Electronic Supplementary Information

A smart sensor for rapid detection of lethal hydrazine in human blood and drinking water

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1. UV absorption spectra and absorption vs. conc. of hydrazine plot:

(a) UV-vis absorption titration spectra of BBHC \((c = 2.0 \times 10^{-5} \text{ M})\) in the presence of 1 equiv. of hydrazine \((c = 2.0 \times 10^{-4} \text{ M})\) at pH 7.1 in CH\(_3\)CN–H\(_2\)O (1: 9, v/v) (b) absorbance ratio changes \((A_{408}/A_{352})\) of BBHC upon gradual addition of hydrazine (1 equiv.)

![UV absorption spectra and absorption vs. conc. of hydrazine plot](image)

**Fig S1:** (a) UV-vis absorption titration spectra of BBHC \((c = 2.0 \times 10^{-5} \text{ M})\) in the presence of 1 equiv. of hydrazine \((c = 2.0 \times 10^{-4} \text{ M})\) at pH 7.1 in CH\(_3\)CN–H\(_2\)O (1: 9, v/v) (b) absorbance ratio changes \((A_{408}/A_{352})\) of BBHC upon gradual addition of hydrazine (1 equiv.)

2. Calculation of the detection limit:

![Calculation of the detection limit](image)

**Fig S2:** Fluorescence change at 464 nm of BBHC upon gradual addition of hydrazine.

The detection limit DL of BBHC for Hydrazine was determined from the following equation\(^1\):

\[
DL = K \times Sb1/S
\]

Where \(K = 2\) or 3 (we take 2 in this case); \(Sb1\) is the standard deviation of the blank solution; \(S\) is the slope of the calibration curve.

From the graph, we get slope = 4.443, and \(Sb1\) value is 0.9552

Thus using the formula we get the Detection Limit = 0.43 \(\mu\)M i.e. BHC can detect hydrazine in this minimum concentration.
3. Calculation of rate constant:

From the time vs. absorbance at fixed wavelength (530 nm) plot using first order rate equation (Figure S3), we get rate constant \( (K) = \text{Slope} \times 2.303 = 0.0782 \times 2.303 = 18 \times 10^{-2} \text{ s}^{-1} \).

![Fig S3](image)

**Fig S3:** The time vs. fluorescence at a fixed wavelength (464 nm) plot using first order rate equation.

4. Bar Diagram of BBHC towards different metal ions and anions in fluorescence spectra:

![Bar Diagram](image)

**Fig S4:** Fluorescence response of BBHC \( (2.0 \times 10^{-5} \text{ M}) \) toward various (a) cations and (b) anions (1equiv.) at pH 7.1 in CH\(_3\)CN–H\(_2\)O (1:9, v/v).
5. Bar diagram of BBHC towards different amine-containing compound in fluorescence titration methods:

(a) ![Bar chart illustrating fluorescence response of free probe and one equivalent of (a) other amine-containing compounds and (b) amino acids in CH$_3$CN-H$_2$O (1:9, v/v, 25 °C).](image)

Fig S5: Bar chart is illustrating fluorescence response of free probe and one equivalent of (a) other amine-containing compounds and (b) amino acids in CH$_3$CN-H$_2$O (1:9, v/v, 25 °C).

6. Fluorescence life time data of BBHC:

<table>
<thead>
<tr>
<th>Entry</th>
<th>$\phi$</th>
<th>$\tau$ (ns)</th>
<th>$K_r$ (10$^8$ X s$^{-1}$)</th>
<th>$K_{nr}$ (10$^8$ X s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BBHC</td>
<td>0.02</td>
<td>0.675</td>
<td>8.34</td>
<td>6.47</td>
</tr>
<tr>
<td>BBHP</td>
<td>0.82</td>
<td>6.035</td>
<td>0.927</td>
<td>0.735</td>
</tr>
</tbody>
</table>

7. Determination of fluorescence quantum yield:

Here, the quantum yield $\phi$ was measured by using the following equation,

$\phi_x = \phi_s (\frac{F_x}{F_s})(\frac{A_x}{A_s})(\frac{n_x^2}{n_s^2}).$

Where, X and S indicate the unknown and standard solution respectively, $\phi = $ quantum yield, $F = $ area under the emission curve, $A = $ absorbance at the excitation wavelength, $n = $ index of refraction of the solvent. Here $\phi$ measurements were performed using anthracene in ethanol as standard [$\phi = 0.27$] (error $\sim$ 10%).

The quantum yield of BBHC itself is 0.2 which is remarkably changed into 0.82, an enhancement around 4 fold is observed.

8. Method for the preparation of TLC plate sticks:

It was easily prepared by immersing a TLC plate into the solution of BBHC (2 X 10$^{-4}$ M) in CH$_3$CN (1 mM) and exposing it to air to evaporate the solvent. The detection of
hydrazine was carried out by inserting the TLC plate to the different concentration of hydrazine (1 mM) and evaporating the solvent to dryness.

![Image](image.png)

**Fig S6:** (a) Color changes on the test paper (i) BBHC and (ii) BBHC in the presence of hydrazine.

9. Application with drinking water and pond water

![Image](image.png)

**Fig S7:** Fluorescence detection of hydrazine in drinking water and pond water by BBHC.
10. $^1$H NMR, $^{13}$C NMR and HR-MS spectra of BBHC and corresponding hydrazone Product (BBHP):

$^1$H NMR spectrum of 2-(benzo[$d$]thiazol-2-yl)-4-bromophenol:

$^{13}$C NMR spectrum of 2-(benzo[$d$]thiazol-2-yl)-4-bromophenol:
HRMS spectrum of 2-(benzo[d]thiazol-2-yl)-4-bromophenol:

\[ \text{HRMS spectrum of 2-(benzo[d]thiazol-2-yl)-4-bromophenol:} \]

\[ \text{1H NMR spectrum of 3-(benzo[d]thiazol-2-yl)-5-bromo-2-hydroxybenzaldehyde:} \]
$^{13}$C NMR spectrum of 3-(benzo[d]thiazol-2-yl)-5-bromo-2-hydroxybenzaldehyde:

HRMS spectrum of 3-(benzo[d]thiazol-2-yl)-5-bromo-2-hydroxybenzaldehyde:
$^1$H NMR spectrum of the receptor (BBHC):

$^{13}$C NMR spectrum of the receptor (BBHC):
HRMS spectrum of the receptor (BBHC):

$^1$H NMR spectrum of BBHC-hydrazine adducts (BBHP):

$^{13}$C NMR spectrum of BBHC-hydrazine adducts (BBHP):
HRMS spectrum of BBHC-hydrazine adducts (BBHP):

\[1^1\text{H NMR titration spectrum of the receptor (BBHC) in the presence of 1 eq. hydrazine:}\]
11. References: