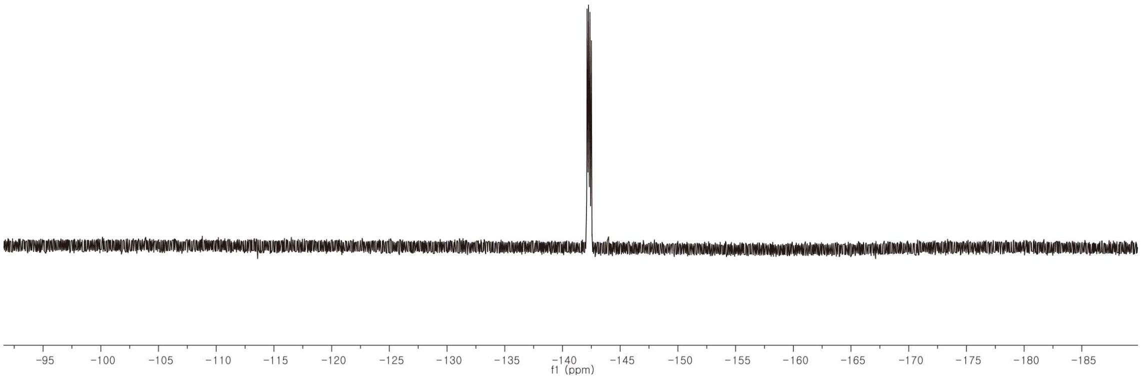


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **10b** in Acetone-d_6

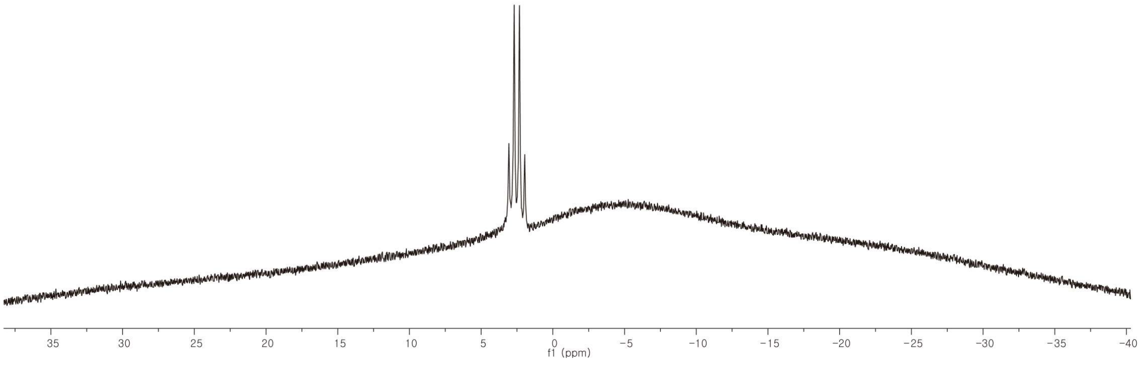
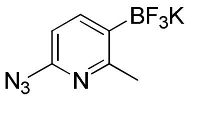


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **10b** in Acetone-d_6



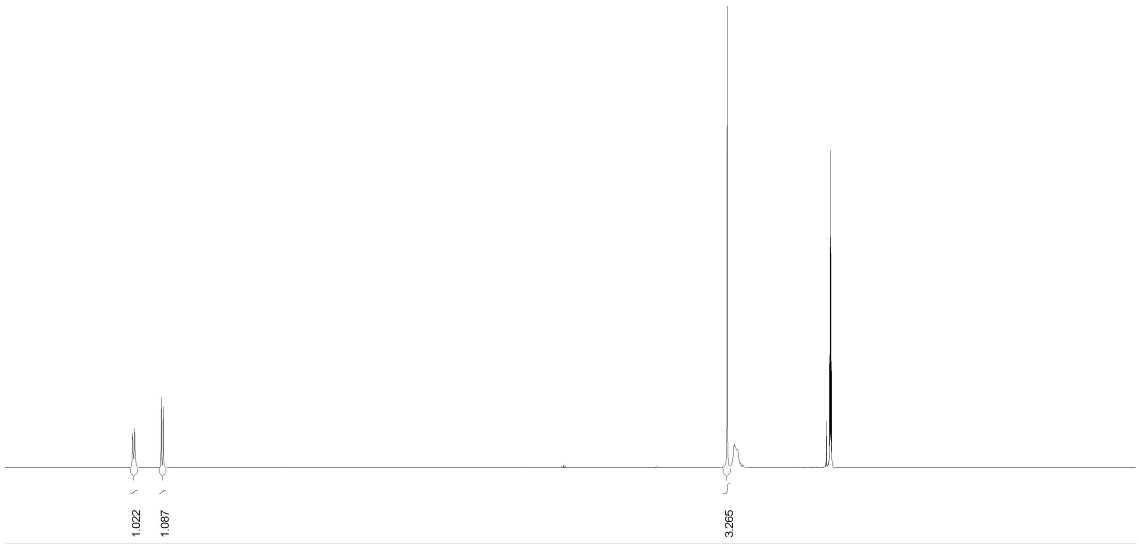


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **11b** in Acetone-d_6

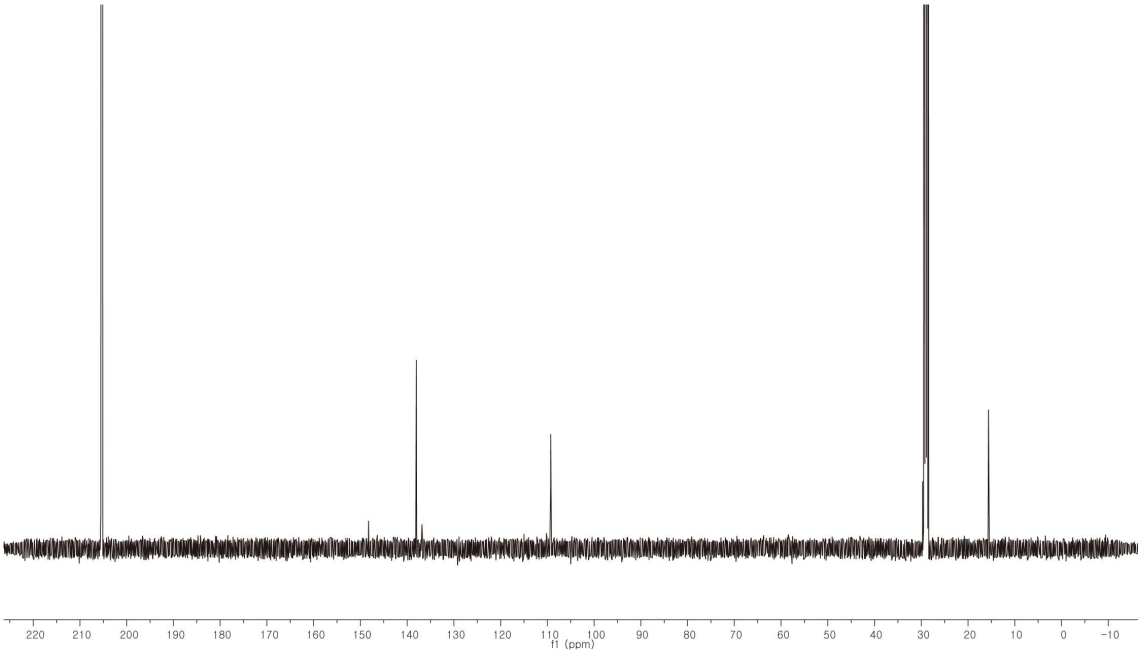
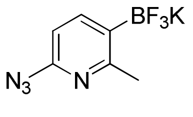


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **11b** in Acetone-d_6



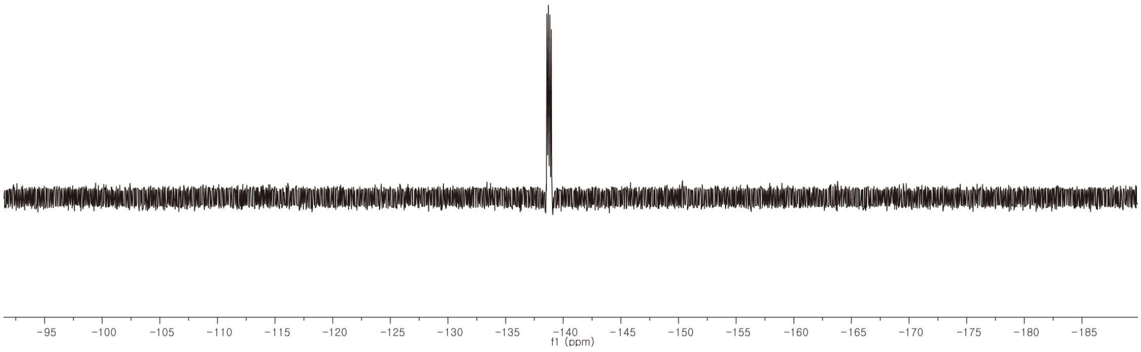


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **11b** in Acetone-d_6

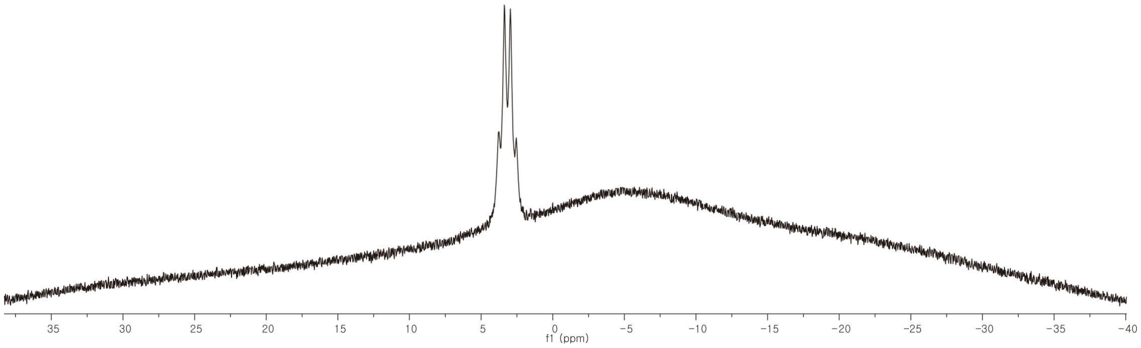
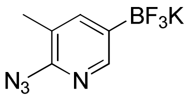


