Increasing solubility and film-forming properties in imidazo[1,5-*a*]pyridine derivatives used as blue emissive materials in optoelectronic devices

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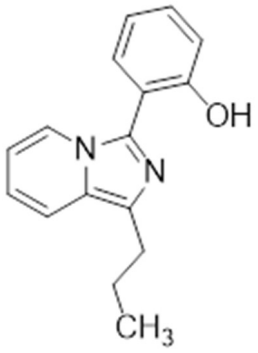


C3: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.44 (t, *J* = 7.4, 1H), 7.73 (d, *J* = 7.8, 1H), 7.43 (t, *J* = 11.4, 1H), 7.31 – 7.21 (m, 1H), 7.14 (t, *J* = 8.6, 1H), 7.02 – 6.90 (m, 1H), 6.67 (m, 1H), 6.59 (t, *J* = 6.4, 1H), 2.87 (t, *J* = 7.4, 2H), 1.94 – 1.65 (m, 2H), 0.99 (t, *J* = 7.4, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 156.59, 134.59, 131.71, 129.50, 127.31, 123.90, 122.10, 118.95, 118.78, 117.89, 117.84, 114.58, 113.88, 28.86, 23.08, 14.08.

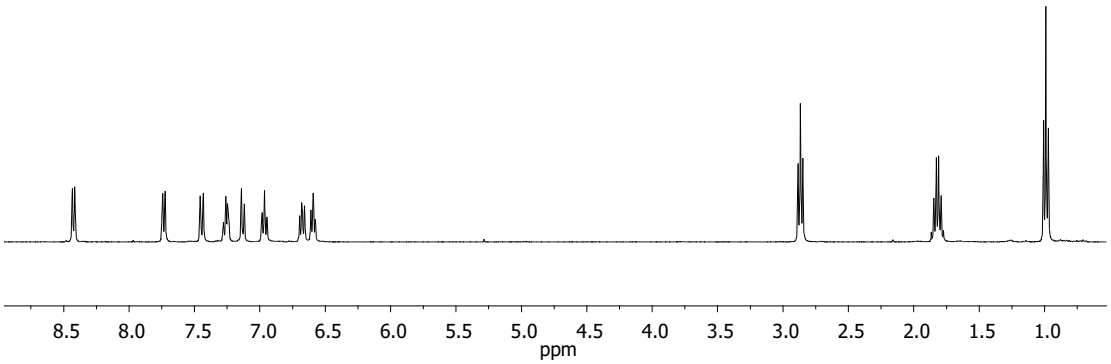


Figure S1: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C3**.

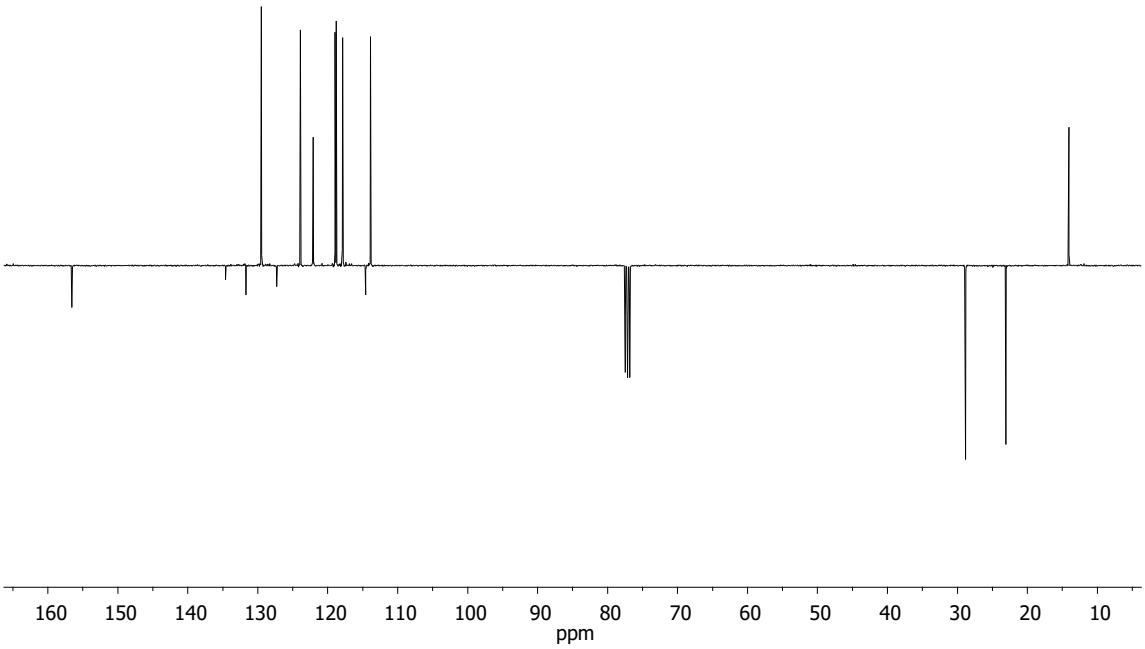
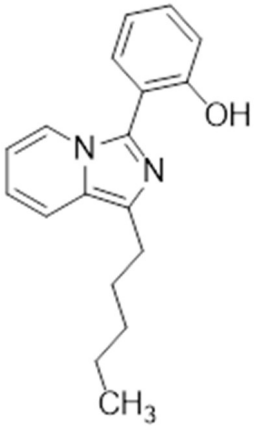


Figure S2: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C3**.



C5: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.42 (d, *J* = 7.3, 1H), 7.66 (d, *J* = 7.8, 1H), 7.44 (d, *J* = 9.1, 1H), 7.18 (t, *J* = 7.1, 1H), 7.14 (d, *J* = 7.5, 1H), 6.89 (t, *J* = 7.0, 1H), 6.69 (m, 1H), 6.52 (t, *J* = 7.2, 1H), 2.89 (t, *J* = 7.5, 2H), 1.80 (m, 2H), 1.42 – 1.30 (m, 4H), 0.90 (t, *J* = 7.0, 3H).^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 156.57, 134.51, 131.81, 129.56, 127.16, 124.03, 122.14, 118.97, 118.75, 117.93, 117.83, 114.49, 113.92, 31.70, 29.49, 26.74, 22.65, 14.18.

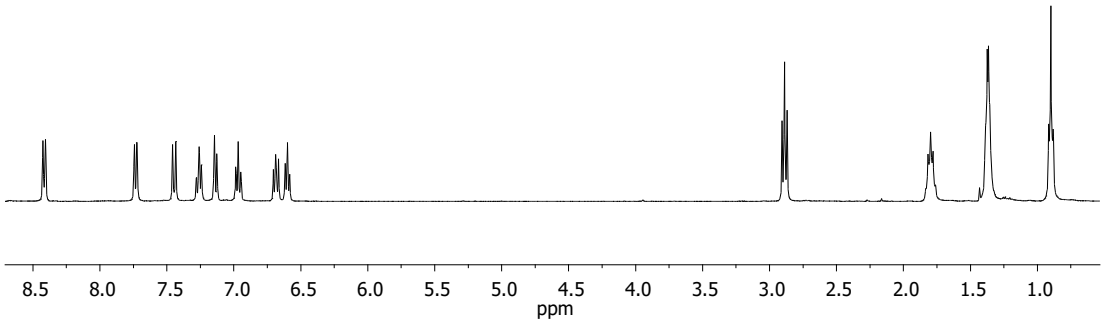


Figure S3: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C5**.

