Electronic Supplementary Information

The high fluorescence sensitivity property and quenching mechanism of one-dimensional Cd-HCIA-1 sensor for nitrobenzene

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Table S1. Crystal data and structure refinement for Cd-HCIA-1

	Cd-HCIA-1
Empirical formula	$C_{52}H_{48}Cd_2N_4O_{19}$
M	1257.75
Crystal system	Triclinic
Space group	$P\bar{1}$
a,(Å)	10.116(3)
b,(Å)	10.401(4)
c,(Å)	13.707(5)
α(°)	92.118(5)
β(°)	106.385(5)
γ(°)	116.737(5)
V(Å^3)	1212.9(7)
Z	1
ρ calcd, g/cm^{-3}	1.722
μ , mm^{-1}	0.963
F(000)	636.0
2θ range for data collected/°	4.724 to 57.092
Reflections collected/unique	7705
GOF	1.062
Final R indexes [I>=2σ(I)]	R_1=0.0289,wR_2=0.0713
Final R indexes [all data]	R_1=0.0332,wR_2=0.0736
Largest diff,peak/hole/e Å^3	0.69/-0.61

Table S2 Selected bonds and angles for Cd-HCIA-1 (Å and °).

Cd-HCIA-1					
Bond lengths(Å)					
Cd1-O1	2.578(2)	Cd1-O4	2.352(2)	Cd1-N2	2.303(2)
Cd1-O2	2.2602(18)	Cd1-O6	2.344(2)	_	_
Cd1-O3	2.4965(19)	Cd1-N1	2.306(2)	_	_
Bond angles(°)					
O1-Cd1-C1	26.52(7)	O3-Cd1-O1	160.64(7)	N1-Cd1-O4	101.07(8)
O2-Cd1-O1	53.30(6)	O4-Cd1-O1	135.28(6)	N1-Cd1-O6	161.58(8)
O2-Cd1-O3	135.91(6)	O4-Cd1-O3	52.90(6)	N1-Cd1-C1	96.77(7)
O2-Cd1-O4	83.04(7)	O4-Cd1-C1	109.11(7)	N2-Cd1-O1	91.03(6)
O2-Cd1-O6	96.15(7)	O6-Cd1-O3	86.78(7)	N2-Cd1-O3	81.58(6)
O2-Cd1-N1	95.84(8)	O6-Cd1-O4	94.21(8)	N2-Cd1-O4	133.69(7)
O2-Cd1-N2	142.06(7)	O6-Cd1-C1	87.76(7)	N2-Cd1-O6	90.80(7)
O2-Cd1-C1	26.87(7)	O6-Cd1-O1	82.70(7)	N2-Cd1-N1	71.22(8)
O3-Cd1-C1	167.06(6)	N1-Cd1-O1	93.38(7)	N2-Cd1-C1	170.8(7)
		N1-Cd1-O3	94.24(7)		

Symmetry transformations used to generate equivalent atoms: #1 -1+x,+y,+z; #2 -x,-y,1-z;#3 1+x,+y,+z

Table S3 HOMO, LUMO and energy gap (E_g) calculated by the B3LYP, CAM-B3LYP, M06-2X and ω-B97XD methods and related experimental results of Cd-HCIA-1 in eV.

	HOMO	LUMO	E_g (theoretical)	E_g (experiment)
B3LYP	-6.28	-2.48	3.80	3.64
CAM-B3LYP	-7.97	-0.98	6.99	
M06-2X	-8.01	-1.29	6.72	
ω-B97XD	-8.54	-0.39	8.15	

Table S4 The maximum absorption peak (S0->S4) for Cd-HCIA-1 by different density functionals in Time-Dependent DFT (TDDFT) and experimental result.

Functional	Theoretical result (nm)	Oscillator strength (*f*)	Experimental result (nm)
B3LYP	305.11	0.0817	286.00
CAM-B3LYP	272.73	0.4308	
M06-2X	268.62	0.4200	

ω-B97XD	270.67	0.4332

Table S5. Calculated (Calcd value) and experimental (Explt value) geometric parameters of periodic structure and cluster model in the S_0 state.

