Triarylborane-Triphenylamine Based Luminophore for Mitochondria Targeted Live Cell Imaging and Colorimetric Detection of Aqueous Fluoride

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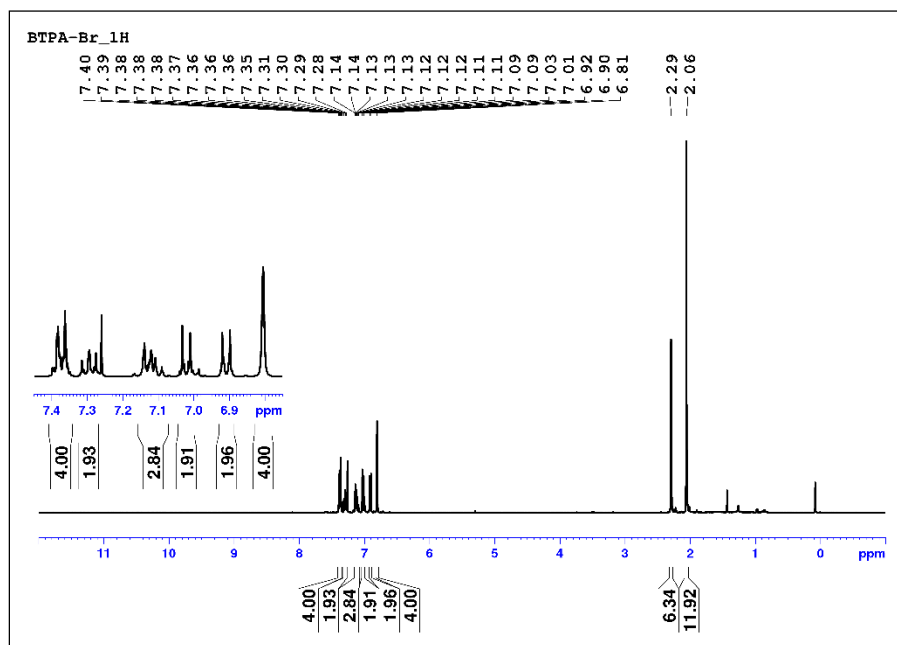
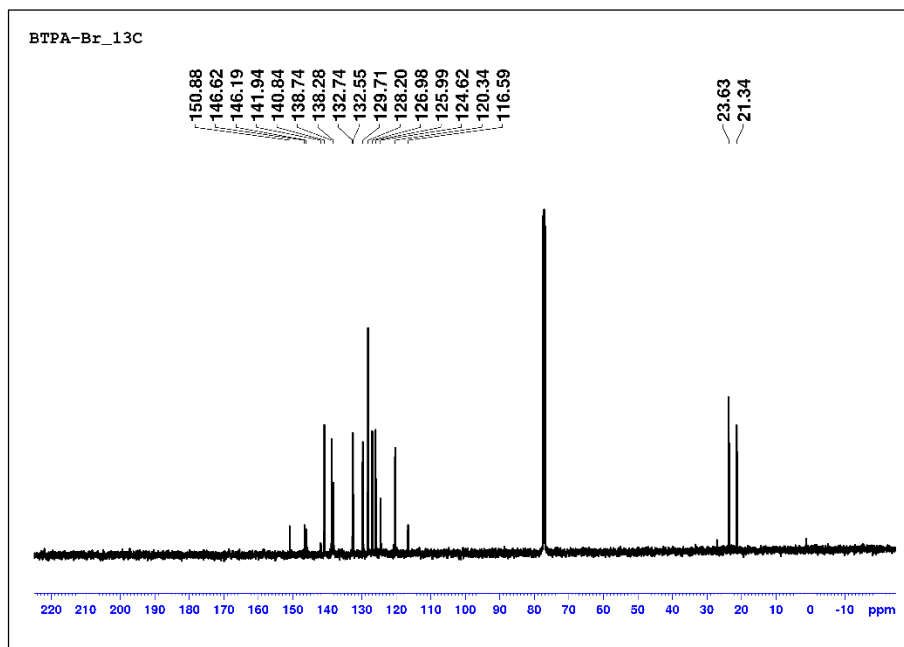**Figure S1.** ^{1}H NMR spectra of **BTPA-Br**

