

Electronic Supplementary Information

Highly Sensitive and Selective Detection of Hg²⁺ in Aqueous Solution with Mercury Specific DNA and Sybr Green I

Experimental Section

MSD (5'-TTCTTTCTTCCCCTTGTTTGTT-3') and the non-cognate oligonucleotide sequence (5'-AAGAAAGAAGGGGAACAAACAA-3') were synthesized and HPLC purified from research biolab Inc. (Singapore). SG (10000×) was purchased from invitrogen inc. When in use, it was diluted to 250× with DMSO, then to 125× with water to make a stock solution. The concentration of 125× SG solution is calculated to be 2.45×10^{-4} M according to the research from Vitzthum, et al in 2004.¹ Other chemicals were all ordered from Sigma. 1.58×10^{-8} M MSD was first incubated with different amount of Hg²⁺ in 3 mL of 10 mM MOPS buffer containing 0.1 M NaNO₃, pH 7.5. 1 uL of 125× SG was then added to the solution. After incubation for two minutes, the mixture was used for the fluorescence study with a Perkin-Elmer LS-55 fluorometer equipped with a xenon lamp excitation source and a Hamamatsu (Japan) 928 PMT. CD measurements were carried out using Jasco J-810 spectropolarimeter (Japan) with a 1 mm optical path cell.

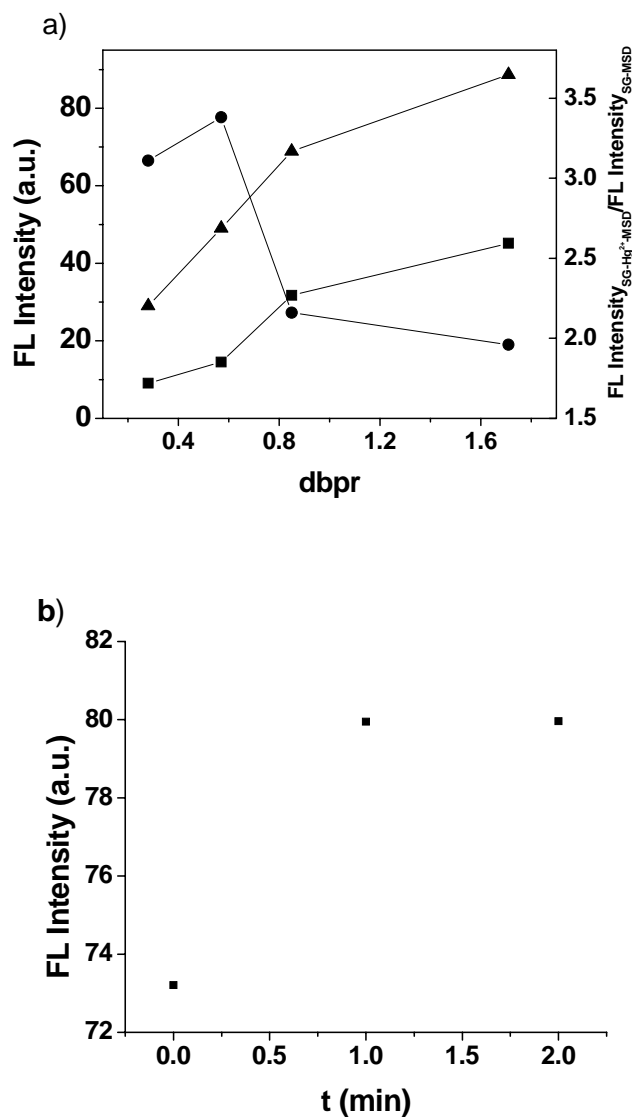


Figure S1. a) Relationship between fluorescence intensity and dbpr for SG-Hg²⁺-MSD and SG-MSD. Squares and triangles represent the fluorescence intensities of SG-MSD and SG-Hg²⁺-MSD, respectively; circles are the ratios of the fluorescence intensity of SG-Hg²⁺-MSD to that of SG-MSD. b) Relationship between the fluorescence intensity and incubation time for SG to interact with Hg²⁺-MSD. [MSD] = 1.58×10^{-8} M and [Hg²⁺] = 9.96 nM were used for optimization of dbpr. [MSD] = 1.58×10^{-8} M, [Hg²⁺] = 16.61 nM and [SG] = 8.14×10^{-8} M were used for (b). 10 mM MOPS, 0.1 M NaNO₃, pH 7.5 was used as the buffer.

