# **Electronic Supplementary Information**

## Water-soluble diboronic acid-based fluorescent sensors

## recognizing D-sorbitol

Guiqian Fang,<sup>‡a, b, c, d</sup> Zhancun Bian,<sup>‡a, b, c, d</sup> Daili Liu, <sup>a, b, c, d</sup> Guiying Wu,<sup>a, b, c, d</sup> Hao Wang,<sup>a, b, c, d</sup> Zhongyu Wu<sup>\*a, b, c, d</sup> and Qingqiang Yao<sup>\*a, b, c, d</sup>

a. School of Medicine and Life Sciences, University of Jinan-Shandong Academy of Medical Sciences, Jinan 250200, Shandong, China

b. Institute of Materia Medica, Shandong Academy of Medical Sciences, Jinan 250062, Shandong, China

c. Key Laboratory for Biotech-Drugs Ministry of Health, Jinan 250062, Shandong, China

d. Key Laboratory for Rare & Uncommon Diseases of Shandong Province, Jinan 250062, Shandong, China

\*Corresponding authors: E-Mail: wu\_med@foxmail.com (Zhongyu Wu), yao\_imm@163.com (Qingqiang Yao).

These author contributed equally.

## **Table of Contents**

- 1. UV-vis absorption spectra of sensor 1, 2 and 15c
- 2. Fluorescence properties of sensors
- 3. Copies of NMR (<sup>1</sup>H and <sup>13</sup>C) and HRMS spectra

#### UV-vis absorption spectra of sensor 1, 2 and 15c



Fig. S1 UV-vis absorption spectra of sensor 1, 2 and 15c DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature.

### **Fluorescence properties of sensors**



**Fig. S2** A) Fluorescence spectra of sensor **1** ( $1 \times 10^{-5}$  M) in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **1** linear range. C) Benesi-Hildebrand plot of sensor **1**1/(*I* - *I*<sub>0</sub>) *versus* 1/[D-sorbitol].

The calculation process of LOD :

*I*=9545110*c*+247.19996

 $R^2 = 0.98522$ 

S=9545110

$$\delta = \sqrt{\frac{\Sigma (F_i - F_0)^2}{N - 1}} = 4.87 \text{ (N=5) K=3}$$

LOD =K ×  $\delta/S$ =1.53×10<sup>-6</sup> M



**Fig. S3** A) Fluorescence spectra of sensor **15a** ( $1 \times 10^{-5}$  M) in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **15a** linear range. C) Benesi-Hildebrand plot of sensor **15a**1/(*I* - *I*<sub>0</sub>) *versus* 1/[D-sorbitol].

The calculation process of LOD:

*I*=18502600*c*+482.6485

 $R^2 = 0.9763$ 

S=18502600

$$\delta = \sqrt{\frac{\Sigma (F_i - F_0)^2}{N - 1}} = 5.02 \text{ (N=5) K=3}$$

LOD =K ×  $\delta/S$ =8.14×10<sup>-7</sup> M



**Fig. S4** A) Fluorescence spectra of sensor **15b** ( $1 \times 10^{-5}$  M) in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **15b** linear range. C) Benesi-Hildebrand plot of sensor **15b** 1/(*I* - *I*<sub>0</sub>) versus 1/[D-sorbitol].

The calculation process of LOD :

*I*=17165000*c*+442.93993

 $R^2 = 0.98234$ 

*S*=17165000

$$\delta = \sqrt{\frac{\Sigma (F_i - F_0)^2}{N - 1}} = 4.37 \text{ (N=5) K=3}$$

LOD =K ×  $\delta/S$ =7.64×10<sup>-7</sup> M



**Fig. S5** A) Fluorescence spectra of sensor **15c** ( $1 \times 10^{-5}$  M) in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **15c** linear range. C) Benesi-Hildebrand plot of sensor **15c**1/(*I* - *I*<sub>0</sub>) *versus* 1/[D-sorbitol].

