Electronic supplementary information

Solvent-dependent and highly selective anion sensing and molecular logic application of bisindolylmaleimide derivatives

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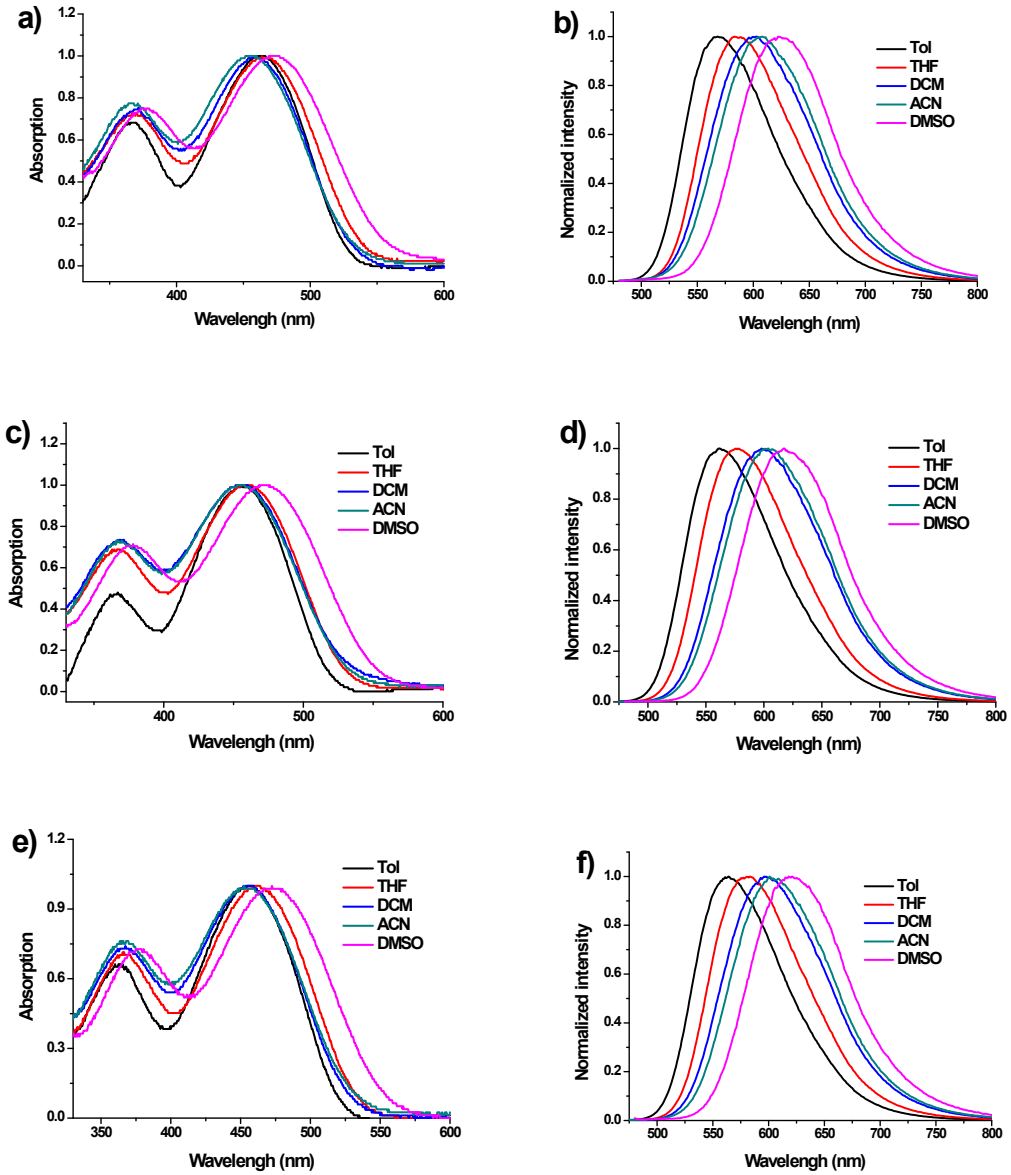

Fig. S1 Normalized absorption and emission spectra of IM-PFB (a, b), IM-TBA (c, d) and IM-MB (e, f) in various solvents.

Table S1 Physical data of sensors in THF.

Compound	λ_{abs} (nm)	λ_{em} (nm)	$\lambda_{0\text{-}0}$ (nm)	Φ_{em} (%)
IM-PFB	371, 459	602	528	30
IM-TBA	370, 456	599	531	34
IM-MB	367, 457	597	524	33
IMC-MB	320, 403	490	461	39

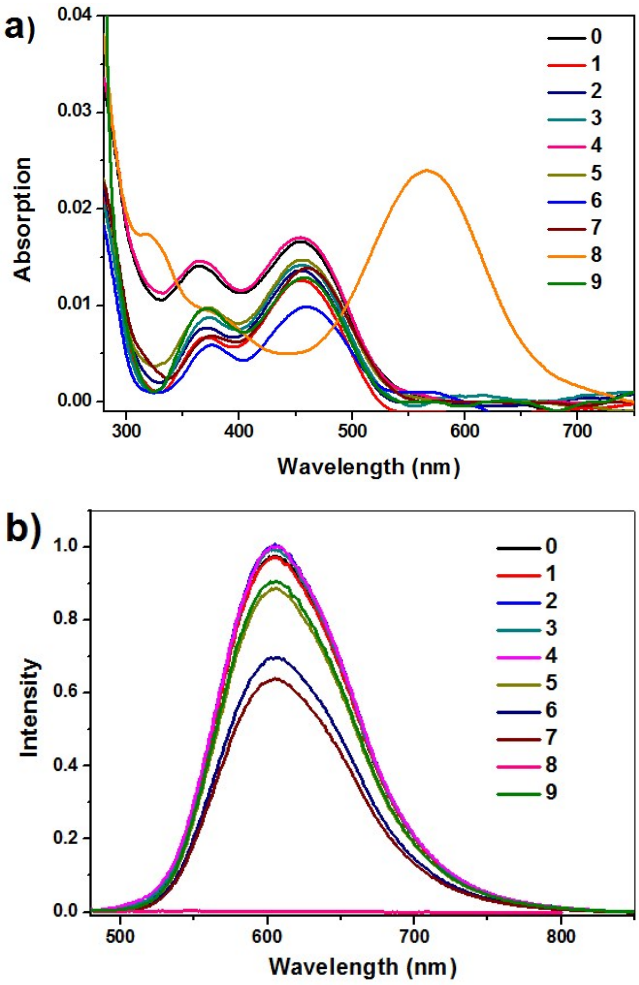

Fig. S2 Absorption (a) and emission (b) spectra of IM-TBA (50 μM in ACN) in the presence of anions (100 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