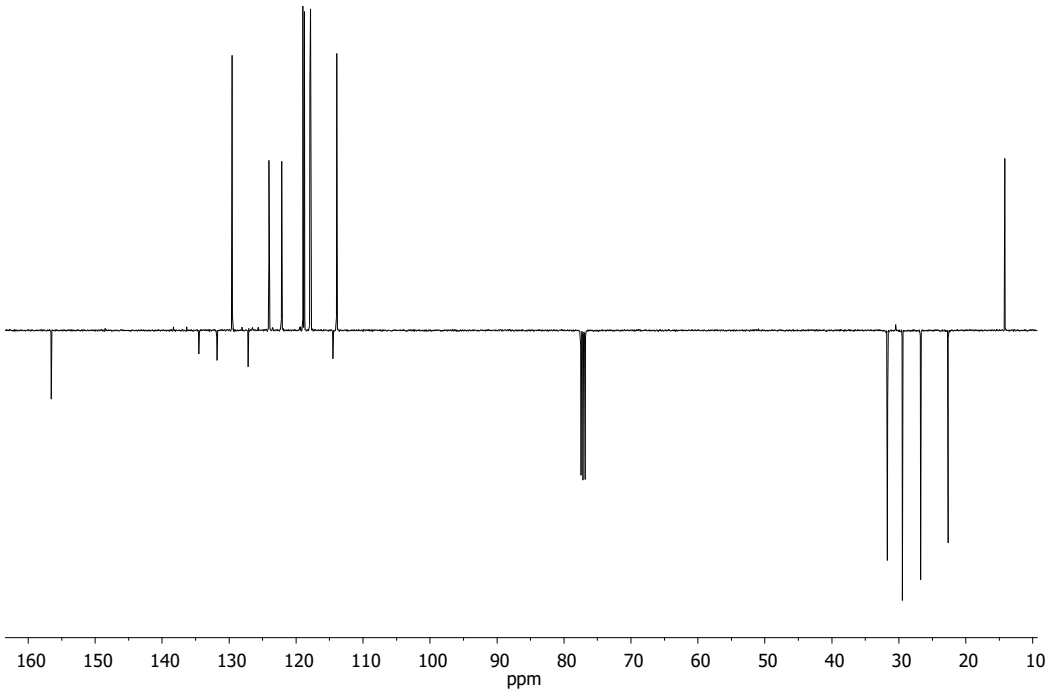
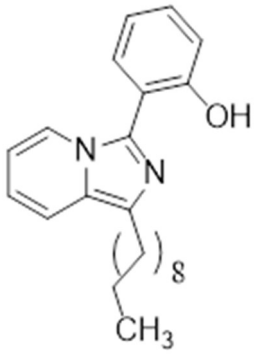


Figure S4: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C5**.



C10: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.40 (d, *J* = 7.2, 1H), 7.73 (d, *J* = 7.7, 1H), 7.45 (d, *J* = 7.7, 1H), 7.25 (t, *J* = 7.5, 1H), 7.14 (d, *J* = 8.1, 1H), 6.96 (t, *J* = 7.5, 1H), 6.71 (m, 1H), 6.62 (t, *J* = 6.7, 1H), 2.91 (t, *J* = 7.5, 2H), 1.80 (m, 2H), 1.45 – 1.12 (m, 14H), 0.87 (t, *J* = 6.6, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 156.59, 134.44, 129.75, 127.17, 122.28, 119.02, 118.75, 118.12, 117.89, 114.05, 110.04, 32.05, 29.84, 29.77, 29.75, 29.62, 29.56, 29.47, 26.75, 22.85, 14.26.

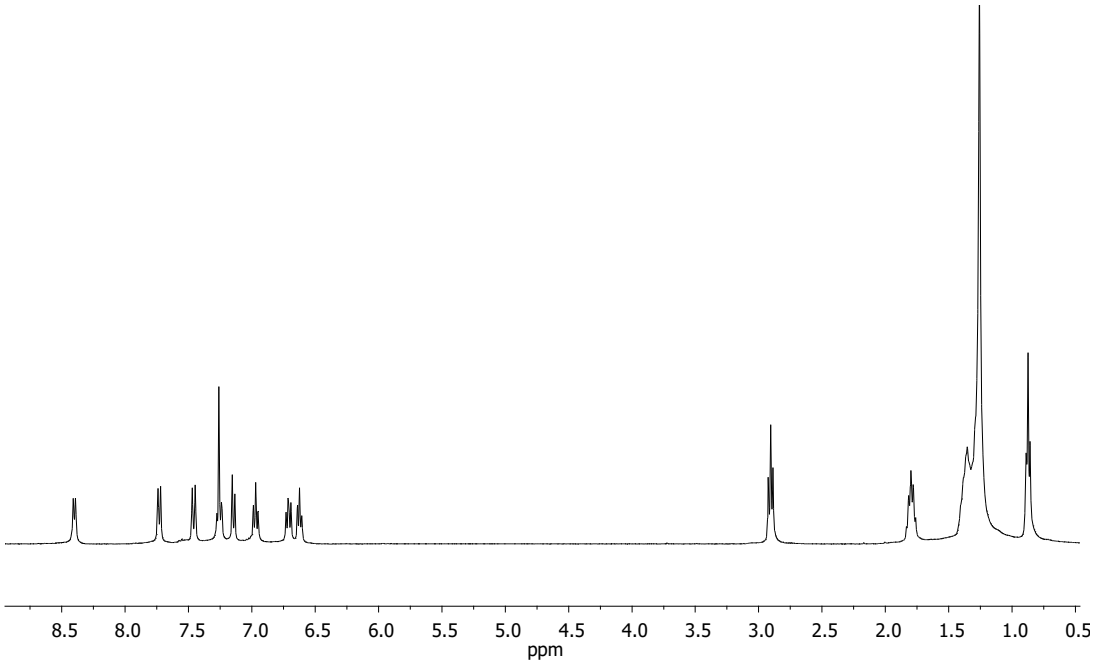


Figure S5: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C10**.

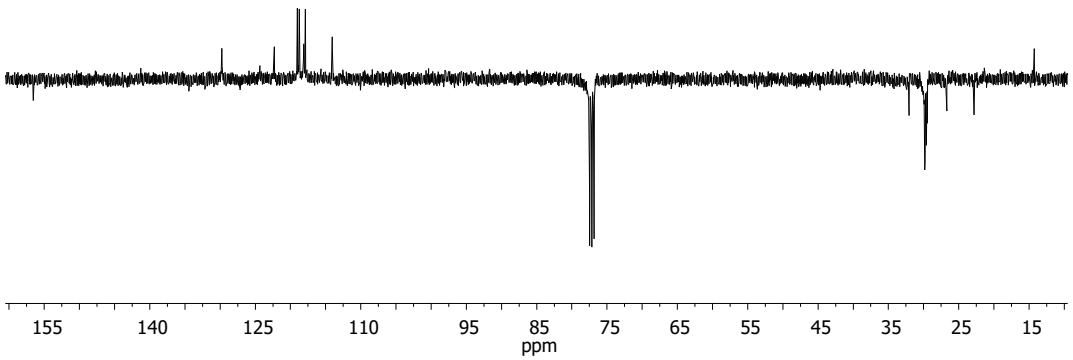
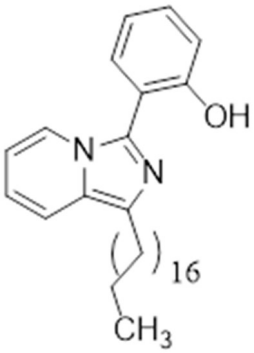


Figure S6: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C10**.



C18: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.36 (d, *J* = 7.3, 1H), 7.67 (d, *J* = 7.9, 1H), 7.37 (d, *J* = 9.1, 1H), 7.22 – 7.16 (m, 1H), 7.06 (d, *J* = 7.9, 1H), 6.89 (t, *J* = 7.3, 1H), 6.61 (m 1H), 6.53 (t, *J* = 6.5, 1H), 2.81 (t, *J* = 7.5, 2H), 2.01 – 1.93 (m, 2H), 1.76 – 1.67 (m, 2H), 1.21 (m, 28H), 0.81 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 156.65, 131.98, 129.51, 127.18, 123.91, 122.13, 118.94, 118.82, 117.88, 117.83, 114.60, 114.22, 113.87, 32.10, 29.88, 29.84, 29.54, 22.86, 14.26.

