

## Supporting Information

### **An aryl-triazole foldamer containing 1, 8-naphthalimide fluorescent motif for monitoring and enhancing the anion- induced folding**

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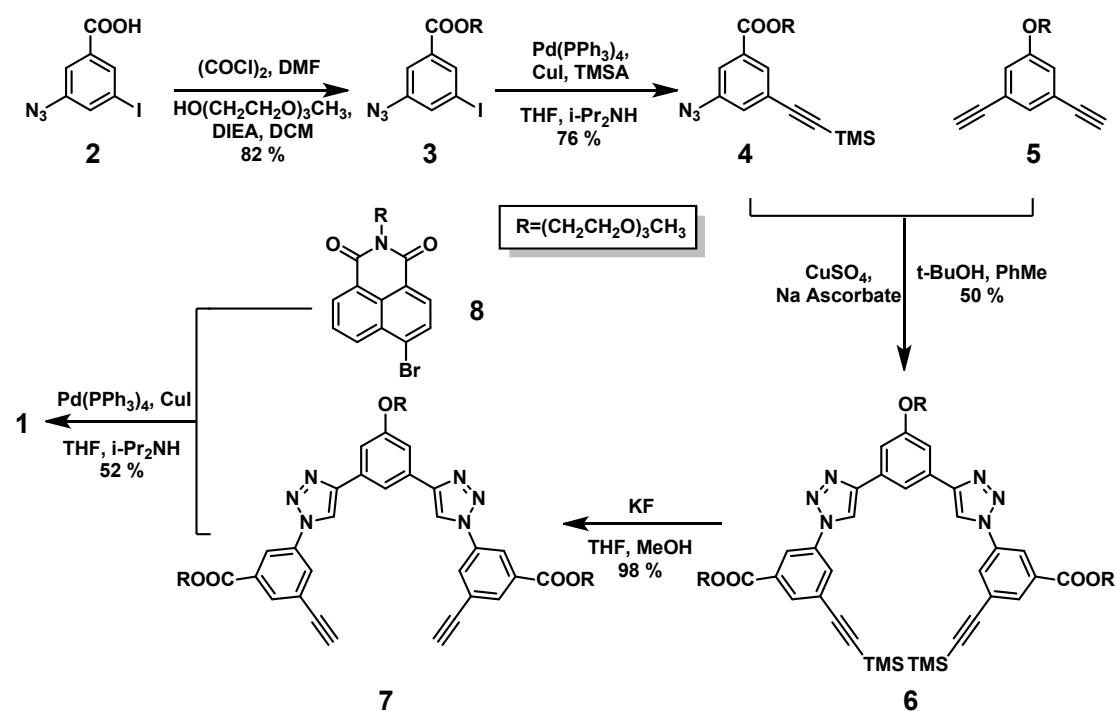
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## 1. Materials and methods

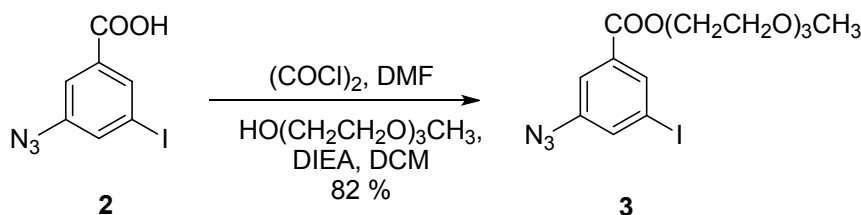
All starting compounds and solvents were obtained from commercial suppliers and used as received unless otherwise indicated. Per-deuterated solvents for NMR spectroscopy were obtained from Cambridge Isotope Laboratories. Anhydrous dichloromethane (DCM) and diisopropylamine (*i*-Pr<sub>2</sub>NH) were distilled over calcium hydride (CaH<sub>2</sub>), and anhydrous tetrahydrofuran (THF) was distilled over sodium benzophenone. Column chromatography was carried out on flash grade silica gel, using 0 – 20 psig pressure.

1D NMR spectra were recorded on BRUKER AVANCE 400 MHz and 2D NMR Spectrum were performed on BRUKER AVANCE 600 MHz at 298 K. Chemical shifts were reported relative to the standard solvent signals on literature. The chemical shift references were as follows: (<sup>1</sup>H) chloroform-*d*, 7.26 ppm; (<sup>13</sup>C) chloroform-*d*, 77.16 ppm; (<sup>1</sup>H) THF-*d*<sub>8</sub>, 1.72 ppm. Typical 1D FID was subjected to exponential multiplication with an exponent of 0.3 Hz. High-resolution mass spectra were recorded on Thermo Fisher Scientific Exactive spectrometer. UV-vis spectra were obtained on a Shimadzu UV-2600 spectrophotometer. The fluorescent spectra were probed on a F-4600 FL Spectrophotometer.

## 2. Synthesis of 1,8-naphthalimide incorporated aryl-triazole foldamer 1

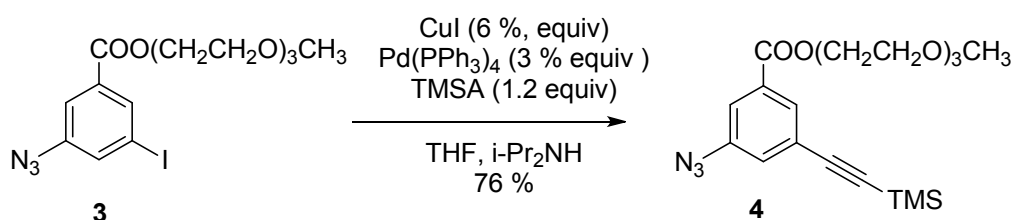


Compound **2**<sup>S1</sup>, **5**<sup>S2</sup>, **8**<sup>S3</sup> were prepared according to literature procedure.

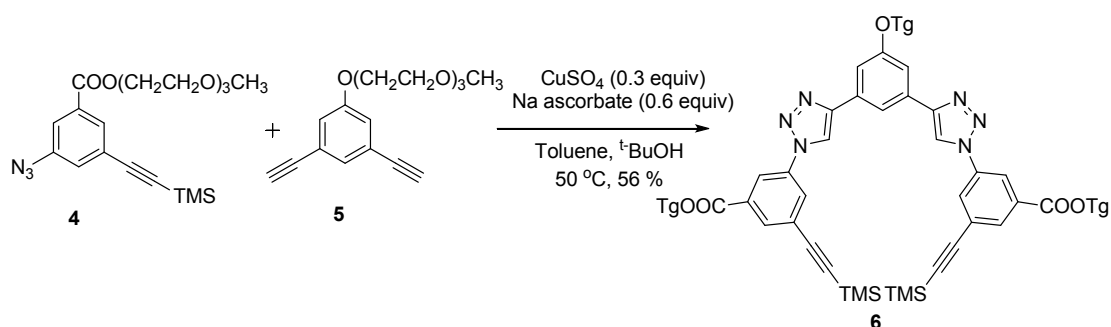


**Compound 3.** Compound **2** (2.20 g, 7.60 mmol) was dried in vacuo, and then dissolved in  $\text{CH}_2\text{Cl}_2$  (5 mL). Oxalyl chloride (0.96 mL, 11.40 mmol) was added. The reaction mixture was stirred at room temperature for 2 h resulting in a homogeneous solution, and then evaporated to provide the corresponding acid chloride. To a solution of the 2-(2-(2-methoxyethoxy)ethoxy)ethanol (1.44 mL, 9.12 mmol) in  $\text{CH}_2\text{Cl}_2$  (5 mL) containing DIEA (2.64 mL, 15.21 mmol) was added a solution of acid chloride in  $\text{CH}_2\text{Cl}_2$  (5 mL) via cannula. The reaction mixture was stirred at room temperature overnight. The solution was evaporated and the product was purified by flash chromatography. The crude product was purified by silica gel flash column chromatography (ethyl acetate /dichloromethane) to give the compound **3** as a brown oil 2.72 g (6.24 mmol, 82 %).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.13 (t,  $J = 1.3$  Hz, 1H), 7.69 – 7.62 (m, 1H), 7.54 – 7.49 (m, 1H), 4.54 – 4.41 (m, 2H), 3.88 – 3.78 (m, 2H), 3.75 – 3.61 (m, 6H), 3.54 (dd,  $J = 5.7, 3.6$  Hz, 2H), 3.37 (s, 3H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz, 298K):  $\delta$  164.2, 141.8, 134.9, 133.2, 132.0, 119.6, 94.2, 72.0,

70.7, 70.7, 70.6, 69.1, 64.8, 59.1. ESI-MS ( $m/z$ ), calcd. for  $C_{14}H_{18}IN_3O_5$  (M) 435.0, found 458.0 (M + Na<sup>+</sup>).

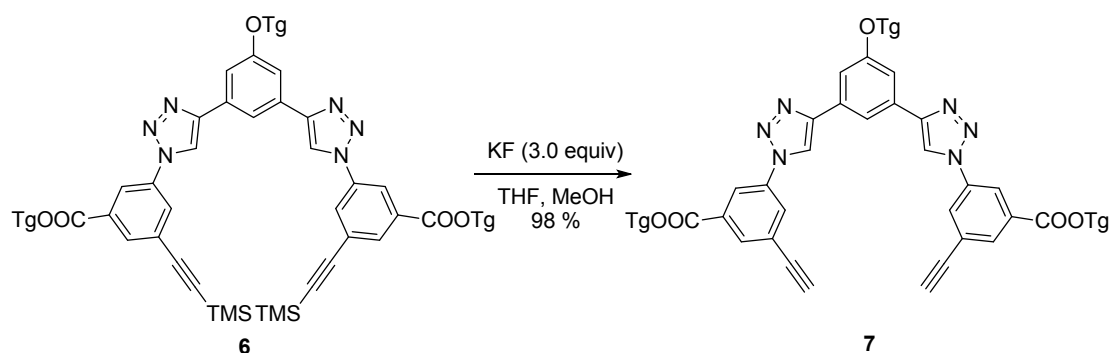


**Compound 4.** The aryl iodic compound **3** (1.99 g, 4.57 mmol), copper(I) iodide (CuI) (17 mg, 0.09 mmol) and tetrakis(triphenylphosphine) palladium ( $Pd(PPh_3)_4$ ) (53 mg, 0.045 mmol) was added to anhydrous tetrahydrofuran (40 ml) under Ar atmosphere. This suspended solution became pellucid when anhydrous diisopropylamine (20 ml, 142 mmol) was added. While stirring, trimethylsilylethyne (0.78 ml, 5.52 mmol) was injected through syringe. The reaction mixture was stirred at 30 ~ 35 °C overnight under Ar atmosphere and was monitored by TLC. Upon completion, the solution was evaporated in vacuo and the residue was re-dissolved with DCM. Organic solution was washed with saturated aqueous  $NH_4Cl$ , brine, dried over sodium sulfate and evaporated in vacuo to dryness. The crude product was purified by silica gel flash column chromatography (ethyl acetate /dichloromethane) to give the compound **4** as a black brown oil 1.41 g (3.48 mmol, 76 %).  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.89 (t,  $J$  = 1.4 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.29 – 7.26 (m, 1H), 4.53 – 4.44 (m, 2H), 3.86 – 3.80 (m, 2H), 3.74 – 3.62 (m, 6H), 3.54 (dd,  $J$  = 5.7, 3.6 Hz, 2H), 3.37 (s, 3H), 0.27 – 0.25 (m, 9H);  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  165.0, 140.8, 132.1, 129.6, 126.2, 125.2, 120.2, 102.8, 96.8, 72.0, 70.8, 70.7, 70.7, 69.1, 64.7, 59.1, -0.1. ESI-MS ( $m/z$ ), calcd. for  $C_{19}H_{27}N_3O_5Si$  (M) 405.2, found 428.2 (M + Na<sup>+</sup>).



