Electronic Supporting Information

for

Discrimination of *cis*-diol containing molecules via fluorescent boronate affinity probes by principal component analysis

Fenying Wang^{a,*}, Shuqing Xiong^b, Tingting Wang^b, Yadan Hou^b, and Qianjin Li^{b,*}

^a School of Chemistry and Chemical Engineering, Nanchang University, Nanchang 330031, China

^b School of Food Science and Pharmaceutical Engineering, Nanjing Normal University, Nanjing 210023, China

*Emails of corresponding authors: Fenying Wang: <u>wangfenying@ncu.edu.cn</u> Qianjin Li: liqianjinnju@163.com & <u>qianjin_li@njnu.edu.cn</u>



Figure S1. UV absorption spectra of FITC-APBA (left) and RBITC-APBA (right). Fluorescent probe concentration: 0.5 µM; solvent: PBS (pH 8.0, 10 mM).



Figure S2. ¹H NMR spectra of FITC-APBA (a) and RBITC-APBA (b) comparing with that of their corresponding substrates.



Figure S3. Fluorescence spectra of FITC (a), FITC-APBA (b), RBITC (c) and RBITC-APBA (d). Fluorescent probe concentration: 0.5μ M; solvent: PBS (pH 8.0, 10 mM).



Figure S4. Dose-fluorescence spectra of FITC-APBA in the co-solvents of PBS/MeOH = 7/3 (v/v) with pH value of 8.0 (a), 7.4 (b), 6.0 (c) and 4.0 (d). Testing molecule: adenosine; FITC-APBA concentration: 0.1 μ M.



Figure S5. Dose-fluorescence spectra of FITC-APBA in the co-solvents of PBS/MeOH = 7/3 (v/v) with pH value of 4.0 to adenosine, deoxyadenosine and glucose. FITC-APBA concentration: 0.1 μ M.



Figure S6. Dose-fluorescence spectra of RBITC-APBA in the co-solvents of PBS/MeOH = 7/3 (v/v) with pH value of 8.0 (a), 7.4 (b), 6.0 (c) and 4.0 (d). Testing molecule: adenosine; RBITC-APBA concentration: 0.5 μ M.



Figure S7. Dose-fluorescence spectra of FITC-APBA (0.1 μ M) to nucleosides of A (a),

G (b), C (c), U (d), DA (e), and AMP (f), in PBS (10 mM, pH 8.0).



Figure S8. Dose-fluorescence spectra of RBITC-APBA (0.5 μ M) to nucleosides of A (a), G (b), C (c), U (d), DA (e), and AMP (f), in PBS (10 mM, pH 8.0)/MeOH = 7/3 (v/v).



Figure S9. Dose-fluorescence spectra of FITC-APBA (0.1 μ M) to monosaccharides of Glu (a), Fru (b), Gal (c), and Man (d), in PBS (10 mM, pH 8.0).



Figure S10. Dose-fluorescence spectra of RBITC-APBA (0.5 μ M) to monosaccharides of Glu (a), Fru (b), Gal (c), and Man (d), in PBS (10 mM, pH 8.0)/MeOH = 7/3 (v/v).



Figure S11. Dose-fluorescence spectra of FITC-APBA (0.1 μ M) to proteins of HRP (a), OVA (b), LF (c), and BSA (d), in PBS (10 mM, pH 8.0).



Figure S12. Dose-fluorescence spectra of RBITC-APBA (0.5 μ M) to proteins of HRP (a), OVA (b), LF (c), and BSA (d), in PBS (10 mM, pH 8.0)/MeOH = 7/3 (v/v).



Figure S13. Principal component analysis of different sugars based on their dosefluorescence responses, binding affinities, and molecular weights using FITC-APBA (a) and RBITC-APBA (b) and both of them (c).



Figure S14. Principal component analysis of glycoprotein and non-glycoprotein based on their dose-fluorescence responses, binding affinities, and molecular weights using FITC-APBA (a) and RBITC-APBA (b) and both of them (c).