Figure S2. ^{13}C NMR spectra of **BTPA-Br**
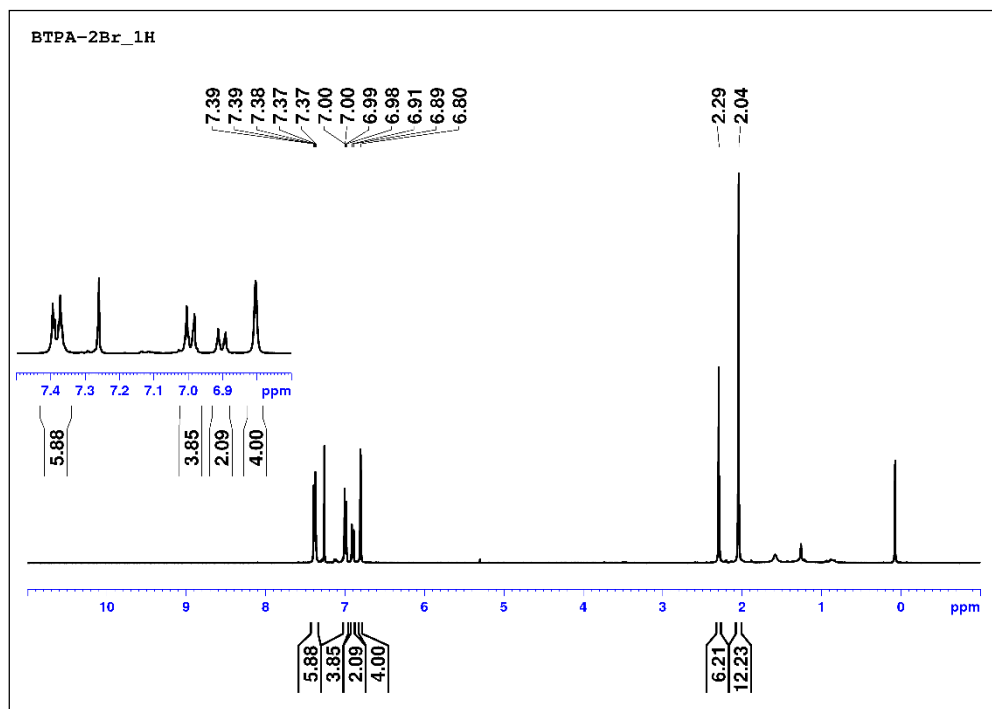
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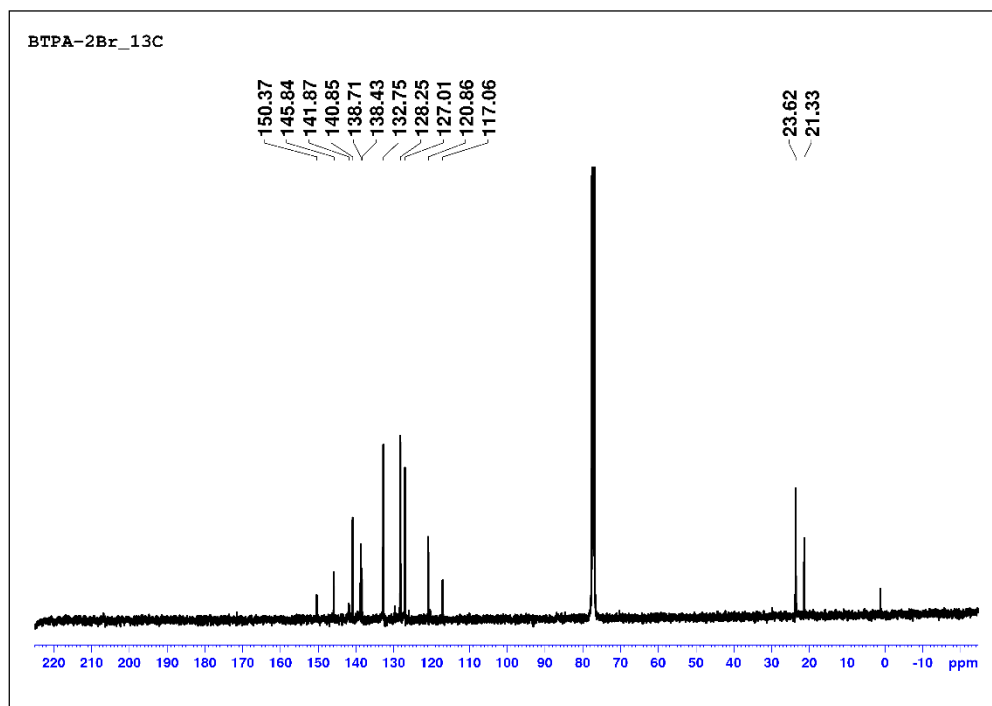
Figure S4. ^{13}C NMR spectra of **BTPA-2Br**
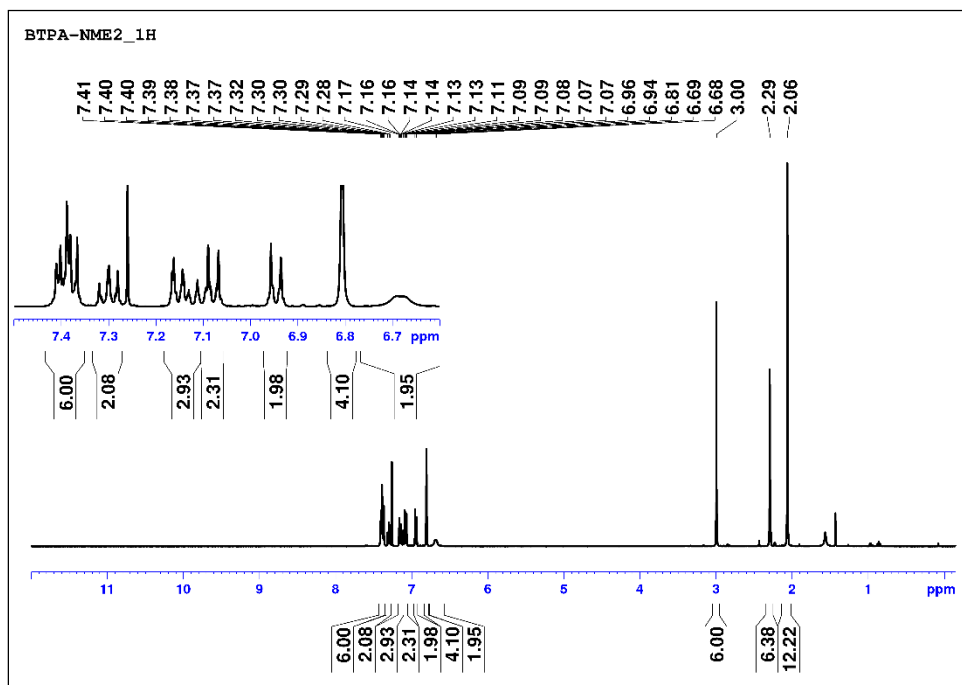
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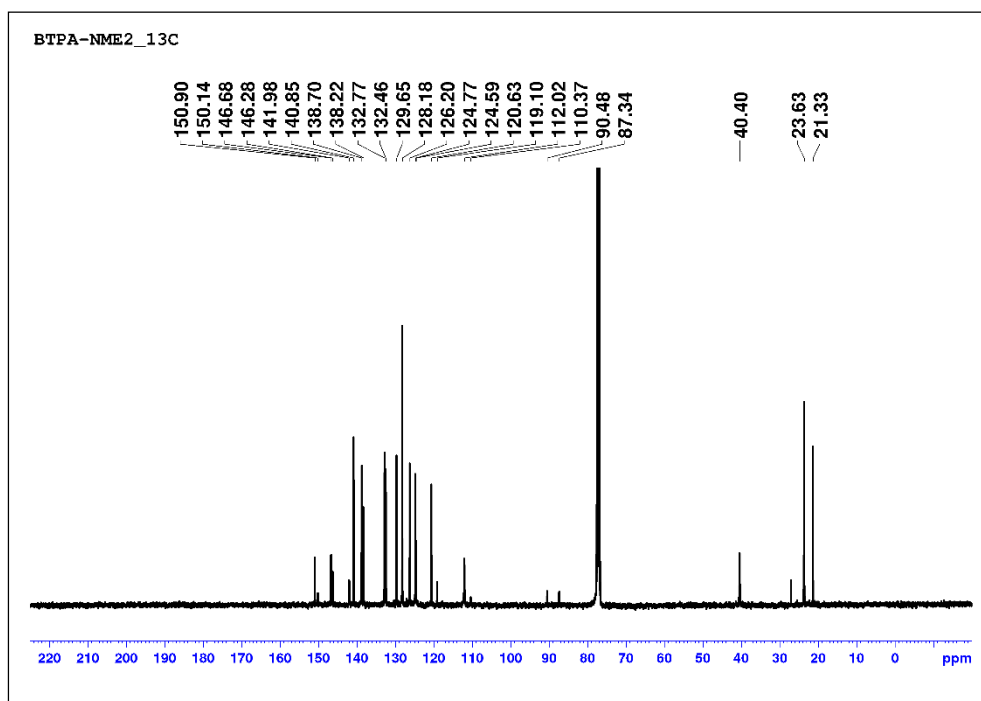
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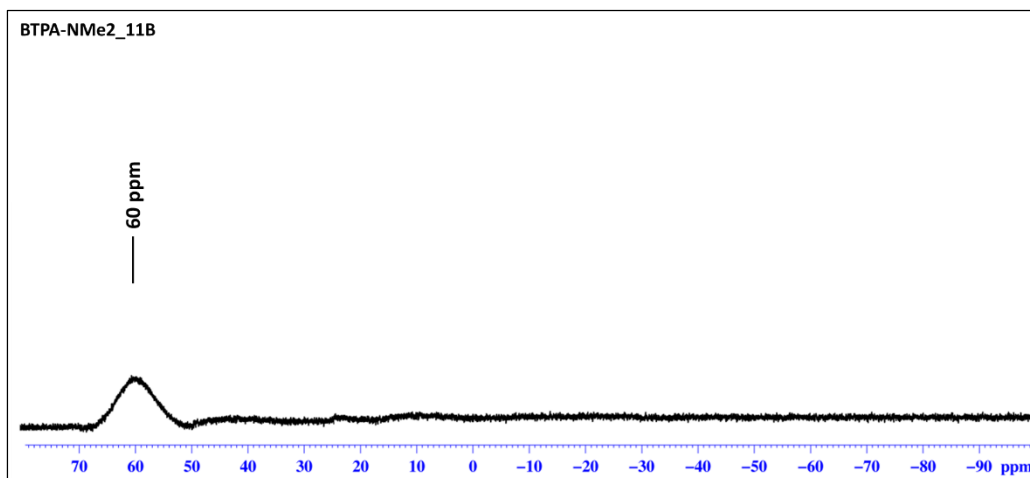
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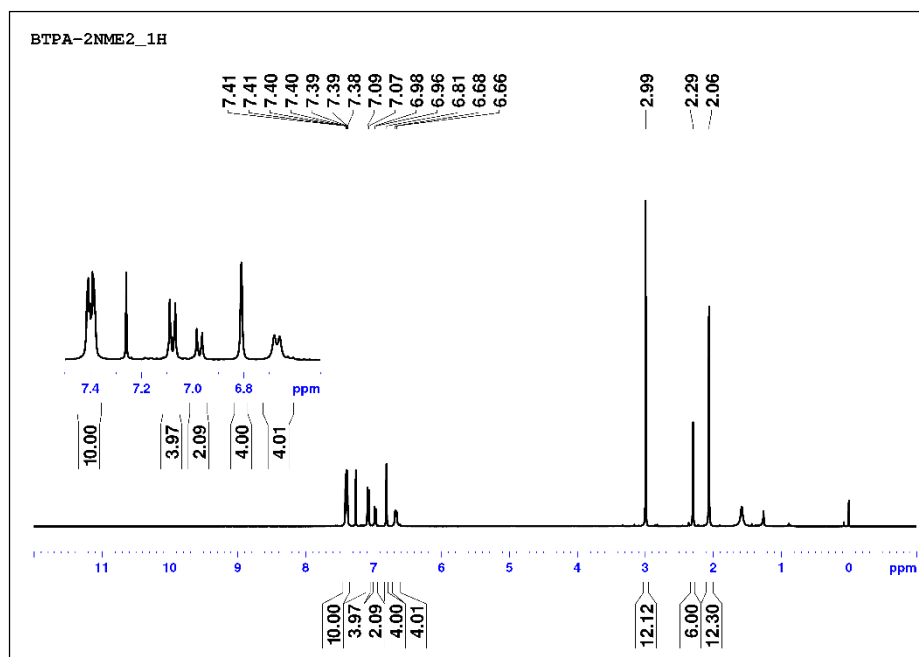
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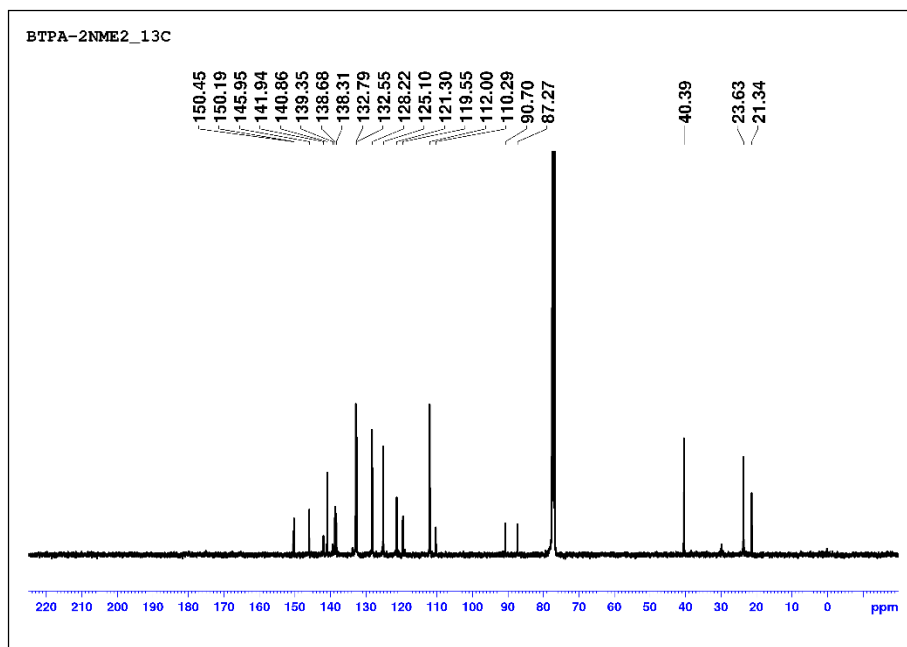
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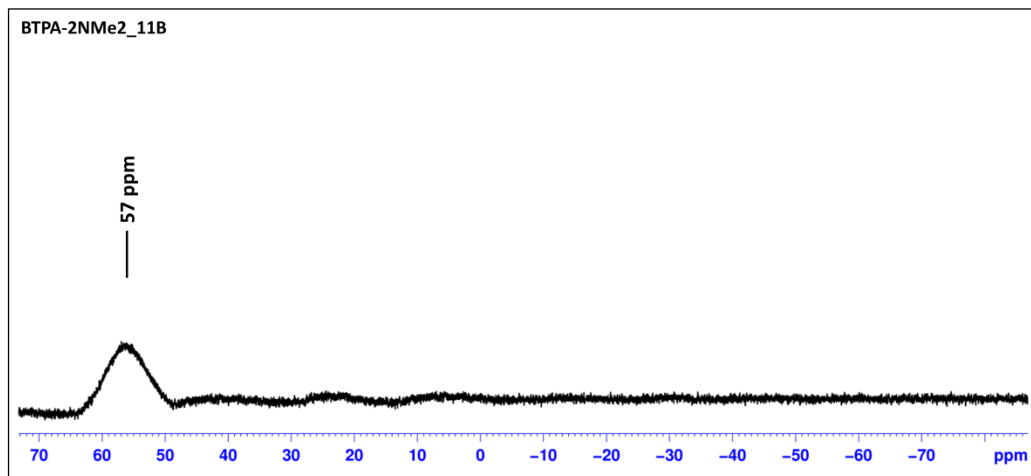
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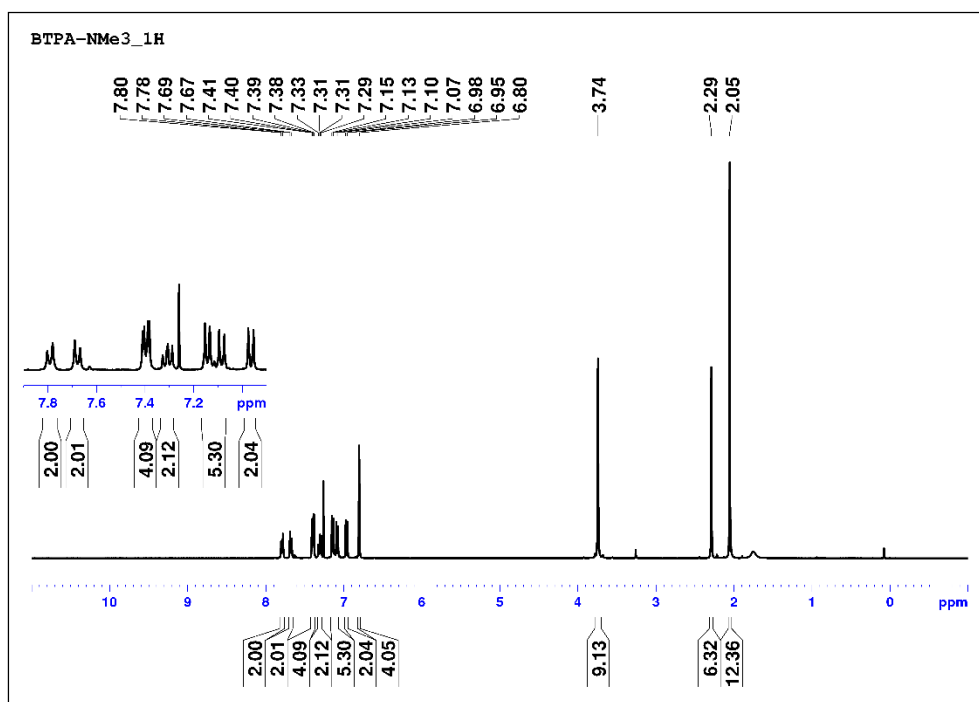
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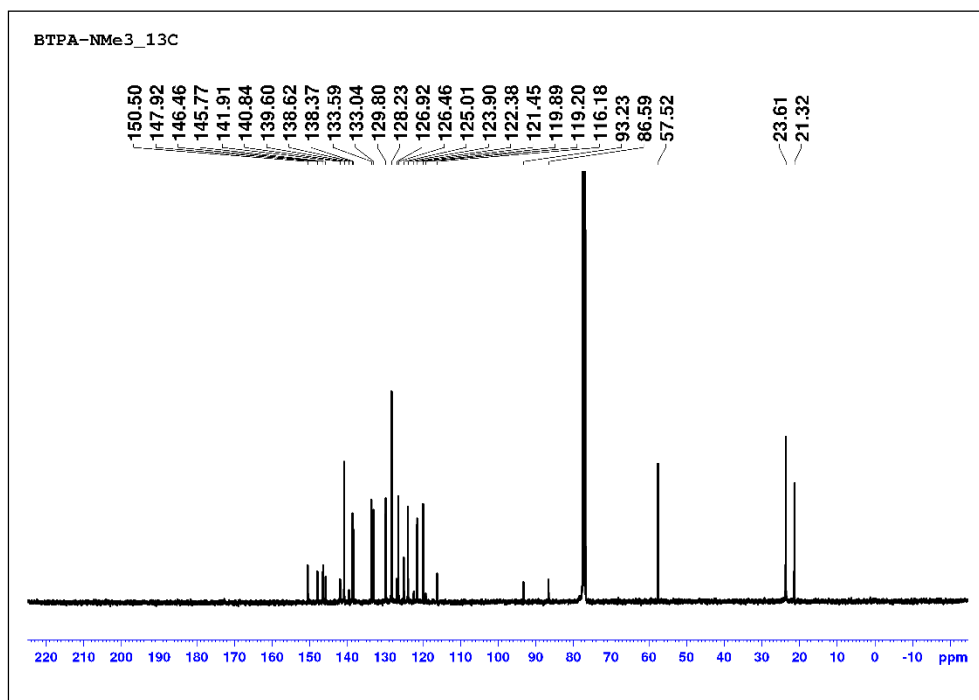
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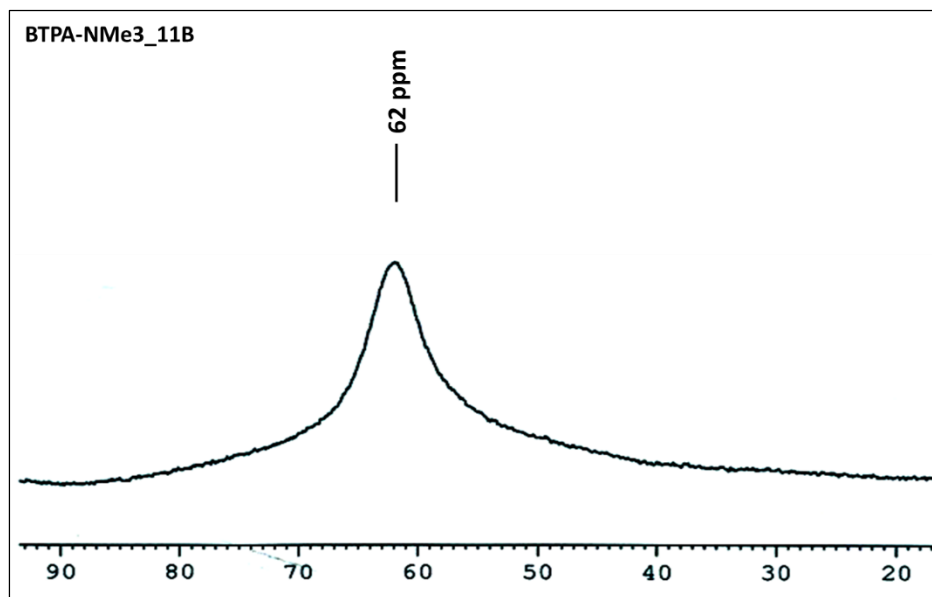
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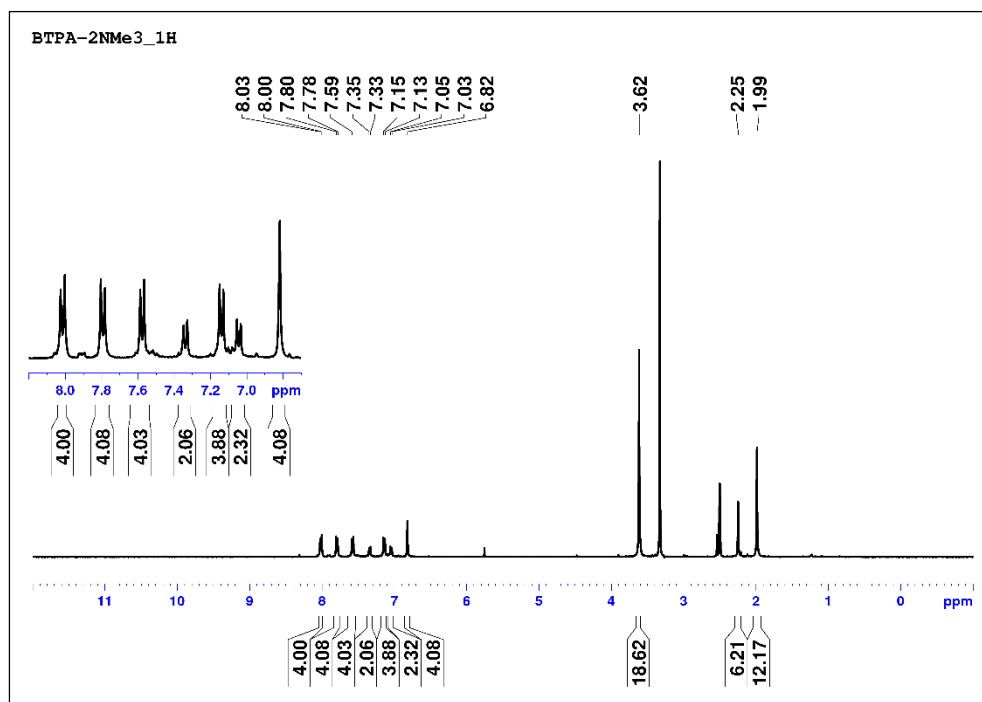
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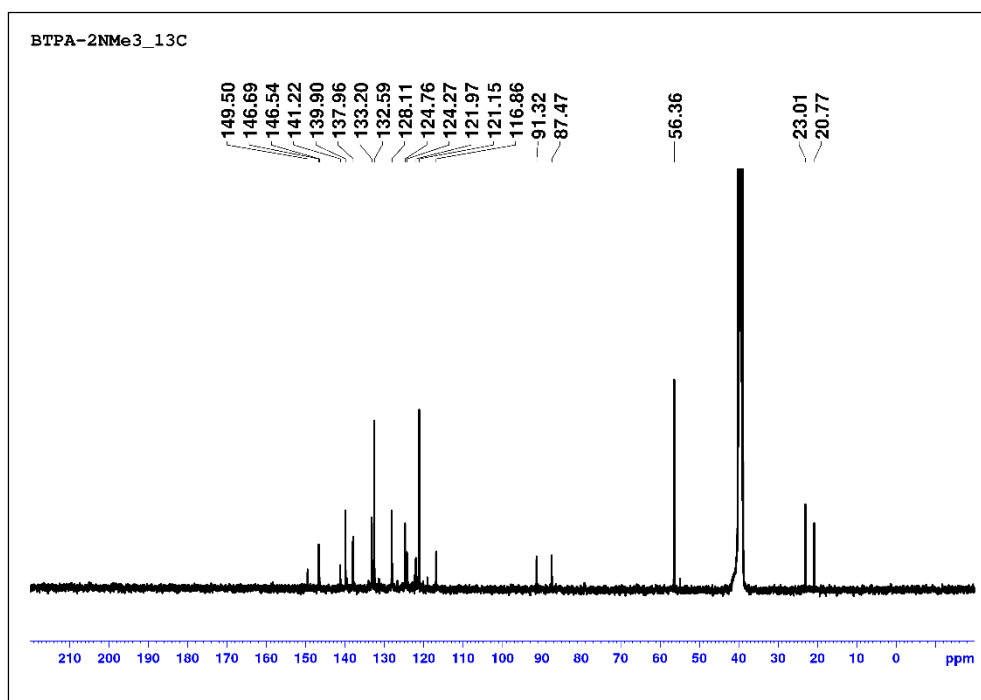
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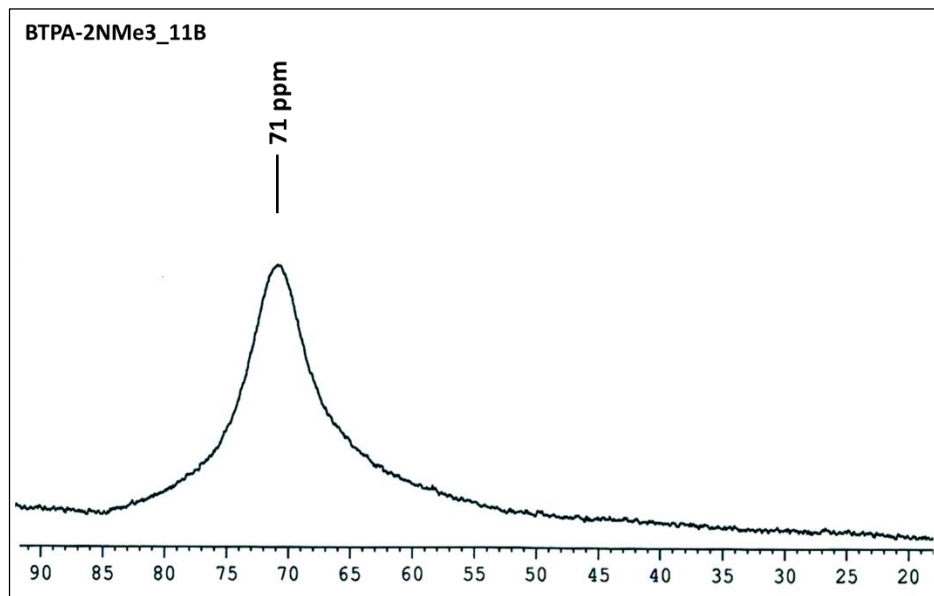
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HRMS Characterization
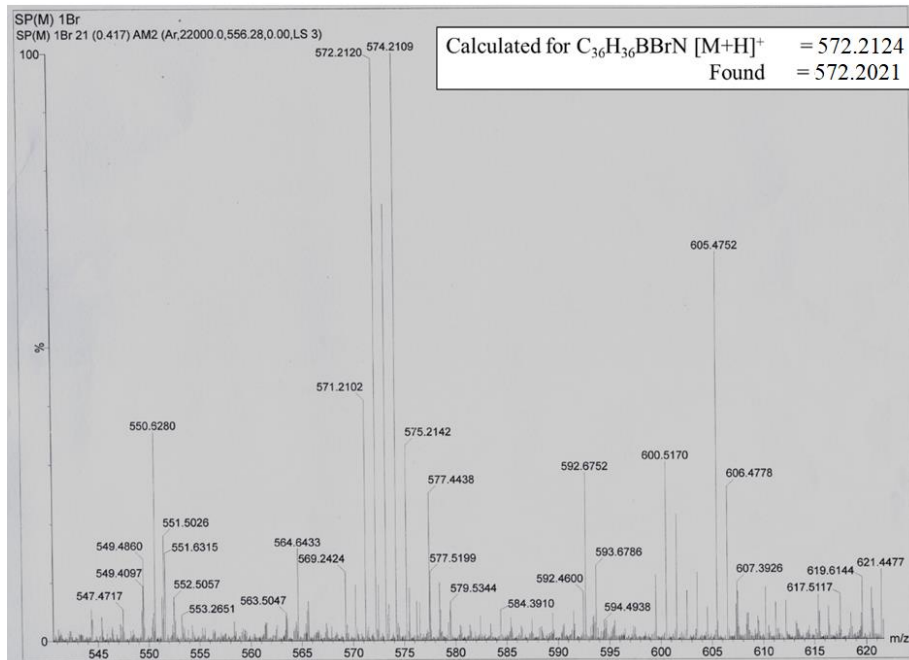
Figure S17. HRMS of **BTPA-Br**
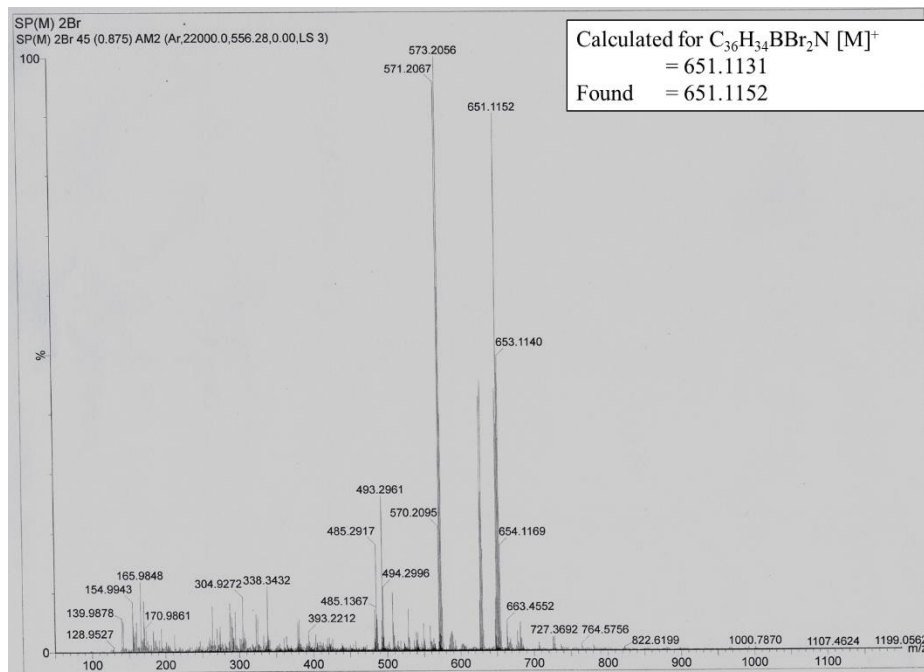
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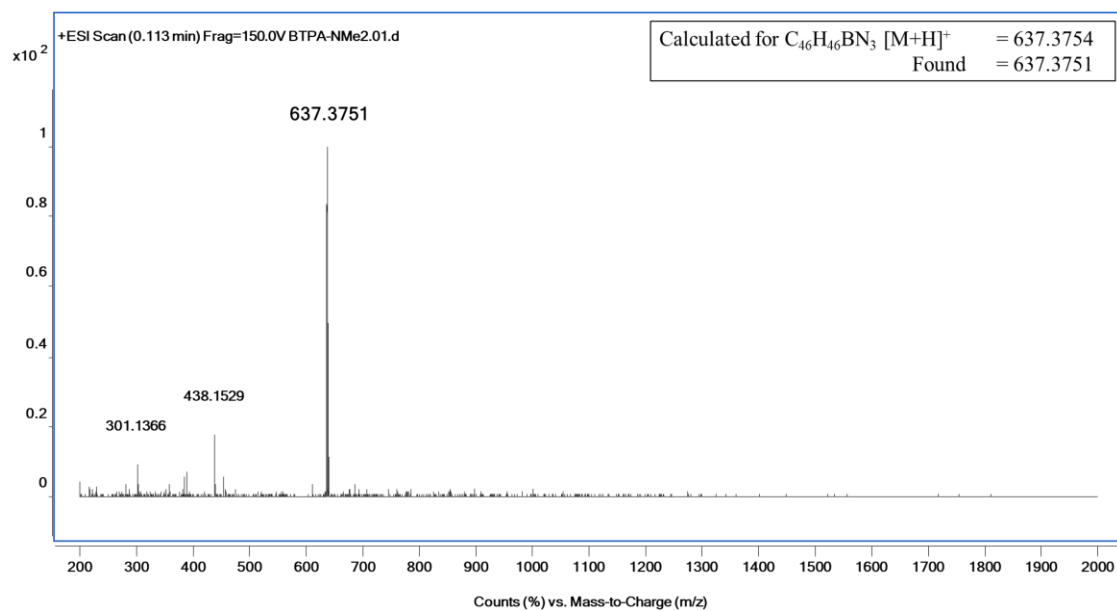
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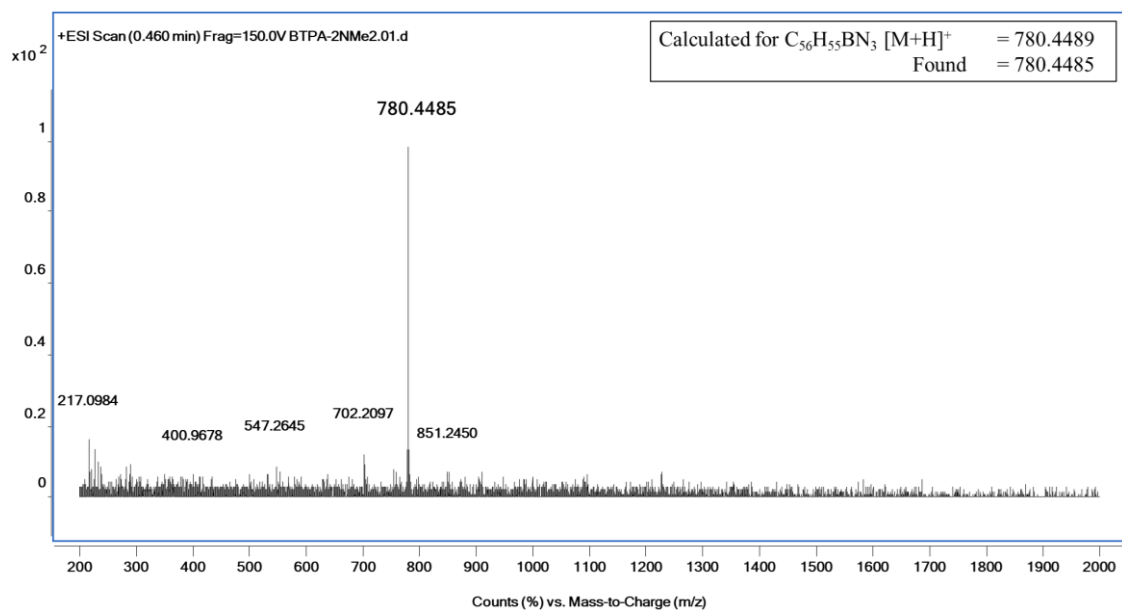
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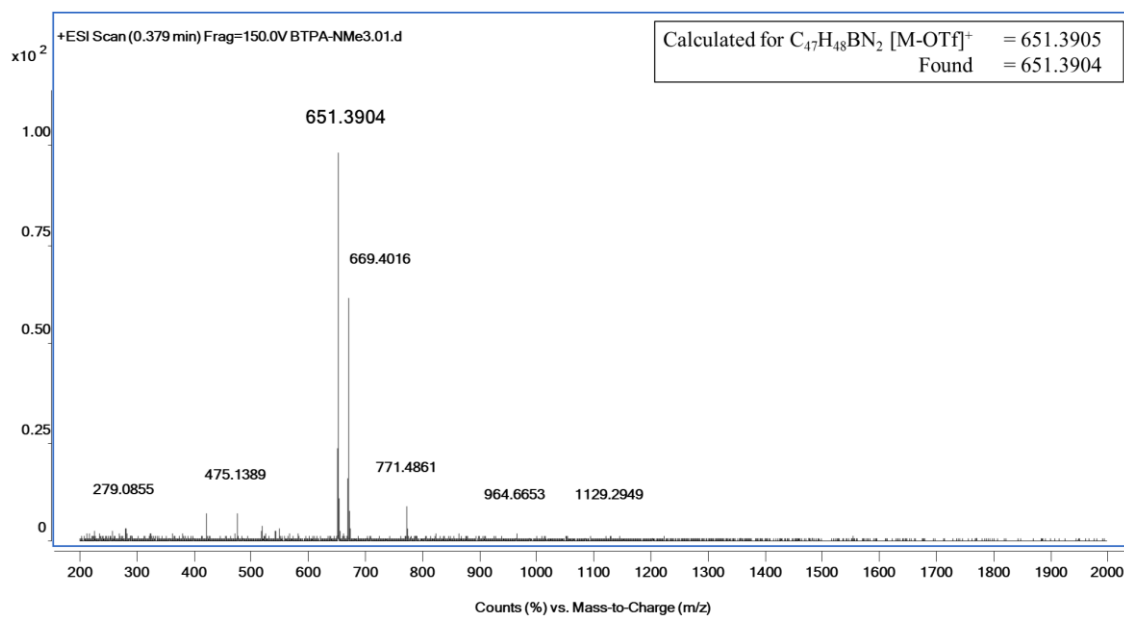
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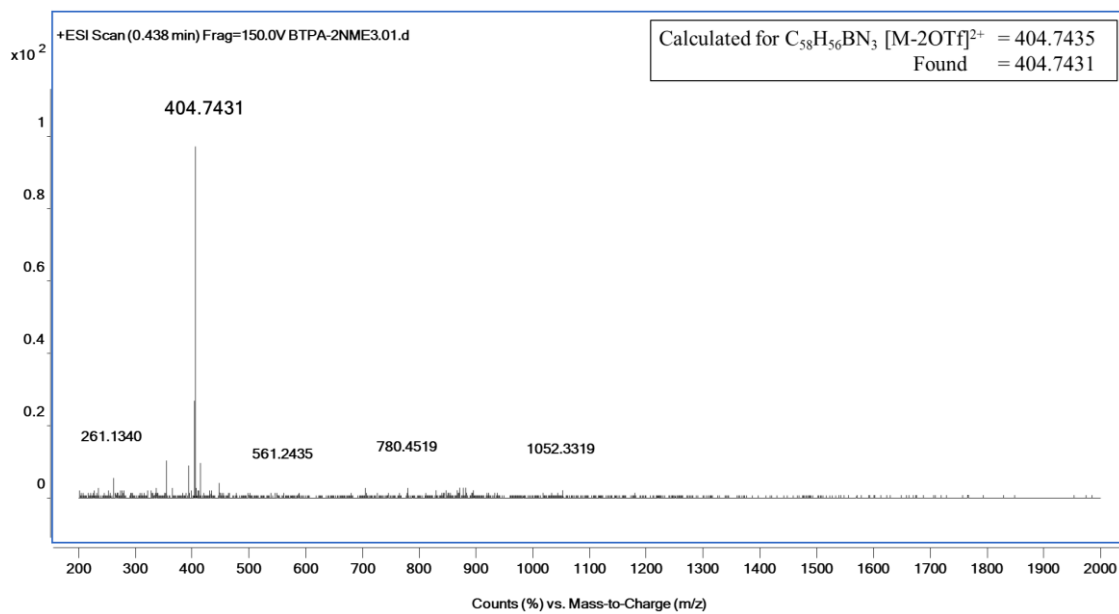
Figure S22. HRMS of **2**

