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Electronic Supporting Information for:

## A H-aggregating fluorescent probe for recognizing both mercury and

# copper ions based on a dicarboxyl-pyridyl bifunctionalized

### difluoroboron dipyrromethene

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Compound	2,6-diCO <sub>2</sub> Bzl-BODIPY			
CCDC code	1484737			
empirical formula	$C_{34}H_{30}BF_2N_3O_4$			
formula weight	593.42			
<i>T</i> (°K)	293(2)			
$\lambda$ (Å)	0.71073 (Mo– <i>Kα</i> )			
Crystal system, Space group, Z	Triclinic, <i>P</i> ī, 2			
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.0378(7), 13.014(1),14.511(1)			
$\alpha, \beta, \gamma$ (°)	114.894(8), 96.065(6), 100.583(7)			
V (Å <sup>3</sup> )	1489.5(2)			
$ \rho_{\text{calcd}} \left( \text{g} \cdot \text{cm}^3 \right) $	1.323			
$\mu (\mathrm{mm}^{-1})$	0.095			
F(000)	620			
Crystal size (mm)	0.50×0.20×0.16			
$\theta$ Range (°)	2.8 - 25.0			
Collected reflections	9721			
Unique reflections	5121			
Observed reflections	2432			
R <sub>int</sub>	0.0629			
Data / restraints / parameters	5121 / 0 / 398			
GOF	1.022			
R indices (for obs.):				
$R_1^{a}, wR_2^{b}$	0.0707, 0.1625			
R indices (for all):				
$R_1, wR_2$	0.1592, 0.2124			
Largest diff. peak/hole (e.Å <sup>-3</sup> )	0.29/-0.22			
$ {}^{a}\mathbf{R}_{1} = \sum(  F_{o}  -  F_{c}  ) / \sum  F_{o} ,  \mathbf{w}\mathbf{R}_{2} = \{\sum w[(F_{o}^{2} - F_{c}^{2})^{2}] / \sum w[(F_{o}^{2})^{2}]\}^{1/2};  {}^{b}w = \{\sum w[(F_{o}^{2} - F_{c}^{2})^{2}] / \sum w[(F_{o}^{2})^{2}]\}^{1/2};  {}^{b}w = \{\sum w[(F_{o}^{2} - F_{c}^{2})^{2}] / \sum w[(F_{o}^{2} - F_{c}^{2})^{2}] $				
$1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ , where $P = (F_o^2 + 2F_c^2)/3]$ .				

TableS1. Crystal Data Collections and Structure Refinement Parameters for 2,6-diCO<sub>2</sub>Bzl-BODIPY

Selected bond lengths and angles						
Bond leng	gths		Bond angle	S		
B-F(1)	1.376(5)	F(1)	-B-F(2)	109.2(4)		
B-F(2)	1.371(5)	F(1)	-B-N(2)	110.2(3)		
B-N(2)	1.535(5)	F(1)	-B-N(3)	110.1(4)		
B-N(3)	1.540(5)	F(2)	-B-N(2)	110.4(4)		
N(1)-C(16)	1.330(6)	F(2)	-B-N(3)	109.7(3)		
N(1)-C(20)	1.310(6)	N(2)	)-B-N(3)	107.2(3)		
N(2)-C(5)	1.344(5)	B-N	(2)-C(5)	125.4(3)		
N(2)-C(9)	1.398(4)	B-N	(2)-C(9)	125.9(3)		
N(3)-C(3)	1.339(5)	B-N	(3)-C(3)	125.8(3)		
N(3)-C(4)	1.395(4)	B-N	(3)-C(4)	125.5(3)		
O(1)-C(10)	1.196(5)					
O(2)-C(10)	1.309(5)					
O(3)-C(11)	1.203(5)					
O(4)-C(11)	1.323(5)					
Hydrogen bonds						
D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)		
C(13)-H(13A)O(2)	0.96	2.25	2.912(6)	125.6		
C(13)-H(13B)F(2)	0.96	2.58	3.089(5)	113.2		
C(13)-H(13C)F(1)	0.96	2.63	3.101(5)	110.4		
C(15)-H(15A)O(3)	0.96	2.30	3.008(6)	129.6		
C(15)-H(15B)F(1)	0.96	2.60	3.067(5)	110.3		
C(17)-H(17A)O(3a)	0.93	2.58	3.419(6)	151.0		
C(19)-H(19A)F(1b)	0.93	2.51	3.289(5)	141.8		
C(34)-H(34B)O(1c)	0.97	2.64	3.495(7)	146.7		

Table S2. Geometrical Parameters for 2,6-diCO<sub>2</sub>Bzl-BODIPY [Å and °].

