Electronic Supplementary Material (ESI) for Dalton Transactions
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Modified mesoporous silica nanoparticles as a reusable, "naked-eye" selective sensor of mercury(II)

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ELECTRONIC SUPPLEMENTARY INFORMATION

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NMR spectra

^{1}H-NMR and ^{13}C-NMR spectra of 1

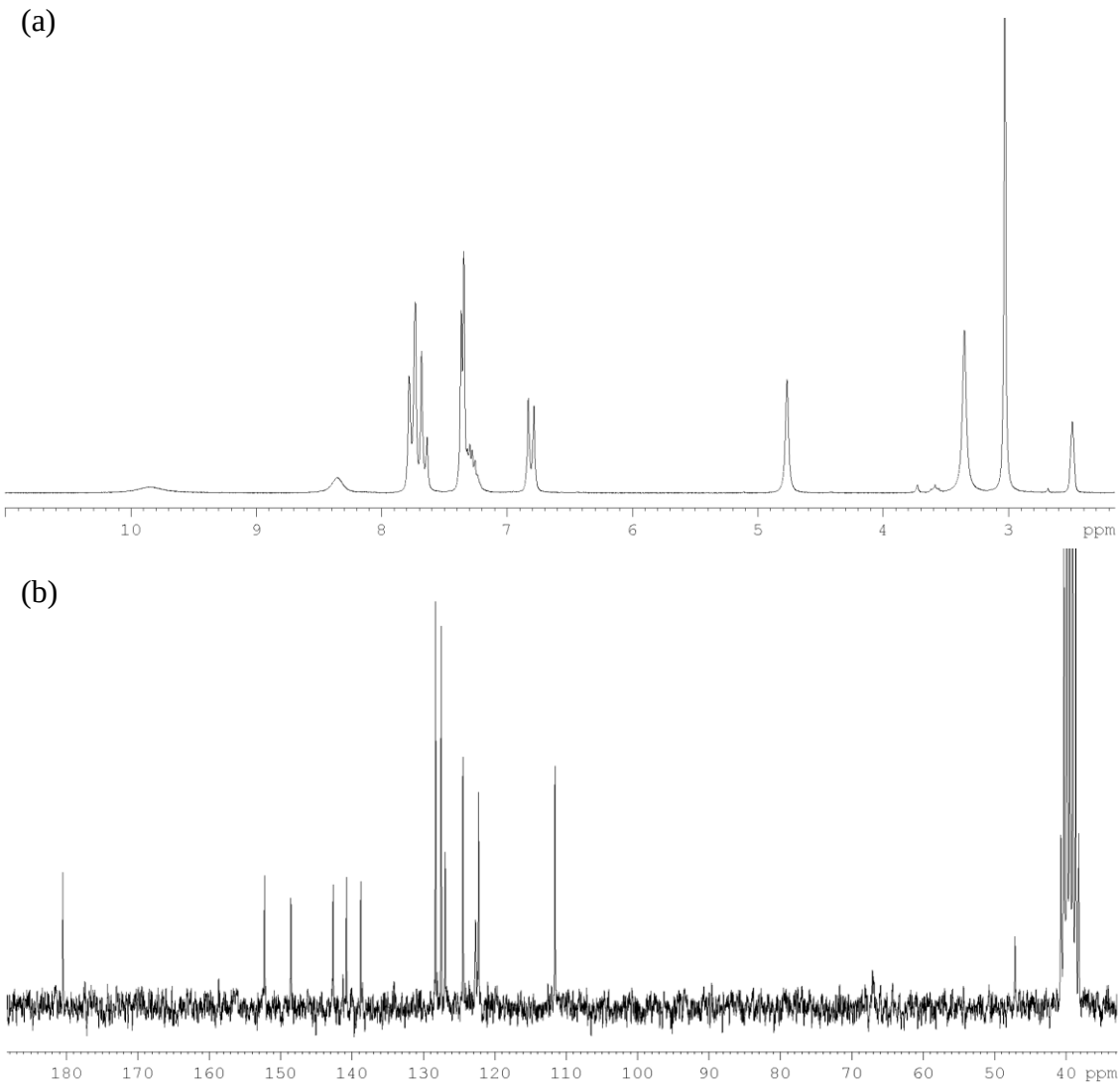

Figure S1. ^{1}H-NMR (a) and ^{13}C-NMR (b) spectra of **1**.

