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# Supporting Information

# Alkyl Chain Length and Anion Effects of AIE-active α-Cyanostilbene-containing Triphenylamine Derivatives on Optical and Electrochemical Properties

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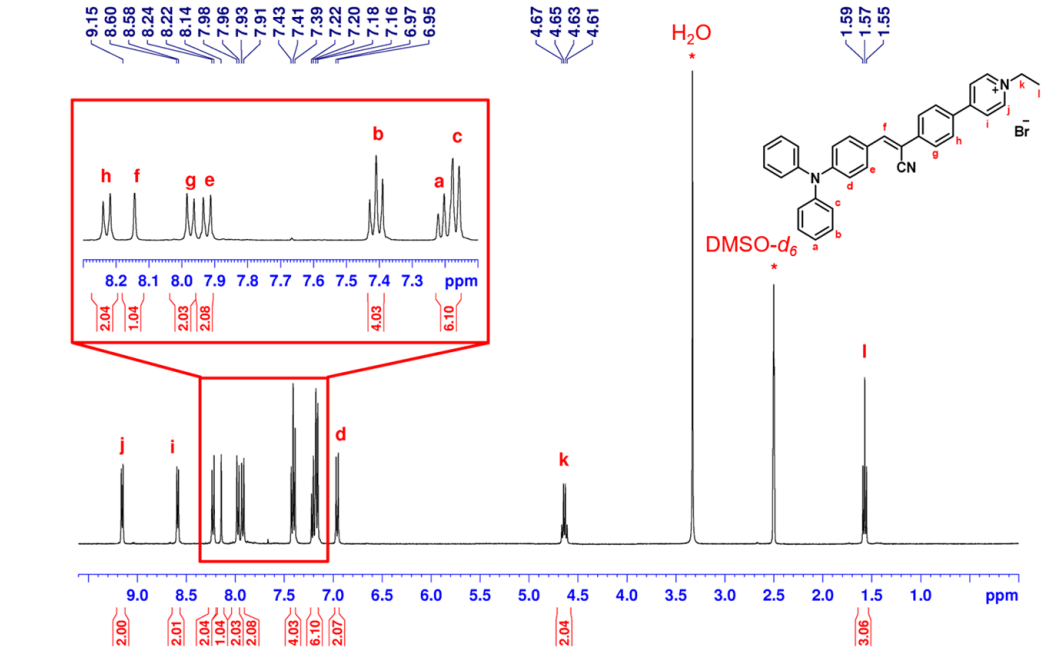