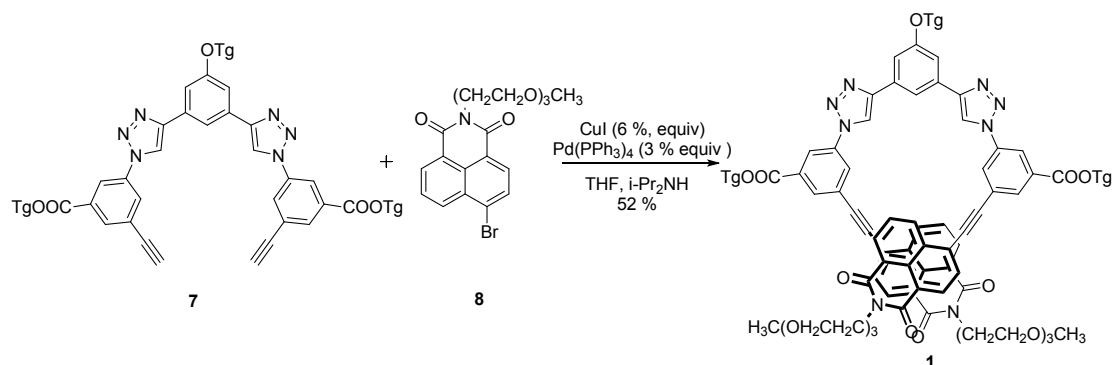
**Compound 6.** Aryl azido compound **4** (0.53 g, 1.30 mmol) and aryl ethynyl compound **5** (0.15 g, 0.52 mmol) was dissolved in 40 ml 1:1 t-BuOH/toluene mix solvents.  $CuSO_4$  (33.34 mg, 0.21 mmol) dissolved in 1 ml water was added into the mixture, followed by the addition of sodium

ascorbate (83.16 mg, 0.42 mmol). The reaction mixture was degassed and stirred overnight under Ar at 50 °C with being protected from light. Upon completion, the solution was evaporated in vacuo and the residue was re-dissolved with DCM. Organic solution was washed with saturated aqueous NH<sub>4</sub>Cl, brine, dried over sodium sulfate and evaporated in vacuo to dryness. The crude product was purified by silica gel flash column chromatography(methanol/dichloromethane) to give the compound **6** as a white solid 0.32 g (0.29 mmol, 56 %). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.42 (d, *J* = 4.8 Hz, 2H), 8.41 – 8.38 (m, 2H), 8.21 (t, *J* = 1.4 Hz, 2H), 8.18 – 8.14 (m, 2H), 8.01 (s, 1H), 7.57 (d, *J* = 1.3 Hz, 2H), 4.59 – 4.51 (m, 4H), 4.37 – 4.27 (m, 2H), 3.93 (dd, *J* = 13.1, 8.6 Hz, 2H), 3.91 – 3.84 (m, 4H), 3.83 – 3.77 (m, 2H), 3.77 – 3.62 (m, 16H), 3.60 – 3.49 (m, 6H), 3.37 (s, 3H), 3.34 (s, 6H), 0.36 – 0.25 (m, 18H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 164.4, 159.5, 147.9, 136.9, 132.4, 131.9, 131.6, 126.9, 125.2, 120.4, 118.3, 115.6, 111.6, 102.2, 97.5, 71.7, 70.8, 70.5, 70.5, 70.4, 70.4, 69.6, 68.9, 67.6, 64.7, 58.8, -0.3. MALDI (*m/z*), calcd. for C<sub>55</sub>H<sub>74</sub>N<sub>6</sub>O<sub>14</sub>Si<sub>2</sub> (M) 1099.4, found 1121.4 (M + Na<sup>+</sup>).



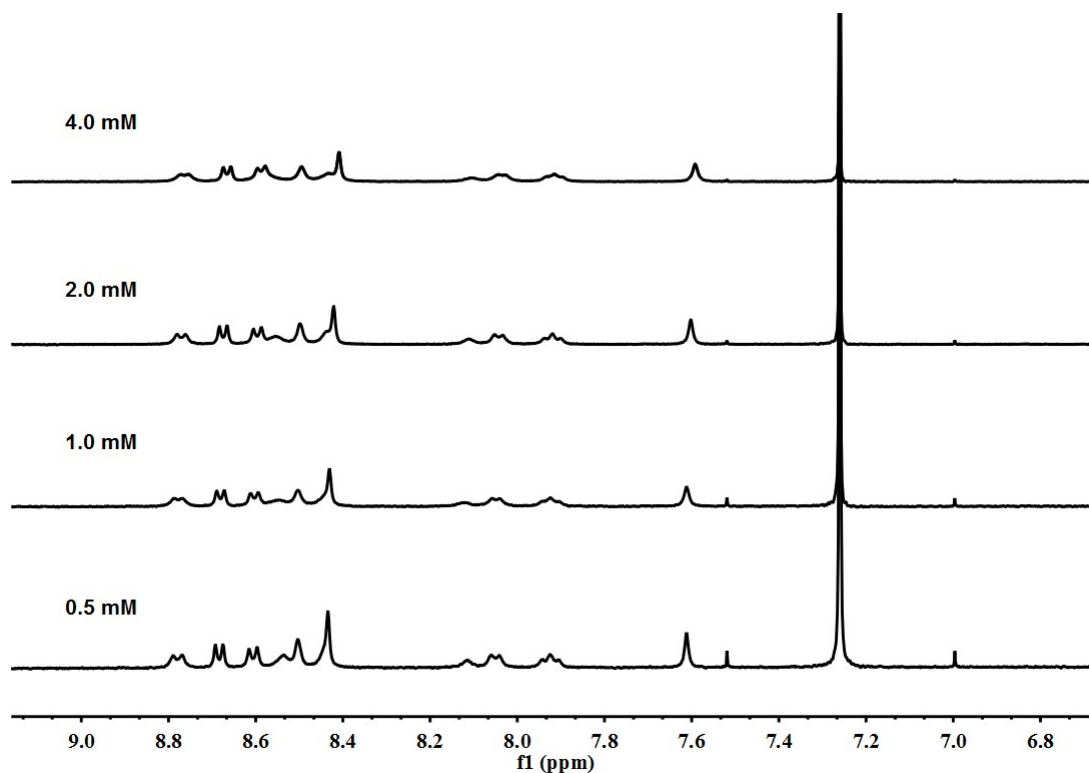
**Compound 7.** To the solution of compound **6** (0.32 g, 0.29 mmol) in the solution of 1:1 THF/MeOH (30 mL), KF (82 mg, 0.87 mmol) was added. The reaction was monitored by TLC. When the reaction finished, most of the solvents were removed under reduced pressure and the residue was poured into H<sub>2</sub>O. It was extracted by DCM (50 mL × 2) and the combined organic layer was washed with brine (100 mL), dried over Na<sub>2</sub>SO<sub>4</sub>, concentrated under reduced pressure. The crude product was purified by flash chromatography (methanol/dichloromethane) to provide compound **7** 0.27 g (0.27 mmol, 98 %) as a grey solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.45 (s, 2H), 8.41 (s, 2H), 8.25 – 8.11 (m, 4H), 7.99 (s, 1H), 7.54 (s, 2H), 4.60 – 4.48 (m, 4H), 4.36 – 4.24 (m, 2H), 3.97 – 3.91 (m, 2H), 3.91 – 3.84 (m, 4H), 3.82 – 3.76 (m, 2H), 3.76 – 3.62 (m, 16H), 3.54 (ddd, *J* = 11.0, 5.6, 3.7 Hz, 6H), 3.35 (d, *J* = 6.3 Hz, 3H), 3.33 (s, 6H), 3.28 (s, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 164.5, 159.7, 148.1, 137.1, 132.9, 132.2, 131.7, 127.4, 124.4, 120.9, 118.3,

115.7, 111.9, 81.3, 80.3, 71.9, 70.9, 70.7, 70.6, 70.6, 69.7, 69.0, 67.8, 64.9, 58.9. ESI-MS ( $m/z$ ), calcd. for  $C_{49}H_{58}N_6O_{14}$  (M) 954.4, found 977.3 (M + Na<sup>+</sup>).

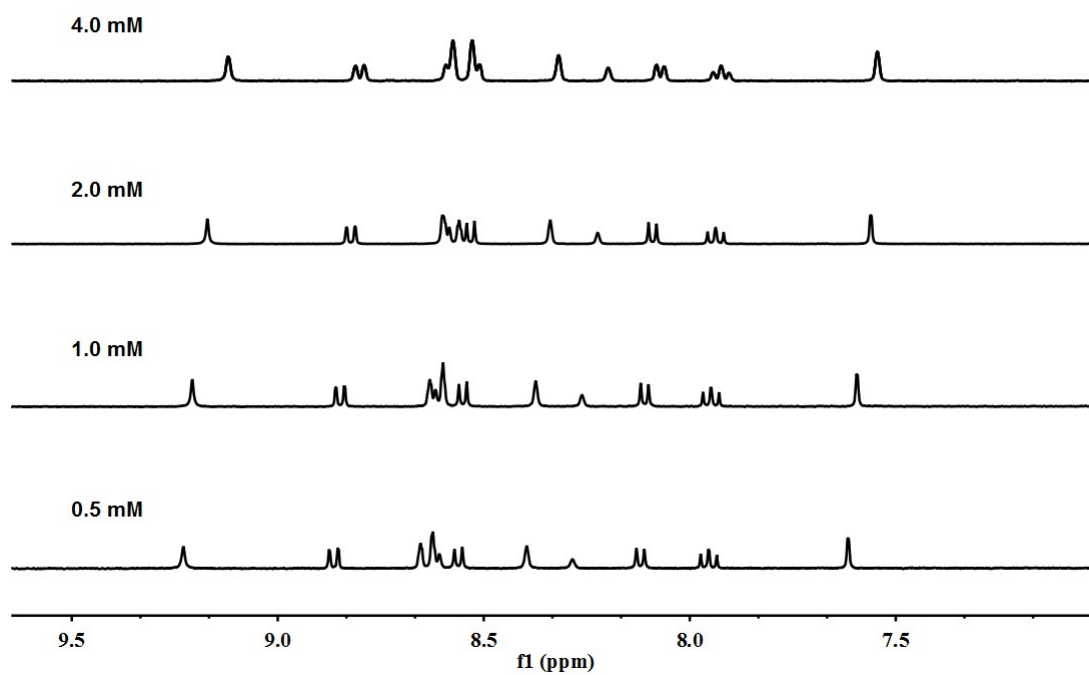


**Compound 1.** The compound **7** (0.12 g, 0.13 mmol), compound **8** (0.16 g, 0.39 mmol), copper (I) iodide CuI (4.97 mg, 0.026 mmol) and tetrakis(triphenylphosphine) palladium ( $Pd(PPh_3)_4$ ) (15.02 mg, 0.013 mmol) was added to anhydrous tetrahydrofuran (20 ml) under Ar. This suspended solution became pellucid when anhydrous diisopropylamine (5 ml, 35.50 mmol) was added. The reaction mixture was stirred at 78 °C overnight under Ar atmosphere and was monitored by TLC. Upon completion, the solution was evaporated in vacuo and the residue was re-dissolved with DCM. Organic solution was washed with saturated aqueous  $NH_4Cl$ , brine, dried over sodium sulfate and evaporated in vacuo to dryness. The crude product was purified by silica gel flash column chromatography(methanol/dichloromethane) to give the compound **1** as a yellow solid 107.97 mg (0.066 mmol, 52 %).  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.78 (d,  $J$  = 8.4 Hz, 2H), 8.69 (d,  $J$  = 6.9 Hz, 2H), 8.61 (d,  $J$  = 7.6 Hz, 2H), 8.51 (d,  $J$  = 9.2 Hz, 4H), 8.44 (s, 4H), 8.11 (s, 1H), 8.05 (d,  $J$  = 7.6 Hz, 2H), 7.97 – 7.86 (m, 2H), 7.61 (s, 2H), 4.68 – 4.54 (m, 4H), 4.46 (t,  $J$  = 6.0 Hz, 4H), 4.41 – 4.27 (m, 2H), 4.03 – 3.88 (m, 6H), 3.88 – 3.78 (m, 6H), 3.78 – 3.50 (m, 35H), 3.49 – 3.41 (m, 3H), 3.37 (d,  $J$  = 11.3 Hz, 3H), 3.33 (d,  $J$  = 3.0 Hz, 12H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ ):  $\delta$  164.5, 163.8, 163.5, 159.8, 148.2, 137.3, 132.5, 132.1, 131.8, 131.7, 131.5, 131.4, 130.3, 128.0, 127.9, 126.9, 126.2, 124.6, 123.0, 122.8, 121.0, 118.2, 115.7, 112.1, 96.0, 88.6, 72.0, 71.9, 71.0, 70.8, 70.7, 70.6, 70.3, 69.8, 69.1, 68.0, 67.9, 65.1, 59.0, 39.3. HR-MALDI ( $m/z$ ), calcd. for  $C_{87}H_{96}N_8O_{24}$  (M) 1636.6537, found 1659.6430 (M + Na<sup>+</sup>).

