Electronic Supplementary Information

Effective Ensemble System for Identification of CN⁻, Based on Cobalt (II) Complex: Mimicking Logic Gate†

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ESI Fig. S1: Interaction of 2a with 10 eq. of metal ions (a) absorption spectra (b) emission spectra in H₂O-DMF (1:9, v/v, HEPES buffer 7.4).

ESI Fig. S2: Benesi-Hilderbrand Plot for the binding constant of 2a towards Co²⁺ (a) absorbance (b) emission spectra.

ESI Fig. S3: Effect of pH (a) and water content (b) on emission intensity of 2a+Co²⁺ complex.

ESI Fig. S4: Benesi-Hilderbrand Plot for the binding constant of 2a+Co³⁺ complex towards CN⁻ absorbance spectra (a) (0-1.4) eq. CN⁻ (b) (1.4-3.0) eq. CN⁻ and (c) emission spectra.

ESI Fig. S5: (a) Calibration curve for 2a+Co²⁺ complex and (b) calibration sensitivity for CN⁻ ion in H₂O-DMF (1:9, v/v, HEPES buffer 7.4).

ESI Fig. S6: IR spectra of (a) 2a+Co²⁺ complex and (b) 2a +Co²⁺+CN⁻ complex.

ESI Fig. S7: Mass spectrum of 2a+Co²⁺ complex.

ESI Fig. S8: Mass spectrum of 2a +Co²⁺+CN⁻ adduct.

ESI Fig. S9: FTIR spectrum of 2a.

ESI Fig. S10: ¹H NMR spectrum of 2a in DMSO- d₆.

ESI Fig. S11: ¹³C spectrum of 2a in CDCl₃

ESI Fig. S12: Mass spectrum of 2a.

ESI Fig. S13: ¹H NMR spectrum of 2b in CDCl₃

ESI Fig. S14: ¹³C spectrum of 2b in CDCl₃.

ESI Fig. S15: ¹H NMR spectrum of 1 in CDCl₃.

ESI Fig. S16: ¹³C spectrum of 1 in CDCl₃.

ESI Fig. S17: (a) Absorption titration spectra (b) Emission titration spectra of 2b upon addition of Co²⁺ in H₂O-DMF (1:9, v/v, HEPES buffer 7.4).

Table S1: Recovery analysis of spiked CN⁻ concentration in deionized water, river water and tap water samplesª.
Experimental Section

Chemical and Instrumentation

All reagents and solvents for experimental work were taken from Sigma–Aldrich. DMF solvent was dried with the help of CaCl₂ as drying agent and then stored on molecular sieve after distillation process (under reduced pressure). CHNS (carbon, hydrogen, nitrogen, sulfur) elemental analysis was supported by using a vireo MICROV3.1.1. IR spectra were recorded with Perkin Elmer FT-IR 1000 spectrophotometer (KBr solid film). Specord S600 Thermo-Scientific PC double beam spectrophotometer used for absorption spectra with quartz cuvette of path length 1 cm. Horiba RF-5301PC was used for emission spectra with standard quartz cell of path length 3 cm. The NMR spectra were recorded in JEOL 400 MHz spectrophotometer by applying tetramethylsilane (TMS) as an internal standard. The cyclic voltammograms were note down with a CHI760E Electro analyzer three-electrode cell with glassy carbon as the working electrode, Hg/HgCl₂ as the reference electrode, Pt wire as the counter electrode and 0.1 M tetrabutylammonium perchlorate (TBAP) was used as the supporting electrolyte on 0.1V s⁻¹ scan rate.

**ESI Fig. S1:** Interaction of 2a with 10 eq. of metal ions (a) absorption spectra (b) emission spectra in H₂O-DMF (1:9, v/v, HEPES buffer 7.4).
**ESI Fig. S2**: Benesi-Hilderbrand Plot for the binding constant of 2a towards Co^{2+} (a) absorbance (b) emission spectra.

