

Supplementary Information

Reaction-based dual signaling of fluoride ions by resorufin sulfonates

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Fig. S1.	Changes in absorbance ratio A_{587}/A_{433} of 1 in the presence of various anions.	S3
Fig. S2.	Fluorescence intensity ratio I/I_0 at 591 nm of 1 in the presence of various anions.	S3
Fig. S3.	UV-vis spectra of 1 , 1 + tetrabutylammonium fluoride, resorufin + tetrabutylammonium fluoride.	S4
Fig. S4.	Fluorescence spectra of 1 , 1 + tetrabutylammonium fluoride, resorufin + tetrabutylammonium fluoride.	S4
Fig. S5.	Time trace for the changes in UV-vis absorbance of 1 at 587 nm in the presence of fluoride ions.	S5
Fig. S6.	UV-vis spectral changes of 1 upon titration with fluoride ions.	S5
Fig. S7.	Competitive signaling of fluoride ions by 1 in the presence of common anions as background.	S6
Fig. S8.	UV-vis spectral changes of 1-F⁻ in the presence of common anions as background.	S6
Fig. S9.	Time trace for the changes in UV-vis absorbance of 2 at 587 nm in the presence of fluoride ions.	S7
Fig. S10.	Concentration dependent fluorescence signaling behavior of 2 for fluoride ions.	S7
Fig. S11.	Changes in UV-vis spectra of 2 in the presence of various anions.	S8
Fig. S12.	Changes in absorption intensity ratio A_{587}/A_{433} of 2 in the presence of various anions.	S8
Fig. S13.	Time trace for the changes in UV-vis absorbance of 3 at 587 nm in the presence of fluoride ions.	S9
Fig. S14.	Concentration dependent fluorescence signaling behavior of 3 for fluoride ions.....	S9
Fig. S15.	Changes in fluorescence intensity ratio (I/I_0) at 591 nm of 1 , 2 and 3 in the presence of fluoride and sulfide ions.	S10

Fig. S16.	Changes in fluorescence intensity ratio (I/I_0) at 591 nm of 1 and 1 + fluoride as a function of water content in CH ₃ CN.	S10
Fig. S17.	Fluorescence intensity ratio I/I_0 at 591 nm of 1 in the presence of various anions.	S11
Fig. S18.	¹ H NMR spectrum of 1 in DMSO-d ₆	S11
Fig. S19.	¹³ C NMR spectrum of 1 in DMSO-d ₆	S12
Fig. S20.	¹ H NMR spectrum of 3 in DMSO-d ₆	S12
Fig. S21.	¹³ C NMR spectrum of 3 in DMSO-d ₆	S13

Fig. S1. Changes in absorbance ratio A_{587}/A_{433} of **1** in the presence of various anions. [**1**] = 1.0×10^{-5} M, $[A^{n-}]$ in TBA salt = 1.0×10^{-4} M in CH_3CN .

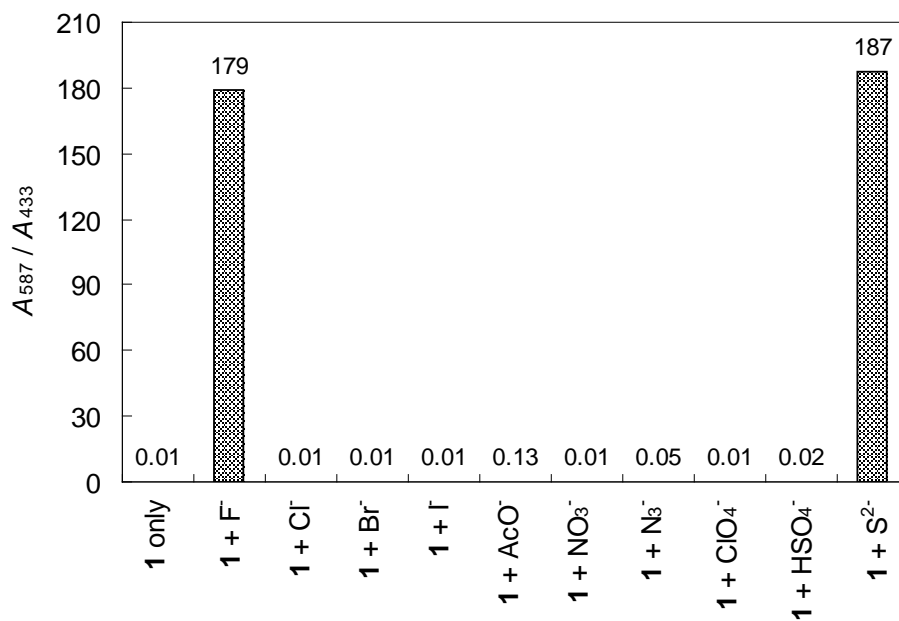


Fig. S2. Fluorescence intensity ratio I/I_0 at 591 nm of **1** in the presence of various anions. [**1**] = 5.0×10^{-6} M, $[A^{n-}]$ in TBA salt = 5.0×10^{-5} M in CH_3CN . $\lambda_{\text{ex}} = 485$ nm.