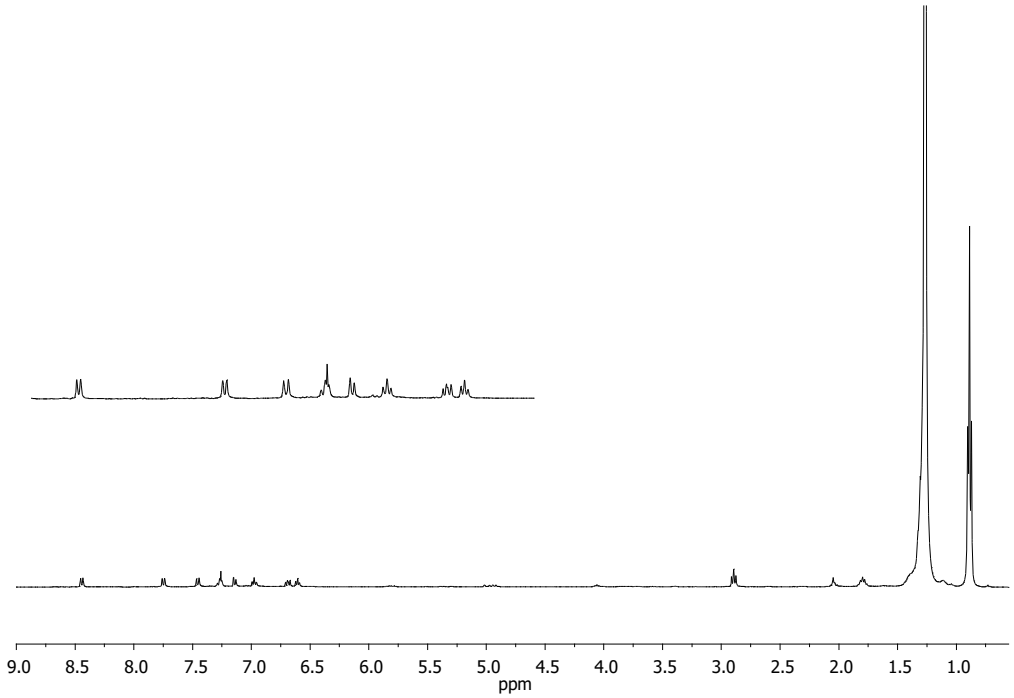


Figure S7: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C18**.

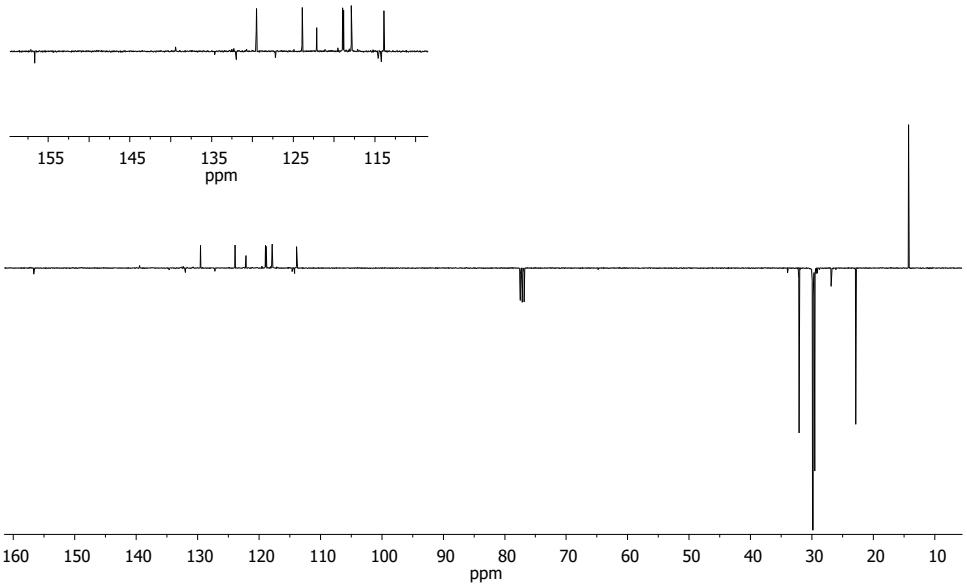
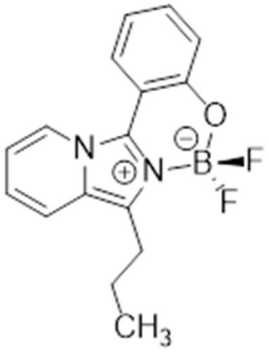


Figure S8: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C18**.



C3-BF$_2$: ^1H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.51 (d, *J* = 6.1, 1H), 7.80 (d, *J* = 7.9, 1H), 7.57 (d, *J* = 7.5, 1H), 7.4 (t, *J* = 7.7, 1H), 7.22 (d, *J* = 8.2, 1H), 7.00 (t, *J* = 7.6, 1H), 6.97 – 6.84 (m, 2H), 3.14 (t, *J* = 7.6, 2H), 1.94 – 1.78 (m, 2H), 1.01 (t, *J* = 7.3, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ =155.19, 131.98, 127.71, 127.40, 122.41, 122.18, 120.76, 120.61, 119.86, 119.38, 117.26, 111.13, 26.41, 23.08, 14.15. FT-IT (ATR) (cm^{-1}): $\tilde{\nu}$ = 1034 – 1147 (BF_2), 2877 – 2980 (aliphatic C-H).

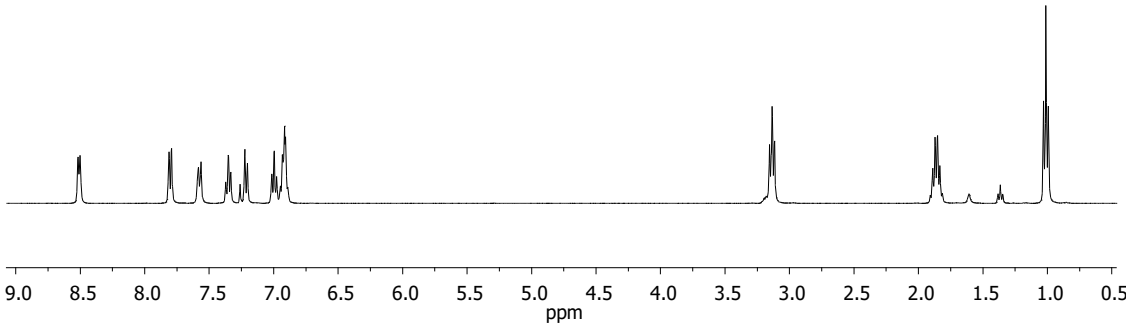


Figure S9: ^1H NMR spectrum ($CDCl_3$, 298 K) of **C3-BF$_2$**.