**Figure S1.** $^{1}$H-NMR spectrum of **TPA-Py-2-Br** in DMSO-$d_6$.

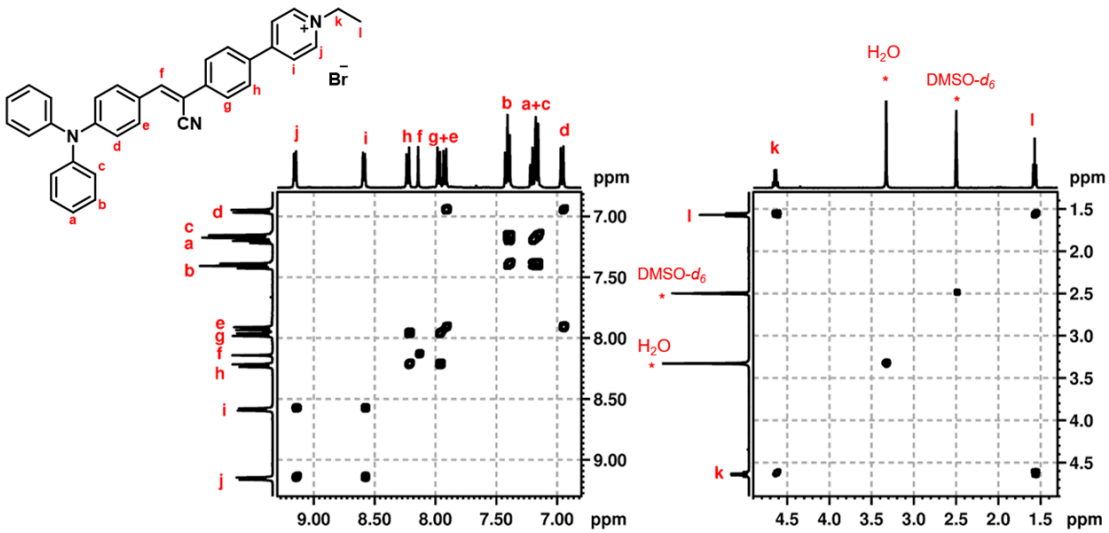



**Figure S2.** $^{1}$H-$^{1}$H COSY spectrum of **TPA-Py-2-Br** in DMSO-$d_6$.

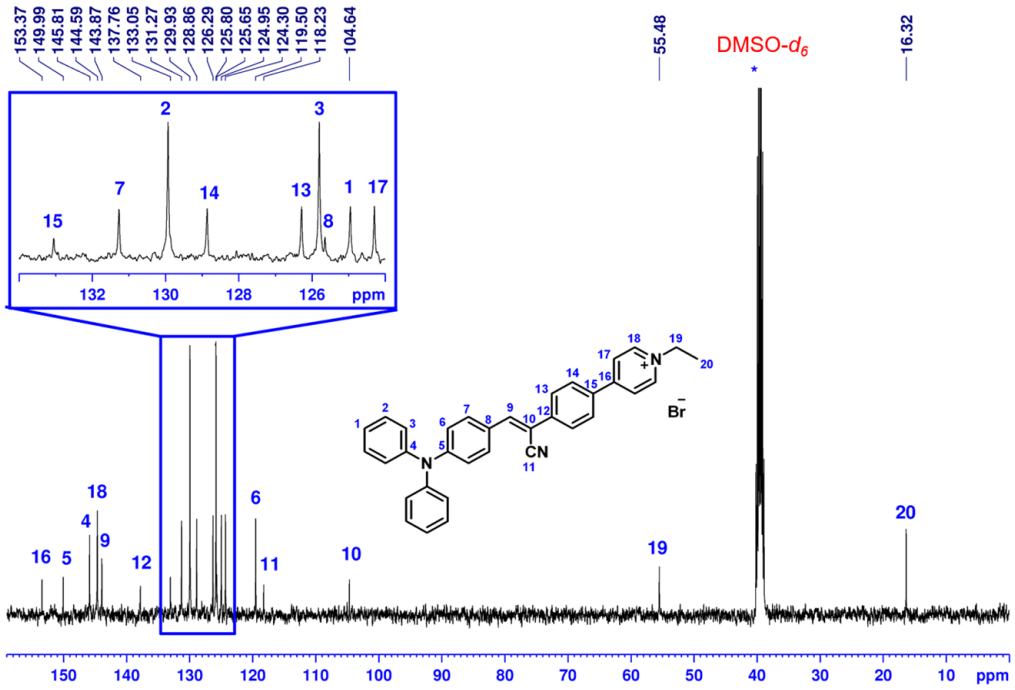



**Figure S3.** $^{13}$C-NMR spectrum of **TPA-Py-2-Br** in DMSO-$d_6$.

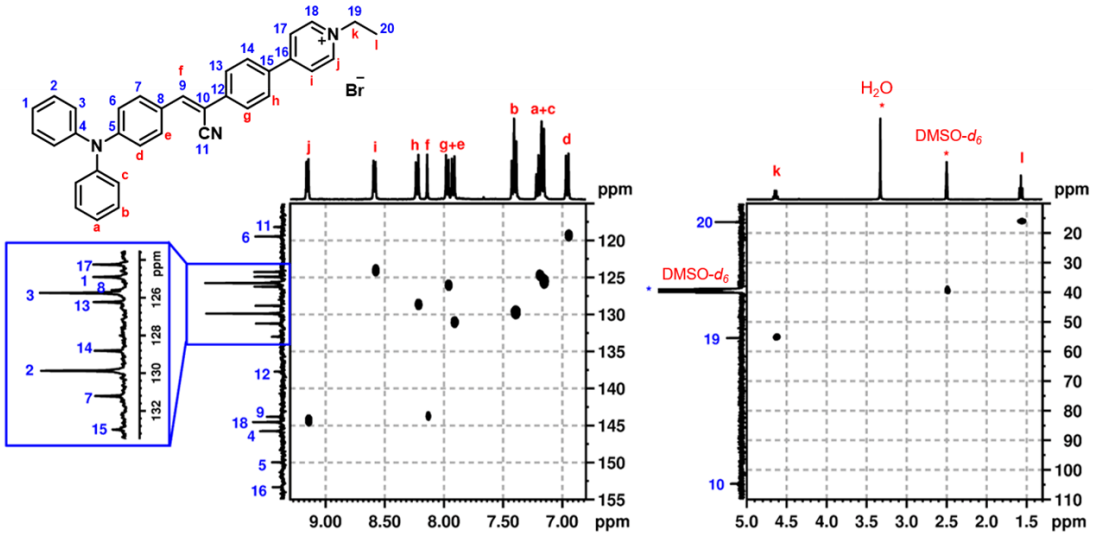



**Figure S4.** $^{1}$H-$^{13}$C HSQC spectrum of **TPA-Py-2-Br** in DMSO-$d_6$.

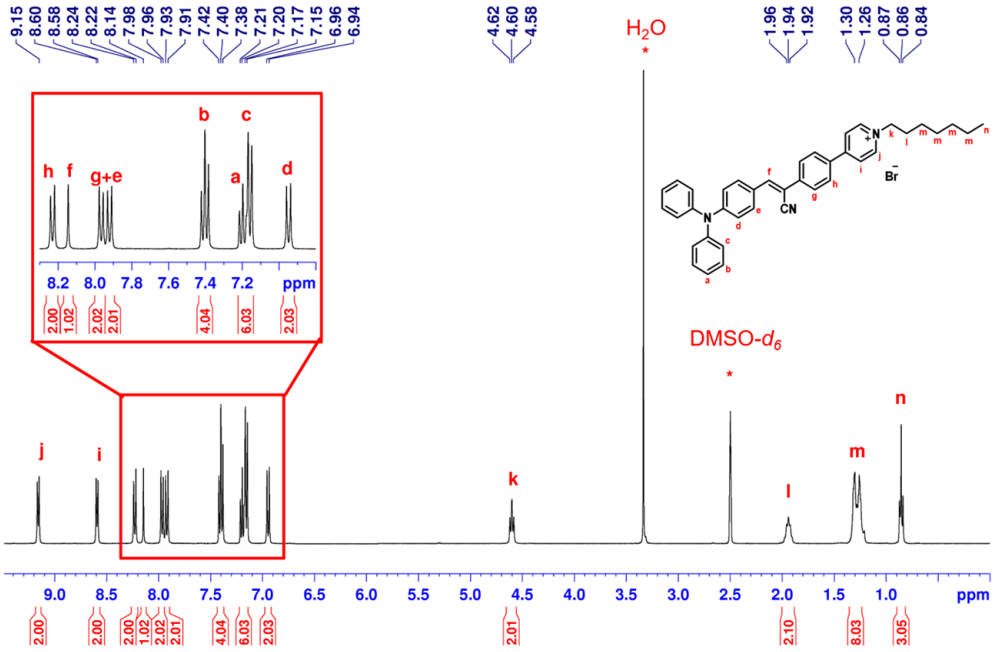



**Figure S5.** $^{1}$H-NMR spectrum of **TPA-Py-7-Br** in DMSO-$d_6$.

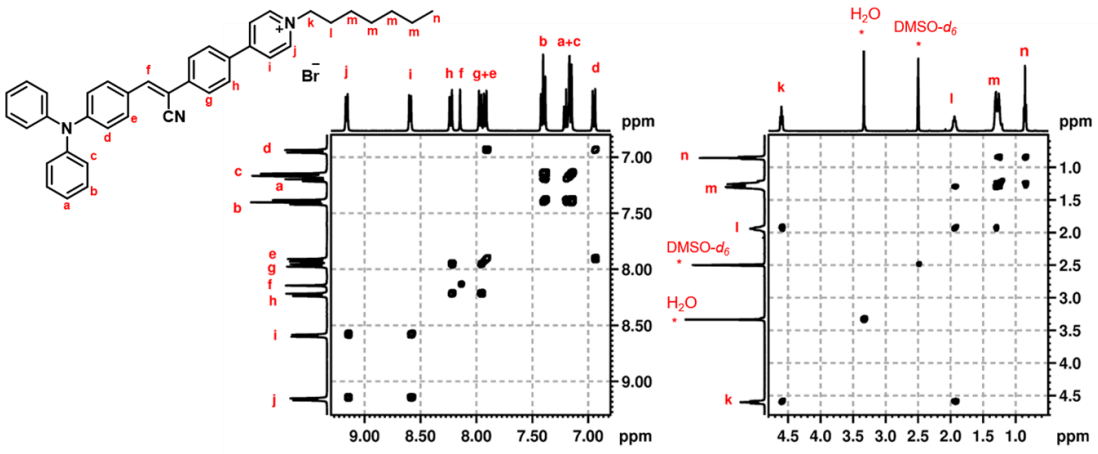



**Figure S6.** $^{1}$H-$^{1}$H COSY spectrum of **TPA-Py-7-Br** in DMSO-$d_6$.

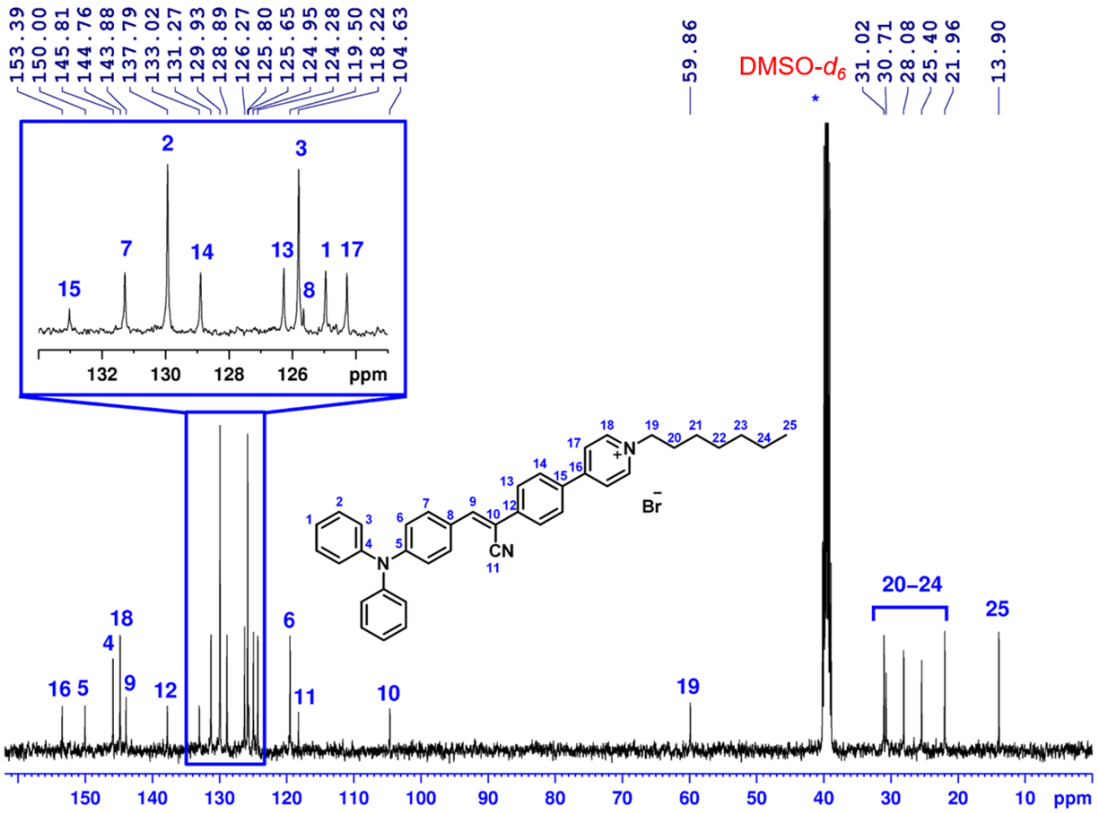



**Figure S7.** $^{13}$C-NMR spectrum of **TPA-Py-7-Br** in DMSO-$d_6$.

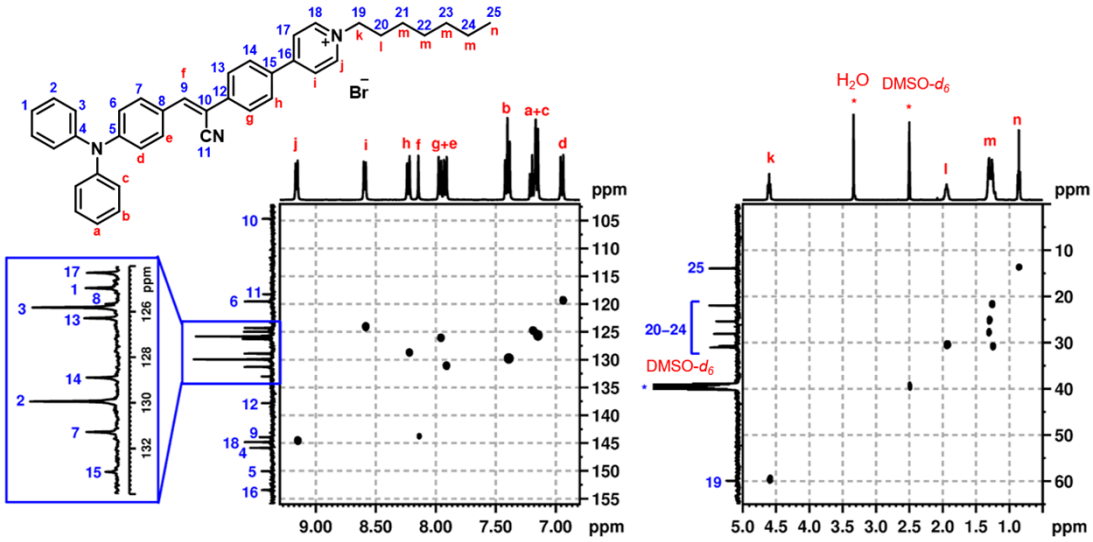



**Figure S8.** $^{1}$H-$^{13}$C HSQC spectrum of **TPA-Py-7-Br** in DMSO-$d_6$.

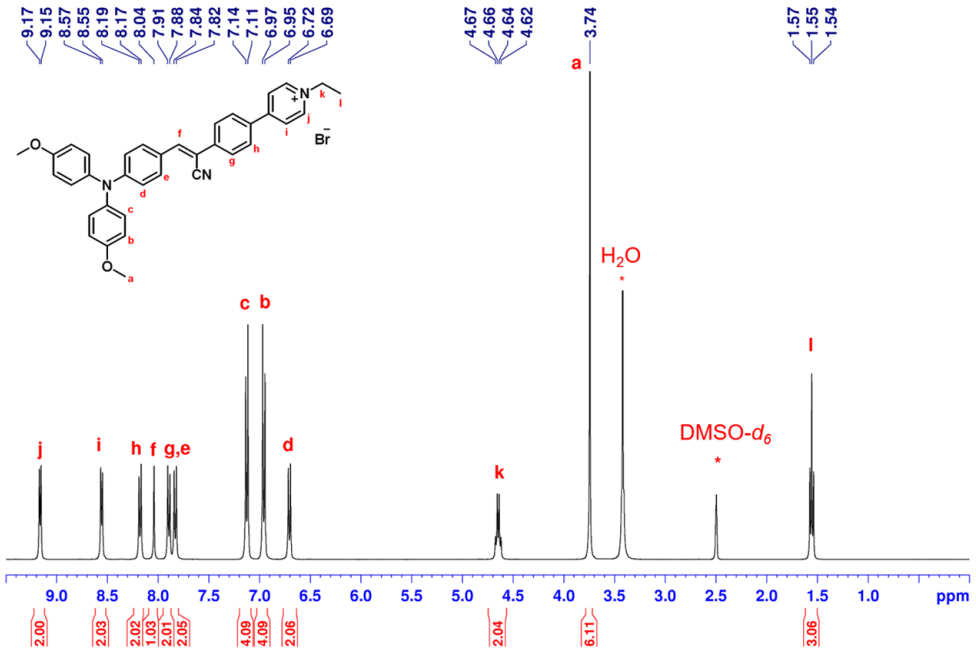



**Figure S9.** $^{1}$H-NMR spectrum of **diOMe-TPA-Py-2-Br** in DMSO-$d_6$.

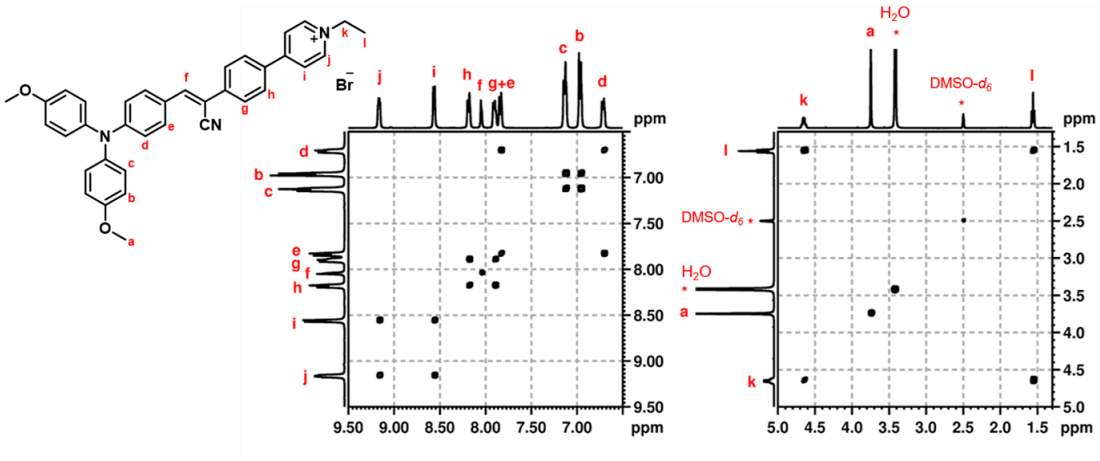



**Figure S10.** $^{1}$H-$^{1}$H COSY spectrum of **diOMe-TPA-Py-2-Br** in DMSO-$d_6$.

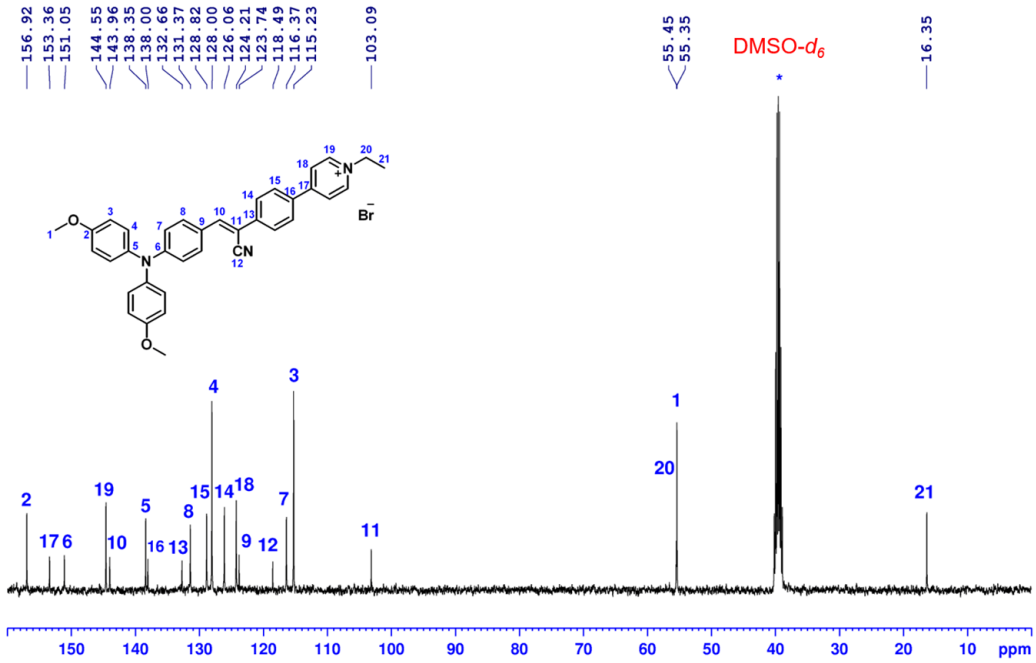



**Figure S11.** $^{13}$C-NMR spectrum of **diOMe-TPA-Py-2-Br** in DMSO-$d_6$.

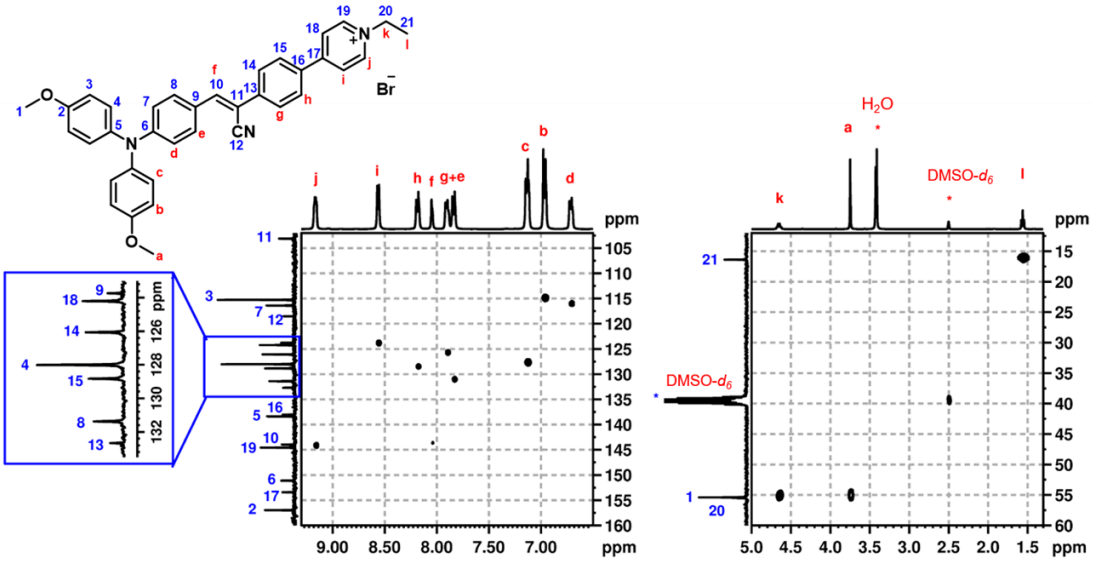



