Supporting Information (SI)

Yutao Yang,a,b† Fangjun Huo,b † Caixia Yin,a* Ming Xu,c Ying Hu,d Jianbin Chao,b Yongbin Zhang,b Timothy E. Glass*c and Juyoung Yoon*d

aInstitute of Molecular Science, Shanxi University, Taiyuan 030006, China; bResearch Institute of Applied Chemistry, Shanxi University, Taiyuan 030006, China; cDepartment of Chemistry, University of Missouri 601 South college Avenue, Columbia, Missouri 65211, United States; dDepartment of Chemistry and Nano Science, Ewha Womans University, Seoul 120-750, Korea

*Correspondence - yincx@sxu.edu.cn; glasst@missouri.edu; jyoon@ewha.ac.kr

Figure S1: The characterization data, 1H NMR, 13C NMR, ESI-MS of the probe and probe-ClO−

Figure S2: The characterization data, 1H NMR, 13C NMR, ESI-MS of probe-ClO−

Figure S3: UV–vis spectra of 1 (25 µM) in HEPES (10 mM, pH 7.4) upon addition of various concentrations of ClO−

Figure S4: The corresponding fluorescence intensity of 1 upon addition of sodium hypochlorite disinfectant.

Figure S5: Choice of pH range for the measurements
Experimental Section..

Synthesis of probe 1: The heterocyclic compound was obtained as shown in Scheme 1. Salicylhydroxamic acid (compound 1, 1 mmol,) was dissolved in methanol (20 mL), then excess sodium hypochlorite was poured into the solution. The mixture was placed at ambient temperature for 30 s to complete the reaction. The final mixture was diluted by water (20 ml) and extracted with ethyl acetate (3×30 mL). The organic layer was concentrated under reduced pressure to give the desired product as a pale-yellow solid (compound 2, 110 mg, 82% yield)

\[ {^{1}} \text{H NMR (300 MHz, 25 °C, DMSO-d_6): \delta 7.58 (d, 1H, J=2.7), 7.23 (d, 1H, J=2.8), 7.08 (m, 2H, J=23.7), 6.61 (d, 1H, J = 8.7 Hz);} \]

\[ {^{13}} \text{C NMR (75 MHz, DMSO-d_6): \delta 168.9, 159.8 131.3, 128.9, 123.7, 121.7, 117.6, 113.8 ESI-MS m/z [probe+Na] 158.33; Elemental analysis (calcd. %) for C_7H_5NO_2: C, 62.22; H, 3.73; N, 10.37; Found: C, 62.35; H, 3.68; N, 10.24.} \]

Methods. All spectroscopic measurements were performed in HEPES (10 mM, pH 7.4) buffer. HEPES buffer solutions were obtained by adding 1 M NaOH solution into 10 mM aqueous HEPES using a pH meter. The probe was dissolved in absolute CH_3OH to prepare the stock solutions with concentrations of 2.0 mM. The UV-Visible spectra and fluorescence spectra were recorded at 25 °C.

Measurement procedure The UV-Vis procedures were shown as follows: into a HEPES (10 mM, pH 7.4) buffer solution containing 25 μM probe, ClO^- sample was gradually titrated. All UV-Vis spectra data were recorded at 30 s after the ClO^- addition.

The fluorescence procedures were as follows: into a HEPES (10 mM, pH 7.4) buffer solution containing 2.5 μM probe 1, ClO^- sample was gradually titrated. All fluorescence spectra data were recorded at 30 s after the ClO^- addition.

The HepG2 cells were grown in 1×SPP medium (1% proteose peptone, 0.2% glucose, 0.1% yeast extract, 0.003% EDTA ferric sodium salt) at 30 °C. The HepG2 were treated with 2.5 μM of probe 1 in culture media for 30 min at 37 °C and washed three times with phosphate-buffered saline (PBS).
Figure S1: 1D $^1$H NMR, $^{13}$C NMR, and ESI-MS of the probe

The $^1$H NMR (300MHz) spectra of the probe in DMSO-$d_6$.

The $^{13}$CNMR (75MHz) spectra of the probe in DMSO-$d_6$. 
Figure S1: $^1$H NMR (300 MHz, 25 °C, DMSO-$d_6$): δ 12.21 (s, 1H), 11.41 (s, 1H), 9.31 (s, 1H), 7.68 (d, 1H, $J = 9.9$ Hz), 7.39 (m, 1H, $J = 15.5$ Hz), 6.91 (m, 2H, $J = 25.2$ Hz), $^{13}$C NMR (75 MHz, DMSO-$d_6$): δ 166.1, 159.2, 133.1, 126.8, 145.7, 118.5, 117.1, 113.8 ESI-MS m/z 152.50; Elemental analysis (calcd. %) for C$_7$H$_7$NO$_3$: C, 54.91; H, 4.61; N, 9.15; Found: C, 54.68; H, 4.39; N, 9.21.

Figure S2: The characterization data, $^1$H NMR, $^{13}$C NMR, ESI-MS of probe-ClO$^-$. 
The $^1$H NMR (300MHz) spectra of the probe-ClO$^{-}$ in DMSO-$d_6$.

The $^{13}$CNMR (75MHz) spectra of the probe-ClO$^{-}$ in DMSO-$d_6$.
Figure S2: $^1$H NMR (300 MHz, 25 °C, DMSO-$d_6$): δ 7.58 (d, 1H, J=2.7), 7.23 (d, 1H, J=2.8), 7.08 (m, 2H, J=23.7), 6.61 (d, 1H, J= 8.7 Hz) $^{13}$C NMR (75 MHz, DMSO-$d_6$): δ 168.9, 159.8 131.3, 128.9, 123.7, 121.7, 117.6, 113.8 ESI-MS m/z [probe+Na] 158.33; Elemental analysis (calcd. %) for C$_7$H$_5$NO$_2$: C, 62.22; H, 3.73; N, 10.37; Found: C, 62.35; H, 3.68; N, 10.24.
Figure S3: UV-Vis spectra of probe (25 μM) in HEPES (10 mM, pH = 7.4) upon addition of various concentrations of ClO\(^-\) (0 – 250 μM).
Figure S4: The corresponding fluorescence intensity of 1 upon addition of sodium hypochlorite disinfectant with different volumes: 0, 7, 12, 29 μL, respectively.

<table>
<thead>
<tr>
<th>Added ClO$^-$ (μM) $^b$</th>
<th>Found ClO$^-$ (μM)$^c$</th>
<th>% Recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2</td>
<td>1.23±0.01</td>
<td>98.4</td>
</tr>
<tr>
<td>1.5</td>
<td>1.50±0.03</td>
<td>96.8</td>
</tr>
<tr>
<td>1.8</td>
<td>1.86±0.02</td>
<td>100.5</td>
</tr>
</tbody>
</table>

$^a$Initial solution contained 100,000 fold diluted disinfectant, 2.5 μM probe in 10 mM HEPES, pH 7.4. $^b$Concentration of pure NaOCl solution added. $^c$Calculated by fluorescence.
Figure S5: Choice of pH range for the measurements

(a) Intensity (a.u.) vs. Wavelength (nm)

(b) Intensity (a.u.) vs. Wavelength (nm)
Figure S5: (a) Fluorescence intensity of free probe (2.5 μM) under different pH conditions. b) Fluorescence intensity of free probe+ClO⁻ under different pH conditions. (c) The fluorescence intensity of probe at 415 nm in the absence and presence of Cys under different pH (λex = 300 nm; Slit: 5nm/5 nm).