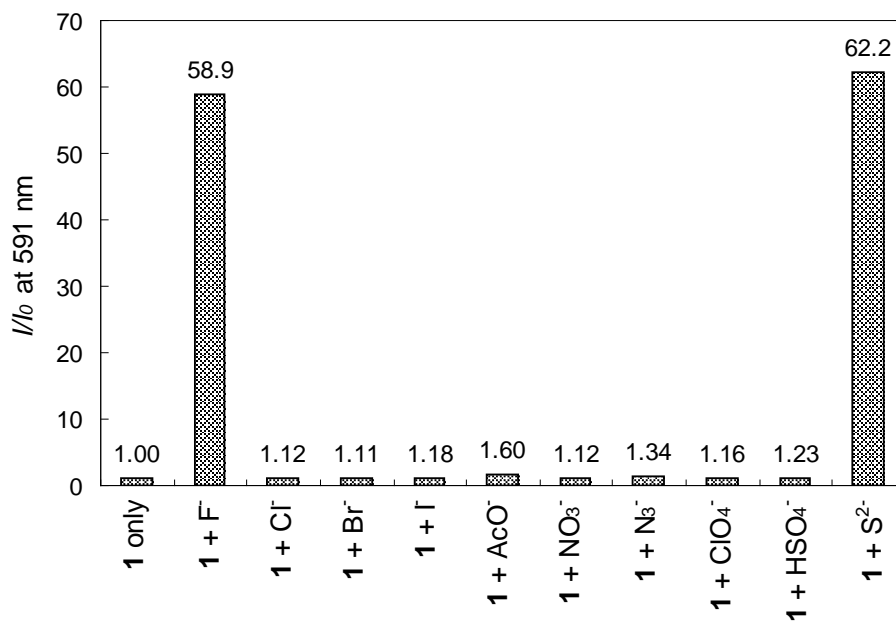


Fig. S3. UV-vis spectra of **1**, **1** + tetrabutylammonium fluoride, resorufin + tetrabutylammonium fluoride. [**1**] = [Resorufin] = 1.0×10^{-5} M, [TBA⁺F⁻] = 1.0×10^{-4} M in CH₃CN.

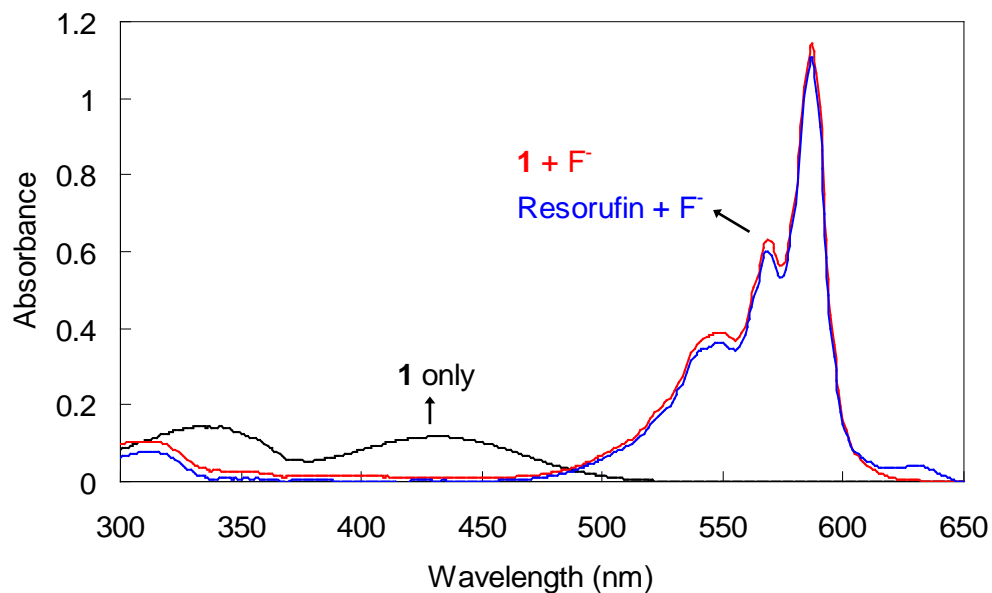


Fig. S4. Fluorescence spectra of **1**, **1** + tetrabutylammonium fluoride, resorufin + tetrabutylammonium fluoride. [**1**] = [Resorufin] = 5.0×10^{-6} M, [TBA⁺F⁻] = 5.0×10^{-5} M in CH₃CN. λ_{ex} = 485 nm.

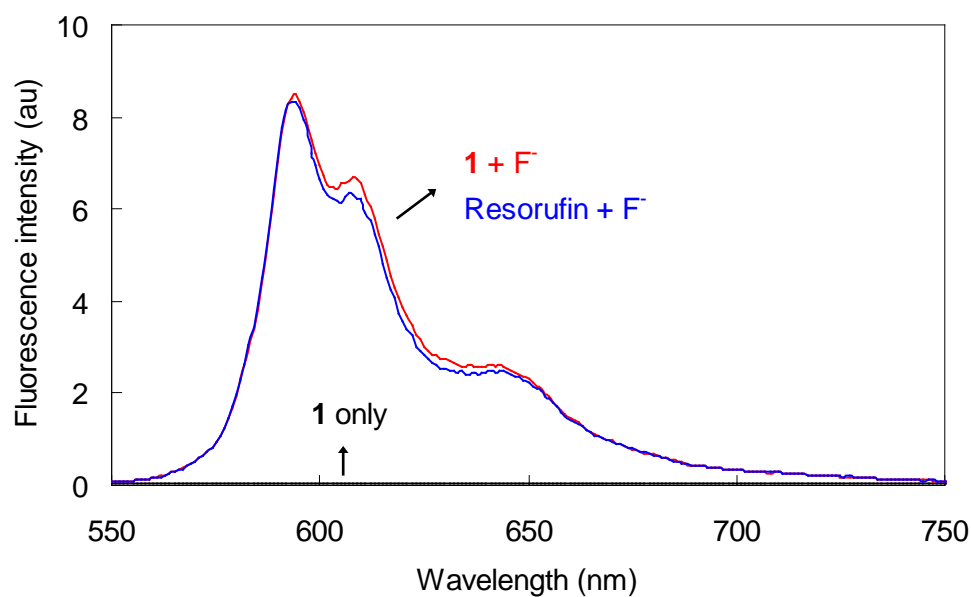


Fig. S5. Time trace for the changes in UV-vis absorbance of **1** at 587 nm in the presence of fluoride ions. $[1] = 1.0 \times 10^{-5}$ M, $[TBA^+F^-] = 1.0 \times 10^{-4}$ M in CH_3CN .