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **11b** in Acetone-d_6



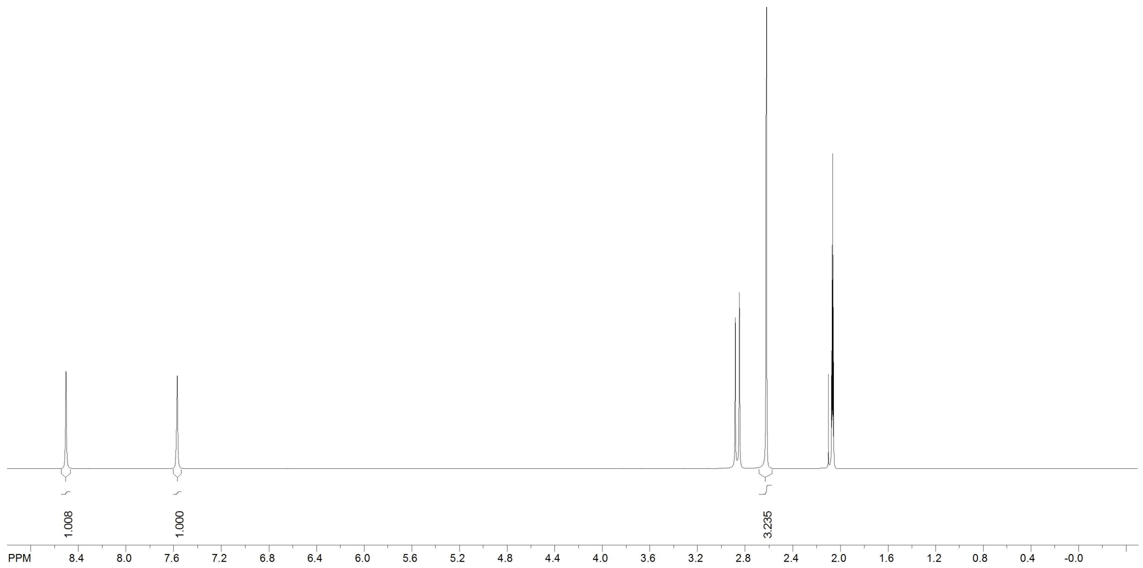


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **12b** in Acetone-d_6

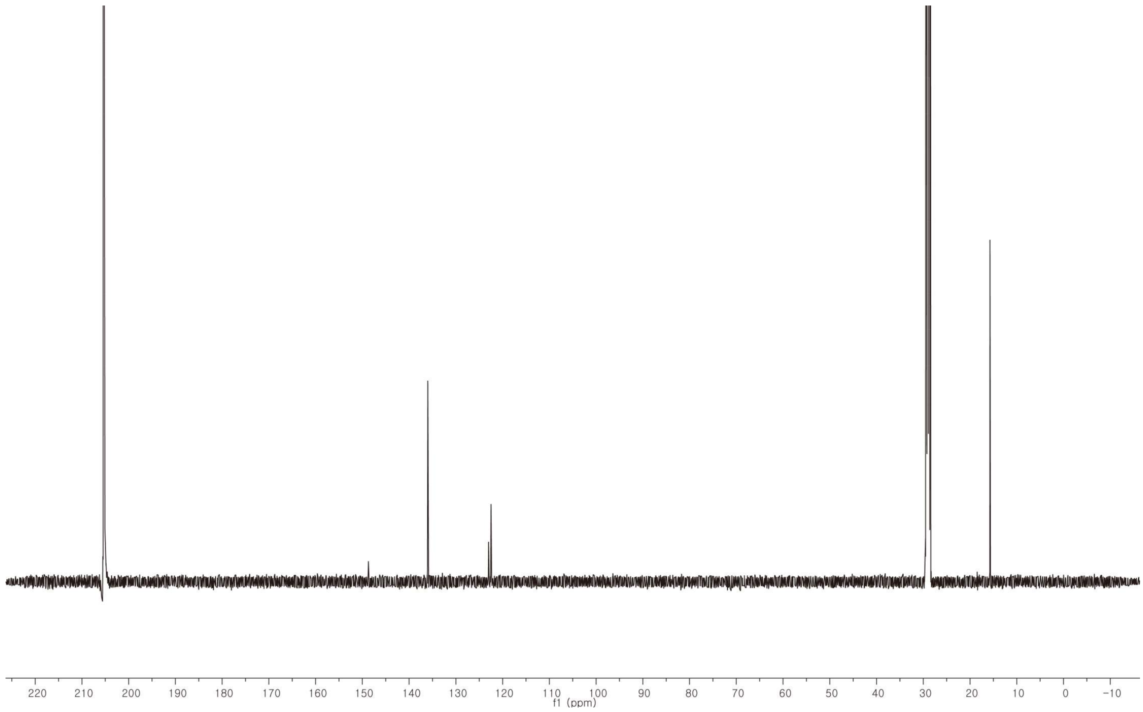
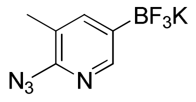


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **12b** in Acetone-d_6



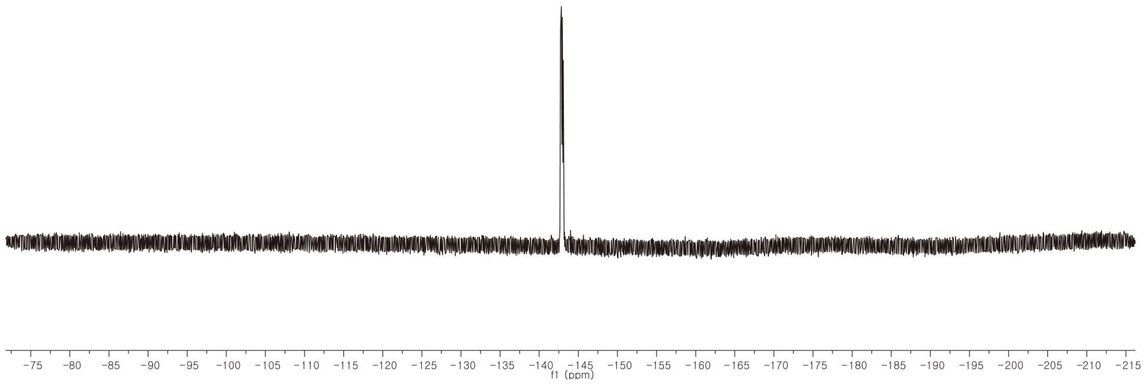


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **12b** in Acetone-d_6

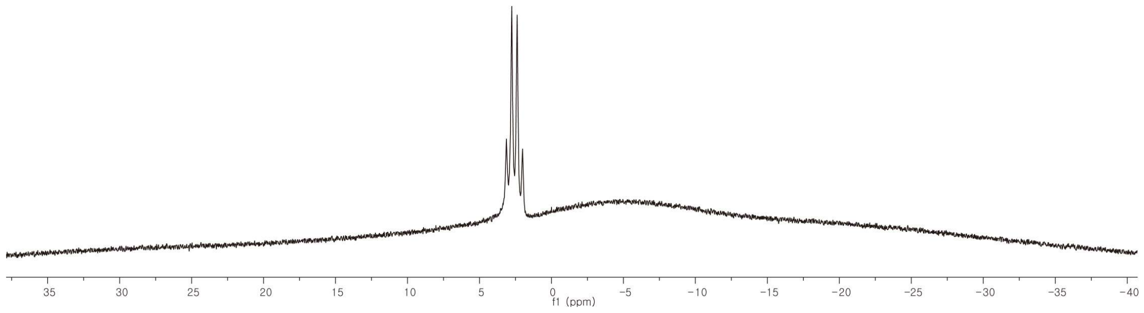
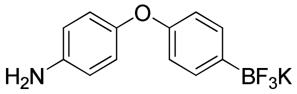


