Synthesis and evaluation of a boronate-tagged 1,8-naphthalimide probe for fluoride recognition

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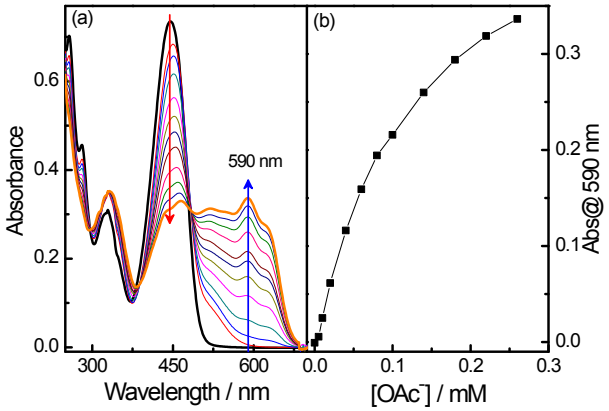
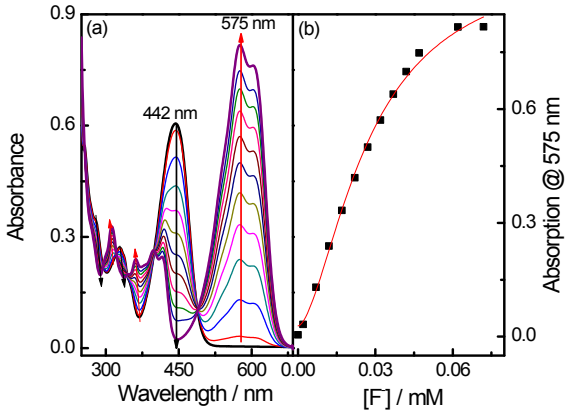
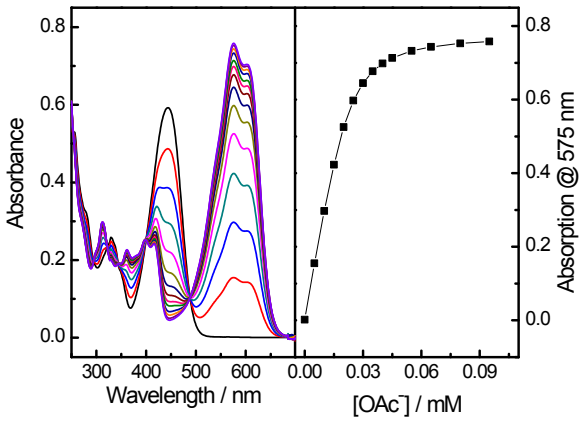


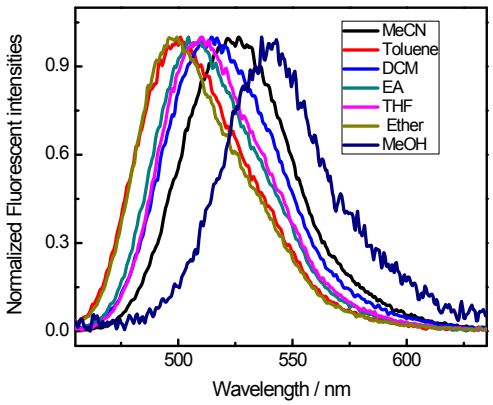
S 1 (a) Absorption spectra changes of probe **1** along with addition of TBAOAc in MeCN. [**1**] = 12 μM (b) absorption changes at 590 nm of probe **1** with different concentration of TBAOc



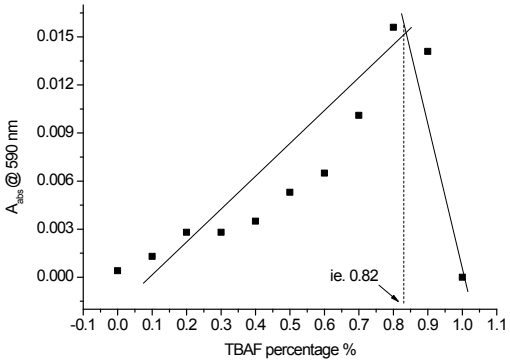
S 2 (a) Absorption spectral changes of probe **2** along with addition of TBAF in MeCN. [**2**] = 21.4 μM (b) absorption changes at 575 nm of probe **2** with different concentrations of TBAF



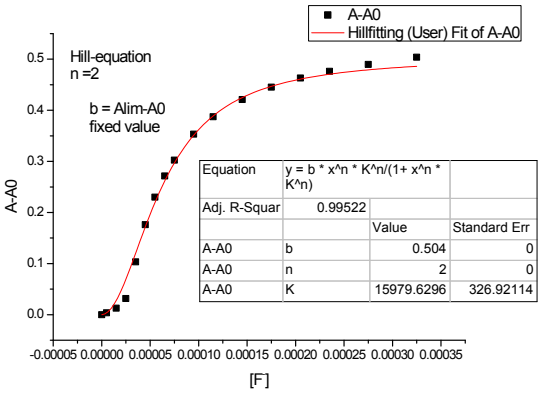
S 3 (a) Absorption spectral changes of probe **2** along with addition of TBAOAc in MeCN. [**2**] = 21.4 μM (b) absorption changes at 575 nm of probe **2** with different concentrations of TBAOc