	Periodic (Calcd)	Cluster (Calcd)	Complex (Explt)
Bond length (Å)			
Cd1-O1	2.63	2.46	2.57
Cd1-O3	2.47	2.63	2.50
Cd1-O6	2.35	2.35	2.34
Cd1-N1	2.30	2.31	2.31
Cd1-N2	2.35	2.35	2.30
Bond angle (°)			
O3-Cd1-O1	169.5	169.5	160.6
O2-Cd1-O4	76.80	77.10	83.04
N2-Cd1-N1	71.92	71.99	71.22
N1-Cd1-O6	161.4	161.4	161.6
Dihedral angle (°)			
C17-N1-Cd1-N2	177.6	177.6	176.6
C8-O3-Cd1-O2	-3.44	-3.34	-3.51
C1-O1-Cd1-O6	98.16	100.3	99.70

Table S6 MOFs for the determination of NB

MOFs	Analyte	K_{sv} (M^{-1})	LOD (μM)	Refs.
Cd-HCIA-1	NB	6.30×10^{6}	0.00303	This work
[Zn $(L)_{0.5}(bpb)_{0.5}(H_2O)_2$]n	NB	8.53×10^{4}	0.2	[1]
Eu^{3+}@MIL-121	NB	2.68×10^{6}	0.00156	[2]
[Zn(HNTB)(phen)] n	NB	60.75	753	[3]
Cd-MOF	NB	4.19×10^{6}	0.0716	[4]
$[Eu_2(MPDA)_3(H_2O)_2]\cdot2H_2O$	NB	1.03×10^{4}	5.69	[5]
$Zn_3(BCT)_2$: 4% Eu(III)	NB	2.05×10^{3}	0.00788	[6]
Eu-MOF	NB	1.33×10^{4}	0.028	[7]
Cu-MOF-1	NB	1.31×10^{5}	7.6×10^{-4}	[8]

Table S7 Quenching response time of different concentrations of NB to Cd-HCIA-1

	2×10^{-4} mol/L	1×10^{-4} mol/L	2×10^{-5} mol/L	1×10^{-5} mol/L	2×10^{-6} mol/L
Reaction time (s)	75	121	159	188	198

Table S8. Average excited state lifetime values (<τ>) of Cd-HCIA-1 before and after addition of NB.

	a_1(%)	a_2(%)	τ_1(ns)	τ_2(ns)	<τ>*(ns)
Cd-HCIA-1	99.22	0.78	0.44	3.88	0.447
Treated by NB	97.51	2.49	0.20	1.55	0.234

where <τ>* represents the actual average fluorescence lifetime.

Table S9. Absorption wavelength (λ/nm), electronic transition and oscillator strengths (*f*) of Cd-HCIA-1 at the CAM-B3LYP theory level with LR or SS relative to experimental data (λ_{Exp}/nm).

	electronic transition	λ/ nm	*f*	λ_{Exp}/nm
LR	$S_0\rightarrow S_1$	280	0.0826	286
	$S_0\rightarrow S_4$	273	0.4308	
SS	$S_0\rightarrow S_1$	281	0.0627	

Table S10 Hole-electron analysis index of Cd-HCIA-1.

	Energy (eV)	D (Å)	Sr	H (Å)	t (Å)	Δ σ (Å)
NB@Cd-HCIA-1	3.571	2.306	0.369	2.641	0.901	-0.556
PhOH@Cd-HCIA-1	4.186	1.363	0.480	2.944	-0.199	0.253