### 3. NMR experiments on the foldamer 1

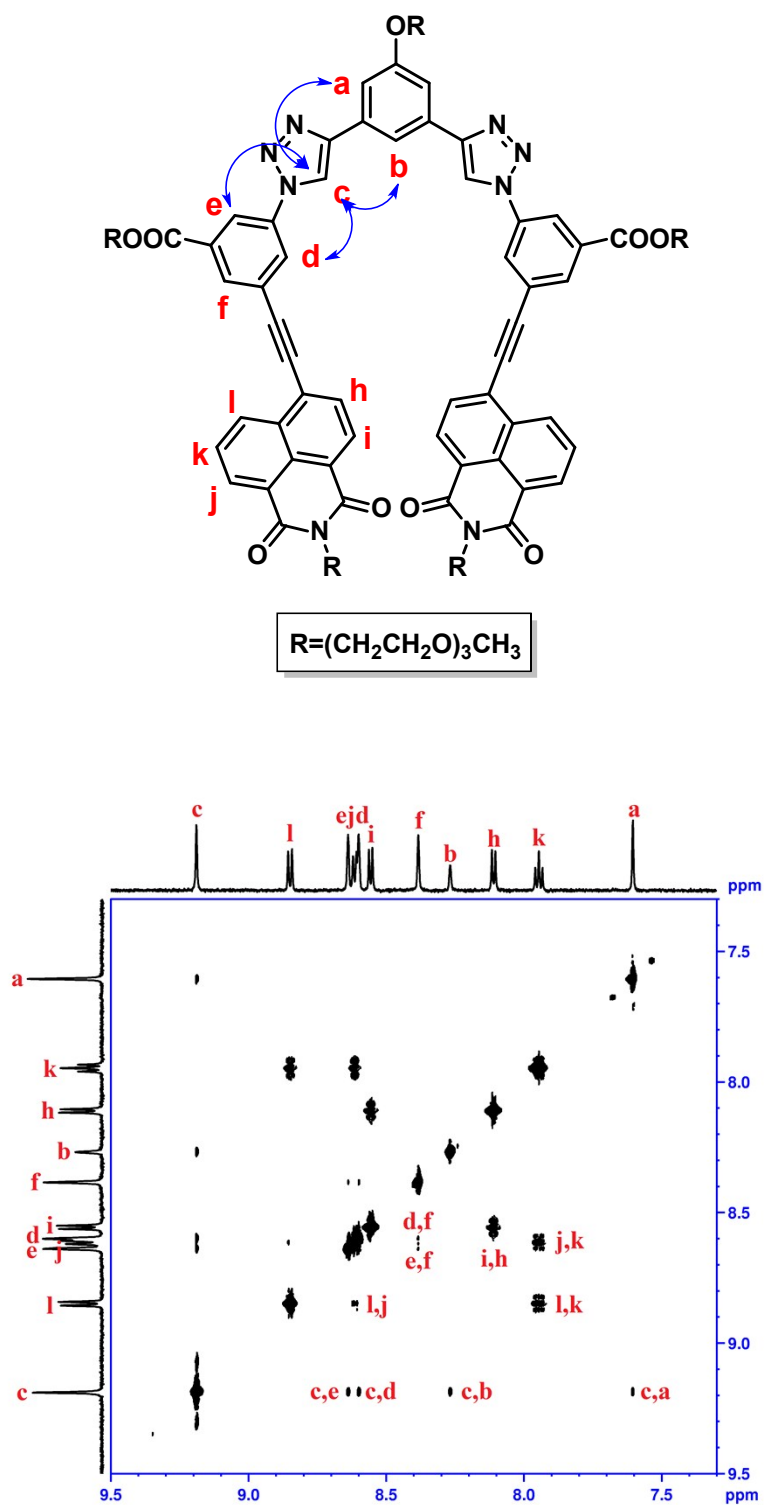


**Fig. S1** Partial  $^1\text{H}$  NMR (400MHz, 298 K) spectra of receptor 1 upon changing the concentration in  $\text{CDCl}_3$ .

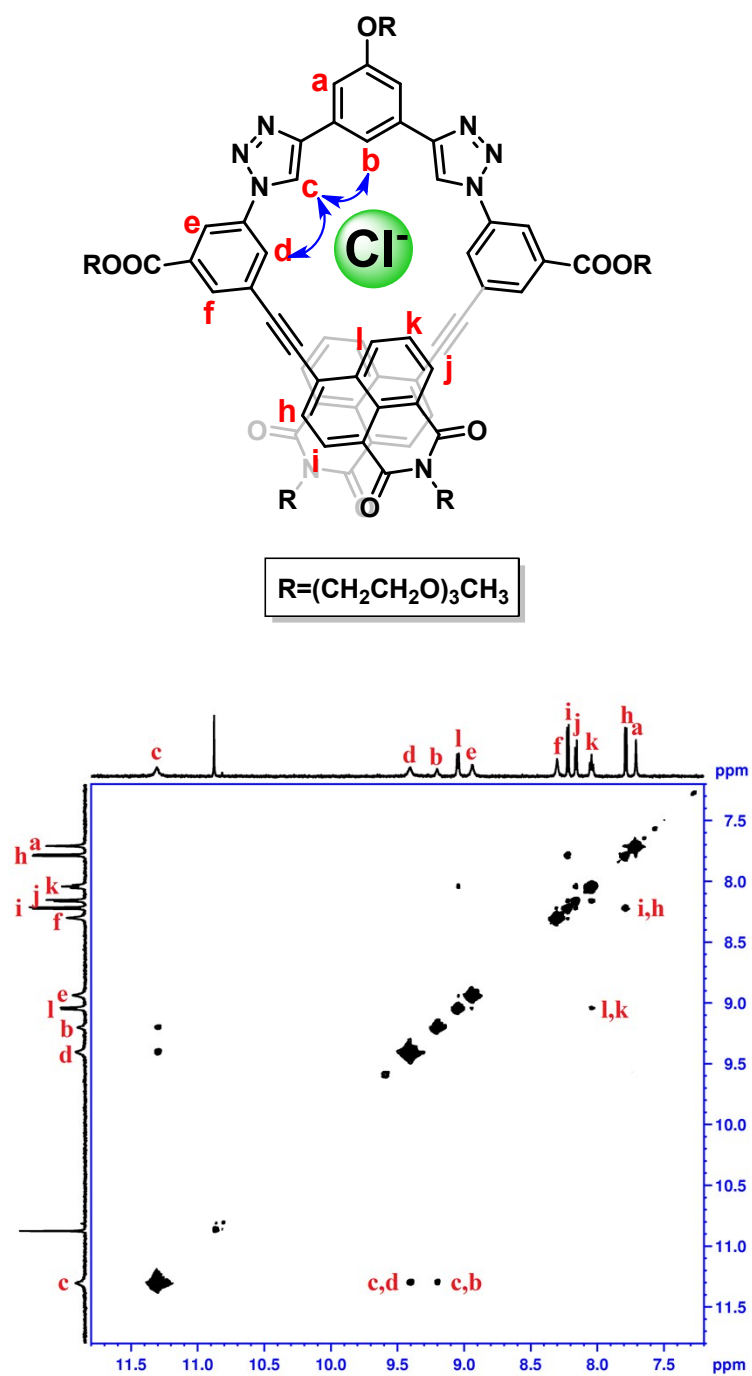


**Fig. S2** Partial  $^1\text{H}$  NMR (400MHz, 298 K) spectra of receptor 1 upon changing the concentration in  $\text{THF}-d_8$ .

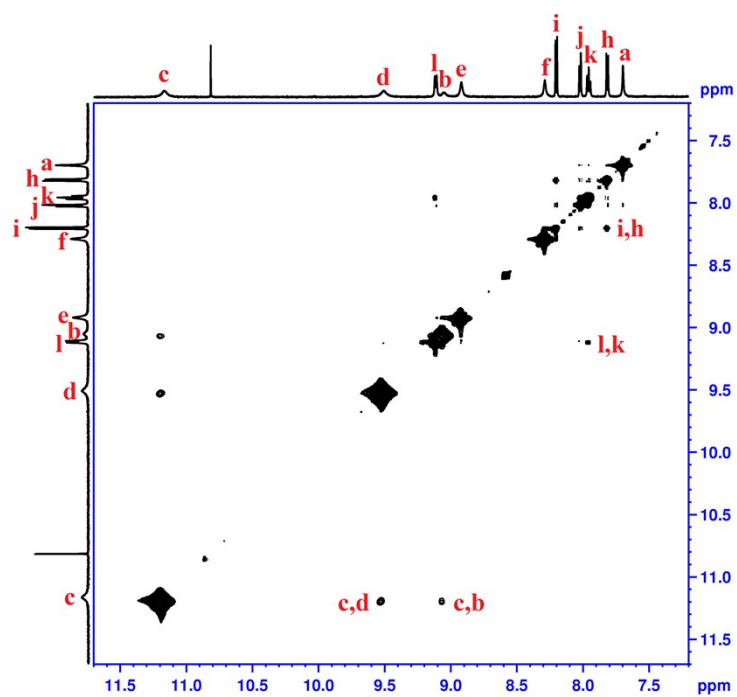
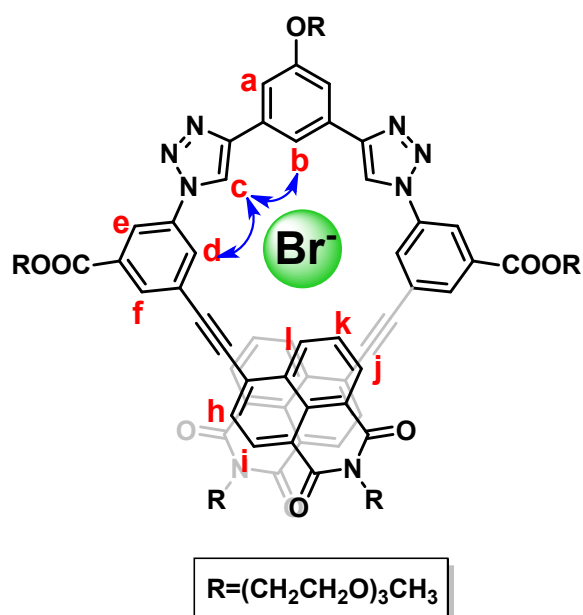




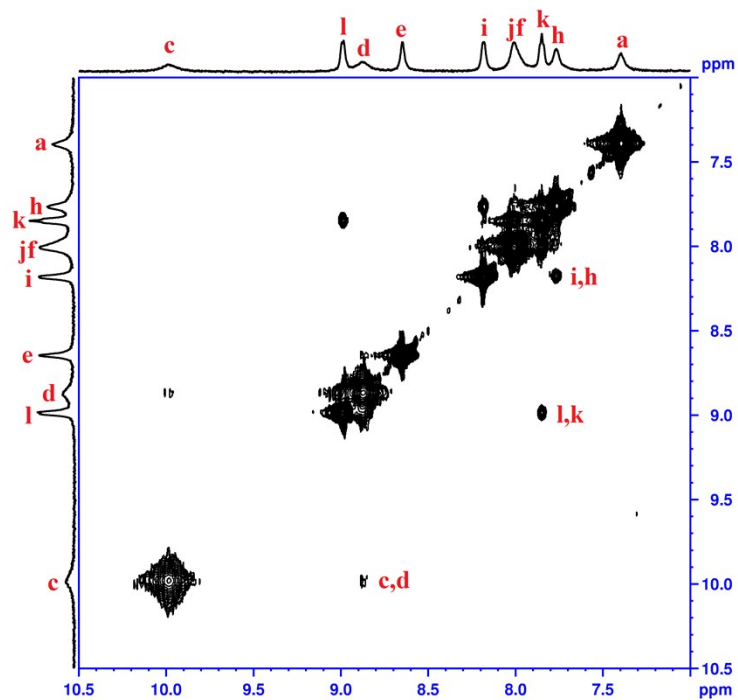
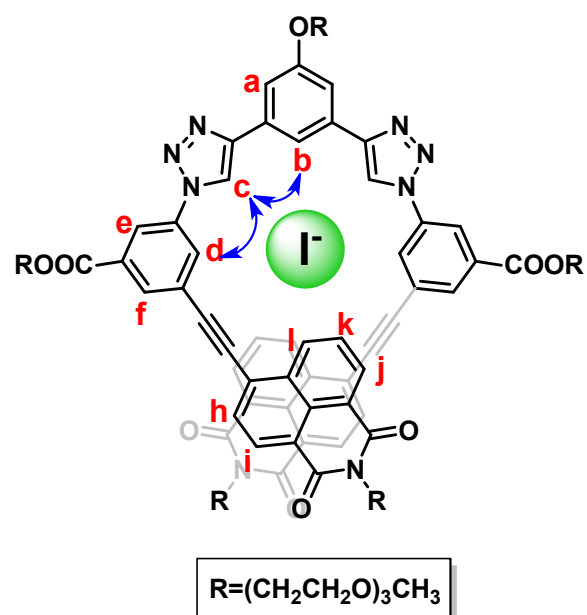
**Fig. S3** Partial  $^1\text{H}$ - $^1\text{H}$  NOESY NMR spectra of receptor **1**. ( $[\mathbf{1}] = 1 \text{ mM}$ , 600MHz, 298 K,  $\text{THF-}d_8$ ).



