Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information

Experimental details

A Reaction-based Chromogenic and Fluorescent Chemodosimeter for Fluoride Anion

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Materials. All reactions were carried out under an argon atmosphere by using standard Schlenk techniques. Solvents were dried and distilled from appropriate drying agents under an inert atmosphere prior to use. Glassware was oven-dried at about 120 ^{o}C. All reagents and chemicals, unless otherwise stated, were purchased from commercial sources and used without further purification.

Apparatus. NMR spectra were measured in appropriate deuterated solvents on a JEOL EX270 or a Varian Inova 400 MHz FT-NMR spectrometer, with ^{1}H NMR chemical shifts quoted relative to $SiMe_4$. Fast-atom bombardment (FAB) mass spectra were recorded on a Finnigan MAT SSQ710 mass spectrometer in m-nitrobenzyl alcohol matrices. Fluorescence spectra were measured using a Perkin-Elmer LS-55 spectrofluorophotometer. A UNICO 4802 UV-vis double-beam spectrophotometer was used to measure absorption spectra.

Spectroscopic titrations with anions. Stock solutions of the anions (0.5 mM) such as Cl^-, Br^-, I^-, ClO_4^-, $H_2PO_4^-$, CH_3COO^-, SCN^-, CO_3^{2-}, NO_3^- and SO_4^{2-} here were prepared in the form of K^+ salts in de-ionized water. Stock solution of BODIPY **dye 3** (0.6 mM) and TBAF (1.5 mM) was prepared in acetone. For absorptive and fluorometric measurements, 8 μM of BODIPY **dye 3** was used. The emission spectra were obtained by excitation at 400 nm, and emission was collected from 400-700 nm. Both excitation and emission slit widths were 10 mm. All the spectroscopic data were collected after 5 min of equilibrium.

Limit of detection (LOD). At 550 nm, the enhanced intensity has linear regression relationship with the concentration of F^- within the range of 4-16 μM. The linear regression equation was $\Delta I = -80.39 + 28.49\ C_{F^-}$ (μM), where $\Delta I = I - I_0$ and C_{F^-} is the concentration of F^-, with correlation coefficient $R^2 = 0.9737$. The limit of detection was 67.4 nM calculated by 3σ/S, where σ represents the standard deviation of 10 blank determinations, and S is the slope of the calibration curve. That is corresponding to 1.28 ppb ($67.4\times10^{-9}\times19/1000 = 1.28\times10^{-9}$).

Preparation of BODIPY dyes

BODIPY dye 1 2,4,6-Trimethylbenzaldehyde (19 mmol, 2.81g) and 2,4-dimethylpyrrole (38 mmol, 3.61g) were dissolved in 500 mL of dry CH_2Cl_2. After

1 mL of TFA was added to the reaction mixture, the mixture was stirred for 3 h at room temperature under Argon atmosphere. DDQ (19 mmol, 4.3 g) was then added. After stirring for 30 min, triethylamine (40 mL) and $BF_3{\cdot}OEt_2$ (40 mL) were added. After the mixture was stirred overnight, it was washed twice with water and the organic phase was concentrated. The crude product was purified by column chromatography on silica gel using petroleum ether/dichloromethane (70/30, v/v) to obtain an orange crystalline solid (3.3 g, 20%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.94 (s, 2H), 5.95 (s, 2H), 2.55 (s, 6H), 2.33 (s, 3H), 2.09 (s, 6H), 1.38 (s, 6H). MS: 366 (M^+).

BODIPY dye 2 BODIPY **dye 1** (8.7 mmol, 3.2 g) and N-iodosuccinimide (NIS, 35.2 mmol, 7.92 g) were dissolved in 50 mL of CH_2Cl_2. After the mixture was stirred for 12 h, it was concentrated under reduced pressure and purified by column chromatography on silica gel using petroleum ether/dichloromethane (70/30, v/v) to obtain a dark red solid (4.5 g, 80%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.97 (s, 2H), 2.64 (s, 6H), 2.36 (s, 3 H), 2.06 (s, 6H), 1.39 (s, 6H). MS: 618 (M^+).