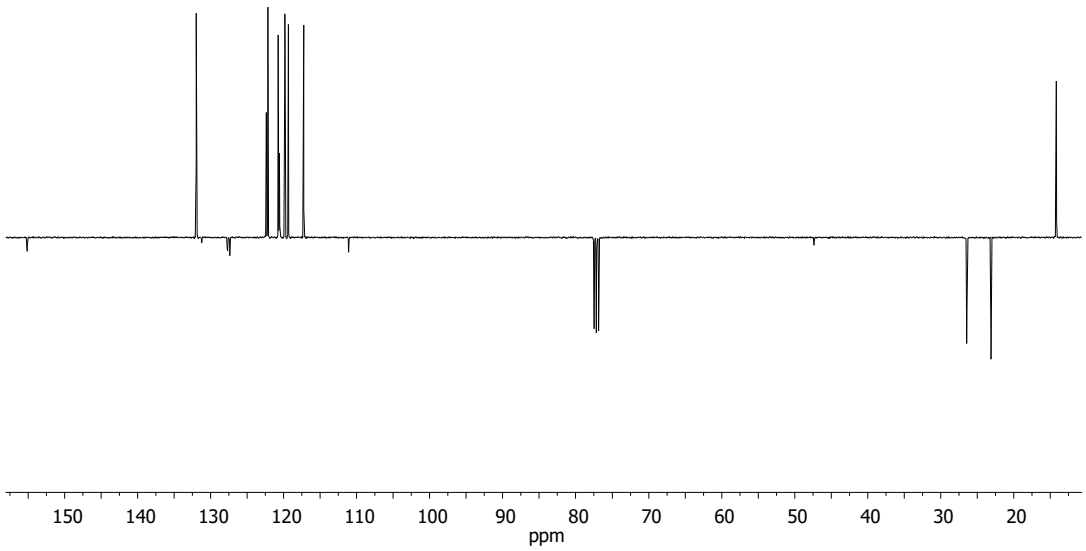
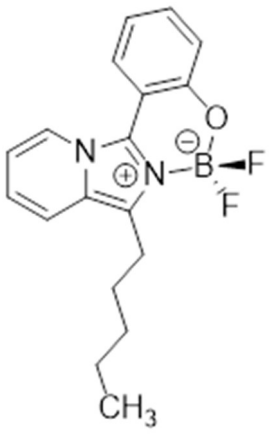


Figure S10: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C3-BF$_2$**.



C5-BF$_2$: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.41 (d, *J* = 7.2 1H), 7.78 (d, *J* = 7.9, 1H), 7.62 – 7.48 (m, 1H), 7.32 (t, *J* = 7.6, 1H), 7.19 (d, *J* = 8.2, 1H), 7.04 – 6.83 (m, 3H), 3.14 (t, *J* = 7.7, 2H), 1.81 (m, 2H), 1.38 (m, 4H), 0.89 (t, *J* = 6.7, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 155.10, 131.88, 131.11, 127.61, 127.54, 122.40, 122.16, 120.74, 120.53, 119.81, 119.28, 117.25, 111.11, 31.78, 29.45, 24.47, 22.46, 14.07. FT-IT (ATR) (cm^{-1}): ṽ = 1005 – 1131 (BF_2), 2869 – 2960 (aliphatic C-H).

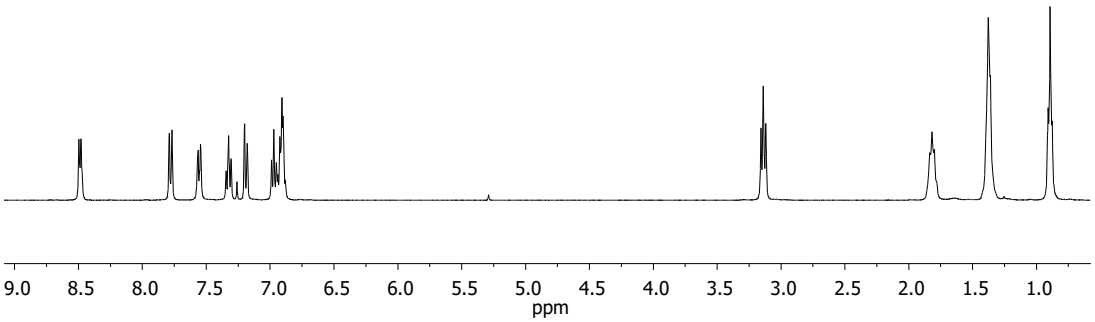


Figure S11: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C5-BF$_2$**.

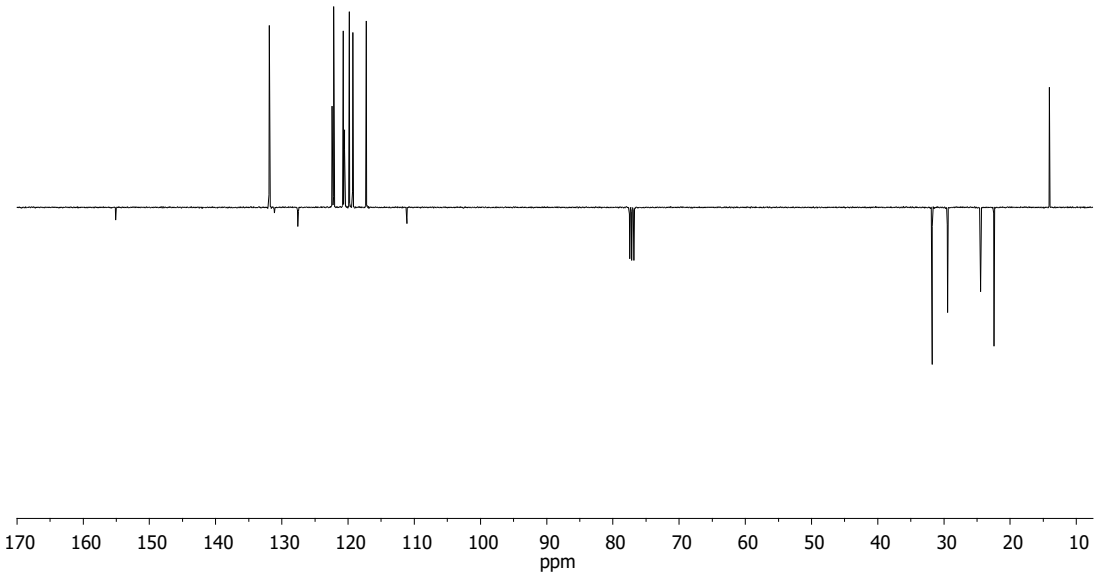
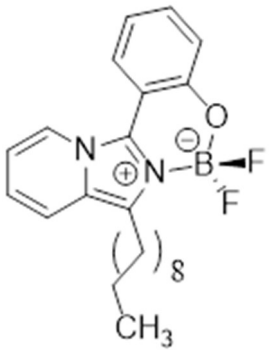


Figure S12: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C5-BF$_2$**.



C10-BF$_2$: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.49 (d, *J* = 7.7, 1H), 7.78 (d, *J* = 7.2, 1H), 7.60 (m, 1H), 7.35 (t, *J* = 7.2, 1H), 7.27 (d, *J* = 9.4, 1H), 7.11 – 7.02 (m, 1H), 6.99 – 6.84 (m, 2H), 3.28 – 3.11 (m, 5H), 1.88 – 1.76 (m, 2H), 1.38 (m, 8H), 1.35 – 1.17 (m, 13H), 0.87 (t, *J* = 6.7, 3H). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 155.34, 132.15, 127.90, 127.58, 122.42, 122.17, 120.81, 120.61, 119.93, 119.54, 117.24, 111.25, 47.22, 32.03, 29.84, 29.73, 29.71, 29.47, 29.45, 24.61, 22.82, 14.25. FT-IT (ATR) (cm^{-1}): ṽ = 1012 – 1154 (BF_2), 2845 – 2949 (aliphatic C-H).