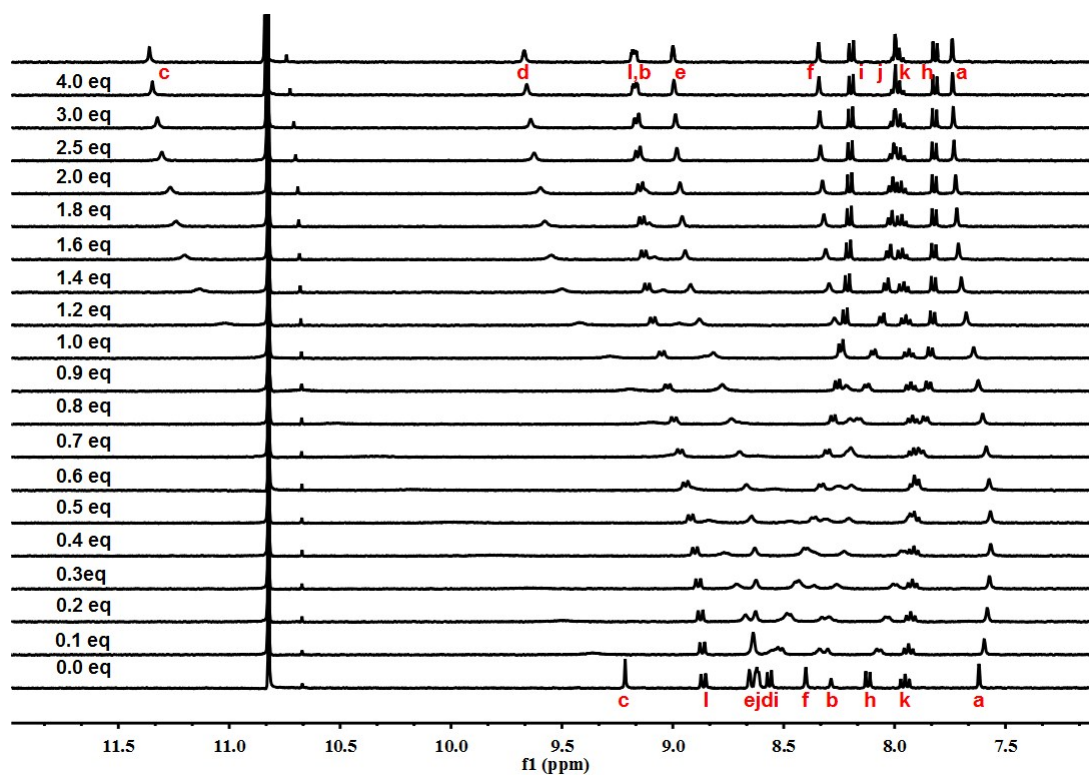
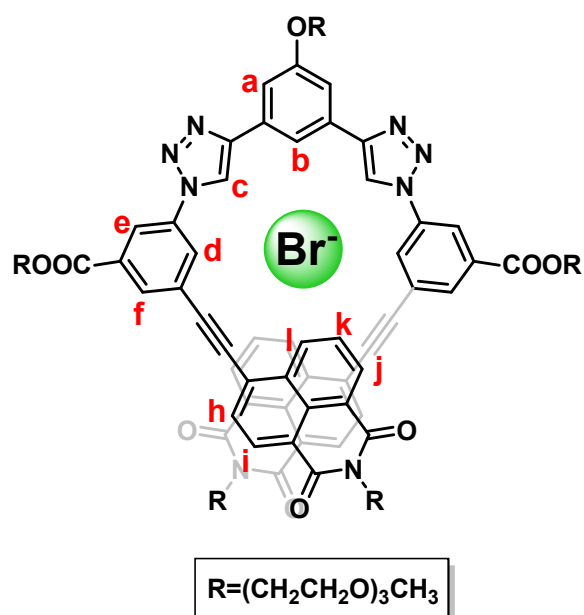
**Fig. S4** Partial <sup>1</sup>H-<sup>1</sup>H NOESY NMR spectra of receptor **1** with 1.6 equivalents of *n*Bu<sub>4</sub>N<sup>+</sup>Cl<sup>-</sup>. ([**1**] = 1 mM, 600MHz, 298 K, THF-*d*<sub>8</sub>).



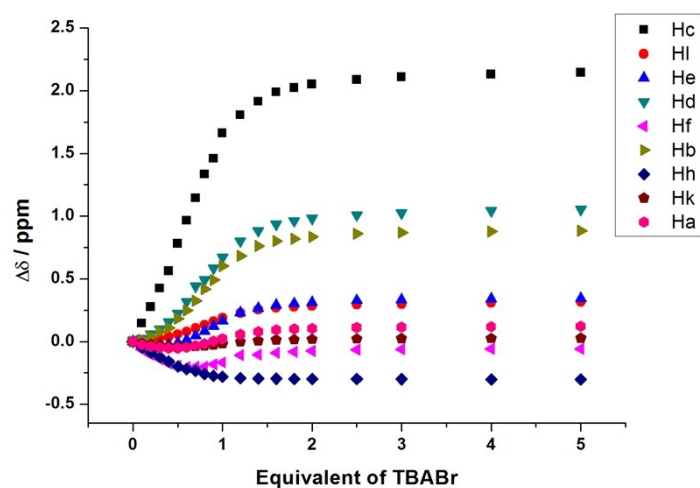
**Fig. S5** Partial  $^1\text{H}$ - $^1\text{H}$  NOESY NMR spectra of receptor **1** with 1.4 equivalents of  $n\text{Bu}_4\text{N}^+\text{Br}^-$ . ( $[\mathbf{1}] = 1 \text{ mM}$ , 600MHz, 298 K,  $\text{THF-}d_8$ ).



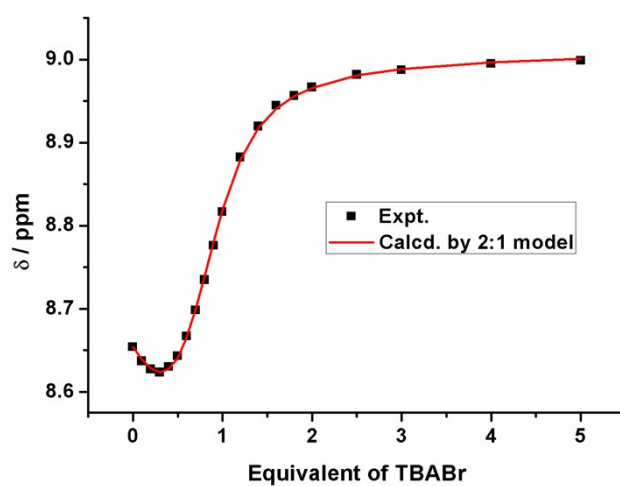
**Fig. S6** Partial  $^1\text{H}$ - $^1\text{H}$  NOESY NMR spectra of receptor **1** with 1.2 equivalents of  $n\text{Bu}_4\text{N}^+\text{I}^-$ . ( $[\mathbf{1}] = 1 \text{ mM}$ , 600MHz, 298 K,  $\text{THF-}d_8$ ).



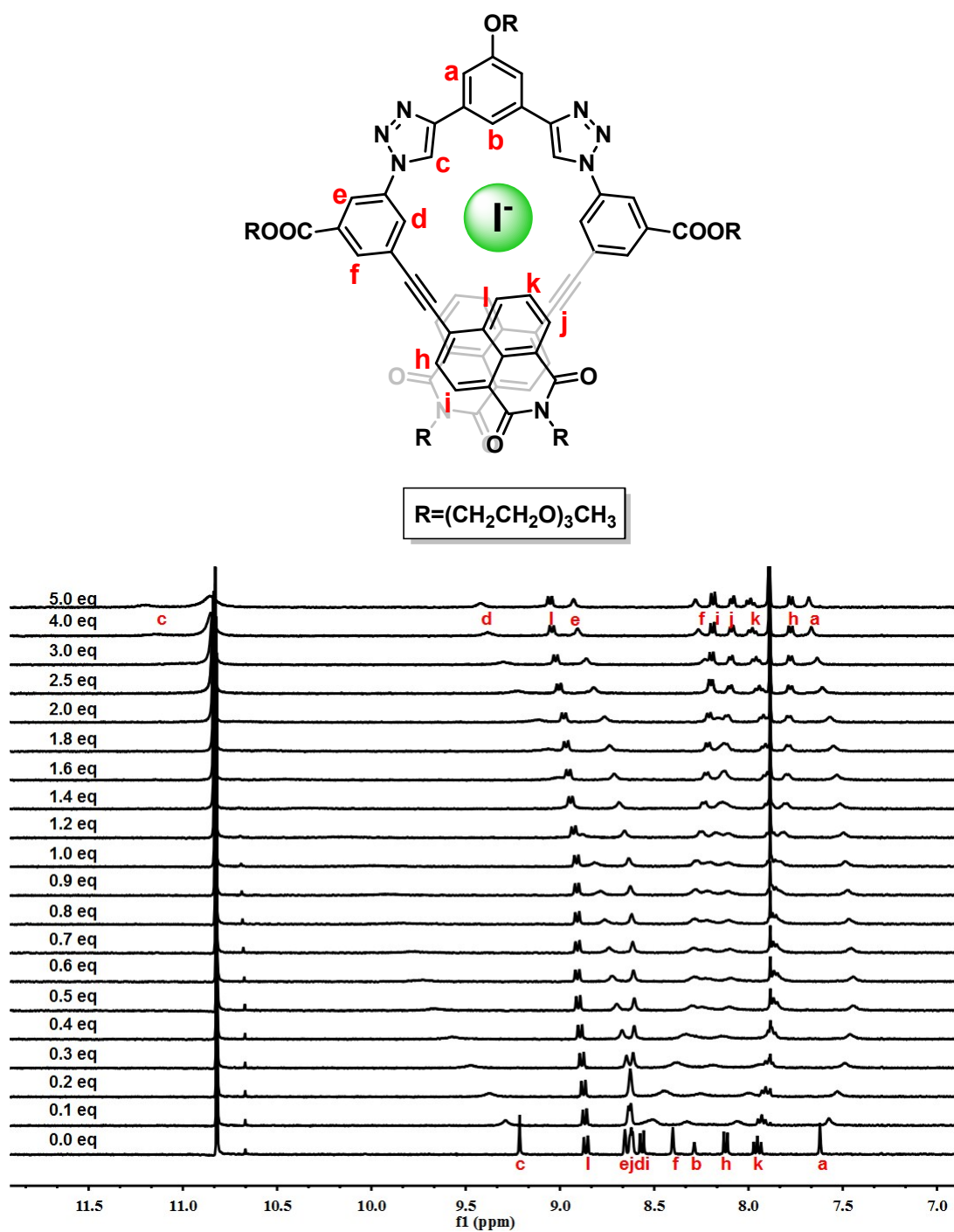
**Fig. S7** Partial  $^1\text{H}$  NMR spectra recorded during the titration of receptor **1** (0.5 mM) with TBABr in  $\text{THF-}d_8$  at 298K.



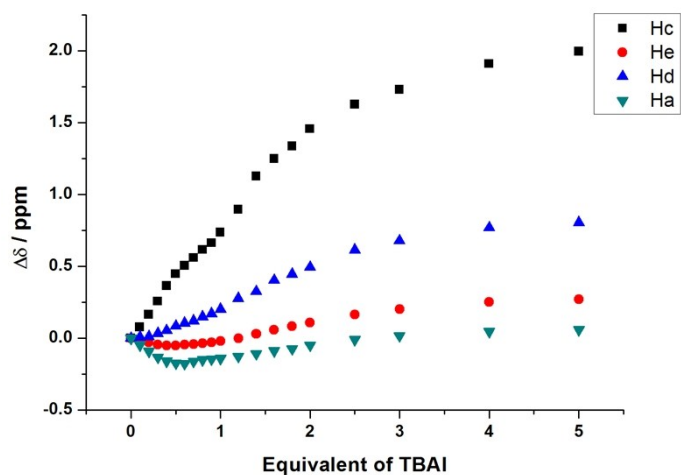
**Fig. S8** Changes in  $^1\text{H}$  chemical shifts of some protons in **1** with increasing concentration of TBABr in  $\text{THF-}d_8$  at 298 K.



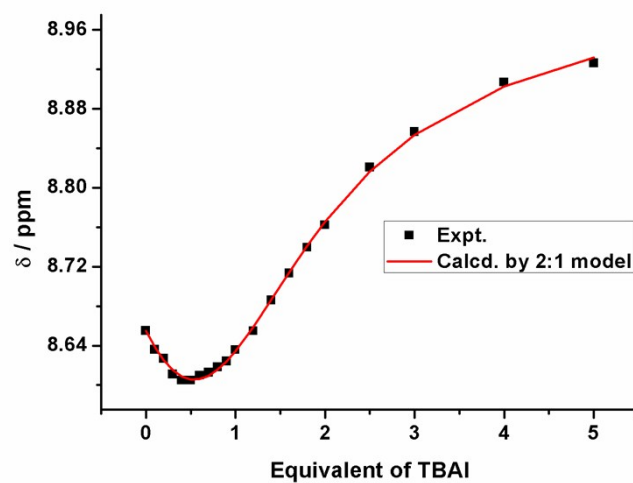
**Fig. S9** Change in  $^1\text{H}$  chemical shift of the  $\text{H}_c$  in Receptor **1** (0.5 mM, 298 K) on addition of TBABr in  $\text{THF-}d_8$ . The data (■) were curve-fitted to 2:1 binding model (fitting-curve was represented by line).



