Supplementary Materials for

Acetylated Trifluoromethyl Diboronic Acid Anthracene with a Large Stokes Shift and Long Excitation Wavelength as a Glucose-Selective Probe

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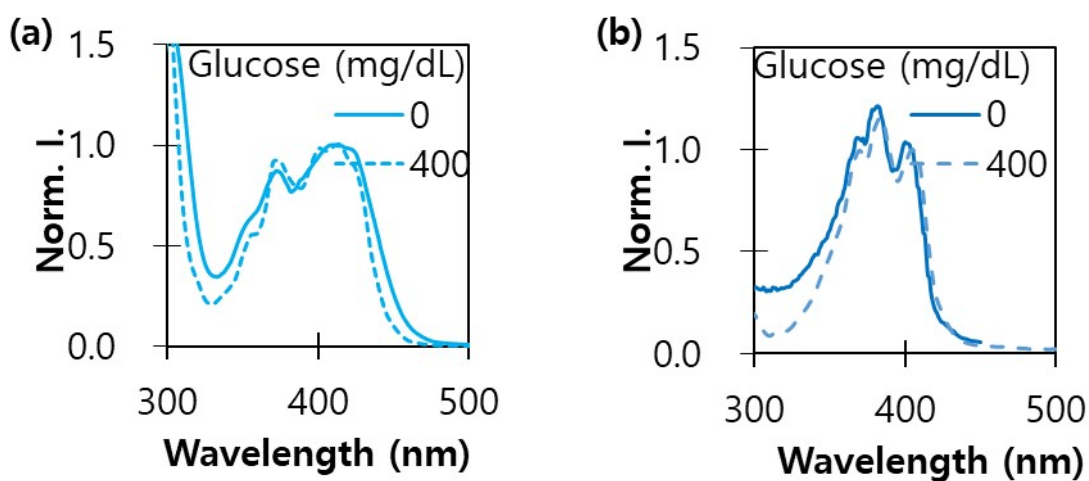
Figure S1. Glucose dependence of excitation spectra of AcTDA (a), and TDA (b). Excitation intensity was normalized at the maximum excitation of each dye. The fixed emission wavelength for AcTDA and TDA was 490 nm and 430 nm respectively.
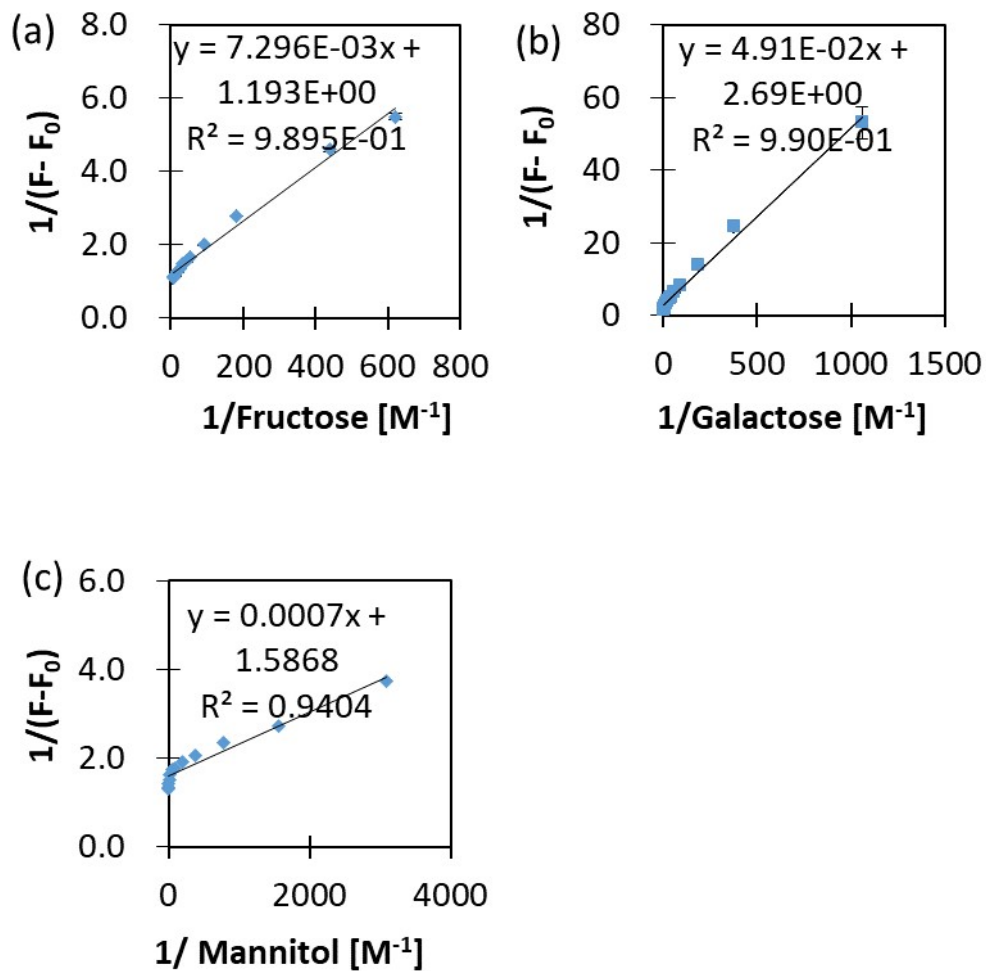
Figure S2. The modified Benesi-Hildebrand plot of AcTDA with fructose (a), galactose (b), and mannitol (c)

