Supporting Information

Novel Sulfonamido Spirobifluorene as Fluorescent Sensorsfor Mercury(II) Ion and Glutathione

Komthep Silpcharu^a, Mongkol Sukwattanasinitt^a, Paitoon Rashatasakhon^{a,*}

^aDepartment of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330,

Thailand



Figure S1. Fluorescence emission spectra of (A) DSS (10μ M)and (B)TSS(10μ M) in various solvents



Figure S2. Fluorescence spectra of (A) $DSS(10\mu M)$ and (B) $TSS(10\mu M)$ in various water/DMSO ratios.



Figure S3. Absorption spectra of (A) **DSS**(10μ M) and (B) **TSS**(10μ M) in various water/DMSO ratios.



Figure S4. Fluorescence responses of (A) **DSS**(10 μ M) and (B) **TSS**(10 μ M) in the presence of Hg(II) (100 μ M) andforeign ions (1000 μ M)



Figure S5. UV spectra of (A) 10 μ M **DSS**, (B) 1000 μ M Fe(OAc)₂, and (C) 10 μ M **DSS** + 1000 μ M Fe(OAc)₂in 50% of 10 mM HEPES buffer in DMSO, pH 7.0.



Figure S6. pH effects on emission intensities of (A) **DSS**(10μ M) and (B)**TSS** (10μ M) before and after addition of Hg(II) (100μ M)



Figure S7. Fluorescence spectra of (A) DSS (10μ M) and (B) TSS (10μ M) with Hg(II) (100μ M) and various amounts of EDTA



Figure S8. UV spectra for **DSS** before and after addition of $Hg(OAc)_2$ (5 and 10 eq.) in 50% of 10 mM HEPES buffer in DMSO, pH 7.0. Inset is the photographed image showing the Tyndall effect.



Figure S9. Stern-Volmer plots for (A) DSS (10µM) and (B)TSS (10µM) at 25 and 50°C.



Figure S10. Fluorescence spectra of mixtures between **DSS** (10 μ M) and Hg(II) (100 μ M) in the presence of type of some beverage ingredients (300 μ M).

Table S1. Statistic data

Quantitative Analysis of DSS Sensor

| Туре | [Hg(II)] (ppm) | [Hg(II)] in sample (ppm) | | | | | |
|---------------|-------------------|--------------------------|--------|--------|---------|-------|--|
| | | 1st | 2nd | 3rd | Average | SD | |
| Bottled water | 0.00 | 0.029 | -0.020 | -0.020 | -0.003 | 0.028 | |
| | 0.50 | 0.517 | 0.588 | 0.536 | 0.547 | 0.037 | |
| | 1.00 | 1.000 | 1.053 | 1.012 | 1.022 | 0.028 | |
| Rain water | 0.00 | 0.032 | -0.020 | -0.021 | -0.003 | 0.031 | |
| | 0.50 | 0.423 | 0.523 | 0.500 | 0.482 | 0.052 | |
| | 1.00 | 1.096 | 1.017 | 1.009 | 1.041 | 0.048 | |
| Tap water | 0.00 | 0.006 | -0.005 | -0.013 | -0.004 | 0.009 | |
| | 0.50 | 0.486 | 0.557 | 0.473 | 0.506 | 0.045 | |
| | 1.00 | 1.122 | 1.027 | 1.016 | 1.055 | 0.058 | |
| P-value | | 0.12 | 0.12 | 0.12 | 0.13 | | |

Quantitative Analysis of TSS Sensor

| Туре | [Hg(II)] (ppm) | [Hg(II)] in sample (ppm) | | | | | |
|---------------|-------------------|--------------------------|--------|--------|---------|-------|--|
| | | 1st | 2nd | 3rd | Average | SD | |
| | 0.00 | 0.017 | -0.011 | -0.034 | -0.009 | 0.026 | |
| Bottled water | 0.50 | 0.597 | 0.532 | 0.568 | 0.565 | 0.032 | |
| | 1.00 | 0.971 | 1.104 | 0.996 | 1.024 | 0.071 | |
| Rain water | 0.00 | 0.019 | 0.010 | -0.060 | -0.011 | 0.043 | |

| | 0.50 | 0.515 | 0.435 | 0.471 | 0.474 | 0.040 |
|-----------|------|-------|--------|-------|--------|-------|
| | 1.00 | 1.197 | 1.034 | 1.072 | 1.101 | 0.085 |
| | 0.00 | 0.009 | -0.106 | 0.071 | -0.009 | 0.090 |
| Tap water | 0.50 | 0.576 | 0.518 | 0.441 | 0.512 | 0.067 |
| | 1.00 | 1.086 | 1.226 | 1.036 | 1.116 | 0.099 |
| P-value | | 0.10 | 0.15 | 0.15 | 0.13 | |

Quantitative Analysis of ICP-OES

| | | [Hg(II)] in sample (ppm) | | | | | |
|---------------|-------|--------------------------|-------|---------|-------|--|--|
| Туре | (ppm) | Hg1 | 849 | Hg1942 | | | |
| | | Average | SD | Average | SD | | |
| Bottled water | 0.00 | 0.025 | 0.001 | 0.027 | 0.002 | | |
| | 0.50 | 0.571 | 0.011 | 0.559 | 0.012 | | |
| | 1.00 | 1.082 | 0.019 | 1.071 | 0.016 | | |
| Rain water | 0.00 | 0.032 | 0.006 | 0.040 | 0.005 | | |
| | 0.50 | 0.504 | 0.032 | 0.500 | 0.034 | | |
| | 1.00 | 1.118 | 0.022 | 1.096 | 0.015 | | |
| Tap water | 0.00 | 0.028 | 0.004 | 0.033 | 0.004 | | |
| | 0.50 | 0.513 | 0.030 | 0.507 | 0.033 | | |
| | 1.00 | 1.185 | 0.036 | 1.173 | 0.031 | | |
| P-value | | 0.09 | | 0.09 | | | |



Figure S11.¹H-NMR spectrum of compound 2a.



Figure S12.¹³C-NMR spectrum of compound 2a.



Figure S13.Mass spectrum of compound 2a.



Figure S14.¹H-NMR spectrum of compound 2b.



Figure S15.¹³C-NMR spectrum of compound 2b.



Figure S16.Mass spectrum of compound 2b.



Figure S17.¹H-NMR spectrum of compound 3a.



Figure S18.¹³C-NMR spectrum of compound 3a.



Figure S19. Mass spectrum of compound 3a.



Figure S20.¹H-NMR spectrum of compound 3b.



Figure S21.¹³C-NMR spectrum of compound 3b.



Figure S22. Mass spectrum of compound 3b.



Figure S23.¹H-NMR spectrum of compound CH₃SO₂NH-C₆H₄-I.



Figure S24.¹³C-NMR spectrum of compound CH₃SO₂NH-C₆H₄-I.

Figure S25. High resolution mass spectrum of compound CH₃SO₂NH-C₆H₄-I.

Figure S26.¹H-NMR spectrum of DSS.

Figure S27.¹³C-NMR spectrum of DSS.

Figure S28.Mass spectrum of DSS.

Figure S29.¹H-NMR spectrum of TSS.

Figure S30.¹³C-NMR spectrum of TSS.

Figure S31.Mass spectrum of TSS.