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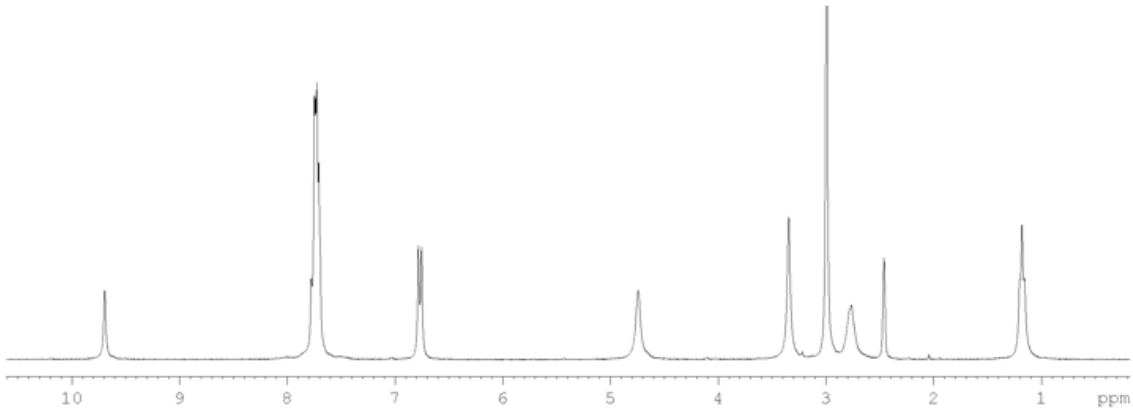
^{1}H-NMR and ^{13}C-NMR spectra of 2

(a)



(b)

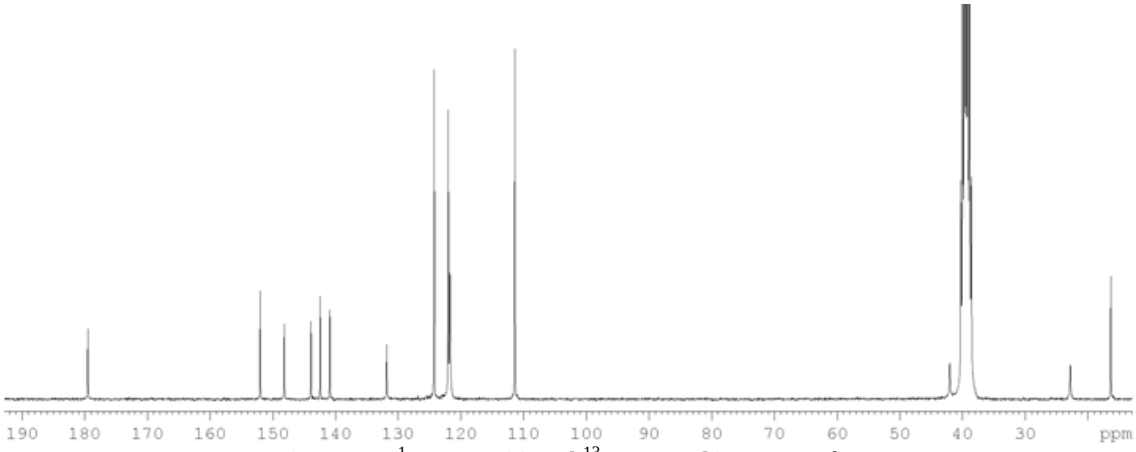


Figure S2. ^{1}H-NMR (a) and ^{13}C-NMR (b) spectra of **2**.

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UV-Vis spectrum of 2

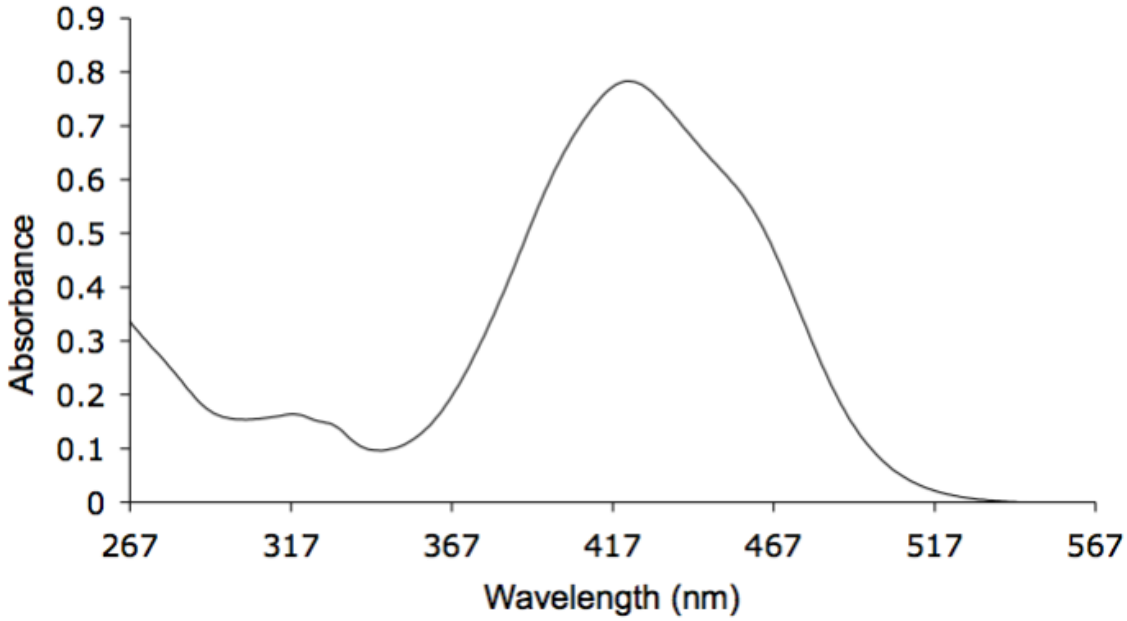

Figure S3. Absorption spectrum of **2** ($c = 10^{-5}$ *M*).