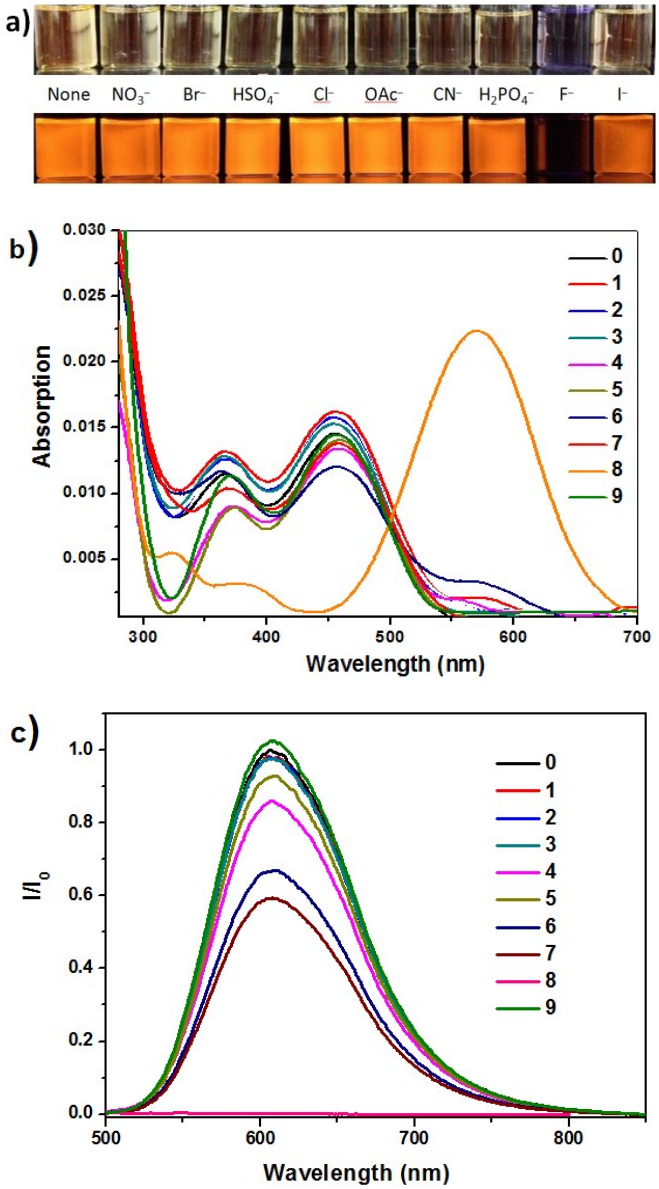

Fig. S3 a) Photograph of IM-PFB (50 μM in ACN) in the presence of various anions (100 eq) under daylight (top) and UV light (bottom). Absorption (b) and emission (c) spectra of IM-PFB (50 μM in ACN) in the presence of anions (100 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

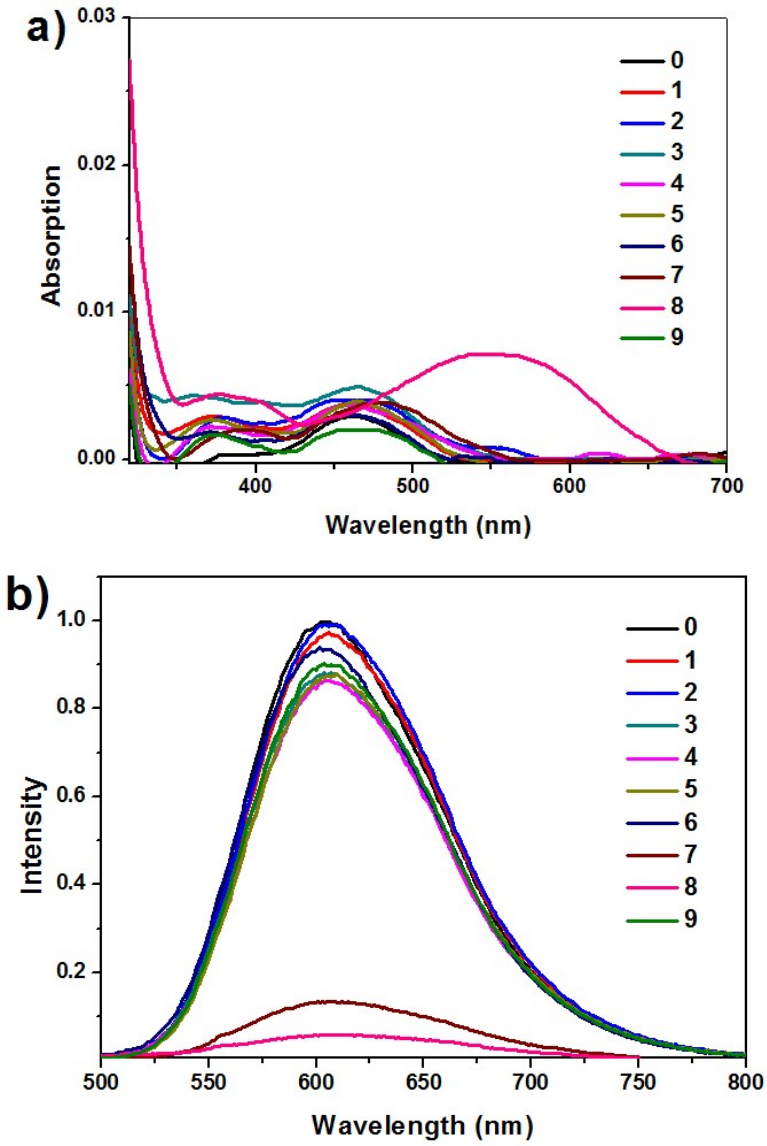

Fig. S4 Absorption (a) and emission (b) spectra of IM-PFB (50 μM in DCM) in the presence of anions (100 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