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **12b** in Acetone-d_6



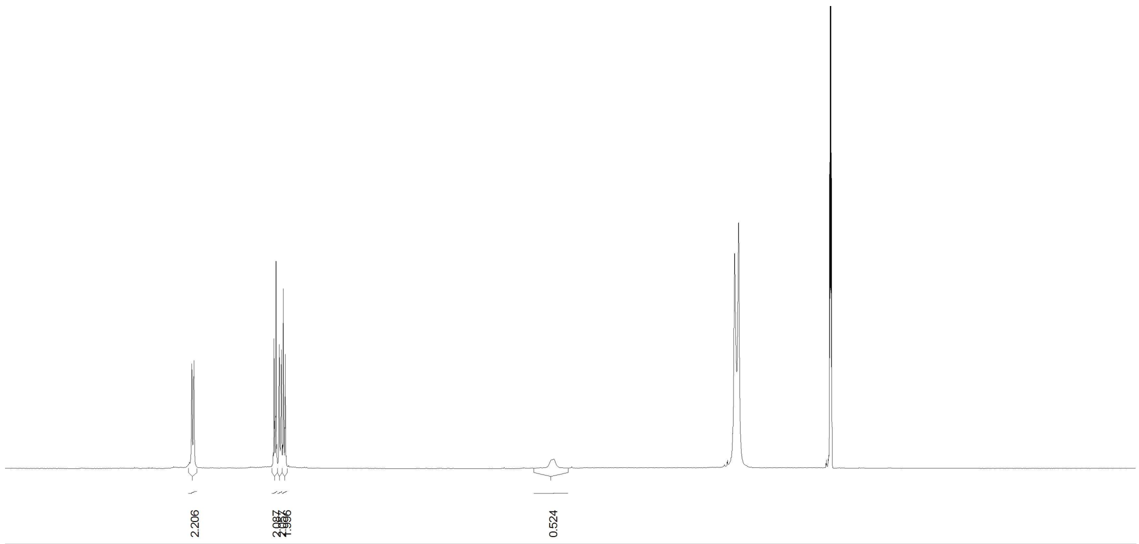


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **13b** in Acetone-d_6

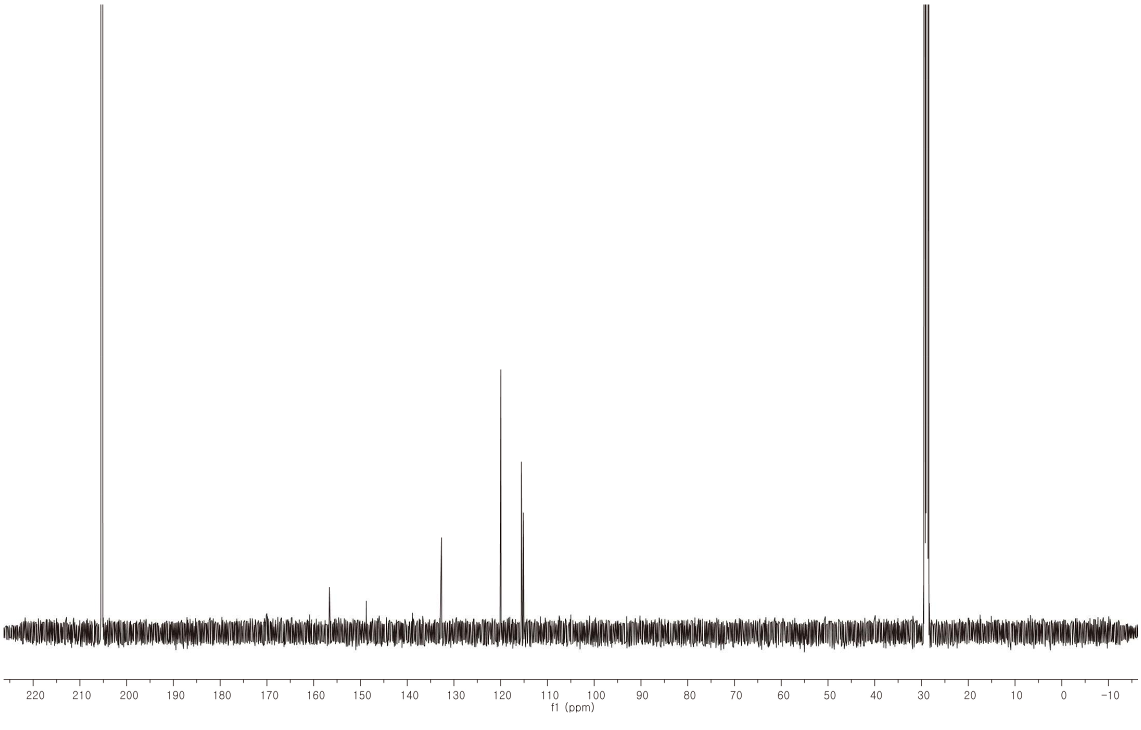
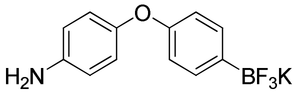


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **13b** in Acetone-d_6



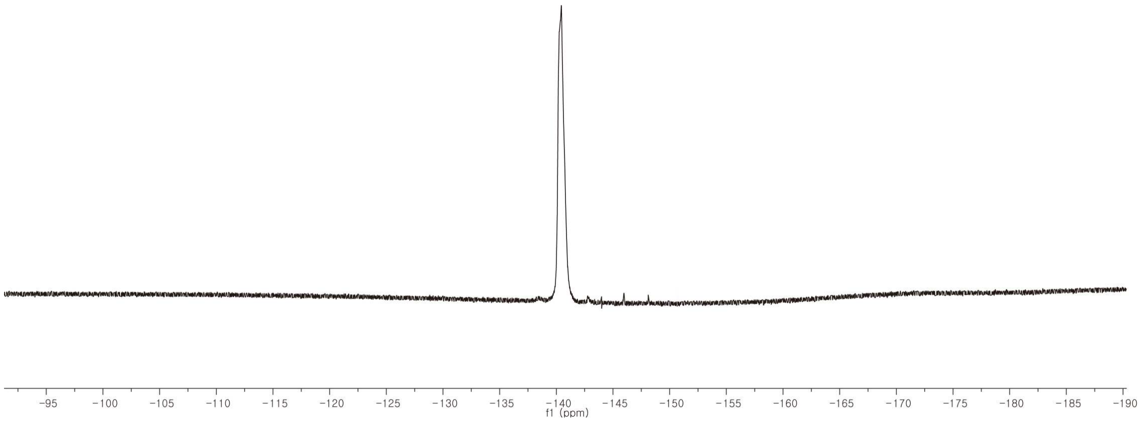


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **13b** in Acetone-d_6

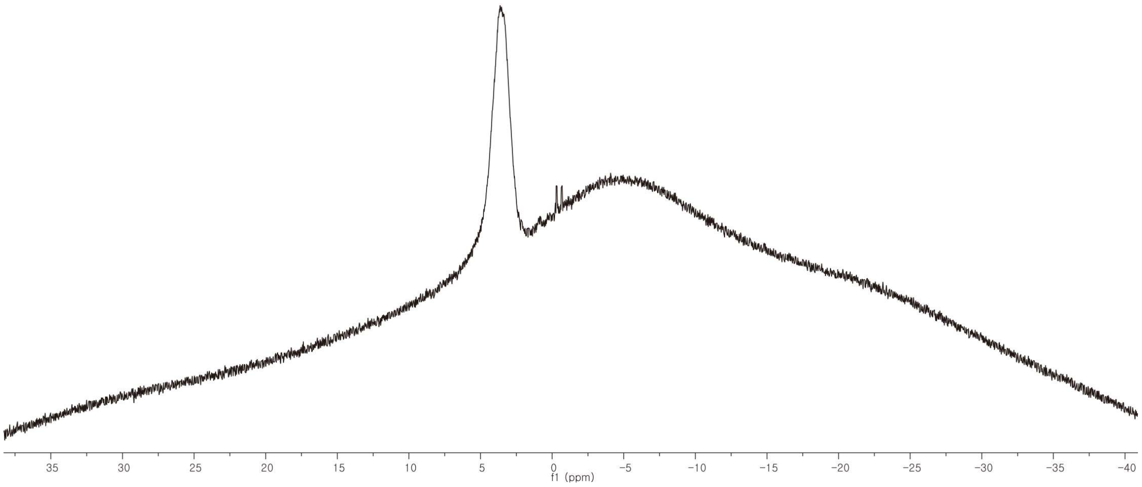
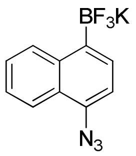


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **13b** in Acetone-d_6



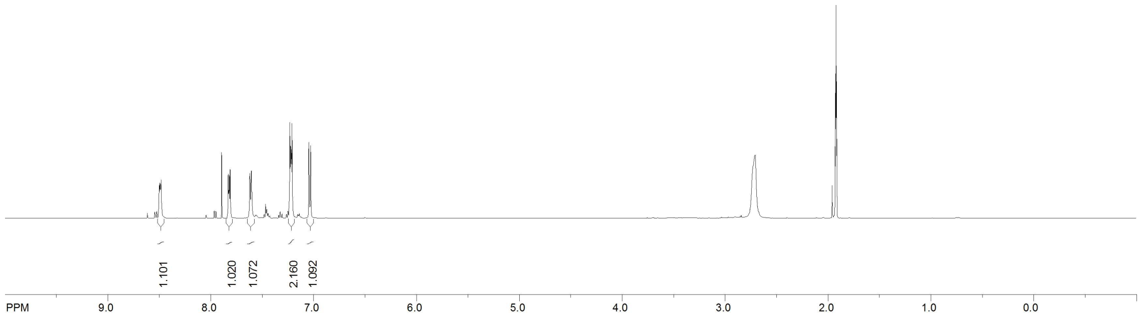


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **14b** in Acetone-d_6

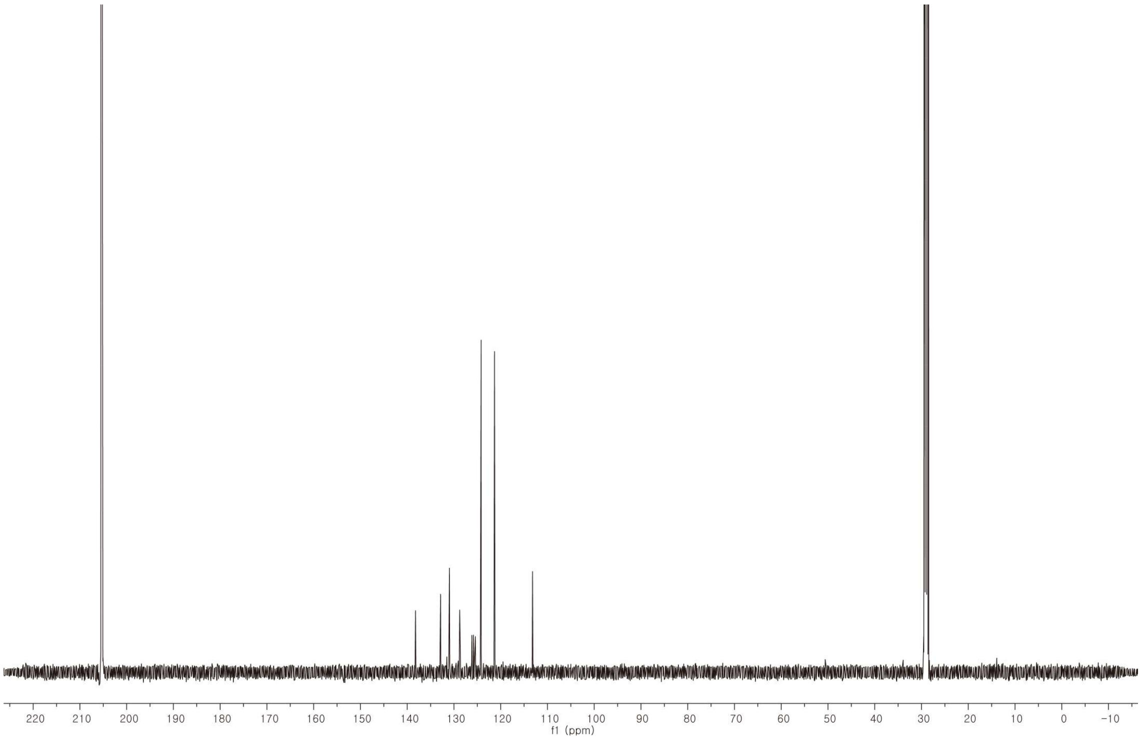
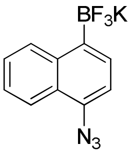