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Irradiation experiments on 2

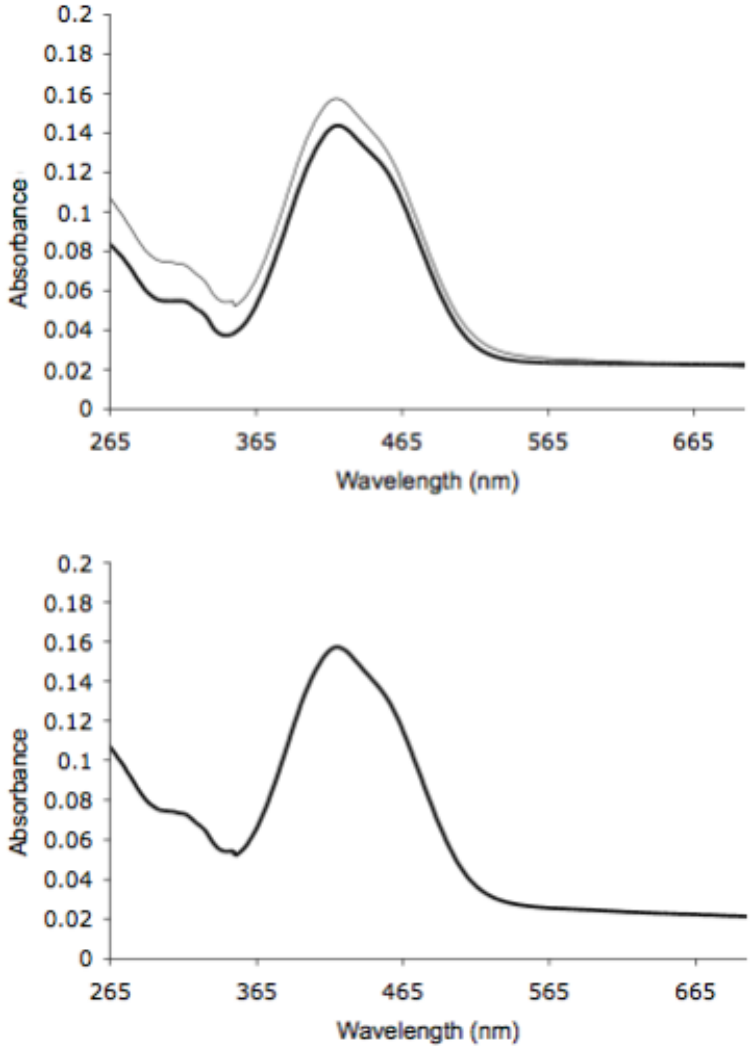

Figure S4. Top: spectrum of **2** (thick line) and spectrum of **2** after irradiation with λ = 500 nm (30 min, thin line, [**2**] = 10^{-5} *M*). Bottom: UV-Vis spectra of **2** before (thick line) and after (thin line, overlapped) irradiation with λ = 360 nm.