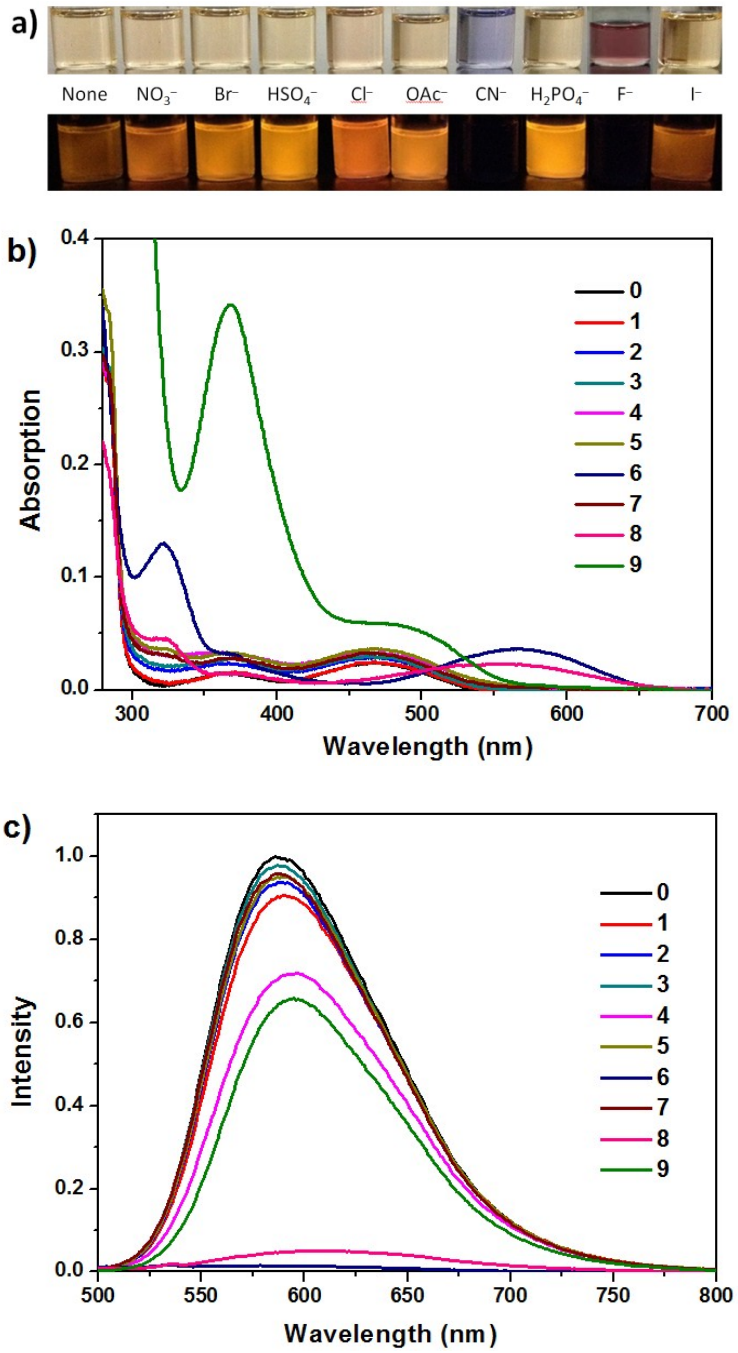

Fig. S5 a) Photograph of IM-PFB (50 μM in THF) in the presence of various anions (100 eq) under daylight (top) and UV light (bottom). Absorption (b) and emission (c) spectra of IM-PFB (50 μM in THF) in the presence of anions (100 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

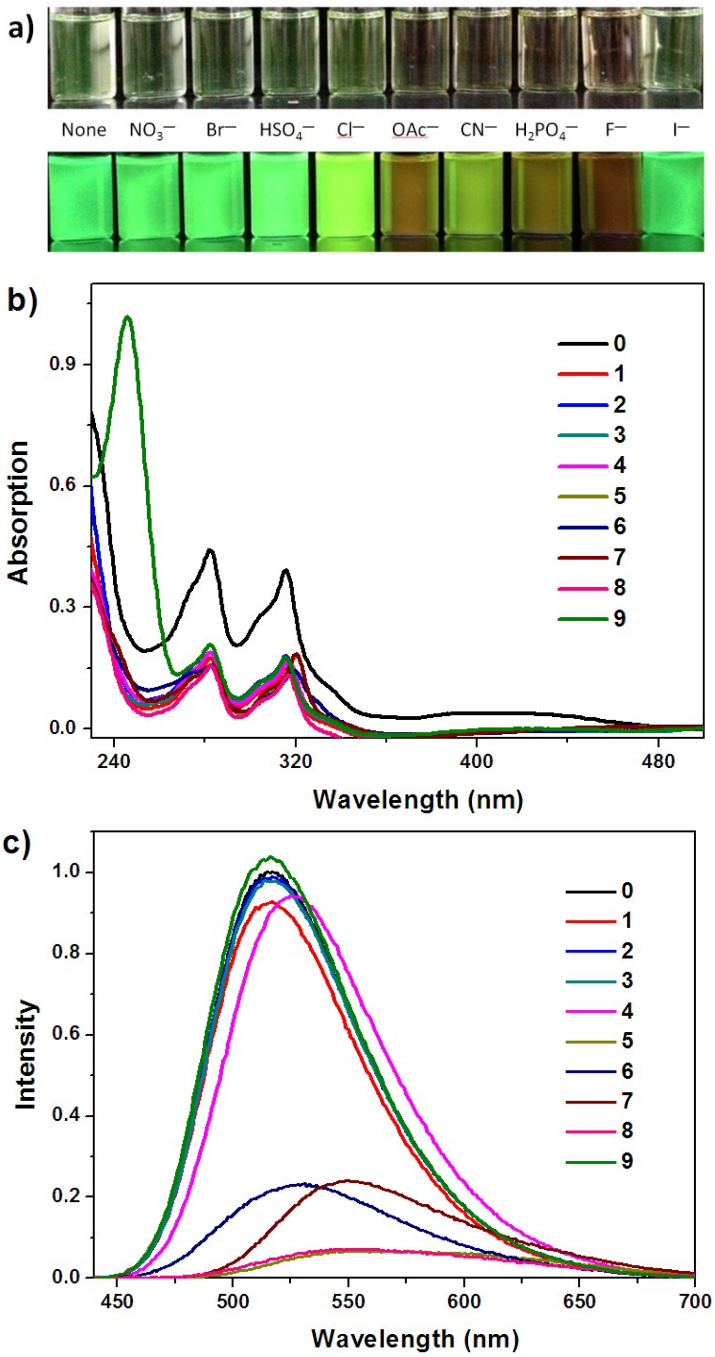

Fig. S6 a) Photograph of IMC-MB (50 μM in ACN) in the presence of various anions (20 eq) under daylight (top) and UV light (bottom). Absorption (b) and emission (c) spectra of IMC-MB (50 μM in ACN) in the presence of anions (20 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