**Figure S12.** $^{1}$H-$^{13}$C HSQC spectrum of **diOMe-TPA-Py-2-Br** in DMSO-$d_6$.

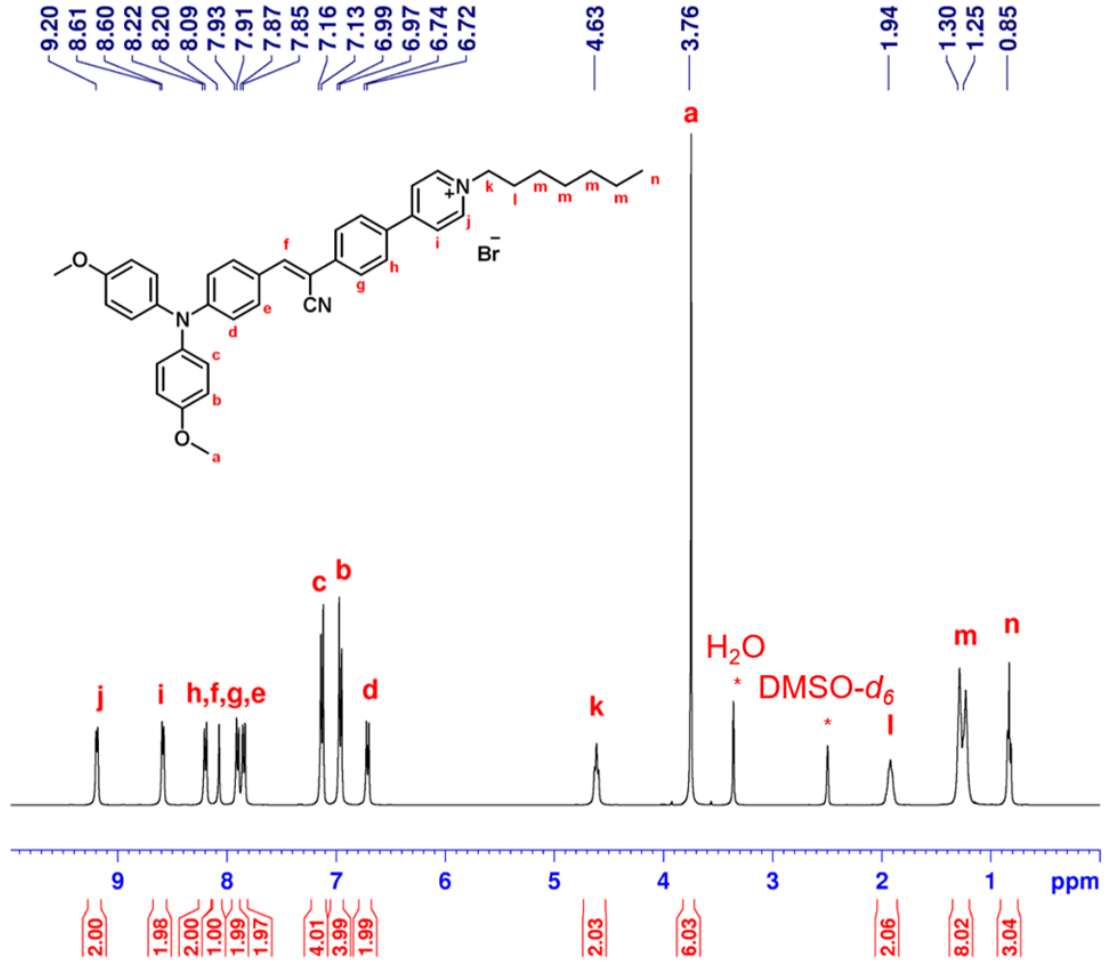



**Figure S13.** $^{1}$H-NMR spectrum of **diOMe-TPA-Py-7-Br** in DMSO-$d_6$.

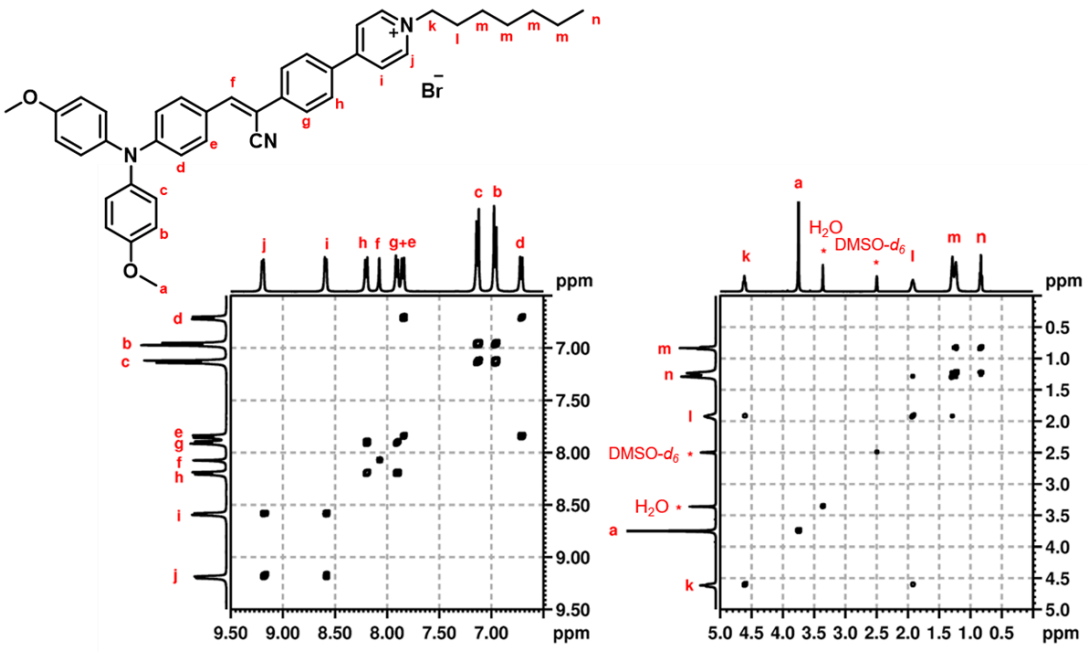



**Figure S14.** $^{1}$H-$^{1}$H COSY spectrum of **diOMe-TPA-Py-7-Br** in DMSO-$d_6$.

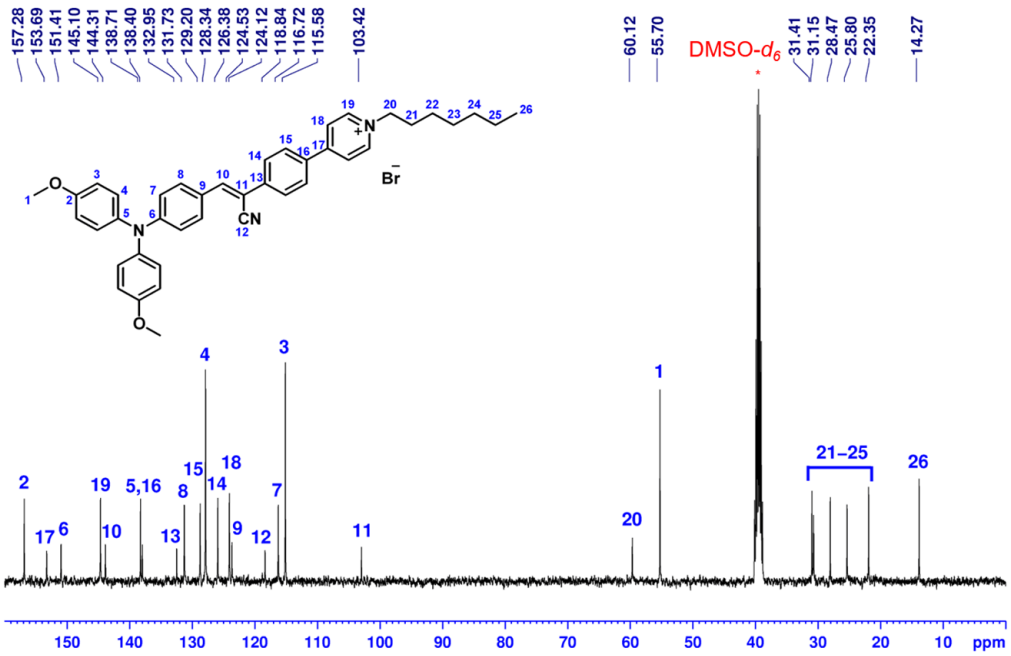



**Figure S15.** $^{13}$C-NMR spectrum of **diOMe-TPA-Py-7-Br** in DMSO-$d_6$.

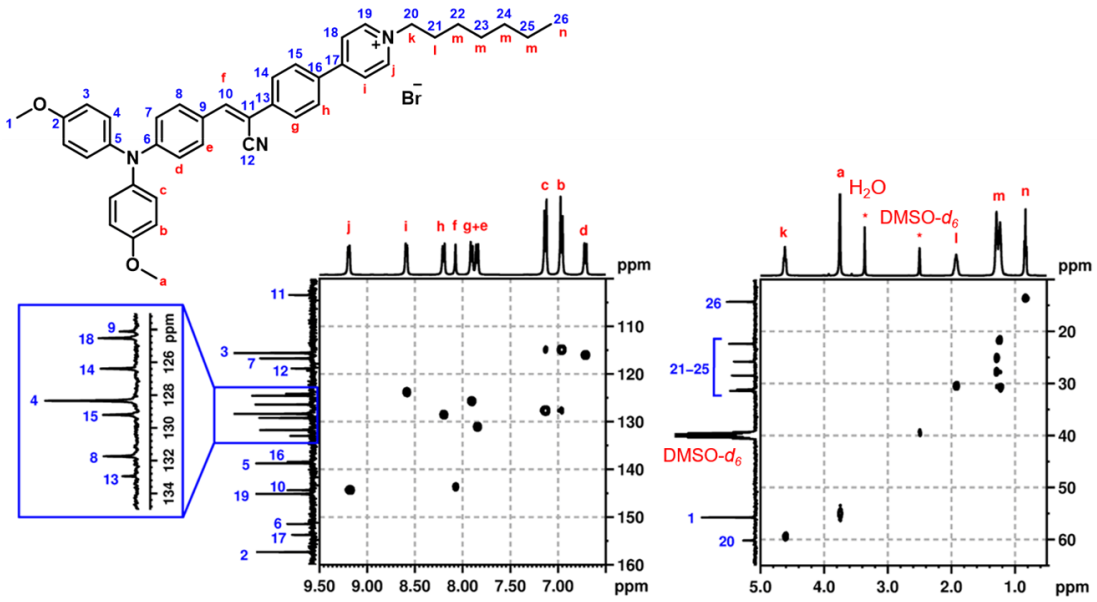



**Figure S16.** $^{1}$H-$^{13}$C HSQC spectrum of **diOMe-TPA-Py-7-Br** in DMSO-$d_6$.

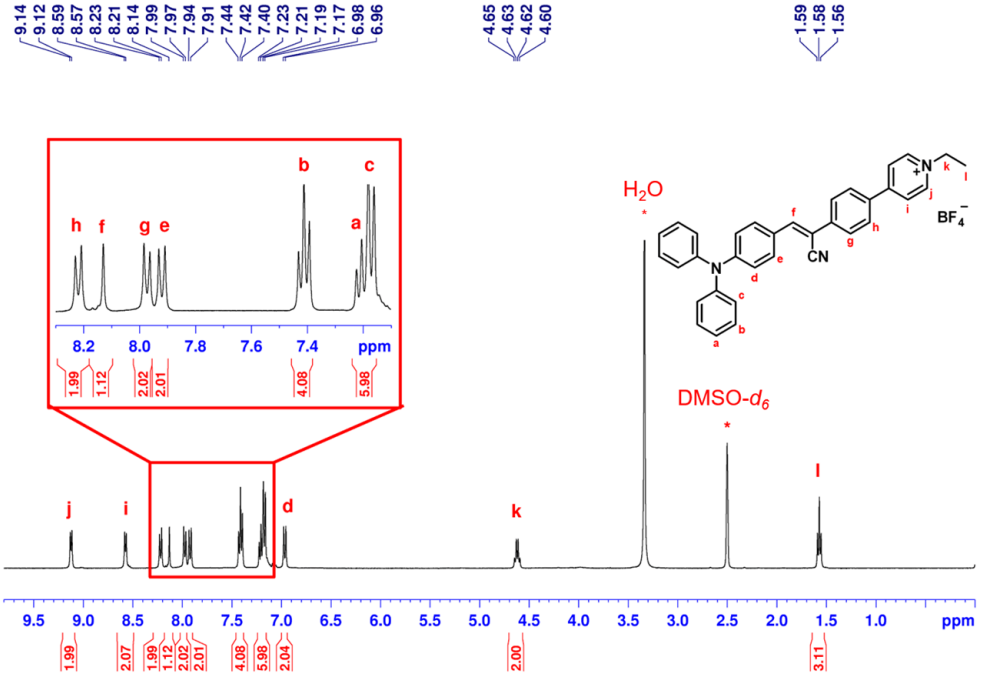