BODIPY dye 3 BODIPY **dye 2** (7.1 mmol, 4.4 g), CuI (0.7 mmol, 0.14 g) and $Pd(PPh_3)_4$ (0.38 mmol, 0.44 g) were added to a 250 mL two-neck round-bottom flask and were kept at inert atmosphere. When anhydrous THF (100 mL), anhydrous triethylamine (50 mL) and trihexylsilylacetylene (32.4 mmol, 10 mL) were added to the flask, the mixture was refluxed for 4 h under nitrogen atmosphere. After the completion of the reaction (which was monitored by TLC), the reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel using petroleum ether/dichloromethane (80/20, v/v) to obtain a red oily solid (5.1 g, 74%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.96 (s, 2H), 2.64 (s, 6H), 2.34 (s, 3H), 2.05 (s, 6H), 1.46 (s, 6H), 1.34-1.26 (m, 48H), 0.88-0.84 (m, 18H), 0.64-0.59 (m, 12H). MS: 979 (M^+).

Calculations

Calculations were performed with Gaussian 09[1] at the Université de Sherbrooke with Mammouth super computer supported by le Réseau Québécois de Calculs de Haute Performances. The DFT[2-5] and TD-DFT[6-8] were calculated with the B3LYP[9-11] method. 6-31G(d)[12-21] basis sets were used for all the atoms. The default Gaussian 09 SCRF Polarizable Continuum Model (PCM) for acetone was included to the final

TD-DFT calculation. The calculated absorption spectra were obtained from GaussView 05[22] and the related MO contributions from gausssum 2.1[23].

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GaussView 05

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Gaussum 2.1

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Experimental section for the X-ray structure:

The crystals were grown by slow evaporation of a MeOH/chlorobenzene solution at room temperature**.** One single crystal of 0.30 X 0.40 X 0.50 mm^3 was mounted using a glass fiber at 293(2) K on the goniometer. Data were collected on an Enraf-Nonius CAD-4 automatic diffractometer at the Université de Sherbrooke using ω scans. The DIFRAC[1] program was used for centering, indexing, and data collection. One standard reflection was measured every 100 reflections, 12% intensity decay was observed during data collection. The data were corrected for absorption by empirical methods based on psi scans and reduced with the NRCVAX[2] programs. They were solved using SHELXS-97[3] and refined by full-matrix least squares on F^2 with SHELXL-97[4]. The non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed at idealized calculated geometric position and refined isotropically using a riding model.

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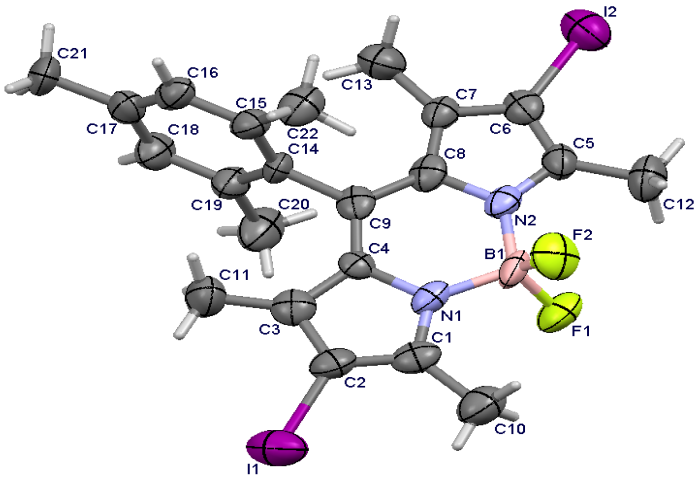

Fig. S1 The X-ray crystal structure of BODIPY **dye 2**. Selected bond length (Å) and bond angles (°): C(1)-N(1) 1.342(10), B(1)-N(1) 1.529(12), C(4)-N(1) 1.410(9), C(2)-I(1) 2.082(9), B(1)-F(1) 1.376(10), N(1)-C(1)-C(2) 107.3(8), C(1)-N(1)-C(4) 109.4(7), N(1)-B(1)-N(2) 108.4(7), F(1)-B(1)-F(2) 108.9(7), F(1)-B(1)-N(1) 111.9(8), C(4)-C(9)-C(8) 120.3(8).

Table S1 Crystal data and structure refinement for BODIPY dye 3.

