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Electronic Supplementary Information

A pyridine based Schiff base as a selective and sensitive fluorescent

probe for cadmium ions with "turn-on" fluorescence responses

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Figure S1. ¹H NMR spectrum of probe PMPA in CDCl₃.



Figure S2. ¹³C NMR spectrum of probe PMPA in CDCl₃.



Figure S3. FT–IR spectra of (a) probe PMPA and (b) complex $PMPA-CdCl_2$.



Figure S4. ESI–MS spectrum of probe PMPA.



Figure S5. Absorption spectra (black line) and fluorescence emission spectra (blue line) of probe PMPA in acetonitrile solvent. The concentration was maintained at 10 μM.



Figure S6. Fluorescence decay profile for probe PMPA in acetonitrile solution ($\lambda_{ex} = 380 \text{ nm}$, $\lambda_{em} = 468 \text{ nm}$).



Figure S7. The fluorescence intensity of PMPA and PMPA+Cd²⁺ at different pH (1–12).



Figure S8. The effect of response time on the fluorescence intensity of PMPA over the addition of Cd^{2+} (at 506 nm).



Figure S9. The excitation spectrum of probe PMPA upon addition of Cd^{2+} .



Figure S10. ESI–MS spectrum of the complex PMPA–CdCl₂.



Figure S11. Coordination geometry of cadmium(II) ions in the complex PMPA-CdCl₂.



Figure S12. The binuclear unit of the complex PMPA-CdCl₂.



Figure S13. Depiction of the dihedral angle between the pyridine ring and the phenyl ring in the complex PMPA-CdCl₂.



Figure S14. ¹H NMR spectrum of the complex PMPA-CdCl₂ in CDCl₃.



Figure S15. ¹³C NMR spectrum of the complex PMPA-CdCl₂ in CDCl₃.

Standard deviation and detection limit calculation

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, fluorescence intensity of **PMPA** without Cd^{2+} was measured by five times and the standard deviation of blank measurements was determined. To gain the slop, the fluorescence intensity data at 479 nm for Cd^{2+} , were plotted as a concentration of Cd^{2+} . So the detection limit was calculated with the follow equation (1):

Detection limit =
$$3\sigma/m$$
 (1)

Where σ is the standard deviation of blank measurements, and m is the slop of fluorescence versus Cd^{2+} concentration.

	Fluorescence intensity
Test 1	32.24
Test 2	28.67
Test 3	38.95
Test 4	32.27
Test 5	33.03
Standard Deviation (σ)	3.72

Table S1. Standard deviation calculation.