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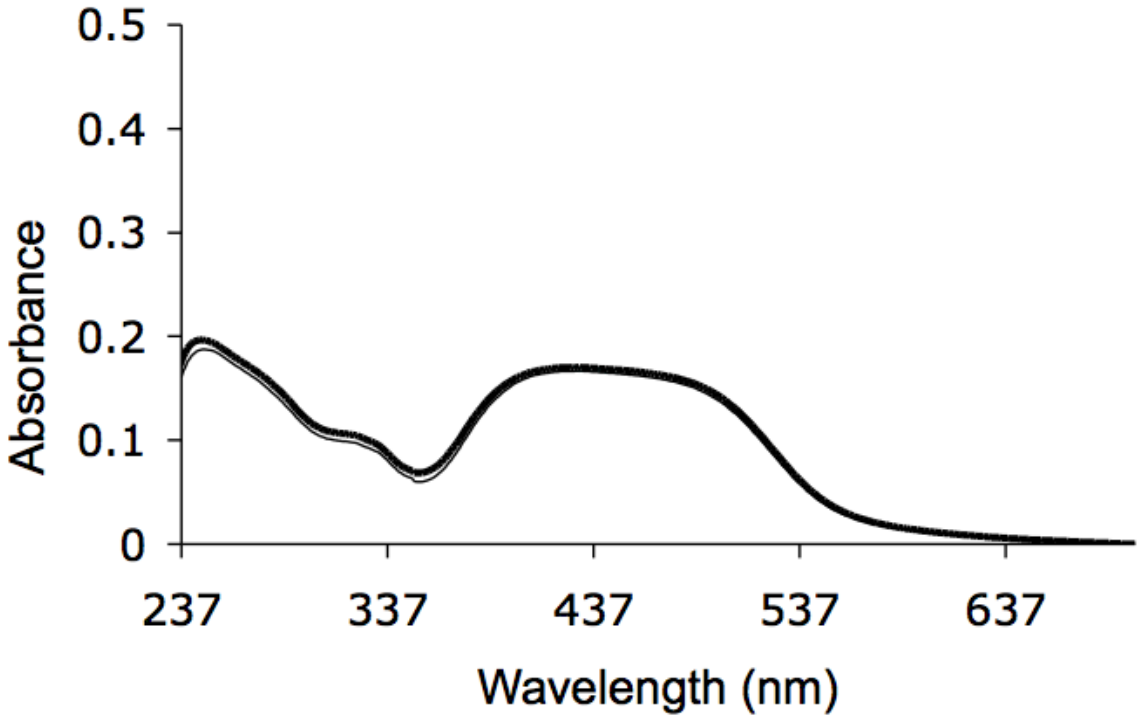

Figure S5. UV-Vis spectrua of the complex [**2**·βCD] before (thick line) and after (thin line) irradiation with λ = 360 nm ([**2**] = 10^{-5} *M*).

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Titrations at different concentrations