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **14b** in Acetone-d_6



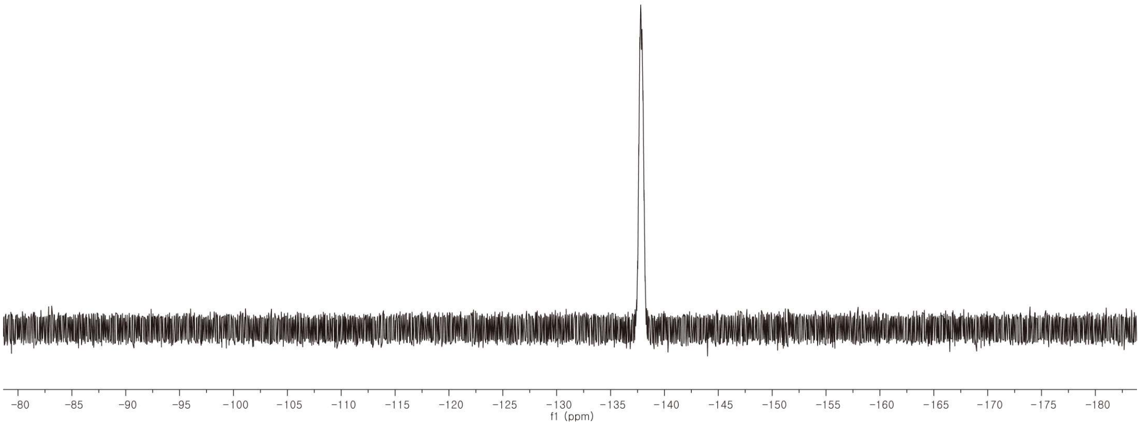


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **14b** in Acetone-d_6

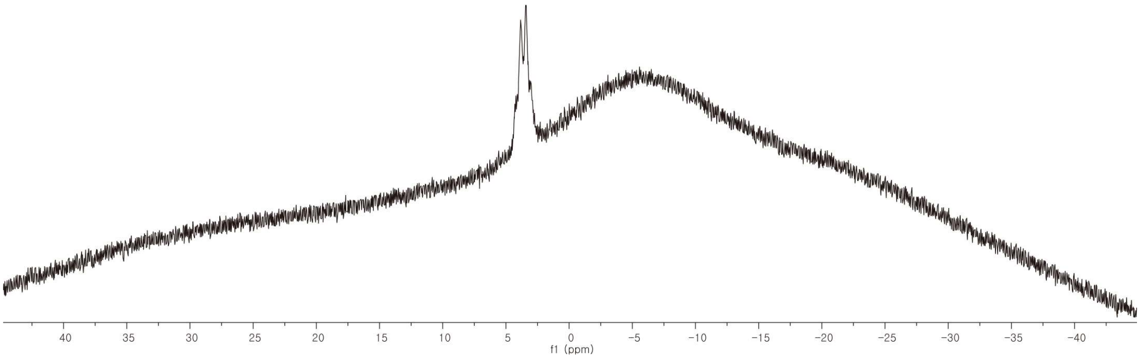
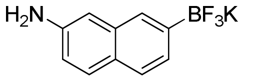


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **14b** in Acetone-d_6



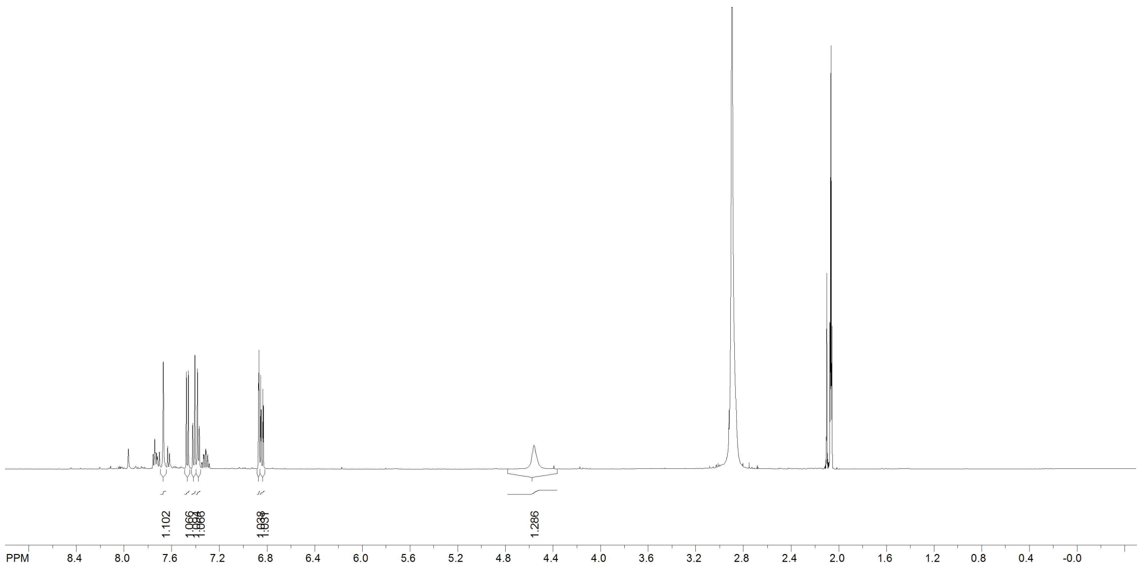


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **15b** in Acetone-d_6

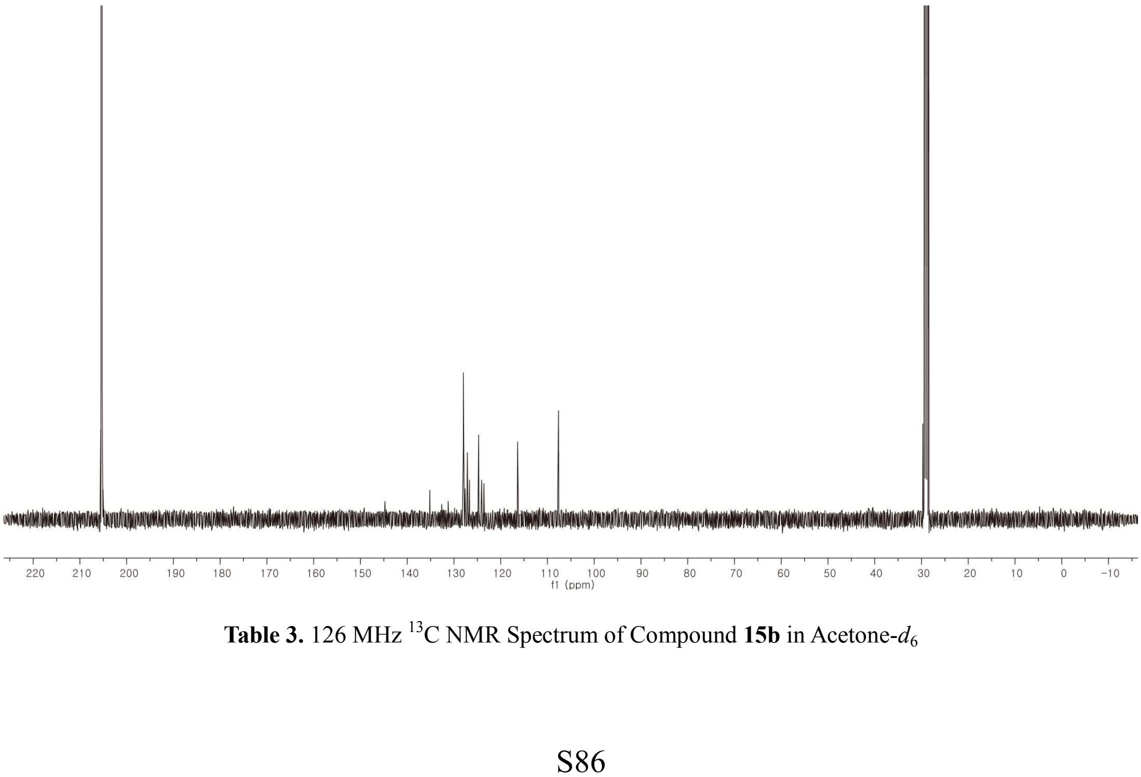
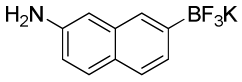


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **15b** in Acetone-d_6



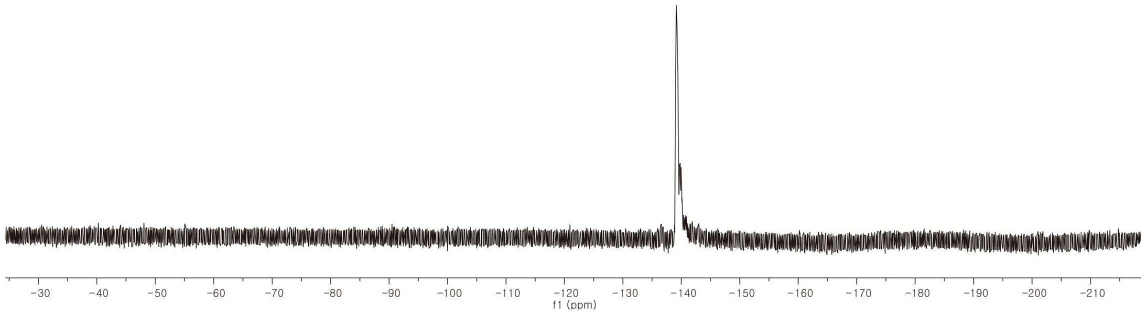


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **15b** in Acetone-d_6

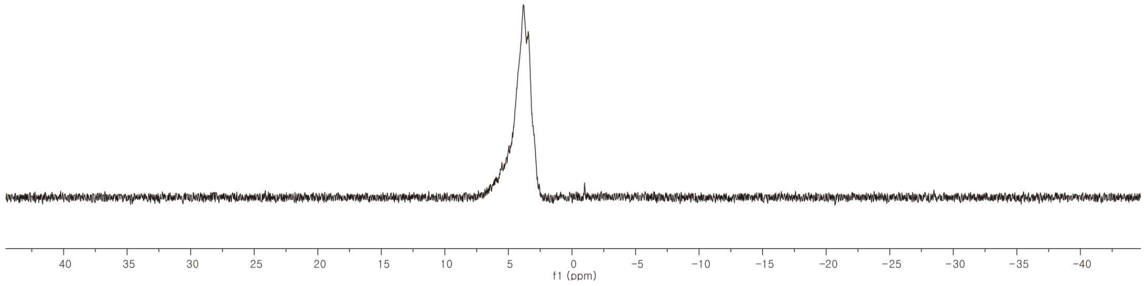
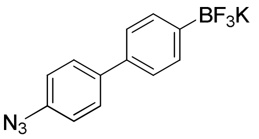