**Figure S17.** $^{1}$H-NMR spectrum of **TPA-Py-2-BF$_4$** in DMSO-*d*$_6$.

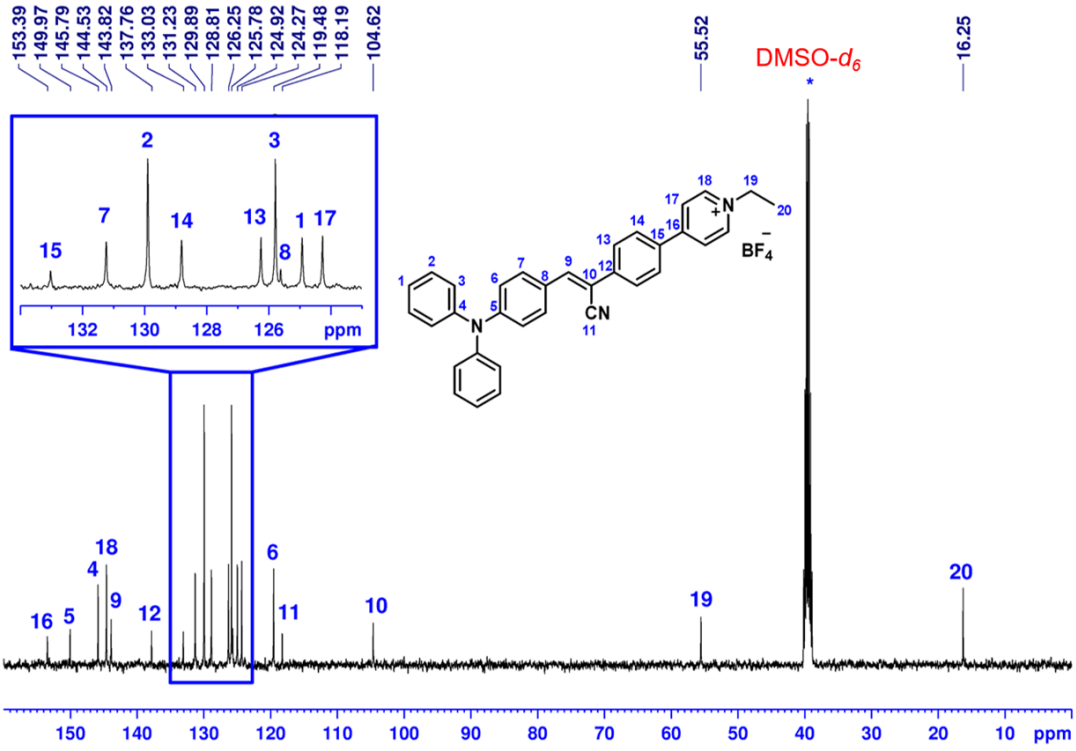



**Figure S18.** $^{13}$C-NMR spectrum of **TPA-Py-2-BF$_4$** in DMSO-*d*$_6$.

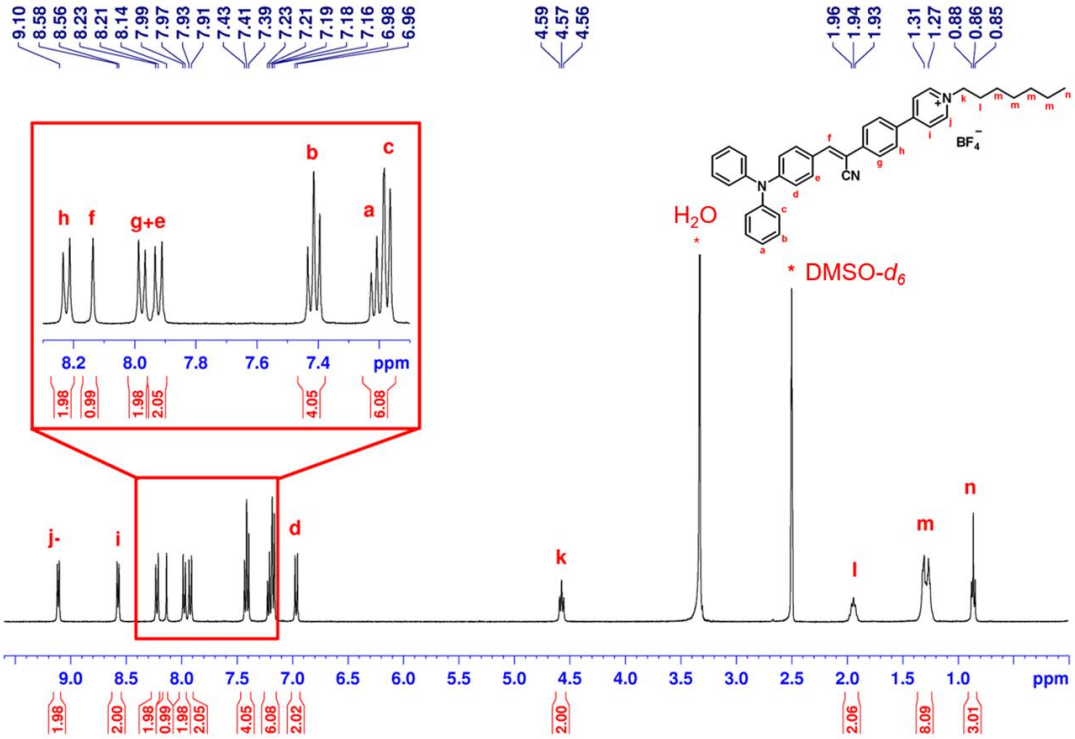



**Figure S19.** $^{1}$H-NMR spectrum of **TPA-Py-7-BF$_4$** in DMSO-*d*$_6$.

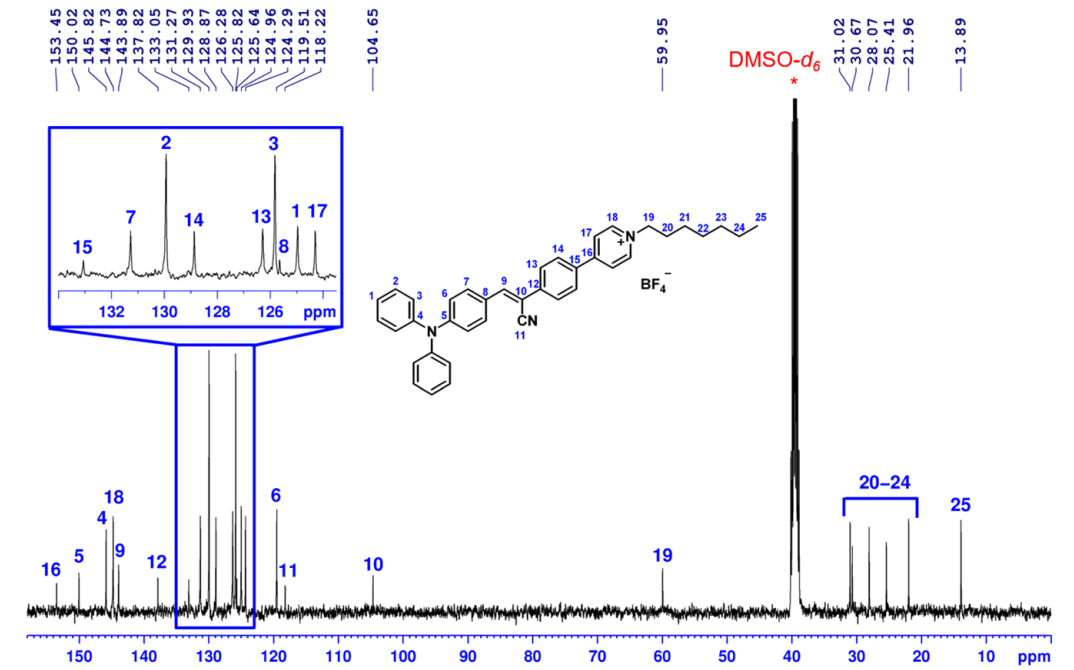



**Figure S20.** $^{13}$C-NMR spectrum of **TPA-Py-7-BF$_4$** in DMSO-*d*$_6$.

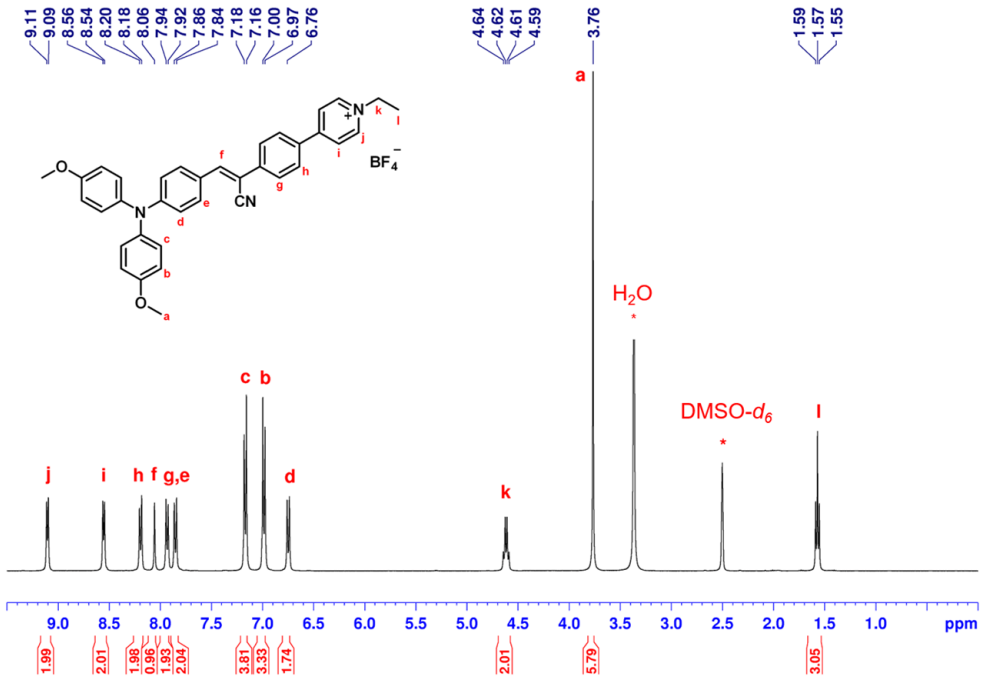



**Figure S21.** [1]H-NMR spectrum of **diOMe-TPA-Py-2-BF$_4$** in DMSO-*d*$_6$.

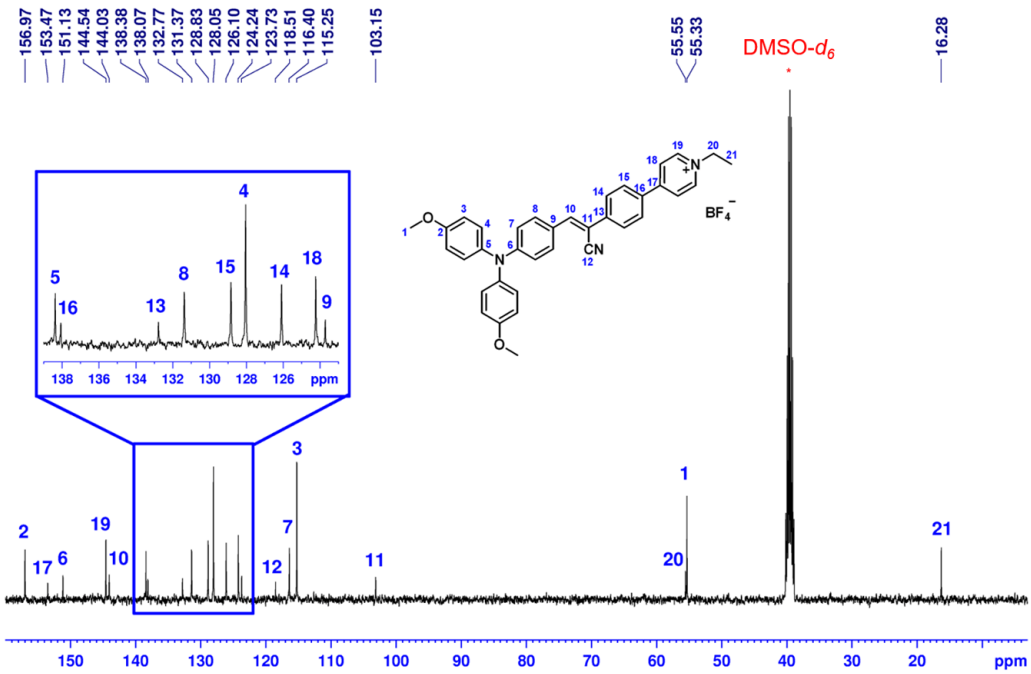
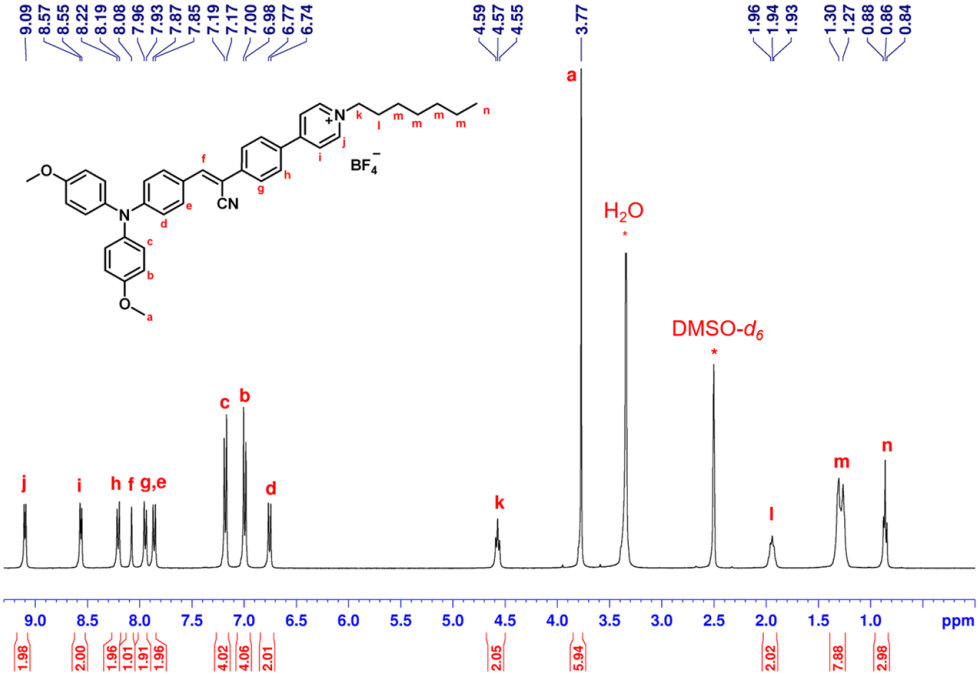