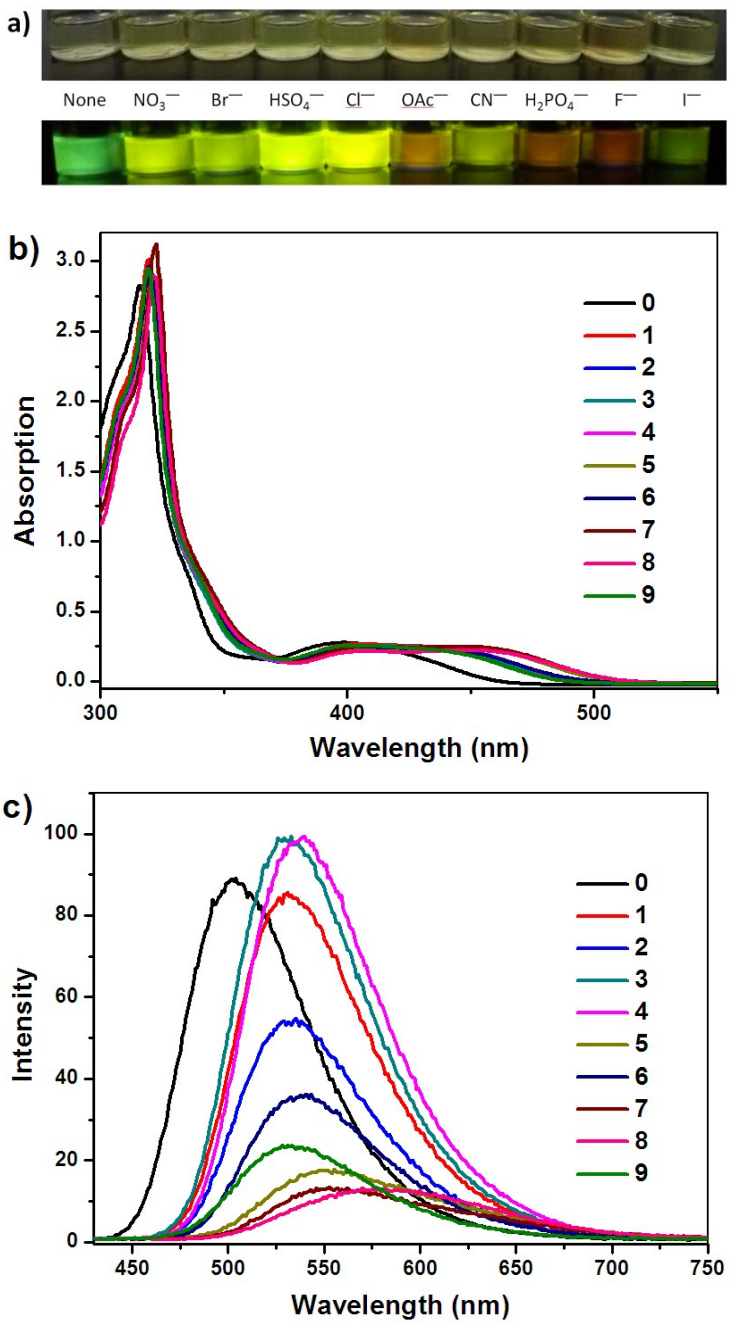

Fig. S7 a) Photograph of IMC-MB (50 μM in DCM) in the presence of various anions (20 eq) under daylight (top) and UV light (bottom). Absorption (b) and emission (c) spectra of IMC-MB (50 μM in DCM) in the presence of anions (20 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