Identification code	BODIPY 3	
Empirical formula	C22 H23 B F2 I2 N2	
Formula weight	618.03	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.918(7) Å	α= 90°.
	b = 10.565(6) Å	β= 108.26(3)°.
	c = 21.838(10) Å	γ = 90°.
Volume	4583(4) $Å^3$	
Z	8	
Density (calculated)	1.791 Mg/m^3	
Absorption coefficient	2.771 mm^{-1}	
F(000)	2384	
Crystal size	0.50 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.96 to 25.60°.	
Index ranges	-25<=h<=24, 0<=k<=12, 0<=l<=26	
Reflections collected	4272	
Independent reflections	4272 [R(int) = 0.0000]	
Completeness to theta = 25.50°	99.3 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.4902 and 0.3379	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4272 / 0 / 262	
Goodness-of-fit on F^2	0.934	
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1234	
R indices (all data)	R1 = 0.1613, wR2 = 0.1460	
Largest diff. peak and hole	0.718 and -0.647 $e.Å^{-3}$	

Table S2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for BODIPY dye 3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9397(4)	7671(8)	4362(5)	53(2)
C(2)	9358(4)	7465(8)	3721(4)	54(2)
C(3)	9062(4)	8488(8)	3335(4)	53(2)
C(4)	8924(3)	9371(7)	3775(4)	37(2)
C(5)	8658(4)	11659(9)	5226(4)	51(2)
C(6)	8419(4)	12749(9)	4875(4)	52(2)
C(7)	8377(4)	12552(8)	4239(4)	46(2)
C(8)	8598(4)	11294(9)	4214(4)	48(2)
C(9)	8651(4)	10584(8)	3684(4)	47(2)
C(10)	9675(5)	6824(9)	4940(4)	73(3)
C(11)	8938(5)	8591(9)	2636(4)	70(3)
C(12)	8800(5)	11416(10)	5933(4)	70(3)
C(13)	8108(5)	13502(9)	3712(4)	70(3)
C(14)	8410(4)	11141(7)	3024(3)	39(2)
C(15)	7739(4)	10967(8)	2656(4)	50(2)
C(16)	7528(5)	11450(8)	2024(4)	52(2)
C(17)	7951(5)	12021(8)	1748(4)	53(2)
C(18)	8617(4)	12180(9)	2124(4)	59(2)
C(19)	8856(4)	11730(8)	2766(4)	51(2)
C(20)	9582(4)	11946(11)	3169(4)	80(3)
C(21)	7714(5)	12481(10)	1054(4)	74(3)
C(22)	7246(4)	10362(9)	2931(4)	65(3)
B(1)	9055(5)	9421(11)	5003(4)	54(3)
F(1)	9658(2)	9463(5)	5494(2)	71(2)
F(2)	8591(3)	8747(5)	5213(2)	73(2)
I(1)	9719(1)	5834(1)	3407(1)	86(1)
I(2)	8158(1)	14389(1)	5268(1)	76(1)
N(1)	9129(3)	8814(6)	4393(3)	43(2)
N(2)	8786(3)	10810(7)	4836(3)	45(2)

Table S3 Bond lengths [Å] and angles [°] for BODIPY dye 3.

C(1)-N(1)	1.342(10)
C(1)-C(2)	1.393(11)
C(1)-C(10)	1.508(11)
C(2)-C(3)	1.390(11)
C(2)-I(1)	2.082(9)
C(3)-C(4)	1.432(11)
C(3)-C(11)	1.471(11)
C(4)-C(9)	1.392(10)
C(4)-N(1)	1.410(9)
C(5)-N(2)	1.321(10)
C(5)-C(6)	1.388(12)
C(5)-C(12)	1.501(11)
C(6)-C(7)	1.379(10)
C(6)-I(2)	2.080(9)
C(7)-C(8)	1.414(11)
C(7)-C(13)	1.498(11)
C(8)-N(2)	1.388(10)
C(8)-C(9)	1.413(11)
C(9)-C(14)	1.491(10)
C(14)-C(19)	1.380(10)
C(14)-C(15)	1.394(10)
C(15)-C(16)	1.406(11)
C(15)-C(22)	1.493(11)
C(16)-C(17)	1.358(11)
C(17)-C(18)	1.388(11)
C(17)-C(21)	1.520(10)
C(18)-C(19)	1.415(11)
C(19)-C(20)	1.514(11)
B(1)-F(1)	1.376(10)
B(1)-F(2)	1.391(11)
B(1)-N(1)	1.529(12)
B(1)-N(2)	1.573(12)
N(1)-C(1)-C(2)	107.3(8)
N(1)-C(1)-C(10)	123.3(9)
C(2)-C(1)-C(10)	129.4(9)