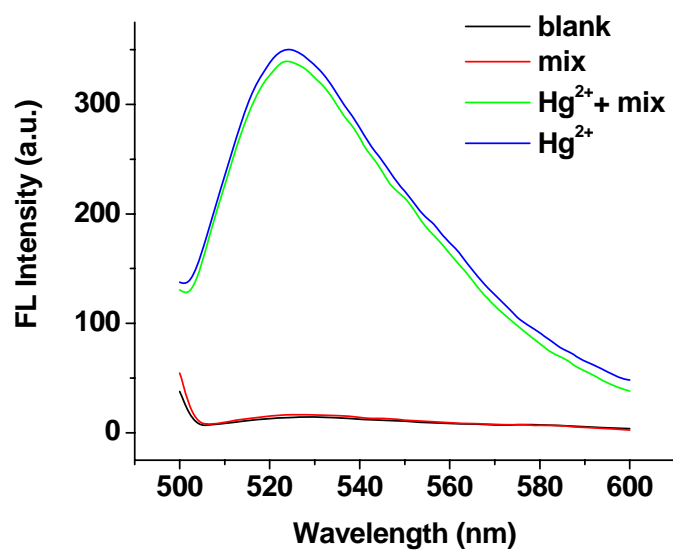


Figure S2. Fluorescence spectra of solutions containing MSD only (blank), MSD with mixture of Co^{2+} , Cu^{2+} , Ni^{2+} , Pb^{2+} , Cd^{2+} , Ca^{2+} , Mg^{2+} , Ba^{2+} , Zn^{2+} ions in the presence and absence of Hg^{2+} , and MSD with Hg^{2+} only. $[\text{MSD}] = 1.58 \times 10^{-8} \text{ M}$; $[\text{Hg}^{2+}] = 132.87 \text{ nM}$; $[\text{non-specific ion}] = 1.00 \text{ }\mu\text{M}$ each.

Table S1 Fluorescence data of MSD and non-cognate oligonucleotide (DNAnc) in the absence and presence of Hg²⁺ ^a

MSD: 5'-TTCTTTCTTCCCCTTGTTTGTT-3'

Concentration of Hg ²⁺ /nM	0	33.2	66.4	99.6	166.1
FI	14.5	141.8	280.5	346.8	329.3
Wavelength/nm	528.2	526.2	523.0	524.0	525.1

Non-cognate oligonucleotide: 5'-AACAAACAAGGGGAAGAAAGAA-3'

Concentration of Hg/nM	0	33.2	66.4	332.0	664.0
FI	7.9	11.4	22.0	33.0	23.4
Wavelength/nm	529.0	529.0	529.0	529.2	530.0

a: [MSD] = [DNAnc] = 1.58×10^{-8} M, [SG] = 8.14×10^{-8} M. A buffer of 10 mM MOPS, 0.1 M NaNO₃, pH 7.5 was used.