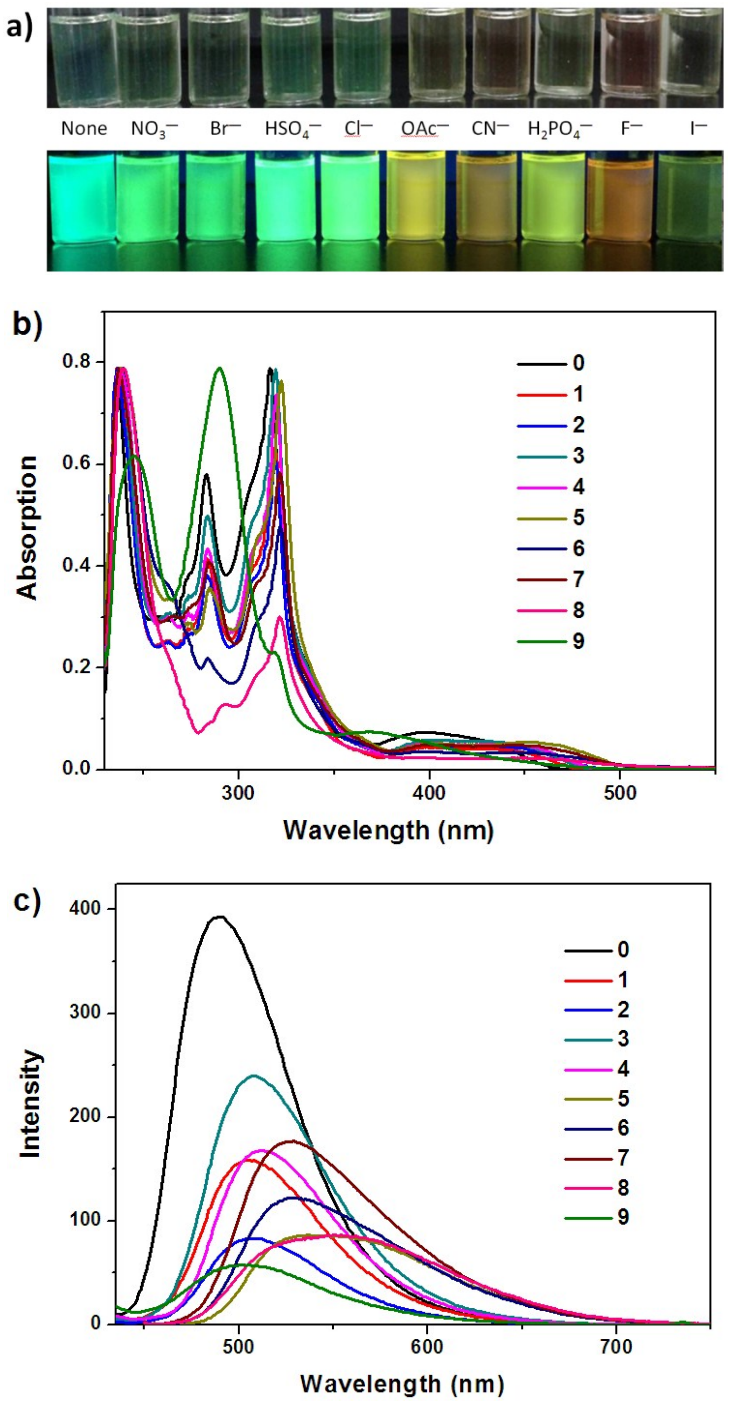

Fig. S8 a) Photograph of IMC-MB (50 μM in THF) in the presence of various anions (20 eq) under daylight (top) and UV light (bottom). Absorption (b) and emission (c) spectra of IMC-MB (50 μM in THF) in the presence of anions (20 eq). Anions arrangement: 0-none, 1-NO_3^-, 2-Br^-, 3-HSO_4^-, 4-Cl^-, 5-OAc^-, 6-CN^-, 7-$H_2PO_4^-$, 8-F^-, 9-I^-.

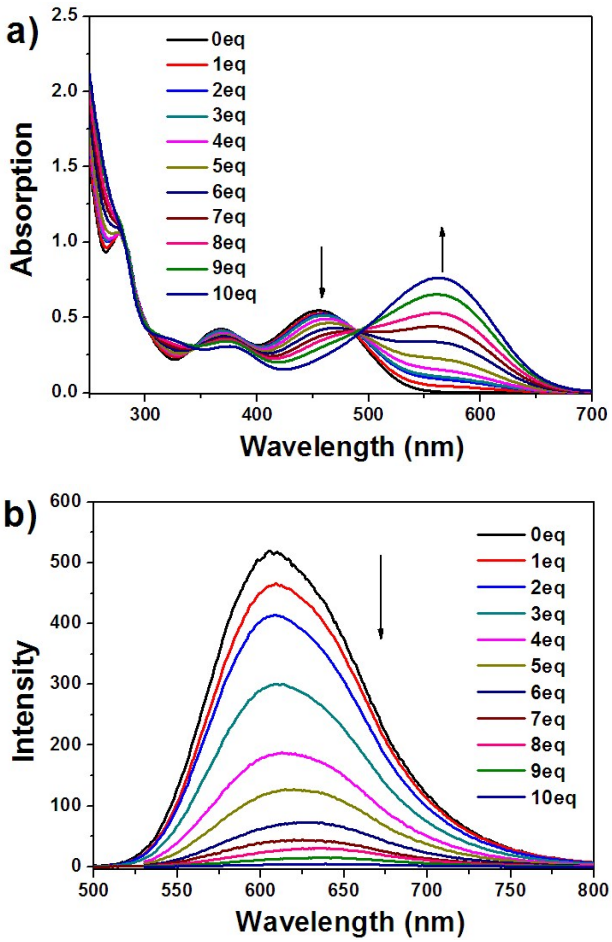

Fig. S9 Absorption (a) and emission (b) spectra of IM-MB (5 μM) in ACN upon titration of F^-.

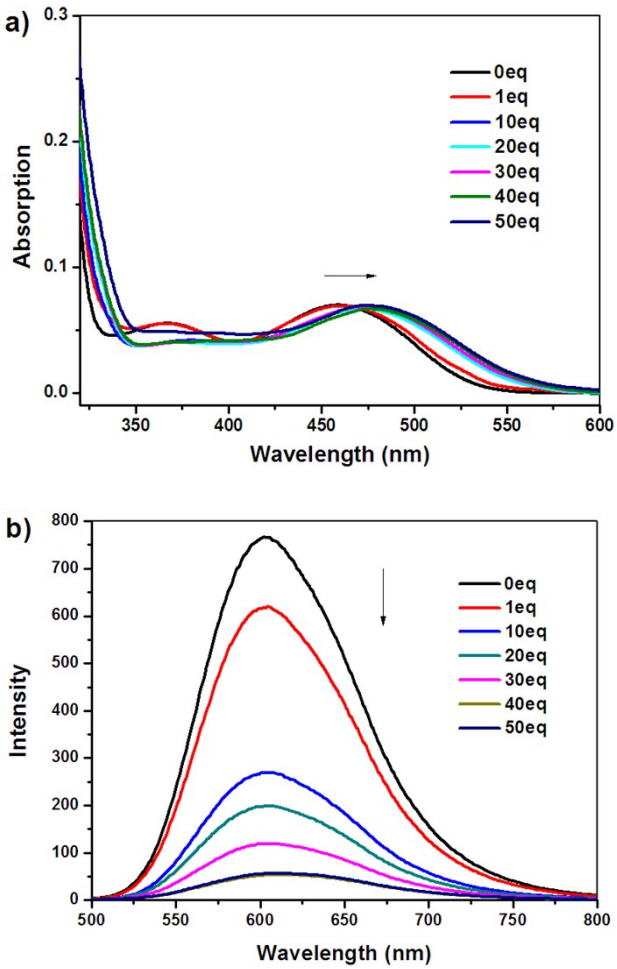

Fig. S10 Absorption (a) and emission (b) spectra of IM-PFB (5 μM) in DCM upon titration of $H_2PO_4^-$.

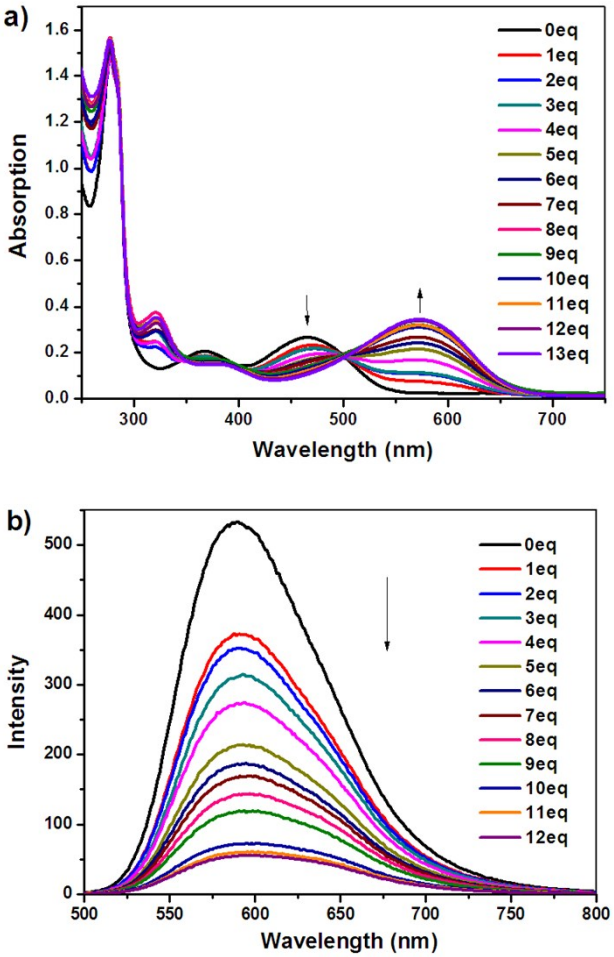

Fig. S11 Absorption (a) and emission (b) spectra of IM-PFB (5 μM) in THF upon titration of CN^-.

