**Electronic Supplementary Information**

# Ultrafast Fluorescent Detection of Mercury(II) Ions in Aqueous and Biological Systems Using a Boronic Acid–Based Reaction Probe

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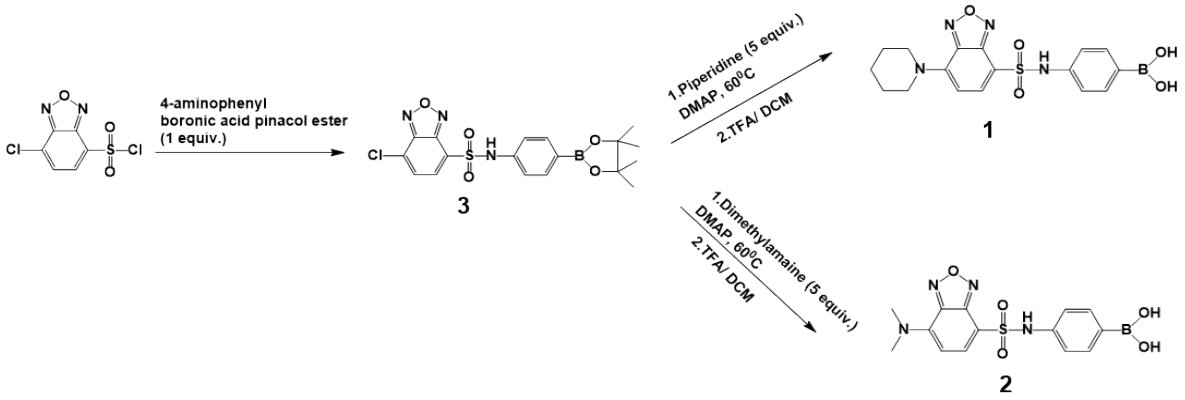



Scheme S1. Synthesis scheme of probe **1** and probe **2**.

