Supporting Information

for

Fluoride-driven 'turn on' ESPT in the binding with a novel benzimidazole-based sensor

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1. Binding constants determination by UV–vis and fluorescence methods

Binding constants (K) were calculated by non-linear least-square analysis of the titration curves according to the following relation for 1:1 complexation.

$$\Delta X = A\left\{C_H + C_G + B - \left[\left(C_H + C_G + B\right)^2 - 4C_H C_G\right]^{\frac{1}{2}}\right\}$$

where ΔX is the difference value between the absorbance (or emission intensity) of the whole system and the absorbance of free host, A is a floating parameter in the analysis, B is the ratio between 1 to k (binding association), C_H and C_G are the concentration of host and guest, respectively.
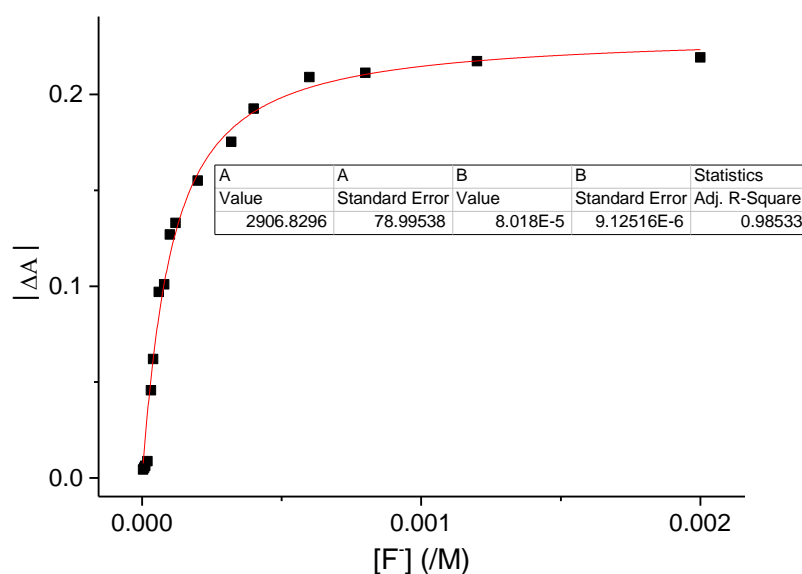

A	A	B	B	Statistics
Value	Standard Error	Value	Standard Error	Adj. R-Square
2906.8296	78.99538	8.018E-5	9.12516E-6	0.98533

Figure S1: Non-linear curve fit of absorbance changes at 410 nm as a function of fluoride concentration.

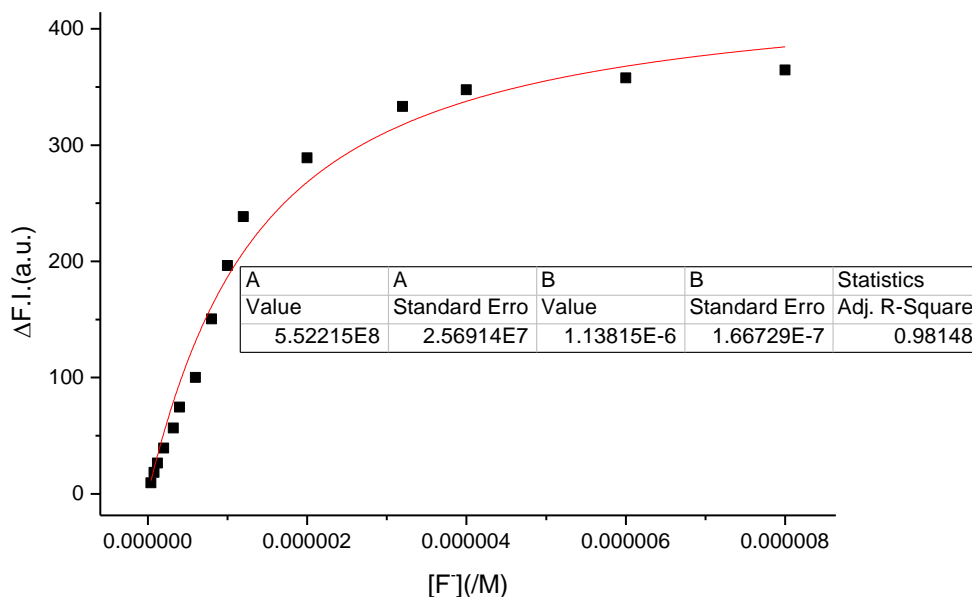| A	A	B	B	Statistics
Value	Standard Erro	Value	Standard Erro	Adj. R-Square
5.52215E8	2.56914E7	1.13815E-6	1.66729E-7	0.98148

Figure S2: Non-linear curve fit of emission intensity at 376 nm as a function of fluoride concentration.