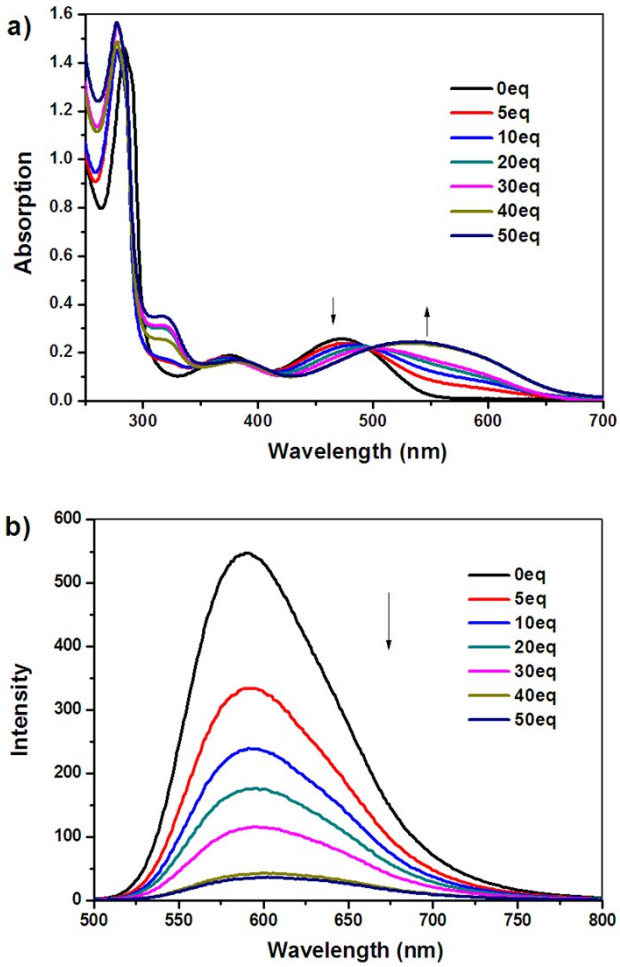

Fig. S12 Absorption (a) and emission (b) spectra of IM-PFB (5 μM) in THF upon titration of F^-.

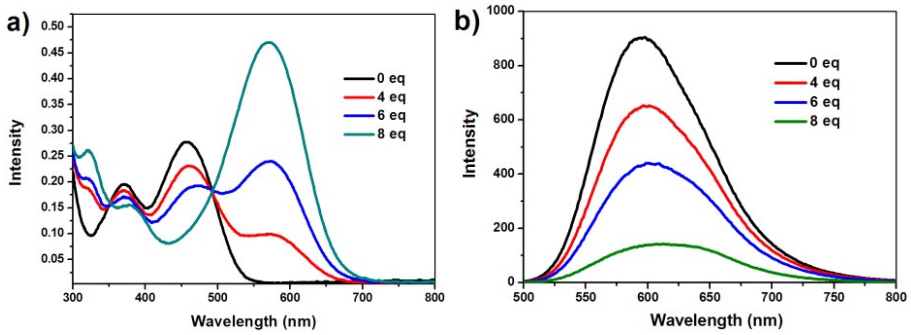

Fig. S13 Absorption (a) and fluorescence (b) spectra of IM-PFB (50 μM) in DCM upon the addition of different amounts of $N(Et)_4OH$.

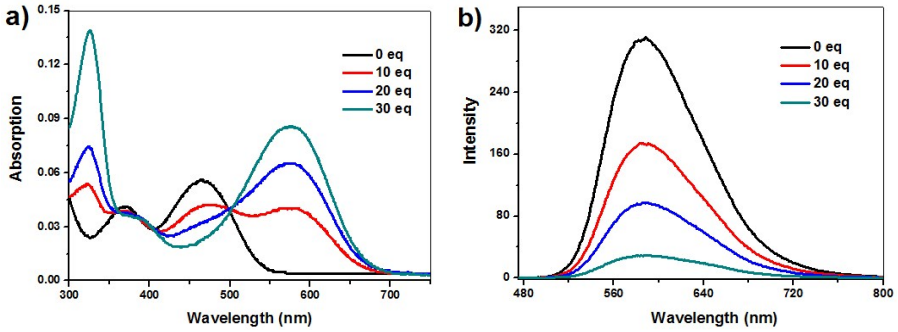

Fig. S14 Absorption (a) and fluorescence (b) spectra of IM-PFB (10 μM) in THF upon the addition of different amounts of $N(Et)_4OH$.

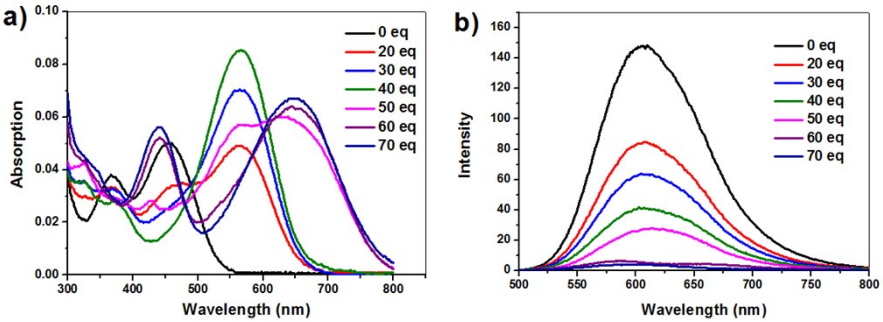

Fig. S15 Absorption (a) and fluorescence (b) spectra of IM-PFB (10 μM) in ACN upon the addition of different amounts of $N(Et)_4OH$.