Single Crystal XRD Characterization:
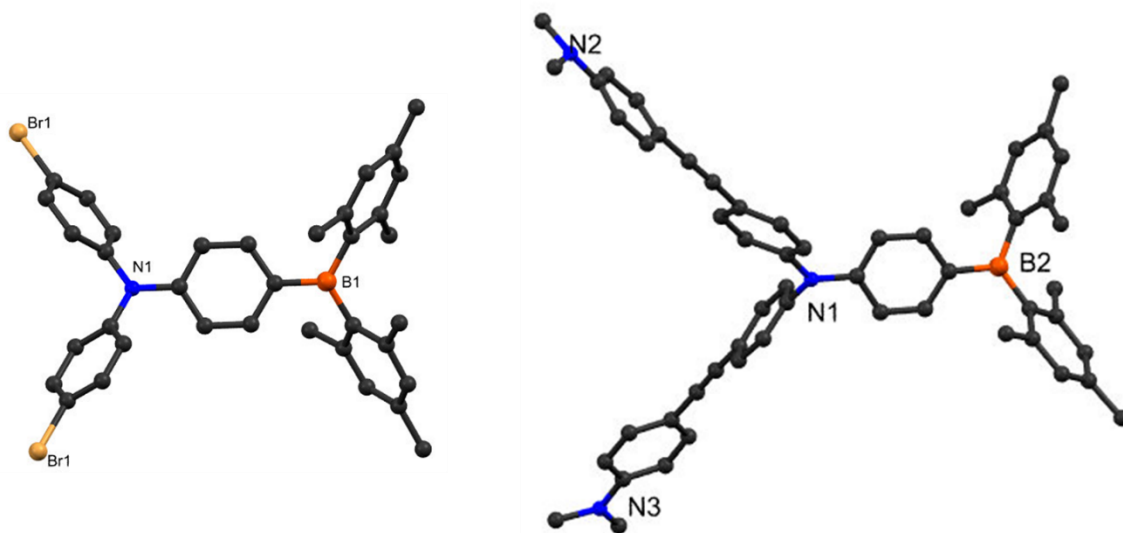
Figure S23. Molecular structures of **BTPA-2Br** (left) and **BTPA-2NMe₂** (right) obtained from Single Crystal X-Ray Diffraction measurements (**H** atoms are omitted for clarity).

Table S1. Selected crystallographic data for structures **BTPA-2Br** and **BTPA-2NMe₂**.

	BTPA-2Br	BTPA-2NMe₂
Empirical formula	$C_{18} H_{17} B_{0.50} Br N_{0.50}$	$C_{112} H_{108} B_2 N_6$
Formula weight	325.64	1559.66
Temperature	295(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic
Space group	$C\,2/c$	P -1
Unit cell dimensions	a = 19.682(5) Å; α = 90°	a = 13.122(2) Å; α = 76.429(4)°
	b = 14.346(3) Å; β = 104.682(6)°	b = 19.080(4) Å; β = 77.166(4)°
	c = 12.215(3) Å; γ = 90°	c = 19.964(4) Å; γ = 76.851(4)°.
Volume	3336.2(13) Å³	4655.6(15) Å³

Z	8	2
Density(calculated)	1.297 Mg/m^3	1.113 Mg/m^3
Theta range for data collection	3.323 to 27.559°	2.993 to 25.000°
Index ranges	-25<=h<=25, -18<=k<=18, -15<=l<=15	-15<=h<=15, -22<=k<=22, -23<=l<=23
Reflections collected	49667	56898
Independent reflections	3839 [R(int) = 0.1495]	14778 [R(int) = 0.1088]
Completeness to theta = 24.999°	99.8 %	90.0 %
Goodness-of-fit on F^2	0.994	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.0977	R1 = 0.1235, wR2 = 0.3115
R indices (all data)	R1 = 0.1952, wR2 = 0.1323	R1 = 0.2470, wR2 = 0.3456
Largest diff. peak and hole	0.410 and -0.407 e.Å^{-3}	0.467 and -0.371 e.Å^{-3}
CCDC number	1975082	1975083

Optical Properties
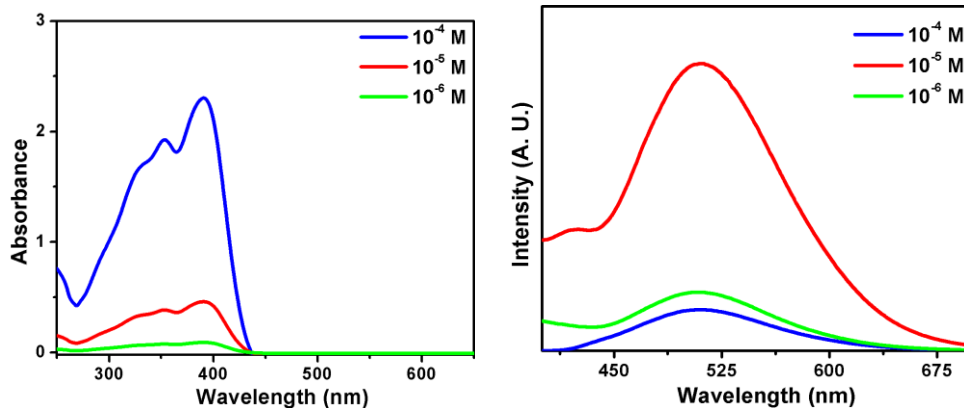
Figure S24: UV-Visible (left) and fluorescence (right) spectra of **BTPA-NMe₂** in CH₃CN at various concentrations (λ_{ex} at 375 nm)
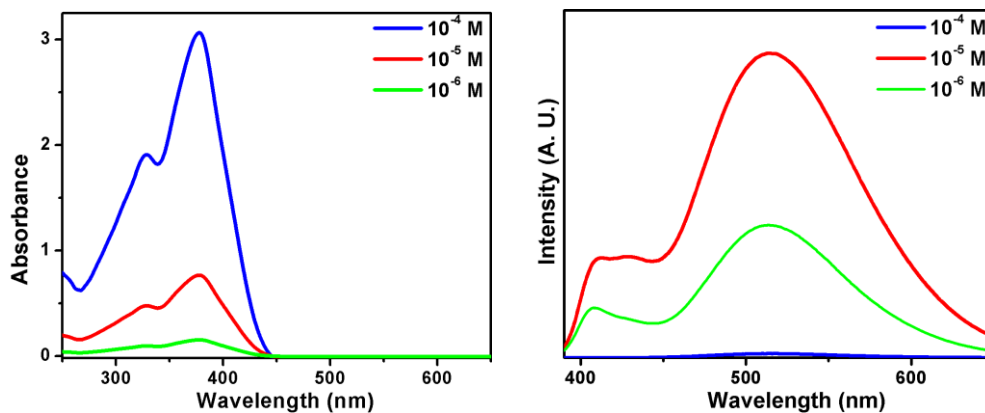
Figure S25: UV-Visible (left) and fluorescence (right) spectra of **BTPA-2NMe₂** in CH₃CN at various concentrations (λ_{ex} at 375 nm)
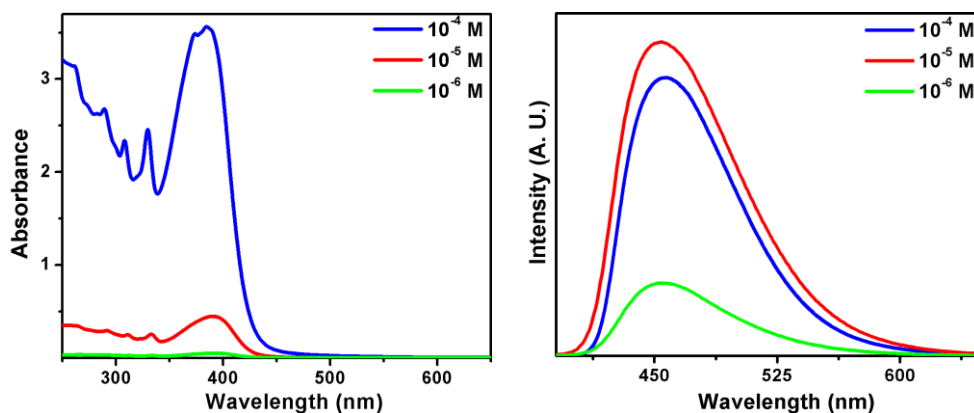
Figure S26: UV-Visible (left) and fluorescence (right) spectra of **1** in CH₃CN at various concentrations (λ_{ex} at 375 nm)
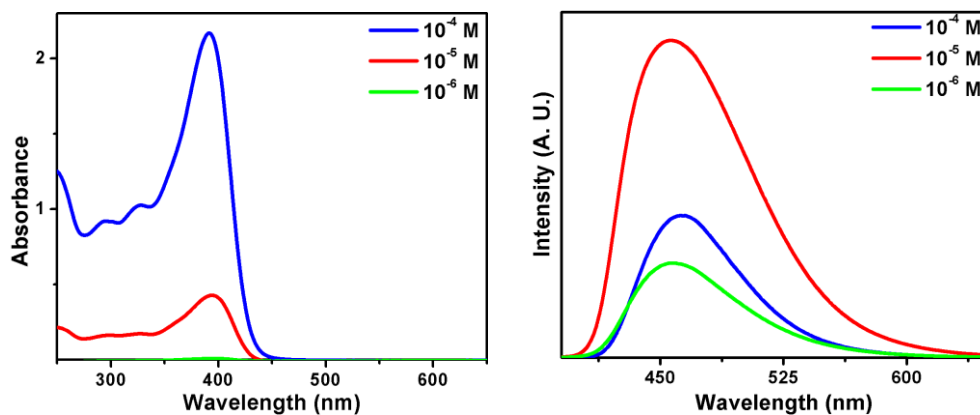
Figure 27: UV-Visible (left) and fluorescence (right) spectra of **1** in CH$_3$CN at various concentrations (λ_{ex} at 375 nm)
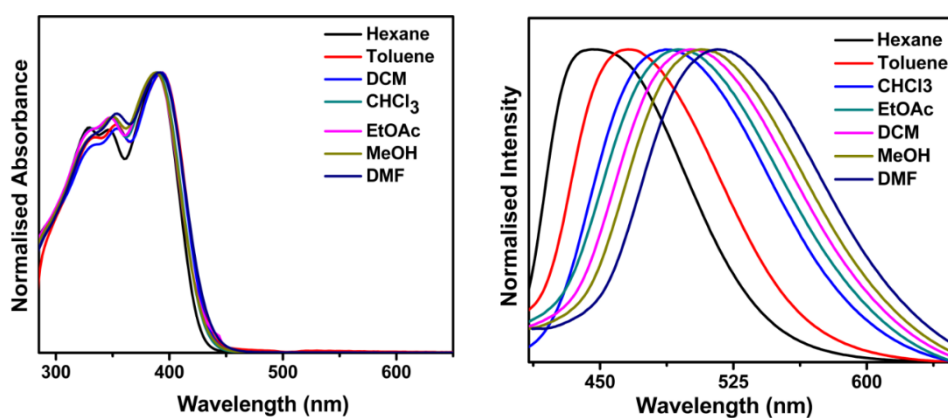
Figure 28: Normalized UV-Visible (right) and Fluorescence (left) spectra of **BTPA-NMe₂** in solvents with different polarity (10 µM; λ_{ex} at 375 nm)
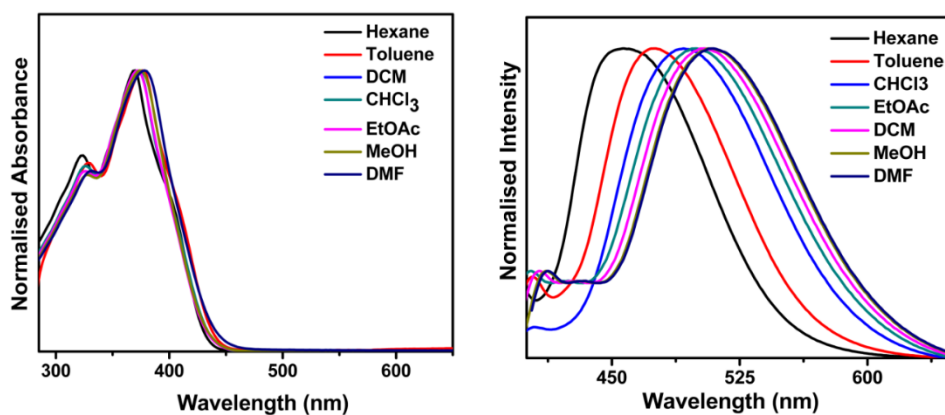
Figure 29: Normalized UV-Visible (right) and Fluorescence (left) spectra of **BTPA-2NMe₂** in solvents with different polarity (10 µM; λ_{ex} at 375 nm)
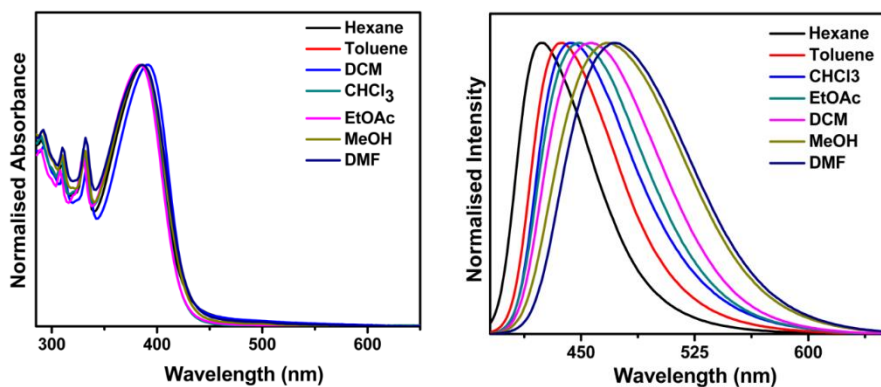
Figure 30: Normalized UV-Visible (right) and Fluorescence (left) spectra of **1** in solvents with different polarity (10 μM; λ_{ex} at 375 nm)
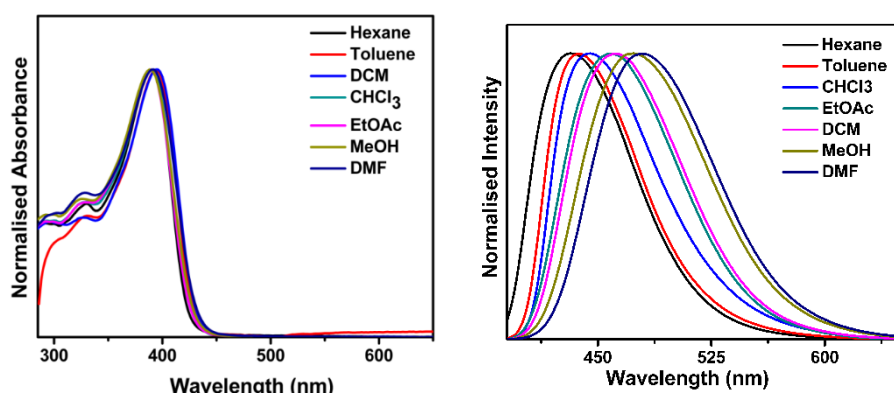
Figure 31: Normalized UV-Visible (right) and fluorescence (left) spectra of **2 in** solvents with different polarity (10 μM; λ_{ex} at 375 nm)

Table S2: Optical data of **BTPA-NMe₂** in different solvents

Solvents	λ_{abs}	λ_{em}	λ_{abs}- λ_{em} (nm); (cm^{-1})	Quantum yields (%)	Life time (ns)	Radiative decay constant $(10^8/s)$	Non-radiative decay constant $(10^8/s)$
Hexane	389	446	57; (3291)	68	1.53	4.43	2.09
Toluene	393	466	73; (3986)	66	1.14	5.79	2.98
CHCl₃	393	486	97; (4849)	62	1.72	3.61	2.21
EtOAc	389	496	107; (5131)	41	1.95	2.15	3.31
CH₂Cl₂	387	501	114; (5879)	21	2.39	1.13	3.31
CH₃CN	390	505	115; (5840)	16	2.45	0.65	3.43
MeOH	387	508	121; (6154)	2	2.01	0.099	4.86
DMF	391	515	124; (6158)	1	2.59	0.033	3.98

Table S3: Optical data of **BTPA-2NMe₂** in different solvents

Solvents	λ_{abs} (nm)	λ_{em} (nm)	λ_{abs}- λ_{em} (nm); (cm⁻¹)	Quantum yields (%)	Life time (ns)	Radiative decay constant (10^8/s)	Non-radiative decay constant (10^8/s)
Hexane	384	455	71; (4063)	66	1.86	3.51	1.82
Toluene	384	475	91; (4989)	65	1.87	3.40	1.87
CHCl₃	391	492	101; (5250)	63	1.52	4.15	2.43
EtOAc	384	498	114; (5962)	38	1.97	1.92	3.15
CH₂Cl₂	384	503	119; (6161)	15	2.47	0.61	3.34
CH₃CN	391	507	116; (6299)	13	2.51	0.51	3.47
MeOH	384	510	126; (6351)	3	1.86	0.16	4.21
DMF	390	517	127; (6435)	2	2.57	0.078	3.81

Table S4: Optical data of **1** in different solvents

Solvents	λ_{abs}	λ_{em}	λ_{abs}- λ_{em} (nm); (cm⁻¹)	Quantum yields (%)	Life time (ns)	Radiative decay constant (10^8/s)	Non-radiative decay constant (10^8/s)
Hexane	368	417	49; (3196)	74	1.28	5.78	2.03
Toluene	376	423	47; (2955)	75	1.39	5.39	1.79
CHCl₃	372	437	65; (3998)	73	1.38	5.29	1.96
EtOAc	372	443	71; (4308)	72	1.39	5.18	2.03
CH₂Cl₂	372	448	76; (4560)	73	1.52	4.85	1.78
CH₃CN	378	457	79; (4574)	73	1.81	4.03	1.49
MeOH	374	467	93; (5314)	72	1.31	5.49	2.14
DMF	378	473	99; (5324)	71	1.79	3.97	1.62

Table S5: Optical data of **2** in different solvents

Solvents	λ_{abs}	λ_{em}	$\lambda_{abs} - \lambda_{em}$ (nm); (cm^{-1})	Quantum yields (%)	Life time (ns)	Radiative decay constant (10^8/s)	Non-radiative decay constant (10^8/s)
Hexane	374	431	57; (3536)	71	1.26	5.63	2.34
Toluene	372	438	66; (4050)	70	1.38	5.07	2.17
CHCl$_3$	375	444	69; (4144)	70	1.45	4.84	2.06
EtOAc	377	457	80; (4644)	69	1.57	4.40	2.04
CH$_2$Cl$_2$	376	462	86; (4950)	70	1.73	4.04	1.73
CH$_3$CN	378	470	92; (5179)	69	1.26	5.48	2.46
MeOH	378	478	100; (5553)	67	2.06	3.25	1.60
DMF	374	480	106; (5904)	67	2.01	3.33	1.65