**Fig. S10** Partial  $^1H$  NMR spectra recorded during the titration of receptor **1** (0.5 mM) with TBAI in  $THF-d_8$  at 298K.



**Fig. S11** Changes in  $^1\text{H}$  chemical shifts of some protons in **1** with increasing concentration of TBAI in  $\text{THF-}d_8$  at 298 K.

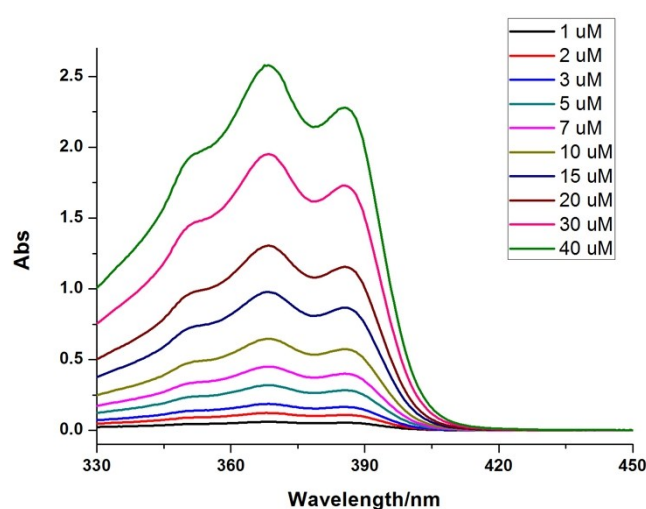


**Fig. S12** Change in  $^1\text{H}$  chemical shift of the  $\text{H}_e$  in receptor **1** (0.5 mM, 298 K) on addition of TBAI in  $\text{THF-}d_8$ . The data (■) were curve-fitted to 2:1 binding model (fitting-curve was represented by line).

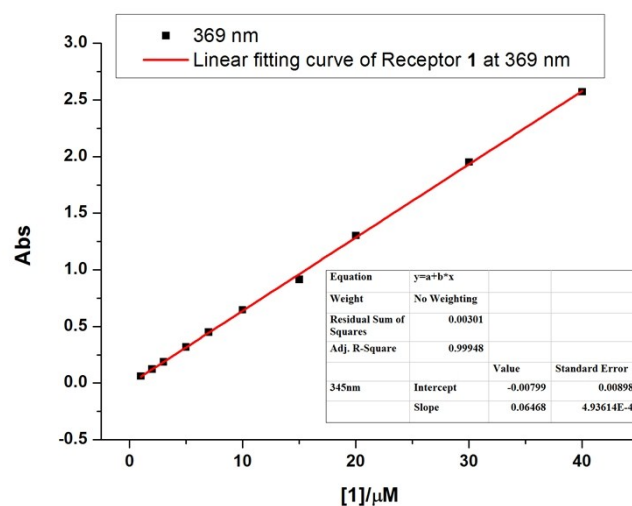


#### 4. UV-Vis titration of foldamer 1

Summary of data analysis. The UV-Vis titration data were fitted with ReactLab™ EQUILIBRIA, in a 1:1 binding model with all halogen anions to give the association constants. Typically, six sets of data, i.e., data points at six different wavelengths, were employed for the fitting. To estimate the standard deviation, the data were fitted for totally five times. At each run, association constants were generated from only five data sets with one set of data excluded in turn. The titration experiments have been repeated three times with each anion. The association constants obtained are summarized in Table S1.

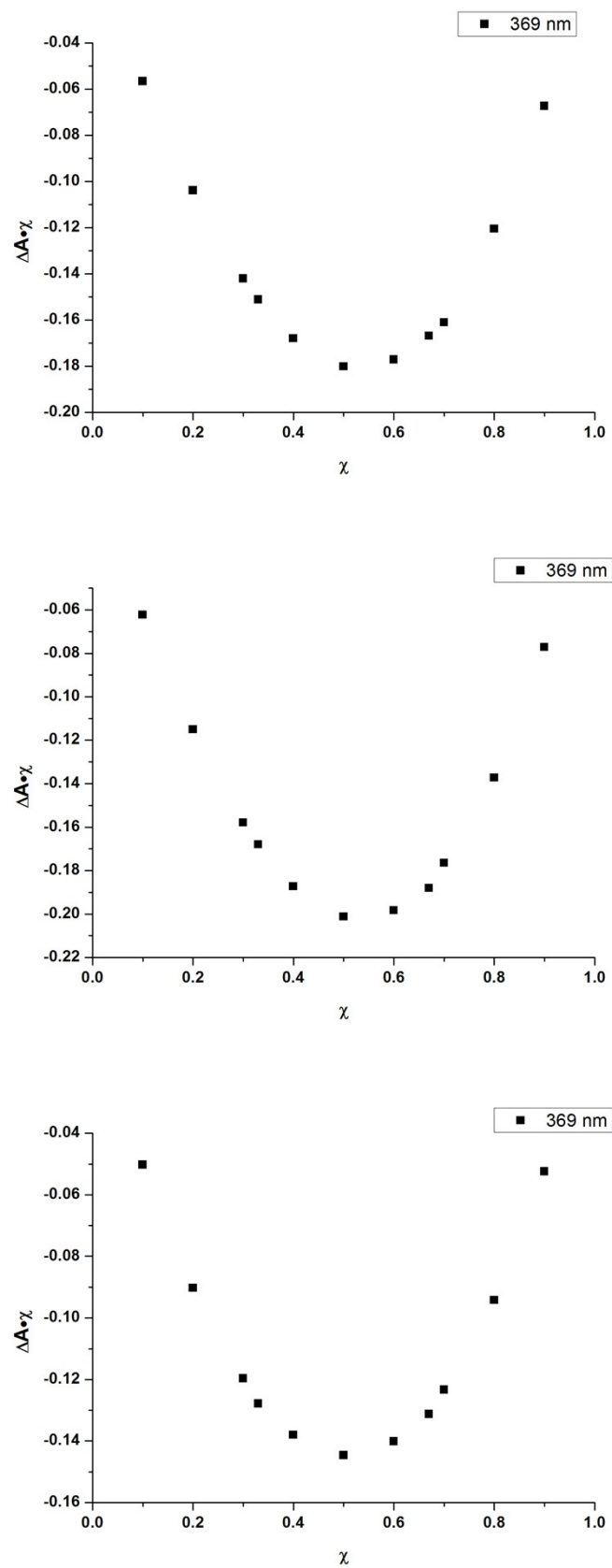


(a)

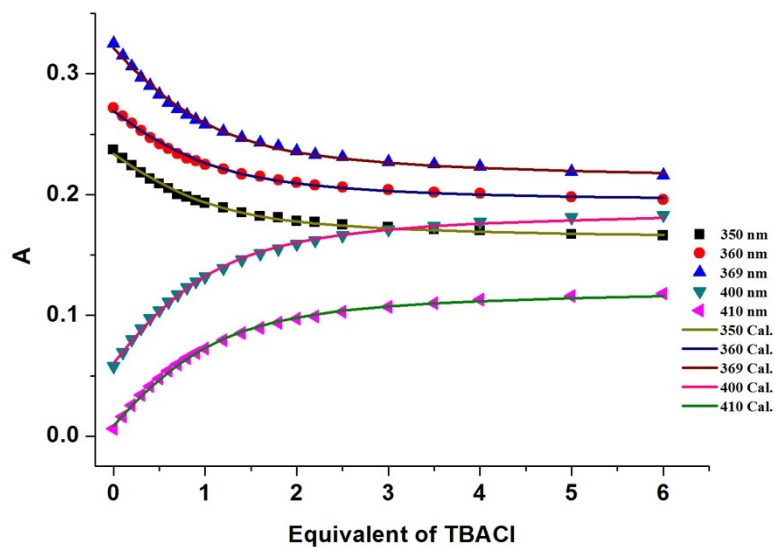


(b)

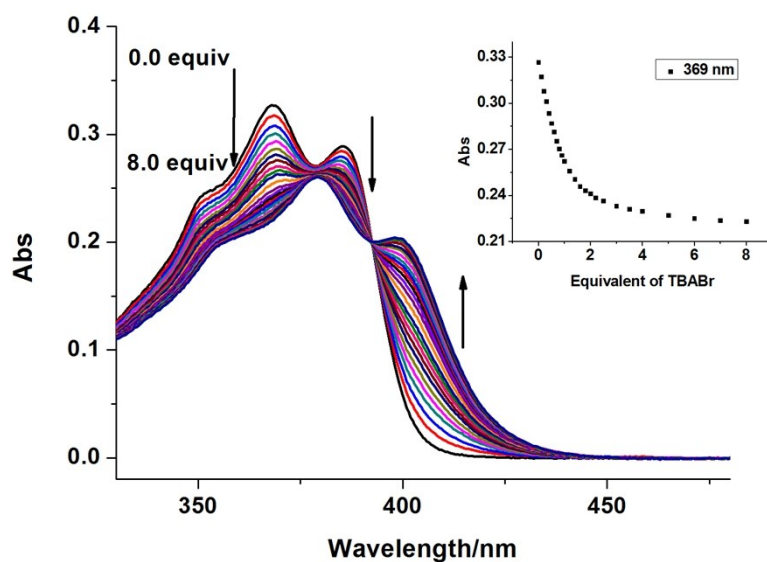
**Fig. S13** (a) Concentration-dependent UV-vis spectra of **1** in THF (SG) at 298 K; (b) the linear fitting curve of receptor **1** at 369 nm.



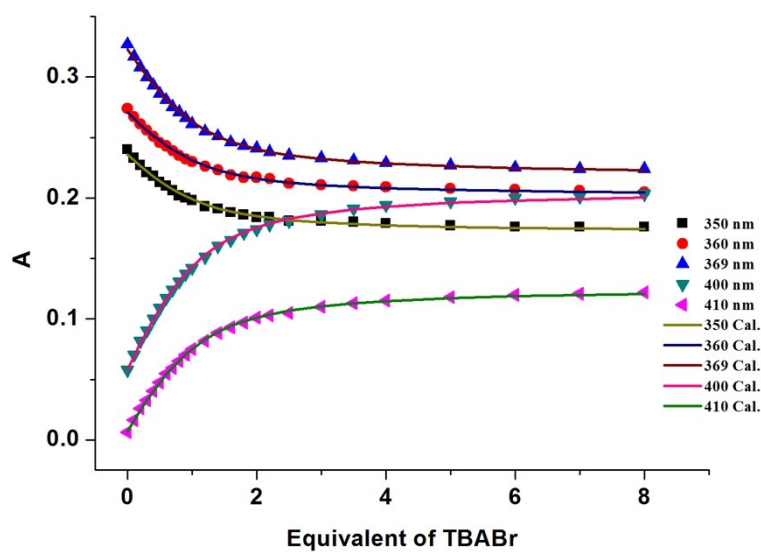
**Fig. S14** Job's Plot of receptor **1** with halogen anions, up: TBACl; middle: TBABr; down: TBAI in THF(SG) at 298 K.



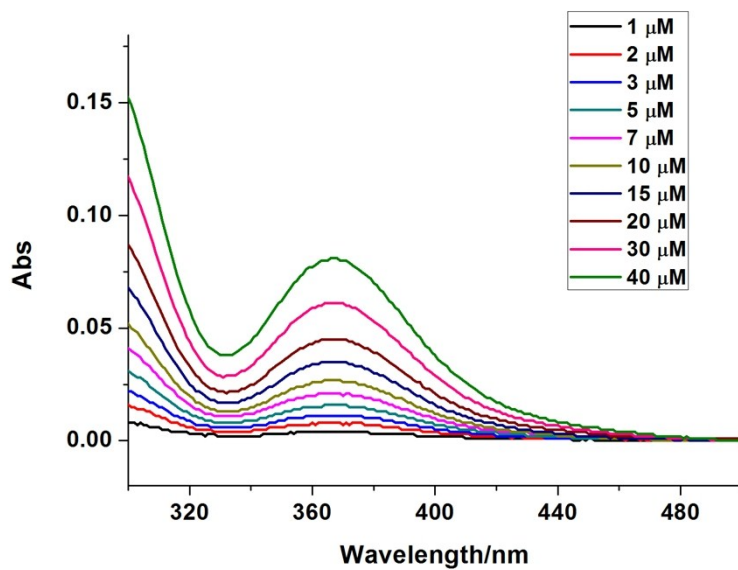
**Fig. S15** The corresponding changes of UV-Vis absorption intensity at  $\lambda = 350, 360, 369, 400$  and  $410$  nm, in which the experimental data (*points*) were curved-fitted (*lines*) to 1:1 (1 to TBACl) model by ReactLabTM Equilibria.