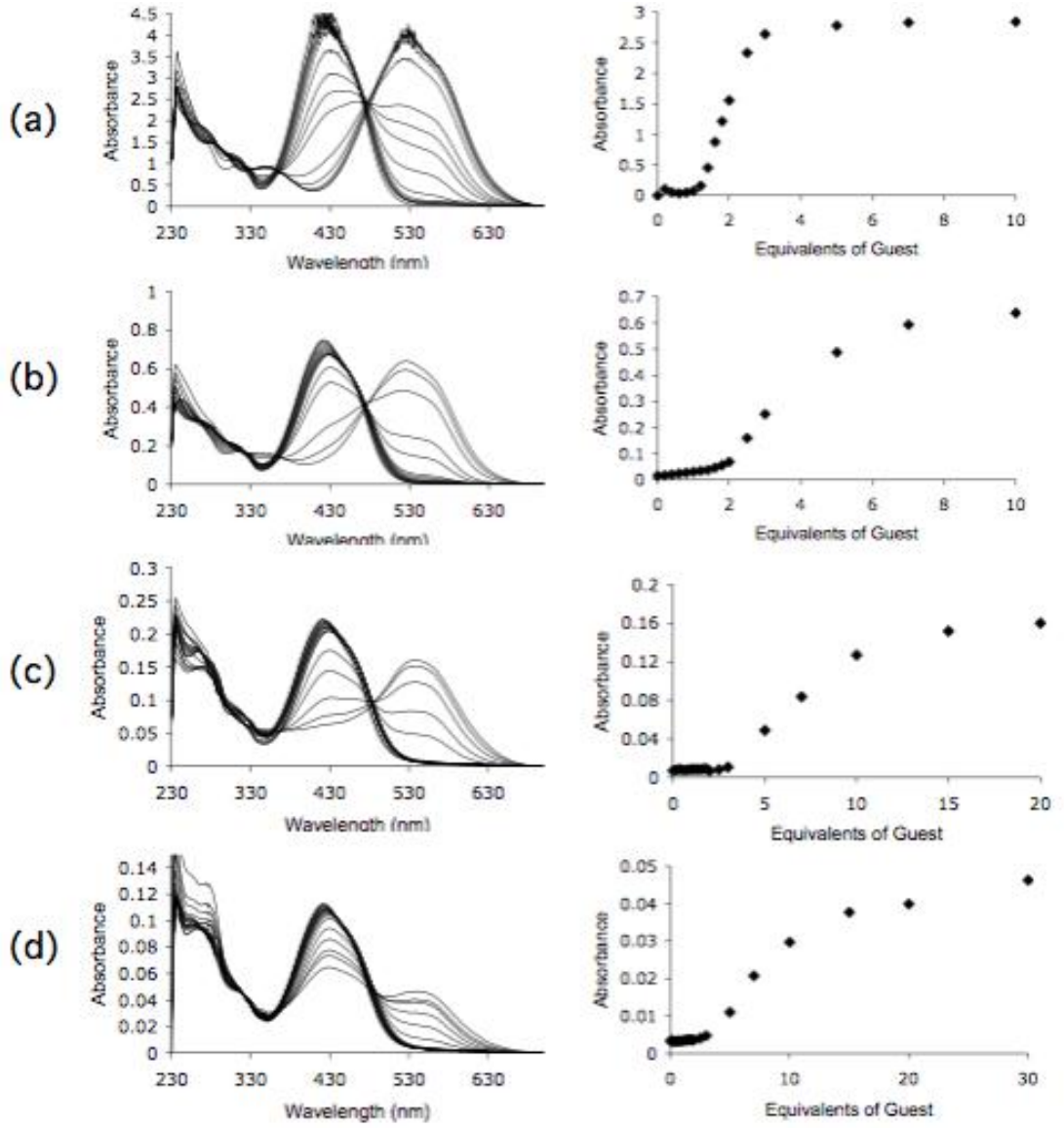

Figure S6. Titrations at different concentrations of host. (a) $5x10^{-5}$ *M*, (b) $5x10^{-6}$ *M*, (c), 10^{-6} *M*, (d) and $5x10^{-7}$ *M*.

Job Plot of [2·Hg]

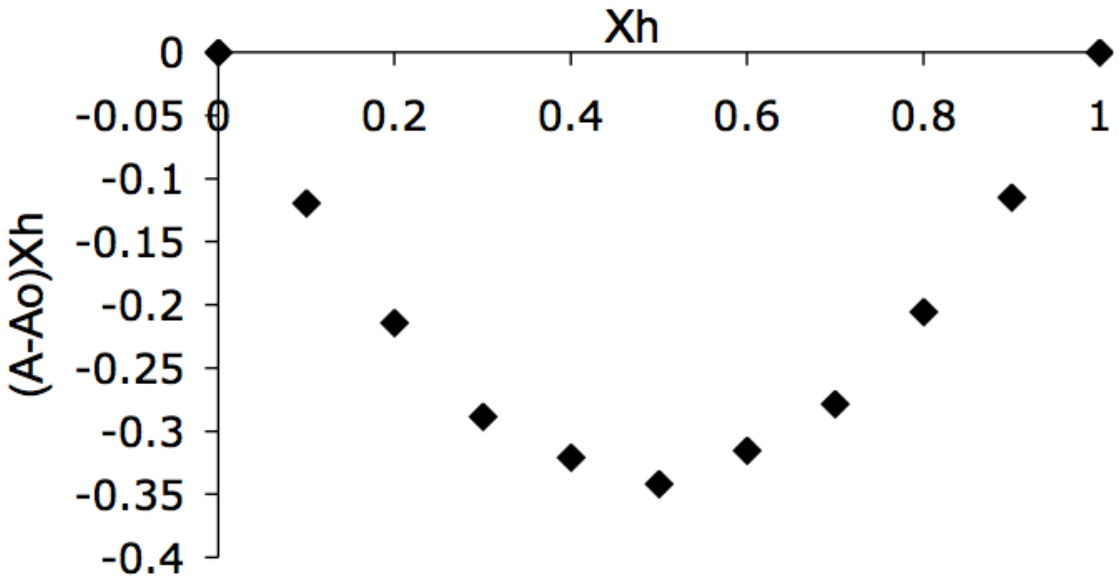

Figure S7. Job Plot of the complex [**2**·Hg] ($c = 10^{-5}$ *M*)

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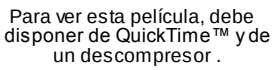
Mass spectra

(a)



(b)

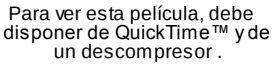


Figure S8. Mass spectra corresponding to the complexes (a) [**2**·Hg] and (b) [**2**·Hg_2]

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Absorption titrations

General procedure

Stock solutions were prepared with HPLC grade solvents. In the case of receptors **1** and **2**, 3 mL of a freshly prepared 10 μ*M* solution were placed in a 1 cm cuvette and a UV spectrum was recorded. Then, aliquots of guest (all the cations as their triflate salts) were added and a spectrum was recorded immediately after each addition giving a set of spectra showing the behavior of the receptor towards each analyte.

For the nanoparticles **3** the same procedure was followed but working with 3 mL of a suspension of solid in the corresponding solvent (1 mg per mL).