Anion Binding studies in Acetonitrile

Acetonitrile solutions of **1** and **2** (1×10^{-5} M) were titrated independently against incremental addition of solution of TBAF.
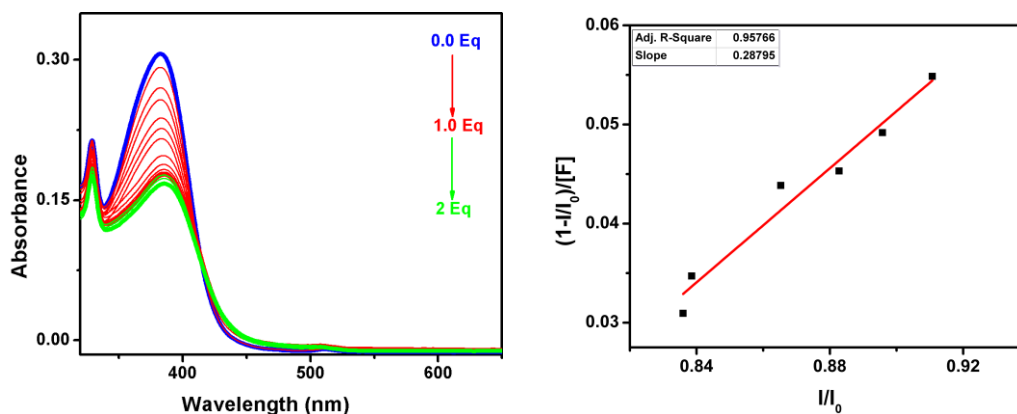
Figure S32: Left: changes associated with UV-Vis spectrum of **1** (acetonitrile, 10 µM) in the presence of fluoride ions (TBAF, 1.5×10^{-3} M) (λ_{ex} at 375 nm); right: plot of I/I$_0$ Vs (1-I/I$_0$)/[F$^-$] (λ_{abs} at 385 nm). Calculated binding constant K = 2.8×10^5 M^{-1}
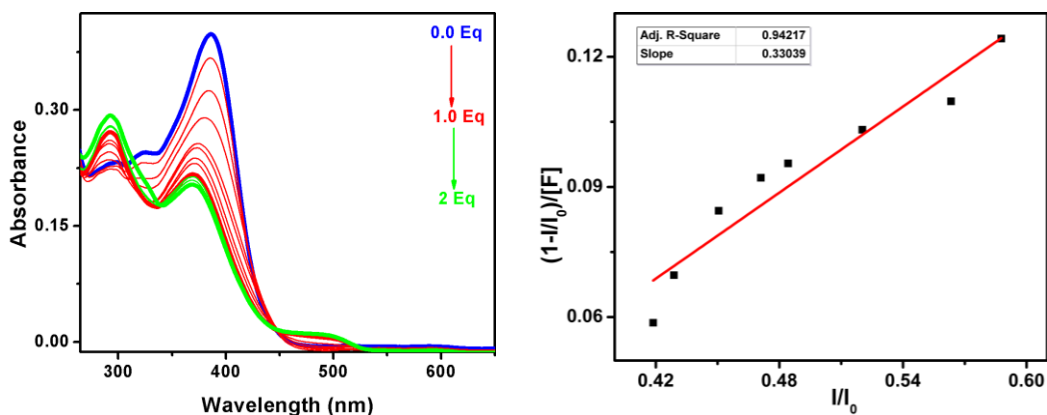
Figure S33: Left: changes associated with UV-Vis spectrum of **2** (10 µM in water (1% CH_3CN was added to enhance the solubility) in the presence of fluoride ions (1.5×10^{-3} M) (KF dissolved in HEPES buffer and pH maintains 7.0) (λ_{ex} at 375 nm); right: plot of I/I_0 Vs $(1-I/I_0)/[F^-]$ (λ_{abs} at 385 nm). Calculated binding constant K = 3.3×10^5 M^{-1}.
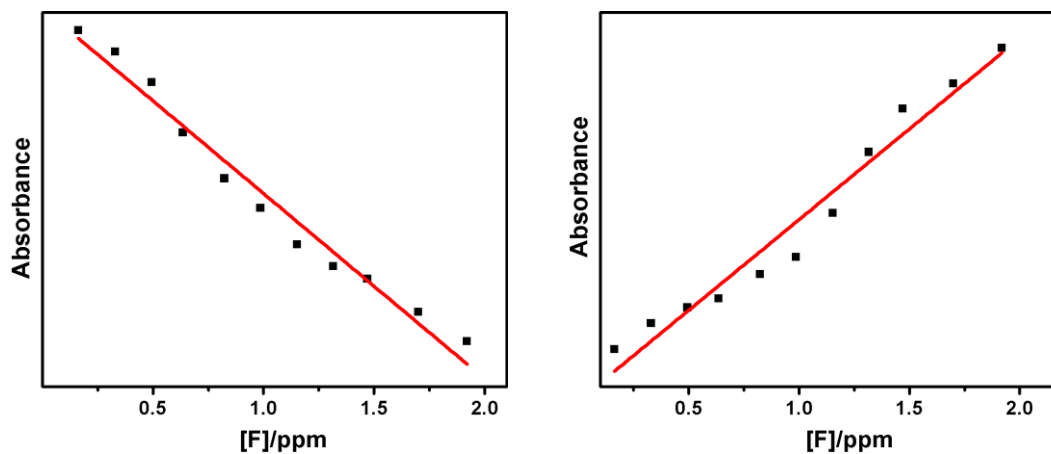
Figure S34: Linear plots between the changes in absorbance of **2** at 385 nm (left) and 485 nm (right) *vs* concentration of fluoride (in ppm) in CH_3CN solvent.
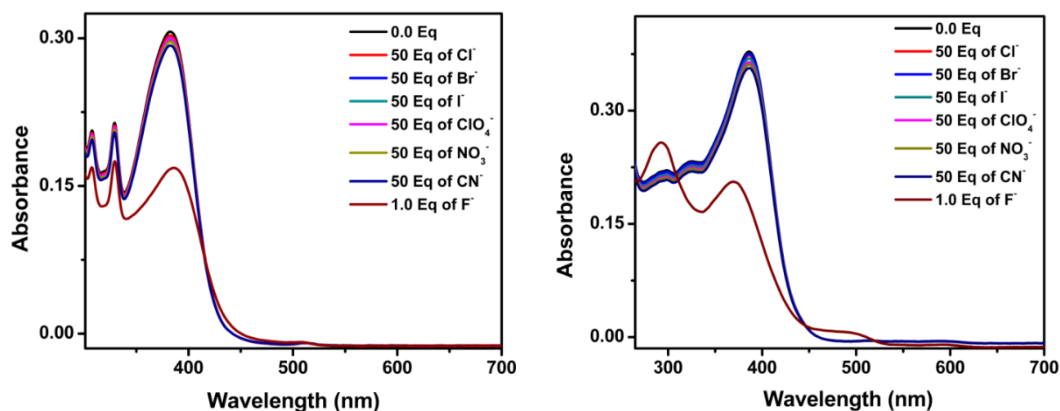
Figure S35: Changes associated with UV-Visible spectra of **1** (left) and **2** (right) in presence of various anions (CH_3CN, 10 µM)

Figure S36: Photograph demonstrating the color changes of **1** (above) and **2** (down) associated with the addition of different anions under ambient light. Concentration: 10 μM in acetonitrile; Fluoride was added in 1 equv amount and other anions were used in greater than 50 equv amount.

Fluorescence titrations study in organic medium (CH₃CN)

Fluorescence titration studies were carried by placing 2 mL of compounds **1** and **2** were in 1×10^{-5} M stock solution in CH₃CN. A septum screw capped quartz cuvette of 1 cm width and followed by gradual incremental addition of 1×10^{-3} M CH₃CN solution of anions. The experiment was repeated for at least three times at 298 K to obtain concordant value. Compounds **1** or **2** were excited at 375 nm and the emissions were monitored in the range of 400-700 nm (2 nm slit width kept constant for both source and detector).

Figure S37: Changes associated with PL spectra of **1** (left) and **2** (right) in the presence of fluoride ions (TBAF, 1.5×10^{-3} M ,acetonitrile) (λ_{ex} at 375 nm)
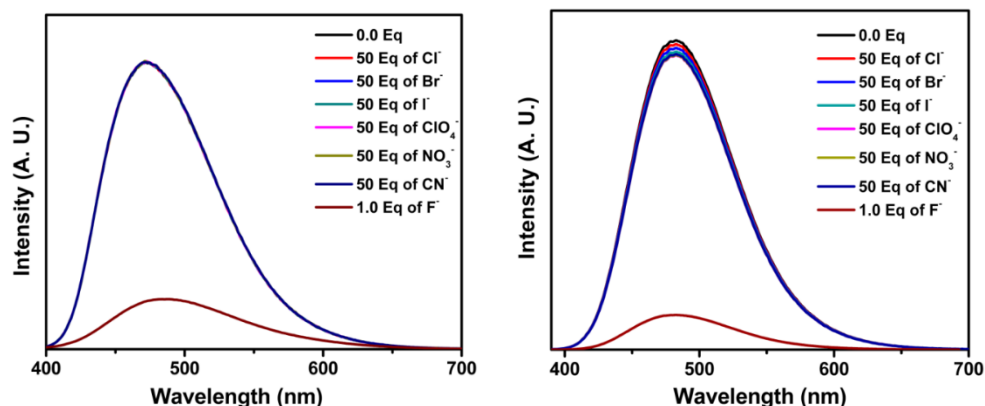
Figure S38: Changes associated with PL spectra of **1** (left) and **2** (right) in presence of various anions (CH$_3$CN, 10 µM)(λ_{ex} at 375 nm).

Figure S39: Photograph demonstrating the emission color changes associated with **1** (above) and **2** (down) with different anions under UV-light. Solution concentration was 10 µM in acetonitrile solvent. Fluoride was added in 1equv amount and other anions were used in greater than 50equv amount.

UV-visible titration studies in CH$_3$CN: H$_2$O (1:1)

Respective Lewis acid (**1/2**) (1 × 10^{-5} M) was dissolved in CH$_3$CN: H$_2$O in 1:1 ratio. The pH of solution was maintained at pH 7.0 using HEPES buffer (6 mM). Aqueous solutions of potassium fluoride used as a fluoride source.
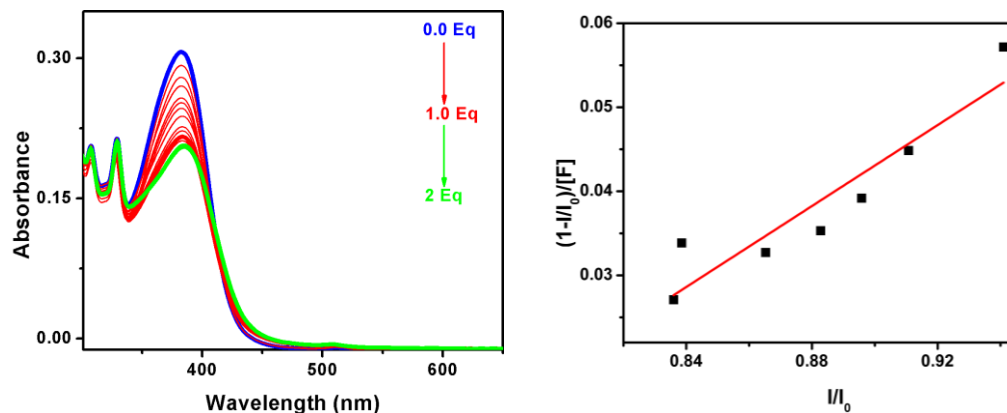
Figure S40: Left: Changes associated with UV-Vis absorption spectrum of **1** (1:1 ratio of CH_3CN/H_2O mixture 10 µM) in presence of fluoride ions (KF, 1×10^{-3} M). right: plot of I/I_0 Vs $(1-I/I_0)/[F^-]$ (λ_{abs} at 385 nm). Calculated binding constant K = 2.4×10^5 M^{-1}
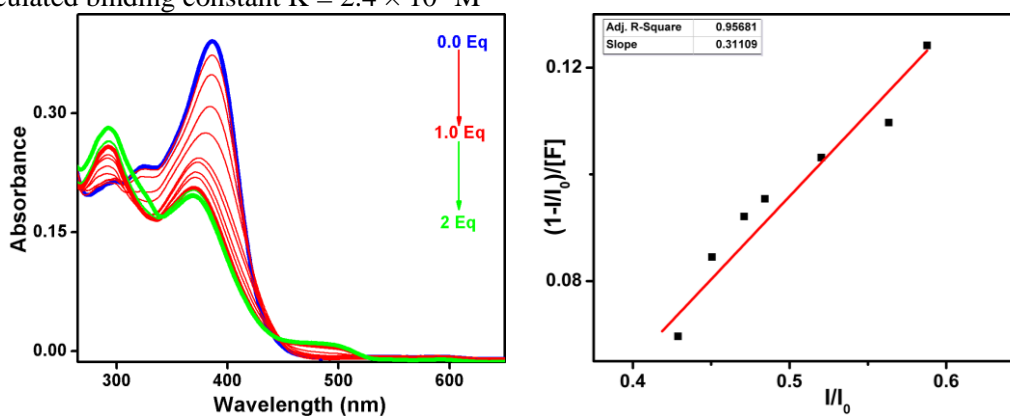
Figure S41: Left: Changes associated with UV-Vis absorption spectrum of **2** (1:1 ratio of CH_3CN/H_2O mixture 10 µM) in presence of fluoride ions (KF, 1×10^{-3} M,). right: plot of I/I_0 Vs $(1-I/I_0)/[F^-]$ (λ_{abs} at 385 nm). Calculated binding constant K = = 3.1×10^5 M^{-1}
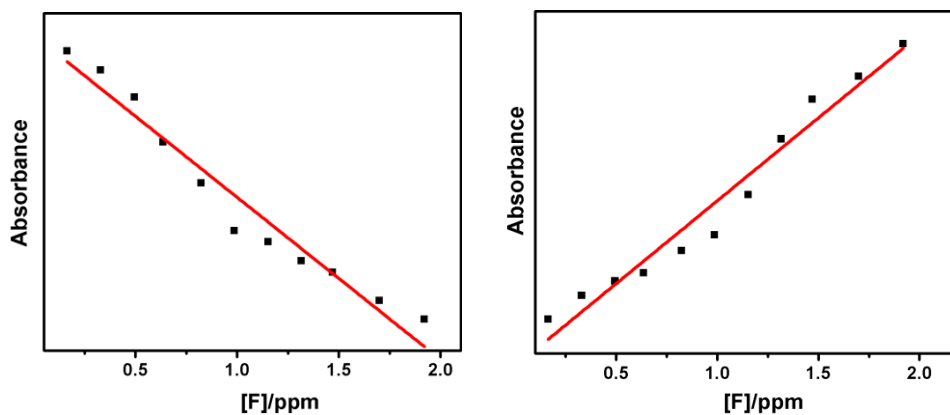
Figure S42: Linear plot between the changes in absorbance of **2** at 385 nm (left) and 485 nm (right) *vs* concentration of fluoride (ppm) in 1:1 mixture of CH_3CN and H_2O.
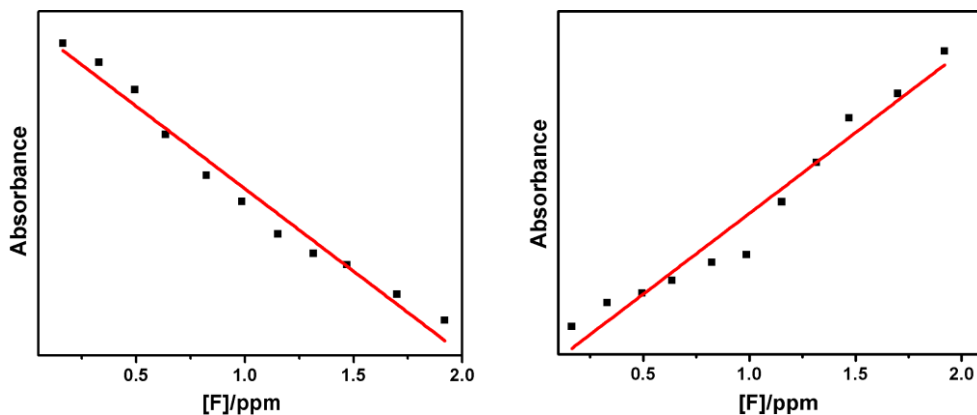
Figure S43: Linear plot between the changes in absorbance of **2** at 385 nm (left) and 485 nm (right) *vs* concentration of fluoride in water (1% CH₃CN was added to enhance the solubility).
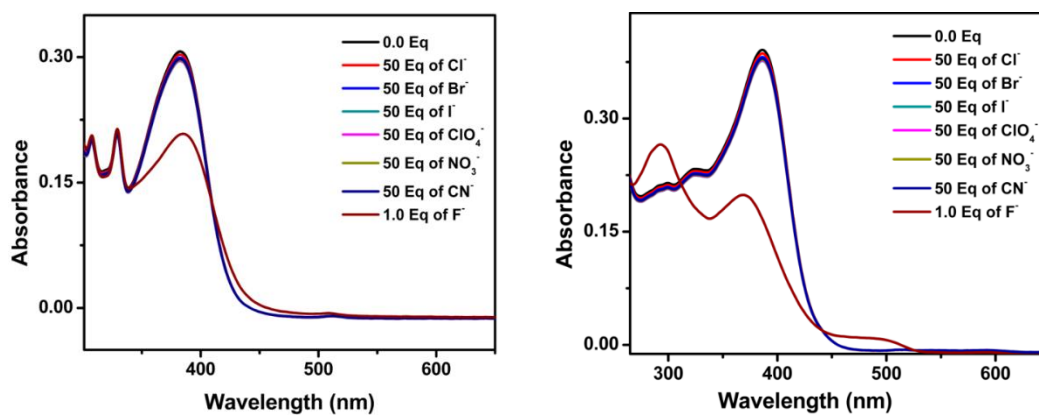
Figure S44: UV-Visible absorbance spectra of **1** (left) and **2** (right) in presence of various anions (in 1:1 mixture of CH₃CN and H₂O)

Fluorescence titration studies in CH₃CN: H₂O (1:1)

Respective Lewis acid (**1/2**) (1×10^{-5} M) was dissolved in CH₃CN:H₂O mixture in the ratio 1:1. The pH of solution was maintained at pH 7.0 using HEPES buffer. Aqueous solutions of potassium fluoride used as a fluoride source (1×10^{-3} M in HEPES buffer, pH = 7). The experiment was repeated for at least three times at 298 K to obtain concordant value. Compounds **1** or **2** were excited at 375 nm and the emissions were monitored in the range of 400-700 nm (2 nm slit width kept constant for both source and detector).
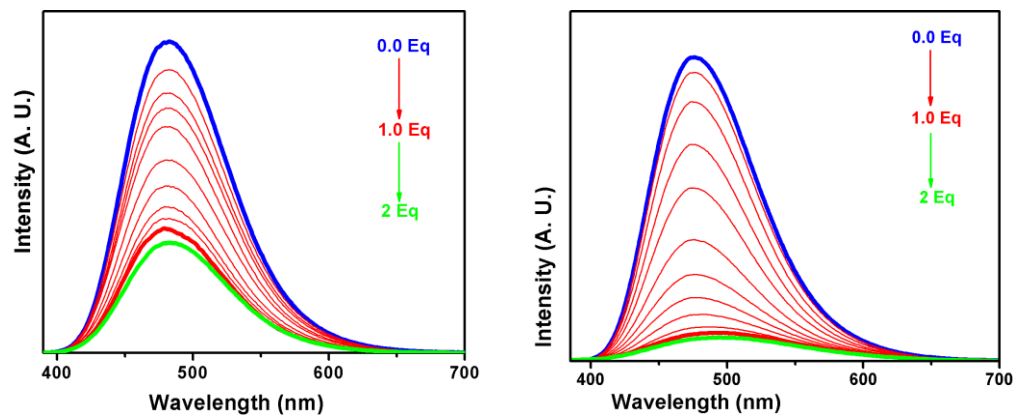
Figure S45: Changes associated with PL spectrum of **1** (left) and **2** (right) (1:1 ratio of CH_3CN/H_2O mixture, 10 μM) in the presence of fluoride ions (KF, 1×10^{-3} M,) (λ_{ex} at 375 nm)
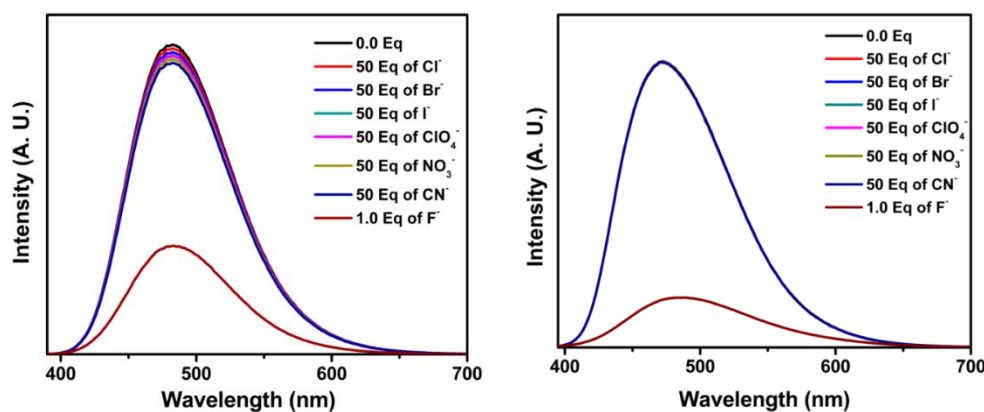
Figure S46: Changes associated with PL spectra of **1** (left) and **2** (right) in presence of various anions (1:1 ratios of H_2O and CH_3CN, 10 μM)(λ_{ex} at 375 nm).