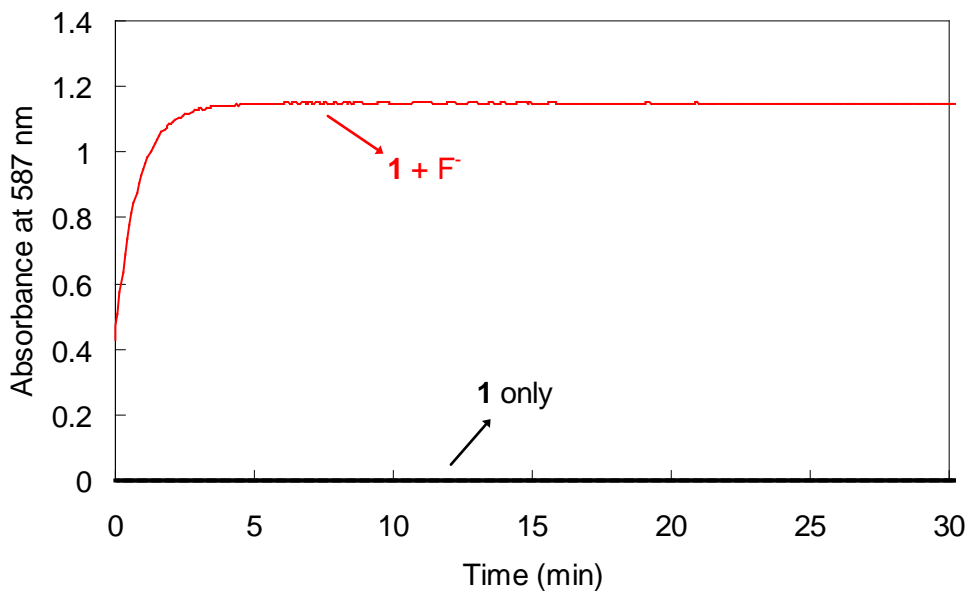


Fig. S6. UV-vis spectral changes of **1** upon titration with fluoride ions. $[1] = 1.0 \times 10^{-5}$ M, $[TBA^+F^-] =$ from 0 to 5.5×10^{-5} M in CH_3CN .

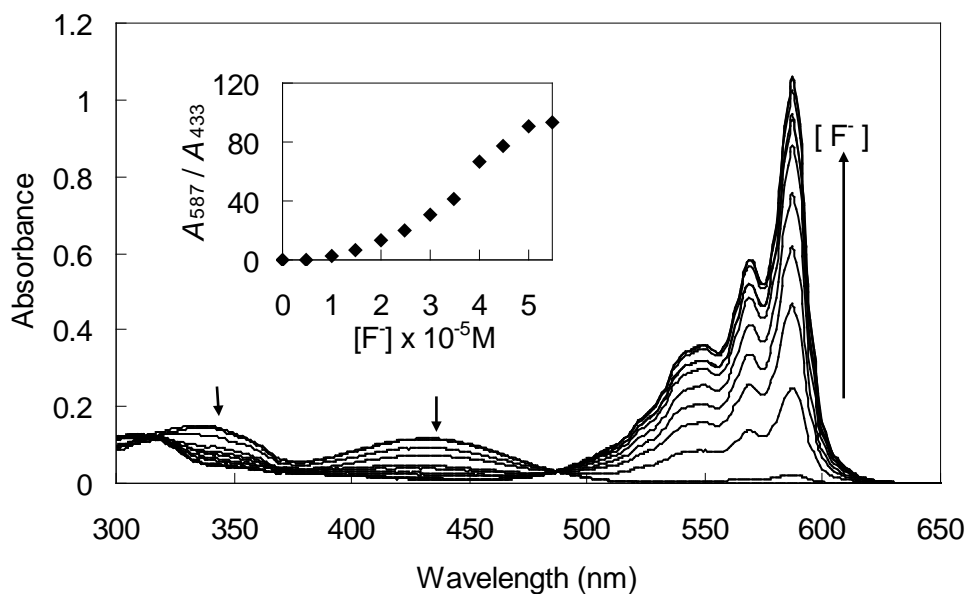


Fig. S7. Competitive signaling of fluoride ions by **1** in the presence of common anions as background. $[1] = 5.0 \times 10^{-6}$ M, $[F^-] = [A^-]$ in TBA salt = 5.0×10^{-5} M in CH_3CN . $\lambda_{ex} = 485$ nm. Other anions = Cl^- , Br^- , I^- , AcO^- , NO_3^- , N_3^- , ClO_4^- , and HSO_4^- .

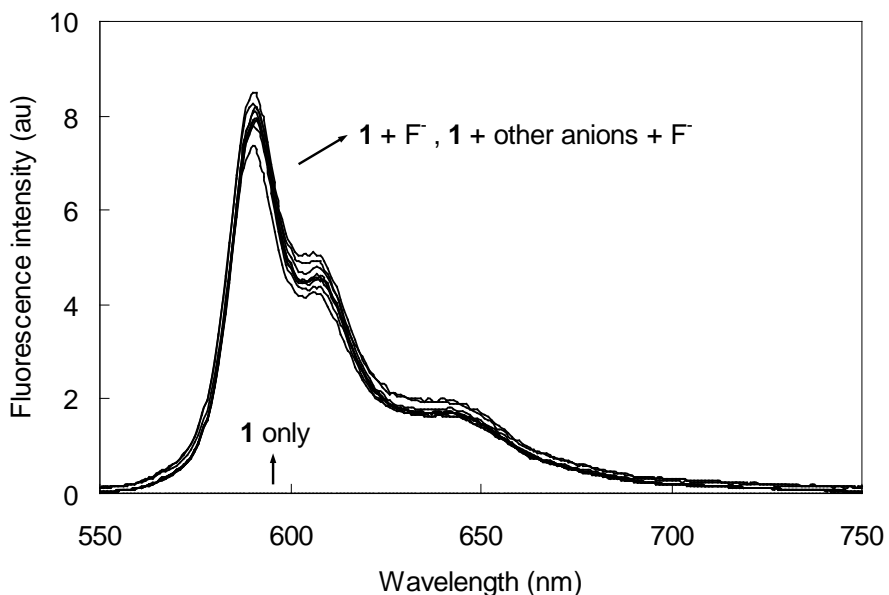


Fig. S8. UV-vis spectral changes of **1-F⁻** in the presence of common anions as background. $[1] = 1.0 \times 10^{-5}$ M, $[F^-] = [A^-]$ in TBA salt = 1.0×10^{-4} M in CH_3CN . Other anions = Cl^- , Br^- , I^- , AcO^- , NO_3^- , N_3^- , ClO_4^- , and HSO_4^- .

