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Supporting Information

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Novel Highly Selective Mercury Sensing in Aqueous Solutions: Fluorescence Resonance Energy Transfer associated with Hairpin Structure Formation of Oligonucleotide Derivatives derived by Mercury-Mediated Thymine-Hg-Thymine Pair Formation

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EXPERIMENTAL SECTION

Preparation of ODN-based sensors

The ODN-based sensors were synthesized using phosphoramidite chemistry on a DNA synthesizer (Applied Biosystems DNA/RNA Synthesizer 392) with commercially available reagents, including a Dabcyl-amidite unit (Glen Research, VA) and Fluorescein-attached-CPG (Glen Research). The ODNs were deprotected and purified using established procedures. Each ODN prepared in this study exhibited a sharp major peak in an HPLC analysis.

Fluorescence spectroscopy

Fluorescence spectra were measured on an RF-5300PC Spectrofluorophotometer (Shimadzu, Japan) at an excitation wavelength of 480 nm with an excitation slit width of 5 nm, and an emission slit width of 5 nm at room temperature.

Preparation of sensors that can detect Hg^{II} ion at various concentrations

In addition to **D-ODN-F** (Figure 1), the ODN-based Hg sensors **D-(T_{21})-F** and **D-($T_4C_4T_4$)-F** (Figure S-1) were synthesized. Figure S-2 shows the fluorescence emission spectra of the sensors in the presence of different concentrations of Hg^{II} ion. As with **D-ODN-F** (Figure 3), the fluorescence intensities of the sensors decreased as the Hg^{II} concentration increased (Figure S-2a and c). However, **D-(T_{21})-F** and **D-($T_4C_4T_4$)-F** were less sensitive to Hg^{II} ion than was **D-ODN-F**. While the fluorescence intensity of **D-ODN-F** was linearly correlated with Hg^{II} over the concentration range from 20 to 100 nM (Figure 3), the intensities of **D-(T_{21})-F** and **D-($T_4C_4T_4$)-F** were linearly correlated with Hg^{II} over concentration ranges from 100 ~ 300 nM and 200 ~ 400 nM, respectively (Figure S-2b and d).

D-(T_{21})-F 5'-Dabcyl-d(**TTTTTTTTTTTTTTTTTTTTT**)-(6-Fluorescein)-3'

D-($T_4C_4T_4$)-F 5'-Dabcyl-d(**TTTTCCCCTTTT**)-(6-Fluorescein)-3'

Figure S-1. Structures of **D-(T_{21})-F** and **D-($T_4C_4T_4$)-F**.

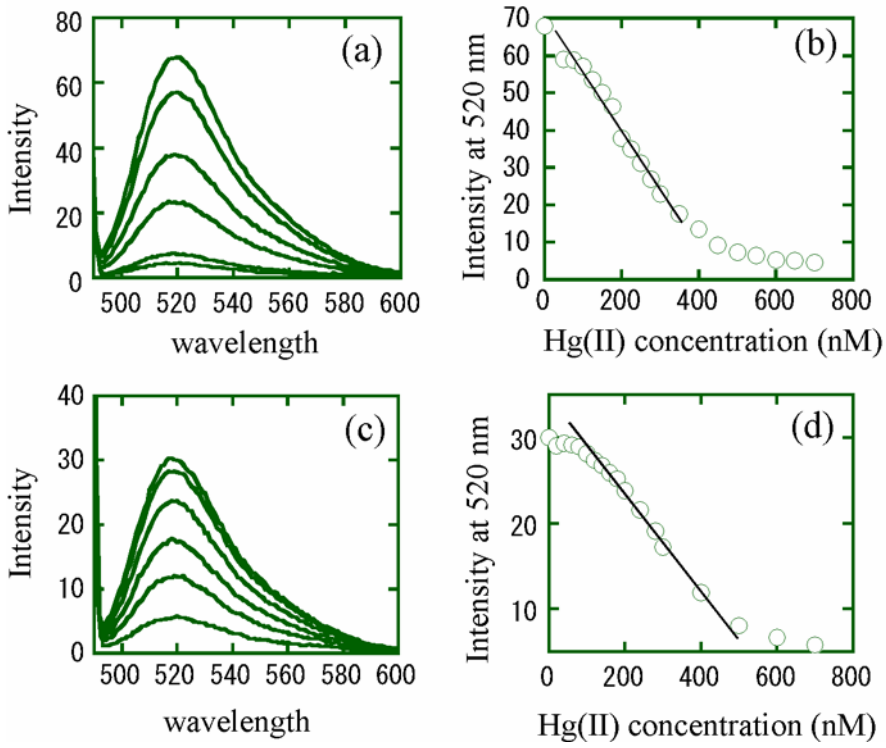

Figure S-2. (a) Fluorescence response of **D-T$_{21}$-F** (10 nM) to Hg^{II} ion at 0, 100, 200, 300, 500, and 700 nM. (b) Fluorescence emission intensity (520 nm) of **D-T$_{21}$-F** vs. Hg^{II} concentration. (c) Fluorescence response of **D-T$_4$C$_4$T$_4$-F** (10 nM) to Hg^{II} ion to 0, 100, 200, 300, 400, and 700 nM. (b) Fluorescence emission intensity (520 nm) of **D-T$_4$C$_4$T$_4$-F** vs. Hg^{II} concentration. A buffer containing 10 mM MOPS (pH 7.0), 25 mM $NaCl_2$, 500 mM $NaNO_3$, and 0.1 mM ethylenediamine was used.