UV-visible titration studies in water

Respective Lewis acid (**1/2**) (1×10^{-5}M) were dissolved in water (1% of CH_3CN was added to enhance the solubility). The pH of solution was maintained at pH 7.0 using HEPES buffer. Aqueous solutions of potassium fluoride used as a fluoride source
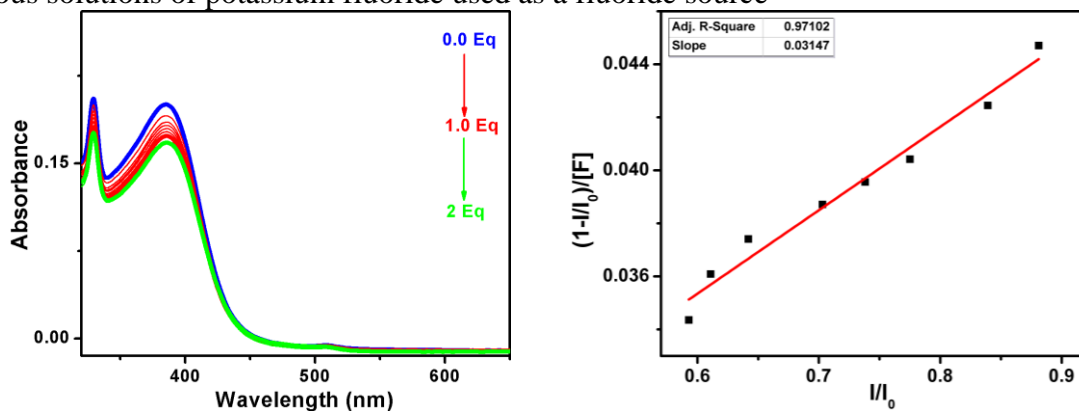
Figure S47: Left: Changes associated with UV-Vis absorption spectrum of **1** (aqueous solution (1% of CH_3CN was added to enhance the solubility), 10 μM) in presence of fluoride ions (KF, 1.5×10^{-3} M). right: plot of I/I_0 Vs $(1-I/I_0)/[F^-]$ (λ_{abs} at 385 nm). Calculated binding constant $K = 3.0 \times 10^4$ M^{-1}

S25
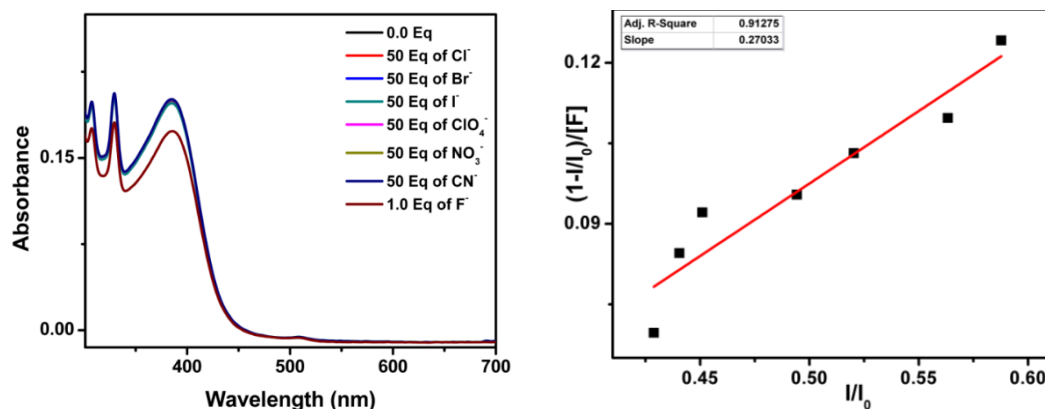
Figure S48: Left: Changes associated with UV-Vis absorption spectrum of **1** (aqueous solution (1% of CH₃CN was added to enhance the solubility), 10 μM) in presence of various anions. right: plot of I/I_0 Vs $(1-I/I_0)/[F^-]$ (λ_{abs} at 385 nm) for compound **2**. Calculated binding constant $K = 2.7 \times 10^3$ M^{-1} for **2.**
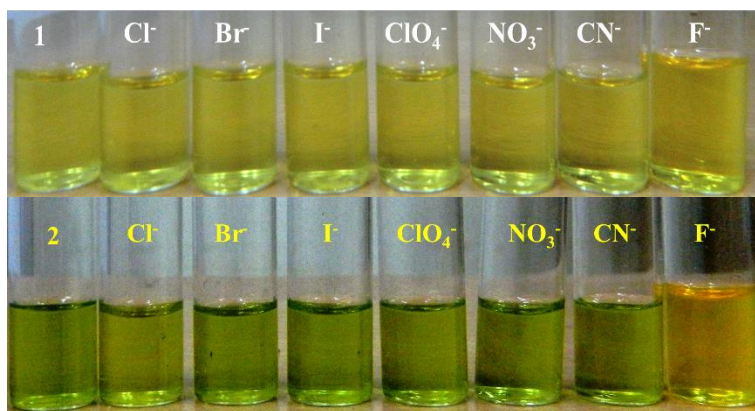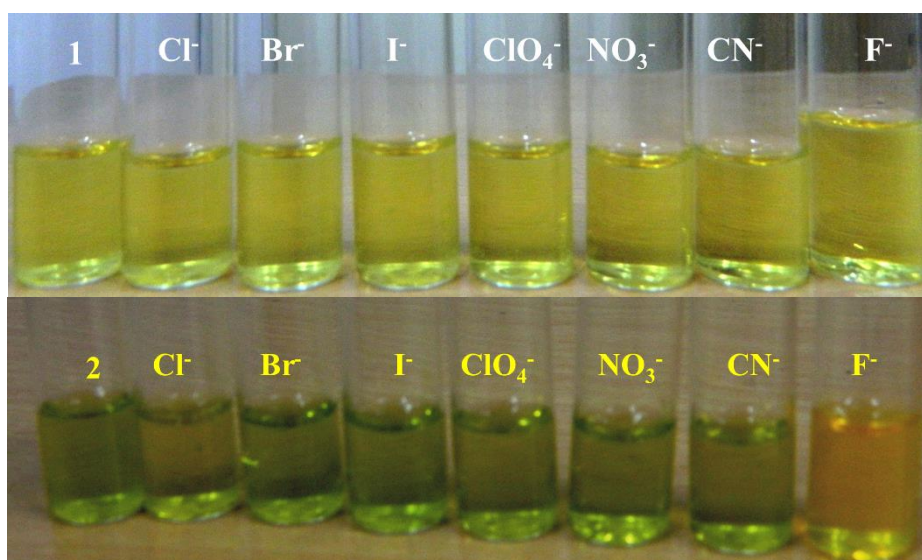

Figure S49: Photograph demonstrating the color changes of **1** (above) and **2** (down) associated with the addition of different anions under normal light. 10 μM solutions were prepared by dissolving respective compounds aqueous solution (1% of CH₃CN); Fluoride was added in 1 equv amount and other anions were used in greater than 50 equv amount.

Fluorescence titration studies in water

Respective Lewis acid (**1/2**) (1×10^{-5} M) was dissolved in water (1% of CH₃CN was added to enhance the solubility). The pH of solution was maintained at pH 7.0 using HEPES (6 mM) buffer. Aqueous solutions of potassium fluoride used as a fluoride source (1×10^{-3} M in HEPES buffer, pH = 7). The experiment was repeated for at least three times at 298 K to obtain concordant value. Compounds **1** or **2** were excited at 375 nm and the emissions were monitored in the range of 400-700 nm (2 nm slit width kept constant for both source and detector)
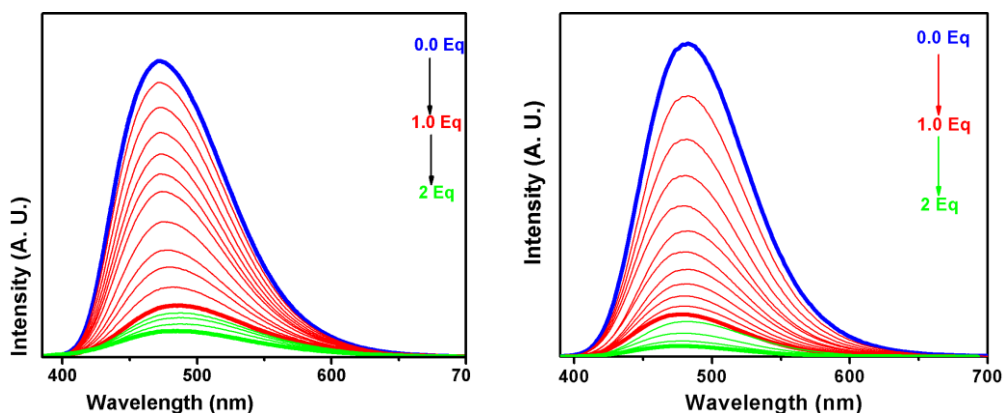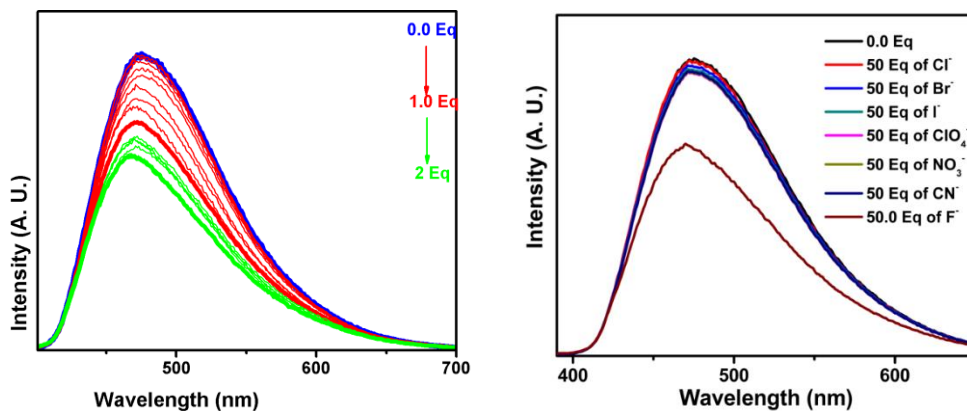
Figure S50: Changes associated with PL spectra of **1** (aqueous solution (1% of CH$_3$CN was added to enhance the solubility), 10 µM) in the presence of fluoride ions (KF, 1.5×10^{-3} M)(λ_{ex} at 375 nm) (left). Changes associated with PL spectra of **1** (right) in presence of various anions (λ_{ex} at 375 nm) (right).
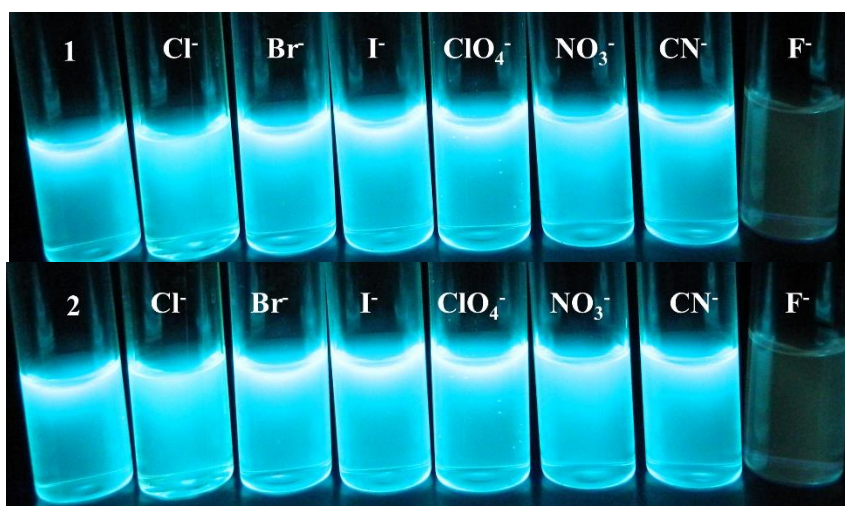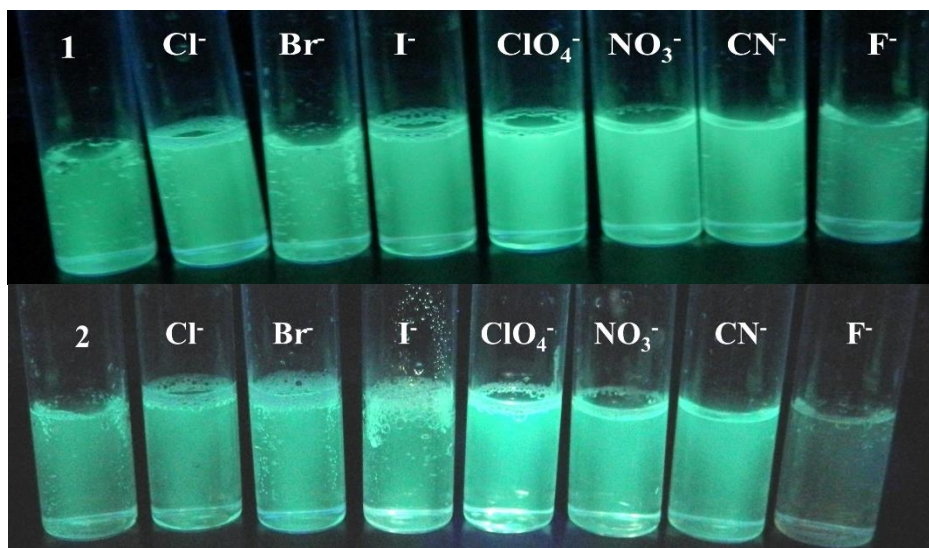

Figure S51: Photograph demonstrating the emission changes associated with **1** (above) and **2** (down) in presence of different anions under UV-light. Concentrations of solutions were 10 µM in aqueous solution (1% of CH$_3$CN was added to enhance the solubility). Fluoride was added in 1 equv amount and other anions were used in greater than 50 equv amount.
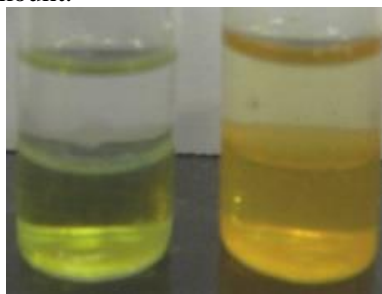
Figure S52: Demonstration of extraction of aqueous inorganic fluoride. Left side vial (before shaking)**:** bottom green layer is the DCM solution of compound **2**, colorless top layer is the aqueous KF. Right side vial (after shaking): Visible colour change for the DCM layer from green to yellow clearly indicates that fluoride ions are extracted from aqueous layer.

Determination of Binding Constant[2]

Solution of (Solvent, Acetonitrile or 1:1 Acetonitrile and water (1% CH3CN was added to enhance the solubility) compounds **1** or **2** (2 mL, 1×10^{-5} M) were placed in a septa screw capped quartz cuvette and was titrated against incremental amount of fluoride ions. The change in absorbance of the band at 395 nm with respect to fluoride concentration was used for calculations.

Sensor + F$^-$ $\leftrightarrow$ F• **sensor**; here sensor is compound **1** or **2**

$I = Ks[$**sensor**$] + Kp[$F• **sensor**$]$

$I_0 = Ks[$**sensor**$]_0$

$[$**sensor**$]_0 = [$**sensor**$] + [$F• **sensor**$]$

$K = [$F• **sensor**$]/ [$**sensor**$][F]$

$I/I_0 = (1 + (Kp/Ks)K[F])/(1 + K[F]) (1 - I/I_0)/[F] \rightarrow K(I/I_0) - K(Kp/Ks)I/I_0 = 1 + K (1 - I/I_0)/[F]$

Here, I_0 is initial absorbance of respective band (395 nm), I is absorbance of respective band upon addition of 1.0 equv of Fluoride. The association constant was obtained from the slope of $(1 - I/I_0)/[F]^-$ Vs I/I_0.

Determination of quenching efficiency

Solution of (Acetonitrile or 1:1 ratios of CH_3CN and H_2O or in water (1% CH_3CN was added to enhance the solubility)) compounds **1** or **2** (2 mL, 1×10^{-5} M) were placed in a septa screw capped quartz cuvette and was titrated against incremental amount of fluoride ions and monitored change in fluorescence band at ~495 nm. Fluorescence quenching efficiency for **1** and **2** were calculated by the following equation.

$$\eta = (I_0\text{-}I)/I_0 \text{ x } 100\%$$

Where, I_0 is the initial PL intensity of the sensors (**1** or **2**) and **I** is the intensity after addition of 1 equivalent of fluoride.

Table S6: The quenching efficiency of **1** and **2**

Compounds	Quenching efficiency (%)		
	CH_3CN	1:1 /(H_2O:CH_3CN)	Water
1	89	60	23
2	96	92	83

Calculation of Limit of Detection (LoD)

The limit of detection of compound **1** and **2** were calculated from the fluorescence quenching titration experiment (compounds **1** or **2** were dissolved in Acetonitrile or 1:1 ratios of CH_3CN and H_2O or in water (1% CH_3CN was added to enhance the solubility)). The intercept to X-axis ($\log[F^-]$) was obtained by linear fitting of the $(I_{max}-I)/(I_{max}-I_{min})$ vs $\log[F^-]$, where I_{max}, I and I_{min} are the initial fluorescence intensity, PL intensity at particular concentration and PL intensity at saturation point respectively. Limit of detection were calculated using the formula, $([F] \times MWPA)/1000$ (multiplied by 10^9 to get the values in ppb), where MWPA is the molecular weight of F^- source. The LoD of **1** and **2** is given in Table S6.

Table S7: The LoD and association constants of **1** and **2**

Compounds	limit of detection (ppm)		
	CH_3CN	1:1/ H_2O:CH_3CN	water
1	6.2	8.1	87.2
2	0.03	0.05	0.1
Compounds	Association constants ($\times 10^5$ M^{-1})		
	CH_3CN	1:1 /(Water:CH_3CN)	Water
1	2.8	2.4	0.3
2	3.3	3.1	2.7
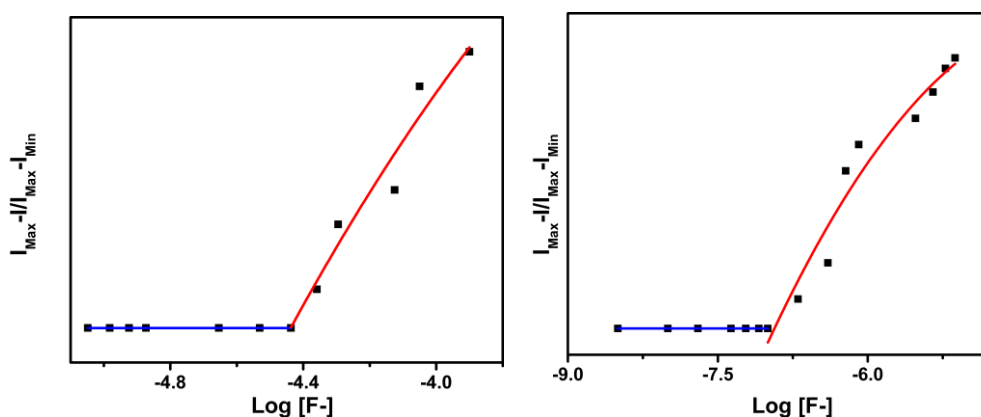
Figure S53: $(I_{max}-I)/(I_{max}-I_{min})$ vs $\log[F]^-$ plots for PL data obtained for acetonitrile solutions of **1** (left) and **2** (right). For **1** and **2**, the lowest detection limits ($[F^-]$) were found to be 6.2 and 0.03 ppm respectively.
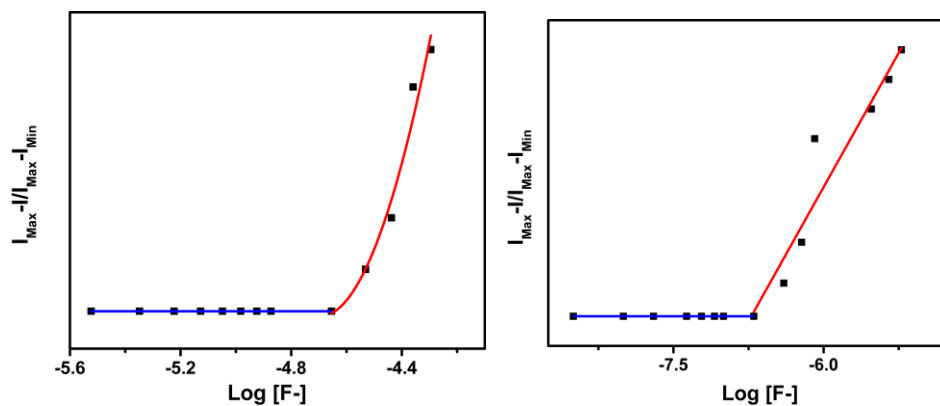
Figure S54: $(I_{max}-I)/(I_{max}-I_{min})$ vs log[F]$^-$ plots for PL data obtained for **1** (left) and **2** (right) in 1:1 ratio of CH$_3$CN:H$_2$O. For **1** and **2**, the lowest detection limits ([F$^-$]) were found to be 8.1 and 0.05 ppm respectively.
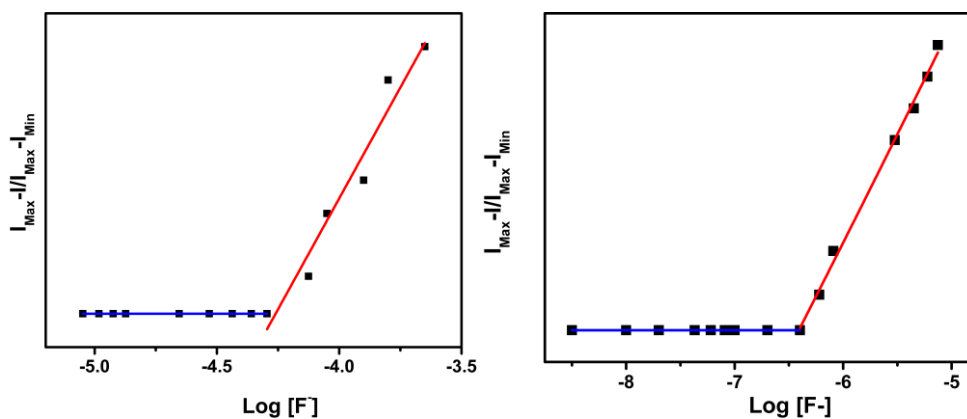
Figure S55: $(I_{max}-I)/(I_{max}-I_{min})$ vs log[F$^-$] plots for PL data obtained for **1** (left) and **2** (right) in aqueous medium. For **1** and **2**, the lowest detection limits ([F$^-$]) were found to be 87.2 and 0.1 ppm respectively.