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **15b** in Acetone-d_6



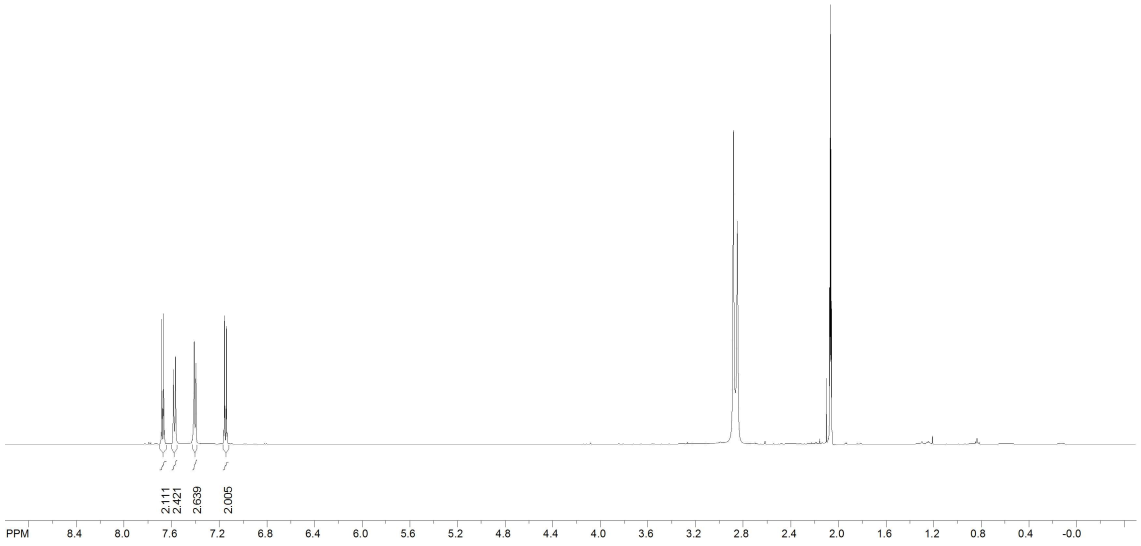


Table 3. 500 MHz ^{1}H NMR Spectrum of Compound **16b** in Acetone-d_6

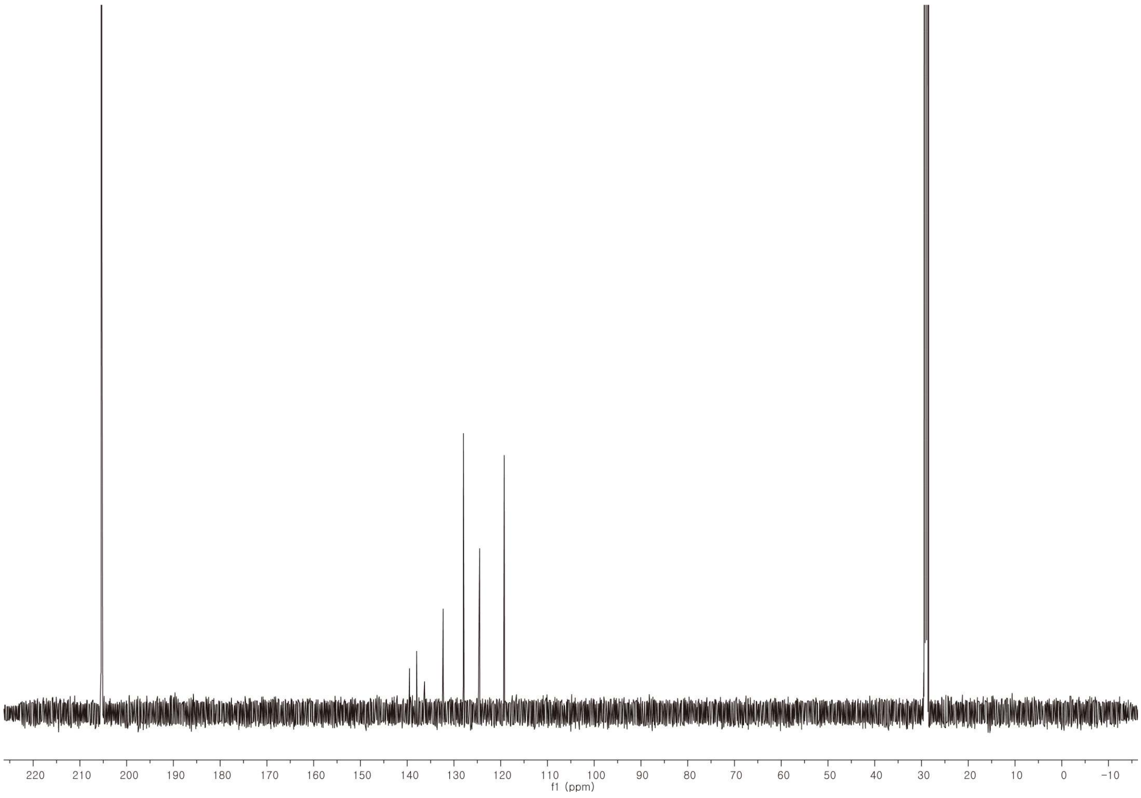


Table 3. 126 MHz ^{13}C NMR Spectrum of Compound **16b** in Acetone-d_6

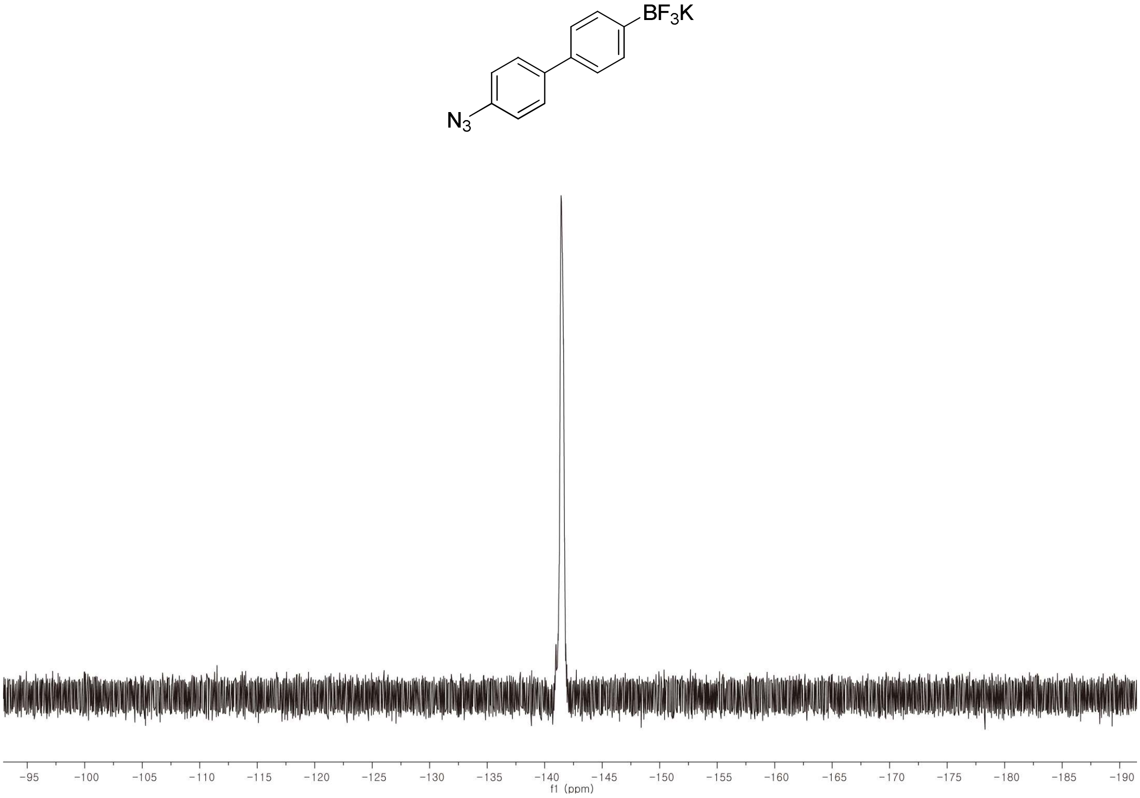


Table 3. 376 MHz ^{19}F NMR Spectrum of Compound **16b** in Acetone-d_6

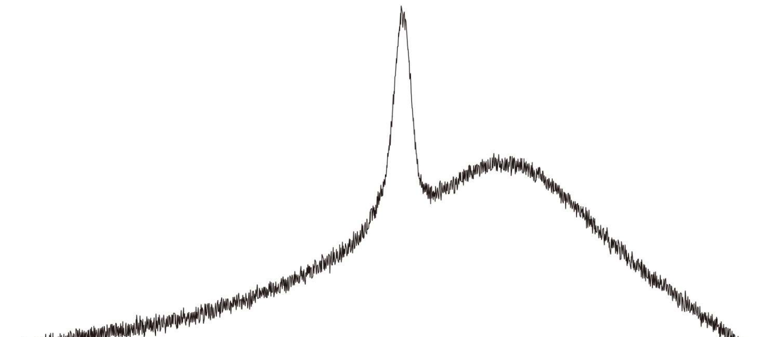
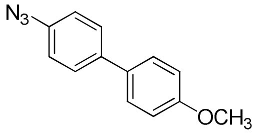