M+DA = M·DA   (1)

,where M is free mannitol, DA is free Diboronic acid anthracene, and M·DA is M-DA complex.

Dissociation constant $Kd = [M·DA]/([M]+[DA])$ (2)

Fraction bound $DA = [M·DA]/([DA]+[[M·DA]]$ (3)

From (1), (2) and (3)

Fraction bound $DA = [M]/(Kd+[M])$ (4)

(4) becomes

$[M]/$Fraction bound $DA = Kd+[M]$ (5)

Plotting [M]/Fraction bound DA vs [M] gives a straight line with slope 1 and intercept Kd

$$[M \cdot DA] = \alpha F_{bound} \quad (6)$$

where α is a coefficient, which is a function of a fluorescence measuring instrument, a container where a sample is placed, and the complex

$$F_{total} = F_{bound} + F_{unbound} \quad (7)$$

$$F_{bound} = F_{total} - F_{unbound} \quad (8)$$

$$[M \cdot DA] = \alpha (F_{total} - F_{unbound}) \quad (9)$$

When M is 5000 mg/dL, $F_{total} = F_{sat} = 8044927$.

When M is 0, $F_{total} = F_{unbound} = 480810$ and $F_{unbound}/F_{sat} = 0.06$. Since $F_{unbound}$ at saturation should be smaller than 480810, $F_{unbound}/F_{sat}$ is much smaller than 0.06. Therefore, we could assume when F total is saturated, $F_{total} \gg F_{unbound}$. In addition, we assumed when $M_0 \gg DA_0$, most of DA forms the complex with M at saturation

Then

$$\alpha = [DA]_0 / F_{sat} \quad (10)$$

From (10), the calculated α was 2.49×10^{-13}

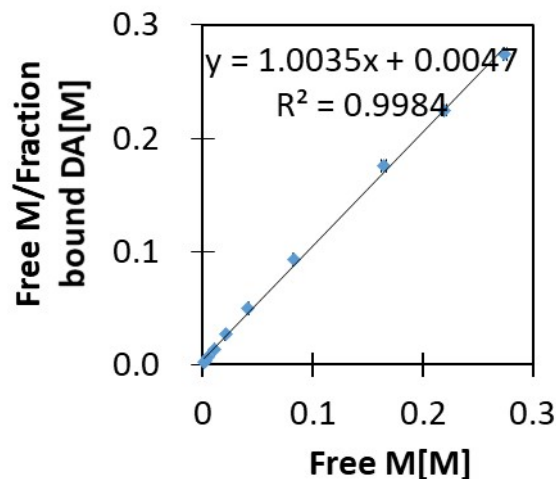Using α, we calculated [M]/Fraction bound DA and obtained a liner plot as shown in Figure S3

Figure S3. Association constant of AcTDA for mannitol. In order to minimize contribution of unbound DA to the total fluorescence, we used fluorescence value at least 10 fold higher than fluorescence at M = 0. Since the amount of mannitol is always much higher than the dye, we assumed $[M]_0$ was equal to [M]