C(3)-C(2)-C(1)	111.2(8)
C(3)-C(2)-I(1)	125.6(7)
C(1)-C(2)-I(1)	123.1(7)
C(2)-C(3)-C(4)	104.1(8)
C(2)-C(3)-C(11)	125.9(9)
C(4)-C(3)-C(11)	129.9(8)
C(9)-C(4)-N(1)	120.7(7)
C(9)-C(4)-C(3)	131.5(8)
N(1)-C(4)-C(3)	107.8(7)
N(2)-C(5)-C(6)	108.5(7)
N(2)-C(5)-C(12)	122.2(8)
C(6)-C(5)-C(12)	129.1(9)
C(7)-C(6)-C(5)	109.2(8)
C(7)-C(6)-I(2)	126.8(7)
C(5)-C(6)-I(2)	124.0(7)
C(6)-C(7)-C(8)	105.3(8)
C(6)-C(7)-C(13)	124.2(9)
C(8)-C(7)-C(13)	130.4(8)
N(2)-C(8)-C(9)	122.4(8)
N(2)-C(8)-C(7)	107.7(7)
C(9)-C(8)-C(7)	129.9(8)
C(4)-C(9)-C(8)	120.3(8)
C(4)-C(9)-C(14)	120.1(7)
C(8)-C(9)-C(14)	119.6(8)
C(19)-C(14)-C(15)	120.8(7)
C(19)-C(14)-C(9)	120.4(7)
C(15)-C(14)-C(9)	118.7(7)
C(14)-C(15)-C(16)	117.9(8)
C(14)-C(15)-C(22)	121.5(7)
C(16)-C(15)-C(22)	120.4(8)
C(17)-C(16)-C(15)	123.2(9)
C(16)-C(17)-C(18)	117.7(8)
C(16)-C(17)-C(21)	122.0(9)
C(18)-C(17)-C(21)	120.3(8)
C(17)-C(18)-C(19)	121.6(8)
C(14)-C(19)-C(18)	118.7(8)
C(14)-C(19)-C(20)	120.9(7)
C(18)-C(19)-C(20)	120.3(8)

F(1)-B(1)-F(2)	108.9(7)
F(1)-B(1)-N(1)	111.9(8)
F(2)-B(1)-N(1)	110.1(8)
F(1)-B(1)-N(2)	108.9(8)
F(2)-B(1)-N(2)	108.6(7)
N(1)-B(1)-N(2)	108.4(7)
C(1)-N(1)-C(4)	109.4(7)
C(1)-N(1)-B(1)	125.5(7)
C(4)-N(1)-B(1)	125.1(7)
C(5)-N(2)-C(8)	109.2(7)
C(5)-N(2)-B(1)	127.8(7)
C(8)-N(2)-B(1)	122.9(7)

Symmetry transformations used to generate equivalent atoms.