Table 3. 128 MHz ^{11}B NMR Spectrum of Compound **16b** in Acetone-d_6



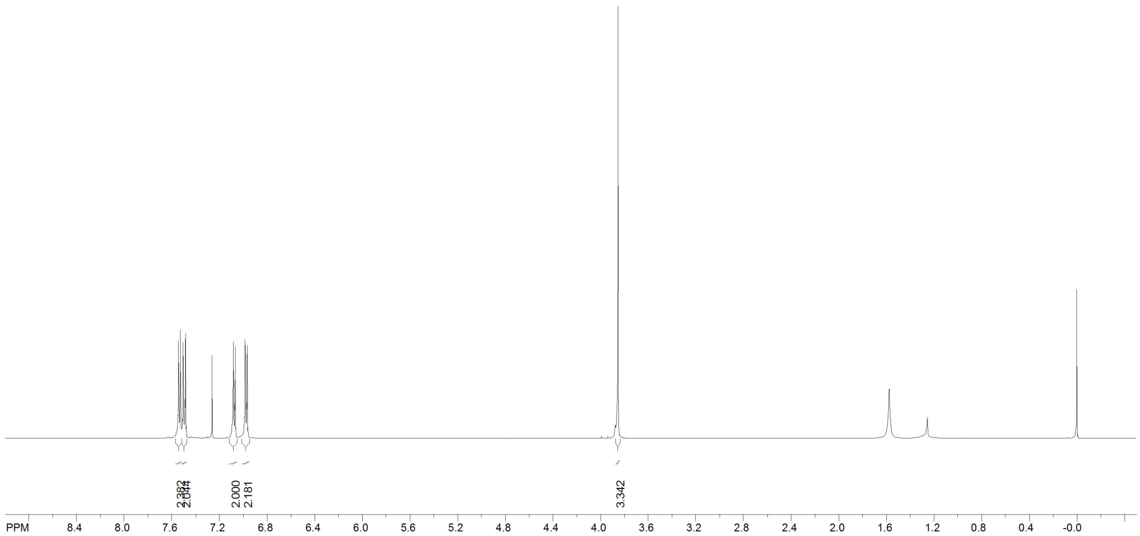


Table 4. 500 MHz ^{1}H NMR Spectrum of Compound **17** in Acetone-d_6

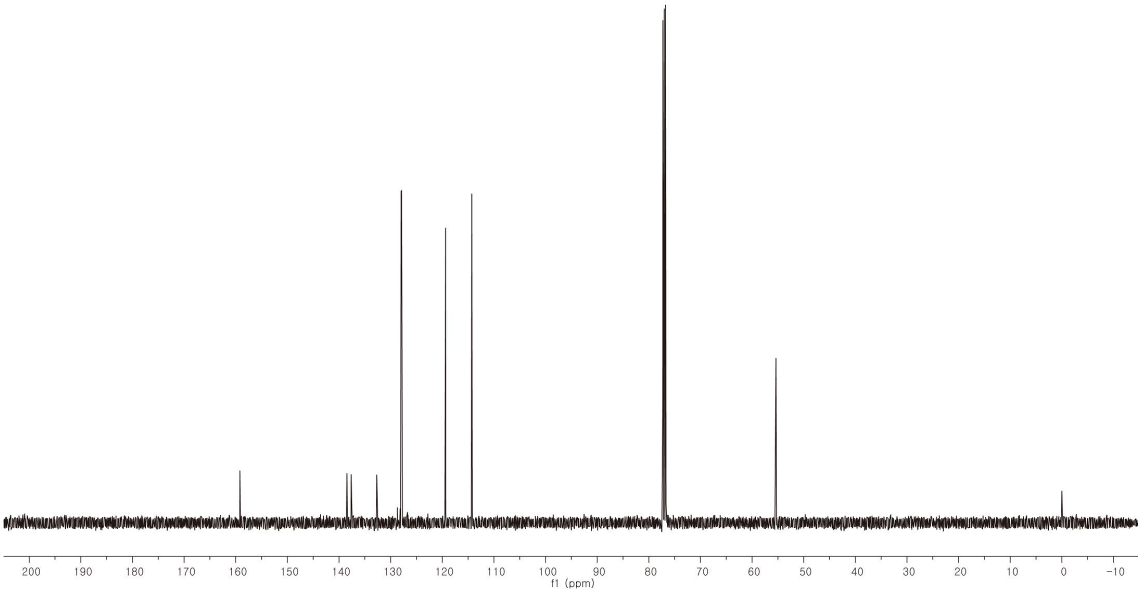
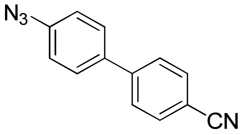


Table 4. 126 MHz ^{13}C NMR Spectrum of Compound **17** in Acetone-d_6



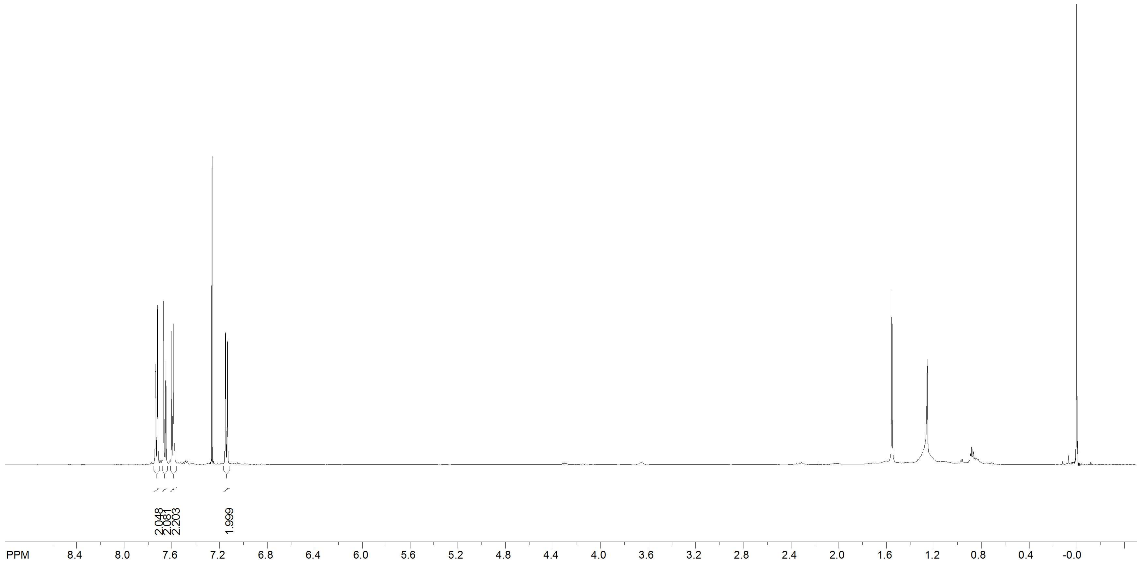


Table 4. 500 MHz ^{1}H NMR Spectrum of Compound **18** in Acetone-d_6

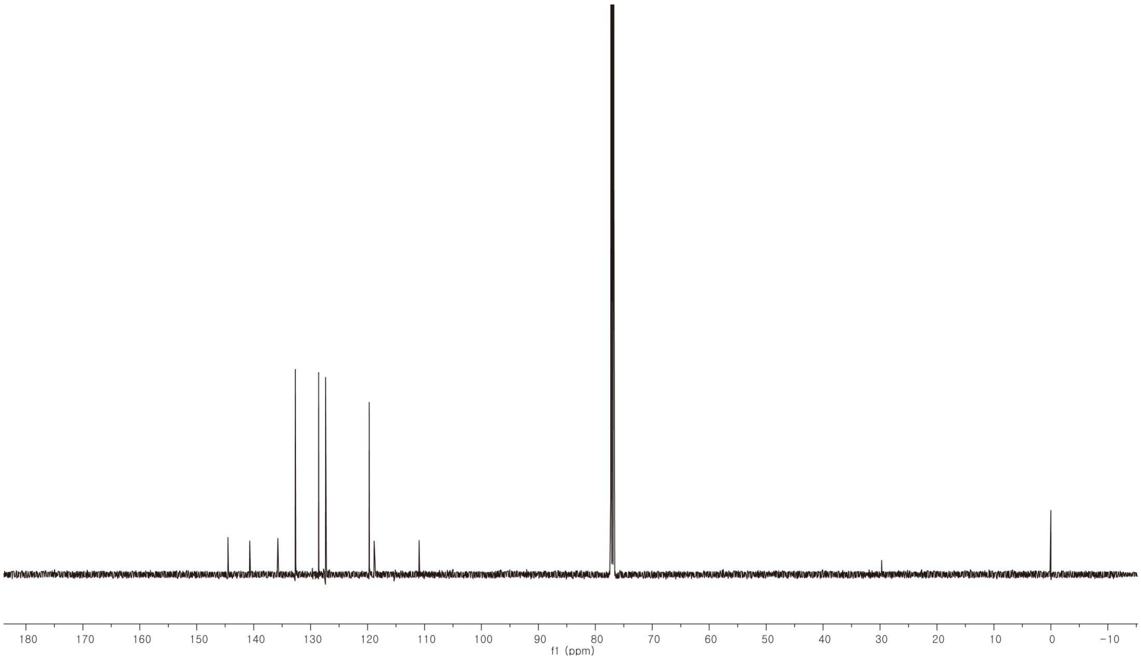
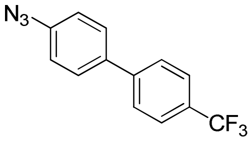


