Supporting Information

Using Natural Potential of Chromone: Development of Small Molecules as Multi-ion Detectors

Palwinder Singh*, Matinder Kaur
Department of Chemistry, UGC Sponsored Centre for Advanced Studies, Guru Nanak Dev University, Amritsar-143005, India
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Equation for calculation of binding constants

Binding constants of compound-anion complex were calculated using Benesi-Hildebrand Equation. \[
\frac{1}{(A_f - A_{obs})} = \frac{1}{(A_f - A_{fc})} + \frac{1}{K (A_f - A_{fc})} [\text{Ligand}]
\]

Where \(A_f\) is absorbance of free host, \(A_{obs}\) is absorbance observed, \(A_{fc}\) is absorbance at saturation, \(K\) is the binding constant.

EXPERIMENTAL SECTION

Melting points were determined in capillaries and are uncorrected. \(^1\)H and \(^{13}\)C NMR spectra were recorded on JEOL 300 MHz and 75 MHz NMR spectrometer, respectively using CDCl\(_3\) and/or DMSO-d\(_6\) as solvent. Chemical shifts are given in ppm with TMS as internal reference. \(J\) values are given in Hertz. Signals are abbreviated as singlet, s; doublet, d; double-doublet, dd; triplet, t; multiplet, m. In \(^{13}\)C NMR spectral data, +ve, -ve terms correspond to CH\(_3\), CH, CH\(_2\) signals in DEPT-135 NMR spectra. Chromatography was performed with silica 100-200 mesh and reactions were monitored by thin layer chromatography (TLC) with silica plates coated with silica gel HF-254. Element analysis was performed on Thermoelectron FLASH EA1112 CHN analyzer. Reactions under microwaves were performed using microwave oven (INALSA model 1MW17EG) with microwave power 700 W and operating frequency 2450 MHz. IR and UV spectral data were recorded on Varian 660-IR FT-IR Spectrometer and BioTek PowerWave XS instruments respectively.

Equation for calculation of correlation coefficient from linear regression analysis

\[
r = \frac{\sum[(X_i - \bar{X})(Y_i - \bar{Y})]}{\sqrt{\sum(X_i - \bar{X})^2 (Y_i - \bar{Y})^2}}
\]

Equation for calculation of correlation coefficient from partial regression analysis

\[
r_{12.3} = \frac{r_{12} - r_{13}r_{23}}{\sqrt{(1-r_{13}^2)(1-r_{23}^2)}}
\]

Here, 1= compound 1, 2= Fe\(^{3+}\), 3= Hg\(^{2+}\)
r\(_{12}\) = partial correlation between compound 3 and Fe\(^{3+}\)
r\(_{13}\) = partial correlation between compound 3 and Hg\(^{2+}\)
r\(_{12.3}\) = partial correlation between compound 3 and Fe\(^{3+}\) eliminating the effect of Hg\(^{2+}\)
r\(_{13.2}\) = partial correlation between compound 3 and Hg\(^{2+}\) eliminating the effect of Fe\(^{3+}\) (same formula as for r\(_{12.3}\))
1,3-Dimethyl-5-((4-oxo-4H-chromen-3-yl)methylene)pyrimidine-2,4,6(1H,3H,5H)-trione (3): Creamish solid, 83% yield, mp 185 °C; νmax (KBr): 1685, 1659, 1612 (C=O). 1H NMR (300 MHz, CDCl3): δ 3.45 (s, 3H, 2xCH3), 7.46-7.71 (m, 2H, ArH), 7.73-7.77 (m, 1H, ArH), 8.28 (dd, J1 = 3.4 Hz, 1H, ArH), 8.88 (s, 1H, 1H, ArH), 8.87 (s, 1H, 2-H). 13C NMR (normal/DEPT-135) (CDCl3): δ 28.4 (+ve, CH3), 30.0 (+ve, CH3), 117.9 (+ve, CH), 118.3 (+ve, CH), 118.3 (+ve, CH), 126.3 (+ve, CH), 126.5 (+ve, CH), 134.5 (C), 148.7 (C), 151.0 (C), 155.6 (C), 161.2 (C), 161.7 (C), 163.50 (C), 175.2 (C). FAB mass m/z 312 (M+1); (Found: C 61.56, H 4.13, N 9.27; C16H12N2O5 requires C 61.54, H 3.87, N 8.97).