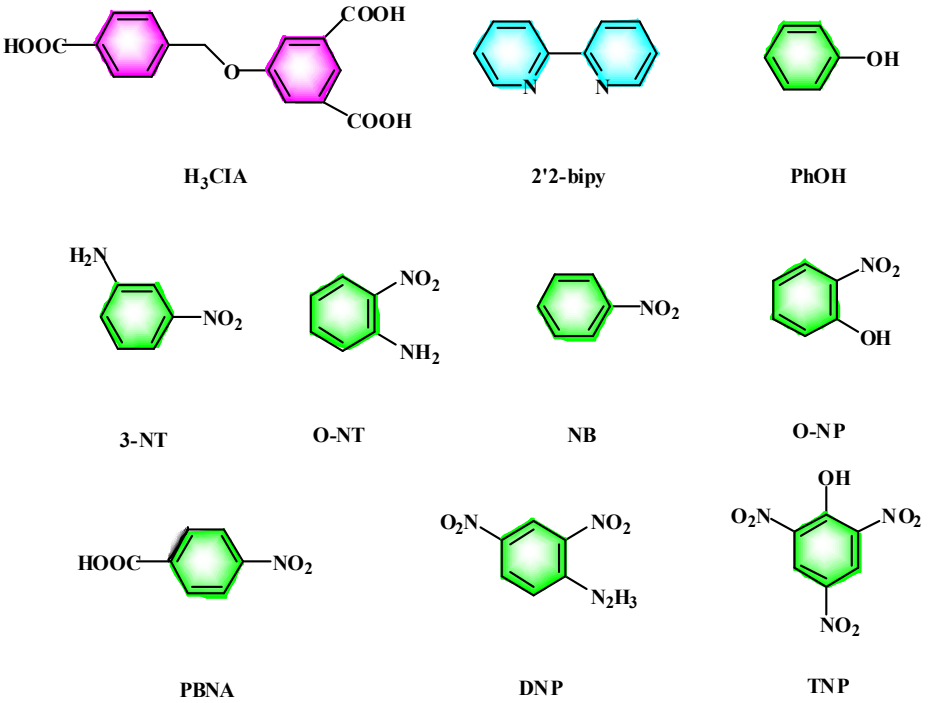

Fig. S1 Molecular structures of ligand structure in Cd-HCIA-1 and the selected nitro-detection species.

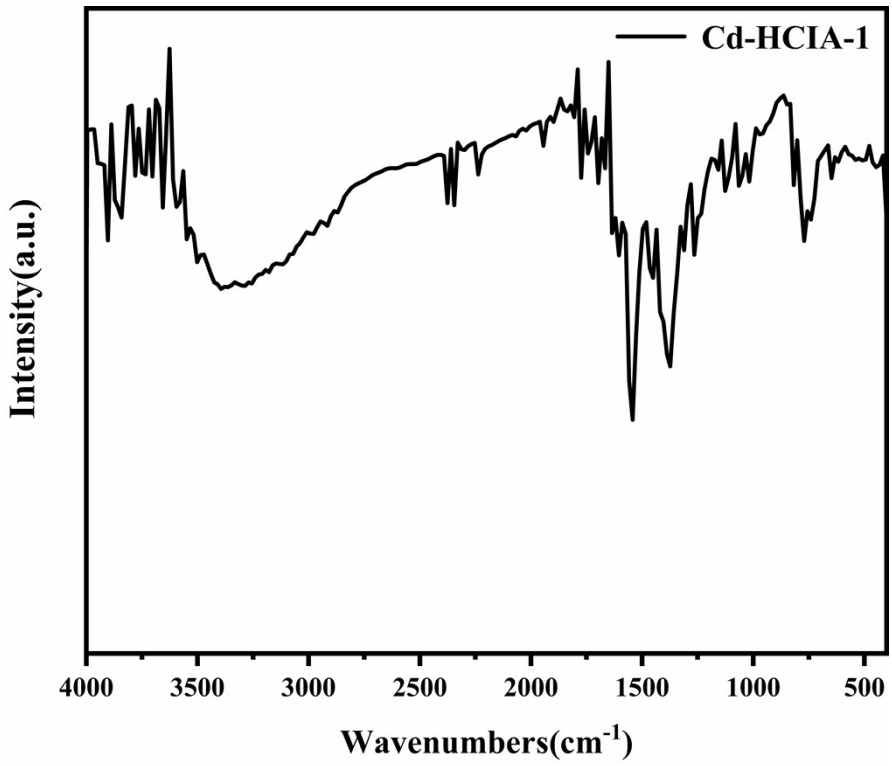

Fig. S2 The FI-IR spectra of Cd-HCIA-1.