Table 4. 126 MHz ^{13}C NMR Spectrum of Compound **18** in Acetone-d_6



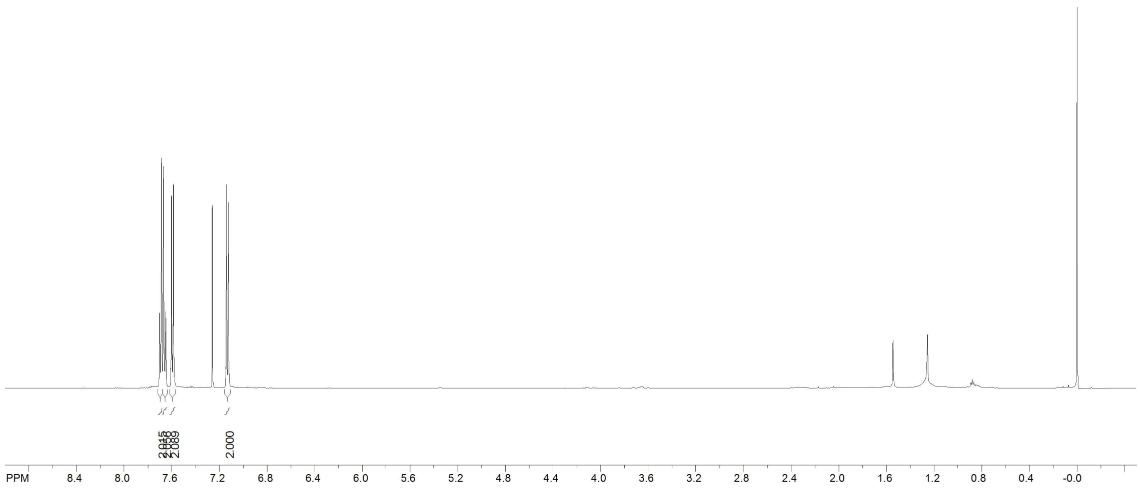


Table 4. 500 MHz ^{1}H NMR Spectrum of Compound **19** in Acetone-d_6

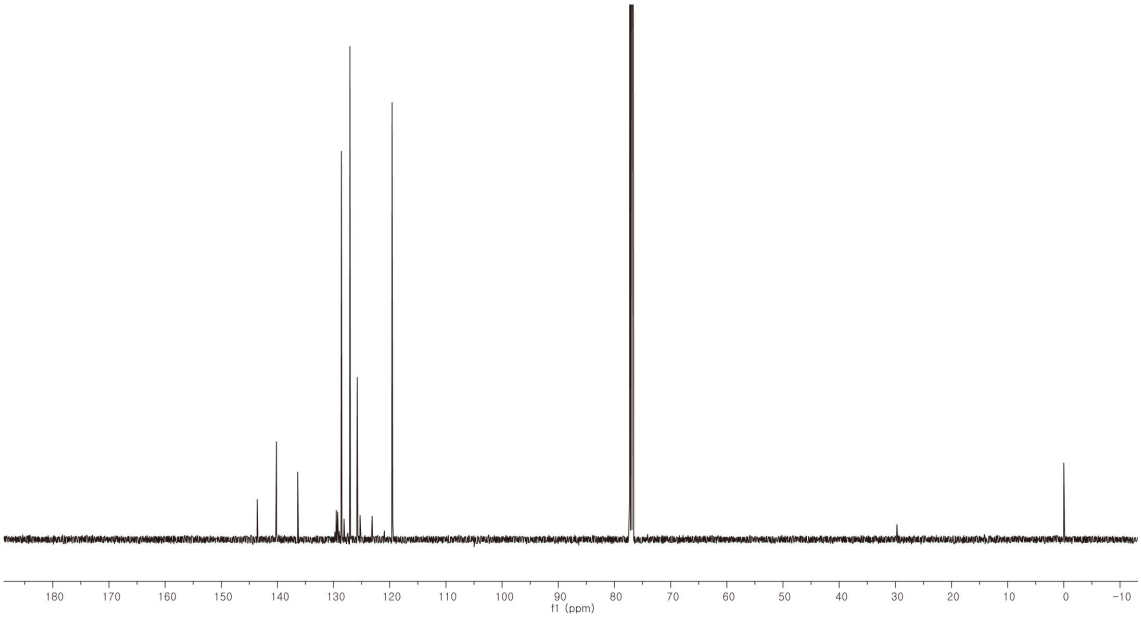
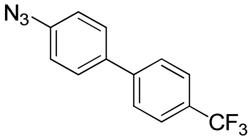


Table 4. 126 MHz ^{13}C NMR Spectrum of Compound **19** in Acetone-d_6



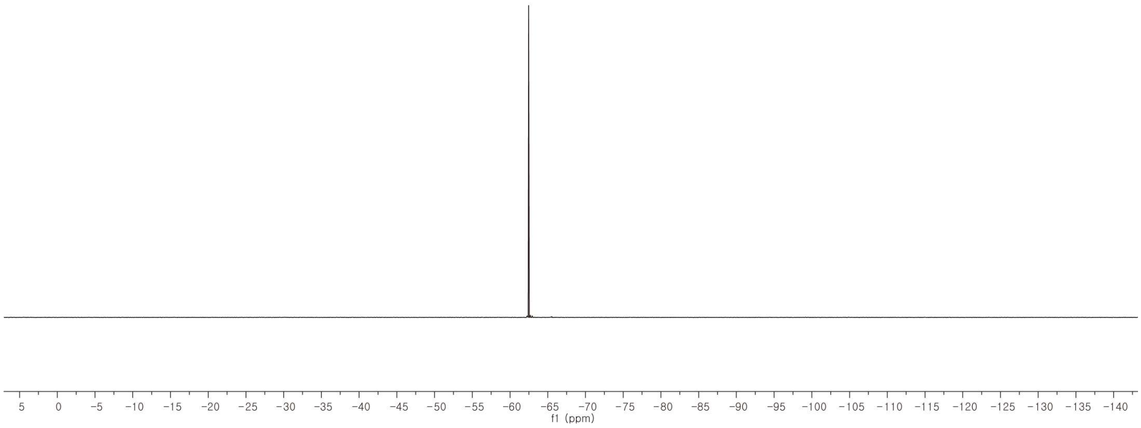
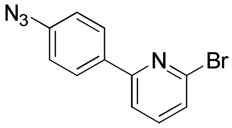