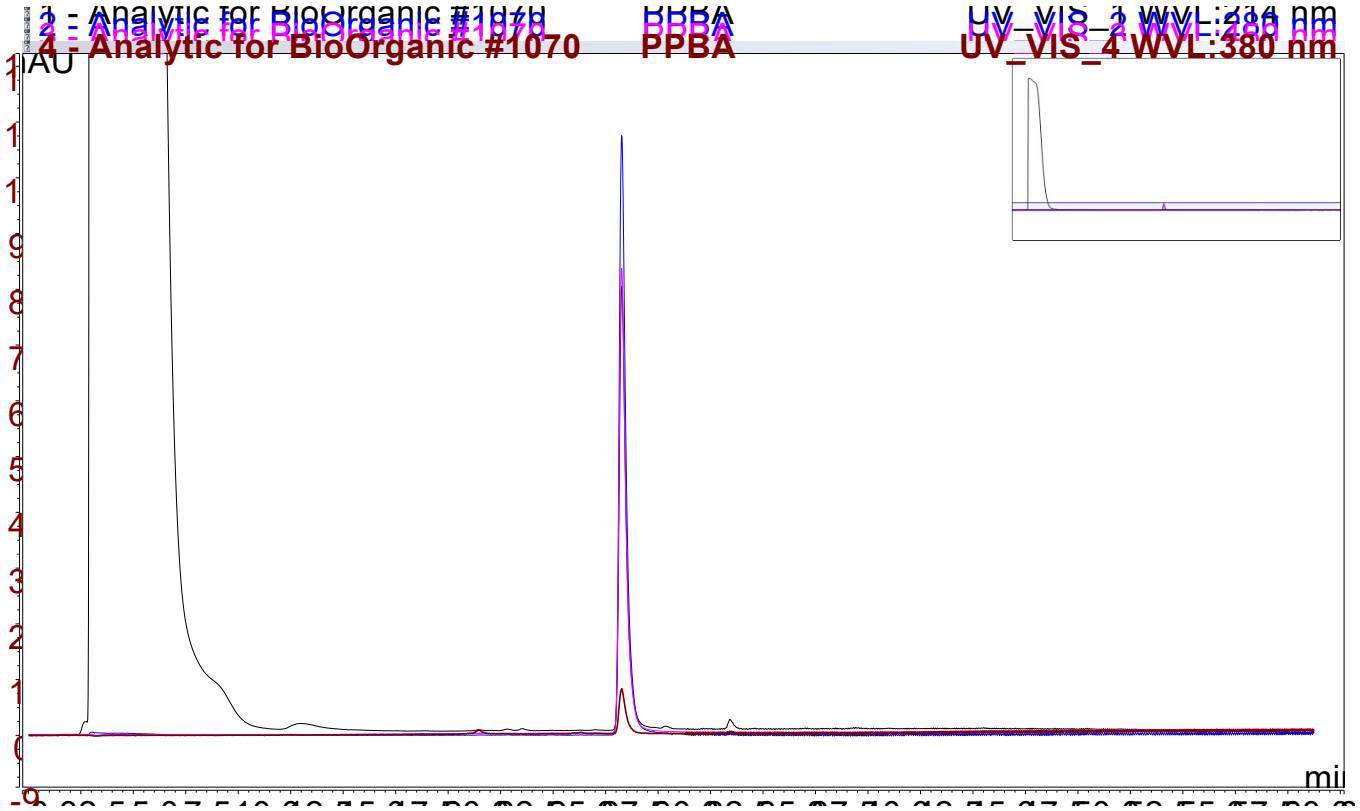



**Figure S1**. HPLC chromatogram of **1**.

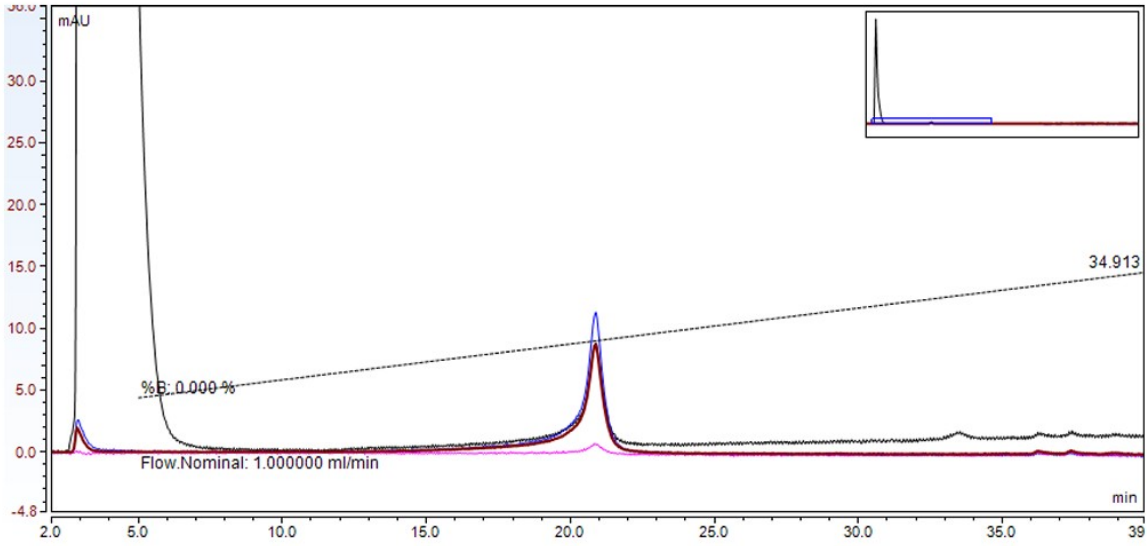



**Figure S2**. HPLC chromatogram of **2**.

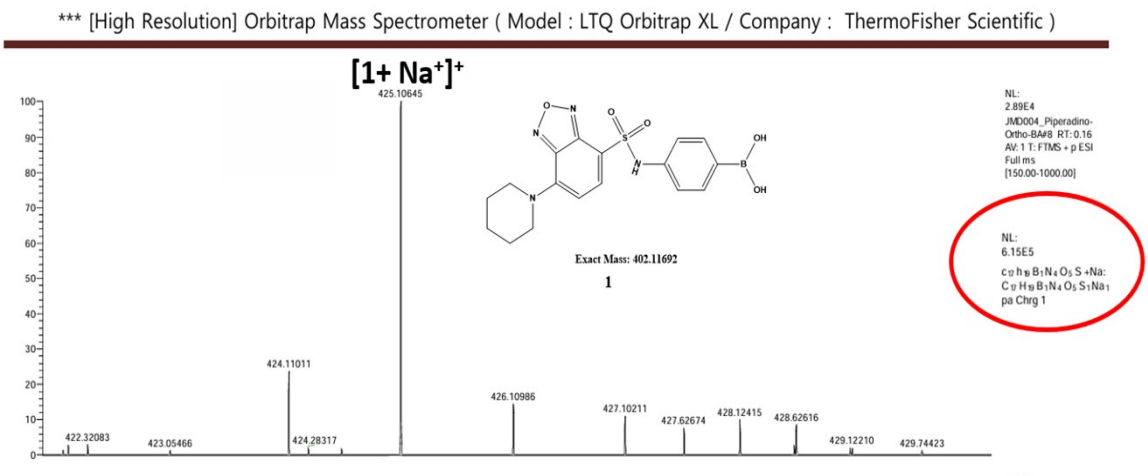



**Figure S3**. HR-mass spectrum of **1**.

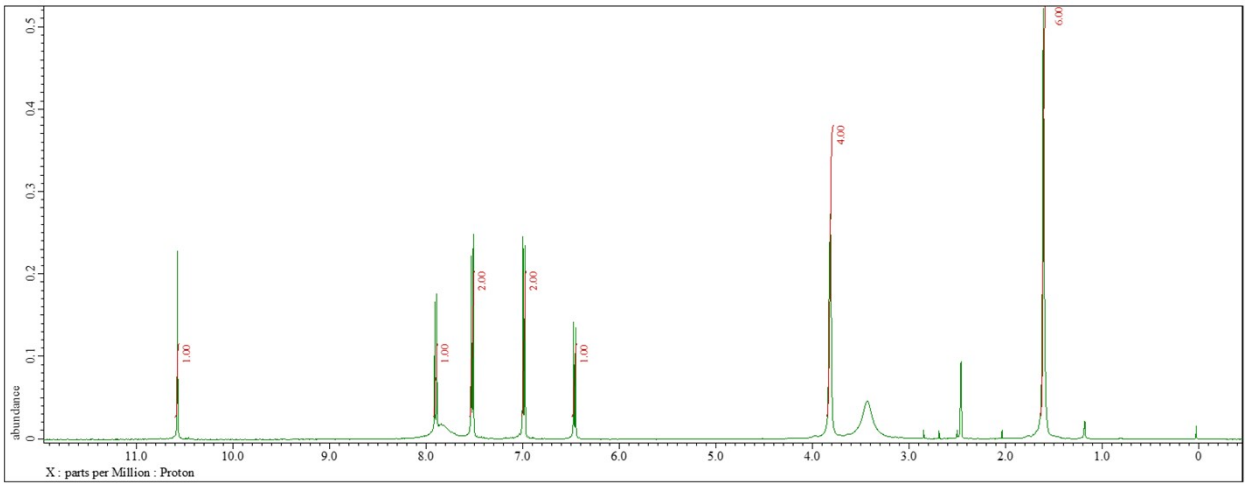



**Figure S4**. $^{1}$H NMR of **1**.

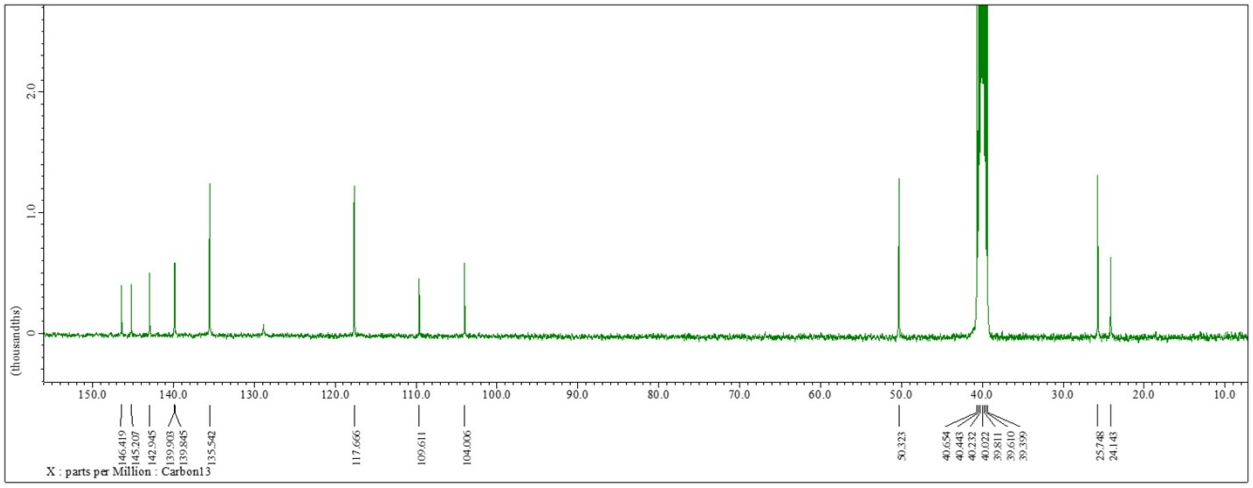



**Figure S5**. $^{13}C$ NMR of **1**.

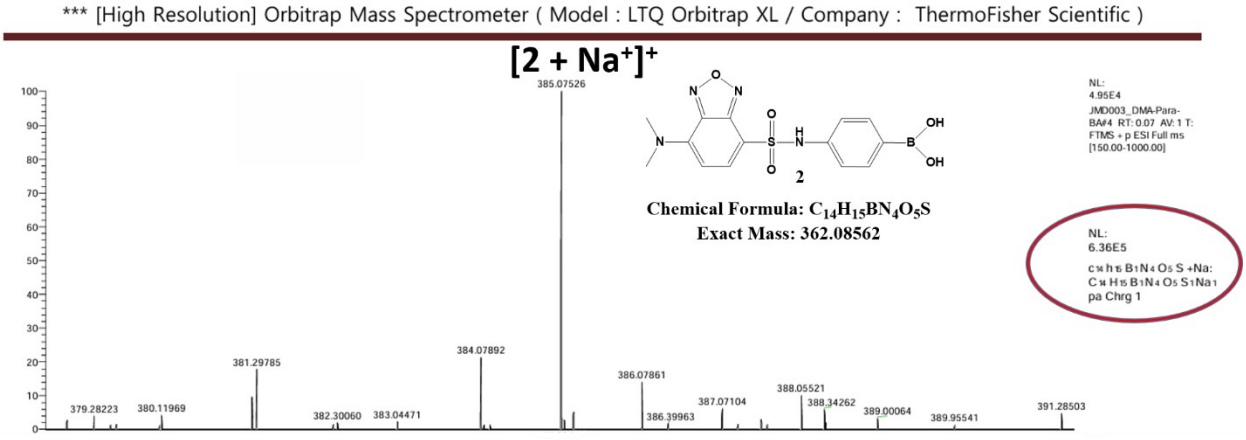



**Figure S6**. HR-mass spectrum of **2**.

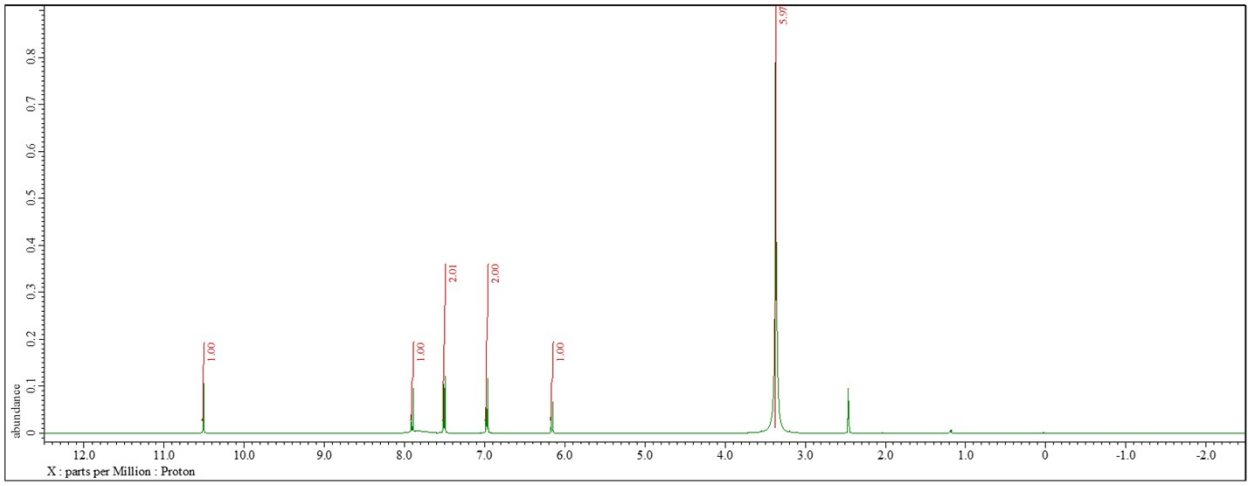