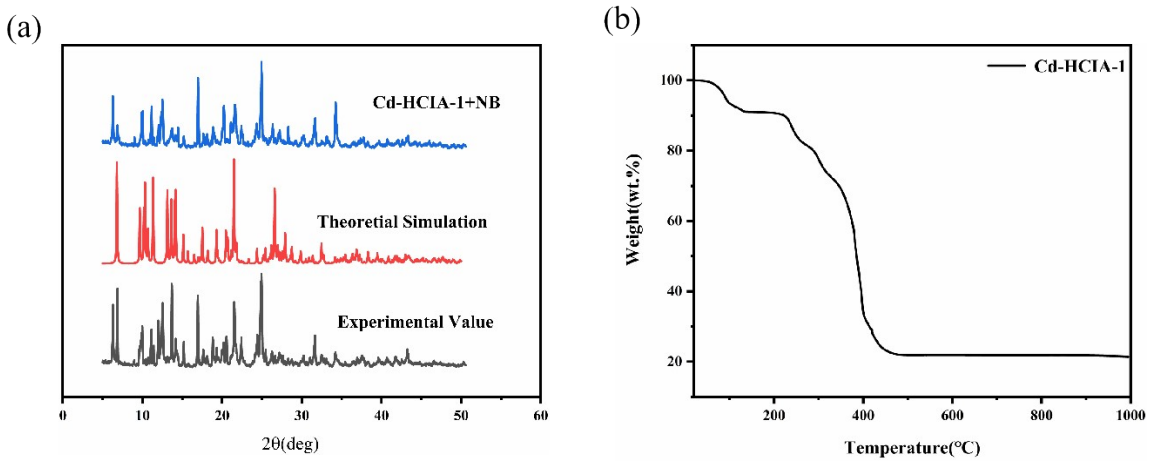

Fig. S3 (a) PXRD patterns of simulated, experimental and Cd-HCIA-1 after selective experiments of NB.(b) The TGA curve for Cd-HCIA-1

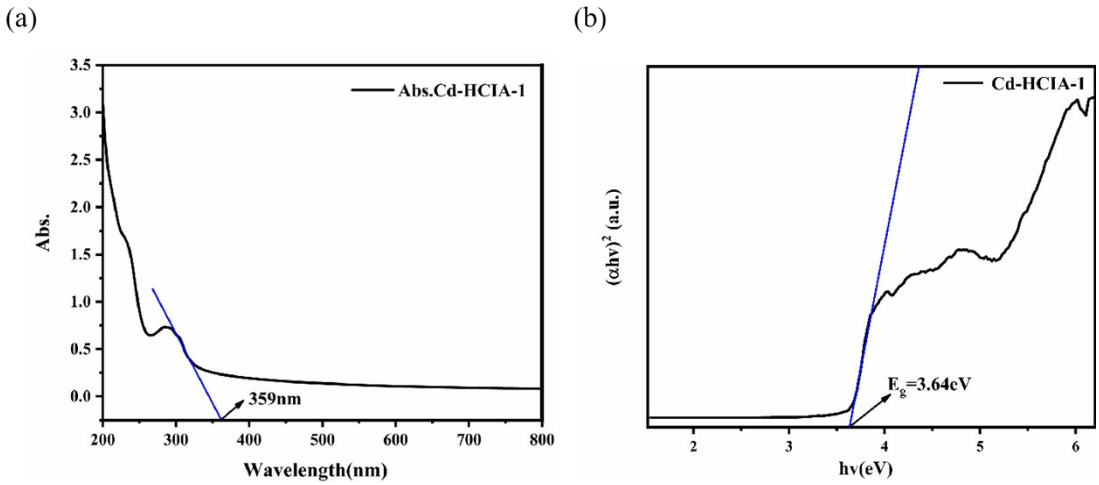

Fig. S4 UV–visible absorption spectra of Cd-HCIA-1. (b) Optical band gap energy plots of Cd-HCIA-1.