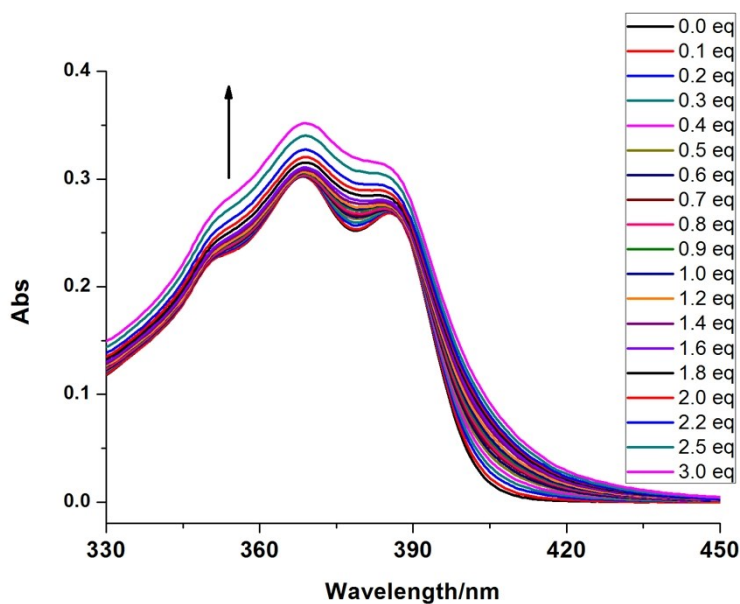
**Fig. S16** UV-Vis spectroscopic titration of receptor **1** ( $[1] = 5 \mu\text{M}$ ) with TBABr in THF. Insert: Change in UV absorption intensity at 369 nm of **1** on titration with TBABr in THF.



**Fig. S17** The corresponding changes of UV-Vis absorption intensity at  $\lambda = 350, 360, 369, 400$  and  $410$  nm, in which the experimental data (*points*) were curved-fitted (*lines*) to 1:1 (1 to TBABr) model by ReactLabTM Equilibria.



**Fig. S18** Concentration-dependent UV-vis spectra of TBAI in THF (SG) at 298 K.



**Fig. S19** UV-Vis spectroscopic titration of receptor **1** ( $[1] = 5 \mu\text{M}$ ) with TBAI in THF. Insert: Change in UV absorption intensity at 369 nm of **1** on titration with TBAI in THF.

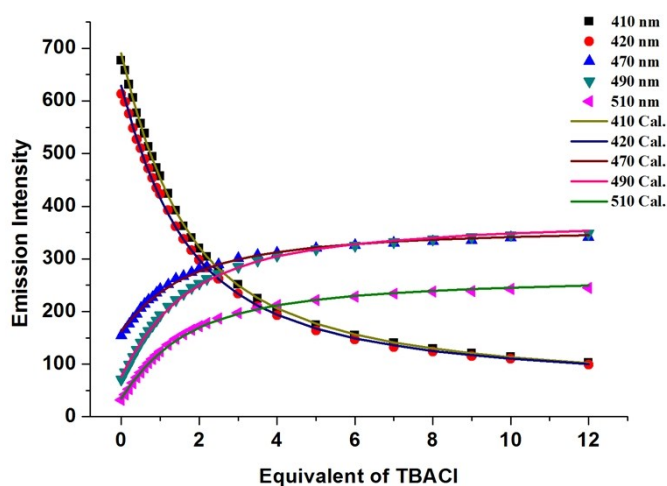
**Table S1.** Summary of association constants of **1** to chloride, bromide, iodide in THF derived from UV-Vis titration experiments.<sup>a</sup>

Anion	$K_a(\text{UV})$			
	Run 1	Run 2	Run 3	Average value
$\text{Cl}^-$	$590,000 \pm 19,000$	$620,000 \pm 16,000$	$540,000 \pm 17,000$	$580,000 \pm 19,000$
$\text{Br}^-$	$630,000 \pm 14,000$	$720,000 \pm 17,000$	$690,000 \pm 18,000$	$680,000 \pm 18,000$
$\text{I}^-$ <sup>b</sup>				

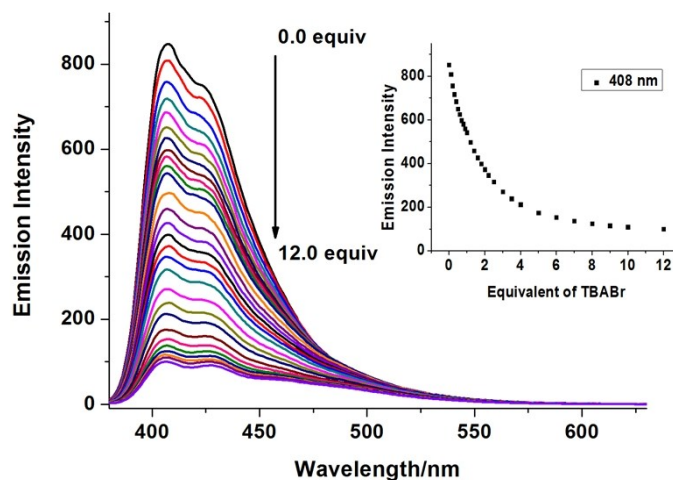
<sup>a</sup> The UV-Vis titration data were fitted with ReactLabTM EQUILIBRIA, in a 1:1 binding model with all halogen anions to give the association constants. The data were obtained by repeating three times with each anion to reduce errors. Throughout the table, the unit of association constants are  $\text{L/mol (M}^{-1}\text{)}$ ,  $[1] = 5 \mu\text{M}$ . <sup>b</sup> The binding constant could not be obtained through UV-Vis titration experiment.

## 5. Fluorescent titration of foldamer 1

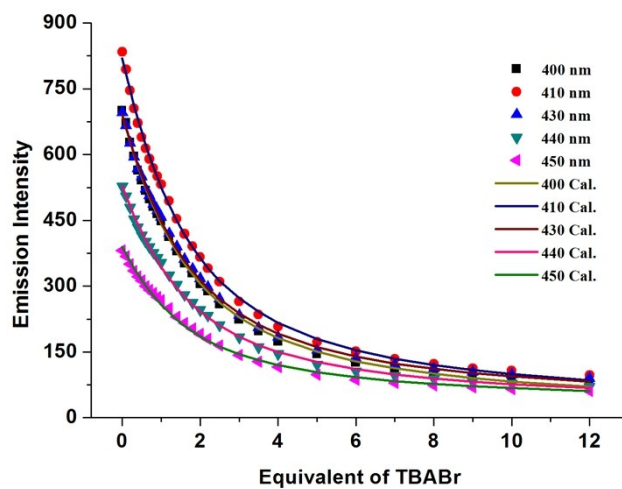
Summary of data analysis. The fluorescence titration data were fitted with ReactLab<sup>TM</sup> EQUILIBRIA, in a 1:1 binding model with all halogen anions to give the association constants. Typically, six sets of data, i.e., data points at six different wavelengths, were employed for the fitting. To estimate the standard deviation, the data were fitted for totally five times. At each run, association constants were generated from only five data sets with one set of data excluded in turn. The titration experiments have been repeated three times with each anion. The association constants obtained are summarized in Table S2.



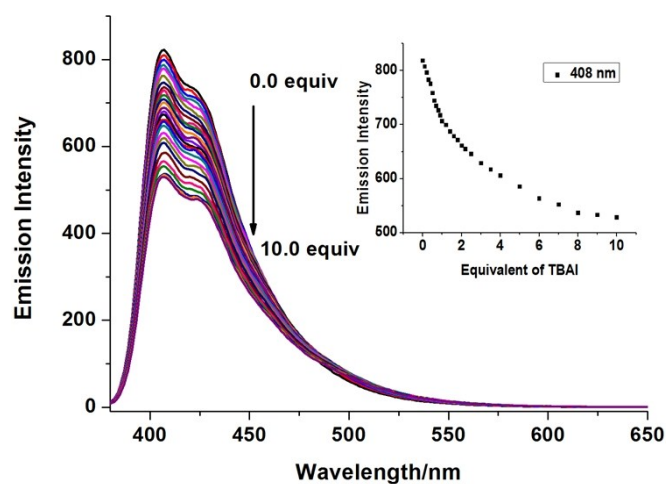
**Fig. S20** The corresponding changes of emission intensities at  $\lambda = 410, 420, 470, 490$  and  $510$  nm, in which the experimental data (*points*) were curved-fitted (*lines*) to 1:1 (**1** to TBACl) model by ReactLab<sup>TM</sup> Equilibria.



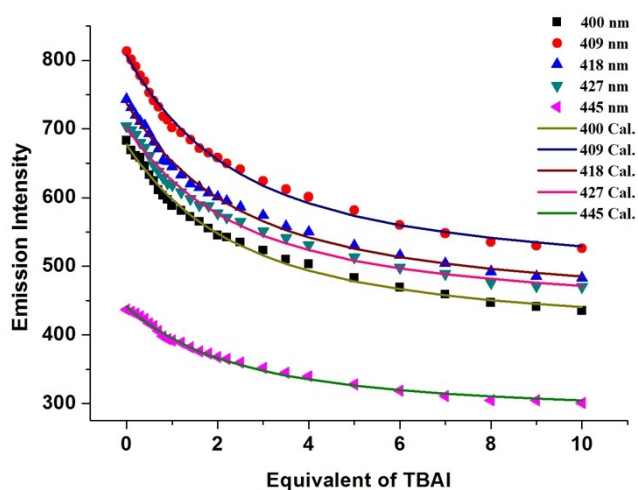
**Fig. S21** Fluorescent spectroscopic titration of Receptor **1** ( $[1] = 1$   $\mu$ M) with TBABr in THF. Insert: Change in fluorescent emission intensity at 408 nm of **1** on titration with TBABr in THF.



**Fig. S22** the corresponding changes of emission intensities at  $\lambda = 400, 410, 430, 440$  and  $450$  nm, in which the experimental data (*points*) were curved-fitted (*lines*) to 1:1 (**1** to TBABr) model by ReactLabTM Equilibria.



**Fig. S23** Fluorescent spectroscopic titration of **1** ( $[1] = 1 \mu\text{M}$ ) with TBAI in THF. Insert: Change in fluorescent emission intensity at 408 nm of **1** on titration with TBAI in THF.



**Fig. S24** the corresponding changes of emission intensities at  $\lambda = 400, 409, 418, 427$  and  $445$  nm, in which the experimental data (*points*) were curved-fitted (*lines*) to 1:1 (**1** to TBAI) model by ReactLabTM Equilibria.

**Table S2.** Summary of association constants of **1** to chloride, bromide, iodide in THF fluorescence titration experiments.<sup>a</sup>

Anion	$K_a(\text{FL})$			
	Run 1	Run 2	Run 3	Average value
Cl <sup>-</sup>	910,000±13,000	940,000±12,000	840,000±15,000	900,000±15,000
Br <sup>-</sup>	900,000±15,000	860,000±16,000	920,000±13,000	890,000±16,000
I <sup>-</sup>	540,000±19,000	480,000±17,000	590,000±16,000	540,000±19,000

<sup>a</sup> The Fluorescence titration data were fitted with ReactLabTM EQUILIBRIA, in a 1:1 binding model with all halogen anions to give the association constants. The data were obtained by repeating three times with each anion to reduce errors. Throughout the table, the unit of association constants are L/mol ( $\text{M}^{-1}$ ), [**1**] =  $\mu\text{M}$ .



## 6. $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra of new compounds

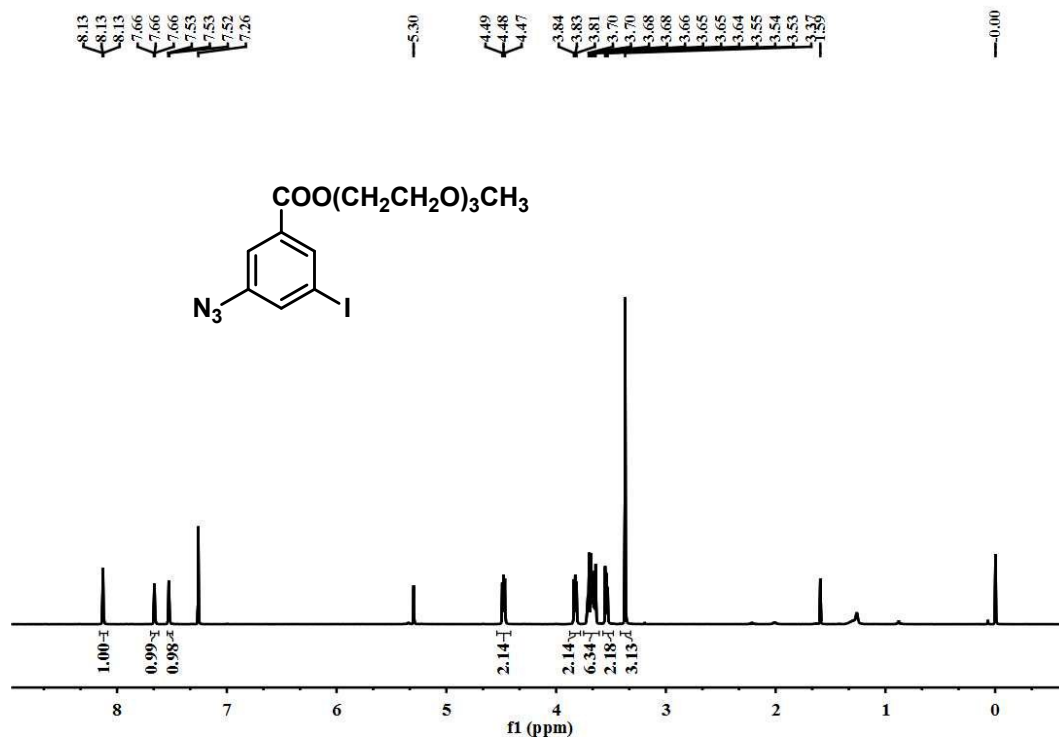


Fig. S25  $^1\text{H}$  NMR (400 MHz, 298K) spectra of compound **3** in  $\text{CDCl}_3$ .