Cytotoxicity Study:
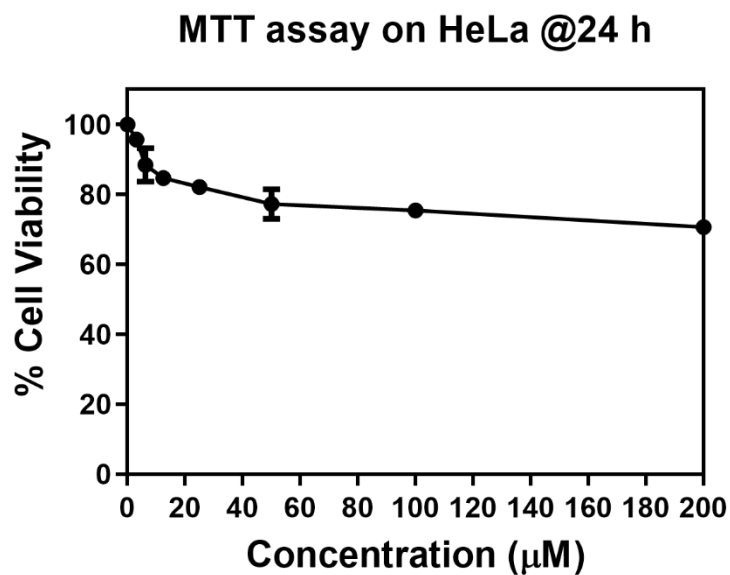
Figure S56a: Cell viability of Hela cells treated with different concentrations of **2** for 24 h.
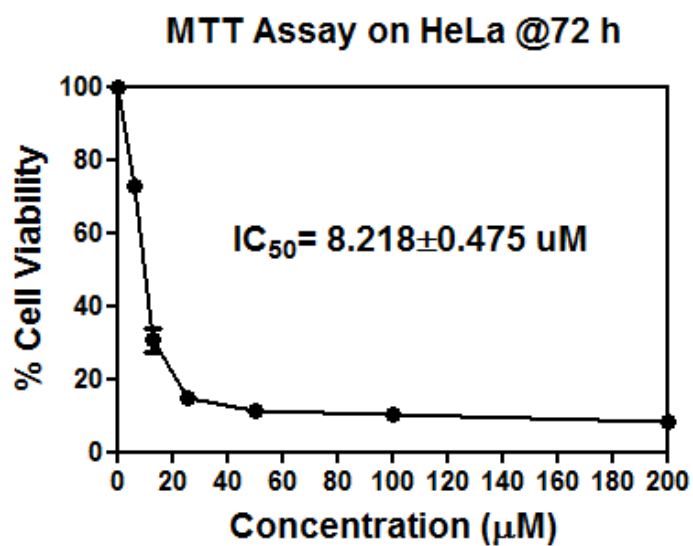
Figure S56b: Cell viability of Hela cells treated with different concentrations of **2** for 72 h.
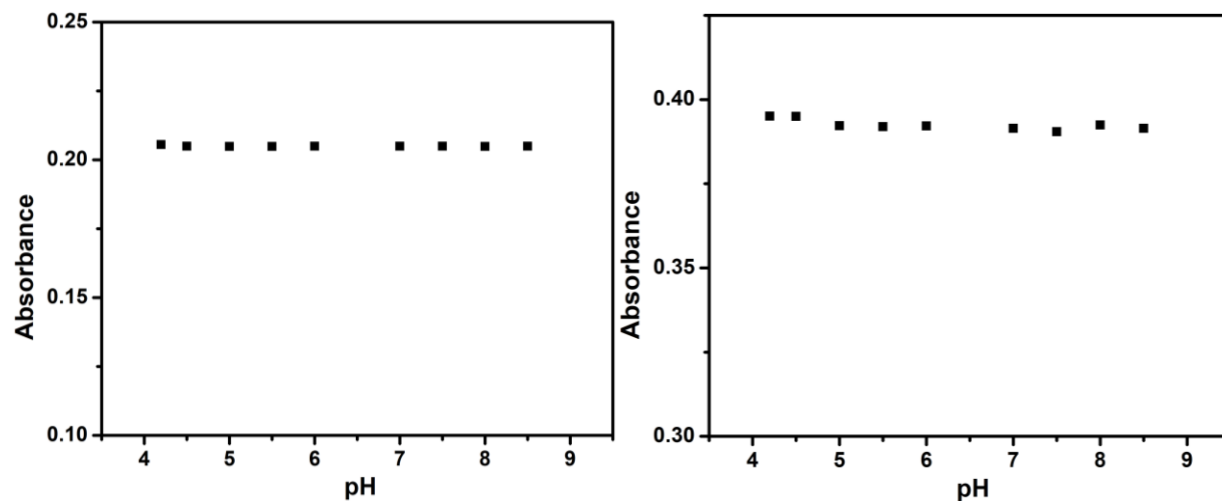
Figure 57: The absorption spectra of compounds **1** and **2** with various pHs.
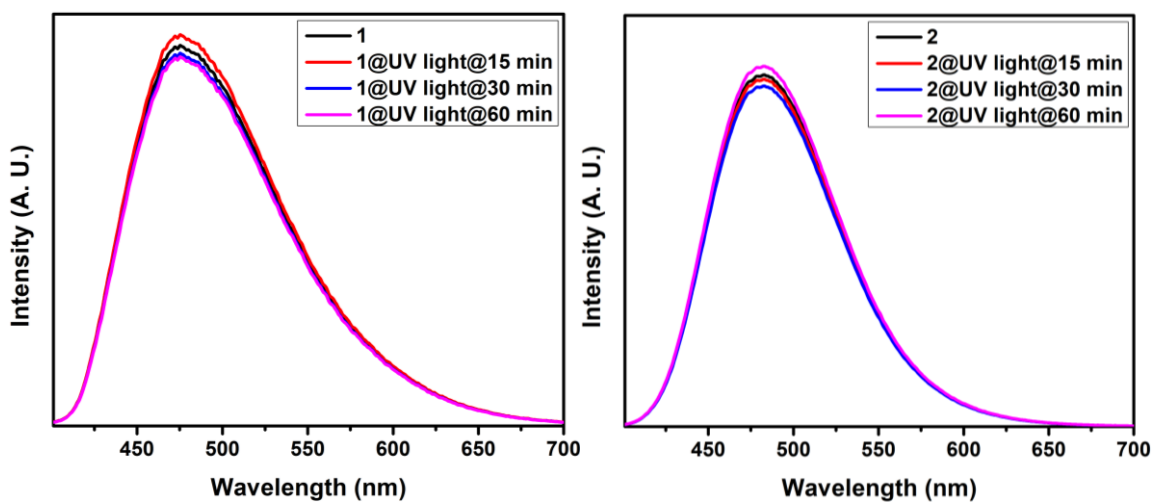
Figure 58: The fluorescence spectra of compounds **1** and **2** under exposure to UV light conditions with varying time period.

DFT calculations:[3]
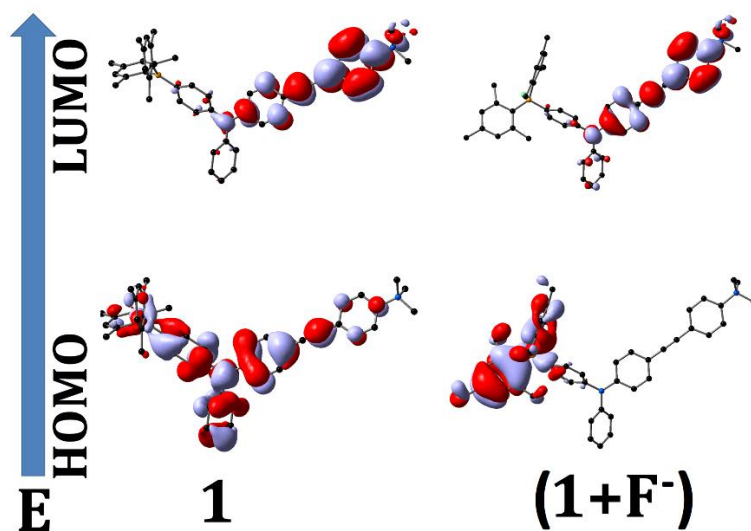
Figure S59: HOMO and LUMO of **1** (left) and **(1+F⁻)** (right) plotted with a 0.02 iso-contour value.
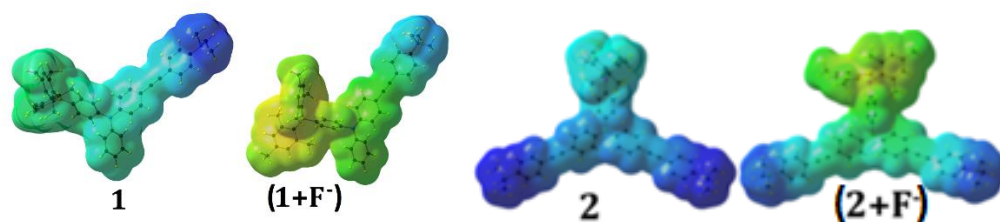
Figure S60: ESP surfaces of **1** and **(1+F⁻) and 2** and **(2+F⁻)** (iso value = 0.0004, range = ± 0.15).
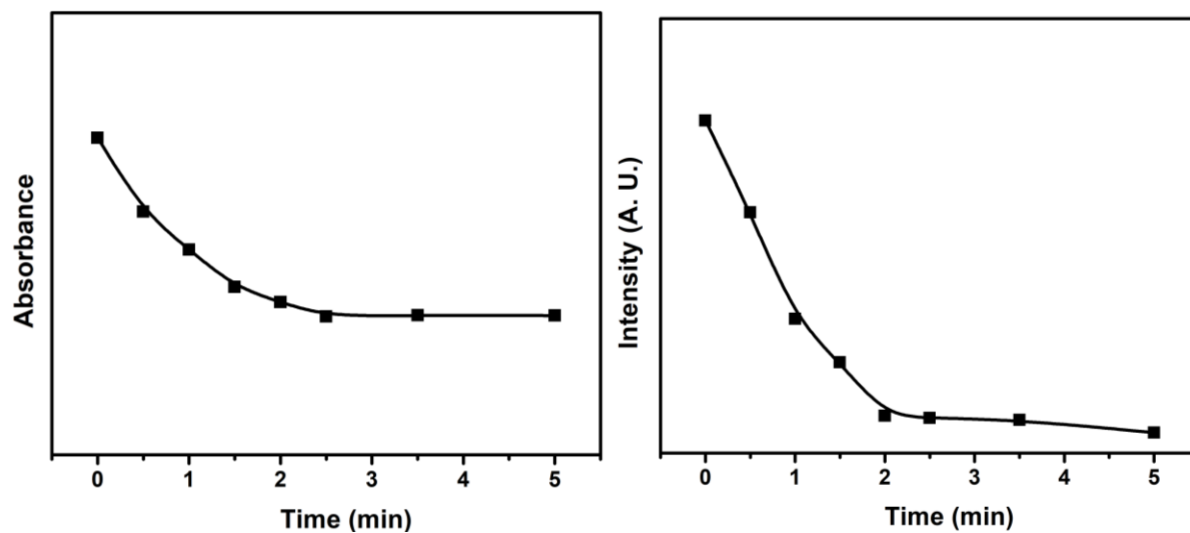
Figure S61: Change of Absorption (left) and fluorescence (right) with time upon addition of 1 eq of fluoride ions to receptor **1**
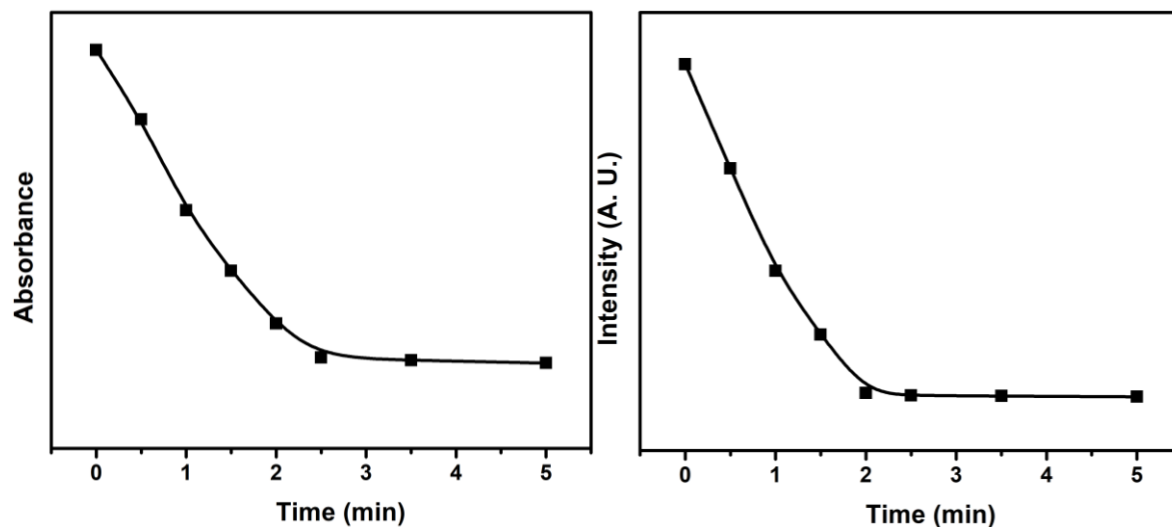
Figure S62: Change of Absorption (left) and fluorescence (right) with time upon addition of 1 eq of fluoride ions to receptor **2**

Table S8: Coordinates of **BTPA-NMe₂**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.270759	6.662450	-1.376822
2	6	0	-1.023091	5.711688	-2.070022
3	6	0	0.623696	6.241262	-0.390554
4	6	0	-0.880024	4.354169	-1.789046
5	1	0	-1.716560	6.024871	-2.846028
6	6	0	0.760494	4.886958	-0.090805
7	1	0	1.211550	6.970776	0.160229
8	6	0	0.009791	3.930108	-0.790191
9	1	0	-1.454994	3.616055	-2.339324
10	1	0	1.447926	4.562586	0.684138
11	6	0	-0.969186	1.712211	-0.355277
12	6	0	-0.929238	0.363097	-0.759458
13	6	0	-2.165707	2.212217	0.194746
14	6	0	-2.052717	-0.441118	-0.625895
15	1	0	-0.017805	-0.039748	-1.188875
16	6	0	-3.271790	1.385141	0.335497
17	1	0	-2.212546	3.245946	0.521330
18	6	0	-3.265179	0.032317	-0.074518
19	1	0	-1.995928	-1.473244	-0.962395
20	1	0	-4.173360	1.794454	0.783634
21	5	0	-4.520526	-0.885758	0.073352
22	6	0	-4.624524	-2.198552	-0.815589
23	6	0	-5.659691	-0.471407	1.101368
24	6	0	-4.770669	-3.479762	-0.216699
25	6	0	-4.558291	-2.138212	-2.232661
26	6	0	-5.386848	-0.305029	2.482840
27	6	0	-6.990516	-0.218683	0.659257
28	6	0	-4.832466	-4.627580	-1.011130
29	6	0	-4.828598	-3.657276	1.287336
30	6	0	-4.652827	-3.309675	-2.994251
31	6	0	-4.397440	-0.833904	-2.994142
32	6	0	-6.401741	0.099316	3.362824
33	6	0	-4.038953	-0.617916	3.106156
34	6	0	-7.968322	0.194239	1.564833

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35	6	0	-7.386924	-0.342228	-0.798157
36	6	0	-4.784882	-4.567352	-2.406416
37	1	0	-4.927016	-5.597792	-0.525908
38	1	0	-5.686534	-3.136448	1.724517
39	1	0	-4.907976	-4.717258	1.549715
40	1	0	-3.930998	-3.265383	1.780553
41	1	0	-4.619368	-3.233578	-4.080204
42	1	0	-3.339707	-0.583820	-3.142149
43	1	0	-4.856982	-0.910208	-3.985838
44	1	0	-4.850769	0.017446	-2.480808
45	6	0	-7.697723	0.360367	2.928107
46	1	0	-6.164416	0.208188	4.420426
47	1	0	-4.098263	-1.532722	3.711035
48	1	0	-3.249899	-0.761241	2.367012
49	1	0	-3.721721	0.187790	3.779145
50	1	0	-8.973630	0.393880	1.196513
51	1	0	-6.876530	0.402303	-1.422626
52	1	0	-7.141100	-1.326560	-1.207592
53	1	0	-8.462986	-0.182798	-0.921531
54	6	0	-4.903411	-5.818105	-3.245100
55	6	0	-8.778489	0.807625	3.884003
56	1	0	-5.953797	-6.110625	-3.378898
57	1	0	-4.476071	-5.673970	-4.243105
58	1	0	-4.391279	-6.665754	-2.775926
59	1	0	-9.644043	0.133931	3.853993
60	1	0	-8.413092	0.837120	4.915533
61	1	0	-9.146253	1.810569	3.631736
62	6	0	1.474990	2.010467	-0.357918
63	6	0	2.487712	2.363014	-1.264597
64	6	0	1.786259	1.136387	0.696797
65	6	0	3.773152	1.857701	-1.120756
66	1	0	2.258378	3.036362	-2.084398
67	6	0	3.067831	0.619501	0.831886
68	1	0	1.014597	0.865118	1.410332
69	6	0	4.092720	0.969938	-0.072098
70	1	0	4.545414	2.135952	-1.831257
71	1	0	3.294695	-0.054194	1.652430
72	7	0	0.162614	2.542668	-0.498134
73	1	0	-0.379511	7.719239	-1.603451
74	6	0	5.405975	0.444207	0.069065
75	6	0	6.530408	-0.008677	0.188344
76	6	0	7.841150	-0.539973	0.327306
77	6	0	8.853384	-0.250291	-0.609064
78	6	0	8.179242	-1.385022	1.402977
79	6	0	10.132030	-0.771317	-0.480823
80	1	0	8.622703	0.392511	-1.453526
81	6	0	9.455116	-1.910456	1.540498
82	1	0	7.419355	-1.633066	2.138197
83	6	0	10.475430	-1.612159	0.605335
84	1	0	10.869406	-0.521340	-1.234253
85	1	0	9.657738	-2.560482	2.383285
86	6	0	12.028245	-3.105572	1.779592
87	1	0	11.441838	-4.028502	1.647085
88	1	0	13.087531	-3.367779	1.753842
89	1	0	11.810037	-2.706629	2.777921
90	6	0	12.724950	-1.937710	-0.318654
91	1	0	12.404428	-2.404183	-1.263495
92	1	0	12.908985	-0.873627	-0.511928
93	1	0	13.673981	-2.387409	-0.021076
94	7	0	11.757637	-2.116435	0.750487

Table S9: Coordinates of **BTPA-2NMe₂**

| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |

1	6	0	-3.578029	-2.657912	0.130003
2	6	0	-3.392999	-1.527035	0.952916
3	6	0	-2.533478	-3.013084	-0.749113
4	6	0	-2.217221	-0.789978	0.903319
5	1	0	-4.179917	-1.242154	1.644447
6	6	0	-1.363929	-2.267154	-0.809768
7	1	0	-2.657679	-3.876339	-1.395579
8	6	0	-1.187859	-1.144988	0.015962
9	1	0	-2.088282	0.069268	1.553721
10	1	0	-0.576038	-2.549553	-1.500830
11	6	0	-0.009656	1.017163	-0.038332
12	6	0	1.015412	1.760522	0.579740
13	6	0	-1.064741	1.715796	-0.657411
14	6	0	0.969069	3.147793	0.583941
15	1	0	1.835264	1.240928	1.064528
16	6	0	-1.083438	3.103743	-0.653719
17	1	0	-1.857493	1.161198	-1.148551
18	6	0	-0.076976	3.875167	-0.028679
19	1	0	1.766618	3.692960	1.082337
20	1	0	-1.901457	3.613932	-1.155374
21	5	0	-0.121005	5.436440	-0.011282
22	6	0	0.727859	6.219629	1.080352
23	6	0	-1.027824	6.195799	-1.073806
24	6	0	1.703216	7.182476	0.700961
25	6	0	0.550303	5.975208	2.467706
26	6	0	-0.827293	6.042572	-2.469317
27	6	0	-2.100445	7.034392	-0.652636
28	6	0	2.456640	7.845450	1.673068
29	6	0	1.991129	7.498207	-0.753004
30	6	0	1.306365	6.681380	3.411775
31	6	0	-0.452959	4.970213	3.006754
32	6	0	-1.666608	6.697001	-3.383118
33	6	0	0.324494	5.249157	-3.057778
34	6	0	-2.919905	7.658094	-1.594202
35	6	0	-2.424945	7.246367	0.812332
36	6	0	2.269323	7.618474	3.039227
37	1	0	3.208783	8.565454	1.354323
38	1	0	1.101694	7.870144	-1.271248
39	1	0	2.774174	8.258718	-0.837014
40	1	0	2.335574	6.613409	-1.302145
41	1	0	1.136204	6.488956	4.470210
42	1	0	0.001192	3.979553	3.132375
43	1	0	-0.821979	5.286878	3.988631
44	1	0	-1.316709	4.836612	2.351779
45	6	0	-2.720841	7.506736	-2.971156
46	1	0	-1.482551	6.566210	-4.448735
47	1	0	1.104197	5.924121	-3.436094
48	1	0	0.792529	4.578219	-2.336106
49	1	0	-0.011405	4.643842	-3.908030
50	1	0	-3.742158	8.280344	-1.243889
51	1	0	-2.763952	6.319090	1.291885
52	1	0	-1.558007	7.601168	1.377382
53	1	0	-3.228398	7.980894	0.928590
54	6	0	3.061007	8.384534	4.072747
55	6	0	-3.617484	8.205960	-3.965649
56	1	0	2.617079	9.370909	4.264605
57	1	0	3.094388	7.851342	5.028813
58	1	0	4.092109	8.554991	3.743101
59	1	0	-3.521856	9.297098	-3.892447
60	1	0	-3.374348	7.919706	-4.993988
61	1	0	-4.673726	7.966106	-3.791129
62	6	0	1.260497	-1.091745	-0.081238
63	6	0	1.489333	-2.189086	0.764559
64	6	0	2.270572	-0.705969	-0.977690
65	6	0	2.692066	-2.881130	0.714829
66	1	0	0.716417	-2.494292	1.462826
67	6	0	3.479219	-1.388611	-1.016686
68	1	0	2.100433	0.134225	-1.643437