**Figure S22.** [13]C-NMR spectrum of **diOMe-TPA-Py-2-BF$_4$** in DMSO-*d*$_6$.

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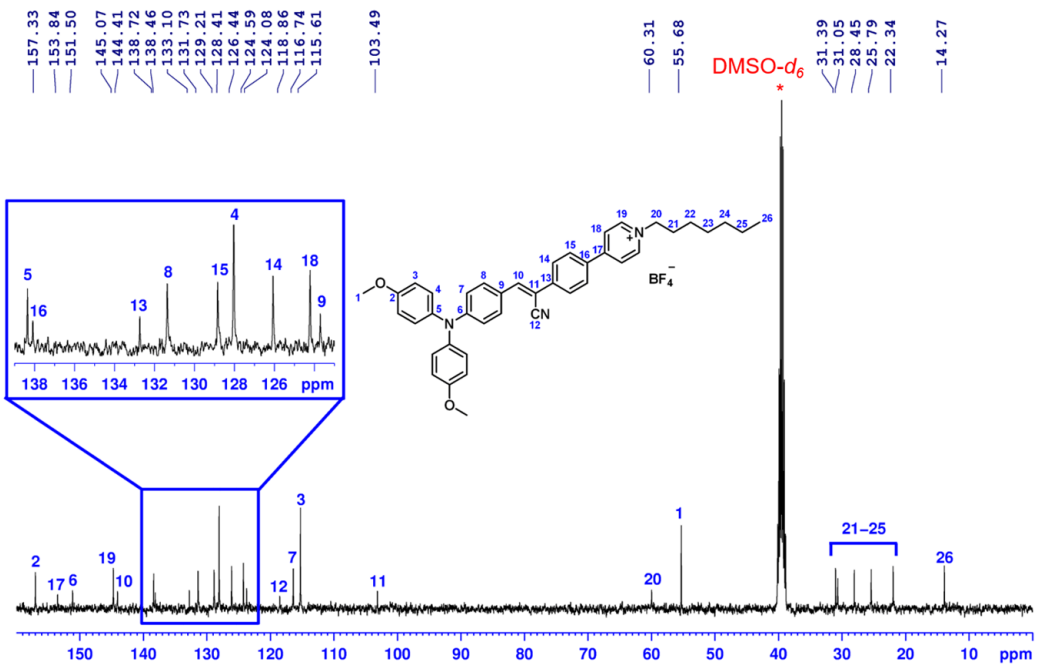
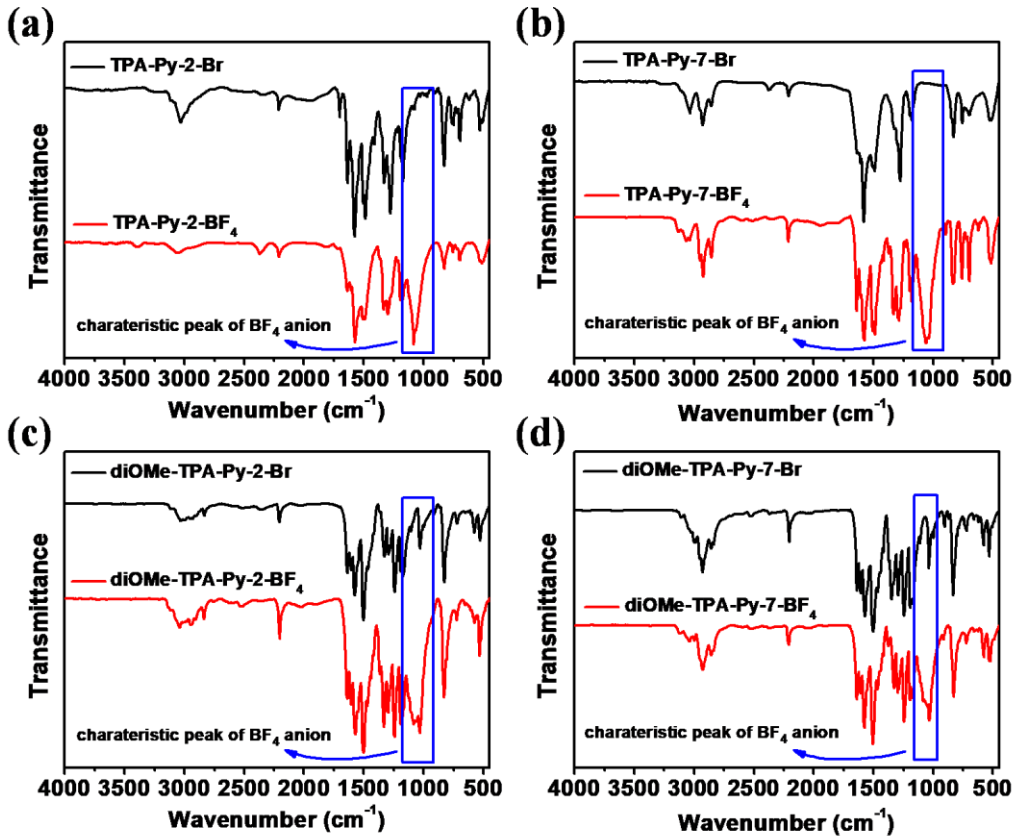



**Figure S24.** [13]C-NMR spectrum of **diOMe-TPA-Py-7-BF$_4$** in DMSO-$d_6$.

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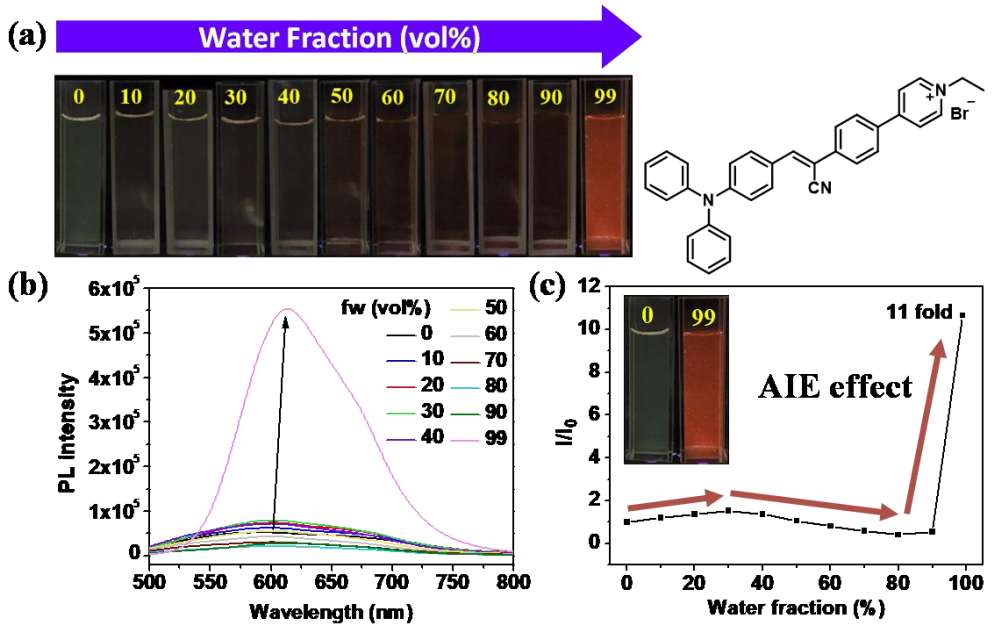


**Figure S26.** (a) Photos taken under UV light of **TPA-Py-2-Br** in different water/DMSO fractions, (b) PL spectra of **TPA-Py-2-Br** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **TPA-Py-2-Br**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$: 449 nm.

