Electronic Supplementary Information (ESI) For

Three Zn(II) Coordination Polymers Constructed with a New Amide-thiophene-derived Bis-pyridyl Ligand as Ultrasensitive Luminescent Sensors for Hg(II) and Purines

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S1. X-ray Crystallography

The single-crystal diffraction data for LCPs **1-3** were collected by using a Bruker SMART APEXII CCD diffractometer at 293 K with Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å). The structures were solved by direct methods and refined by full matrix least-squares on F^2 employing the OLEX2 program.[1] All crystal data and detailed structural refinement results are summarized in Table S1, and selected bond lengths (Å) and angles (°) are listed in Table S2. The single crystal data for LCPs **1-3** have been obtained in the Cambridge Crystallographic Data Center (CCDC no: 2060451, 2089164, and 2089165).

Materials and methods

All chemicals and reagents were purchased from commercial sources and used as received except for 4-bpft (Scheme 1). The single-crystal diffraction data for LCPs **1–3** were collected by using a Bruker SMART APEXII CCD diffractometer at 293 K with Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å). The powder X-ray diffraction (D/teX Ultra diffractometer) and the infrared spectra (Varian 640 FTIR spectrometer) were measured to confirm the structures of LCPs **1–3**. The fluorescent spectra were recorded on a Hitachi F-4500 luminescence/phosphorescence spectrometer. UV−vis absorption spectra were obtained by PerkinElmer Lambda 750. With a FLS1000 transient steady-state fluorescence spectrometer, the fluorescence lifetime could be obtained. The ^{1}H NMR spectra was recorded on Agilent 400-MR spectrometer using DMSO-d_6 as a solvent.

Table S1. Crystallographic data for LCPs **1-3**.

LCP	LCP **1**	LCP **2**	LCP **3**
CCDC	2060451	2089164	2089165
Empirical formula	$C_{52}H_{44}Zn_2N_8O_{14}S_2$	$C_{27}H_{22}ZnN_4O_6S$	$C_{26}H_{20}ZnN_4O_7S$
Formula weight	1199.81	595.91	597.89
Crystal system	Triclinic	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a (Å)	11.9101(5)	10.0385(10)	9.8851(8)
b (Å)	14.8958(6)	11.1557(12)	10.8960(8)
c (Å)	16.5644(7)	12.4792(13)	12.2041(10)
α (°)	106.2430(10)	79.339(2)	82.082(2)
β (°)	109.7700(10)	80.212(2)	80.528(2)
γ (°)	96.0220(10)	68.539(2)	68.643(2)
V (Å^3)	2589.55(19)	1270.1(2)	1203.18(17)
Z	2	2	2
D_{calc} (g/cm^3)	1.539	1.558	1.650
μ/mm^{-1}	1.083	1.101	1.165
$F(000)$	1232	612	612
R_{int}	0.0167	0.0229	0.0317
$R_1{}^a$ [$I>2\sigma(I)$]	0.0419	0.0409	0.0406
$wR_2{}^b$(all data)	0.1077	0.1031	0.0842
GOF	1.018	1.021	1.004
$\Delta\rho_{max}$(e·Å^{-3})	1.334 and -0.620	0.639 and -0.658	0.356 and -0.395

$^a R_1 = \sum|F_o| - |F_c|/\sum|F_o|$. $^b wR_2 = [\sum w(F_o{}^2 - F_c{}^2)^2/\sum w(F_o{}^2)^2]^{1/2}$.

Table S2. Selected bond lengths (Å) and bond angles (°) for LCP **1**.

	LCP **1**		
Zn(2)–O(4)	2.0183(15)	Zn(1)–O(1)	1.9957(15)
Zn(2)–O(9)#1	2.1528(16)	Zn(1)–O(5)#2	2.0269(19)
Zn(2)–O(10)#1	2.2706(19)	Zn(1)–N(1)	2.163(2)
Zn(2)–O(3)	2.0793(17)	Zn(1)–O(2)	2.0329(18)
Zn(2)–N(5)	2.144(2)	Zn(1)–N(4)#2	2.166(2)
Zn(2)–N(8)#1	2.177(2)	O(2)–Zn(1)–N(4)#2	84.37(9)
O(4)–Zn(2)–O(9)#1	153.75(7)	N(5)–Zn(2)–O(9)#1	88.36(7)
O(4)–Zn(2)–O(10)#1	94.55(7)	N(5)–Zn(2)–O(10)#1	93.47(8)