**Figure S7**. $^{1}$H NMR of **2**.

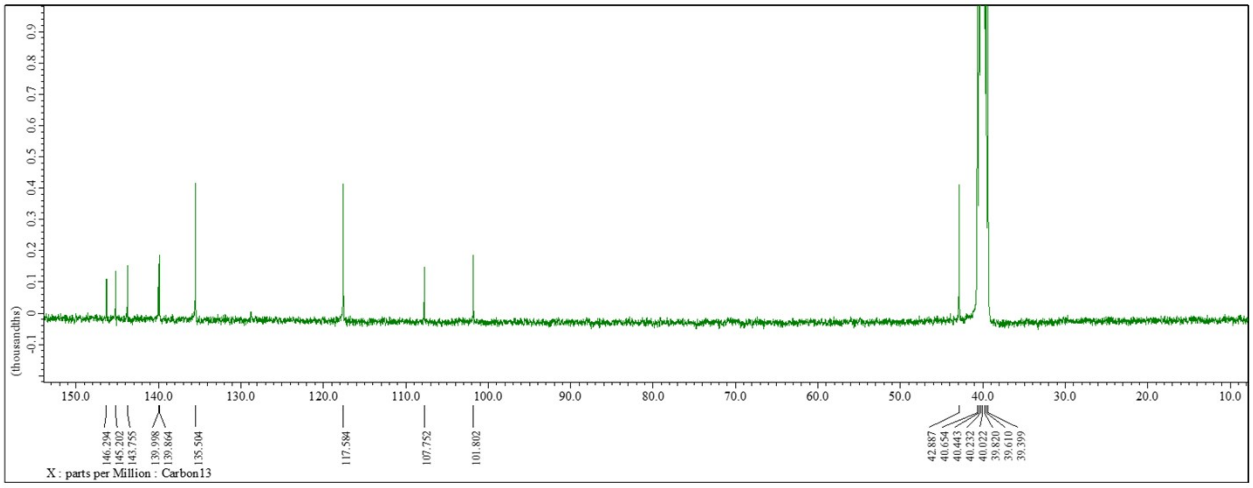
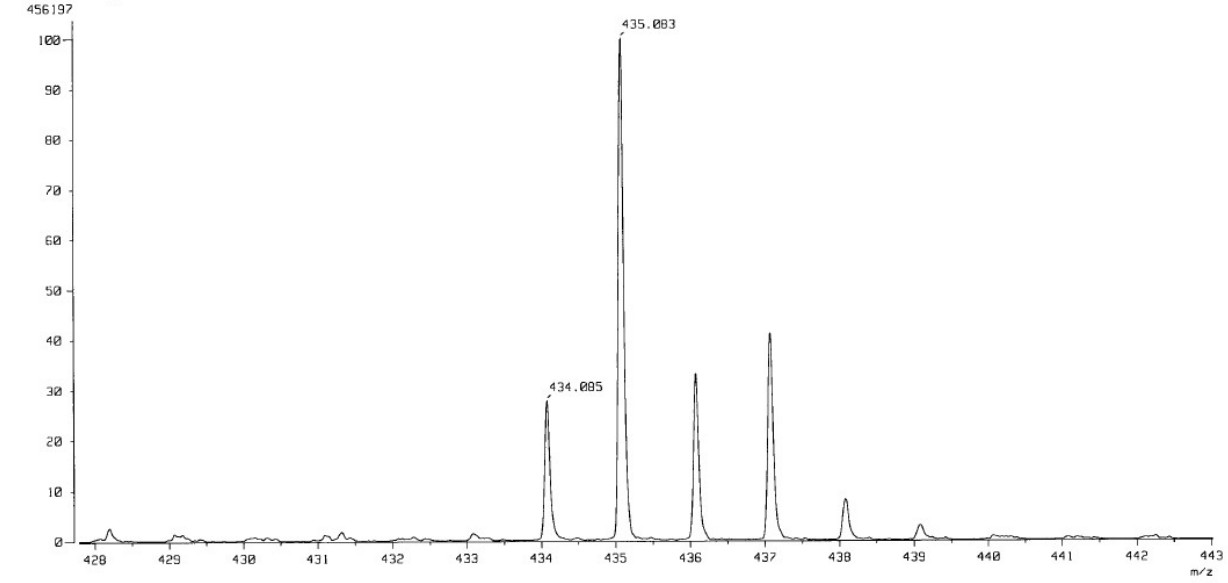



**Figure S8**. $^{13}C$ NMR of **2**.

[ Mass Spectrum ]
Data : 26-YN-1281_Sample4 Date : 11-Mar-2026 10:05
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
Spectrum Type : Normal Ion [EF-Linear]
RT : 0.84 min Scan# : 26
BP : m/z 435.0830 Int. : 41.88
Output m/z range : 427.7893 to 443.0119 Cut Level : 0.00 %




[ Elemental Composition ]
Data : 26-YN-1281_Sample4 Date : 11-Mar-2026 10:05
Sample: -
Note : -
Inlet : Direct Ion Mode : EI+
RT : 0.84 min Scan#: 26
Elements : C 18/0, H 19/0, Cl 1/0, N 3/0, O 5/0, S 1/0, B 1/0
Mass Tolerance : 1mmu
Unsaturation (U.S.) : -0.5 - 1000.0

| Observed m/z | Int% | Err[ppm / mmu] | U.S. | Composition |
|---|---|---|---|---|
| 420.0591 | 43.1 | -0.4 / -0.2 | 12.5 | C 17 H 16 Cl N 3 O 5 S B |
| 421.0652 | 13.1 | | | |
| 422.0723 | 18.6 | | | |
| 423.1115 | 20.3 | | | |
| 434.0854 | 27.8 | | | |
| 435.0830 | 100.0 | +0.6 / +0.3 | 12.0 | C 18 H 19 Cl N 3 O 5 S B |
| 436.0836 | 33.1 | | | |
| 437.0825 | 41.1 | | | |