	PMPA–CdCl ₂					
CCDC No.	2122596					
formula	$C_{18}H_{14}Cl_2N_2OCd$					
Mr	457.61					
A cryst syst	l riclinic					
space group $a \lceil \Delta \rceil$	F = 1 8 0895(2)					
$b \begin{bmatrix} A \end{bmatrix}$	8 7415(2)					
c [Å]	13.3578(3)					
$\alpha [\circ]$	108.358(2)					
β [°]	96.423(2)					
γ[°]	97.449(2)					
Volume [A ³]	8/7.17(4)					
L $D \left[\alpha \cdot cm^{-3} \right]$	2 1 733					
$\mu \text{ [mm^{-1}]}$	12.827					
F(000)	452					
Θ range [°]	3.533 - 68.293					
<i>h</i> range	$-9 \le h \le 6$					
<i>k</i> range	$-10 \le k \le 10$					
l range	$-15 \le l \le 15$ 2102 / 0 / 217					
GOF	1 040					
$R_1, wR_2[I \ge 2\sigma(I)]^a$	0.0474. 0.1220					
R_1, wR_2 [all data] ^a	0.0487, 0.1234					
$\Delta \rho_{\rm max}, \Delta \rho_{\rm min} [e \cdot {\rm \AA}^{-3}]$	0.977, -1.985					
$aR_1 = \sum F_o - F_c / \sum F_o ; wR_2 = \sum [w (F_o^2 - F_c^2)^2] / \sum [w]$	$(F_0^2)^2$]] ^{1/2} .					
Table S3 Selected bond distances (Å) and angles (°) for the complex PMPA –CdCl ₂						
Parameter	PMPA-CdCl ₂					
Parameter Cd(1)-N(1)	PMPA-CdCl2 2.338(4)					
Parameter Cd(1)-N(1) Cd(1)-N(2)	PMPA-CdCl2 2.338(4) 2.423(3)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1)	PMPA-CdCl2 2.338(4) 2.423(3) 2.4090(13)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2)	PMPA-CdCl2 2.338(4) 2.423(3) 2.7424(10)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2) Cd(1)-Cl(2A)	PMPA-CdCl2 2.338(4) 2.423(3) 2.7424(10) 2.5140(11)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2) Cd(1)-Cl(2A) N(2)-C(6)	PMPA-CdCl2 2.338(4) 2.423(3) 2.7424(10) 2.5140(11) 1 265(6)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2) Cd(1)-Cl(2A) N(2)-Cl(6) N(2)-Cd(1)-N(1)	PMPA-CdCl2 2.338(4) 2.423(3) 2.7424(10) 2.5140(11) 1.265(6) 70.93(12)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2) Cd(1)-Cl(2A) N(2)-C(6) N(2)-Cd(1)-N(1) N(1)-Cd(1)-Cl(1)	PMPA-CdCl2 2.338(4) 2.423(3) 2.4090(13) 2.7424(10) 2.5140(11) 1.265(6) 70.93(12) 110.93(10)					
Parameter Cd(1)-N(1) Cd(1)-N(2) Cd(1)-Cl(1) Cd(1)-Cl(2) Cd(1)-Cl(2A) N(2)-C(6) N(2)-Cd(1)-N(1) N(1)-Cd(1)-Cl(1) N(2)-Cd(1)-Cl(1)	PMPA-CdCl2 2.338(4) 2.423(3) 2.7424(10) 2.5140(11) 1.265(6) 70.93(12) 110.93(10) 105.29(9)					
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Parameter $Cd(1)$ -N(1) $Cd(1)$ -N(2) $Cd(1)$ -Cl(2) $Cd(1)$ -Cl(2) $Cd(1)$ -Cl(2A) N(2)-Cd(0) N(2)-Cd(1)-N(1) N(1)-Cd(1)-Cl(1) N(2)-Cd(1)-Cl(1) N(1)-Cd(1)-Cl(2) N(2)-Cd(1)-Cl(2) N(2)-Cd(1)-Cl(2) N(2)-Cd(1)-Cl(2) N(2)-Cd(1)-Cl(2A) N(2)-Cd(1)-Cl(2A) Cl(2)-Cd(1)-Cl(2A) Cl(2)-Cd(1)-Cl(2A) Cl(2)-Cd(1)-Cl(2A) Cl(2A)-Cd(1)-Cl(2A) Cl(2A)-Cd(1)-Cl(1) C(1)-N(1)-Cd(1) C(5)-N(1)-Cd(1) C(6) N(2) Cd(1)	PMPA-CdCl2 2.338(4) 2.423(3) 2.4090(13) 2.7424(10) 2.5140(11) 1.265(6) 70.93(12) 110.93(10) 105.29(9) 86.40(9) 153.76(9) 94.87(4) 109.59(10) 93.19(9) 81.86(3) 139.04(4) 115.7(3) 126.2(3) 112.8(2)					
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 Table S2. Crystallographic and structural determination data for the complex PMPA–CdCl2.

Sample	Added (µM)	Measure (µM)	Recovery (%)	RSD (%)
Tap water	0	0	—	—
	3	2.56	85.33	0.945
Pond water	0	0	_	_
	3	1.85	61.67	1.470
Hun River water	0	0	_	_
	3	1.57	52.67	1.236

Table S4. Determinations of Cd^{2+} in real samples (n = 3).