2. Calculation of detection limit

The detection limit (D) of BIP in emission spectra for fluoride ion was determined according to the followed equation:

$$D = 3S_b / k$$

Where S_b is the standard deviation of the blank solution; k is the slope of the curve.

From the Figure S3, we get the slope, which was 156553000. And the standard deviation S_b was 1.1166. Then the detection limit was obtained to be 0.021μM using the above-mentioned equation.
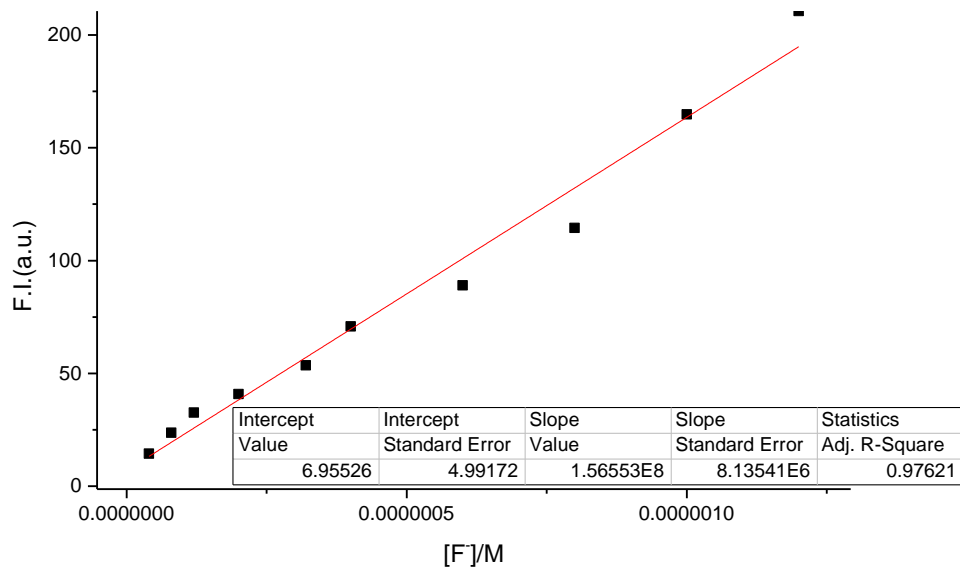
The table embedded in the figure reads:

	Intercept	Intercept	Slope	Slope	Statistics
	Value	Standard Error	Value	Standard Error	Adj. R-Square
	6.95526	4.99172	1.56553E8	8.13541E6	0.97621

Figure S3: Changes of fluorescence intensity of BIP at 376 nm as a function of fluoride concentration.
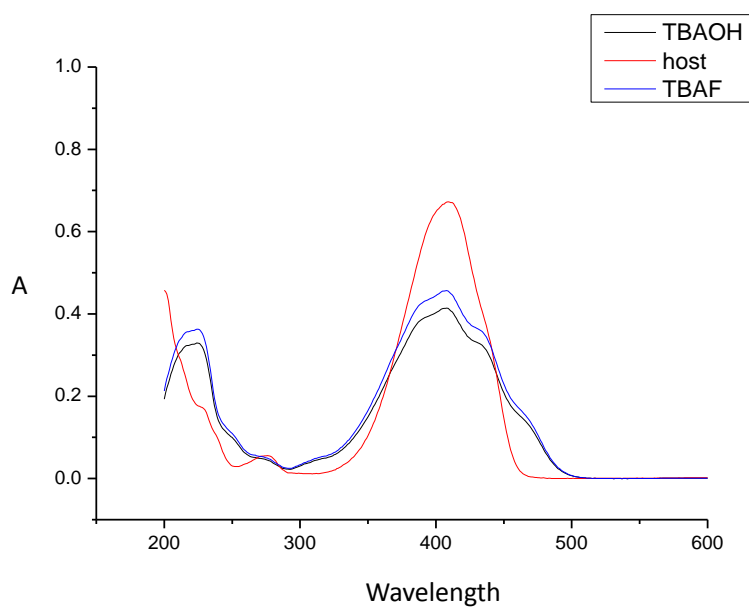
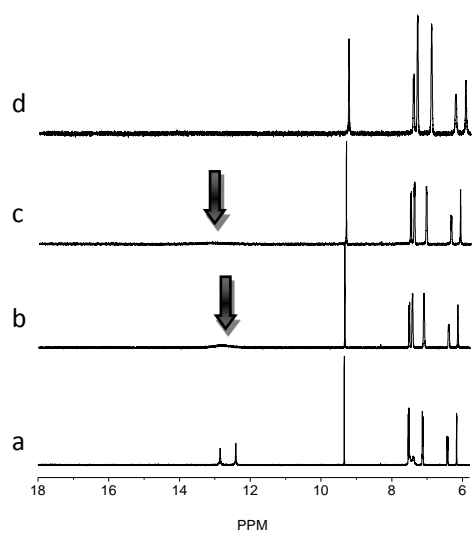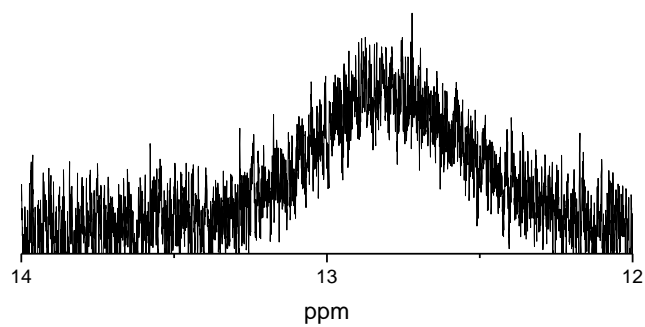**Figure S4:** Spectral changes of BIP upon addition of F^- and OH^-.