**Figure S9**. HR-mass spectrum of **3**.

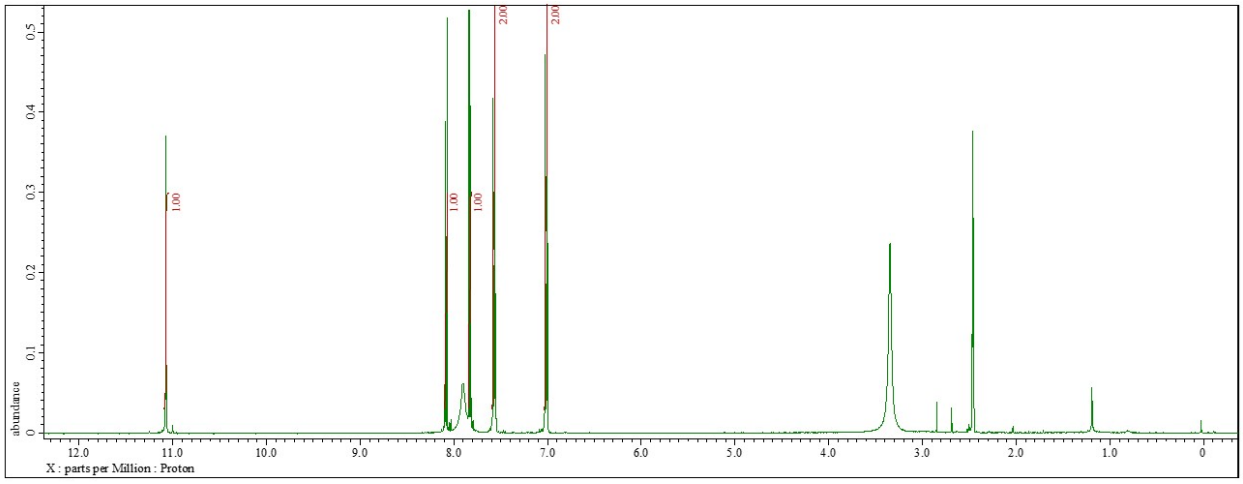



**Figure S10**. $^{1}$H NMR of **3**.

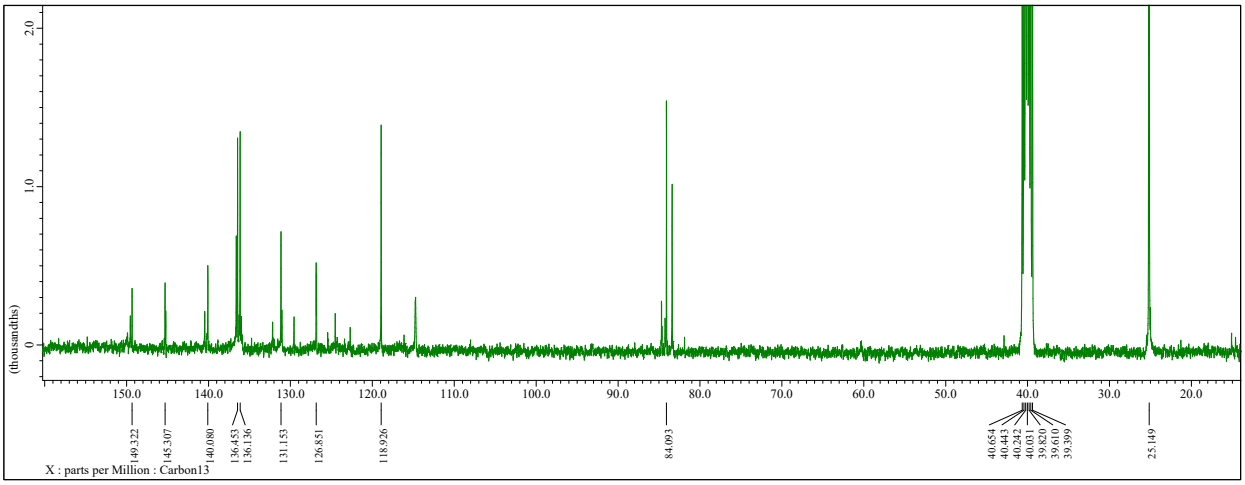



**Figure S11**. $^{13}$C NMR of **3**.

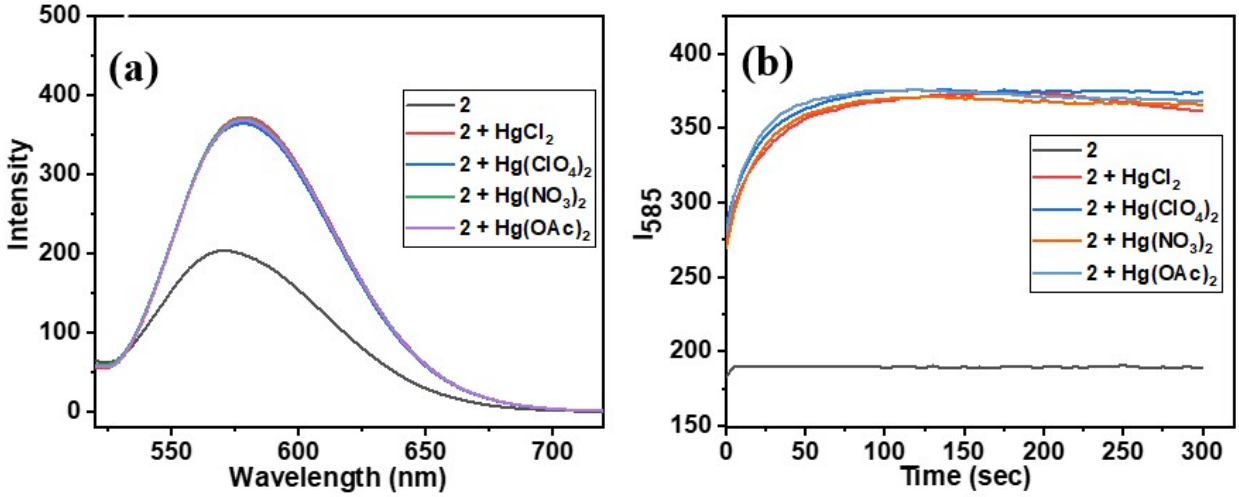



**Figure S12**. (a) Fluorescence emission spectra and (b) time-dependent emission intensity of probe **2** with various mercury salts (5 μM) after 2 min incubation in aqueous buffered solution (pH 7.4) containing 1% DMF.