The calculation process of LOD :

*I*=17508000*c*+394.88005

 $R^2 = 0.98496$ 

S=17508000

$$\delta = \sqrt{\frac{\Sigma(F_i - F_0)^2}{N - 1}} = 4.03 \text{ (N=5) K=3}$$

LOD =K ×  $\delta/S$ =6.91×10<sup>-7</sup> M



**Fig. S6** A) Fluorescence spectra of sensor **15d** ( $1 \times 10^{-5}$  M) in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **15d** linear range. C) Benesi-Hildebrand plot of sensor **15d**1/(*I* - *I*<sub>0</sub>) versus 1/[D-sorbitol].

The calculation process of LOD : *I*=13811700*c*+297.94058 *R*<sup>2</sup>=0.99553 *S*=13811700

$$\delta = \sqrt{\frac{\Sigma (F_i - F_0)^2}{N - 1}} = 5.63 \text{ (N=5) K=3}$$

LOD =K ×  $\delta/S$ =1.22×10<sup>-6</sup> M



**Fig. S7** A) Fluorescence spectra of sensor **15e**  $(1 \times 10^{-5} \text{ M})$  in the presence of different concentrations of D-sorbitol in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature; B) The photograph of sensor **15e** linear range. C) Benesi-Hildebrand plot of sensor **15e** $1/(I - I_0)$  versus 1/[D-sorbitol].

The calculation process of LOD : *I*=17942500*c*+423.81207

 $R^2=0.9815$ 

S=17942500

$$\delta = \sqrt{\frac{\Sigma(F_i - F_0)^2}{N - 1}} = 3.28 \text{ (N=5) K=3}$$

LOD = $K \times \delta/S$ =5.48×10<sup>-7</sup> M



**Fig. S8** Fluorescence spectra of sensor **2** ( $1 \times 10^{-5}$  M) in the presence of different carbohydrates (from 0 to  $13 \times 10^{-5}$  M) in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature.





**Fig. S9** Fluorescence spectra of sensor 1 ( $1 \times 10^{-5}$  M) in the presence of different carbohydrates (from 0 to  $13 \times 10^{-5}$  M) in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature.





**Fig. S10** Fluorescence spectra of sensor **15c**  $(1 \times 10^{-5} \text{ M})$  in the presence of different carbohydrates (from 0 to  $13 \times 10^{-5}$  M) in DMSO/PBS (pH 9, 0.1M) solution (1:99, v/v), at room temperature.



### Copies of NMR (<sup>1</sup>H and <sup>13</sup>C) and HRMS spectra

Fig. S11 <sup>1</sup>H NMR spectrum of 2



Fig. S12 <sup>13</sup>C NMR spectrum of 2



Fig. S13 HRMS spectrum of compound 2



Fig. S14 <sup>1</sup>H NMR spectrum of 3



Fig. S15 <sup>13</sup>C NMR spectrum of 3



Fig. S16 HRMS spectrum of compound 3



Fig. S17 <sup>1</sup>H NMR spectrum of 15a



Fig. S18 <sup>13</sup>C NMR spectrum of 15a



Fig. S19 HRMS spectrum of compound 15a



Fig. S20 <sup>1</sup>H NMR spectrum of 15b



Fig. S21 <sup>13</sup>C NMR spectrum of 15b



Fig. S22 HRMS spectrum of compound 15b



Fig. S23 <sup>1</sup>H NMR spectrum of 15c



Fig. S24 <sup>13</sup>C NMR spectrum of 15c



Fig. S25 HRMS spectrum of compound 15c



Fig. S26 <sup>1</sup>H NMR spectrum of 15d



Fig. S27 <sup>13</sup>C NMR spectrum of 15d



Fig. S28 HRMS spectrum of compound 15d



Fig. S29 <sup>1</sup>H NMR spectrum of 15e



Fig. S30 <sup>13</sup>C NMR spectrum of 15e



Fig. S31 HRMS spectrum of compound 15e