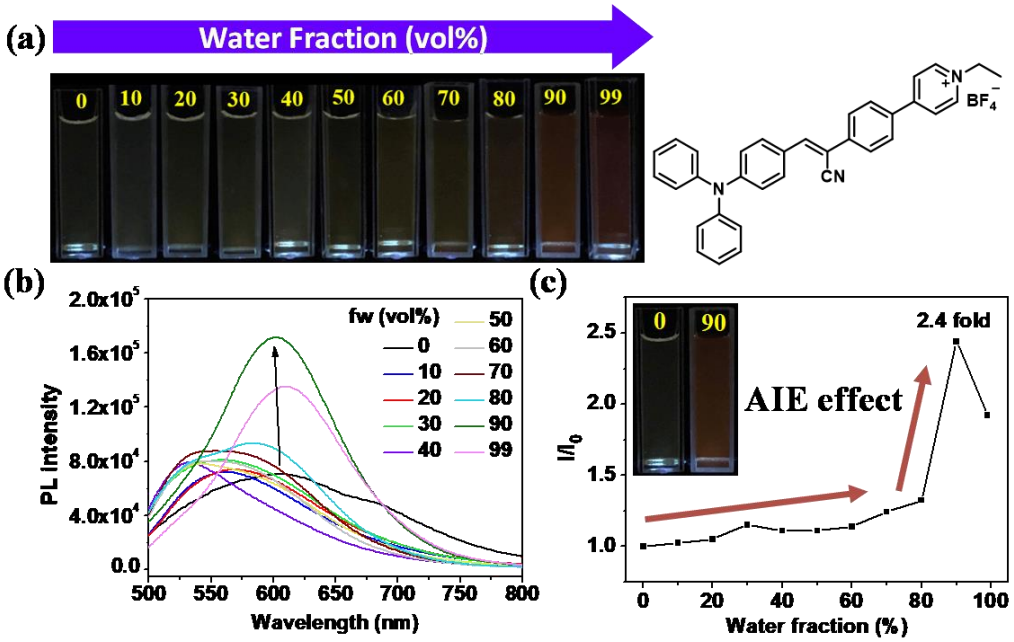


**Figure S27.** (a) Photos taken under UV light of **TPA-Py-2-BF$_4$** in different water/DMSO fractions, (b) PL spectra of **TPA-Py-2-BF$_4$** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **TPA-Py-2-BF$_4$**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$: 449 nm.

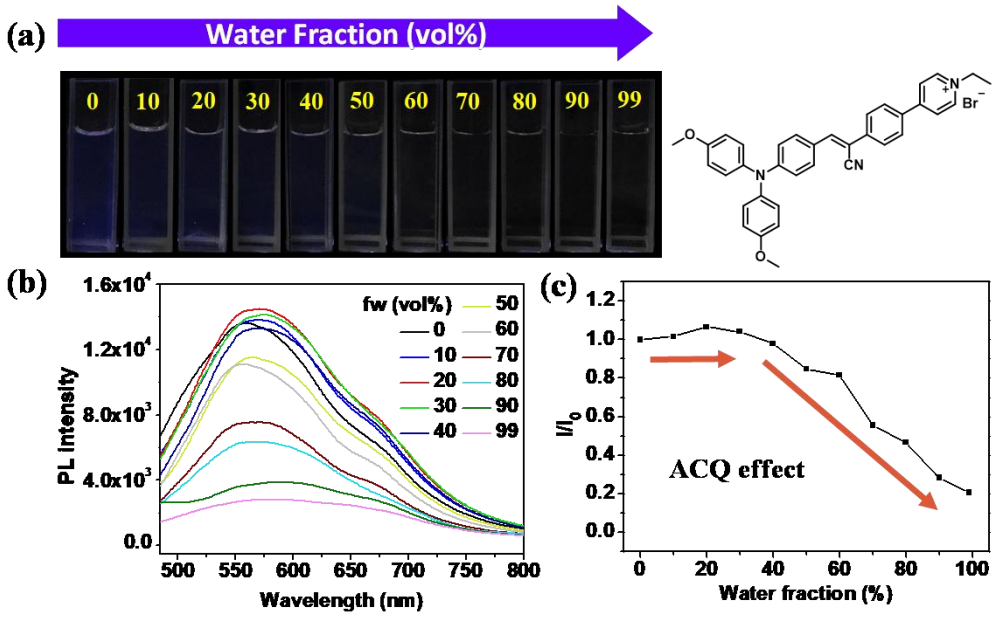


**Figure S28.** (a) Photos taken under UV light of **diOMe-TPA-Py-2-Br** in different water/DMSO fractions, (b) PL spectra of **diOMe-TPA-Py-2-Br** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **diOMe-TPA-Py-2-Br**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$: 463 nm.

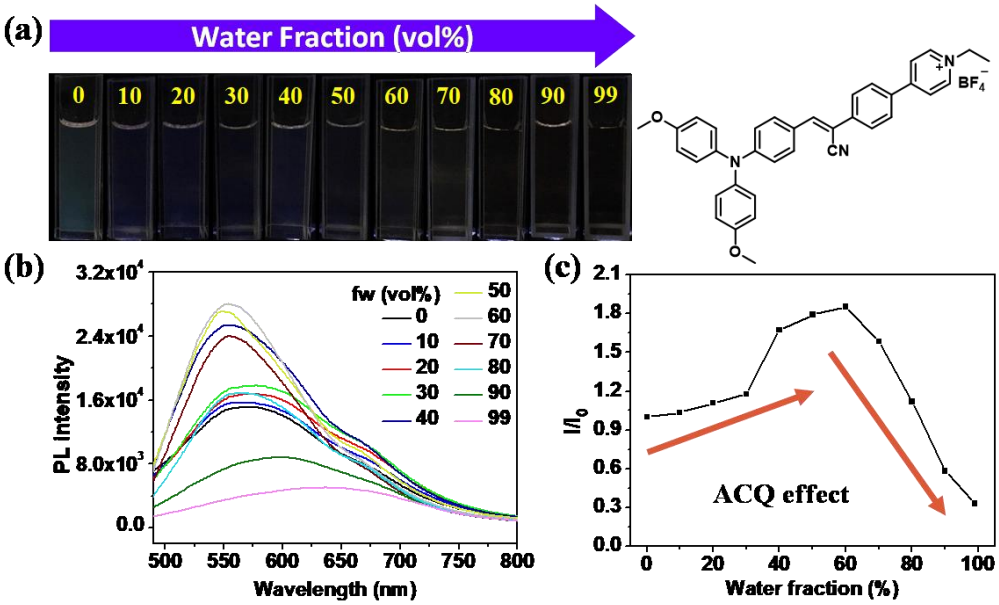


**Figure S29.** (a) Photos taken under UV light of **diOMe-TPA-Py-2-BF$_4$** in different water/DMSO fractions, (b) PL spectra of **diOMe-TPA-Py-2-BF$_4$** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **diOMe-TPA-Py-2-BF$_4$**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$: 463 nm.

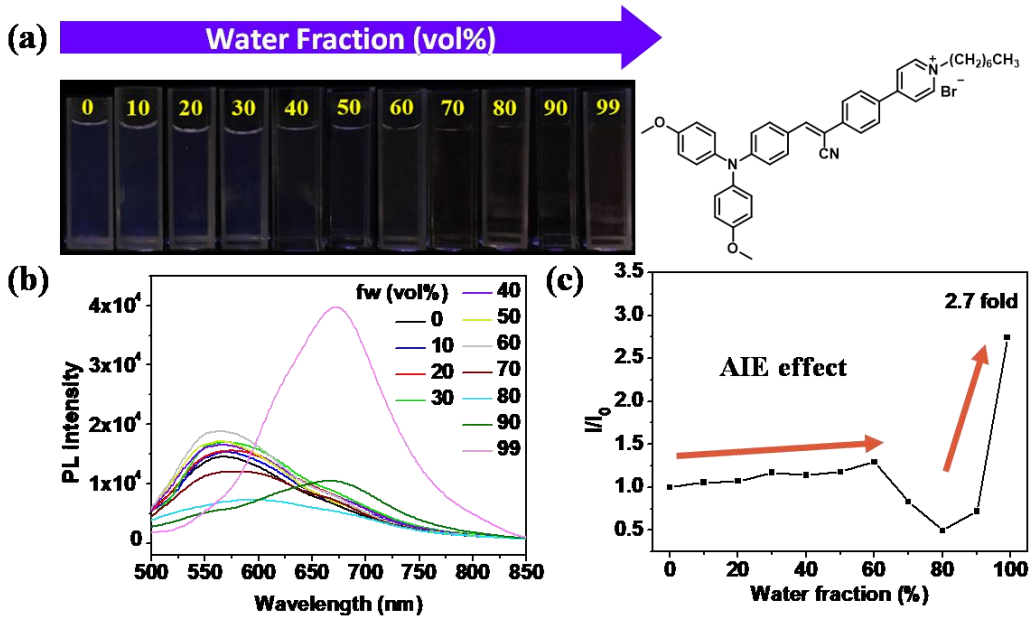


**Figure 30.** (a) Photos taken under UV light of **diOMe-TPA-Py-7-Br** in different water/DMSO fractions, (b) PL spectra of **diOMe-TPA-Py-7-Br** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **diOMe-TPA-Py-7-Br**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$: 466 nm.

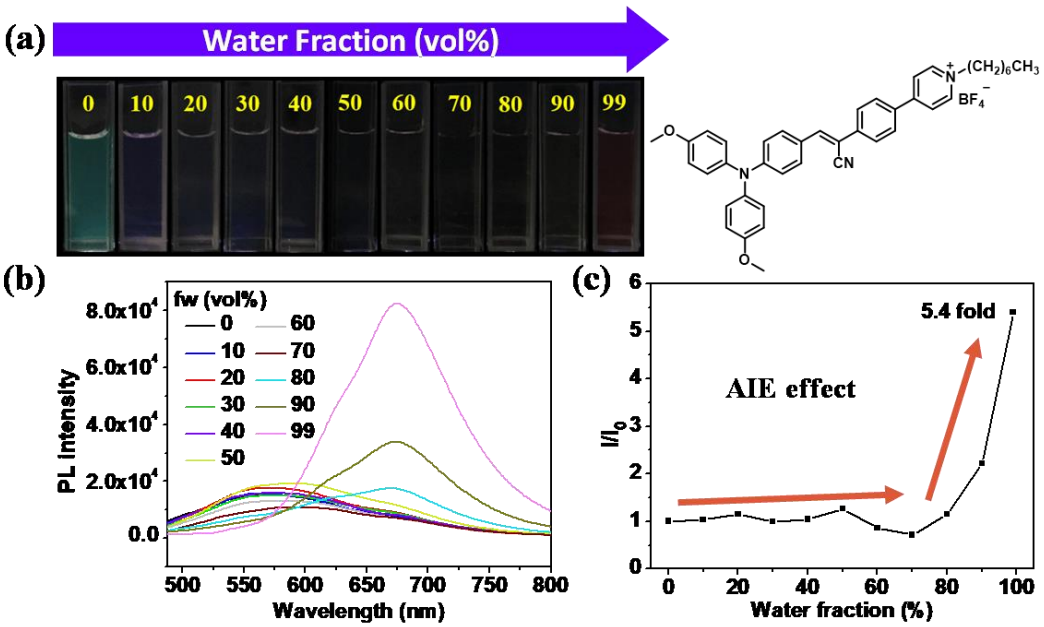


**Figure S31.** (a) Photos taken under UV light of **diOMe-TPA-Py-7-BF$_4$** in different water/DMSO fractions, (b) PL spectra of **diOMe-TPA-Py-7-BF$_4$** in water/DMSO solutions with different water fractions ($f_w$), (c) Plot of relative emission intensity ($I/I_0$) versus different compositions of aqueous mixtures of **diOMe-TPA-Py-7-BF$_4$**. $I_0$ = Emission intensity in pure DMSO solution (10 μM). $\lambda_{ex}$ : 466 nm.