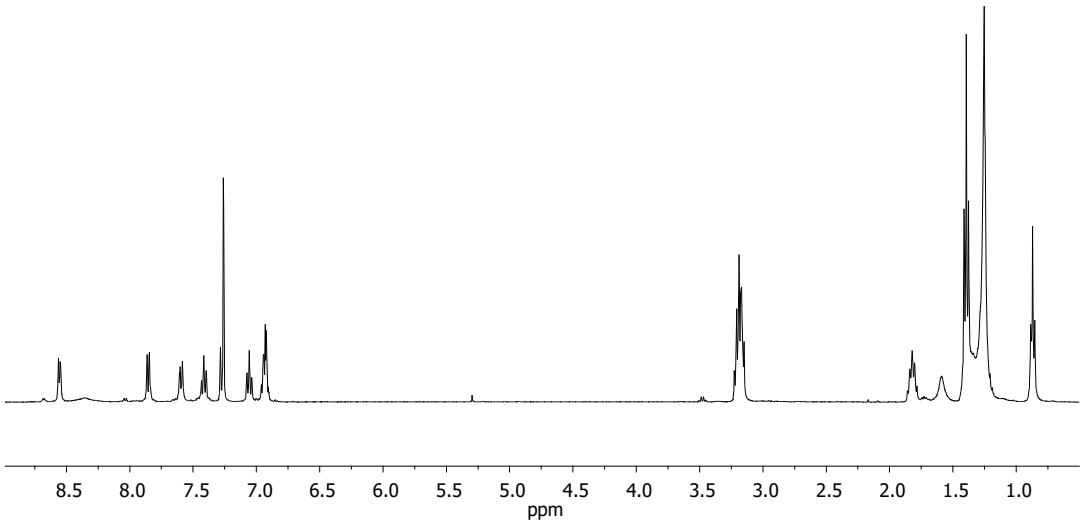


Figure S13: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C10-BF$_2$**.

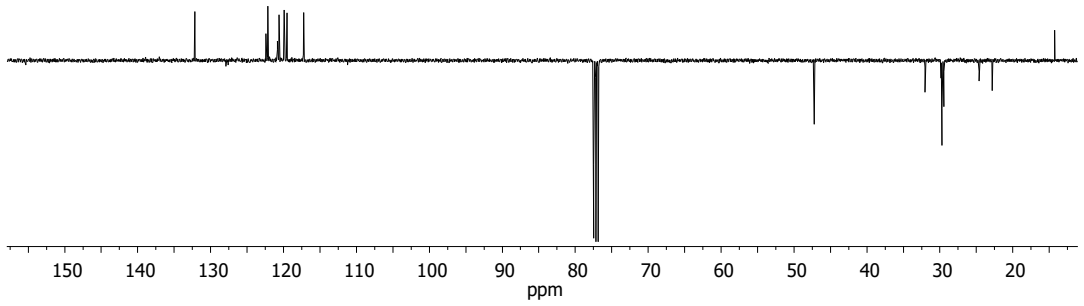
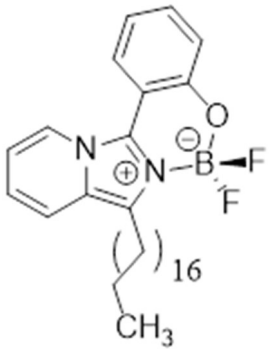


Figure S14: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C10-BF$_2$**.



C18-BF$_2$: ^{1}H NMR (400 MHz, $CDCl_3$, 298 K, *J* [Hz]): δ = 8.54 (d, *J* = 5.9, 1H), 7.83 (d, *J* = 8.0, 1H), 7.62 – 7.55 (m, 1H), 7.39 (t, *J* = 7.8, 1H), 7.26 (t, *J* = 6.6, 1H), 7.02 t, *J* = 7.8, 1H), 6.99 – 6.86 (m, 2H), 3.17 (t, *J* = 7.7, 2H), 1.83 (m, 2H), 1.48 – 1.16 (m, 30H), 0.89 (t, *J* = 6.7, 3H).^{13}C NMR (100 MHz, $CDCl_3$, 298 K): δ = 155.27, 132.04, 131.26, 127.80, 127.56, 122.42, 122.16, 120.71, 120.64, 119.88, 119.44, 117.24, 111.17, 32.07, 29.84, 29.80, 29.74, 29.72, 29.50, 29.48, 24.59, 22.83, 14.25. FT-IT (ATR) (cm^{-1}): ṽ = 1041 – 1152 (BF_2), 2845 – 2956 (aliphatic C-H).

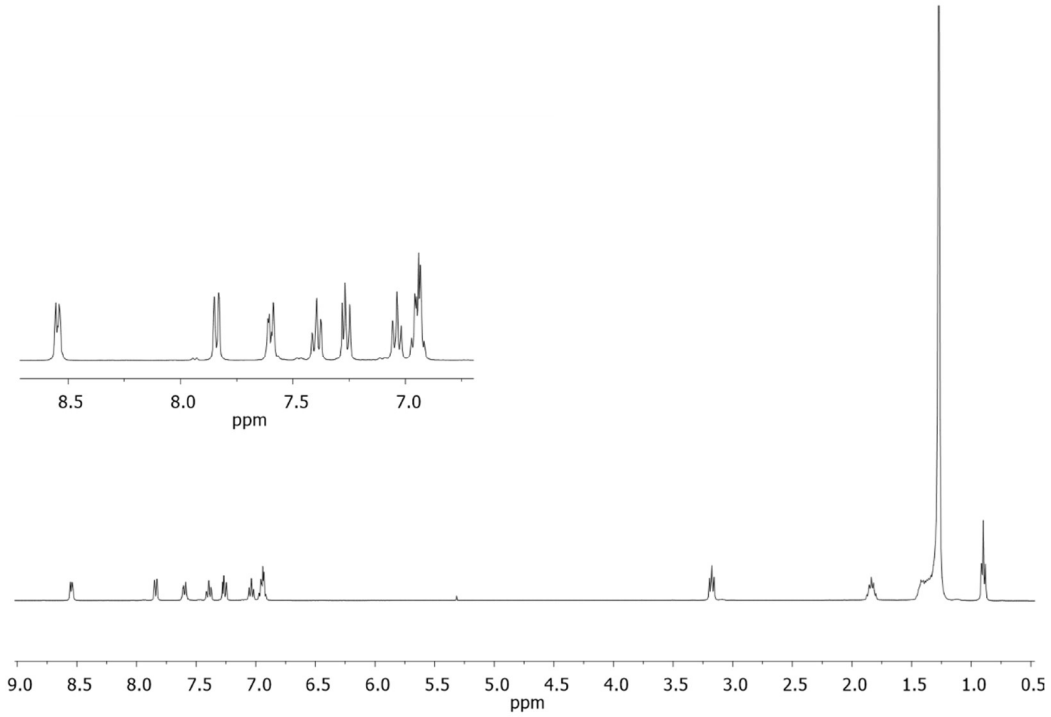


Figure S15: ^{1}H NMR spectrum ($CDCl_3$, 298 K) of **C18-BF$_2$**.

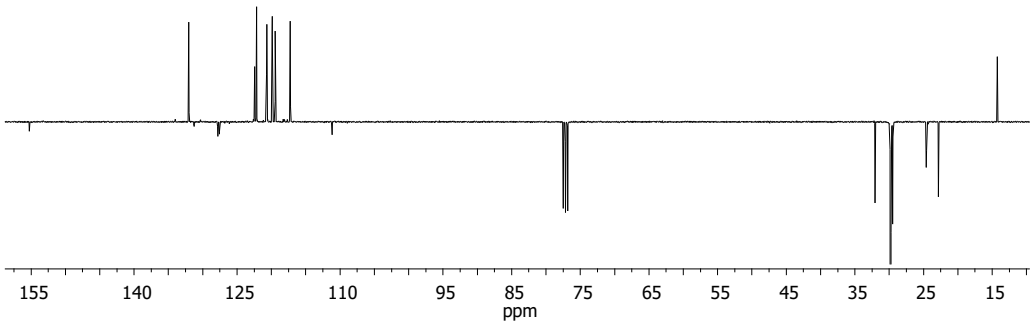


Figure S16: ^{13}C NMR spectrum ($CDCl_3$, 298 K) of **C18-BF$_2$**.