Titration of 2 with water

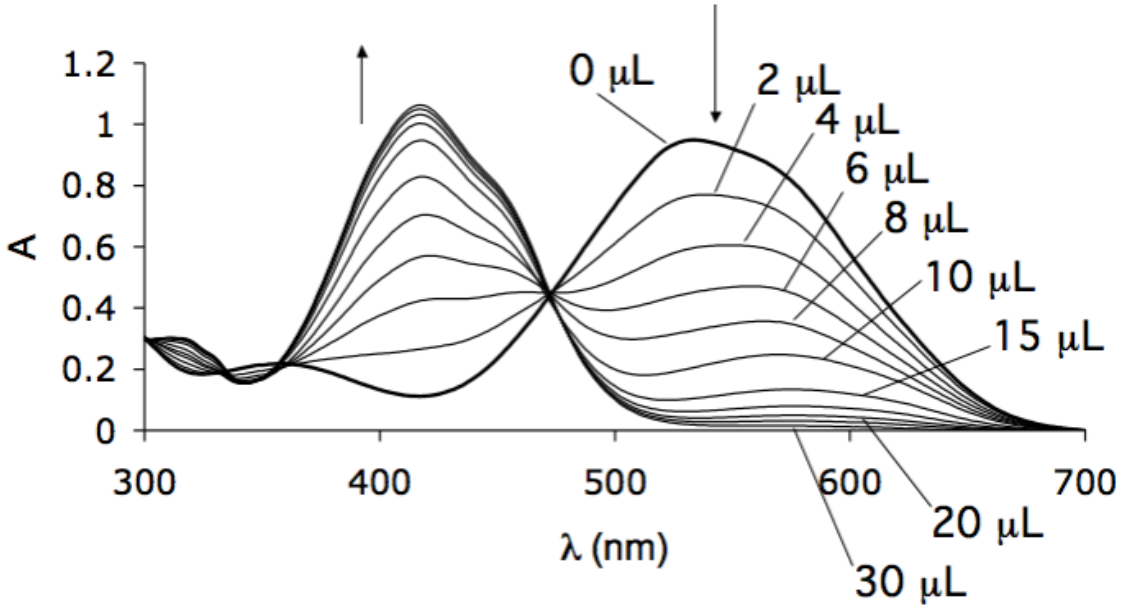

Figure S9. Evolution of absorption spectra of **2** upon addition of various amounts of water.

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Titration of 2 with cadmium and lead

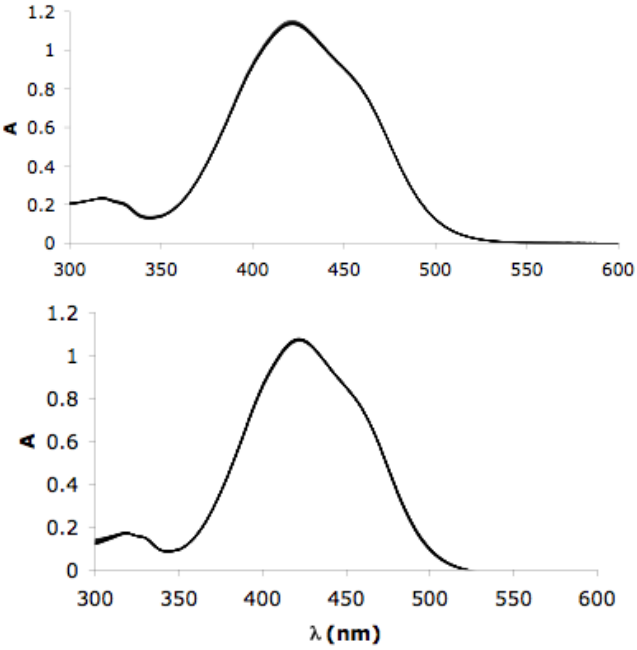

Figure S10. Evolution of absorption spectra of **2** upon titration with $Pb(OTf)_2$ (top) and $Cd(OTf)_2$ (bottom).