5-((6-Isopropyl-4-oxo-4H-chromen-3-yl)methylene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (4): Creamish solid, 92% yield, mp 152 °C; νmax (KBr): 1730, 1675, 1583 (C=O). 1H NMR (300 MHz, CDCl3): δ = 1.27 (s, 3H; CH3), 1.32 (s, 3H; CH3), 3.01-3.05 (m, 1H; CH), 3.37 (s, 3H; CH3), 3.40 (s, 3H; CH3), 7.43 (d, J = 8.4 Hz, 1H; ArH), 7.57 (dd, J3 = 7.8 Hz, J2 = 9 Hz, 1H; ArH), 8.09 (d, J = 2.4 Hz, 1H; ArH), 8.88 (s, 1H; ArH), 9.77 ppm (s, 1H; 2-H); 13C NMR (normal/DEPT-135) (CDCl3): δ 24.2 (+ve, CH3), 28.8 (+ve, CH3), 29.4 (+ve, CH3), 34.2 (+ve, CH3), 118.2 (+ve, CH), 118.5 (C), 118.6 (C), 123.8 (+ve, CH), 133.8 (+ve, CH), 147.9 (+ve, CH), 149.6 (C), 151.5 (C), 154.5 (C), 161.7 (C), 163.9 (+ve, CH), 175.8 (C). FAB mass m/z 355 (M+1); (Found: C 64.40, H 5.12, N 7.91; C19H18N2O5 requires C 64.41, H 5.21, N 7.96).

5-((6-Bromo-4-oxo-4H-chromen-3-yl)methylene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (5): Creamish solid, 97% yield, mp 236 °C; νmax (KBr): 1733, 1668, 1576 (C=O). 1H NMR (300 MHz, CDCl3) δ = 3.40 (s, 3H; CH3), 3.47 (s, 3H; CH3), 7.41 (d, J = 9 Hz, 1H; ArH), 7.79 (dd, J3 = 8.8 Hz, J4 = 2.7 Hz, 1H; ArH), 8.38 (d, J = 2.4 Hz, 1H; ArH), 8.78 (s, 1H; ArH), 9.71 (s, 1H; 2-H); 13C NMR (normal/DEPT-135) (CDCl3): δ 24.7 (+ve, CH3), 25.3 (+ve, CH3), 114.3 (C), 115.1 (C), 116.5 (+ve, CH), 125.3 (+ve, CH), 133.7, (+ve, CH), 144.3 (+ve, CH), 150.6 (C), 157.4 (C), 159.3 (C); FAB mass m/z 392 (M+1). (Found: C 49.13, H 2.83, N 7.16; C16H11BrN2O5 requires C 49.12, H 2.84, N 7.17).

1,3-Dimethyl-5-((6-nitro-4-oxo-4H-chromen-3-yl)methylene)pyrimidine-2,4,6(1H,3H,5H)-trione (6): Creamish solid, 95% yield, mp 200 °C; νmax (KBr): 1734, 1672, 1623 (C=O). 1H NMR (300 MHz, CDCl3): δ = 2.00 (s, 3H; CH3), 7.14-7.41 (m, 2H; ArH), 7.44-7.46 (m, 2H; ArH), 7.89-8.01 (m, 1H; ArH); 13C NMR (normal/DEPT-135) (CDCl3): δ 28.5 (+ve, CH3), 29.1
(+ve, CH₃), 118.7 (C), 120.2 (+ve, CH), 123.1 (+ve, CH), 123.8 (C), 128.7 (+ve, CH), 145.4 (C), 146.7 (+ve, CH), 150.8 (C), 158.4 (C), 161.0 (C), 161.3 (C), 162.4 (+ve, CH), 173.8 (C); FAB mass m/z 358 (M⁺+1). (Found: C 53.79, H 3.10, N 11.76; C₁₆H₁₁N₃O₇ requires C 53.80, H 3.09, N 11.77).