O(4)–Zn(2)–O(3)	115.78(7)	N(5)–Zn(2)–N(8)#1	174.54(7)
O(4)–Zn(2)–N(5)	93.34(7)	N(8)#1–Zn(2)–O(10)#1	88.50(8)
O(4)–Zn(2)–N(8)#1	91.59(8)	O(1)–Zn(1)–O(5)#2	137.05(9)
O(9)#1–Zn(2)–O(10)#1	59.20(6)	O(1)–Zn(1)–N(1)	93.90(7)
O(9)#1–Zn(2)–N(8)#1	88.27(7)	O(1)–Zn(1)–O(2)	121.98(8)
O(3)–Zn(2)–O(9)#1	90.41(7)	O(1)–Zn(1)–N(4)#2	93.73(8)
O(3)–Zn(2)–O(10)#1	149.33(6)	O(5)#2–Zn(1)–N(1)	88.82(8)
O(3)–Zn(2)–N(5)	89.43(8)	O(5)#2–Zn(1)–O(2)	100.97(9)
O(3)–Zn(2)–N(8)#1	86.30(8)	O(5)#2–Zn(1)–N(4)#2	90.46(8)
O(2)–Zn(1)–N(1)	85.52(9)	N(1)–Zn(1)–N(4)#2	169.54(8)

Symmetry codes: #1 -x,-y+2,-z+1, #2 -x+1,-y+1,-z+1

Table S3. Selected bond lengths (Å) and bond angles (º) for LCP **2**.

LCP **2**			
Zn(1)–O(1)	2.0032(18)	Zn(1)–N(1)#3	2.191(3)
Zn(1)–O(2)#1	2.060(2)	Zn(1)–O(5)#2	2.348(2)
Zn(1)–O(3)#2	2.19(2)	Zn(1)–N(2)	2.177(3)
N(2)–Zn(1)–N(1)#3	171.39(8)	O(2)#1–Zn(1)–O(3)#2	91.2(6)
O(1)–Zn(1)–O(2)#1	117.72(8)	O(2)#1–Zn(1)–N(1)#3	83.52(9)
O(1)–Zn(1)–O(3)#2	150.3(7)	O(2)#1–Zn(1)–O(5)#2	150.35(8)
O(1)–Zn(1)–N(1)#3	91.41(8)	O(2)#1–Zn(1)–N(2)	88.74(9)
O(1)–Zn(1)–O(5)#2	90.34(8)	O(3)#2–Zn(1)–O(5)#2	60.0(7)
O(1)–Zn(1)–N(2)	95.53(9)	N(1)#3–Zn(1)–O(3)#2	84.9(5)
O(1)–Zn(1)–O(10)#2	146.3(7)	N(1)#3–Zn(1)–O(5)#2	86.61(9)
N(2)–Zn(1)–O(5)#2	98.41(9)	N(2)–Zn(1)–O(3)#2	91.6(5)
O(10)#2–Zn(1)–N(2)	84.9(6)		

Symmetry codes: #1 -x+1, -y, -z+1, #2 x-1, y, z, #3 -x, -y, -z+1

Table S4. Selected bond lengths (Å) and bond angles (º) for LCP **3**.

LCP **3**			
Zn(1)–O(1)#1	1.983(2)	Zn(1)–N(1)#2	2.196(3)
Zn(1)–O(2)	1.979(2)	Zn(1)–N(2)	2.179(3)
Zn(1)–O(3)#2	2.034(2)	O(2)–Zn(1)–N(1)#2	88.56(9)
O(1)#1–Zn(1)–O(3)#2	129.41(9)	O(2)–Zn(1)–N(2)	91.57(10)

O(1)#1–Zn(1)–N(1)#2	95.12(10)	O(3)#2–Zn(1)–N(1)#2	87.67(9)
O(1)#1–Zn(1)–N(2)	90.78(10)	O(3)#2–Zn(1)–N(2)	84.86(9)
O(2)–Zn(1)–O(1)#1	128.32(9)	N(2)–Zn(1)–N(1)#2	172.37(10)
O(2)–Zn(1)–O(3)#2	102.21(9)		

Symmetry codes: #1 x+1, y, z, #2 -x+1, -y+2, -z

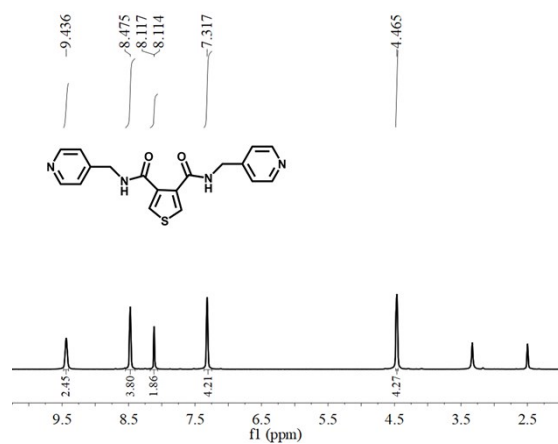**Table S5.** Comparison of fluorescent property of LCPs **1**–**3** for sensing Hg(II).