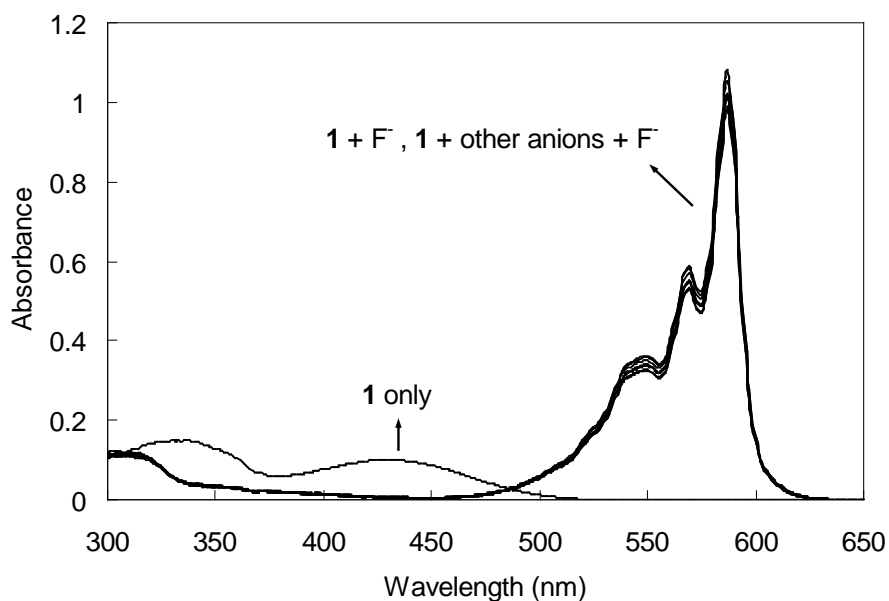


Fig. S9. Time trace for the changes in UV-vis absorbance of **2** at 587 nm in the presence of fluoride ions. $[2] = 1.0 \times 10^{-5}$ M, $[TBA^+F^-] = 1.0 \times 10^{-4}$ M in CH_3CN .

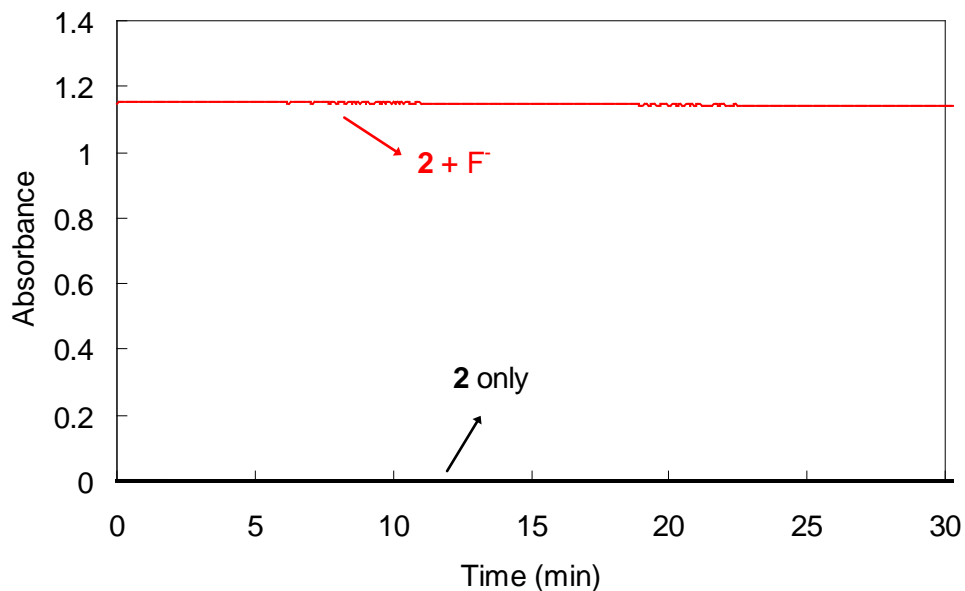


Fig. S10. Concentration-dependent fluorescence signaling behavior of **2** for fluoride ions. $[2] = 5.0 \times 10^{-6}$ M, $[TBA^+F^-] = 0 \sim 1.2 \times 10^{-5}$ M in CH_3CN . $\lambda_{ex} = 485$ nm.

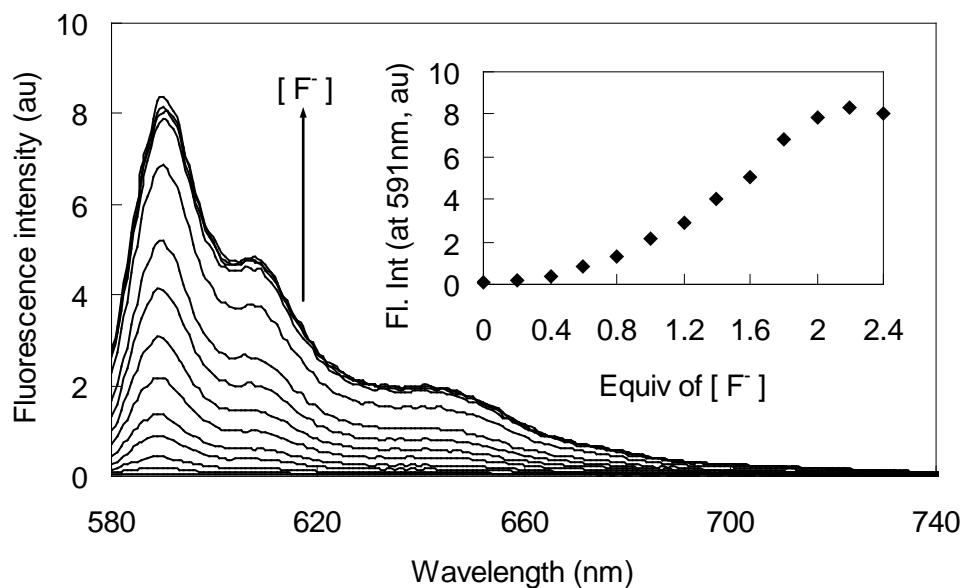


Fig. S11. Changes in UV-vis spectra of **2** in the presence of various anions. $[2] = 1.0 \times 10^{-5}$ M, $[A^-]$ in TBA salt = 1.0×10^{-4} M in CH_3CN .