5-((6-Fluoro-8-nitro-4-oxo-4H-chromen-3-yl)methylene)-1,3-dimethylpyrimidine-2,4,6(1H, 3H,5H)-trione (7): Creamish solid, 97% yield, mp 190 °C; ν max (KBr): 1681, 1593, 1537 (C=O). ¹H NMR (300 MHz, CDCl₃): δ = 3.38 (s, 3H; CH₃), 3.40 (s, 3H; CH₃), 8.12 (dd, ³J = 7.2 Hz, ⁴J = 3 Hz, 1H; ArH), 8.23 (dd, ³J = 6.9 Hz, ⁴J = 3.3 Hz, 1H; ArH), 8.66 (s, 1H; CH), 10.32 (s, 1H; =H); ¹³C NMR (normal/DEPT-135) (CDCl₃): δ 28.5 (+ve, CH₃), 29.1 (+ve, CH₃), 117.6 (+ve, CH), 117.9 (+ve, CH), 118.3 (C), 118.8 (+ve, CH), 119.2 (+ve, CH), 120.5 (C), 126.6 (C), 145.9 (+ve, CH), 150.8 (C), 160.9 (C), 161.2 (C), 161.8 (+ve, CH), 172.6 (C); FAB mass m/z 376 (M⁺+1). (Found: C 51.25, H 2.69, N 11.24; C₁₉H₁₀F₃N₃O₇ requires C 51.20, H 2.68, N 11.21).

5-(4-Oxo-4H-chromen-3-ylmethylene)-pyrimidine-2,4,6-trione (8): Creamish solid, 88% yield, mp >240 °C; ν max (KBr): 3199, 3089 (NH), 1756, 1701 (C=O).

(4Z)-1-(3-Chlorophenyl)-3-methyl-4-((4-oxo-4H-chromen-3-yl)methylene)-1H-pyrazol-5(4H)-one (9): Orange solid, 87% yield, mp 227 °C; ν max (KBr): 1680, 1610 (C=O). ¹H NMR (300 MHz, CDCl₃): δ = 2.39 (s, 3H; CH₃), 7.17-7.18 (m, 1H; ArH), 7.33 (t, ³J = 8.1 Hz, 1H; ArH), 7.50-7.58 (m, 2H; ArH), 7.74-7.79 (m, 1H; ArH), 7.88-7.91 (m, 1H; ArH), 8.01-8.04 (m, 2H; ArH), 8.29 (dd, ³J = 8.1 Hz, ⁴J = 1.5 Hz, 1H; ArH), 10.75 (s, 1H); ¹³C NMR (normal/DEPT-135) (CDCl₃): δ 13.25 (+ve, CH₃), 116.6 (+ve, CH), 118.2 (C), 118.7 (+ve, CH), 118.8 (+ve, CH), 123.6 (C), 124.9 (+ve, CH), 126.4 (+ve, CH), 126.5 (+ve, CH), 127.3 (C), 129.8 (+ve, CH), 134.5 (+ve, CH), 134.6 (+ve, CH), 136.6 (C), 139.2 (C), 151.5 (C), 156.0 (C), 162.5 (C), 164.1 (C), 175.3 (C); FAB mass m/z 365 (M⁺+1), 365:367 (3:1). (Found: C 66.13, H 3.73, N 7.70; C₂₀H₁₃ClN₂O₂ requires C 65.85, H 3.59, N 7.68).

(4Z)-1-(3-Chlorophenyl)-4-((6-isopropyl-4-oxo-4H-chromen-3-yl)methylene)-3-methyl-1H-pyrazol-5(4H)-one (10): Orange solid, 85% yield, mp 190 °C; ν max (KBr): 1705 (C=O). ¹H NMR (300 MHz, CDCl₃): δ = 1.30 (s, 3H; CH₃), 1.31 (s, 3H; CH₃), 2.38 (s, 3H; CH₃), 2.87-3.10 (m, 1H; ArH), 3.00-3.10 (m, 1H; ArH), 7.17-7.18 (m, 1H; ArH), 7.31 (t, ³J = 8.1 Hz, 1H; ArH), 7.45 (d, ³J = 8.4 Hz, 1H; ArH), 7.67-7.78 (m, 2H; ArH), 8.01-8.10 (m, 2H; ArH), 10.72 (s, 1H); ¹³C NMR (normal/DEPT-135) (CDCl₃): δ 13.2 (+ve, CH₃), 23.8 (+ve, CH₃), 33.8 (+ve, CH₃), 116.6 (+ve, CH), 118.0 (+ve, CH), 118.5 (C), 118.8 (C), 123.3 (+ve, CH₃), 145.4 (C), 146.7 (+ve, CH), 150.8 (C), 158.4 (C), 161.0 (C), 161.3 (C), 162.4 (+ve, CH), 173.8 (C); FAB mass m/z 358 (M⁺+1). (Found: C 53.79, H 3.10, N 11.76; C₁₆H₁₁N₃O₇ requires C 53.80, H 3.09, N 11.77).
(4Z)-4-((6-Bromo-4-oxo-4H-chromen-3-yl)methylene)-1-(3-chlorophenyl)-3-methyl-1H-pyrazol-5(4H)-one (11):