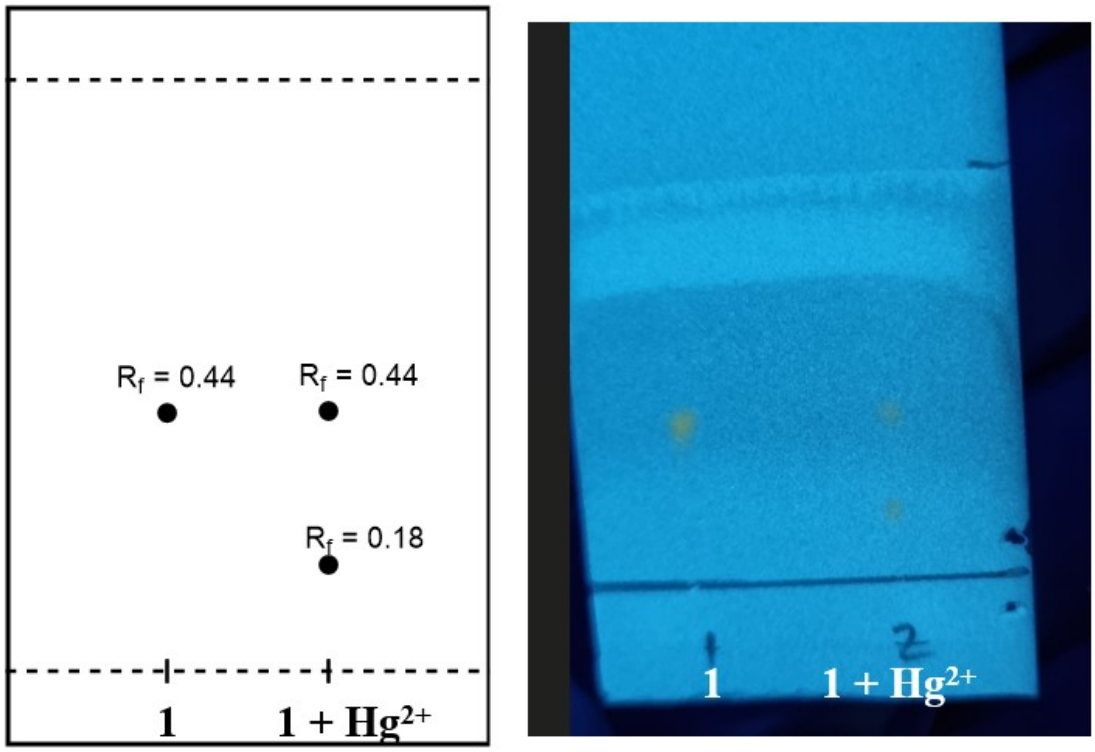



**Figure S13**. $C_{18}$-TLC analysis of probe **1** with Hg(II) in $H_2O$:$CH_3CN$ (80:20)

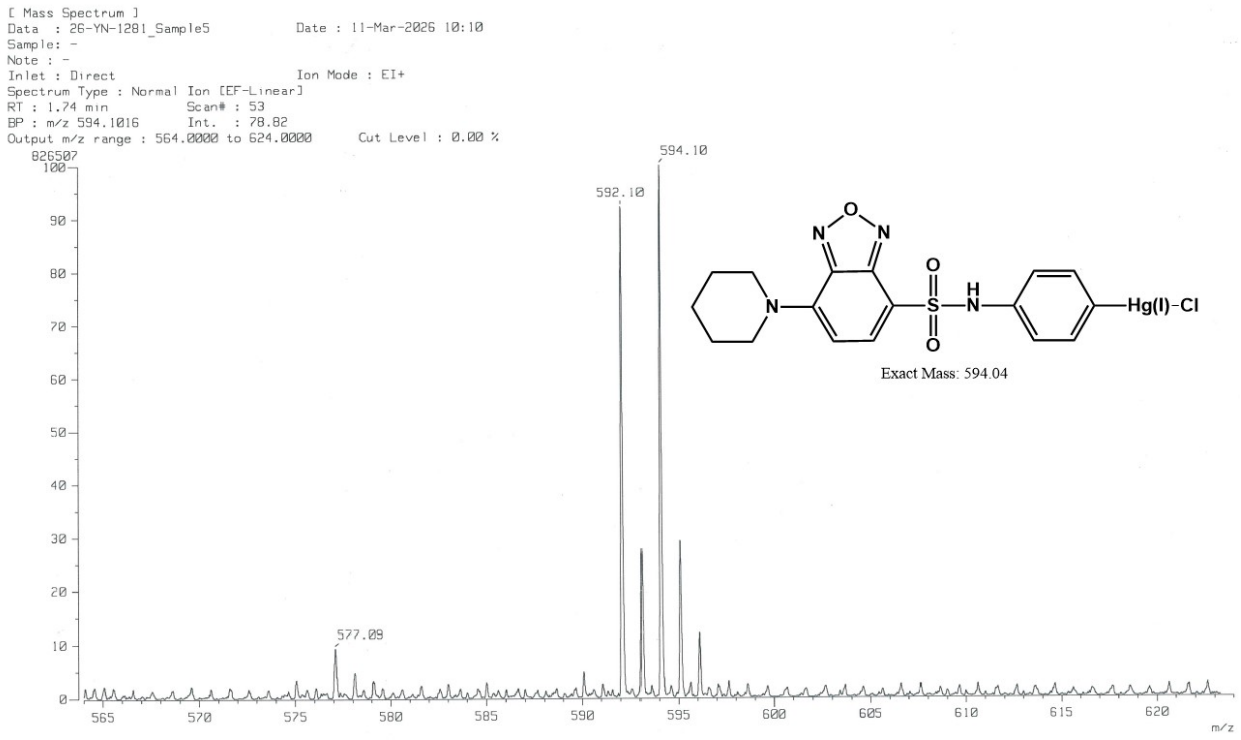



**Figure S14**. mass spectrometric analysis of the reaction product using FAB mass spectrometry.

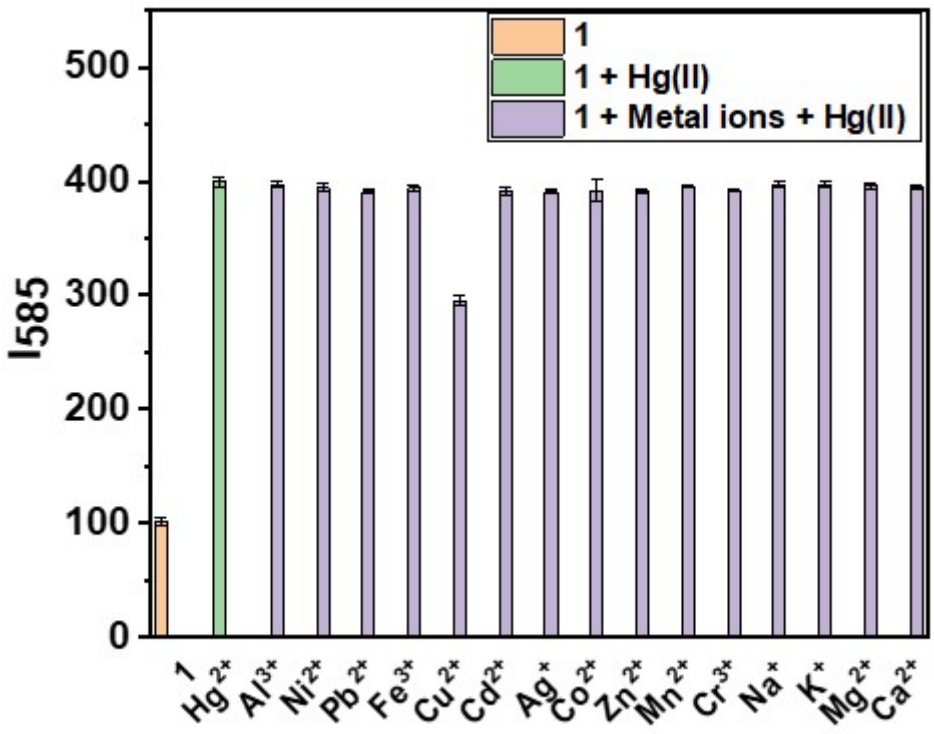



**Figure S15**. Fluorescence emission intensity of **1** with $Hg^{2+}$ in the presence of coexisting metal ions in aqueous buffered solution (10 mM HEPES, pH 7.4) containing 1% DMF. The concentrations of probe **1**, heavy metal ions, and Group I and II metal ions were 5 μM, 10 μM, and 1000 μM, respectively.