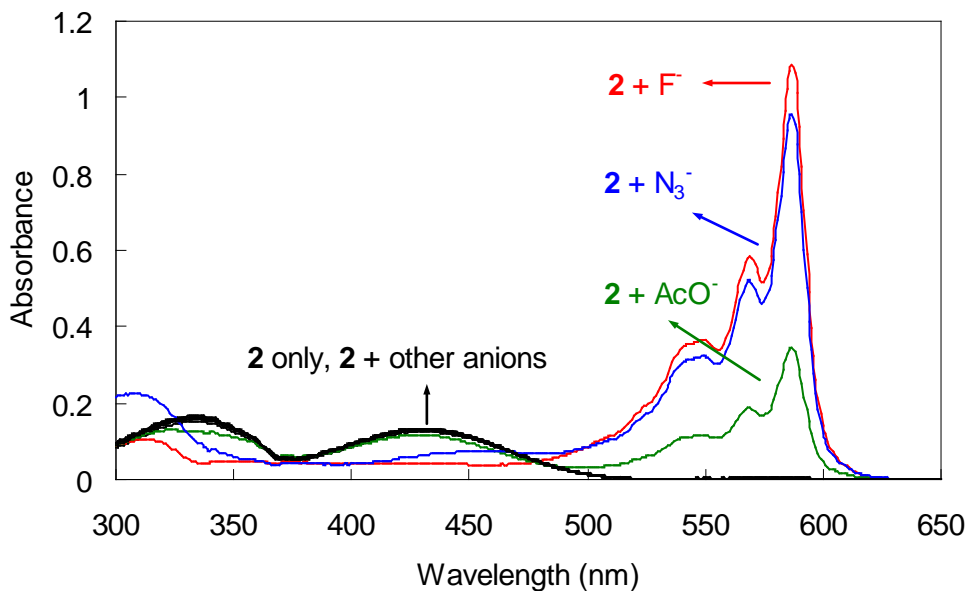


Fig. S12. Changes in absorption intensity ratio A_{587}/A_{433} of **2** in the presence of various anions. $[2] = 1.0 \times 10^{-5}$ M, $[A^-]$ in TBA salt = 1.0×10^{-4} M in CH_3CN .

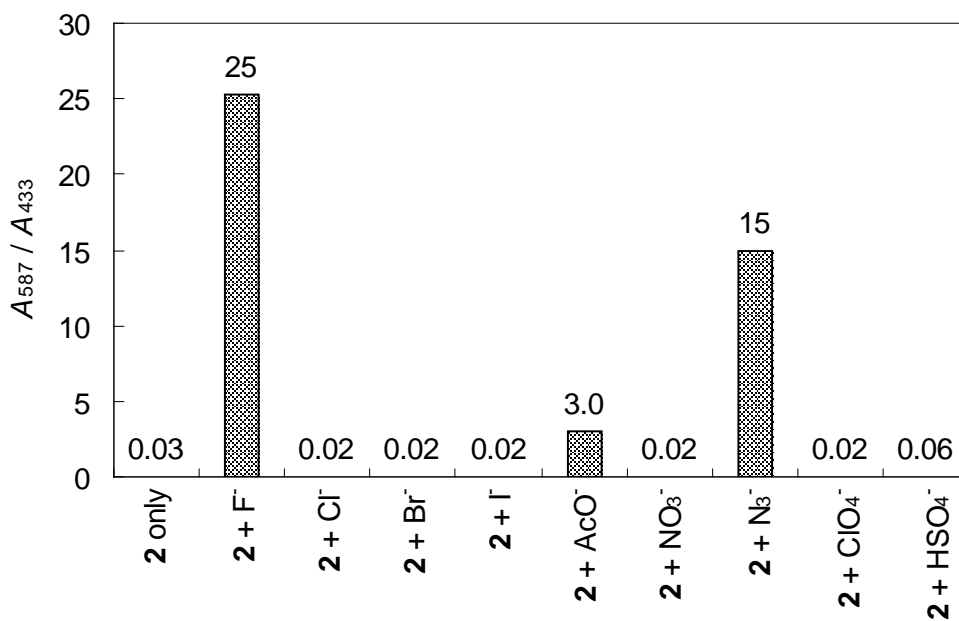


Fig. S13. Time trace for the changes in UV-vis absorbance of **3** at 587 nm in the presence of fluoride ions. $[3] = 1.0 \times 10^{-5}$ M, $[TBA^+F^-] = 1.0 \times 10^{-4}$ M in CH_3CN .