Orange solid, 91% yield, mp 210 °C; v<sub>max</sub> (KBr): 1673, 1624 (C=O); <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ = 2.32 (s, 3H; CH<sub>3</sub>), 7.07-7.10 (m, 1H; ArH), 7.23 (t, J = 8.1 Hz, 1H; ArH), 7.40 (d, J = 8.7 Hz, 1H; ArH), 7.74-7.82 (m, 2H; ArH), 7.87 (s, 1H; ArH), 7.95 (t, J = 2.1 Hz, 1H; ArH), 8.33 (d, J = 2.4 Hz, 1H; ArH), 10.66 (s, 1H); FAB mass m/z 444 (M<sup>+</sup>+1). (Found: C 54.14, H 2.73, N 6.31; C<sub>20</sub>H<sub>12</sub>BrClN<sub>2</sub>O<sub>3</sub> requires C 54.15, H 2.72, N 6.31).

(4Z)-1-(3-Chlorophenyl)-3-methyl-4-((6-nitro-4-oxo-4H-chromen-3-yl)methylene)-1H-pyrazol-5(4H)-one (12):

Orange solid, 87% yield, mp >240 °C; v<sub>max</sub> (KBr): 1684, 1662 (C=O). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ = 2.34 (s, 3H; CH<sub>3</sub>), 7.09-7.13 (m, 1H; ArH), 7.27 (t, J = 8.4 Hz, 1H; ArH), 7.68 (d, J = 9.3 Hz, 1H; ArH), 7.79-7.82 (m, 1H; ArH), 7.85 (d, J = 6.3 Hz, 1H; ArH), 7.95 (t, J = 2.1 Hz, 1H; ArH), 8.51 (dd, <sup>3</sup>J = 9 Hz, <sup>4</sup>J = 2.7 Hz, 1H; ArH), 9.08 (d, J = 2.4 Hz, 1H; ArH), 10.71 (s, 1H); FAB mass m/z 410 (M<sup>+</sup>+1); (Found: C 58.62, H 2.95, N 10.25; C<sub>20</sub>H<sub>12</sub>ClN<sub>3</sub>O<sub>5</sub> requires C 58.63, H 2.95, N 10.24).

(4Z)-1-(3-Chlorophenyl)-4-((6-fluoro-8-nitro-4-oxo-4H-chromen-3-yl)methylene)-3-methyl 1H-pyrazol-5(4H)-one (13):

Orange solid, 89% yield, mp 230 °C; v<sub>max</sub> (KBr): 1730, 1653 (C=O). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ = 2.33 (s, 3H; CH<sub>3</sub>), 7.09-7.13 (m, 1H; ArH), 7.27 (t, J = 8.4 Hz, 1H; ArH), 7.78-7.83 (m, 2H; ArH), 7.94 (t, J = 2.1 Hz, 1H; ArH), 8.08 (dd, <sup>3</sup>J = 7 Hz, <sup>4</sup>J = 3 Hz, 1H; ArH), 8.18 (dd, <sup>3</sup>J = 7.2 Hz, <sup>4</sup>J = 3 Hz, 1H; ArH), 10.73 (s, 1H); FAB mass m/z 427 (M<sup>+</sup>+1); (Found: C 56.15, H 2.59, N 9.82; C<sub>20</sub>H<sub>12</sub>ClFNO<sub>5</sub> requires C 56.16, H 2.60, N 9.83).