Fluorescent sensing materials	K_{sv} (M^{-1})	Detection Limit (M)	Medium	Ref.
LCP **1**	5.44×10^4	9.83×10^{-7}	H_2O	This work
LCP **2**	6.07×10^3	8.84×10^{-6}	H_2O	This work
LCP **3**	2.43×10^3	2.21×10^{-5}	H_2O	This work
CdTe QD	–	1.0×10^{-8}	H_2O/MeCN	2
Au/N–CQDs	–	1.18×10^{-7}	H_2O	3

Table S6. Comparison of fluorescent property of LCP **1** for sensing adenine.

Fluorescent sensing materials	K_{sv} (M^{-1})	Detection Limit (M)	Medium	Ref.
LCP **1**	1.103×10^4	4.83×10^{-6}	H_2O	This work
L–Tryptophan-Cu^{2+}	–	0.046×10^{-6}	H_2O	4
GO–PANI	–	1.3×10^{-5}	H_2O	5
N–GN	–	8.0×10^{-5}	DMA	6

Table S7. Comparison of fluorescent property of LCP **1** for sensing guanine.

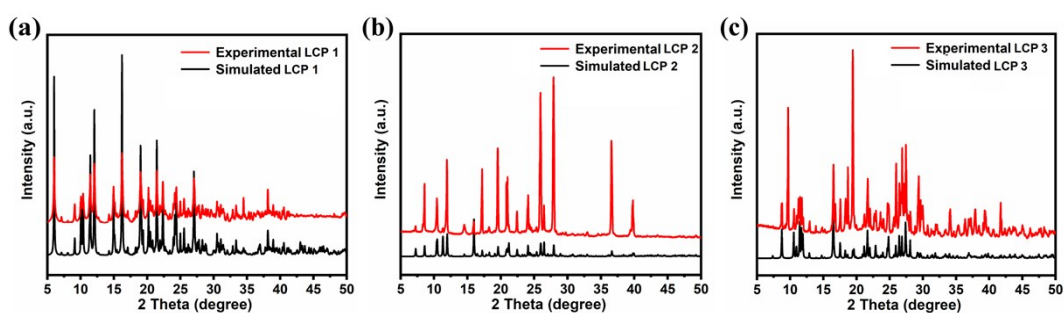| Fluorescent sensing materials	K_{sv} (M^{-1})	Detection Limit (M)	Medium	Ref.
LCP **1**	8.99×10^4	5.97×10^{-6}	H_2O	This work
CDs	–	0.67×10^{-7}	H_2O	7
CdTe nanoparticles	–	8×10^{-8}	H_2O	8
Cu^{2+}-nuclear	–	1.9×10^{-6}	H_2O	9
GO–PANI	–	1.36×10^{-5}	H_2O	10

Fig. S1. ^{1}H NMR spectrum of 4-bpft in DMSO-d_6.
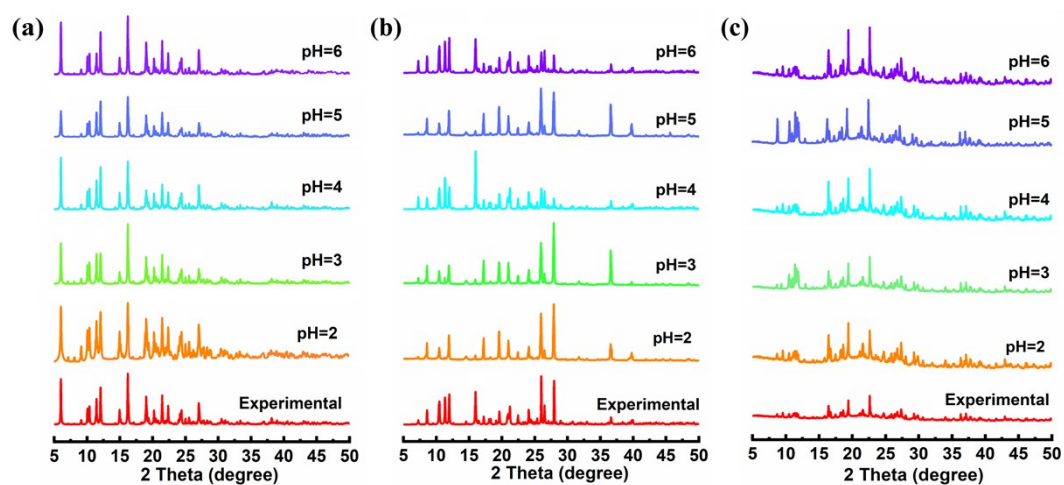