69	6	0	3.717602	-2.494100	-0.173235
70	1	0	2.857361	-3.725458	1.376888
71	1	0	4.251153	-1.080600	-1.715144
72	7	0	0.020221	-0.393852	-0.037528
73	6	0	4.952479	-3.197121	-0.214661
74	6	0	6.009992	-3.800880	-0.243448
75	6	0	7.242908	-4.507110	-0.270660
76	6	0	7.470408	-5.614147	0.570945
77	6	0	8.290170	-4.124835	-1.132309
78	6	0	8.673210	-6.303768	0.554522
79	1	0	6.684944	-5.929791	1.251301
80	6	0	9.496756	-4.808032	-1.156134
81	1	0	8.148428	-3.271350	-1.788786
82	6	0	9.722775	-5.925980	-0.317323
83	1	0	8.796572	-7.143416	1.227802
84	1	0	10.270661	-4.466658	-1.833019
85	6	0	12.031564	-6.106810	-1.128773
86	1	0	12.363768	-5.114468	-0.785100
87	1	0	12.874799	-6.795301	-1.048315
88	1	0	11.769789	-6.026961	-2.191097
89	6	0	11.178747	-7.653239	0.640841
90	1	0	11.180315	-7.259518	1.669511
91	1	0	10.431425	-8.454430	0.586107
92	1	0	12.155319	-8.099956	0.445244
93	7	0	10.918311	-6.625435	-0.352504
94	6	0	-4.778758	-3.416984	0.183821
95	6	0	-5.806606	-4.069300	0.224940
96	6	0	-7.003735	-4.833976	0.266682
97	6	0	-7.176836	-5.966212	-0.554059
98	6	0	-8.068104	-4.488207	1.122752
99	6	0	-8.343619	-6.714656	-0.522374
100	1	0	-6.377433	-6.254848	-1.230157
101	6	0	-9.238994	-5.230348	1.161777
102	1	0	-7.968571	-3.616548	1.762919
103	6	0	-9.409538	-6.374088	0.344992
104	1	0	-8.425368	-7.571407	-1.180357
105	1	0	-10.028272	-4.915393	1.833708
106	7	0	-10.567781	-7.132896	0.397140
107	6	0	-11.705594	-6.656071	1.164526
108	1	0	-12.089671	-5.690091	0.800313
109	1	0	-12.511830	-7.389242	1.101091
110	1	0	-11.447081	-6.539558	2.224248
111	6	0	-10.776476	-8.192342	-0.574826
112	1	0	-10.802936	-7.819718	-1.611027
113	1	0	-9.986795	-8.950774	-0.507870
114	1	0	-11.726841	-8.686986	-0.365859

Table S10: Coordinates of **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.789002	1.057393	-0.143309
2	6	0	2.709767	0.422500	0.512458
3	6	0	3.512359	2.214334	-0.906319
4	6	0	1.422284	0.916141	0.411666
5	1	0	2.900180	-0.458787	1.117332
6	6	0	2.225442	2.709285	-1.012566
7	1	0	4.323450	2.712713	-1.428400
8	6	0	1.146952	2.071069	-0.357110
9	1	0	0.615178	0.419346	0.937255
10	1	0	2.037544	3.590098	-1.615502
11	6	0	-1.292599	1.727680	-0.323766
12	6	0	-2.384728	2.139513	0.454739
13	6	0	-1.350687	0.491451	-0.986133

14	6	0	-3.498121	1.315067	0.579559
15	1	0	-2.349667	3.098410	0.962471
16	6	0	-2.477922	-0.313314	-0.858725
17	1	0	-0.518441	0.176235	-1.608473
18	6	0	-3.584389	0.064115	-0.067990
19	1	0	-4.326997	1.644209	1.200538
20	1	0	-2.511256	-1.257227	-1.395724
21	5	0	-4.851285	-0.860229	0.078179
22	6	0	-5.781250	-0.682189	1.346935
23	6	0	-5.127340	-1.945061	-1.043244
24	6	0	-7.174045	-0.427531	1.201433
25	6	0	-5.258416	-0.753462	2.665316
26	6	0	-5.289982	-1.588193	-2.406647
27	6	0	-5.175084	-3.331317	-0.714201
28	6	0	-7.976229	-0.238685	2.329009
29	6	0	-7.832257	-0.316124	-0.159424
30	6	0	-6.103288	-0.588840	3.769495
31	6	0	-3.793226	-1.028713	2.958175
32	6	0	-5.477781	-2.578827	-3.380754
33	6	0	-5.367846	-0.148926	-2.879463
34	6	0	-5.351799	-4.285933	-1.716341
35	6	0	-4.995124	-3.826669	0.707004
36	6	0	-7.464959	-0.323391	3.627439
37	1	0	-9.035027	-0.027096	2.190129
38	1	0	-7.737843	-1.243886	-0.732433
39	1	0	-8.898356	-0.091474	-0.055576
40	1	0	-7.388958	0.483009	-0.765744
41	1	0	-5.681696	-0.671120	4.770099
42	1	0	-3.212665	-0.099465	3.014200
43	1	0	-3.686152	-1.538153	3.922004
44	1	0	-3.316253	-1.653009	2.198250
45	6	0	-5.509054	-3.933785	-3.061858
46	1	0	-5.609626	-2.274678	-4.418145
47	1	0	-6.412353	0.139192	-3.059328
48	1	0	-4.953464	0.561747	-2.162408
49	1	0	-4.834819	-0.017826	-3.828326
50	1	0	-5.367169	-5.339091	-1.440387
51	1	0	-3.995916	-3.595062	1.097848
52	1	0	-5.719081	-3.375856	1.392085
53	1	0	-5.115716	-4.913486	0.755478
54	6	0	-8.364801	-0.160942	4.829141
55	6	0	-5.718626	-4.990396	-4.120387
56	1	0	-8.974975	-1.059139	4.992598
57	1	0	-7.787089	0.014002	5.742427
58	1	0	-9.058371	0.677873	4.700333
59	1	0	-6.685366	-5.494538	-3.993775
60	1	0	-5.699336	-4.559117	-5.126260
61	1	0	-4.945297	-5.766533	-4.070778
62	6	0	-0.373230	3.970065	-0.705026
63	6	0	0.227404	4.936429	0.113098
64	6	0	-1.212817	4.370849	-1.752098
65	6	0	-0.001581	6.290796	-0.126149
66	1	0	0.865190	4.621864	0.933664
67	6	0	-1.448400	5.726820	-1.975147
68	1	0	-1.677923	3.618670	-2.381733
69	6	0	-0.841472	6.691143	-1.167641
70	1	0	0.465696	7.033754	0.514188
71	1	0	-2.101911	6.029264	-2.788497
72	7	0	-0.151536	2.574711	-0.460434
73	6	0	5.103158	0.550723	-0.038100
74	6	0	6.238797	0.111575	0.052980
75	6	0	7.548516	-0.398801	0.161776
76	6	0	8.639934	0.237744	-0.469511
77	6	0	7.816558	-1.570369	0.909840
78	6	0	9.933146	-0.262390	-0.362538
79	1	0	8.465027	1.136765	-1.050228
80	6	0	9.103832	-2.073154	1.019338
81	1	0	6.998196	-2.081486	1.404988

82	6	0	10.167477	-1.419975	0.383646
83	1	0	10.727174	0.271153	-0.869270
84	1	0	9.255106	-2.974590	1.604754
85	7	0	11.556014	-2.000415	0.531343
86	6	0	11.945734	-2.031731	1.995905
87	1	0	11.239742	-2.653401	2.543047
88	1	0	12.952835	-2.443985	2.082915
89	1	0	11.913480	-1.011661	2.379014
90	6	0	12.602642	-1.196971	-0.198930
91	1	0	13.567370	-1.679066	-0.038521
92	1	0	12.368242	-1.183370	-1.262706
93	1	0	12.623766	-0.184383	0.202308
94	6	0	11.586647	-3.407399	-0.031391
95	1	0	10.879836	-4.028948	0.514811
96	1	0	11.300910	-3.360067	-1.082354
97	1	0	12.596933	-3.806970	0.075650
98	1	0	-1.024648	7.746641	-1.346186

Table S11: Coordinates of (**1**+**F**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.362339	6.989277	-0.227409
2	6	0	-2.034473	6.003263	-0.953538
3	6	0	-0.314781	6.622235	0.619426
4	6	0	-1.659832	4.665686	-0.847647
5	1	0	-2.857209	6.274260	-1.609546
6	6	0	0.060801	5.285187	0.740134
7	1	0	0.203136	7.376560	1.206210
8	6	0	-0.601173	4.297103	-0.004841
9	1	0	-2.186817	3.897516	-1.403581
10	1	0	0.857139	4.999707	1.420583
11	6	0	-1.323169	1.960109	0.235803
12	6	0	-1.486784	0.975095	-0.744614
13	6	0	-2.193362	1.999390	1.329824
14	6	0	-2.511467	0.038414	-0.616446
15	1	0	-0.803541	0.941709	-1.590848
16	6	0	-3.212493	1.053322	1.429939
17	1	0	-2.056638	2.758352	2.097273
18	6	0	-3.419257	0.050430	0.459718
19	1	0	-2.601655	-0.735095	-1.375508
20	1	0	-3.866795	1.068437	2.296822
21	6	0	1.060835	2.485941	0.117976
22	6	0	2.113318	3.264353	-0.437941
23	6	0	1.391643	1.210224	0.652311
24	6	0	3.408359	2.791595	-0.462745
25	1	0	1.888916	4.231378	-0.872029
26	6	0	2.688126	0.748415	0.631138
27	1	0	0.607024	0.600938	1.083489
28	6	0	3.738531	1.520171	0.069635
29	1	0	4.190864	3.395296	-0.913564
30	1	0	2.916281	-0.224705	1.055572
31	7	0	-0.248272	2.920769	0.124338
32	1	0	-1.659268	8.030863	-0.312155
33	6	0	5.049709	1.025551	0.033429
34	6	0	6.186251	0.567790	0.006431
35	6	0	7.469264	0.008570	-0.025939
36	6	0	8.573734	0.699641	-0.585387
37	6	0	7.715177	-1.288118	0.501519
38	6	0	9.842046	0.137119	-0.622914
39	1	0	8.420385	1.691662	-0.996053
40	6	0	8.977813	-1.852060	0.466531
41	1	0	6.891482	-1.843347	0.936782
42	6	0	10.050030	-1.143370	-0.097415

43	1	0	10.641695	0.717413	-1.066290
44	1	0	9.107338	-2.846840	0.882907
45	6	0	-3.994734	-2.537374	0.153016
46	6	0	-3.098242	-3.292081	0.965863
47	6	0	-4.244048	-3.058671	-1.145964
48	6	0	-2.546397	-4.497052	0.510491
49	6	0	-3.667665	-4.266490	-1.570814
50	6	0	-2.825397	-5.015997	-0.753673
51	1	0	-1.868178	-5.044052	1.166905
52	1	0	-3.888343	-4.627962	-2.575686
53	6	0	-2.664174	-2.844363	2.351608
54	1	0	-2.310392	-1.808964	2.352494
55	1	0	-3.486859	-2.880656	3.069820
56	1	0	-1.852220	-3.485834	2.717952
57	6	0	-2.249482	-6.337229	-1.209854
58	1	0	-2.874128	-7.186029	-0.895415
59	1	0	-2.170679	-6.385495	-2.302682
60	1	0	-1.248806	-6.507045	-0.792773
61	6	0	-5.135661	-2.361172	-2.159374
62	1	0	-6.193429	-2.416718	-1.883804
63	1	0	-4.901371	-1.297813	-2.260862
64	1	0	-5.020719	-2.823385	-3.147726
65	9	0	-4.729143	-1.131156	2.161519
66	6	0	-6.145991	-0.706769	0.195203
67	6	0	-6.544276	0.404786	-0.592230
68	6	0	-7.202223	-1.549112	0.659029
69	6	0	-7.897801	0.640262	-0.890219
70	6	0	-8.538866	-1.287552	0.337281
71	6	0	-8.917411	-0.190016	-0.437177
72	1	0	-8.156967	1.504831	-1.501787
73	1	0	-9.309261	-1.965055	0.707101
74	6	0	-5.571712	1.411926	-1.183277
75	1	0	-5.035110	1.973794	-0.412319
76	1	0	-4.806679	0.942471	-1.810795
77	1	0	-6.110316	2.134727	-1.808125
78	6	0	-10.369424	0.087931	-0.752591
79	1	0	-10.889158	-0.814699	-1.099407
80	1	0	-10.917107	0.449205	0.129538
81	1	0	-10.469588	0.851063	-1.533060
82	6	0	-6.948740	-2.772151	1.522060
83	1	0	-6.234040	-3.457584	1.055466
84	1	0	-6.518404	-2.487701	2.484888
85	1	0	-7.882201	-3.320366	1.697346
86	5	0	-4.601520	-1.082424	0.709566
87	6	0	12.463876	-0.931726	-0.751347
88	1	0	12.554338	-0.006221	-0.183984
89	1	0	13.408542	-1.476150	-0.728915
90	1	0	12.180924	-0.720141	-1.781824
91	6	0	11.347469	-3.091102	-0.907833
92	1	0	12.337742	-3.551505	-0.914868
93	1	0	10.626678	-3.760677	-0.443098
94	1	0	11.025231	-2.852066	-1.921306
95	6	0	11.857182	-2.099046	1.299141
96	1	0	11.136819	-2.766531	1.767873
97	1	0	12.842030	-2.570301	1.269503
98	1	0	11.895714	-1.157905	1.847699
99	7	0	11.410665	-1.800890	-0.116851

Table S12: Coordinates of **2**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	3.778976	-2.396512	-0.040267
2	6	0	3.581473	-1.175397	-0.720406
3	6	0	2.682132	-2.965151	0.641880

4	6	0	2.345319	-0.551290	-0.718801
5	1	0	4.409722	-0.726387	-1.259373
6	6	0	1.446181	-2.337395	0.651590
7	1	0	2.816629	-3.895553	1.184680
8	6	0	1.254235	-1.118536	-0.030143
9	1	0	2.212392	0.382579	-1.253087
10	1	0	0.625059	-2.777902	1.206484
11	6	0	-0.000800	0.987063	-0.007567
12	6	0	-0.721024	1.680755	-0.988841
13	6	0	0.701944	1.699214	0.972654
14	6	0	-0.725779	3.073107	-0.986145
15	1	0	-1.261702	1.126205	-1.750497
16	6	0	0.671016	3.091423	0.969878
17	1	0	1.254198	1.158954	1.736296
18	6	0	-0.036539	3.820478	-0.008434
19	1	0	-1.272168	3.600636	-1.763361
20	1	0	1.198295	3.632197	1.750682
21	5	0	-0.064266	5.402368	-0.003517
22	6	0	-0.307075	6.156820	-1.369300
23	6	0	0.167953	6.150188	1.369190
24	6	0	-1.352032	7.115245	-1.493833
25	6	0	0.491669	5.897189	-2.515409
26	6	0	-0.641071	5.898863	2.507369
27	6	0	1.239327	7.080963	1.512279
28	6	0	-1.581520	7.748556	-2.717680
29	6	0	-2.267373	7.466562	-0.336993
30	6	0	0.247458	6.576996	-3.713577
31	6	0	1.652579	4.917168	-2.507094
32	6	0	-0.372310	6.541371	3.723656
33	6	0	-1.879946	5.024130	2.463633
34	6	0	1.480772	7.687330	2.745059
35	6	0	2.171551	7.420729	0.365789
36	6	0	-0.788223	7.503192	-3.842138
37	1	0	-2.398990	8.463162	-2.793529
38	1	0	-1.718923	7.938150	0.484734
39	1	0	-3.047573	8.161815	-0.661727
40	1	0	-2.768455	6.583932	0.077794
41	1	0	0.888845	6.378951	-4.570905
42	1	0	1.330637	3.906827	-2.789713
43	1	0	2.417201	5.227355	-3.227286
44	1	0	2.134192	4.835042	-1.529077
45	6	0	0.684729	7.435955	3.869290
46	1	0	-1.017583	6.339552	4.577343
47	1	0	-2.786012	5.644669	2.448188
48	1	0	-1.915988	4.374644	1.587335
49	1	0	-1.945539	4.389960	3.355702
50	1	0	2.315590	8.380338	2.833786
51	1	0	2.720939	6.541587	0.005857
52	1	0	1.631211	7.832654	-0.491772
53	1	0	2.915479	8.158749	0.680987
54	6	0	-1.023823	8.241734	-5.137666
55	6	0	0.962686	8.125328	5.183463
56	1	0	-0.538331	9.226616	-5.124632
57	1	0	-0.620162	7.691029	-5.993581
58	1	0	-2.091401	8.412125	-5.314152
59	1	0	0.822989	9.210456	5.099736
60	1	0	0.298115	7.764514	5.974563
61	1	0	1.996696	7.961528	5.510515
62	6	0	-1.216762	-1.139561	0.022746
63	6	0	-1.392200	-2.358477	-0.663064
64	6	0	-2.313625	-0.592048	0.717946
65	6	0	-2.618706	-3.004760	-0.652383
66	1	0	-0.566104	-2.784160	-1.222175
67	6	0	-3.540320	-1.234514	0.720668
68	1	0	-2.192699	0.341223	1.256148
69	6	0	-3.721805	-2.455137	0.035215
70	1	0	-2.741044	-3.934694	-1.198847
71	1	0	-4.373486	-0.800406	1.264231

```
72     7     0      0.013207   -0.450313   -0.005337
73     6     0     -4.986772   -3.095379    0.030958
74     6     0     -6.085641   -3.623009    0.032434
75     6     0     -7.373484   -4.209252    0.036012
76     6     0     -7.624696   -5.437739   -0.608466
77     6     0     -8.455111   -3.572511    0.686155
78     6     0     -8.894515   -6.008497   -0.610058
79     1     0     -6.813101   -5.948284   -1.115161
80     6     0     -9.722615   -4.136321    0.687225
81     1     0     -8.289950   -2.626393    1.189763
82     6     0     -9.945180   -5.356681    0.038098
83     1     0     -9.027040   -6.952390   -1.122793
84     1     0    -10.520283   -3.606596    1.198077
85     6     0      5.052217   -3.019975   -0.035999
86     6     0      6.156800   -3.535585   -0.036704
87     6     0      7.449697   -4.110473   -0.039154
88     6     0      7.709222   -5.339425    0.601220
89     6     0      8.527820   -3.462556   -0.684046
90     6     0      8.983459   -5.900143    0.603548
91     1     0      6.900494   -5.858385    1.103934
92     6     0      9.799747   -4.016372   -0.684380
93     1     0      8.356381   -2.515788   -1.184330
94     6     0     10.030446   -5.237536   -0.039617
95     1     0      9.122170   -6.845004    1.112836
96     1     0     10.594347   -3.478271   -1.191236
97     7     0    -11.343149   -5.933736    0.058563
98     7     0     11.432798   -5.803913   -0.059514
99     6     0     11.871650   -6.038773   -1.491971
100    1     0     11.860939   -5.093807   -2.031521
101    1     0     12.881258   -6.453437   -1.484624
102    1     0     11.172939   -6.736694   -1.953661
103    6     0     11.539766   -7.120594    0.670012
104    1     0     12.575723   -7.454543    0.607272
105    1     0     11.260717   -6.977983    1.713416
106    1     0     10.886942   -7.850990    0.193206
107    6     0     12.386406   -4.832992    0.609932
108    1     0     12.378758   -3.889260    0.068081
109    1     0     12.049506   -4.674351    1.634539
110    1     0     13.389565   -5.262970    0.596984
111    6     0    -11.777673   -6.176758    1.490943
112    1     0    -11.773039   -5.233625    2.033779
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114    1     0    -11.073034   -6.871093    1.949028
115    6     0    -11.441525   -7.248704   -0.675256
116    1     0    -11.165482   -7.100480   -1.718679
117    1     0    -10.782344   -7.975783   -0.202126
118    1     0    -12.474833   -7.590686   -0.611813
119    6     0    -12.305246   -4.967727   -0.605900
120    1     0    -11.971310   -4.803002   -1.630513
121    1     0    -13.305075   -5.405375   -0.592711
122    1     0    -12.303782   -4.025857   -0.060757
```

Table S13: Coordinates of (**2**+**F**)

```
---------------------------------------------------------------------
Center   Atomic   Atomic        Coordinates (Angstroms)
Number   Number   Type       X        Y        Z
---------------------------------------------------------------------
  1        6       0     3.952380  -2.623044  -0.038994
  2        6       0     3.704378  -1.323036  -0.539475
  3        6       0     2.867382  -3.342875   0.509483
  4        6       0     2.442359  -0.766494  -0.483625
  5        1       0     4.522296  -0.755408  -0.972003
  6        6       0     1.600167  -2.788683   0.565895
  7        1       0     3.038683  -4.334925   0.916560
  8        6       0     1.359078  -1.485042   0.073034
```