Interfering cations

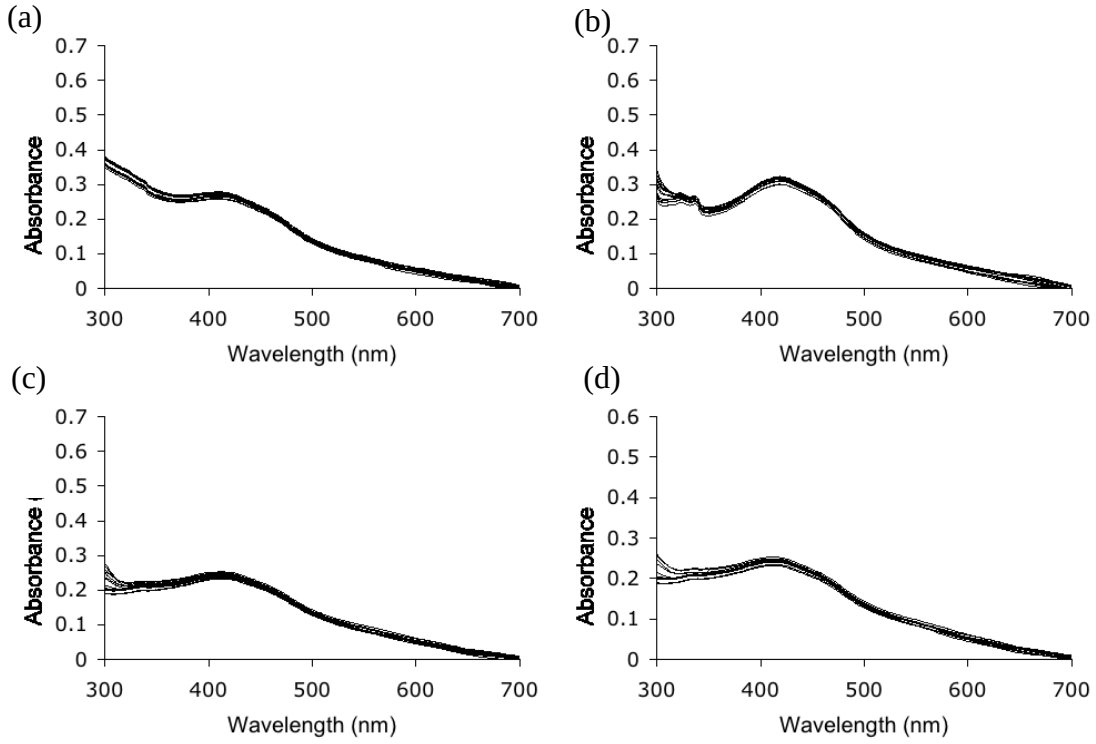

Figure S11. Evolution of absorption spectra upon titration of **3** with (a) Cd(II), (b) Zn(II), (c) Pb(II) and (d) Ag(I).

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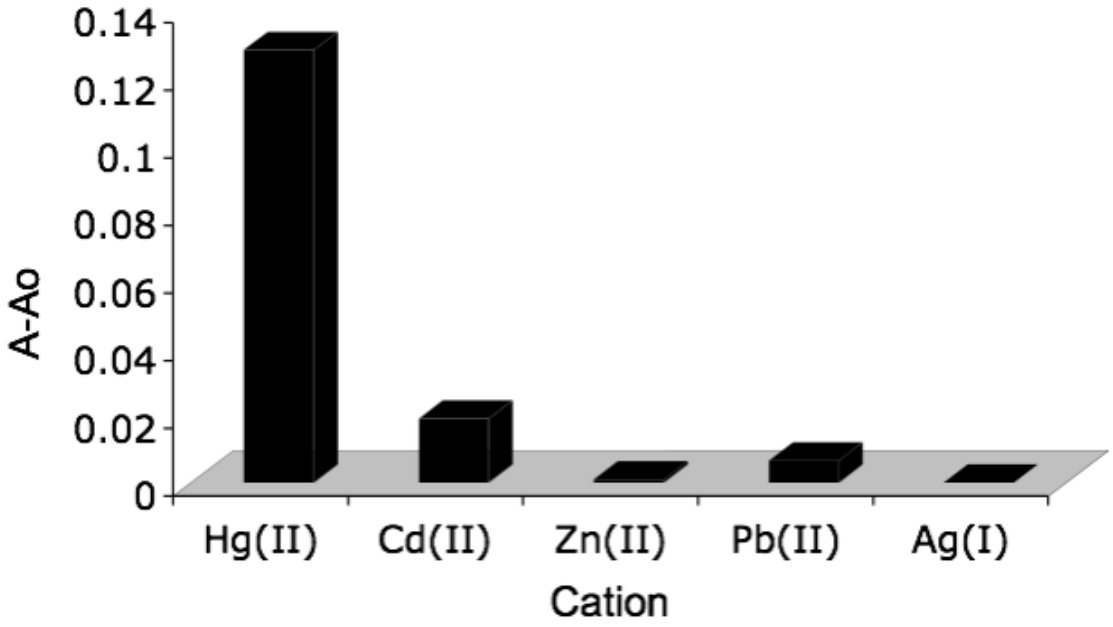

Figure S12. Comparative plot showing the selective response of **3** towards mercury(II).