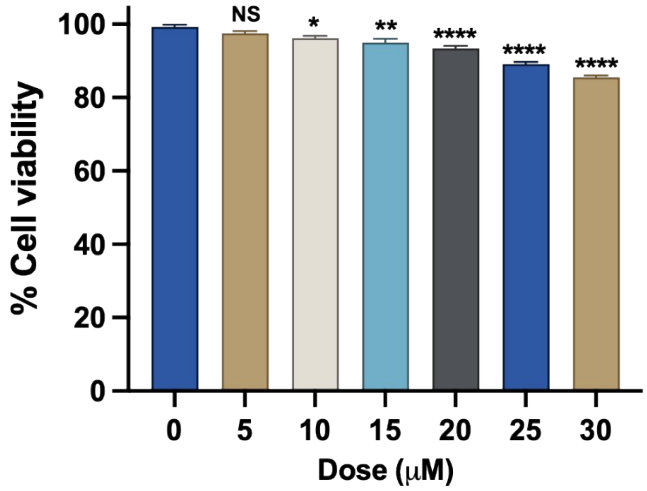



**Figure S16**. Cell toxicity study of probe **1** using an ATP-Glo assay.

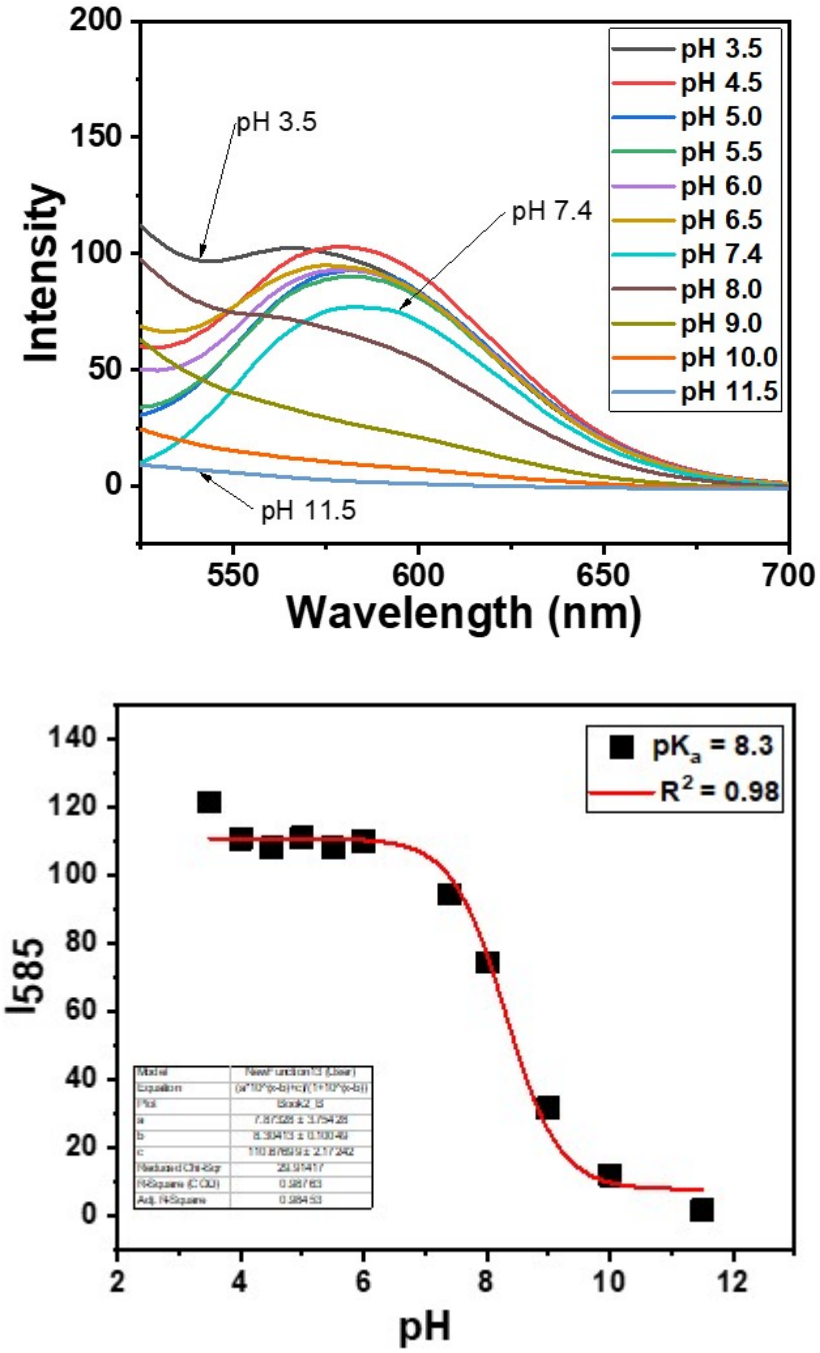



**Figure S17**. Emission intensity changes of probe **1** (5 μM) at different at pHs for determination of p$K_a$ value.

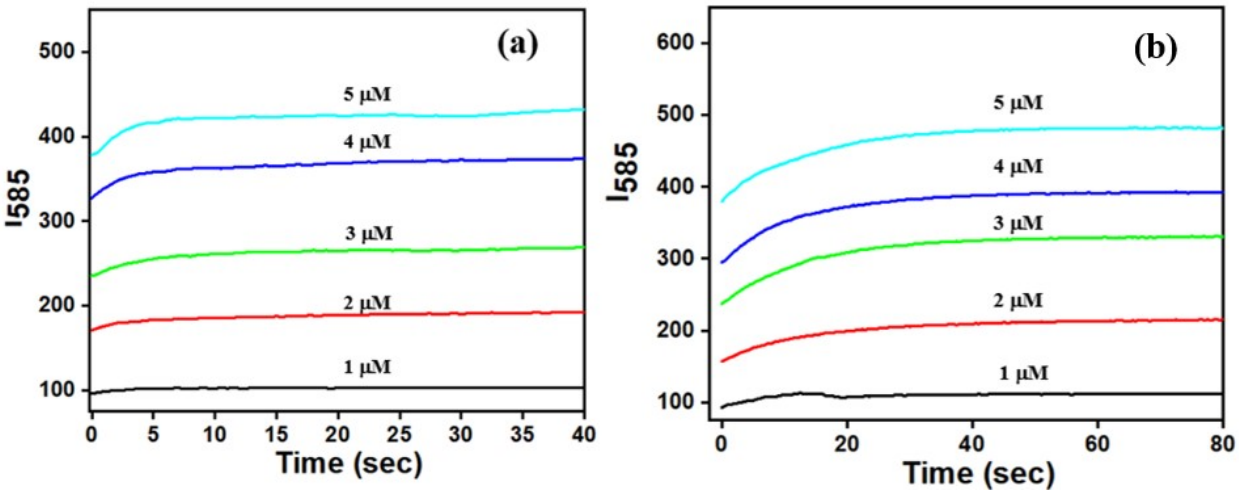
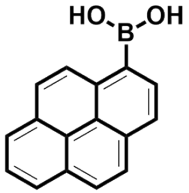
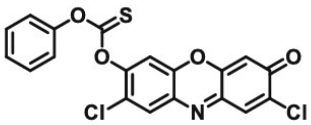
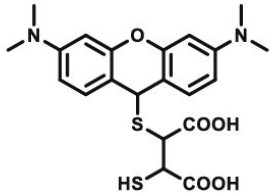
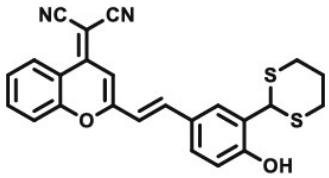


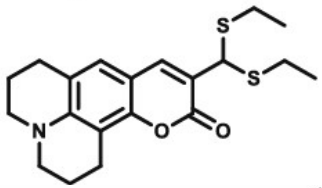
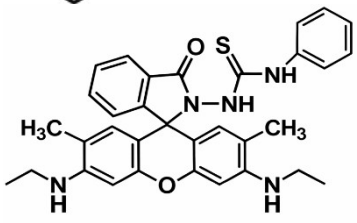
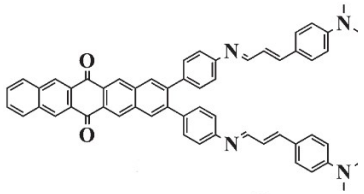
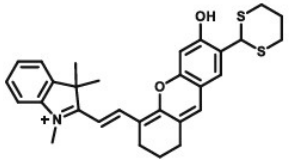
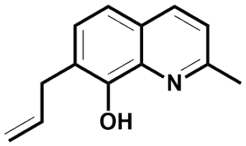

**Figure S18**. Time-dependent fluorescence intensity profiles of probe **1** (1, 2, 3, 4, and 5 μM) with $Hg^{2+}$ (50 μM) in aqueous solution (10 mM HEPES, pH 7.4) including (a) 10% DMF and (b) 20% DMF.

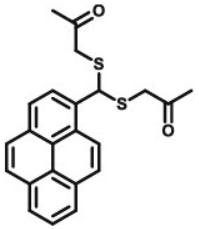
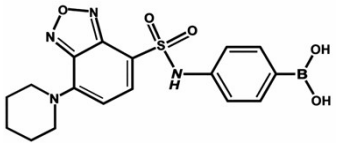
**Table S1.** Recovery of spiked $Hg^{2+}$ in real natural water samples using probe **1**.

| Sample | Spiked $Hg^{2+}$ (nM) | Measured concentration of $Hg^{2+}$ using the probe (nM) | Recovery (%) |
|---|---|---|---|
| Tap water | 0 | 0 | 100 ± 0.1 |
| | 200 | 186.06 | 93.1 ± 0.2 |
| | 400 | 393.48 | 98.4 ± 0.2 |
| | 600 | 557.68 | 92.9 ± 0.2 |
| | 800 | 799.67 | 99.9 ± 0.1 |
| | 1000 | 955.23 | 95.5 ± 0.3 |
| Ground water | 0 | 0 | 100 ± 0.1 |
| | 200 | 194.7109 | 97.3 ± 0.1 |
| | 400 | 393.4837 | 98.3 ± 0.2 |