Fig. S2. The coordination environment of Zn(II) in LCP **2** (a) and LCP **3** (b). The 1D structure of LCP **2** (c) and LCP **3** (d).
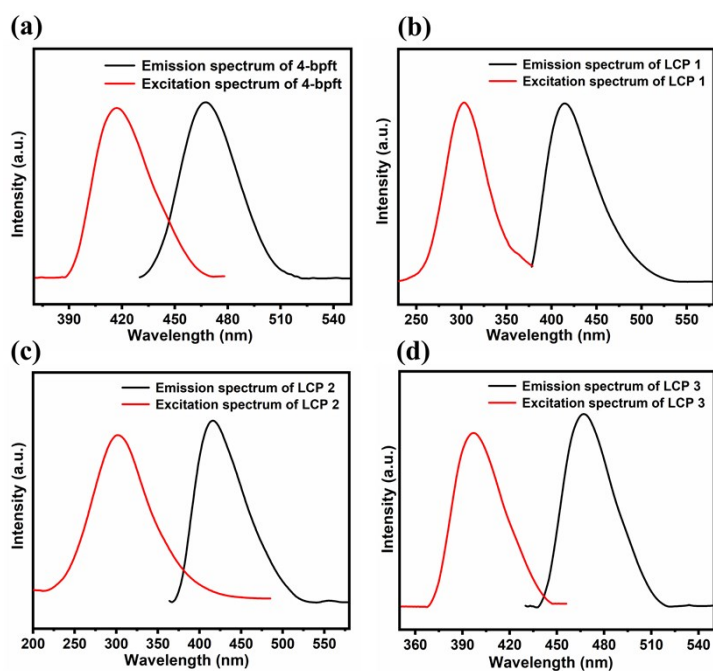

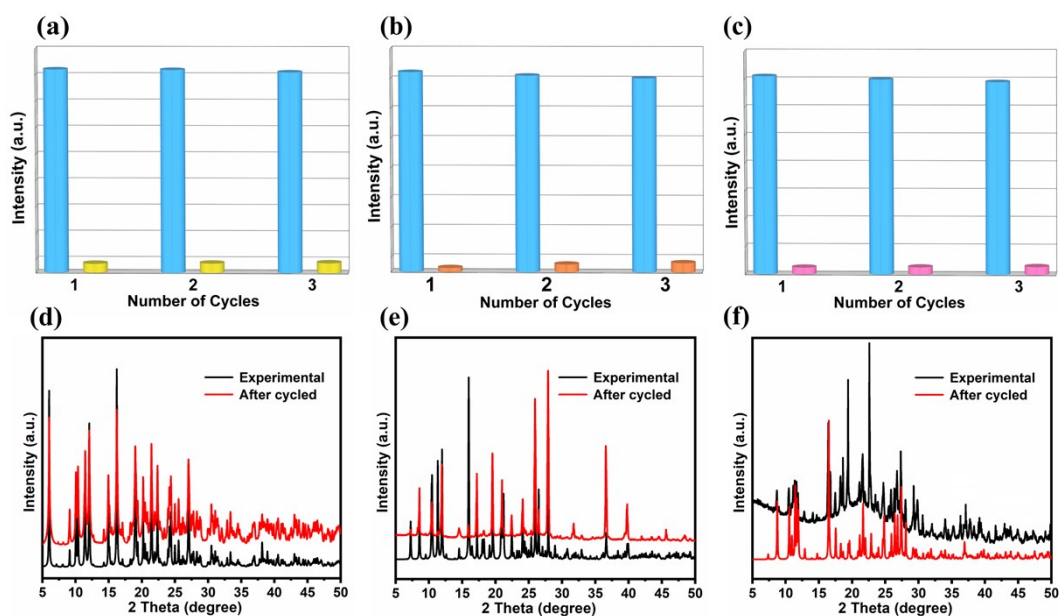**Fig. S3.** The IR spectra of LCPs **1–3**.
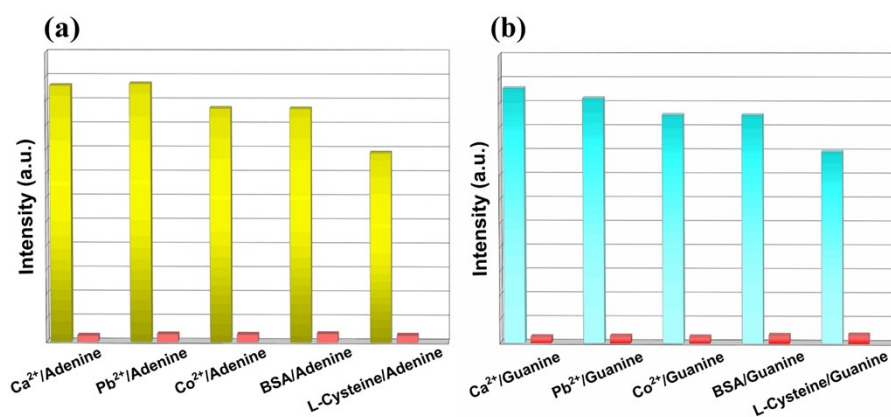
Fig. S4. The PXRD patterns of LCPs **1**–**3**.