Symmetry transformations used to generate equivalent atoms:

a = -x, -y+1, -z; b = -x+1, -y+1, -z; c = x-1, y-1, z-1



Figure S1 FT-IR spectra of benzyl 2,4-dimethyl-1*H*-pyrrole-3-carboxylate



Figure S2 <sup>1</sup>H NMR spectra of benzyl 2,4-dimethyl-1*H*-pyrrole-3-carboxylate



Figure S3 FT-IR spectra of 2,6-diCO<sub>2</sub>Bzl-BODIPY



Figure S4<sup>1</sup>H NMR spectra of 2,6-diCO<sub>2</sub>Bzl-BODIPY



Figure S5 <sup>13</sup>C NMR spectra of 2,6-diCO<sub>2</sub>Bzl-BODIPY



Figure S6 ESI-MS data of 2,6-diCO<sub>2</sub>Bzl-BODIPY



Figure S7 FT-IR spectra of 2,6-diCO<sub>2</sub>H-BODIPY



Figure S8 <sup>1</sup>H NMR spectra of 2,6-diCO<sub>2</sub>H-BODIPY







Figure S10 ESI-MS data of 2,6-diCO<sub>2</sub>H-BODIPY



**Figure S11** (*a*) The ORTEP drawing of 2,6-diCO<sub>2</sub>Bzl-BODIPY molecule; (b) A view showing the 2,6-diCO<sub>2</sub>Bzl-BODIPY molecules parallel packing in the chain-like supramecular aggregates with an alternating head-to-tail orientation in unit cell (righ), in which the alternating H-type to J-type packings (left) are resulted from T-shaped edge-to-face and vertex-to-face C-H... $\pi$  interactions of phenyl-phenyl embraces.





Figure S13 TGA trace of 2,6-diCO<sub>2</sub>H-BODIPY



Figure S14 The solid-state absorbance (gray) and emission (red) spectra of 2,6-diCO<sub>2</sub>H-BODIPY



**Figure S15** (*a*) The absorbance and (*b*) emission ( $\lambda_{ex} = 360 \text{ nm}$ ) spectra of a 10  $\mu$ M solution of 2,6-diCO<sub>2</sub>H-BODIPY in four different solvents.



**Figure S16** (*a*) The absorbance and (*b*) emission ( $\lambda_{ex} = 360 \text{ nm}$ ) spectra of 2,6-diCO<sub>2</sub>H-BODIPY at different concentrations in v/v=1:1 MeOH/H<sub>2</sub>O solution.



**Figure S17** Job's plot of the relationship between fluorescent intensity of 2,6-diCO<sub>2</sub>H-BODIPY probe and the addition of metal ions ranging from 0 to 2.0 eq. (top) and 0 to 10 eq. (bottom)

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Under the Natural Light blank (50 µM Dye) viv 1:1 Dye/H2O	v/v 1:1 Dye/W with Hg <sup>2+</sup>	Vaste Water without Hg <sup>2+</sup>
Under an UV lamp blank v/v 1:1 Dye/H <sub>2</sub> O (50 µM Dye)	v/v 1:1 Dye/V with Hg <sup>2+</sup>	Vaste Water without Hg <sup>2+</sup>

**Figure S18** The photos showing the naked eye visible fluorescent color changes in a 50  $\mu$ M 2,6-diCO<sub>2</sub>H-BODIPY in v/v=1:1 MeOH/H<sub>2</sub>O solution upon addition of isochoric distilled water, the mercury-containing subacidic wastewater (pH = ~6.2) from battery factory (metal ion pollutant: ~14 mg·L<sup>-1</sup> Hg<sup>2+</sup>, ~194 mg·L<sup>-1</sup> Zn<sup>2+</sup>, ~28 mg·L<sup>-1</sup> Mn<sup>2+</sup>), and the same subacidic wastewater (pH = ~6.2) from battery factory but after treatment of mercury removal (metal ion pollutant: <<~0.5  $\mu$ g·L<sup>-1</sup> Hg<sup>2+</sup>, ~146 mg·L<sup>-1</sup> Zn<sup>2+</sup>, ~25 mg·L<sup>-1</sup> Mn<sup>2+</sup>) after exposure on the natural light (upper) and an UV lamp (bottom, 365 nm).

Under the Natu pristine test 1 drop filter strip of paper (blank) H <sub>2</sub> O	ral Light 1 drop 1 drop of of Cu <sup>2+</sup> Hg <sup>2+</sup>	Under an UV lamp (365 nm) pristine test 1 drop 1 drop 1 drop filter strip of of of of paper (blank) H <sub>2</sub> O Cu <sup>2+</sup> Hg <sup>2+</sup>		

**Figure S19** The photos of paper-based test strip containing ~0.03 Mg·cm<sup>-2</sup> of 2,6-diCO<sub>2</sub>H-BODIPY, which fabricated by ~1.0×5.0 cm filter paper dipping in a 50  $\mu$ M 2,6-diCO<sub>2</sub>H-BODIPY in v/v=1:1 MeOH/H<sub>2</sub>O solution, showing the naked eye visible color changes after exposure by 1 drop of 10 eq. of either copper or mercury ion under the natural light (left) and an UV lamp (right, 365 nm).

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**Figure S20** (*a*) The absorbance and (*b*) emission ( $\lambda_{ex} = 360 \text{ nm}$ ) spectra of 2,6-diCO<sub>2</sub>H-BODIPY (10 µM in v/v=1:1 MeOH/H<sub>2</sub>O solution) in a pH range of 2.8-7.41. Inset shows photographs of each pH value under the natural light (upper) or an UV lamp (bottom, 365 nm).