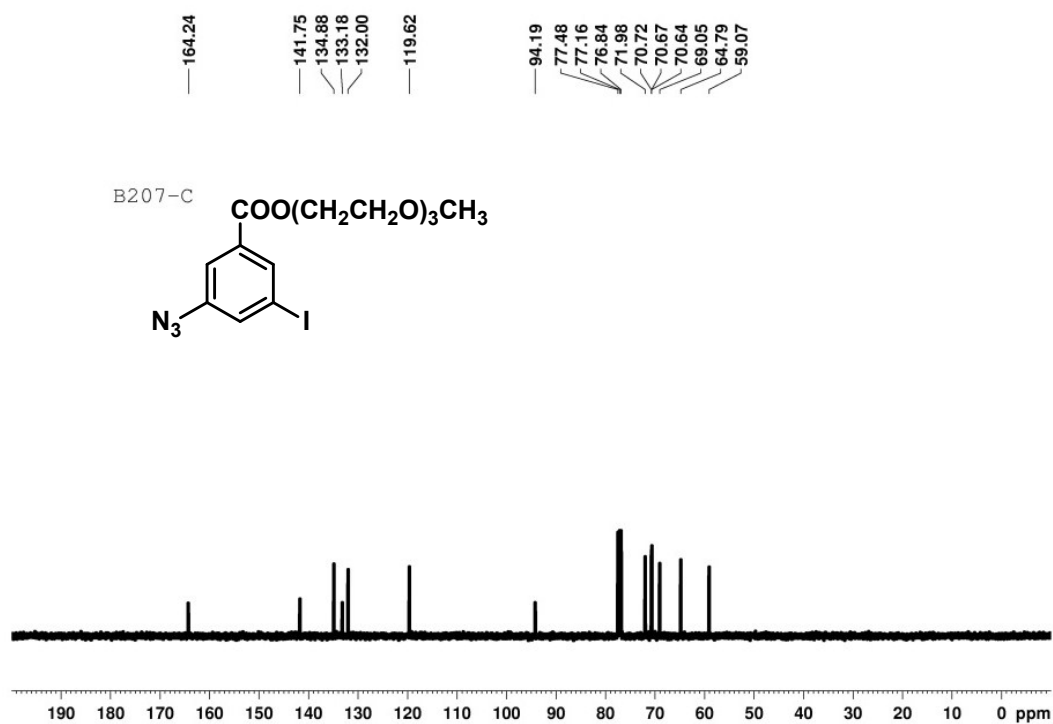


Fig. S26.  $^{13}\text{C}$  NMR (100 MHz, 298K) spectra of compound **3** in  $\text{CDCl}_3$ .

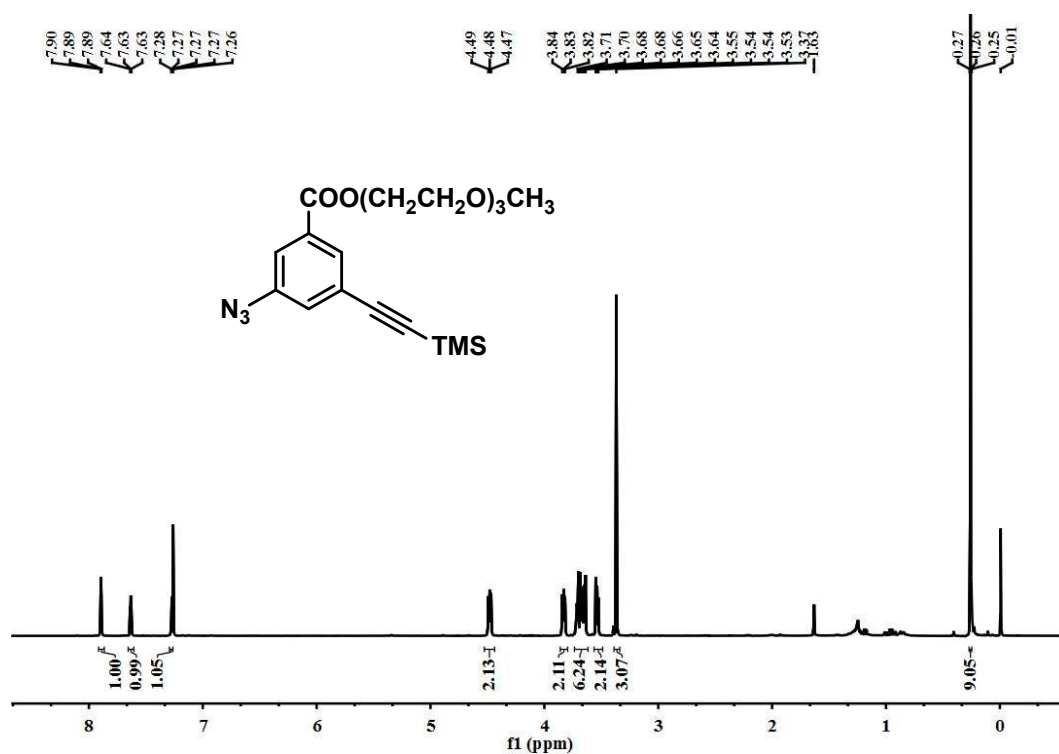


Fig. S27 <sup>1</sup>H NMR (400 MHz, 298K) spectra of compound 4 in CDCl<sub>3</sub>.

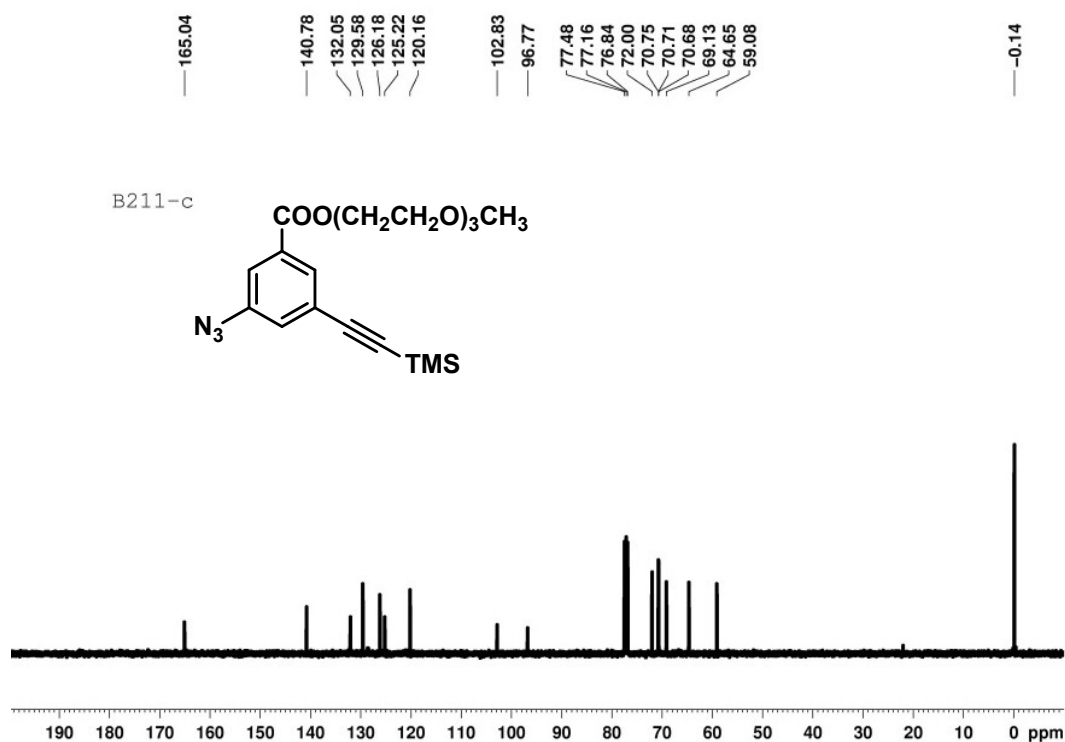


Fig. S28 <sup>13</sup>C NMR (100 MHz, 298K) spectra of compound 4 in CDCl<sub>3</sub>.

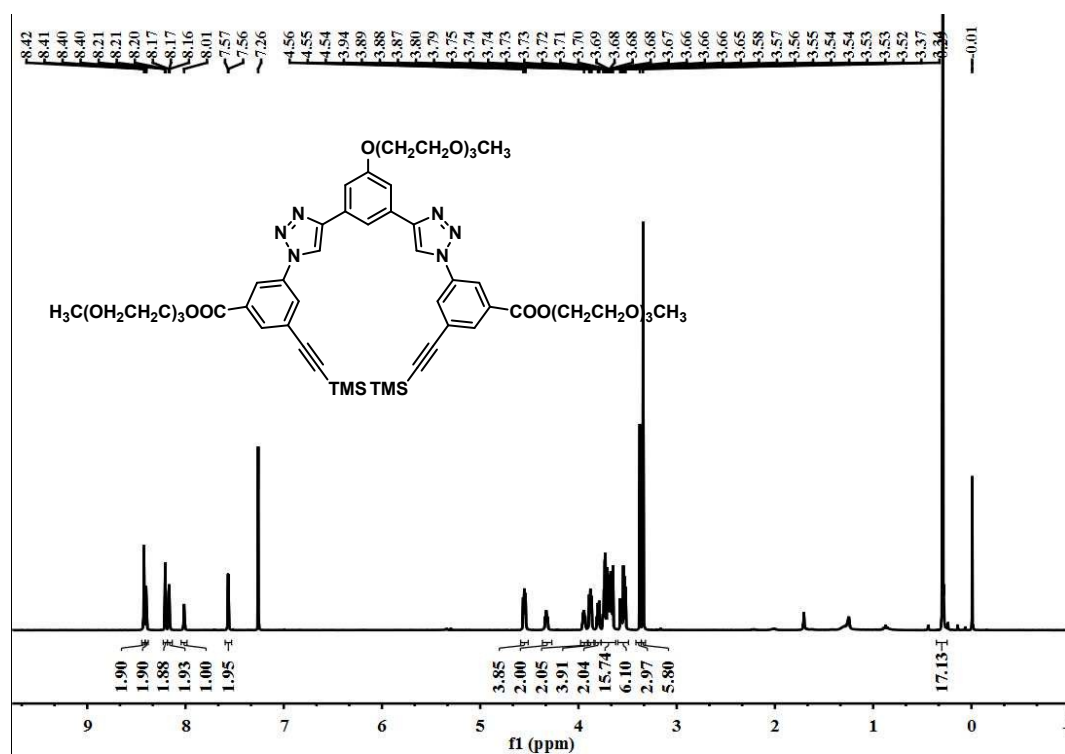


Fig. S29 <sup>1</sup>H NMR (400 MHz, 298K) spectra of compound 6 in CDCl<sub>3</sub>.