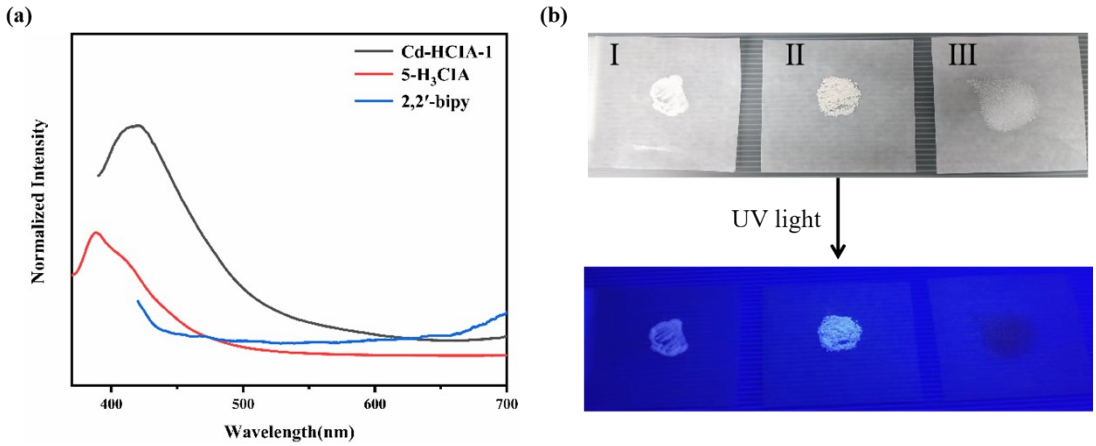

Fig. S5 (a) Solid emission spectra of Cd-HCIA-1 (λ_{ex} = 364 nm) and ligand 5-H_3CIA (λ_{ex} = 364.2 nm), 2-bipy (λ_{ex} = 397.0nm) (b) Color of the sample under natural light and ultraviolet light.I: Cd-HCIA-1, II: 5-H_3CIA, III: 2,2'-bipy.