Fig. S5. The PXRD patterns of LCPs **1**–**3** before and after being soaked in acidic and basic solutions for 12 h with a wide pH range of 2.0 ~ 6.0.
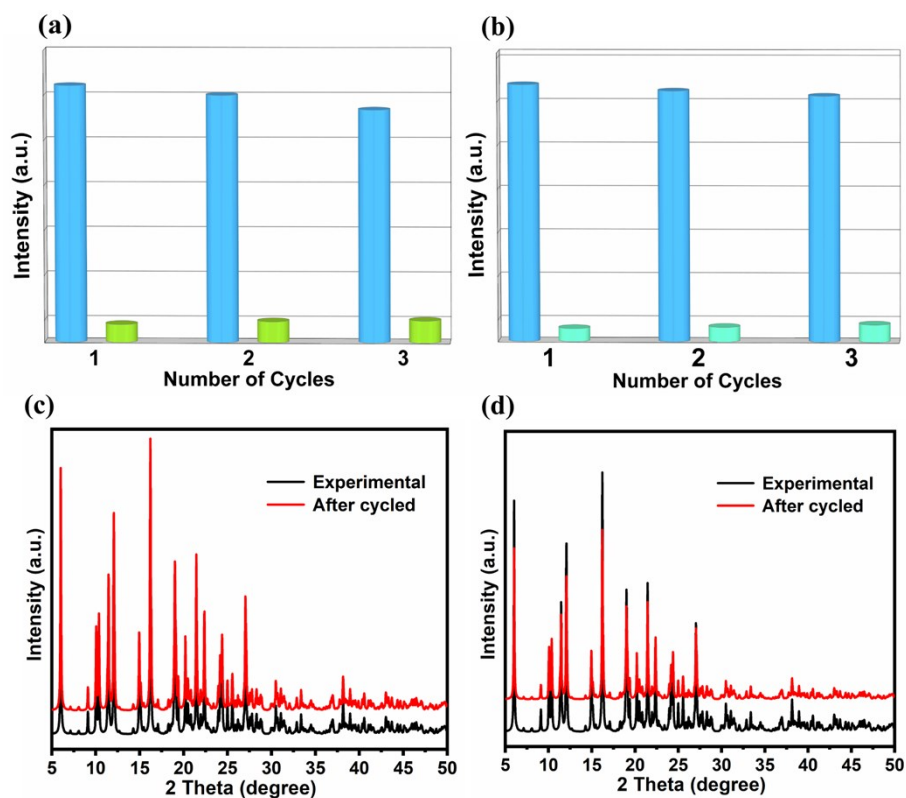

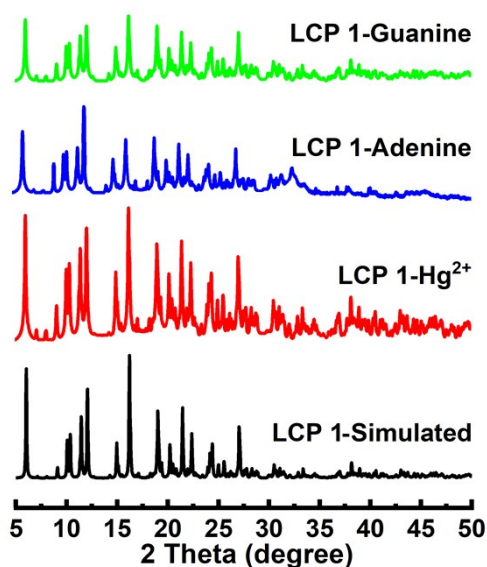**Fig. S6.** The solid excitation and emission spectra of 4-bpft and LCPs **1**–**3**.