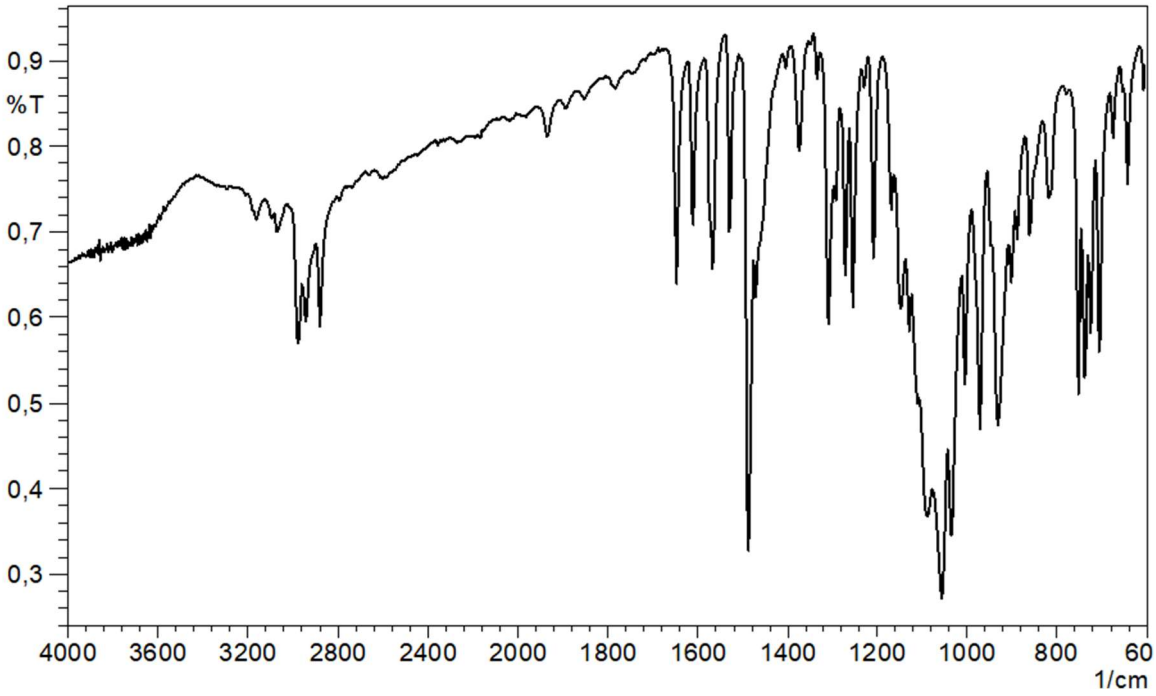


Figure S17: IR spectrum (ATR) of **C3-BF_2**.

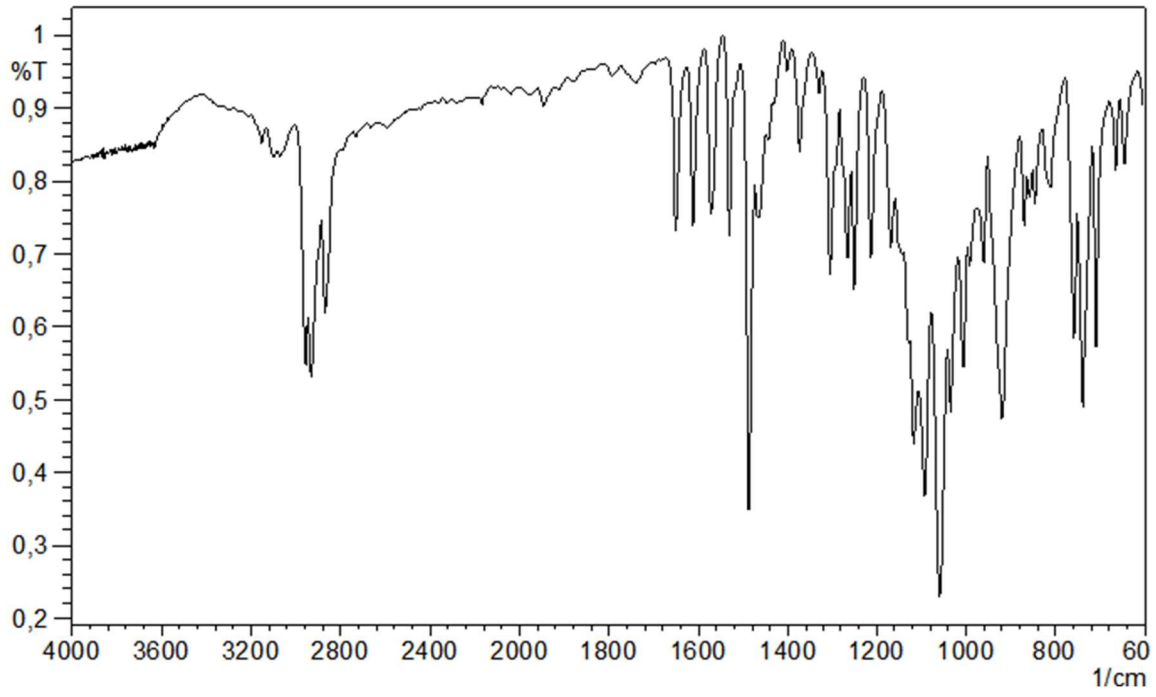


Figure S18: IR spectrum (ATR) of **C5-BF_2**.

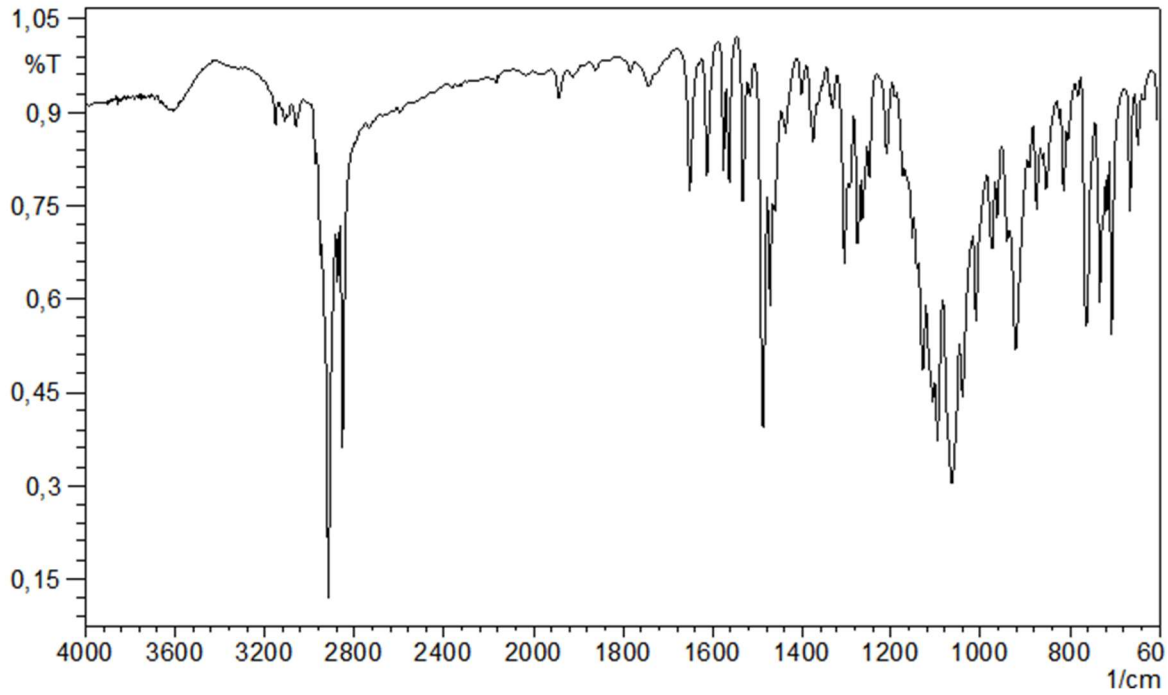


Figure S19: IR spectrum (ATR) of **C10-BF$_2$**.