Figure S5: Partial ^{1}H NMR spectra of BIP in DMSO-d_6 upon the addition of F$^-$: (a) 0 equiv; (b) 0.5 equiv; (c) 2.0 equiv; (d) 5.0 equiv. Arrow marked the NH signal.
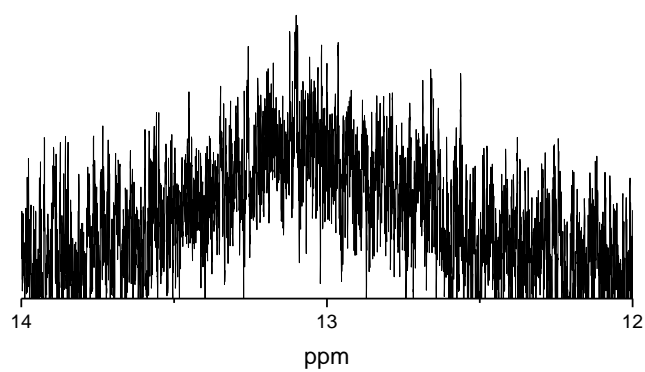
a

b

Figure S6: Partial ^{1}H NMR spectra of BIP in DMSO-d_6 upon the addition of F$^-$:
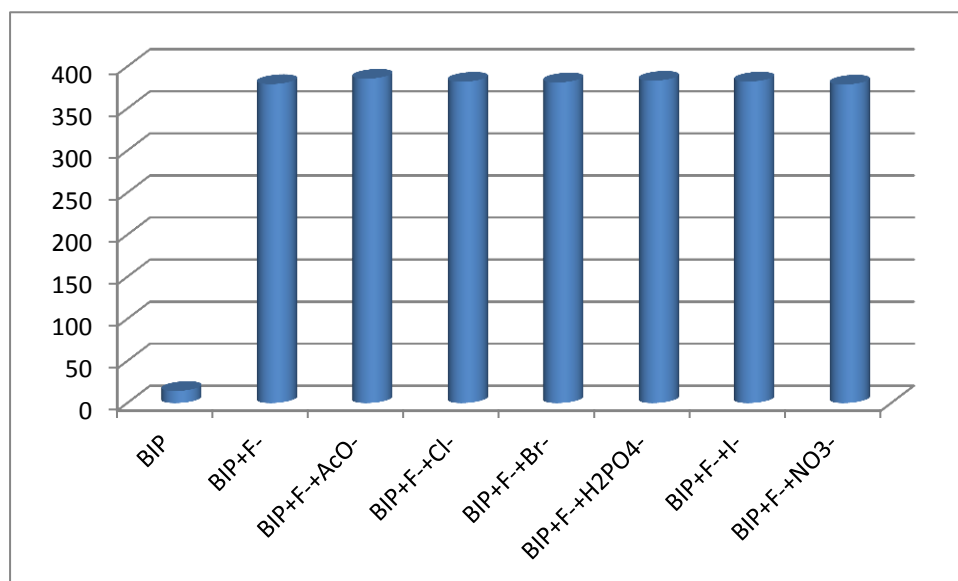(a) 0.5 equiv.; (b) 2.0 equiv.

Figure S7: Emission spectral changes of BIP (4.0 × 10^{-7} mol/l) containing 20.0 equiv fluoride upon the addition of 20.0 equiv other anions (Cl^{-}, Br^{-}, I^{-}, $H_2PO_4^{-}$, NO_3^{-} and AcO^{-}).