Fig. S7. The cyclic response of the luminescence intensities for detecting Hg(II) of LCP **1** (a), LCP **2** (b), and LCP **3** (c); The PXRD patterns treated by Hg(II) of LCP **1** (d), LCP **2** (e), and LCP **3** (f).

Fig. S8. Competitive quenching experiments of LCP **1** for the selective recognition of adenine (a) and guanine (b).
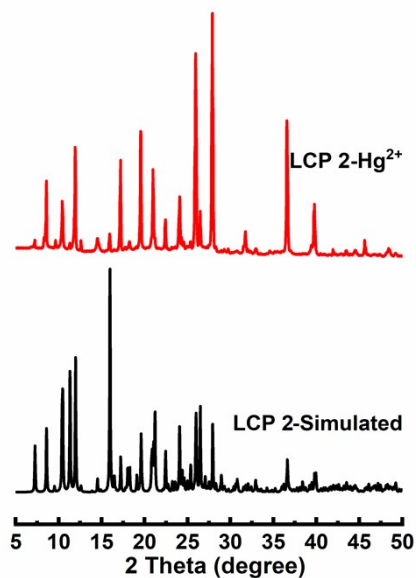
Fig. S9. The cyclic response of the luminescence intensities of LCP **1** for detecting of adenine (a) and guanine (b); The PXRD patterns of LCP **1** treated by adenine (c) and guanine (d).
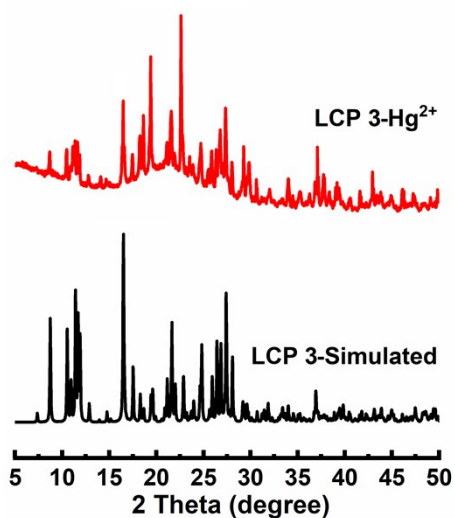

Fig. S10. The PXRD of LCP **1** after soaked in different analytes solution for 24h.
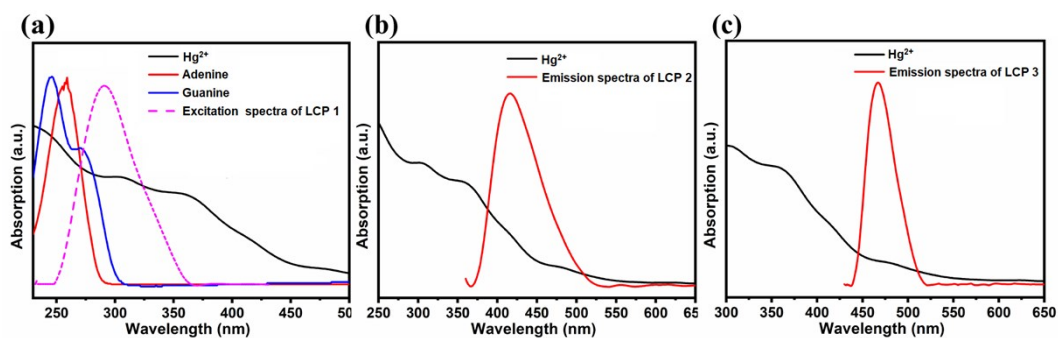
Fig. S11. The PXRD of LCP **2** after immersing in Hg(II) solution for 24h.

Fig. S12. The PXRD of LCP **3** after immersing in Hg(II) solution for 24h.

Fig. S13. UV-vis optical absorption spectra of analytes along with the excitation or emission spectra of LCPs **1**–**3**.

References

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