Cholesterol appended pyridinium ureas: A case of gel making and breaking for selective visual readout of $F^-$

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1. Change in emission of receptor 1 with HSO$_4^-$, Cl$^-$, Br$^-$, I$, ClO_4^-$, AcO$^-$, H$_2$PO$_4^-$ in CH$_3$CN.
2. Change in of absorbance receptor 1 with HSO$_4^-$, Cl$^-$, Br$^-$, I$, ClO_4^-$, AcO$^-$, H$_2$PO$_4^-$ in CH$_3$CN.
3. Change of emission spectra of receptor 1 upon addition of 2 equivalent of different anions in CH$_3$CN.
4. Change in emission of receptor 1 with HSO$_4^-$, Cl$^-$, Br$^-$, I$, ClO_4^-$, AcO$^-$, H$_2$PO$_4^-$ in DMSO.
5. Change in absorbance of receptor 1 with HSO$_4^-$, Cl$^-$, Br$^-$, I$, ClO_4^-$, AcO$^-$, H$_2$PO$_4^-$ in DMSO.
6. Change of emission spectra of receptor 1 upon addition of 15 equivalent of different anion in DMSO.
7. Benesi–Hilderband plot for 1 with fluoride in CH$_3$CN.
8. Benesi–Hilderband plot for 1 with $F^-$ in DMSO.
9. Photograph of formation of gel for receptor 1 with 5 equiv. amounts of Fluoride in DMSO.
10. Job Plot of 1 with TBAF in DMSO.
11. Comparison of IR Spectra.
12. Characterization spectra
13. Comparative $^1$H NMR and FTIR spectra
14. UV-vis titration spectra for 2 with the anions.

1. Change in emission of receptor 1 with various anions in CH$_3$CN.
2. Change in absorbance of receptor 1 with various anions in CH$_3$CN.

Figure 2S. Change in absorbance of receptor 1 (c = 6.32 x 10$^{-5}$ M) with (a) HSO$_4^-$, (b) Cl$^-$, (c) Br$^-$, (d) I$^-$, (e) ClO$_4^-$, (f) AcO$^-$ (g) H$_2$P0$_4^-$ in CH$_3$CN (in all cases [anion] = 1x 10$^{-3}$ M).

Figure 1S. Fluorescence titration spectra for 1 (c = 6.32 x 10$^{-5}$ M) with (a) HSO$_4^-$, (b) Cl$^-$, (c) Br$^-$, (d) I$^-$, (e) ClO$_4^-$, (f) AcO$^-$ (g) H$_2$P0$_4^-$ in CH$_3$CN (in all cases [anion] = 1x 10$^{-3}$ M).
3. Change of emission spectra of receptor 1 upon addition of 2 equivalent of different anion in CH$_3$CN.

![Emission Spectra](image)

**Figure 3S**: Change in emission of receptor 1 ($c = 6.32 \times 10^{-5}$ M) upon addition of 2 eqv. of different Guests ($c = 1 \times 10^{-3}$ M) in CH$_3$CN.

4. Change in emission of receptor 1 with various anions in DMSO.

![Emission Spectra](image)
Figure 4S. Fluorescence titration spectra for 1 (c = 6.01 x 10^{-5} M) with (a) HSO_4^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) ClO_4^-, (f) AcO^- (g) H_2P_0_4^- in DMSO (in all cases [anion] = 1x 10^{-3} M)

5. Change in absorbance of receptor 1 with various anions in DMSO.
6. Change of emission spectra of receptor 1 upon addition of 15 equivalent of different anion in DMSO.

Figure 5S. Change in absorbance of receptor 1 (c = 6.01 x 10⁻⁵ M) with (a) HSO₄⁻, (b) Cl⁻, (c) Br⁻, (d) I⁻, (e) ClO₄⁻ (f) AcO⁻ (g) H₂PO₄⁻ in DMSO (in all cases [anion] = 1x 10⁻³ M).

Figure 6S: Change in emission of receptor 1(c = 6.01x 10⁻⁵ M) upon addition of 15eqv.of Different Guest (c = 1x10⁻³M) in DMSO
7. Benesi–Hilderband plot for 1 with F\(^-\) in CH\(_3\)CN.

![Graph showing Benesi–Hilderband plot](image)

\[ K = 2.07 \times 10^3 \]
\[ R = 0.99 \]

**Figure 7S:** Benesi–Hilderband plot for receptor 1 \((c = 6.32 \times 10^{-5} \text{ M})\) with fluoride \((c = 1 \times 10^{-3} \text{ M})\) at 430 nm in CH\(_3\)CN

8. Benesi–Hilderband plot for 1 with F\(^-\) in DMSO.

![Graph showing Benesi–Hilderband plot](image)

\[ K = 3.21 \times 10^3 \]
\[ R = 0.99 \]

**Figure 8S:** Benesi–Hilderband plot for receptor 1 \((c = 6.01 \times 10^{-5} \text{ M})\) with fluoride \((c = 1 \times 10^{-3} \text{ M})\) at 410 nm in DMSO.
9. Photograph of formation of gel for receptor 1 with 5 equiv. amounts of Fluoride in DMSO.

![Photograph of formation of gel for receptor 1 with 5 equiv. amounts of Fluoride in DMSO.]

Fig 9S. Photograph of Receptor 1 \((c = 3.58 \times 10^{-3} \text{ M})\) with 5 equiv. amounts of Fluoride \((c = 1.5 \times 10^{-2} \text{ M})\) in DMSO.

10. Job plot of 1 with F\(^-\) in DMSO.

![Job plot of 1 with F\(^-\) in DMSO.]

Fig 10S. Job plot for 1 \((c = 5.96 \times 10^{-5} \text{ M})\) with TBAF in DMSO.
11. Comparison of IR- Sepctra.

**Fig 11S.** 1 Partial IR spectrum of **2a**. 2 partial IR spectrum of **2a** in gel state. 3 Partial IR spectrum of **2a** after breaking the gel with fluoride.
12. Characterization spectra

$^1$H NMR (400 MHz, $d_6$-DMSO)
$^{13}$C NMR (100 MHz, d$_6$-DMSO)
Mass
$^1$H NMR (400 MHz, d$_6$-DMSO)
$^{13}$C NMR (100 MHz, d$_6$-DMSO)
Mass
13. Comparative $^1$H NMR and FTIR spectra

Fig 12S. Partial $^1$H NMR (400 MHz, $d_6$DMSO) of (a) $1$ ($X = PF_6^-$, $c = 4.8 \times 10^{-3}$ M) and (b) $X = Cl^-$. 

Fig 13S. Partial $^1$H NMR (400 MHz CDCl$_3$ containing 5% $d_6$DMSO) of (a) $2a$ and (b) $2$. 

Fig 14S. Partial $^1$H NMR (400 MHz, $d_6$DMSO) of (a) $1$ and (b) after addition of 3 equivalent amounts of tetrabutylammonium fluoride.
Fig 15S. Partial FT-IR (in KBr) of (a) 1 and (b) chloride salt of 1.

Fig 16S. Partial FT-IR (in KBr) of (a) 2a and (b) 2
14. UV-vis titration spectra for 2 with the anions.

Fig 17S. Absorption titration spectra for 2 (c = 4.05 x 10^{-5} M) with (a) F-, (b) Cl-, (c) Br-, (d) I-, (e) H_2PO_4^-, (f) HSO_4^-, (g) AcO-, (h) NO_3^-, (i) ClO_4^- in CHCl_3 (in all cases [anion] = 1x 10^{-3} M).