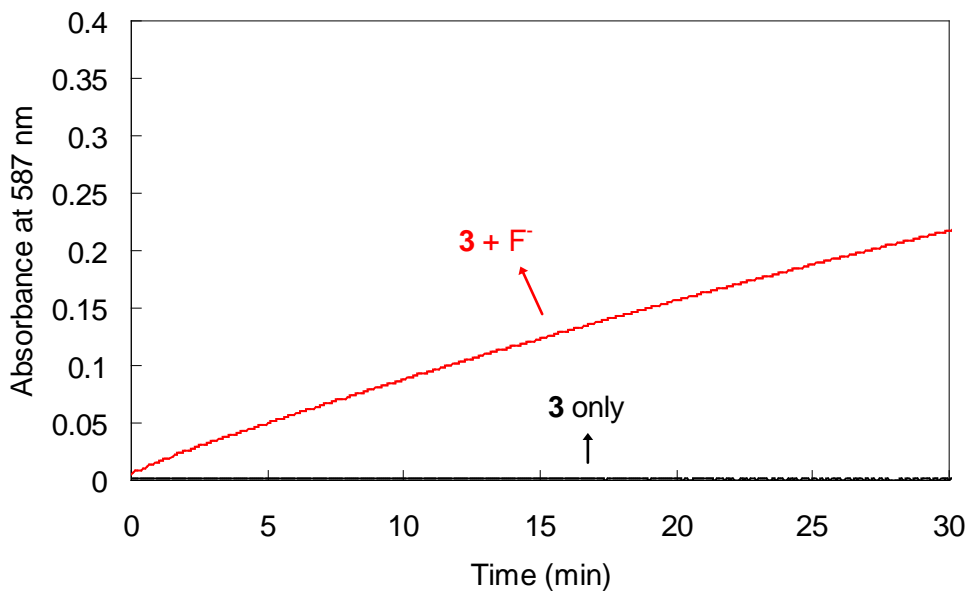


Fig. S14. Concentration dependent fluorescence signaling behavior of **3** for fluoride ions. $[3] = 5.0 \times 10^{-6}$ M, $[TBA^+F^-] = 0 \sim 7.0 \times 10^{-4}$ M in CH_3CN . $\lambda_{ex} = 485$ nm.

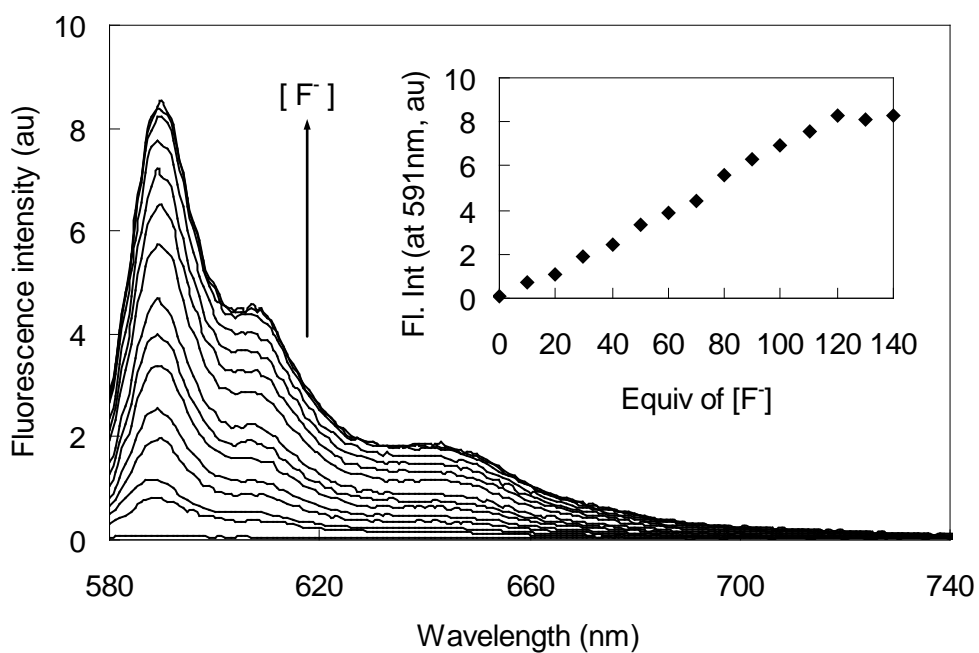


Fig. S15. Changes in fluorescence intensity ratio (I/I_0) at 591 nm of **1**, **2**, and **3** in the presence of fluoride and sulfide ions. [**1**] = [**2**] = [**3**] = 5.0×10^{-6} M, $[\text{TBA}^+\text{F}^-] = [(\text{TBA}^+)_2\text{S}^{2-}] = 5.0 \times 10^{-5}$ M in CH_3CN . $\lambda_{\text{ex}} = 485$ nm.

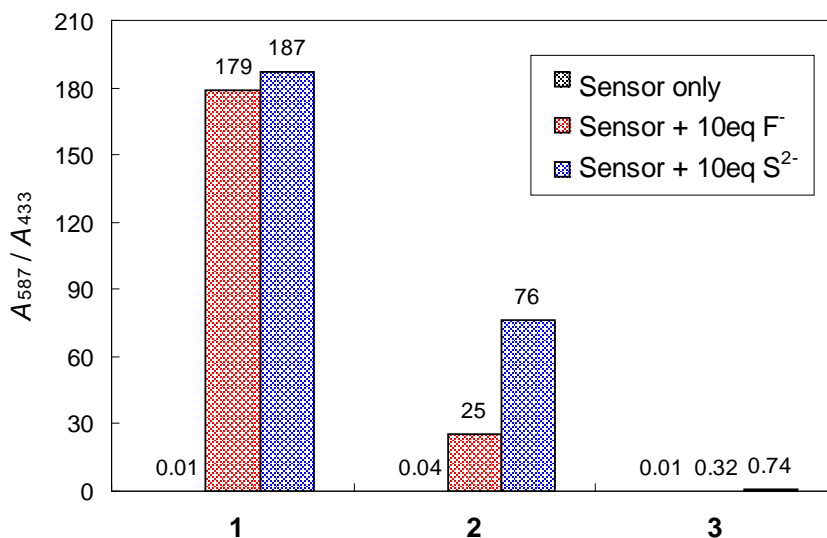


Fig. S16. Changes in fluorescence intensity ratio (I/I_0) at 591 nm of **1** and **1** + fluoride as a function of water content in CH_3CN . [**1**] = 5.0×10^{-6} M, $[\text{TBA}^+\text{F}^-] = 5.0 \times 10^{-5}$ M in aqueous acetonitrile (water content: from 0 to 5%). $\lambda_{\text{ex}} = 485$ nm.