Table 4. 376 MHz ^{19}F NMR Spectrum of Compound **19** in Acetone-d_6



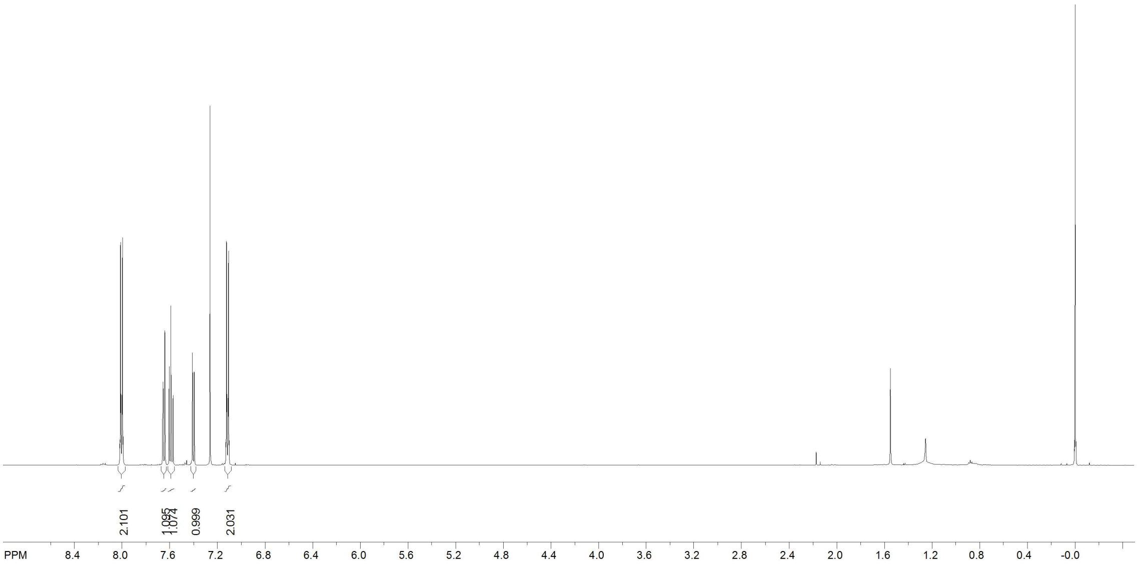


Table 4. 500 MHz ^{1}H NMR Spectrum of Compound **20** in Acetone-d_6

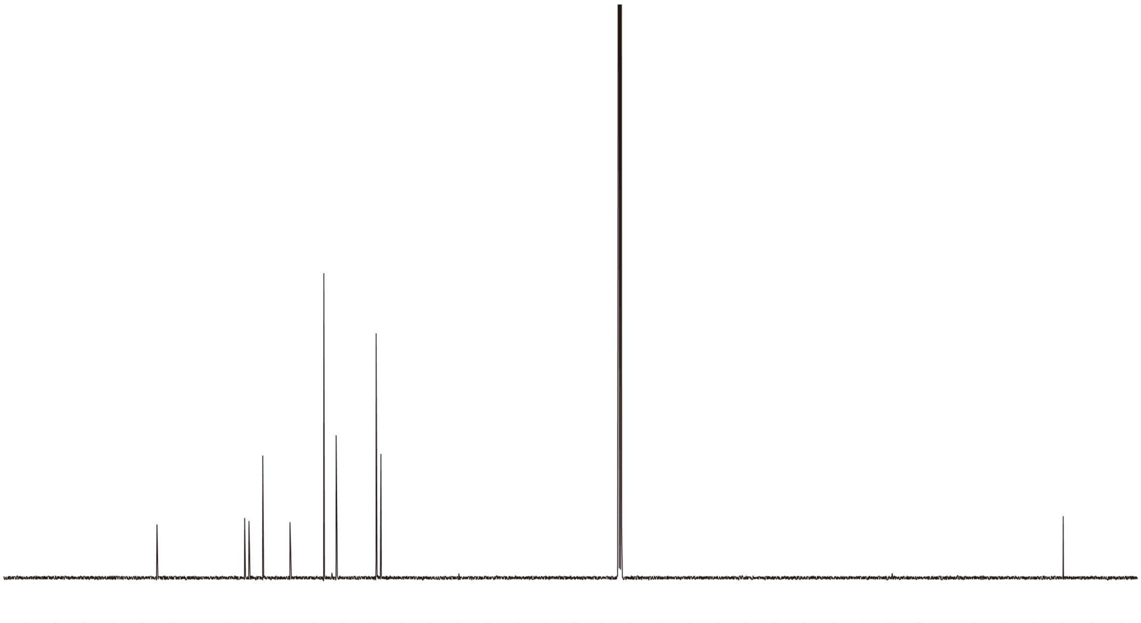
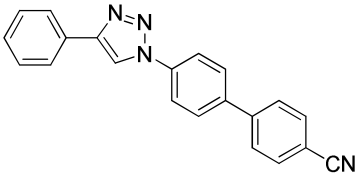
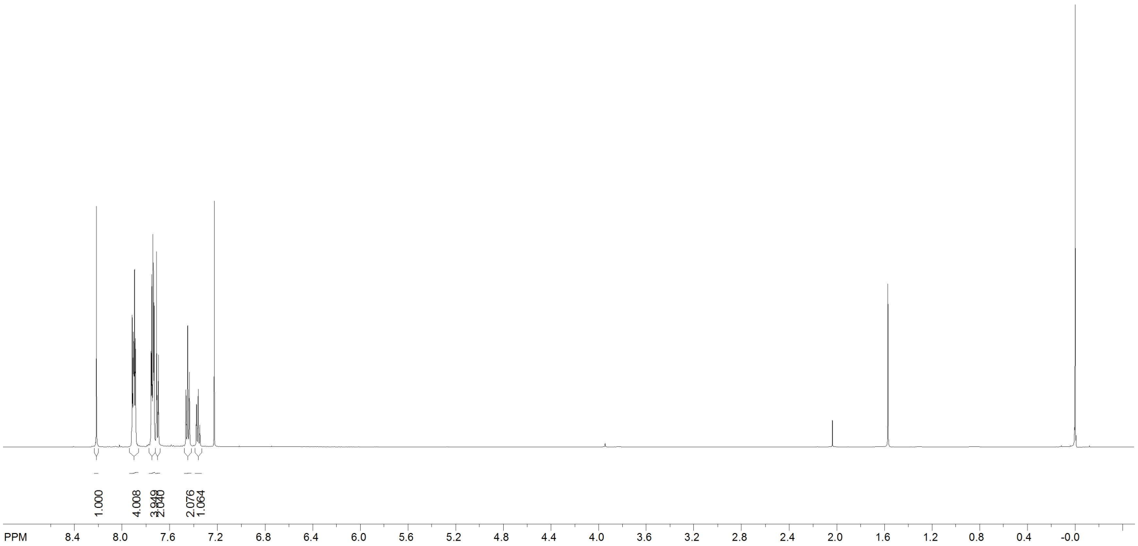
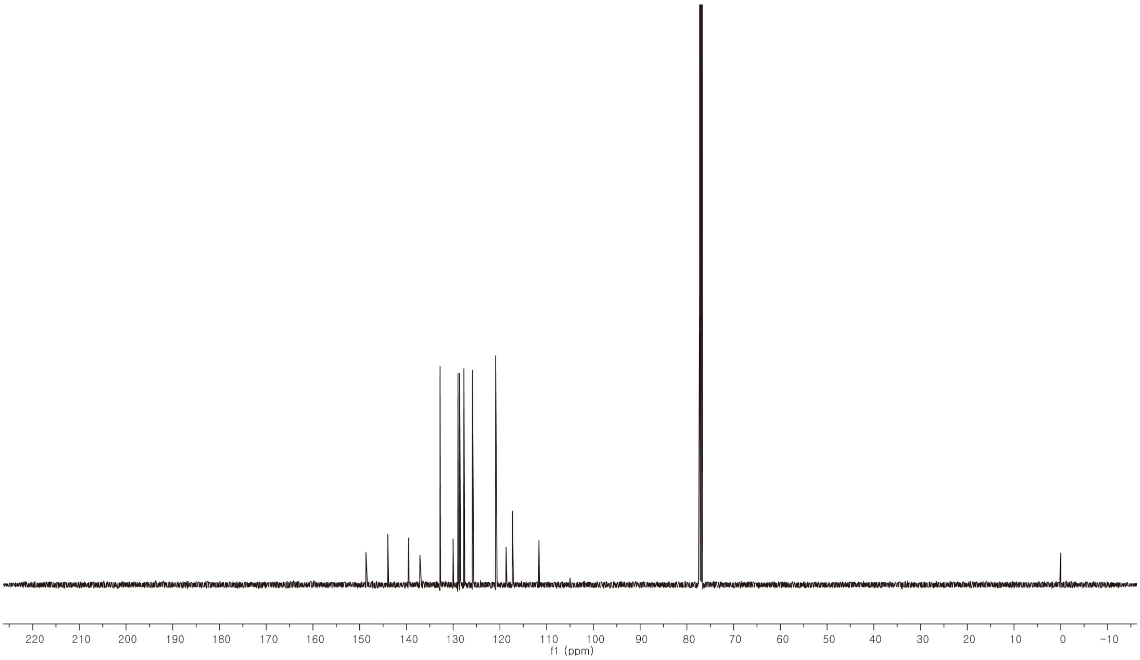


Table 4. 126 MHz ^{13}C NMR Spectrum of Compound **20** in Acetone-d_6

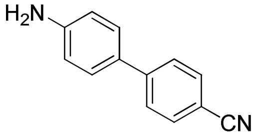


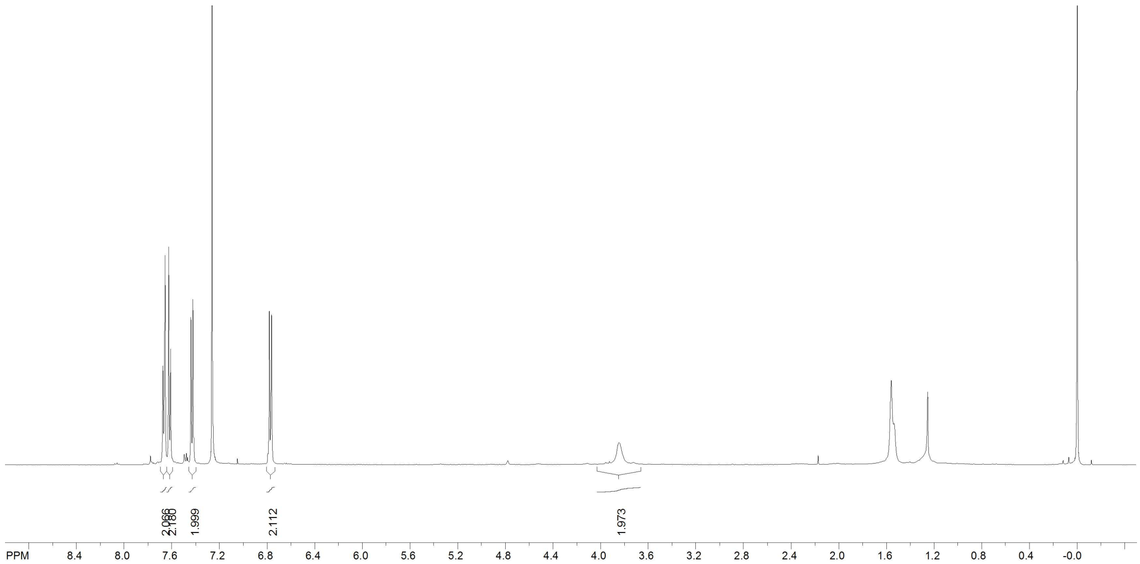


One-pot reaction (eq 1). 500 MHz ^{1}H NMR Spectrum of Compound **21** in Acetone-d_6

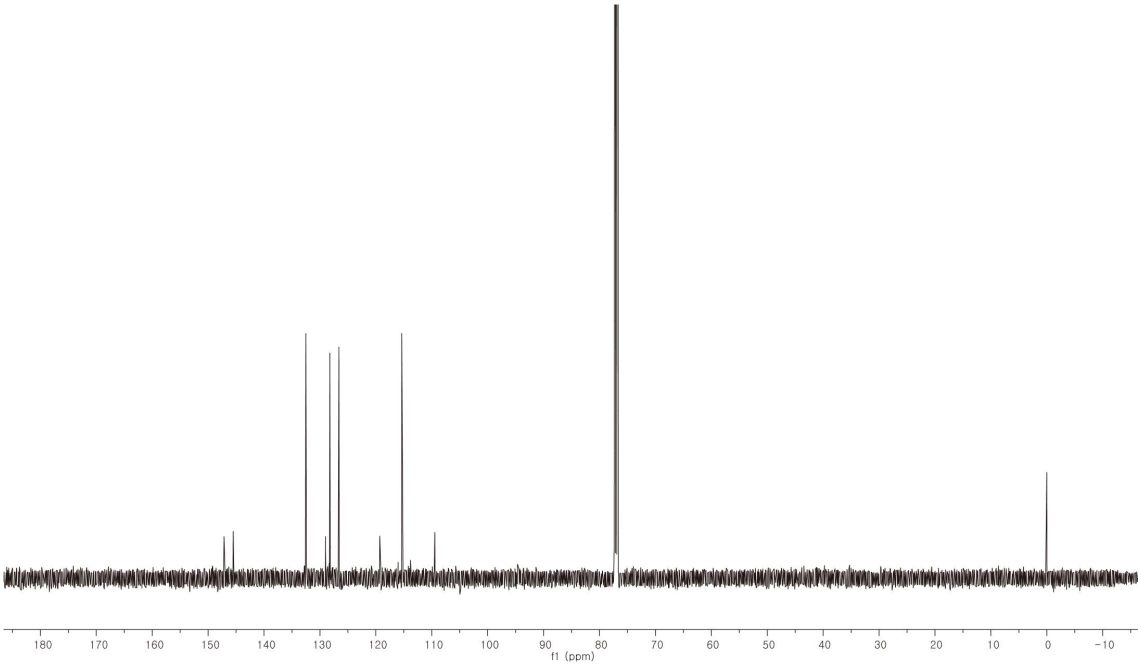


One-pot reaction (eq 1). 126 MHz ^{13}C NMR Spectrum of Compound **21** in Acetone-d_6





One-pot reaction (eq 2). 500 MHz ^{1}H NMR Spectrum of Compound **22** in Acetone-d_6



One-pot reaction (eq 2). 126 MHz ^{13}C NMR Spectrum of Compound **22** in Acetone-d_6