Table S4 Anisotropic displacement parameters ($Å^2 x\ 10^3$)for BODIPY dye 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	33(5)	51(6)	65(7)	4(5)	2(4)	-5(4)
C(2)	38(5)	58(6)	59(6)	9(5)	5(5)	6(4)
C(3)	39(5)	58(6)	58(6)	-4(5)	11(5)	-11(4)
C(4)	27(4)	43(5)	42(5)	2(4)	14(4)	-2(4)
C(5)	44(5)	72(7)	36(5)	-3(5)	12(4)	0(5)
C(6)	37(5)	65(6)	49(6)	-12(5)	8(4)	-6(5)
C(7)	35(5)	61(6)	40(5)	7(5)	10(4)	-3(4)
C(8)	37(5)	61(6)	38(5)	-4(5)	2(4)	-13(4)
C(9)	27(4)	67(6)	41(5)	-6(5)	5(4)	-10(4)
C(10)	60(6)	85(7)	66(6)	17(6)	8(5)	5(6)
C(11)	85(7)	73(7)	47(6)	-3(5)	15(5)	8(6)
C(12)	73(7)	93(8)	45(6)	5(5)	21(5)	-13(6)
C(13)	66(7)	75(7)	75(7)	4(6)	29(6)	16(6)
C(14)	43(5)	47(5)	24(4)	7(4)	7(4)	6(4)
C(15)	42(5)	54(6)	46(5)	2(4)	5(4)	9(4)
C(16)	56(6)	49(5)	42(5)	-2(5)	2(5)	6(5)
C(17)	69(6)	48(5)	43(5)	-3(4)	19(5)	10(5)
C(18)	50(6)	78(7)	55(6)	16(5)	26(5)	1(5)
C(19)	41(5)	68(6)	47(6)	11(5)	16(4)	6(5)
C(20)	52(6)	124(10)	69(7)	28(7)	25(5)	-3(6)
C(21)	89(7)	101(8)	29(5)	12(5)	13(5)	30(6)
C(22)	47(5)	83(7)	61(6)	17(5)	12(5)	-10(5)
B(1)	46(6)	86(8)	25(5)	16(6)	4(5)	1(6)
F(1)	59(3)	89(4)	49(3)	11(3)	-8(3)	6(3)
F(2)	74(4)	81(4)	79(4)	12(3)	44(3)	-18(3)
I(1)	66(1)	77(1)	106(1)	-13(1)	13(1)	17(1)
I(2)	67(1)	85(1)	80(1)	-20(1)	28(1)	-2(1)
N(1)	35(4)	50(4)	39(4)	13(4)	2(3)	-5(3)
N(2)	30(4)	64(5)	39(4)	11(4)	6(3)	0(4)

Table S5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for BODIPY dye 3.

	x	y	z	U(eq)
H(3A)	9853	6067	4812	109
H(3B)	9323	6608	5116	109
H(3C)	10028	7260	5261	109
H(5A)	9091	7836	2481	104
H(5B)	9177	9309	2548	104
H(5C)	8464	8697	2422	104
H(12A)	8662	12136	6129	105
H(12B)	9273	11275	6131	105
H(12C)	8555	10682	5992	105
H(10A)	8105	13141	3308	106
H(10B)	8388	14241	3800	106
H(10C)	7657	13732	3691	106
H(21)	7076	11375	1783	63
H(18)	8913	12592	1950	70
H(17A)	9807	12422	2923	121
H(17B)	9803	11145	3287	121
H(17C)	9596	12408	3551	121
H(20A)	8081	12881	954	111
H(20B)	7354	13079	998	111
H(20C)	7556	11774	770	111
H(23A)	7473	10089	3364	97
H(23B)	7044	9645	2672	97
H(23C)	6902	10963	2934	97

Table S6 Torsion angles [°] for BODIPY dye 3.

N(1)-C(1)-C(2)-C(3)	0.1(10)
C(10)-C(1)-C(2)-C(3)	179.8(8)
N(1)-C(1)-C(2)-I(1)	179.1(5)
C(10)-C(1)-C(2)-I(1)	-1.3(13)
C(1)-C(2)-C(3)-C(4)	0.9(9)
I(1)-C(2)-C(3)-C(4)	-178.0(5)
C(1)-C(2)-C(3)-C(11)	-179.7(8)
I(1)-C(2)-C(3)-C(11)	1.3(13)
C(2)-C(3)-C(4)-C(9)	177.7(8)
C(11)-C(3)-C(4)-C(9)	-1.6(14)
C(2)-C(3)-C(4)-N(1)	-1.5(8)
C(11)-C(3)-C(4)-N(1)	179.1(8)
N(2)-C(5)-C(6)-C(7)	2.1(10)
C(12)-C(5)-C(6)-C(7)	178.9(8)
N(2)-C(5)-C(6)-I(2)	-178.9(5)
C(12)-C(5)-C(6)-I(2)	-2.1(13)
C(5)-C(6)-C(7)-C(8)	0.1(9)
I(2)-C(6)-C(7)-C(8)	-178.9(6)
C(5)-C(6)-C(7)-C(13)	177.0(8)
I(2)-C(6)-C(7)-C(13)	-2.0(12)
C(6)-C(7)-C(8)-N(2)	-2.2(9)
C(13)-C(7)-C(8)-N(2)	-178.8(8)
C(6)-C(7)-C(8)-C(9)	179.1(8)
C(13)-C(7)-C(8)-C(9)	2.5(15)
N(1)-C(4)-C(9)-C(8)	2.4(11)
C(3)-C(4)-C(9)-C(8)	-176.8(8)
N(1)-C(4)-C(9)-C(14)	-177.4(7)
C(3)-C(4)-C(9)-C(14)	3.4(12)
N(2)-C(8)-C(9)-C(4)	-2.6(11)
C(7)-C(8)-C(9)-C(4)	176.0(8)
N(2)-C(8)-C(9)-C(14)	177.2(7)
C(7)-C(8)-C(9)-C(14)	-4.2(13)
C(4)-C(9)-C(14)-C(19)	-83.9(10)
C(8)-C(9)-C(14)-C(19)	96.3(9)
C(4)-C(9)-C(14)-C(15)	91.1(9)
C(8)-C(9)-C(14)-C(15)	-88.7(9)