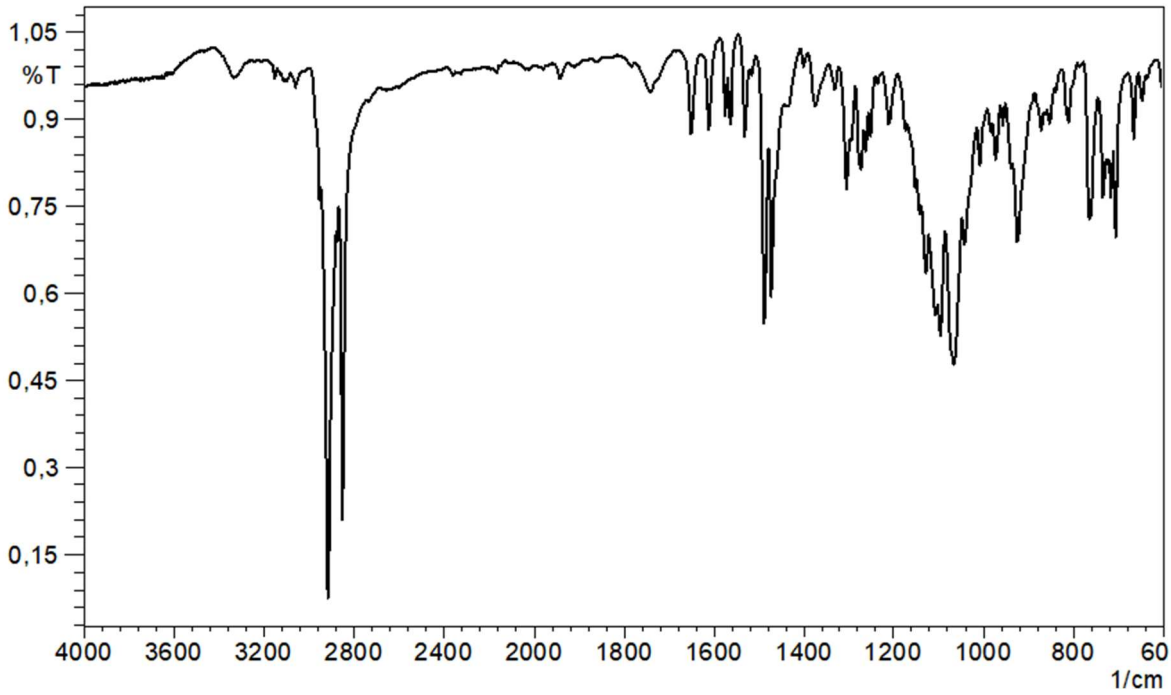


Figure S20: IR spectrum (ATR) of **C18-BF$_2$**.

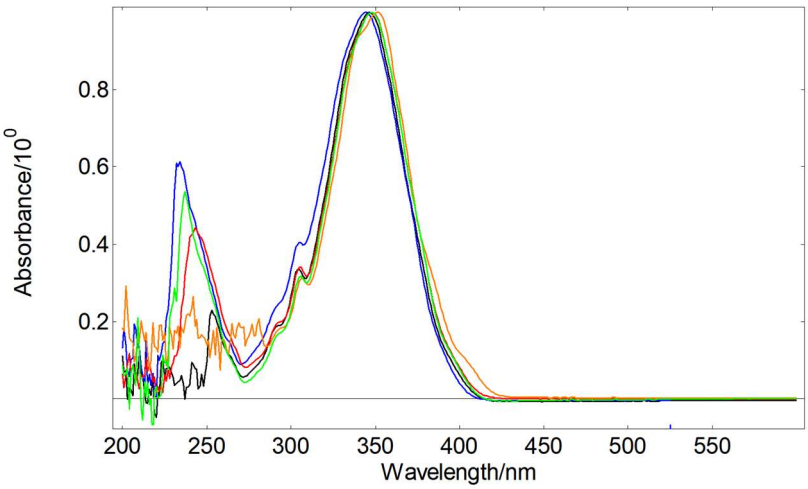


Figure S21: Normalized absorption spectra of **C3-BF$_2$** recorded in solution in different solvents ($5x10^{-5}$ M). Dichloromethane, green; toluene, orange; tetrahydrofuran, red; methanol, blue; ethyl acetate, black.

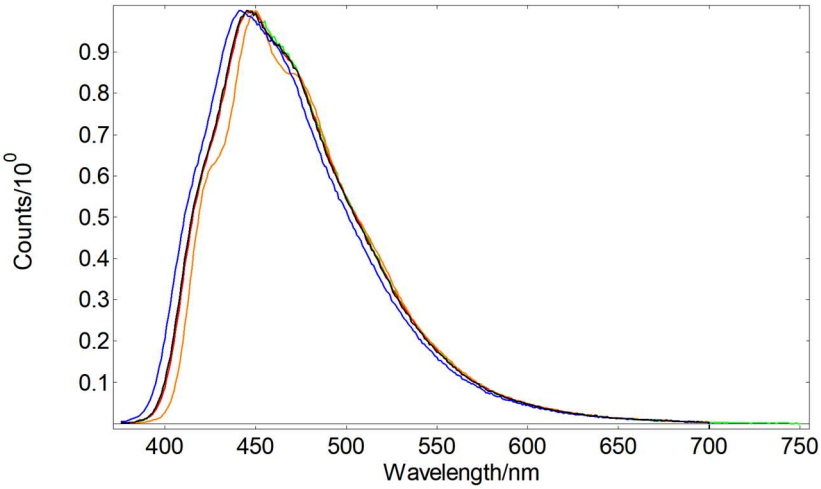


Figure S22: Normalized emission spectra of **C3-BF$_2$** recorded in solution in different solvents ($5x10^{-5}$ M). Dichloromethane, green; toluene, orange; tetrahydrofuran, red; methanol, blue; ethyl acetate, black.

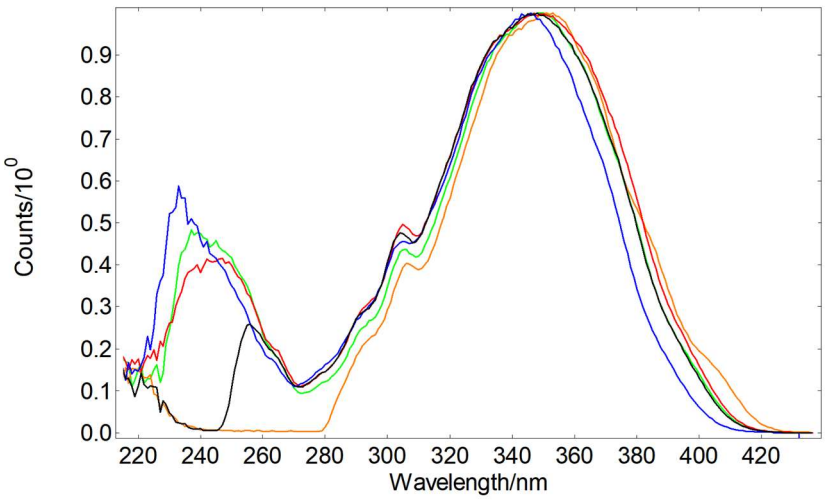


Figure S23: Normalized excitation spectra of **C3-BF$_2$** recorded in solution in different solvents ($5x10^{-5}$ M). Dichloromethane, green; toluene, orange; tetrahydrofuran, red; methanol, blue; ethyl acetate, black.