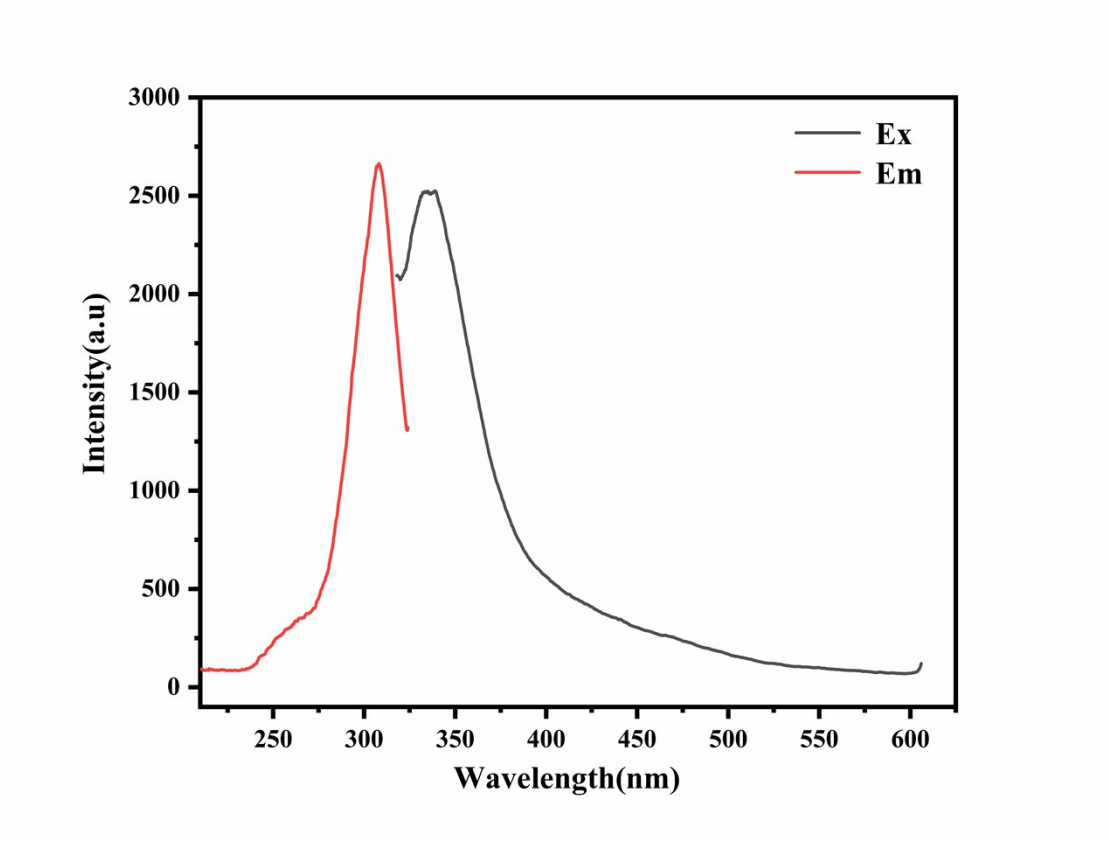

Fig. S6 Fluorescence emission spectrum of Cd-HCIA-1 in water (λ_{ex} = 308.0 nm) and excitation spectrum (λ_{em} = 334.8 nm).

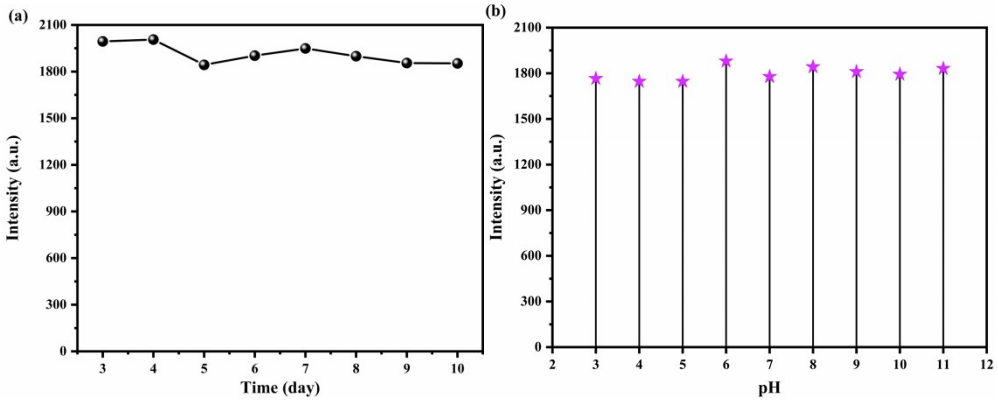

Fig. S7. (a) The intensity of the emission spectrum of Cd-HCIA-1 dispersed over different times and (b) emission intensity after treatment with different pH values solvent at the same time period, λ_{ex} = 308.0 nm.

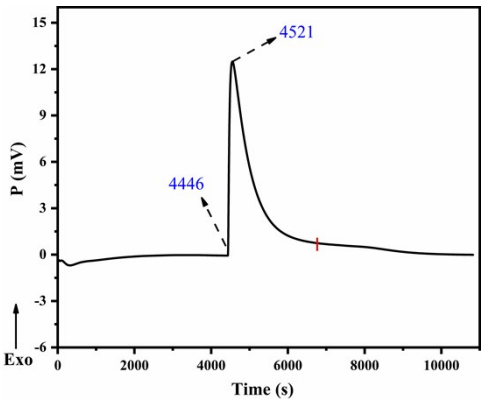

Fig. S8 Heat flow over time in NB@Cd-HCIA-1 system, c(NB) = 2 × 10^{-4} mol/L.