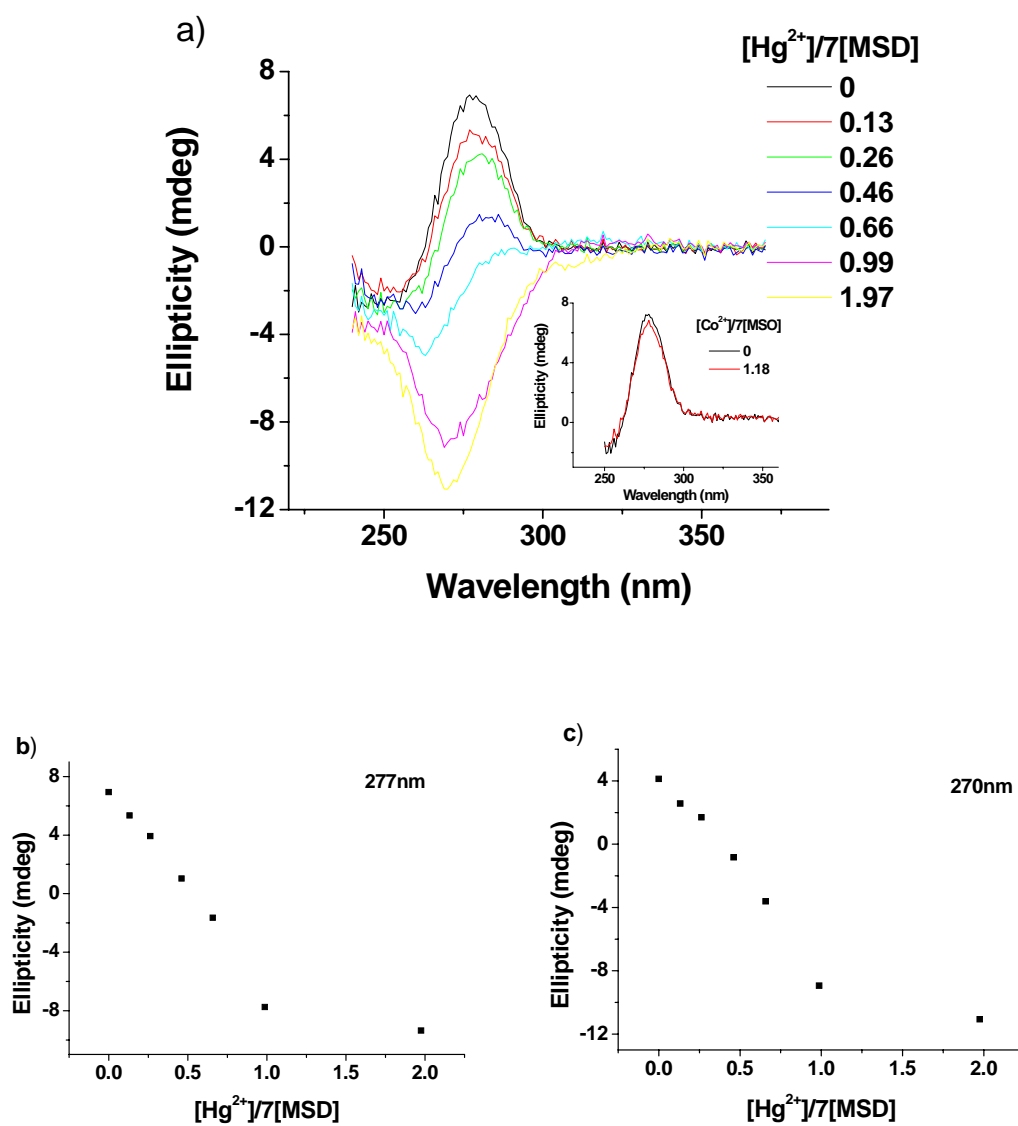


Figure S3. a) CD spectra of MSD upon binding to Hg^{2+} . b), c) Relationships between CD intensities at wavelengths of 277, 270 nm and $[\text{Hg}^{2+}]/7[\text{MSD}]$. $[\text{MSD}] = 18.58 \mu\text{M}$. $[\text{Hg}^{2+}] = 0$ to $256.21 \mu\text{M}$. A buffer of 10 mM MOPS, 0.1 M NaNO_3 , pH 7.5 was used.

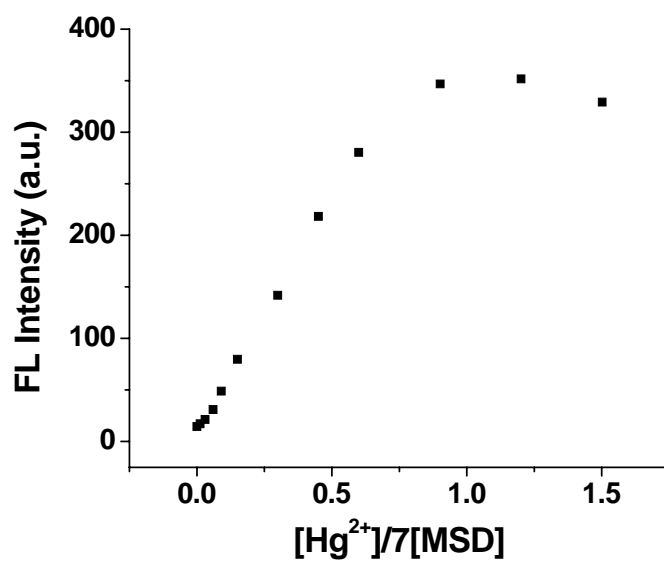


Figure S4. Relationship between the fluorescence intensity of SG-Hg²⁺-MSD vs. [Hg²⁺]/7[MSD]

Reference

- 1 H. Zipper, H. Brunner, J. Bernhagen and F. Vitzthum, *Nucleic Acids Research*, 2004, **32**, e103.