3-(1,3-Dimethyl-2,4,6-trioxotetrahydro-pyrimidin-5-ylidenemethyl)-4-oxo-chroman-2-carbonitrile+3-(1,3-Dimethyl-2,4,6-trioxotetrahydro-pyrimidin-5-ylidenemethyl)-4-hydroxy-2H-chromene-2-carbonitrile (14):

Yellow solid, 75% yield, mp >240 °C; v<sub>max</sub> (KBr): 2177 (C=N), 1638, 1568 (C=O). <sup>1</sup>H NMR (300 MHz, MeOH-d<sub>6</sub>+CDCl<sub>3</sub>): δ = 3.18 (s, 3H; 2×CH<sub>3</sub>), 5.58 (s, 1H; CH), 6.93 (d, J = 8.4 Hz, 1H; ArH), 7.04 (t, J = 7.2 Hz, 1H; ArH), 7.30-7.41 (m, 4H; ArH), 7.61 (t, J = 7.5 Hz, 1H; ArH), 8.18 (dd, <sup>3</sup>J = 7.2 Hz, <sup>4</sup>J = 3 Hz, 1H; ArH), 10.73 (s, 1H); FAB mass m/z 427 (M<sup>+</sup>+1); (Found: C 56.15, H 2.59, N 9.82; C<sub>20</sub>H<sub>12</sub>ClFNO<sub>5</sub> requires C 56.16, H 2.60, N 9.83).
7.84 (d, \( J = 7.8 \) Hz, 1H; ArH), 8.01 (d, \( J = 7.8 \) Hz, 1H; =H), 8.46 (s, 1H; ArH); \( ^{13} \)C NMR (normal/DEPT-135) (MeOH-d\(_4\)+CDCl\(_3\)\): \( \delta \) 23.6 (+ve, CH\(_3\)), 27.5 (+ve, CH\(_3\)), 27.9 (+ve, CH\(_3\)), 67.9 (+ve, CH), 81.9 (+ve, CH), 113.3 (C≡N), 117.9 (C), 118.4 (C), 119.0 (+ve, CH), 119.5 (+ve, CH), 120.5 (C), 122.9 (C), 123.4 (+ve, CH), 125.5 (+ve, CH), 127.5 (+ve, CH), 134.2 (C), 134.9 (C), 141.8 (+ve, CH), 153.6 (C), 156.5 (C), 156.6 (C), 156.7 (C), 157.8 (+ve, CH), 163.2 (C), 164.4 (C), 177.0 (C). FAB mass \( m/\zeta \) 340 (M+1); (Found: C 60.18, H 3.86, N 12.38; C\(_{17}\)H\(_{13}\)N\(_3\)O\(_5\) requires C 60.16, H 3.87, N 12.37).
SI Figure 1. $^1$H NMR spectrum of compound 3.

SI Figure 2. $^{13}$C NMR spectrum of compound 3 (CDCl$_3$).
SI Figure 3. $^{13}$C NMR spectrum of compound 3 in (MeOH-d$_4$+CDCl$_3$). Two tautomers were observed in MeOH.
**SI Figure 4.** IR spectrum of compound 3.

**SI Figure 5.** $^1$H NMR spectrum of compound 4.
SI Figure 6. $^{13}$C NMR spectrum of compound 4.

SI Figure 7. IR spectrum of compound 4.

SI Figure 8. $^1$H NMR spectrum of compound 5.
SI Figure 9. $^{13}$C NMR spectrum of compound 5.

SI Figure 10. IR spectrum of compound 5.
SI Figure 11. $^1$H NMR spectrum of compound 6.
SI Figure 12. $^{13}$C NMR spectrum of compound 6.

SI Figure 13. IR spectrum of compound 6.

SI Figure 14. $^1$H NMR spectrum of compound 7.
SI Figure 15. $^{13}\text{C}$ NMR spectrum of compound 7.

SI Figure 16. IR spectrum of compound 7.
SI Figure 17. IR spectrum of compound 8.

SI Figure 18. $^1$H NMR spectrum of compound 9.
SI Figure 19. $^{13}$C NMR spectrum of compound 9.

SI Figure 20. IR spectrum of compound 9.
SI Figure 21. $^1$H NMR spectrum of compound 10.

SI Figure 22. $^{13}$C NMR spectrum of compound 10.
SI Figure 23. $^1$H NMR spectrum of compound 11.

SI Figure 24. IR spectrum of compound 11.
**SI Figure 25.** $^1$H NMR spectrum of compound 12.