C(19)-C(14)-C(15)-C(16)	-2.3(12)
C(9)-C(14)-C(15)-C(16)	-177.2(7)
C(19)-C(14)-C(15)-C(22)	-178.4(8)
C(9)-C(14)-C(15)-C(22)	6.6(12)
C(14)-C(15)-C(16)-C(17)	3.2(13)
C(22)-C(15)-C(16)-C(17)	179.4(8)
C(15)-C(16)-C(17)-C(18)	-3.0(13)
C(15)-C(16)-C(17)-C(21)	177.2(8)
C(16)-C(17)-C(18)-C(19)	2.0(13)
C(21)-C(17)-C(18)-C(19)	-178.2(8)
C(15)-C(14)-C(19)-C(18)	1.3(13)
C(9)-C(14)-C(19)-C(18)	176.2(8)
C(15)-C(14)-C(19)-C(20)	178.7(8)
C(9)-C(14)-C(19)-C(20)	-6.4(13)
C(17)-C(18)-C(19)-C(14)	-1.2(13)
C(17)-C(18)-C(19)-C(20)	-178.5(9)
C(2)-C(1)-N(1)-C(4)	-1.1(9)
C(10)-C(1)-N(1)-C(4)	179.2(7)
C(2)-C(1)-N(1)-B(1)	178.9(7)
C(10)-C(1)-N(1)-B(1)	-0.8(12)
C(9)-C(4)-N(1)-C(1)	-177.7(7)
C(3)-C(4)-N(1)-C(1)	1.7(8)
C(9)-C(4)-N(1)-B(1)	2.4(11)
C(3)-C(4)-N(1)-B(1)	-178.3(7)
F(1)-B(1)-N(1)-C(1)	54.1(11)
F(2)-B(1)-N(1)-C(1)	-67.2(10)
N(2)-B(1)-N(1)-C(1)	174.2(7)
F(1)-B(1)-N(1)-C(4)	-126.0(8)
F(2)-B(1)-N(1)-C(4)	112.8(8)
N(2)-B(1)-N(1)-C(4)	-5.9(10)
C(6)-C(5)-N(2)-C(8)	-3.5(9)
C(12)-C(5)-N(2)-C(8)	179.4(8)
C(6)-C(5)-N(2)-B(1)	-179.0(7)
C(12)-C(5)-N(2)-B(1)	3.9(13)
C(9)-C(8)-N(2)-C(5)	-177.6(7)
C(7)-C(8)-N(2)-C(5)	3.6(9)
C(9)-C(8)-N(2)-B(1)	-1.8(11)
C(7)-C(8)-N(2)-B(1)	179.3(7)

F(1)-B(1)-N(2)-C(5)	-57.6(11)
F(2)-B(1)-N(2)-C(5)	60.9(11)
N(1)-B(1)-N(2)-C(5)	-179.5(7)
F(1)-B(1)-N(2)-C(8)	127.5(7)
F(2)-B(1)-N(2)-C(8)	-114.0(8)
N(1)-B(1)-N(2)-C(8)	5.5(10)

Symmetry transformations used to generate equivalent atoms.

