Supporting information for

A New Reverse PET Sensor and its Chelatoselective Aromatic Cadmiation

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EXPERIMENTAL

General. NMR spectra were recorded with a Varian Inova Nuity spectrometer at 500 MHz (1H NMR) and at 125 MHz (13C NMR). Chemical shifts were given in ppm using TMS as internal standard. Mass spectra were obtained using a JMS-HX 110A/110A Tandem Mass Spectrometer (JEOL). Fluorescence spectra were obtained using a RF-530/PC Spectrofluorophotometer (Shimadzu). Melting points were determined in open capillaries and are uncorrected. Flash chromatography was carried out with Merck silica gel 60 (230-400 mesh). Thin layer chromatography was carried out with Merck 60 F254 plates with 0.25 mm thickness. CHCl3, CH2Cl2, and MeOH were distilled from CaH2, and THF was distilled from sodium-benzophenone ketyl.

1,8-Bis[(bisdiethylimino)methyl]anthryl tetraacetate (2). 1,8-Bis(bromomethyl)anthracene 1 (789 mg, 2.17 mmol) was added to a stirred solution of diethyl iminodiacetate (1.52 mL, 8.68 mmol) and K2CO3 in CHCl3 (25 mL). After the reaction mixture was stirred at 50°C for 5 hours, the reaction mixture was passed through a celite washing with CHCl3. The filtrate was concentrated under reduced pressure, and the crude product was purified by column chromatography (CHCl3:MeOH = 9:1) to give 2 as a yellow oil in 85% yield (1.07 g): 1H-NMR (CDCl3, 500 MHz) δ 1.22 (t, J = 6.5 Hz, 12H), 3.65 (s, 8H), 4.13 (q, J = 7.5 Hz, 8H), 4.60 (s, 8H), 7.38 (t, J = 7.5 Hz, 2H), 7.43-7.47 (m, 4H), 7.91 (d, J = 8.5 Hz, 2H), 8.40 (s, 1H), 9.55 (s, 1H); 13C-NMR (CDCl3, 125 MHz) δ 14.19, 53.98, 56.41, 60.21, 121.09, 124.78, 126.93, 127.00, 128.29, 130.63, 131.86, 134.51, 171.38; HRMS (FAB) m/z = 581.2861 (M+H)+, calc. for C32H40N2O8 = 581.2863 (M+H)+.

1,8-Bis[(bisimino)methyl]anthryl tetracarboxylic acid (3). KOH was added to a stirred solution of 2 (0.5 g, 0.86 mmol) in distilled water (50 mL). The reaction mixture was then refluxed for 12 h. After the reaction mixture was cooled to room temperature, 1 M HCl solution was added to make pH 2-3. The resulting precipitate was filtered and washed with small amount of cold distilled water. After drying at 90°C in vacuo, compound 3 was obtained as a yellow solid in an analytically pure form (363 mg, 90%), m.p. 233-236 °C dec.; 1H-NMR (DMSO d6, 500 MHz) δ 3.49 (s, 8H), 4.47 (s, 4H), 7.43-7.47 (m, 4H), 8.01 (d, J = 7.0 Hz, 2H), 8.58 (s, 1H),
9.52 (s, 1H); $^{13}$C-NMR (DMSO-d$_6$, 125 MHz) $\delta$ 53.59, 55.71, 120.93, 125.00, 126.89, 126.93, 128.14, 130.05, 131.43, 134.55, 172.46; HRMS (FAB) m/z = 491.1429 (M+Na)$^+$, calc. for C$_{24}$H$_{24}$N$_2$O$_8$ = 491.1430 (M+Na)$^+$.

**Preparation of fluorometric metal ion titration solutions.** Stock solutions (1 mM) of the metal perchlorate salts (for Cd(II), chloride salt was used) were prepared using doubly distilled demineralized water. Stock solutions of 3 were prepared. The solutions were used on the day of preparation. Test solutions were prepared by placing 40 $\mu$L of the probe stock solution into a test tube, adding an appropriate aliquot of each metal stock (0- $\mu$L), and diluting the solution to 4 mL with pH 7 0.1 M HEPES buffer.

For all measurements, excitation was at 367 nm; emission was measured at 420 nm. Both excitation and emission slit widths were 5 nm.

Figure 1. $^{13}$C NMR (125 MHz, CDCl$_3$) spectrum of Compound 2

Figure 2. $^1$H NMR (500 MHz, CDCl$_3$) spectrum of Compound 2

Figure 4. $^1$H NMR (500 MHz, DMSO-d$_6$) spectrum of Compound 2