| | 600 | 566.3296 | 94.3 ± 0.1 |
| | 800 | 808.3139 | 101.1 ± 0.3 |
| | 1000 | 972.5175 | 97.2 ± 0.2 |

**Table S2.** Detection properties of reported turn-on fluorescent chemodosimeters for $Hg^{2+}$ ions.

| Probe Structure | $\lambda_{ex}/\lambda_{em}$ (nm) | Working solvent (v/v) | Saturation concentration of $Hg^{2+}$ | Response time | LOD | Reference |
|---|---|---|---|---|---|---|
|  | 337/387 | $H_2O$:$CH_3OH$ (1:1) | 1 equiv. | 20 min | 6.6 nM | 1 |
|  | 530/595 | 100% $H_2O$ (HEPES Buffer, pH 7.4) | 1 equiv. | 30 min | 0.49 nM | 2 |
|  | 490/570 | 100% $H_2O$ (PBS Buffer, 7.4) | 1 equiv. | ~3 min | 3 nM | 3 |
|  | 514/659 | $H_2O$:DMSO (1:1) (PBS Buffer, pH 7.4) | 15 equiv. | 40 min | 68 nM | 4 |

| | | | | | | |
|---|---|---|---|---|---|---|
|  | 395/500 | $H_2O$:DMSO (9:1) (HEPES Buffer, pH 7.4) | 1 equiv. | 30 min | 90 nM | 5 |
|  | 500/556 | $H_2O$:$CH_3OH$ (20:80) | 1 equiv. | 5 min | 10 nM | 6 |
|  | 380/462 | $H_2O$:THF (0.5:9.5) (HEPES Buffer, pH 7.0) | 200 equiv. | 5 min | 620 nM | 7 |
|  | 630/710 | 100% $H_2O$ (HEPES buffer, pH 7.4) | 1 equiv. | 5 min | 320 nM | 8 |
|  | 322/485 | $H_2O$:$CH_3CN$ (99.8:0.2) | 1 equiv. | NA | 6.2 nM | 9 |

| | | | | | | |
|---|---|---|---|---|---|---|
|  | 375/457 | $H_2O$:$CH_3CH_2OH$ (1:2) (PBS Buffer, pH 7.4) | 1 equiv. | 30 min | 1.49 nM | 10 |
|  | 440/585 | $H_2O$:DMF (99:1) (HEPES Buffer, pH 7.4) | 1 equiv. | 1~2 min | 7.56 nM | This Work |

**References**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