Table S2 Calculated absorption parameters for IM-PFB, IM-PFB^{-} and IMPFB^{2-}.

		Main orbital transition[a] (CIC)	**λ (nm)[b]**	**f[c]**
IM-PFB	$S_0 \rightarrow S_1$	HOMO→LUMO (0.70)	499.5	0.1384
	$S_0 \rightarrow S_2$	HOMO-1→LUMO (0.69)	384.3	0.1096
	$S_0 \rightarrow S_3$	HOMO-3→LUMO (0.66)	374.3	0.0045
IM-PFB^{-}	$S_0 \rightarrow S_1$	HOMO→LUMO (0.67)	544.8	0.1899
	$S_0 \rightarrow S_2$	HOMO→LUMO+1 (0.68)	527.9	0.0435
	$S_0 \rightarrow S_3$	HOMO→LUMO+2 (0.71)	461.0	0.0062
IMPFB^{2-}	$S_0 \rightarrow S_1$	HOMO→LUMO (0.71)	1458.8	0.0066
	$S_0 \rightarrow S_2$	HOMO→LUMO+1 (0.71)	1085.7	0.0051
	$S_0 \rightarrow S_3$	HOMO→LUMO+2 (0.71)	775.8	0.1333

[a] CI expansion coefficients for the main orbital transitions. [b] Wavelength. [c] Oscillator strength.

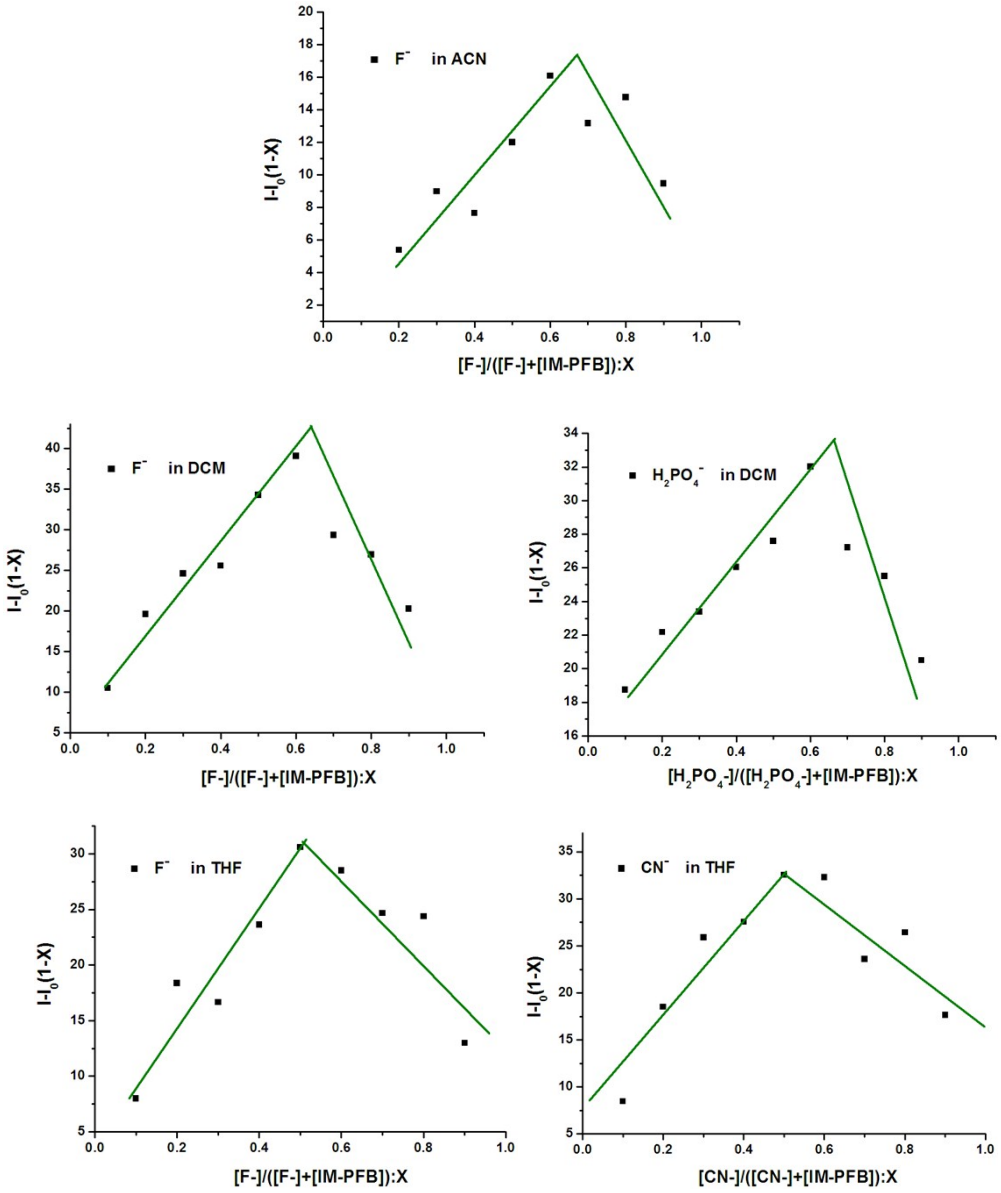

Fig. S16 Job's plot of IM-PFB showing the 1:2 binding stoichiometry in ACN and DCM, and the 1:1 binding stoichiometry in THF with anions. The total concentration of IM-PFB and anion is 20 μM. Emission intensity is recorded at 609 nm.

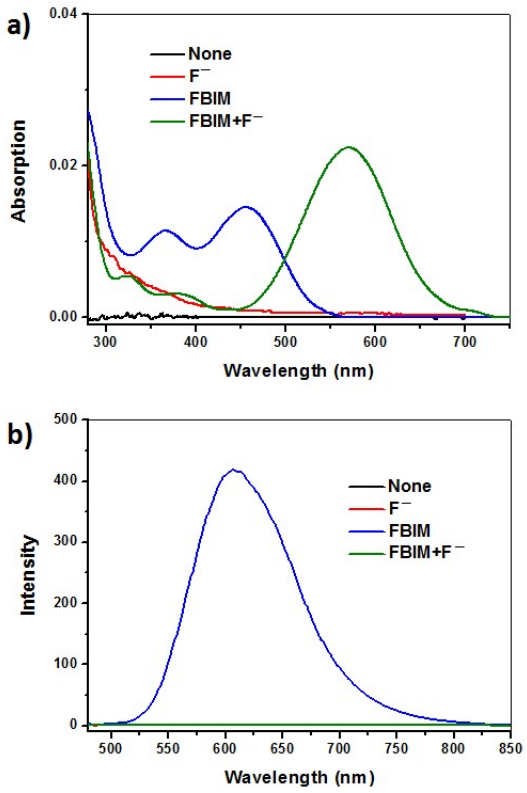

Fig. S17 Absorption (a) and emission (b) spectra of IM-PFB (50 μM) and F^- **(**50 eq**)** in ACN solvent.