**SI Figure 26.** IR spectrum of compound 12.
SI Figure 27. $^1$H NMR spectrum of compound 13.

SI Figure 28. IR spectrum of compound 13.
**SI Figure 29.** $^1$H NMR spectrum of compound 14 (MeOH-d$_4$+CDCl$_3$). Two tautomers were observed in MeOH. Tautomer ‘B’ is major.

**SI Figure 30.** $^{13}$C NMR spectrum of compound 14 (MeOH-d$_4$+CDCl$_3$).
SI Figure 31. DEPT-135 NMR spectrum of compound 14.

SI Figure 32. IR spectrum of compound 14.
SI Figure 33. $^{13}$C NMR spectrum of compound $3+\text{Hg(ClO}_4)_2$ in MeOH-d$_4$+CDCl$_3$.

SI Figure 34. DEPT-135 NMR spectrum of compound $3+\text{Hg(ClO}_4)_2$ in MeOH-d$_4$+CDCl$_3$. 
**UV-vis titrations**

**SI Figure 35.** UV-vis spectra of compound 3 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

**SI Figure 36.** UV-vis spectra of compound 4 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).
**SI Figure 37.** UV-vis spectra of compound 5 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

**SI Figure 38.** UV-vis spectra of compound 6 (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).
**SI Figure 39.** UV-vis spectra of compound 7 (10 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

**SI Figure 40.** UV-vis spectra of compound 8 (10 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).
SI Figure 41. Changes in UV-vis spectra of compound 9 (5 µM) in water-ethanol (9:1 v/v, pH 7.2,) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

SI Figure 42. Changes in UV-vis spectra of compound 10 (5 µM) in water-ethanol (9:1 v/v, pH 7.2,) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).
SI Figure 43. UV-vis spectra of compound 11 (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

SI Figure 44. UV-vis spectra of compound 12 (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).
SI Figure 45. UV-vis spectra of compound 13 (10 μM) in aqueous solution (water-ethanol, pH 7.2, v/v 9:1) upon addition of increasing amount of Hg(ClO₄)₂ (0.1-1 equiv).

SI Figure 46. UV-vis spectra of compound 4 (5 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amounts of Fe(ClO₄)₃ (0.1-1 equiv).
**SI Figure 47.** UV-vis spectra of compound 5 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Fe(ClO$_4$)$_3$ (0.1-1 equiv).

**SI Figure 48.** UV-vis spectra of compound 8 (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Fe(ClO$_4$)$_3$ (0.1 - 1 equiv).
**SI Figure 49.** UV-vis spectra of compound 9 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Fe(ClO₄)₃ (0.1-1 equiv).

**SI Figure 50.** UV-vis spectra of compound 10 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Fe(ClO₄)₃ (0.1-1 equiv).
SI Figure 51. UV-vis spectra of compound 11 (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of Fe(ClO₄)₃ (0.1-1 equiv).

SI Figure 52. Selectivity of compounds 4, 5, 6 and 7 (5µM) towards Hg²⁺ among different cations.
SI Figure 53. Selectivity of compounds 9, 10, 11, 12 and 13 (10 µM) towards Hg$^{2+}$ among different cations.

SI Figure 54. Response of compound 4 (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: 4 (5 µM) in presence of Hg$^{2+}$ (1 µM) and interfering ions Li$^+$, Na$^+$, K$^+$, Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).
**SI Figure 55.** Response of compound 5 (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: 5 (5 µM) in presence of Hg$^{2+}$ (1 µM) and interfering ions Li$^+$, Na$^+$, K$^+$ Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).

**SI Figure 56.** Response of compound 6 (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 434 nm: 6 (2 µM) in presence of Hg$^{2+}$ (2 µM) and interfering ions Li$^+$, Na$^+$, K$^+$ Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).
**SI Figure 57.** Response of compound 7 (10 μM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 434 nm: 7 (10 μM) in presence of Hg$^{2+}$ (2 μM) and interfering ions Li$^+$, Na$^+$, K$^+$ Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).

**SI Figure 58.** Response of compound 8 (10 μM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: 8 (10 μM) in presence of Hg$^{2+}$ (2 μM) and interfering ions Li$^+$, Na$^+$, K$^+$ Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).
SI Figure 59. Response of compound 9 (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: 9 (10 µM) in presence of Hg$^{2+}$ (2 µM) and interfering ions Li$^+$, Na$^+$, K$^+$, Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).