9	1	0	2.272631	0.234829	-0.860786
10	1	0	0.793667	-3.346851	1.028019
11	6	0	0.066861	0.579232	0.278591
12	6	0	-0.510134	1.332621	-0.748383
13	6	0	0.576950	1.218118	1.413796
14	6	0	-0.563234	2.720598	-0.632247
15	1	0	-0.917756	0.828064	-1.621967
16	6	0	0.509640	2.607281	1.502930
17	1	0	1.006074	0.624151	2.218507
18	6	0	-0.042232	3.408172	0.481170
19	1	0	-1.037505	3.289810	-1.427965
20	1	0	0.876317	3.102926	2.397003
21	6	0	-1.109742	-1.554737	0.185335
22	6	0	-1.302435	-2.761494	-0.525326
23	6	0	-2.211937	-0.993693	0.869639
24	6	0	-2.544691	-3.372923	-0.557410
25	1	0	-0.480256	-3.191971	-1.086061
26	6	0	-3.447860	-1.607471	0.838839
27	1	0	-2.079481	-0.065748	1.412799
28	6	0	-3.649153	-2.808462	0.118331
29	1	0	-2.680894	-4.283891	-1.132505
30	1	0	-4.282155	-1.161195	1.370781
31	7	0	0.109710	-0.866153	0.176768
32	6	0	-4.937931	-3.381278	0.059641
33	6	0	-6.079191	-3.815173	0.025686
34	6	0	-7.423965	-4.233106	-0.006959
35	6	0	-7.839258	-5.373579	-0.729358
36	6	0	-8.417959	-3.497644	0.684946
37	6	0	-9.175331	-5.758240	-0.772493
38	1	0	-7.101050	-5.957950	-1.267610
39	6	0	-9.749526	-3.877015	0.645545
40	1	0	-8.127295	-2.618280	1.249088
41	6	0	-10.133873	-5.007949	-0.086777
42	1	0	-9.432381	-6.638206	-1.348184
43	1	0	-10.471568	-3.275477	1.188556
44	6	0	-1.600645	5.524619	0.037049
45	6	0	-2.817164	5.335402	0.756134
46	6	0	-1.731566	6.046909	-1.279023
47	6	0	-4.052564	5.691956	0.198855
48	6	0	-2.987215	6.386673	-1.807065
49	6	0	-4.165859	6.233468	-1.081140
50	1	0	-4.957489	5.534273	0.787040
51	1	0	-3.038888	6.784825	-2.820745
52	6	0	-2.866515	4.727352	2.147792
53	1	0	-2.317780	3.781643	2.198880
54	1	0	-2.408417	5.380408	2.894181
55	1	0	-3.907155	4.537572	2.440284
56	6	0	-5.504062	6.648350	-1.648571
57	1	0	-5.747977	7.690346	-1.396457
58	1	0	-5.518613	6.572456	-2.742489
59	1	0	-6.318359	6.026330	-1.256761
60	6	0	-0.545905	6.273458	-2.201485
61	1	0	0.079085	7.108546	-1.870393
62	1	0	0.112683	5.401968	-2.259932
63	1	0	-0.893068	6.495856	-3.217882
64	9	0	-0.213424	5.175456	2.163988
65	6	0	1.180527	5.960479	0.294990
66	6	0	2.331728	5.536089	-0.417692
67	6	0	1.204144	7.307697	0.768349
68	6	0	3.412896	6.405685	-0.642190
69	6	0	2.295342	8.147924	0.520114
70	6	0	3.421380	7.718922	-0.183984
71	1	0	4.274548	6.038706	-1.200659
72	1	0	2.262562	9.172499	0.891362
73	6	0	2.495051	4.142737	-1.003224
74	1	0	2.522000	3.367847	-0.229621
75	1	0	1.680831	3.872292	-1.684029
76	1	0	3.431542	4.079705	-1.571017

77	6	0	4.596974	8.638130	-0.424588
78	1	0	4.277445	9.608486	-0.825862
79	1	0	5.149078	8.845743	0.502865
80	1	0	5.306546	8.201003	-1.136642
81	6	0	0.062779	7.910922	1.567228
82	1	0	-0.904417	7.750036	1.082137
83	1	0	-0.008649	7.450009	2.555771
84	1	0	0.208419	8.990441	1.691699
85	5	0	-0.149750	5.044541	0.713807
86	6	0	-11.876248	-6.607022	-0.937612
87	1	0	-11.335567	-7.452414	-0.513407
88	1	0	-12.949038	-6.799284	-0.905118
89	1	0	-11.563137	-6.429339	-1.965815
90	6	0	-12.402234	-4.236666	-0.713065
91	1	0	-13.455903	-4.521756	-0.734860
92	1	0	-12.269356	-3.344224	-0.104781
93	1	0	-12.031535	-4.053313	-1.721655
94	6	0	-12.087437	-5.649101	1.295126
95	1	0	-11.953060	-4.755617	1.901649
96	1	0	-13.144457	-5.919445	1.255735
97	1	0	-11.495544	-6.466563	1.707144
98	7	0	-11.600621	-5.375231	-0.113637
99	6	0	5.260539	-3.151582	-0.062711
100	6	0	6.411933	-3.559083	-0.084549
101	6	0	7.760171	-3.965724	-0.094509
102	6	0	8.161206	-5.233963	0.381600
103	6	0	8.770826	-3.097342	-0.576375
104	6	0	9.497966	-5.617422	0.388579
105	1	0	7.409884	-5.921265	0.754824
106	6	0	10.103815	-3.474586	-0.571403
107	1	0	8.492302	-2.117699	-0.948894
108	6	0	10.472899	-4.736278	-0.086224
109	1	0	9.742759	-6.600730	0.769695
110	1	0	10.839034	-2.768969	-0.945832
111	6	0	12.481631	-5.060597	-1.500232
112	1	0	12.359796	-4.057607	-1.904420
113	1	0	13.539495	-5.329497	-1.479242
114	1	0	11.915295	-5.771867	-2.101684
115	6	0	12.196267	-6.481635	0.459743
116	1	0	11.674560	-7.213269	-0.156196
117	1	0	13.270665	-6.663954	0.422323
118	1	0	11.848317	-6.531463	1.490914
119	6	0	12.709892	-4.119419	0.777662
120	1	0	12.588411	-3.115420	0.375953
121	1	0	12.303282	-4.163425	1.788145
122	1	0	13.765067	-4.399818	0.773583
123	7	0	11.940522	-5.099812	-0.085317

Table S14: Molecular orbital of **BTPA-NMe₂**, **BTPA-2NMe₂**, **1** and **2**.

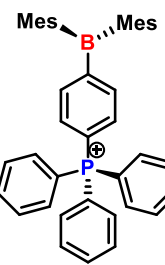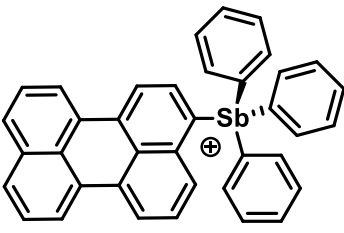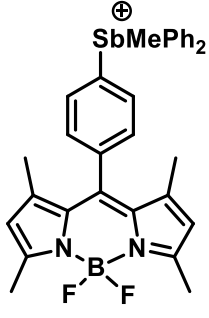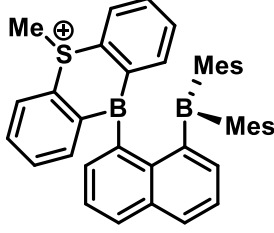| *BTPA-NMe₂*	*BTPA-2NMe₂*	*1*	*2*

LUMO

HOMO

HOMO-1

HOMO-2
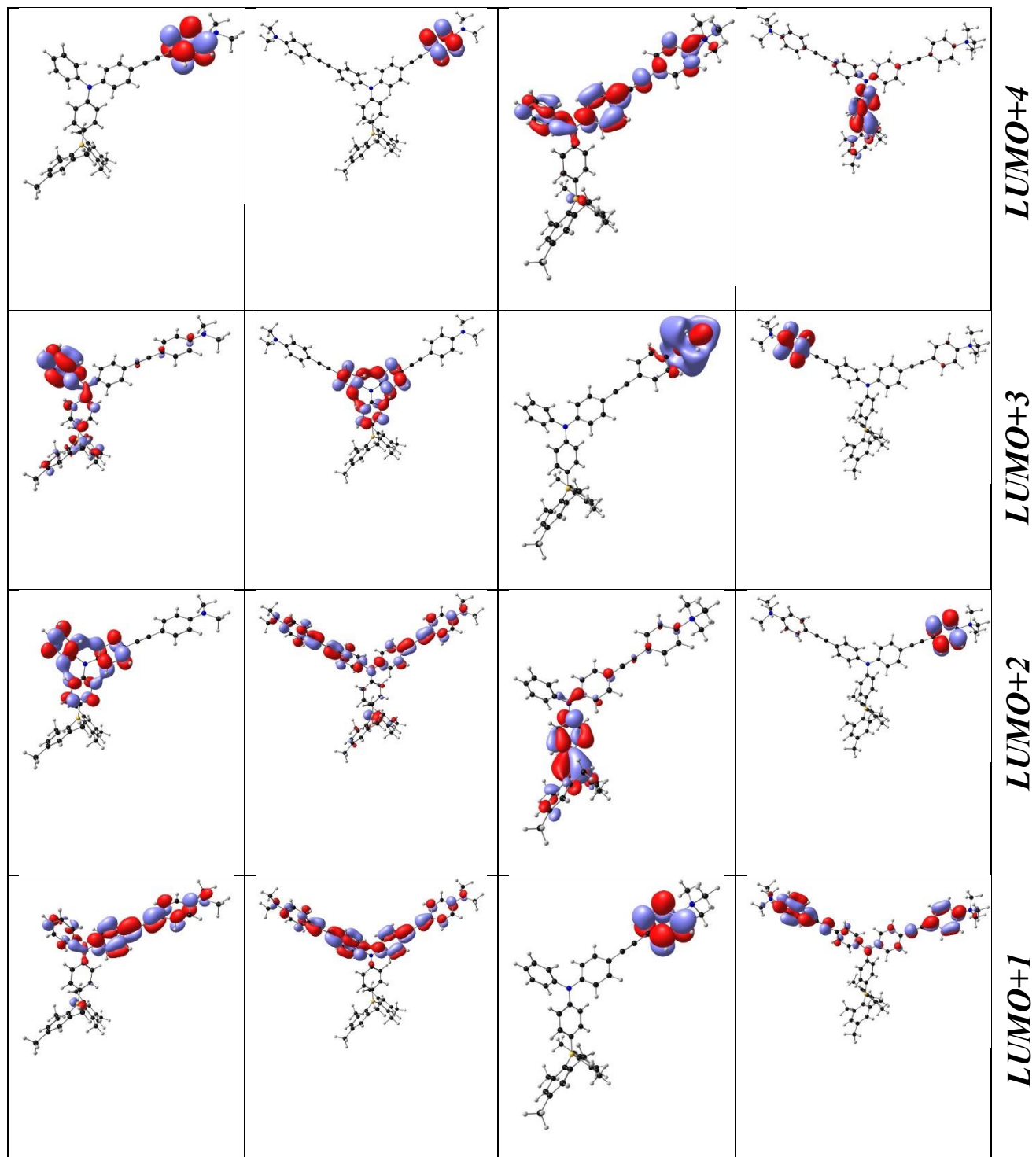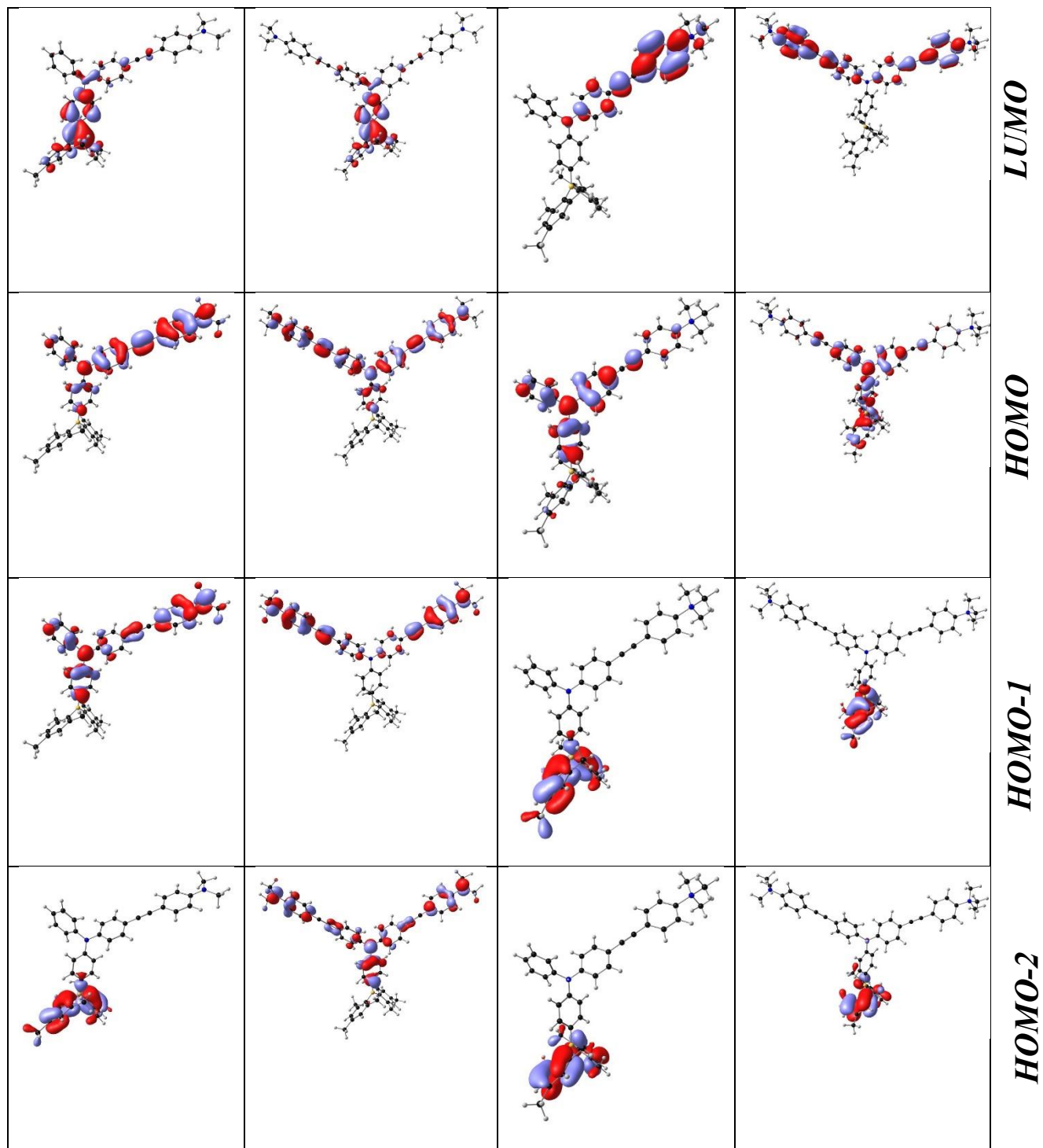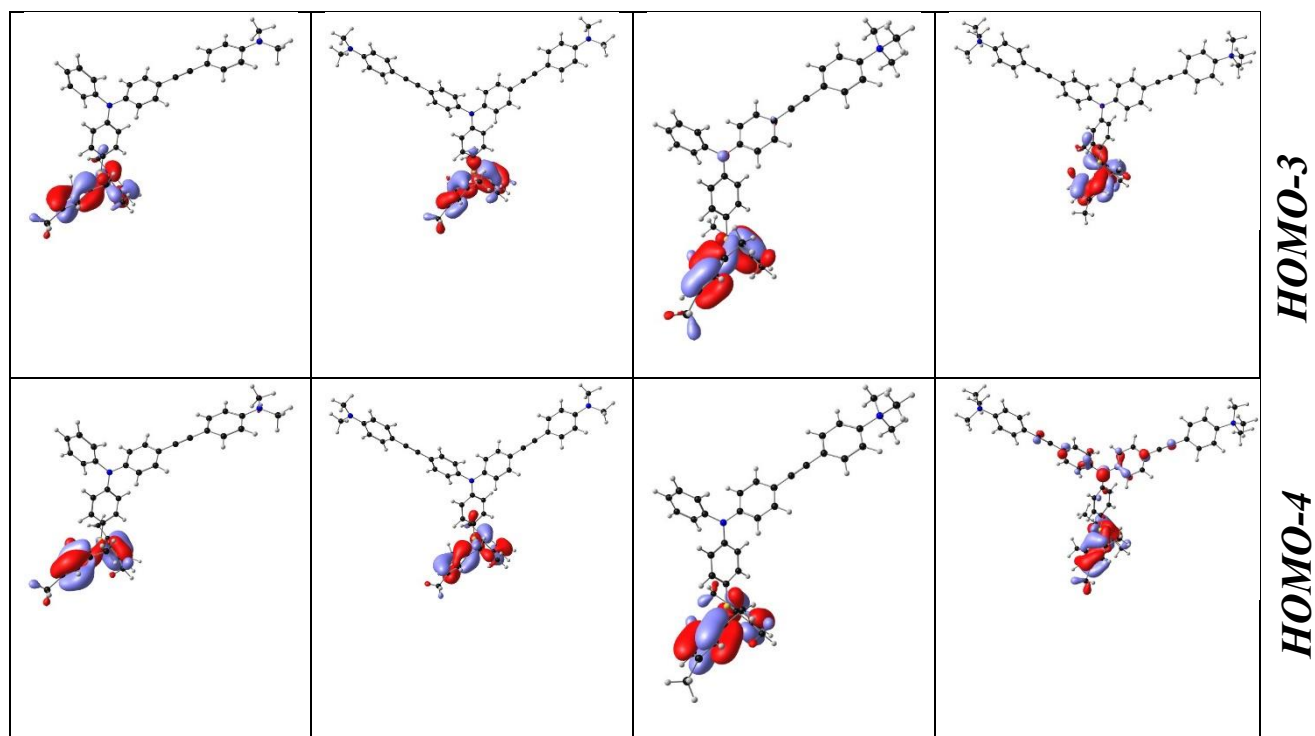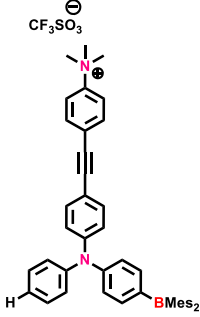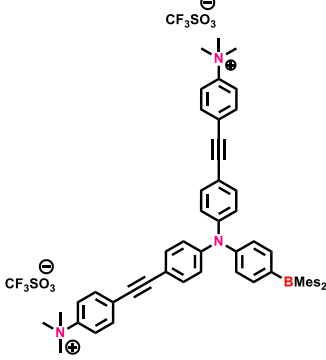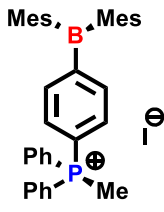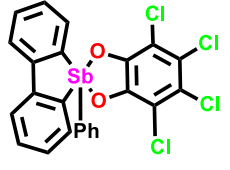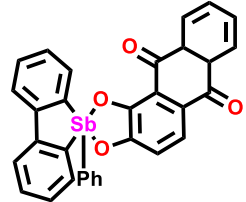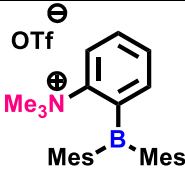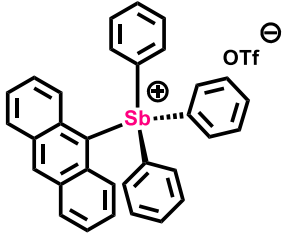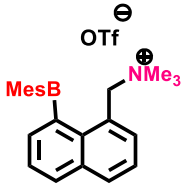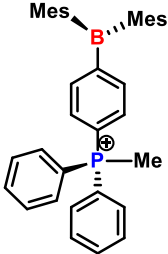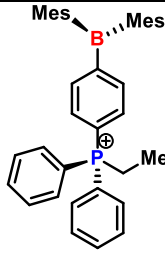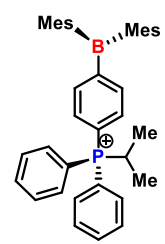
Table S15: Comparison of water soluble main group organometallic compounds (their physical parameters associated with fluoride)

Molecule	Association constant	Detection limit
1)	$0.3 \times 10^5 \, \text{M}^{-1}$	87.2 ppm (this work)
2)	$2.7 \times 10^5 \, \text{M}^{-1}$	0.1 ppm (this work)

1)[4]	$1.0(\pm 0.1) \times 10^3 \text{ M}^{-1}$	-
2)[5]	$13,500\ (\pm 1400\ \text{M}^{-1})$	-
3)[5]	$16,100\ (\pm 1100)\ \text{M}^{-1}$	$5.0 \times 10^{-4} \text{ M}$
4)[6]	$910\ ((50)\ \text{M-1}$	-

5)[7]	$12000 \pm 1100\ \mathrm{M}^{-1}$	1.04 ± 0.01 ppm
6)[8]	$5.0\ (\pm 0.5) \times 10^{6}\ \mathrm{M}^{-1}$	-
7)[9]	$840(\pm 50)\ \mathrm{M}^{-1}$	< 4 ppm
8)[9]	$2500(\pm 200)\ \mathrm{M}^{-1}$	< 4 ppm

9)[9]	4000($\pm$300) M^{-1}	< 4 ppm
10)[9]	10,500($\pm$1000) M^{-1}	< 4 ppm
11)[10]	10 000 $\pm$ 500 M^{-1}	0.48 ($\pm$0.03) ppm (top water)
12)[11]	>10^7 M^{-1}	0.25 μM

13)[12]	$\geq 10^5$ M^{-1}	---

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