Supplementary Information

Fluorescence PET (Photo-induced Electron Transfer) sensor for water based on anthracene-boronic acid ester

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Experimental Section:

General: Melting points were measured with a Yanaco micro melting point apparatus MP model. IR spectra were recorded on a Perkin Elmer Spectrum One FT-IR spectrometer by ATR method. Absorption spectra were observed with a Shimadzu UV-3150 spectrophotometer and fluorescence spectra were measured with a Hitachi F-4500 spectrophotometer. High-resolution mass spectral data by APPI were acquired on a Thermo Fisher Scientific LTQ Orbitrap XL. 1H NMR spectra were recorded on a JNM-LA-400 (400 MHz) FT NMR spectrometer with tetramethylsilane as an internal standard. Column chromatography was performed on silica gel (KANTO CHEMICAL, 60N, spherical, neutral). The determination of water in 1,4-dioxane, THF, acetonitrile and ethanol solution was done with a MKC-610 and MKA-610 Karl Fischer moisture titrator (Kyoto Electronics manufacturing Co., Ltd.) based on Karl Fischer coulometric titration for below 1.5 wt% and volumetric titration for above 1.5 wt%, respectively.

Preparation of 9-[[N-Methyl-N-(2-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-benzyl)amino]methyl]anthracene (2)

A solution of 9-(methylaminomethyl)anthracene (0.19 g, 0.84 mmol) in DMF (70 ml) was treated with sodium hydride (60%, 0.08 g, 2.1 mmol) and stirred for 1 h at room temperature. 2-bromomethylphenylboronic acid pinacol ester (1.0 g, 3.37 mmol) was added dropwise over 20 min and the solution was stirred at room temperature for 1 h. After concentrating under reduced pressure, the resulting residue was dissolved in dichloromethane, and washed with water. The residue was chromatographed on silica gel (dichloromethane–methanol = 10 : 1 as eluent) to give 2 (0.08 g, yield 22 %) as a light yellow solid. M.p. 52–55 °C; IR (ATR): ν =
2976 (m), 1343 (s), 1142 (m) cm$^{-1}$; $^1$H NMR (400 MHz, [D$_2$]dichloromethane, 25 °C, TMS) $\delta$

$= 1.27$ (s, 12H, CH$_3$x4), $2.17$ (s, 3H, CH$_3$), $4.0$ (s, 2H, CH$_2$), $4.36$ (s, 2H, CH$_2$), $7.26$–7.30 (m, 1H), $7.38$–7.47 (m, 6H), $7.8$ (d, $J = 8.2$ Hz, 1H), $7.96$–7.99 (m, 2H), $8.34$ (dd, $J = 1.9$ and 8.9 Hz, 2H), $8.38$ (s, 1H); HRMS (APPI): $m/z$ (%): [M+H$^+$] calcd 438.25989; found 438.25970.