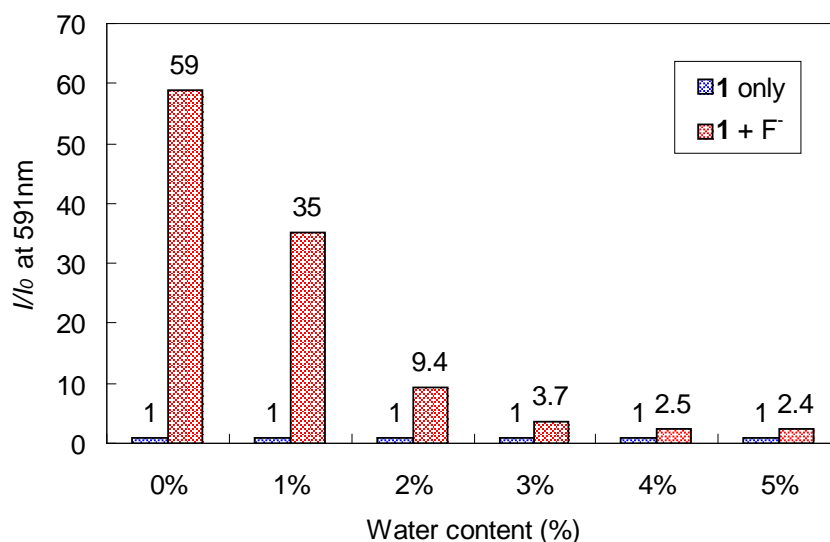


Fig. S17. Fluorescence intensity ratio I/I_0 at 591 nm of **1** in the presence of various anions. $[1] = 1.0 \times 10^{-5}$ M, $[A^-]$ in TBA salt = 1.0×10^{-4} M in 1% aqueous acetonitrile solution. $\lambda_{ex} = 485$ nm.

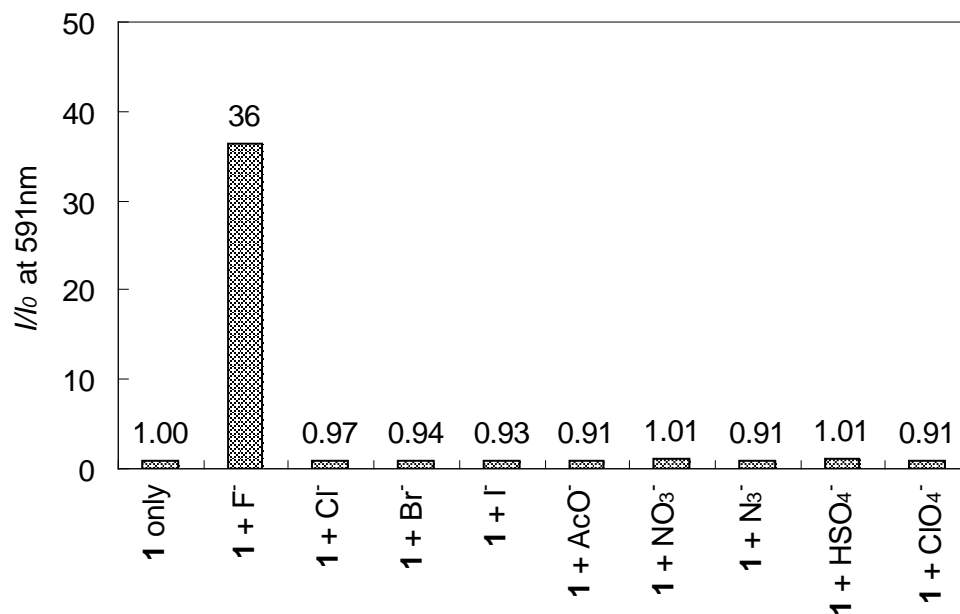


Fig. S18. ¹H NMR spectrum of **1** in DMSO-d₆.

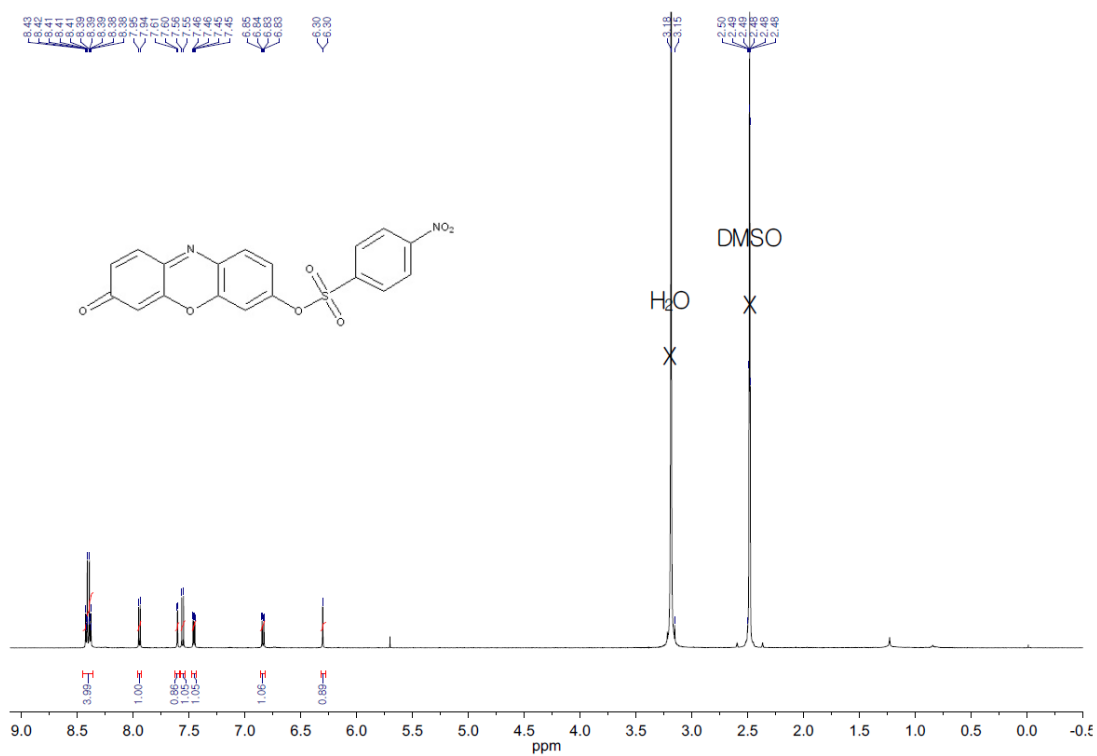


Fig. S19. ^{13}C NMR spectrum of **1** in DMSO-d_6 .