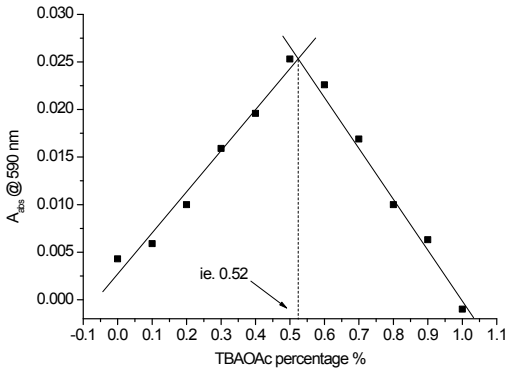
S 4 Normalized fluorescent spectra of probe **1** in different solvent. The polarity of solvent is shown in terms of dielectric constant: toluene 2.38, diethyl ether (Ether) 4.3, ethyl acetate (EA) 6.02, tetrahedrofuran (THF) 7.5, dichloromethane (DCM) 9.1, acetonitrile (MeCN) 37.5 and methanol (MeOH) 33. [**1**] = 2 μM



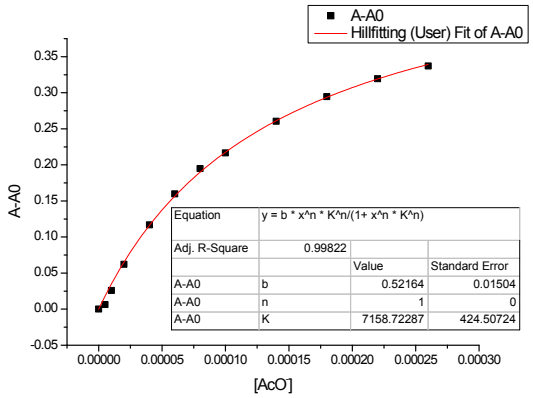
S 5 Job plot diagram for binding interaction between probe **1** and TBAF in MeCN.



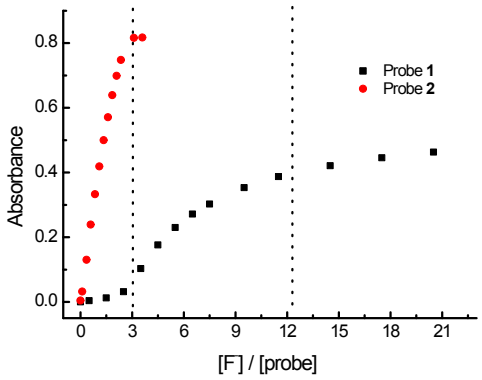
S 6 Non-linear fitting curve of probe **1** with TBAF by Hill equation



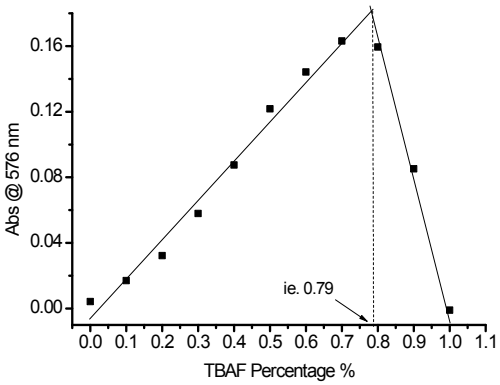
S 7 Job plot diagram for binding interaction between probe **1** and TBAOAc in MeCN..



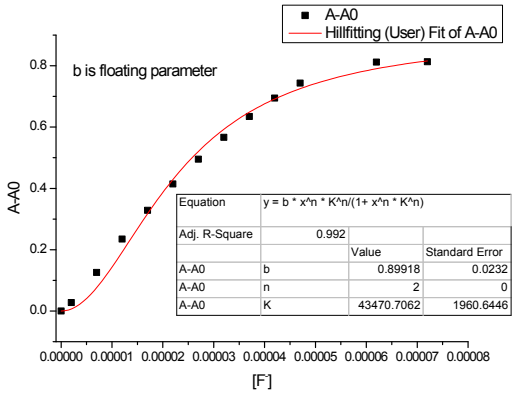
S 8 Non-linear fitting curve of probe **1** with TBAOAc by Hill equation



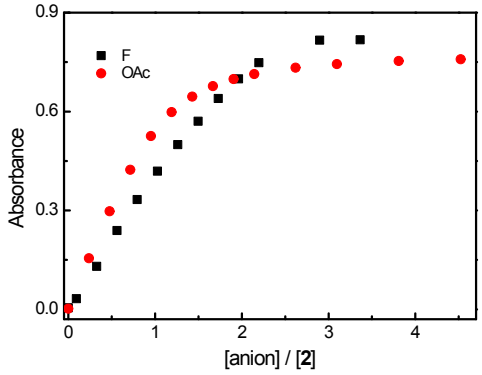
S 9 The ratio of the concentrations of TBAF to that of probe **1**, **2** *versus* the absorption



