Supplementary Material (ESI) for Chemical Communications

Ultraselective Fluorescent Sensing of Hg^{2+} through Metal Coordination-Induced Molecular Aggregation

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Supporting Information

1. Materials and Methods.

Dideoxythymidine-perylene-3,4,9,10-tetracarboxylic diimide (**TT-PTCDI**) was synthesized following the standard condensation method developed by Langhals.[1] Briefly, 3.6 mg (9.2 μmol) 3,4,9,10-perylene-tetracarboxylic dianhydride (Aldrich), 5 mg (21 μmol) 5'-amino-5'-deoxythymidine (Sigma), and 0.6 g imidazole (Fisher) were heated under argon at 120 ^{o}C for 3 h. The reaction mixture was cooled to room temperature and dispersed in 10 mL ethanol, followed by addition of 20 mL 2 M HCl. The mixture was stirred overnight. The resulting red solid was collected by vacuum filtration through a 0.45 μm membrane filter (Osmonics). The solid was then washed thoroughly with distilled water until the pH of washings turned to be neutral. The collected solid was dried in vacuum at 60 ^{o}C. TLC: R_f (silica gel/dioxane:$CHCl_3$ = 75:25) = 0.83. All other chemicals were used as received.

Due to the limited solubility of TT-PTCDI in the common NMR solvents, it was challenging to run NMR measurement on this compound. Mass spectra were run on a MALDI instrument using angiotensin as an external standard. MS ($M+2H^+$), *m/z:* 840.29 (calc. 840.22).

UV-visible absorption spectra were recorded on a Perkin Elmer Lambda 25 spectrophotometer. Fluorescence spectra were measured using a Perkin Elmer LS55 fluorometer.

2. More Spectroscopy Data.

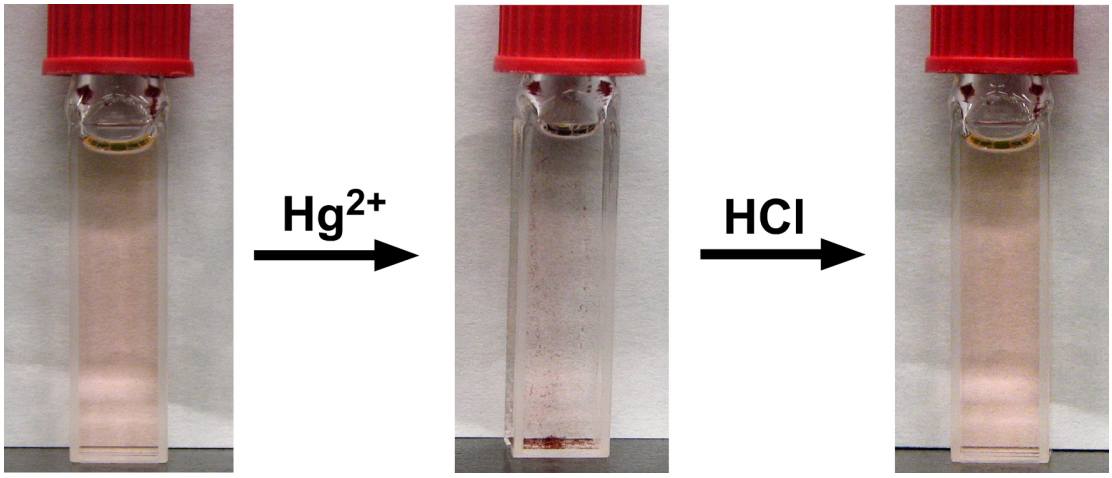

Fig. S1. Addition of 10 μM Hg^{2+} into a 5 μM TT-PTCDI solution in DMF/H_2O (70/30, vol) (*left*) results in complexation and aggregation of the molecules, which eventually leads to formation of redish flocs (*middle*). The floating flocs can be redissolved back to solution by addition of ca. 0.05 M HCl (*right*).

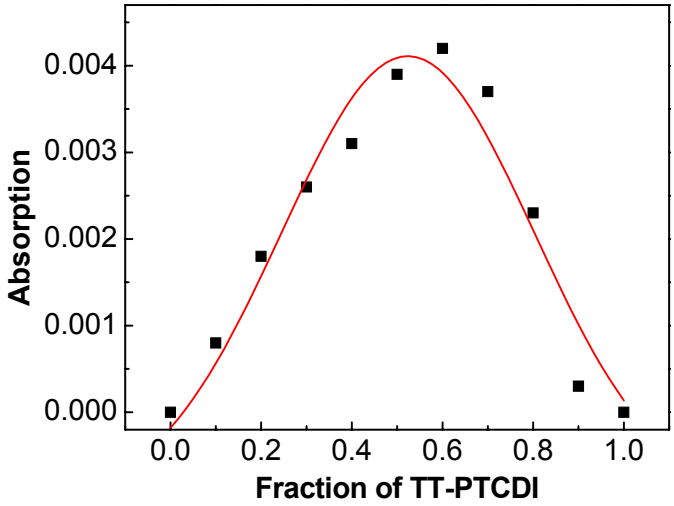

Fig. S2. Job's plot of the complexation between TT-PTCDI and Hg^{2+}. Total concentration of TT-PTCDI and Hg^{2+} was kept constant at 1 μM in DMF/H_2O (70/30, vol) solution.

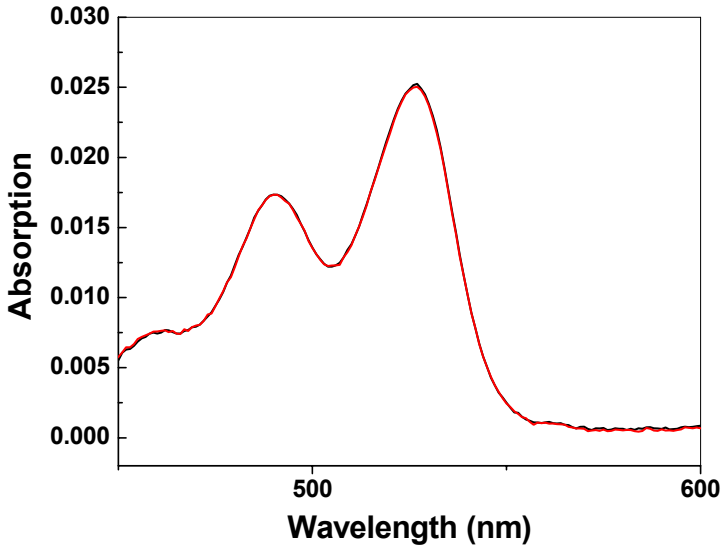

Fig. S3. Absorption spectra of a 1 μM solution of TT-PTCDI in DMF/H_2O (70/30, vol) in the absence (black) and presence of 12.5 μM Cu^{2+} (red), showing no significant change in absorption. Similar results were obtained for all the other environmentally relevant metal ions including Ni^{2+}, Fe^{2+}, Co^{2+}, Pb^{2+}, Cd^{2+}, Zn^{2+}, Mn^{2+}, Cr^{3+}, Mg^{2+}, Ca^{2+}, K^{+} and Na^{+}.

1. H. Langhals, *Heterocycles*, 1995, **40**, 477-500.