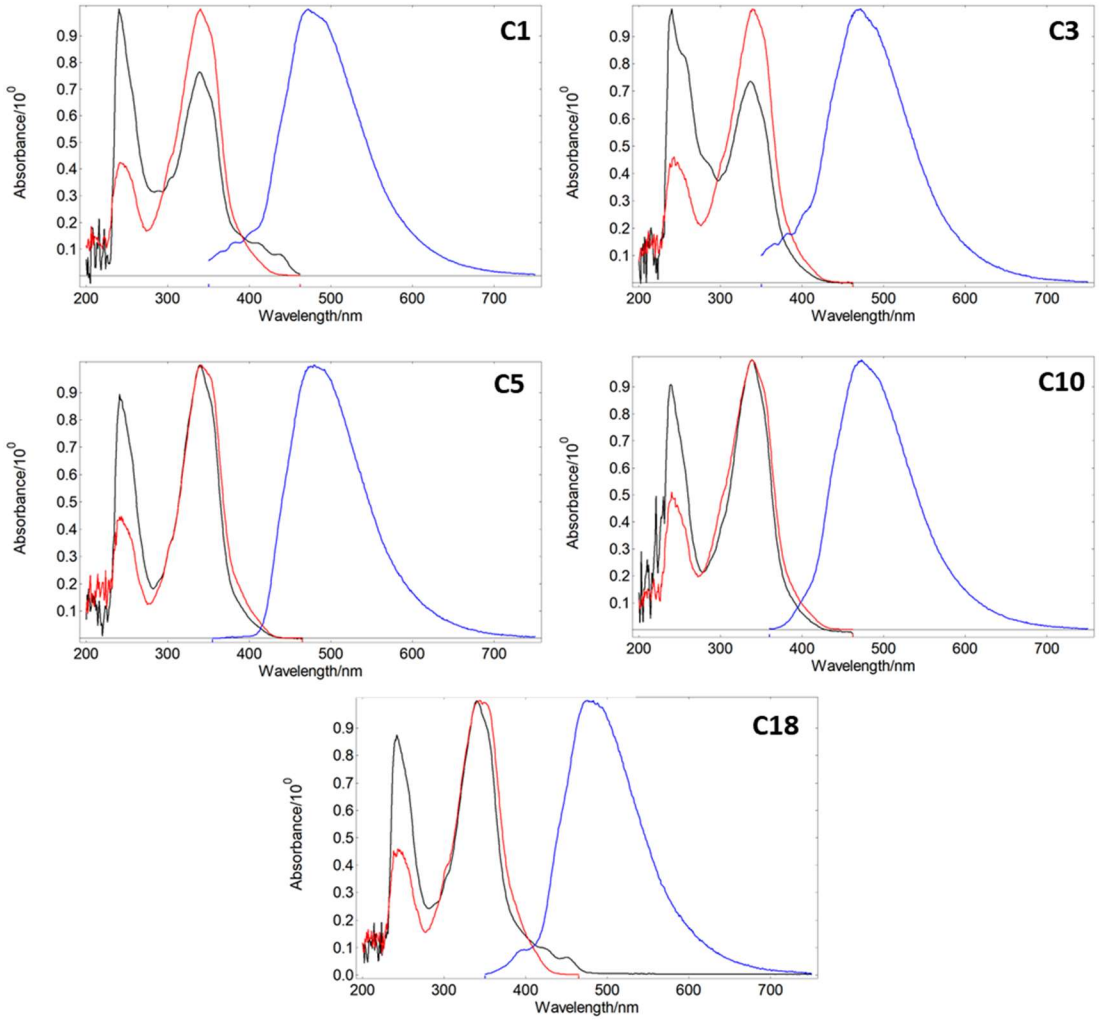


Figure S24: Normalized absorption (black), emission (blue) and excitation (red) spectra of **CX** recorded dichloromethane solution ($5x10^{-5}$ M).

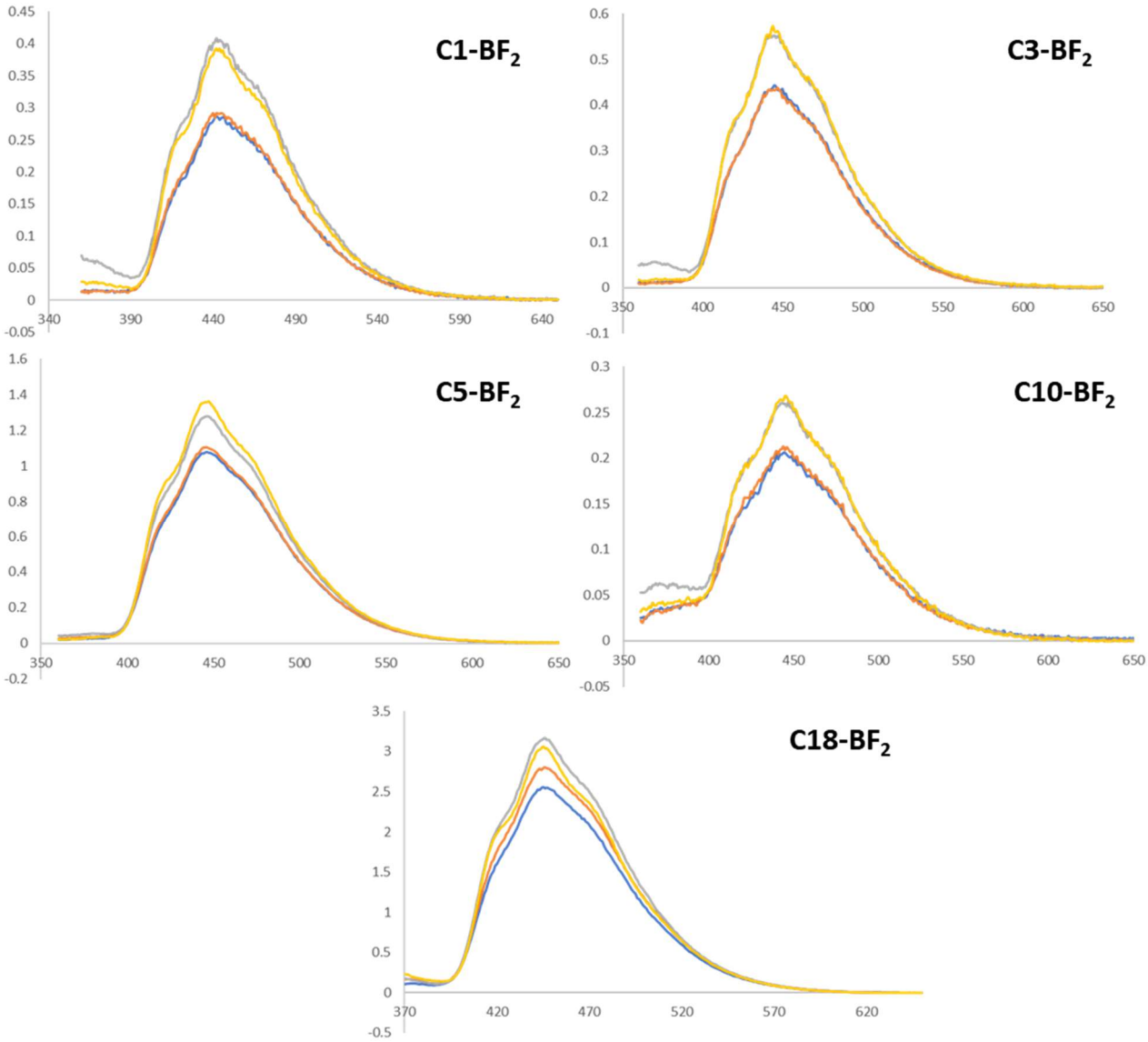


Figure S25: Emission spectra of **CX-BF$_2$** recorded in dichloromethane solution (5x10^{-5} M) at different temperatures: 298 K, blue; 273 K, orange; 233 K, grey; 193 K, yellow.