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FT-IR ATR spectrum of 3

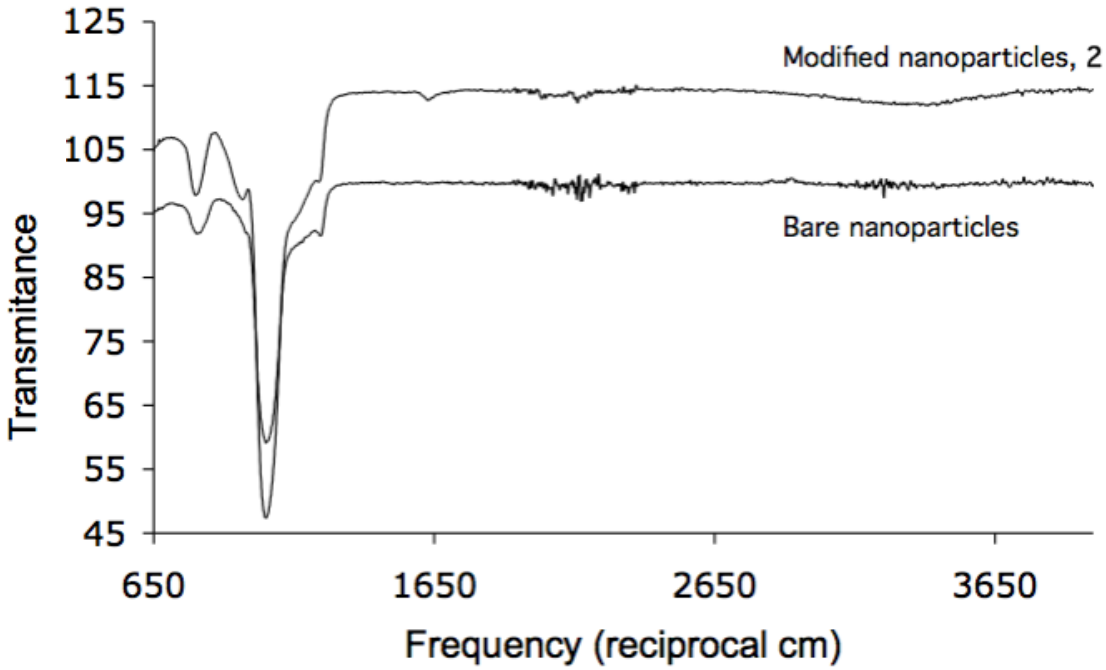

Figure S13. Selected FT-IR ATR spectra.

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UV-Vis spectrum of 3

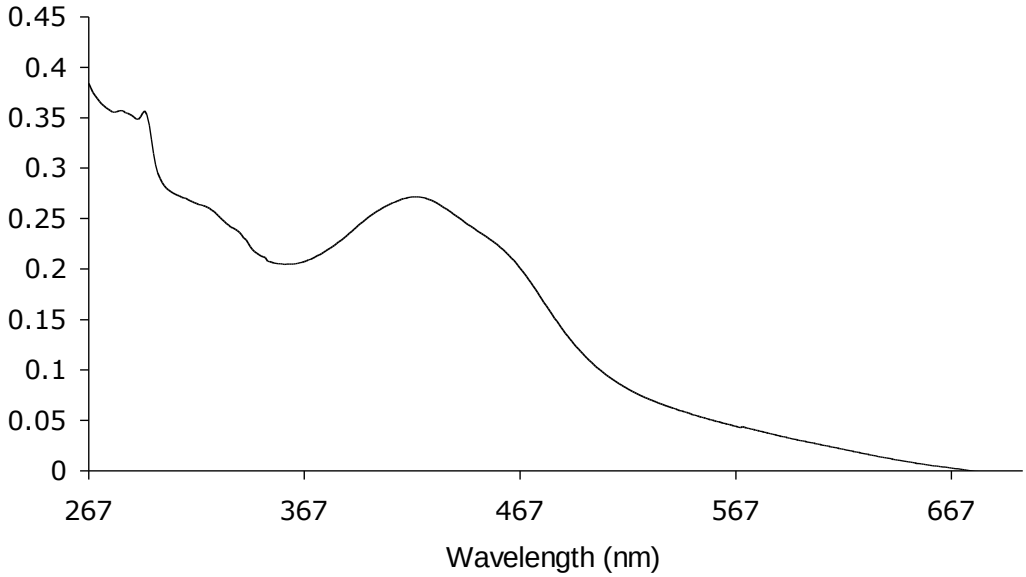

Figure S14. UV-Vis spectrum of a suspension of **3** (1 mg per mL) in THF.

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Fitplot of [3·Hg]

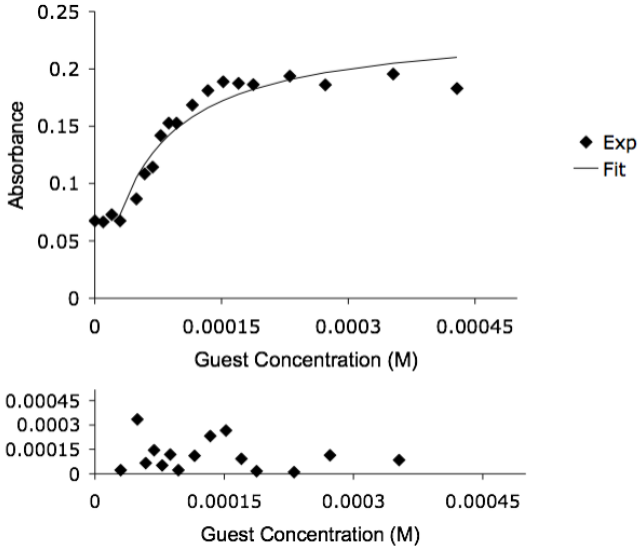

Figure S15. Fitplot of **3** upon titration with mercury(II) and residuals.