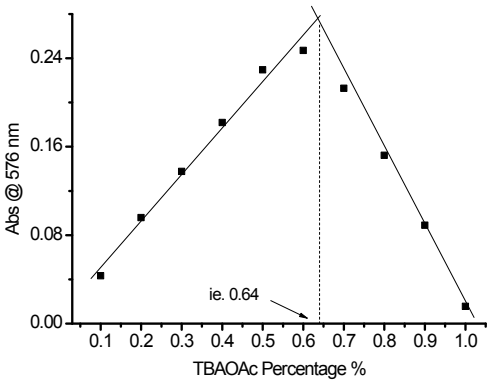
S 10 Job plot diagram for binding interaction between probe **2** and TBAF in MeCN.



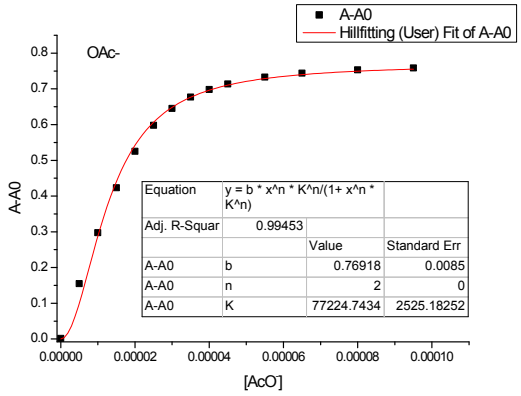
S 11 Non-linear fitting curve of probe **2** with TBAF by Hill equation



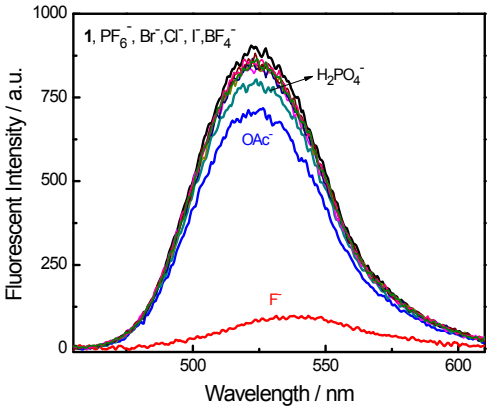
S 12 Absorptions of probe **2** with fluoride and acetate anions *versus* ratios of concentrations of anion to that of probe **2.**



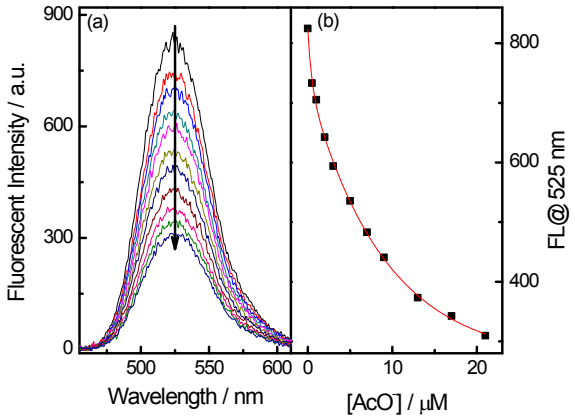
S 13 Job plot diagram for binding interaction between probe **2** and TBAOAc in MeCN



S 14 Non-linear fitting curve of probe **2** with TBAOAc by Hill equation



S 15 Fluorescent spectra changes after addition of 10 μM of different anions in MeCN. [**1**] = 3 uM



S 16 (a) Fluorescent spectra changes of probe **1** along with addition of TBAOAc in MeCN. [**1**] = 3×10^{-6} M, excited wavelength 450 nm; (b) emission changes at 525 nm of probe **1** with different concentration of TBAOAc

S 17 ^{1}H NMR titration of probe **2** with TBAF in DMSO-d_6. [**2**] = 10.7 mM

[TBAF] / [**2**] eq.	H^a ppm (circles)	H^b ppm (triangles)	H^c ppm (stars)
0	11.501	8.806	10.253
0.19		8.774	
0.37		8.749	
0.56		8.724	
1.00		8.687	
1.50		8.648	
2.40		8.575	
3.40		8.521	

S 18 ^{1}H NMR titration of probe **1** with TBAF in DMSO-d_6. [**1**] = 20 mM

[TBAF] / [**1**] eq.	H^a ppm (circles)		H^b ppm (triangles)	
	Original peak	New peak	Original peak	New peak
0	11.660		8.978	
0.25	11.657	11.543	8.978	9.063
0.50	11.659	11.545	8.973	9.060
0.75	11.664	11.550	8.973	9.060
1.00	11.664	11.553	8.972	9.061
1.50		11.558	8.966	9.060
2.00		11.556		9.055
3.00		11.555		9.046