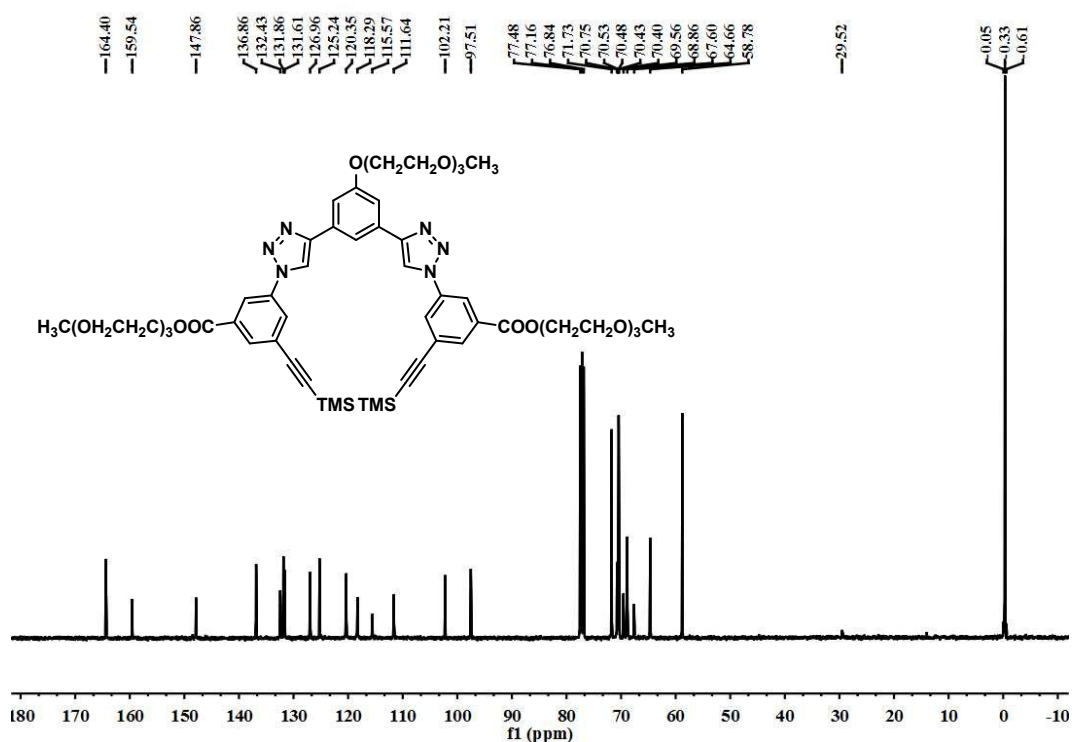
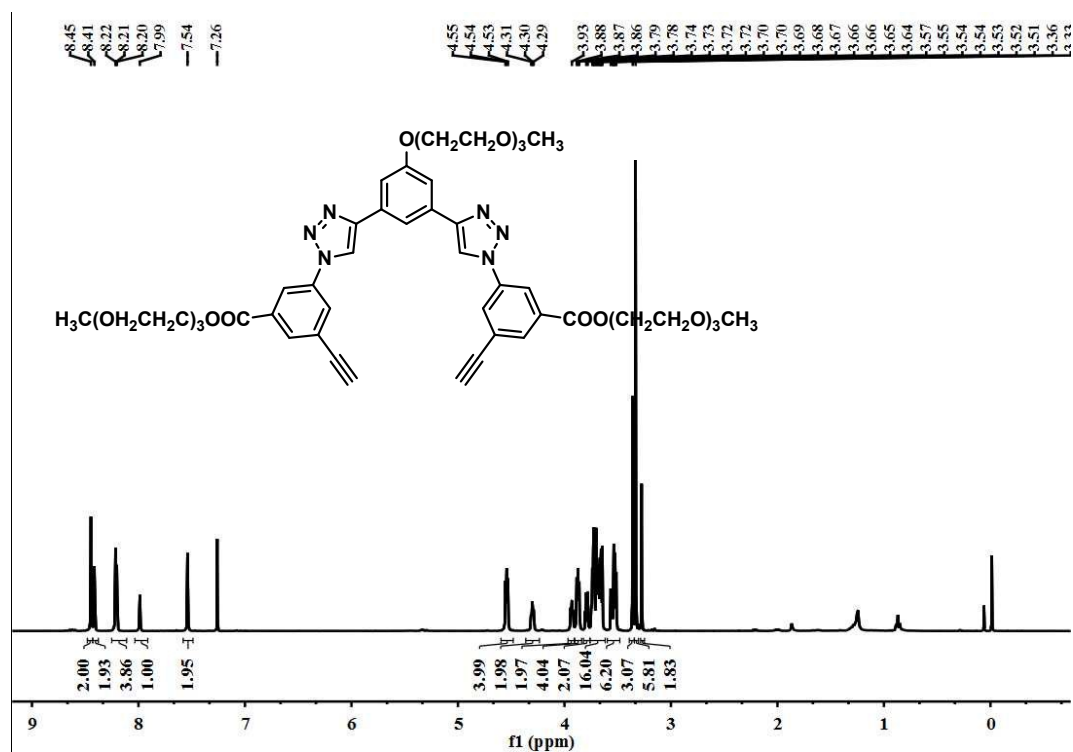
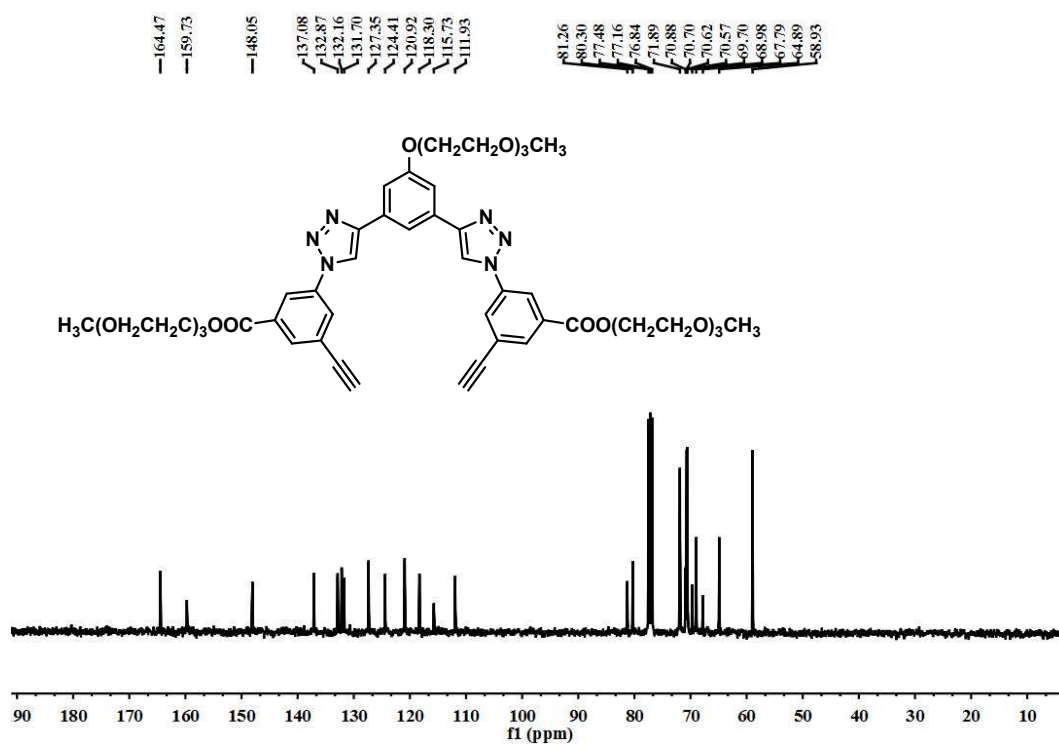


Fig. S30 <sup>13</sup>C NMR (100 MHz, 298K) spectra of compound 6 in CDCl<sub>3</sub>.



**Fig. S31**  $^1\text{H}$  NMR (400 MHz, 298K) spectra of compound **7** in  $\text{CDCl}_3$ .



**Fig. S32**  $^{13}\text{C}$  NMR (100 MHz, 298K) spectra of compound **7** in  $\text{CDCl}_3$ .

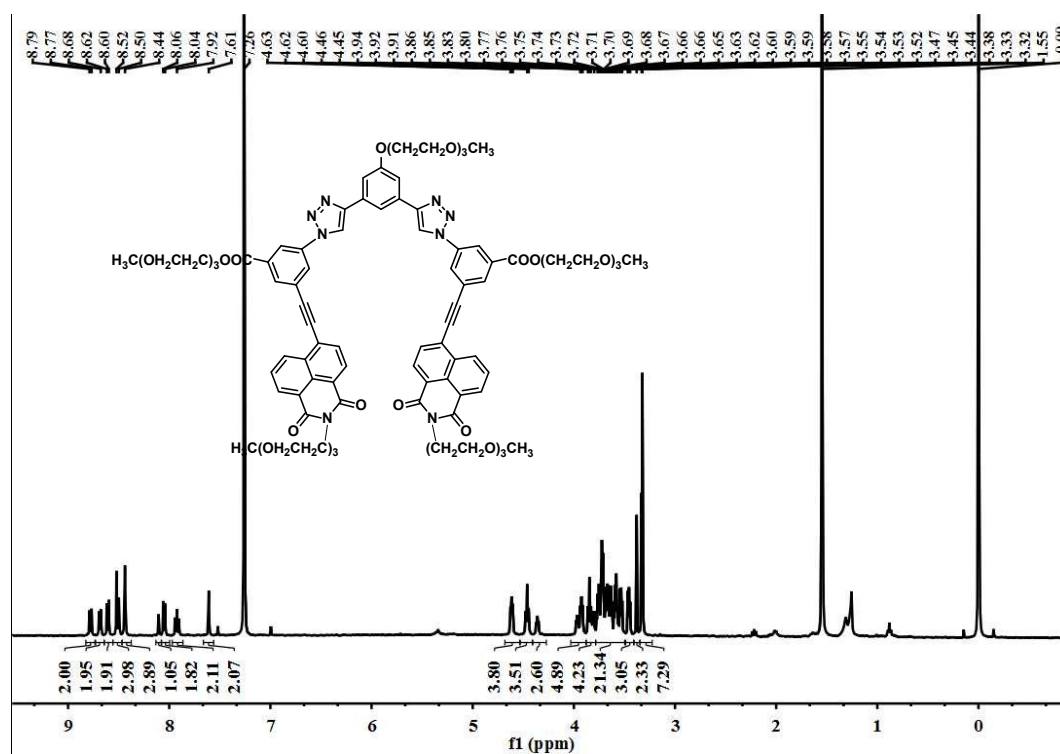


Fig. S33 <sup>1</sup>H NMR (400 MHz, 298K) spectra of compound 1 in  $\text{CDCl}_3$ .

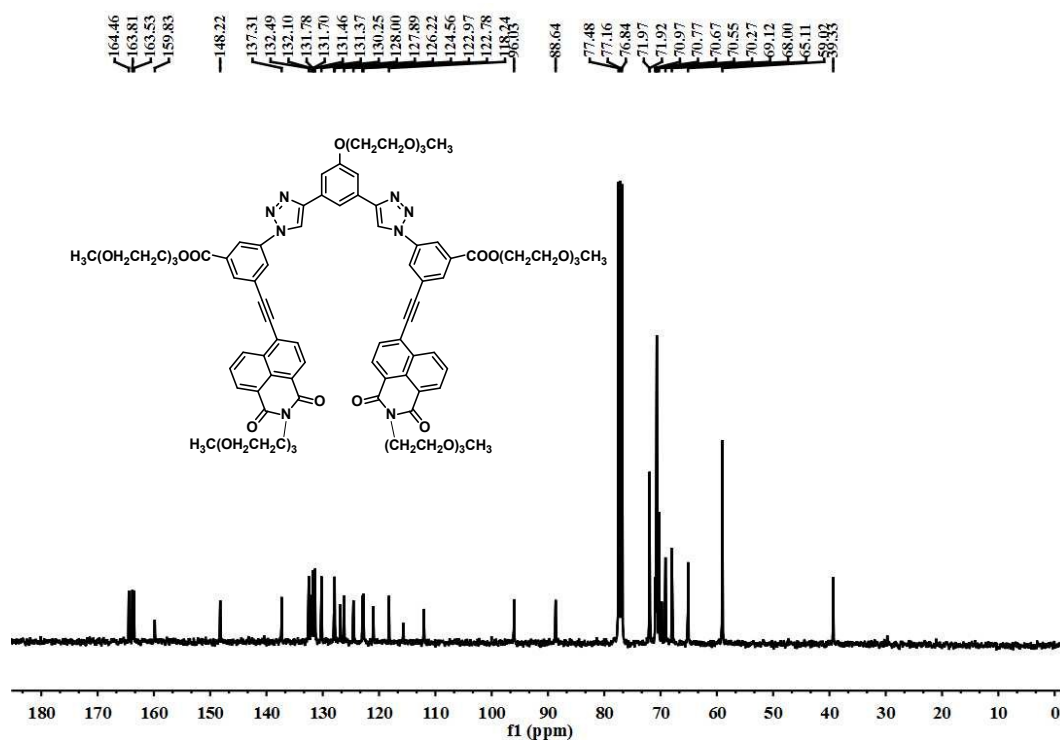


Fig. S34 <sup>13</sup>C NMR (100 MHz, 298K) spectra of compound 1 in  $\text{CDCl}_3$ .

## 7. References

- S1 Y. Wang, F. Li, Y. Han, F.Y. Wang and H. Jiang, *Chem. Eur. J.*, 2009, **15**, 9424.
- S2 Y. Li, M. Pink, J. A. Karty and A. H. Flood, *J. Am. Chem. Soc.*, 2008, **130**, 17293.
- S3 H. Seo, M. E. Jun, K. Ranganathan, K.-H. Lee, K.-T. Kim, W. Lim, Y. M. Rhee and K. H. Ahn, *Org. Lett.*, 2014, **16**, 1374.