SI Figure 60. Response of compound 10 (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 442 nm: 10 (5 µM) in presence of Hg$^{2+}$ (5 µM) and interfering ions Li$^+$, Na$^+$, K$^+$, Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).
SI Figure 61. Response of compound 11 (10 μM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: 11 (10 μM) in presence of Hg$^{2+}$ (2 μM) and interfering ions Li$^+$, Na$^+$, K$^+$, Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).

SI Figure 62. Response of compound 12 (10 μM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 448 nm: 12 (10 μM) in presence of Hg$^{2+}$ (2 μM) and interfering ions Li$^+$, Na$^+$, K$^+$, Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).
**SI Figure 63.** Response of compound 13 (10 μM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 467 nm 13 (10 μM) in the presence of Hg$^{2+}$ (2 μM) and interfering ions Li$^+$, Na$^+$, K$^+$ Mg$^{2+}$, Ba$^{2+}$, Ca$^{2+}$, Cd$^{2+}$, Co$^{2+}$, Cu$^{2+}$, Zn$^{2+}$, Pb$^{2+}$, Ag$^+$, Fe$^{2+}$ and Fe$^{3+}$ (100 equiv).

**SI Figure 64.** Job’s plot for compound 3, absorbance monitored at 417 nm.
SI Figure 65. Job’s plot for compound 4, absorbance monitored at 422 nm.

SI Figure 66. Job’s plot for compound 5, absorbance monitored at 422 nm.
SI Figure 67. Job’s plot for compound 6, absorbance monitored at 434 nm.

SI Figure 68. Job’s plot for compound 7, absorbance monitored at 422 nm.
SI Figure 69. Job’s plot for compound 8, absorbance monitored at 422 nm.

SI Figure 70. Job’s plot for compound 9, absorbance monitored at 422 nm.
**SI Figure 71.** Job’s plot for compound 10, absorbance monitored at 442 nm.

**SI Figure 72.** Job’s plot for compound 11, absorbance monitored at 439 nm.
SI Figure 73. Job’s plot for compound 12, absorbance monitored at 448 nm.

SI Figure 74. Job’s plot for compound 13, absorbance monitored at 467 nm.
SI Figure 75. (a) Change in absorbance of compound 3 at 417 nm with pH, (b) Change in absorbance of compound 3 on addition of 1 equiv of Hg$^{2+}$ (1 µM) at different pH.

SI Figure 76. Bar graph showing the selectivity of compound 6 towards Hg$^{2+}$ in presence of Fe$^{3+}$ monitored at 434 nm.
**SI Figure 77.** Bar graph showing the selectivity of compound 7 towards Hg$^{2+}$ in presence of Fe$^{3+}$ monitored at 439 nm.

**SI Figure 78.** Bar graph showing selectivity of compound 12 towards Hg$^{2+}$ in presence of Fe$^{3+}$ monitored at 448 nm.
**SI Figure 79.** Bar graph showing the selectivity of compound 13 towards Hg$^{2+}$ in presence of Fe$^{3+}$ monitored at 467 nm.

**SI Figure 80.** (a) A part of IR spectrum of compound 3. (b) A part of IR spectrum of compound 3.Hg$^{2+}$. 
**SI Figure 81.** UV-vis spectra of compound 3 (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of sodium cyanide (0.1-1 equiv).

**SI Figure 82.** UV-vis spectra of compound 3 (5 µM) in acetonitrile (ACN) upon addition of increasing amount of TBACN (0.1-1 equiv).
**SI Figure 83.** UV-vis spectra of compound 3 (5 μM) in chloroform (CHCl₃) upon addition of increasing amount of TBACN (0.1-1 equiv).

**SI Figure 84.** Bar graph shows absorbance of compound 3 at 341 nm in presence of 1 equiv of various anions.
**SI Figure 85.** Competitive binding of compound 3 with CN\(^-\) in presence of other anions. Absorbance monitored at 341 nm.

**SI Figure 86.** Change in UV-vis spectrum of compound 3 (black trace) on addition of 1 equiv of CN\(^-\) (1 µM) at pH 6-8.
Table 1. Binding constants for compounds 4-13.

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<tr>
<th>Compound</th>
<th>Binding constant (M⁻¹)</th>
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