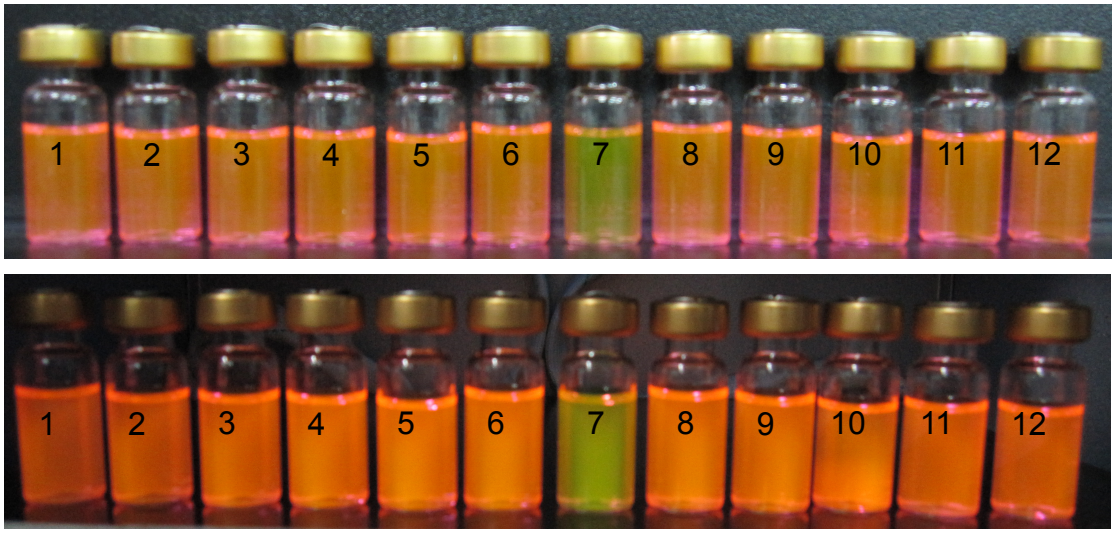

Fig. S2 Color changes of BODIPY **dye 3** with different anions (naked eye, upper; under UV lamp, bottom). From 1 to 12 (left to right): control, Cl^-, Br^-, I^-, ClO_4^-, $H_2PO_4^-$, F^-, CH_3COO^-, SCN^-, CO_3^{2-}, NO_3^- and SO_4^{2-}.

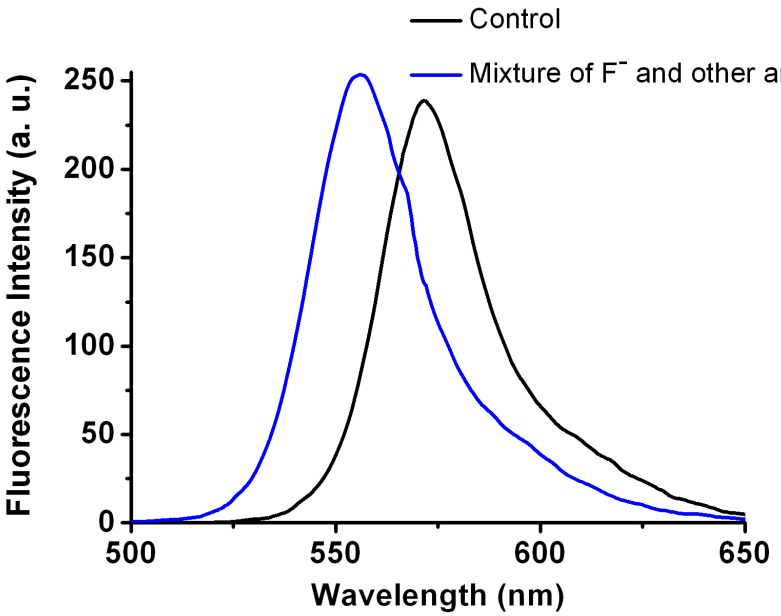

Fig. S3 Interference spectra of BODIPY **dye 3** in acetone. The concentration of BODIPY **dye 3** is 4 μM. The concentration of F^- is 40 μM and each concentration of other interference anions (Cl^-, Br^-, I^-, ClO_4^-, $H_2PO_4^-$, CH_3COO^-, SCN^-, CO_3^{2-}, NO_3^- and SO_4^{2-}) is 16 μM. They are all mixed inside one solution.