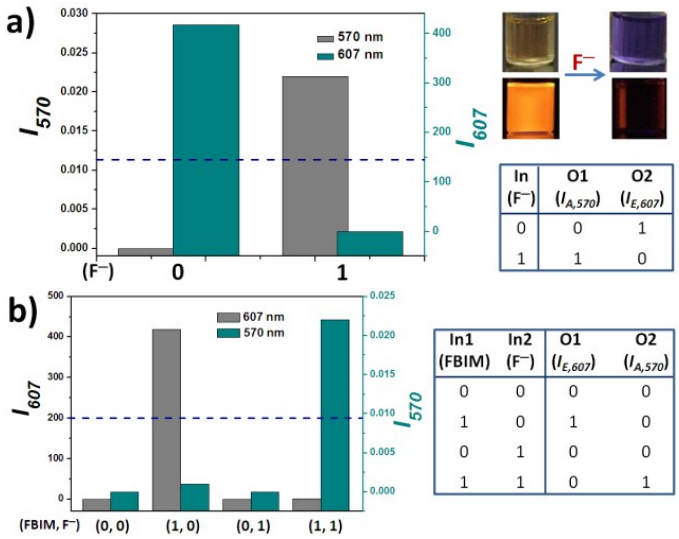

Fig. S18 1-to-2 decoder (a) and 1:2 demultiplexer (b) demonstrated by using the emission intensity at 607 nm ($I_{E,607}$) and the absorption intensity at 570 nm ($I_{A,570}$) in ACN as two outputs (O1 and O2).

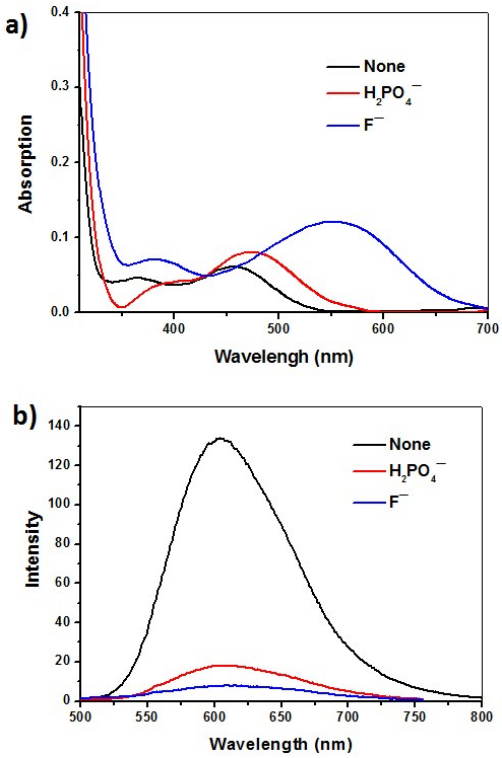

Fig. S19 Absorption (a) and emission (b) spectra of IM-PFB (50 μM) in the presence of F^- and $H_2PO_4^-$ **(**50 eq**)** in DCM solvent.

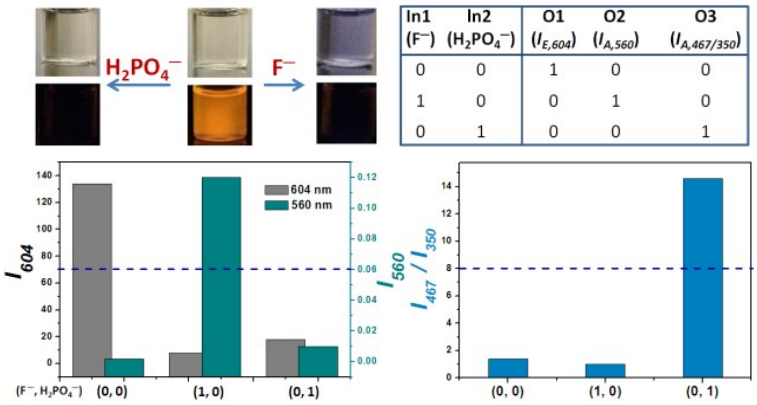

Fig. S20 2-to-3 decoder demonstrated by using F^- and $H_2PO_4^-$ as two inputs, the emission intensity at 604 nm ($I_{E,604}$), the absorption intensity at 560 nm ($I_{A,560}$) and the ratio of the absorption intensity at 467 nm and 350 nm ($I_{A,467/350}$) in DCM as three output.

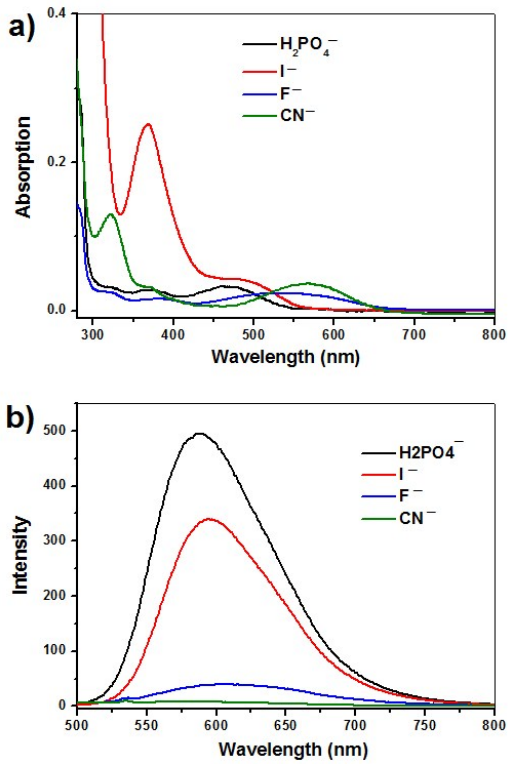

Fig. S21 Absorption (a) and emission (b) spectra of IM-PFB (50 μM) in the presence of F^-, I^-, CN^- and $H_2PO_4^-$ **(**50 eq**)** in THF solvent.