**Table S1.** Crystal data and experimental details for **TPA-Py-2-$BF_4$**.

| Compound | **TPA-Py-2-$BF_4$** |
|---|---|
| Empirical formula | C34 H28 B F4 N3 |
| Formula weight | 565.40 |
| Crystal system | Monoclinic |
| Space group | P 1 21/n 1 |
| Unit cell dimensions | a = 13.1118(7) Å |
| | b = 15.2813(7) Å |
| | c = 13.9655(7) Å |
| | α = 90° |
| | β = 91.365(5)° |
| | γ = 90° |
| Volume | 2797.4(2) $Å^3$ |
| Z | 4 |
| F(000) | 1176 |
| Density (calculated) | 1.342 $Mg/m^3$ |
| Wavelength | 0.71073 Å |
| Cell parameters reflections used | 4441 |
| Theta range for Cell parameters | 3.3730 to 28.9110° |
| Absorption coefficient | 0.097 $mm^{-1}$ |
| Temperature | 150(2) K |
| Crystal size | 0.25 x 0.20 x 0.20 $mm^3$ |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.00000 and 0.97323 |
| No. of measured reflections | 11865 |
| No. of independent reflections | 6141 [R(int) = 0.0292] |
| No. of observed [I>2_igma(I)] | 4280 |
| Completeness to theta = 27.50° | 95.7 % |
| Theta range for data collection | 3.38 to 27.50° |
| Final R indices [I>2sigma(I)] | R1 = 0.0500, wR2 = 0.1366 |
| R indices (all data) | R1 = 0.0805, wR2 = 0.1664 |
| Goodness-of-fit on $F^2$ | 0.987 |
| No. of reflections | 6141 |
| No. of parameters | 379 |
| No. of restraints | 0 |
| Largest diff. peak and hole | 0.297 and -0.229 e.$Å^{-3}$ |

**Table S2.** Crystal data and experimental details for **TPA-Py-7-Br**.

| Compound | **TPA-Py-7-Br** |
|---|---|
| Empirical formula | C39 H38 Br N3 |
| Formula weight | 628.63 |
| Crystal system | Triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 9.5749(6) Å |
| | b = 9.7795(4) Å |
| | c = 35.3728(18) Å |
| | α = 84.999(4)° |
| | β = 89.387(5)° |
| | γ = 82.412(4)° |
| Volume | 3270.7(3) $Å^3$ |
| Z | 4 |
| F(000) | 1312 |
| Density (calculated) | 1.277 $Mg/m^3$ |
| Wavelength | 0.71073 Å |
| Cell parameters reflections used | 3679 |
| Theta range for Cell parameters | 3.0880 to 27.1700° |
| Absorption coefficient | 1.288 $mm^{-1}$ |
| Temperature | 150(2) K |
| Crystal size | 0.25 x 0.20 x 0.15 $mm^3$ |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.00000 and 0.76124 |
| No. of measured reflections | 19095 |
| No. of independent reflections | 13990 [R(int) = 0.0557] |
| No. of observed [I>2_igma(I)] | 8199 |
| Completeness to theta = 27.50° | 93.0 % |
| Theta range for data collection | 2.96 to 27.50° |
| Final R indices [I>2sigma(I)] | R1 = 0.0899, wR2 = 0.2015 |
| R indices (all data) | R1 = 0.1544, wR2 = 0.2542 |
| Goodness-of-fit on $F^2$ | 1.092 |
| No. of reflections | 13990 |
| No. of parameters | 794 |
| No. of restraints | 0 |
| Largest diff. peak and hole | 2.042 and -0.756 e.$Å^{-3}$ |

**Table S3.** Crystal data and experimental details for **TPA-Py-7-$BF_4$**.

| Compound | **TPA-Py-7-$BF_4$** |
|---|---|
| Empirical formula | C39 H38 B F4 N3 |
| Formula weight | 635.53 |
| Crystal system | Triclinic |
| Space group | P-1 |
| Unit cell dimensions | a = 10.0994(2) Å |
| | b = 18.0030(8) Å |
| | c = 19.7095(6) Å |
| | α = 102.494(3)° |
| | β = 94.039(2)° |
| | γ = 103.958(2)° |
| Volume | 3366.85(19) $Å^3$ |
| Z | 4 |
| F(000) | 1336 |
| Density (calculated) | 1.254 $Mg/m^3$ |
| Wavelength | 0.71073 Å |
| Cell parameters reflections used | 6901 |
| Theta range for Cell parameters | 3.0570 to 28.4760° |
| Absorption coefficient | 0.088 $mm^{-1}$ |
| Temperature | 150(2) K |
| Crystal size | 0.25 x 0.20 x 0.15 $mm^3$ |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.00000 and 0.98348 |
| No. of measured reflections | 23237 |
| No. of independent reflections | 14560 [R(int) = 0.0304] |
| No. of observed [I>2_igma(I)] | 8682 |
| Completeness to theta = 27.50° | 94.1 % |
| Theta range for data collection | 3.00 to 27.50° |
| Final R indices [I>2sigma(I)] | R1 = 0.0764, wR2 = 0.1754 |
| R indices (all data) | R1 = 0.1327, wR2 = 0.2218 |
| Goodness-of-fit on $F^2$ | 1.003 |
| No. of reflections | 14560 |
| No. of parameters | 847 |
| No. of restraints | 0 |
| Largest diff. peak and hole | 1.172 and -0.621 e.$Å^{-3}$ |

**Table S4.** Crystal data and experimental details for **diOMe-TPA-Py-2-Br**.

| Compound | **diOMe-TPA-Py-2-Br** |
|---|---|
| Empirical formula | C36 H36 Br N3 O4 |
| Formula weight | 654.59 |
| Crystal system | Monoclinic |
| Space group | P 1 21/n 1 |
| Unit cell dimensions | a = 14.8377(4) Å |
| | b = 10.3068(2) Å |
| | c = 21.2595(5) Å |
| | α = 90° |
| | β = 104.015(2)° |
| | γ = 90° |
| Volume | 3154.42(13) $Å^3$ |
| Z | 4 |
| F(000) | 1360 |
| Density (calculated) | 1.378 $Mg/m^3$ |
| Wavelength | 0.71073 Å |
| Cell parameters reflections used | 7664 |
| Theta range for Cell parameters | 3.5560 to 28.5120° |
| Absorption coefficient | 1.347 $mm^{-1}$ |
| Temperature | 150(2) K |
| Crystal size | 0.30 x 0.25 x 0.20 $mm^3$ |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.00000 and 0.87930 |
| No. of measured reflections | 22809 |
| No. of independent reflections | 7092 [R(int) = 0.0315] |
| No. of observed [I>2_igma(I)] | 5435 |
| Completeness to theta = 27.50° | 97.8 % |
| Theta range for data collection | 2.83 to 27.50°. |
| Final R indices [I>2sigma(I)] | R1 = 0.0368, wR2 = 0.0827 |
| R indices (all data) | R1 = 0.0584, wR2 = 0.0934 |
| Goodness-of-fit on $F^2$ | 0.999 |
| No. of reflections | 7092 |
| No. of parameters | 409 |
| No. of restraints | 0 |
| Largest diff. peak and hole | 0.331 and -0.443 e.$Å^{-3}$ |

**Table S5.** Crystal data and experimental details for **diOMe-TPA-Py-7-Br**.

| Compound | **diOMe-TPA-Py-7-Br** |
|---|---|
| Empirical formula | C41 H42 Br N3 O2 |
| Formula weight | 688.69 |
| Crystal system | Monoclinic |
| Space group | P 1 21/c 1 |
| Unit cell dimensions | a = 14.1460(3) Å |
| | b = 10.3836(2) Å |
| | c = 25.5561(4) Å |
| | $\alpha = 90^{\circ}$ |
| | $\beta = 105.051(2)^{\circ}$ |
| | $\gamma = 90^{\circ}$ |
| Volume | 3625.07(12) $Å^3$ |
| Z | 4 |
| F(000) | 1440 |
| Density (calculated) | 1.262 $Mg/m^3$ |
| Wavelength | 0.71073 Å |
| Cell parameters reflections used | 5835 |
| Theta range for Cell parameters | $2.9840$ to $27.4910^{\circ}$ |
| Absorption coefficient | 1.172 $mm^{-1}$ |
| Temperature | 200(2) K |
| Crystal size | 0.30 x 0.20 x 0.15 $mm^3$ |
| Diffractometer | Xcalibur, Atlas, Gemini |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.00000 and 0.89149 |
| No. of measured reflections | 17089 |
| No. of independent reflections | 7982 [R(int) = 0.0299] |
| No. of observed [I>2_igma(I)] | 5980 |
| Completeness to theta = $27.50^{\circ}$ | 95.7 % |
| Theta range for data collection | $2.98$ to $27.50^{\circ}$ |
| Final R indices [I>2sigma(I)] | R1 = 0.0423, wR2 = 0.0959 |
| R indices (all data) | R1 = 0.0661, wR2 = 0.1098 |
| Goodness-of-fit on $F^2$ | 1.012 |
| No. of reflections | 7982 |
| No. of parameters | 424 |
| No. of restraints | 0 |
| Largest diff. peak and hole | 0.356 and -0.451 $e.Å^{-3}$ |