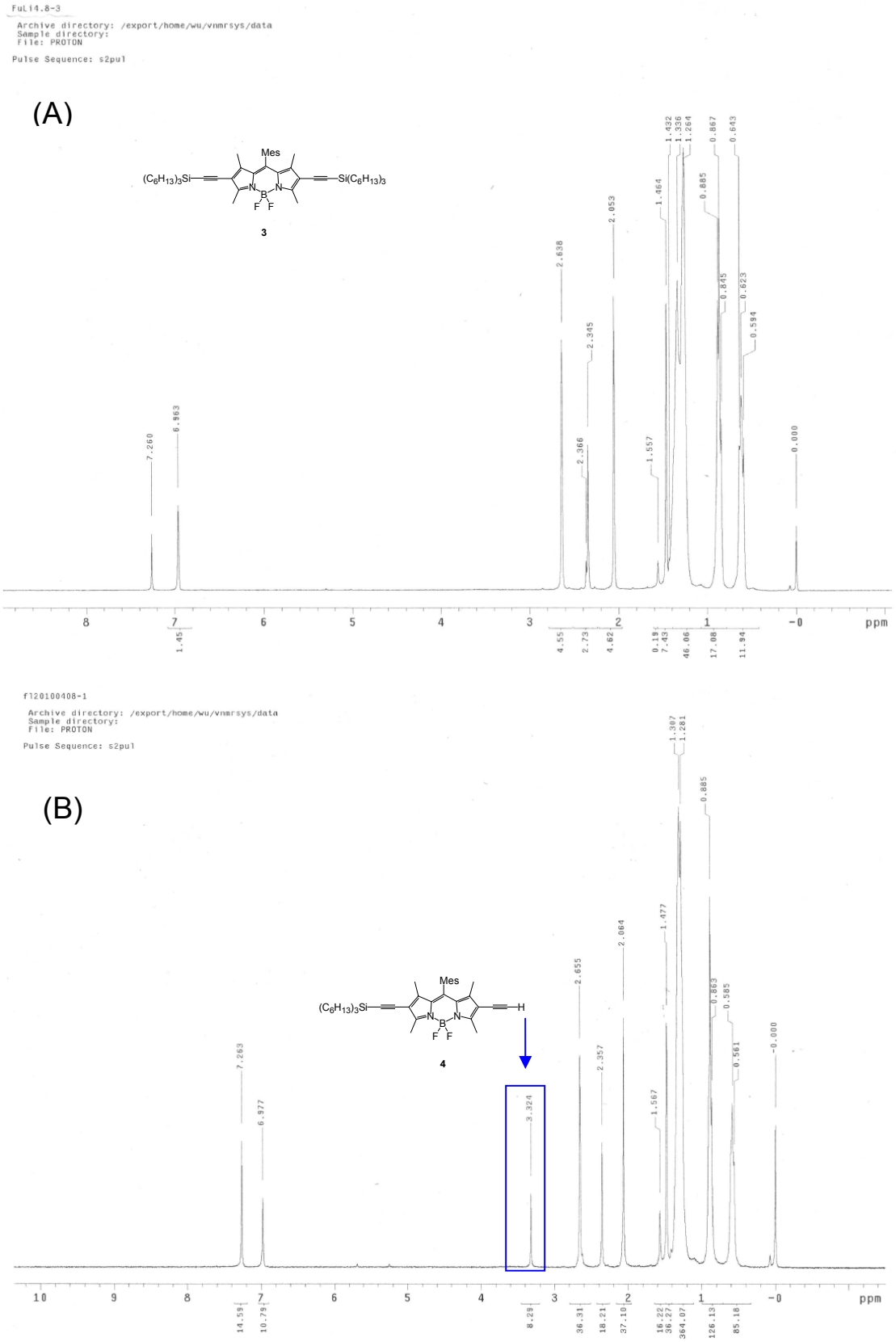

Fig. S4 ^{1}H NMR spectra of BODIPY **dye 3** (A) and that titrated with one equivalent of F^- (B) in $CDCl_3$. The single peak at δ = 3.3 ppm is attributed to the proton of -C≡C-H. The integrations are not corrected.