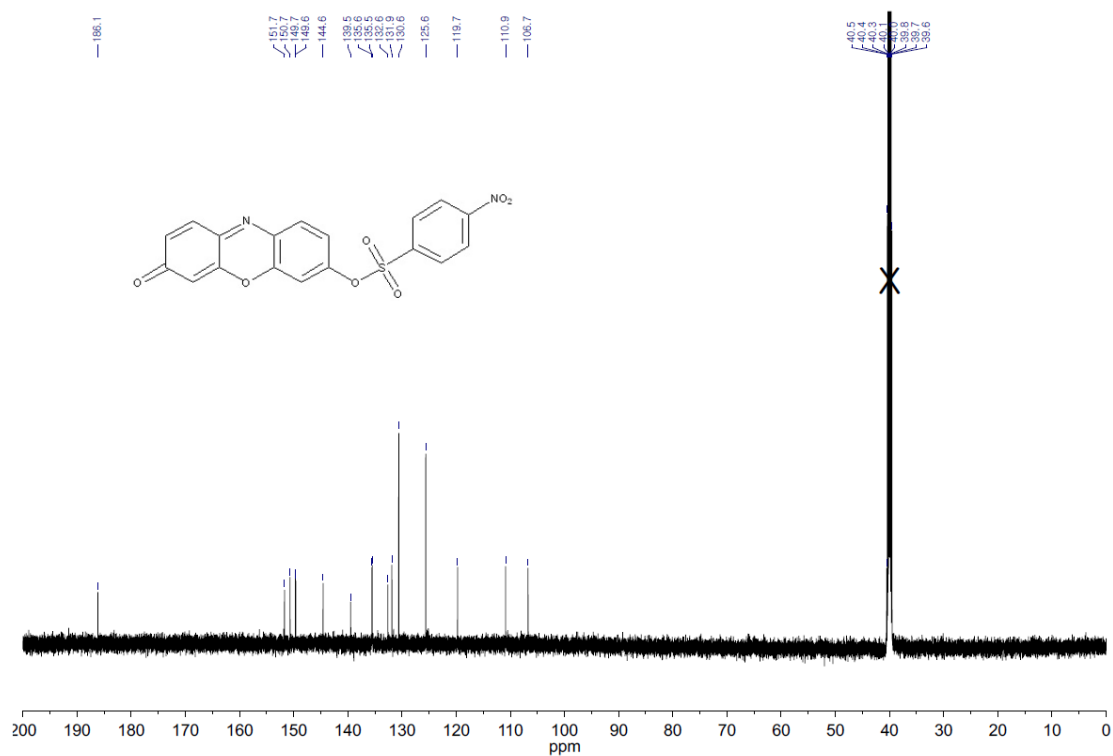


Fig. S20. ^1H NMR spectrum of **3** in DMSO-d_6 .

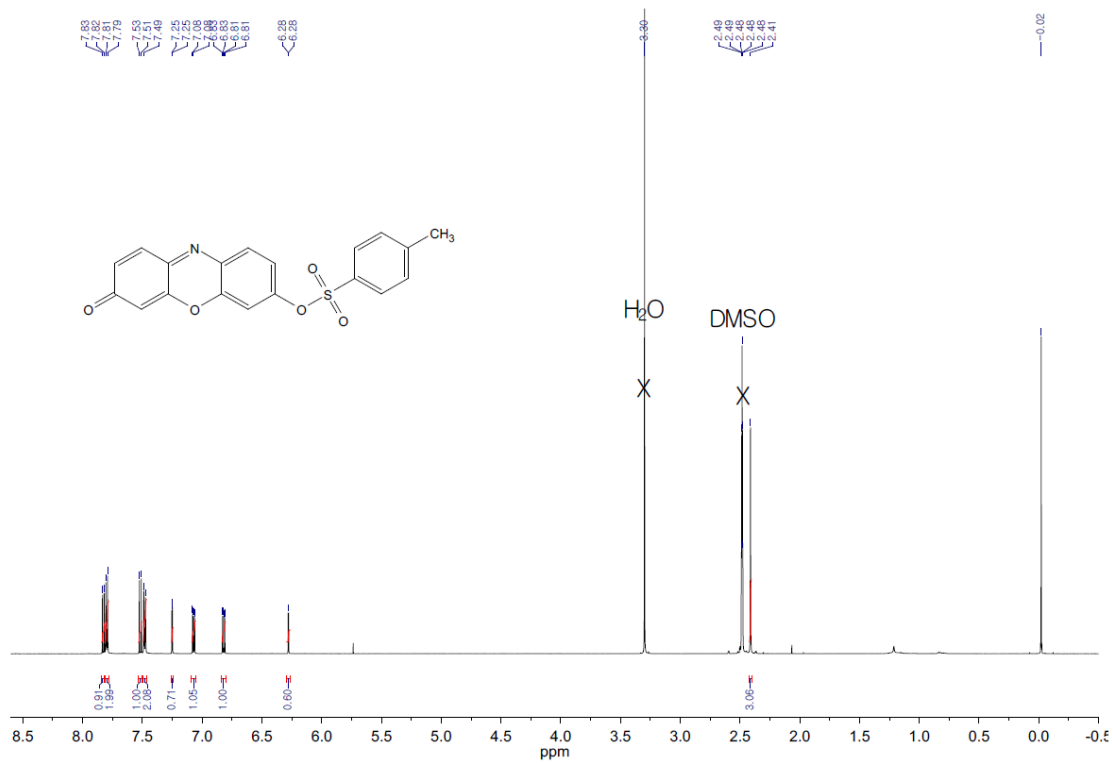


Fig. S21. ^{13}C NMR spectrum of **3** in DMSO-d_6 .