**ESI Fig. 3**: Effect of pH (a) and water content (b) on emission intensity of 2a+Co^{2+} complex.

**ESI Fig. S4**: Benesi-Hilderbrand Plot for the binding constant of 2a+ Co^{2+} complex towards CN\(^-\) absorbance spectra (a) (0-1.4) eq. CN\(^-\) (b) (1.4-3.0) eq. CN\(^-\) and (c) emission spectra.
**Sensitivity and Detection Limit for CN⁻:** For detections limit 7 sample of 2a+Co²⁺ complex (5 μM) was prepared and plot a linear calibration curve which corresponding to change in emission intensities. The estimated standard deviation was found to be 132.84. The calibration sensitivity \( (m = 3222.748) \) for CN⁻ was predictable from the slope of the fluorescence curve obtained between change in fluorescence intensities \( (F-F₀) \) versus CN⁻ concentration. The \( F \) and \( F₀ \) indicate the emission intensities of 2a+Co²⁺ complex in the presence and absence of CN⁻, respectively. Limit of detection (LOD) estimated using equation \( LOD = 3σ/m \). Where, \( σ \) illustrates standard deviation for blank solution of 2a+Co²⁺ and \( m \) calibration sensitivity for CN⁻.

**ESI Fig. S5:** (a) Calibration curve for 2a+Co²⁺ complex and (b) calibration sensitivity for CN⁻ ion in H₂O-DMF (1:9, v/v, HEPES buffer 7.4).

**ESI Fig. S6:** IR spectra of (a) 2a+Co²⁺ complex and (b) 2a +Co²⁺+CN⁻ complex.
ESI Fig. S7: Mass spectrum of 2a+Co$^{2+}$ complex.
ESI Fig. S8: Mass spectrum of 2a +Co$^{2+}$+CN$^-$ adduct.
ESI Fig. S9: FTIR spectrum of 2a.

ESI Fig. S10: $^1$H NMR spectrum of 2a in $d_6$ DMSO.
ESI Fig. S11: $^{13}$C spectrum of 2a in CDCl$_3$
ESI Fig. S12: Mass spectrum of 2a.
**ESI Fig. S13:** $^1$H NMR spectrum of 2b in CDCl$_3$

$^1$H NMR (CDCl$_3$-400MHz) δ/ppm: 15.88 (-OH, s 1H), 7.88-7.97 (m 4H, J-36), 7.54-7.61 (m 3H J-28), 7.38-7.41 (t 2H J-12), 7.26 (s 1H), 2.62 (s 3H), 2.43 (s 3H).
ESI Fig. S14: $^{13}$C spectrum of 2b in CDCl$_3$.

$^{13}$C NMR (CDCl$_3$ -100MHz) δ/ppm: 182.5, 177.6, 162.8, 152.2, 135.5, 134.3, 133.5, 132.8, 129.0, 129.0, 128.7, 127.9, 127.3, 125.9, 125.3, 123.8, 122.2, 119.8, 116.6, 98.4, 21.1, 20.9.
**ESI Fig. S15:** $^1$H NMR spectrum of 1 in CDCl$_3$.

$^1$H NMR (CDCl$_3$-400MHz) $\delta$/ppm: 17.74 (-OH, s 1H) 7.84 (s 1H), 7.48-7.50 (d 1H J-8), 7.19-7.21 (d 1H J-8), 2.78 (s 3H), 2.43 (s 3H).
ESI Fig. S16: $^{13}$C spectrum of 1 in CDCl$_3$.

$^{13}$C NMR (CDCl$_3$, 100MHz) δ/ppm: 206.2, 178.9, 160.4, 153.0, 137.4, 134.5, 125.1, 116.9, 114.9, 101.5, 30.2, 20.9.
ESI Fig. S17: (a) Absorption titration spectra (b) Emission titration spectra of upon addition of Co$^{2+}$ H$_2$O-DMF (1:9, v/v, HEPES buffer 7.4).

Table S1: Recovery analysis of spiked CN$^-$ concentration in deionized water, river water and tap water samples$^a$.

<table>
<thead>
<tr>
<th>Spiked Concentration(μM)</th>
<th>Deionized water</th>
<th>River water</th>
<th>Tap water</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Found (μM)</td>
<td>Recovery (%)</td>
<td>Found (μM)</td>
</tr>
<tr>
<td>0.00</td>
<td>0.01</td>
<td></td>
<td>0.06</td>
</tr>
<tr>
<td>10</td>
<td>10.00</td>
<td>100 ± 1.2</td>
<td>10.16</td>
</tr>
<tr>
<td>20</td>
<td>19.98</td>
<td>99.9 ± 2.1</td>
<td>20.26</td>
</tr>
</tbody>
</table>

$^a$Mean value ± standard deviation (triplicate measurements)