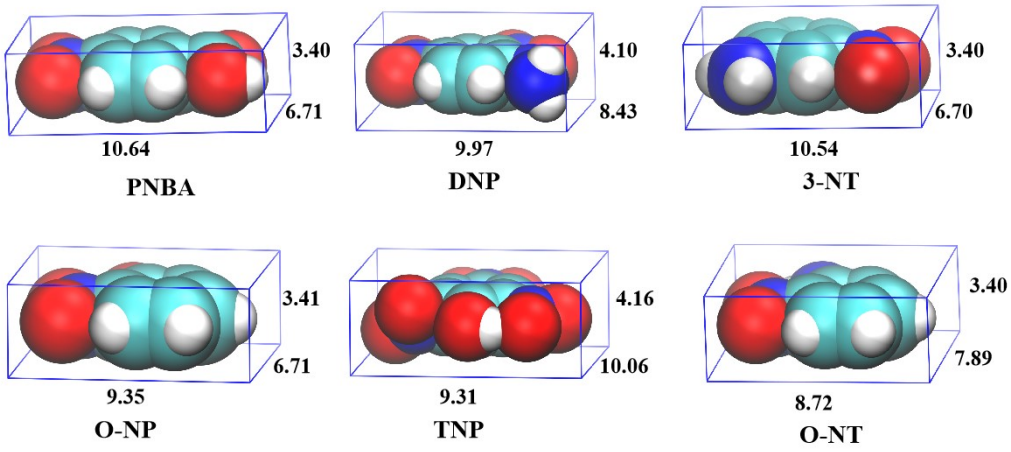

Fig. S9 The blue cuboids marked with width, height, and depth (Å) represent the volumes of nitro-detection species, respectively.

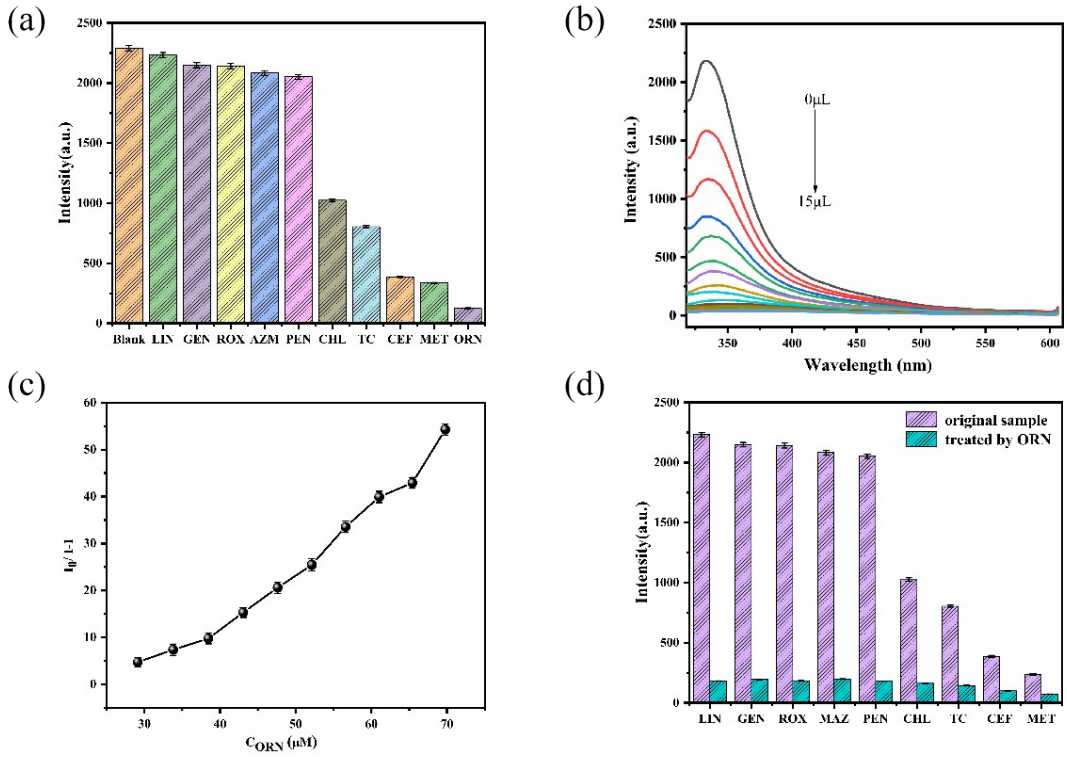

Fig. S10 (a) Fluorescence intensity of Cd-HCIA-1 in different antibiotic solutions. (b) Fluorescence quenching of Cd-HCIA-1 dispersed by gradually increasing the concentration of ornidazole. (c) Linear Stern–Volmer curve of $I_0 / I - 1$ of ornidazole at a low concentration range. (d) After addition of other antibiotic solutions and ornidazole, the fluorescence intensity of Cd-HCIA-1 changes.

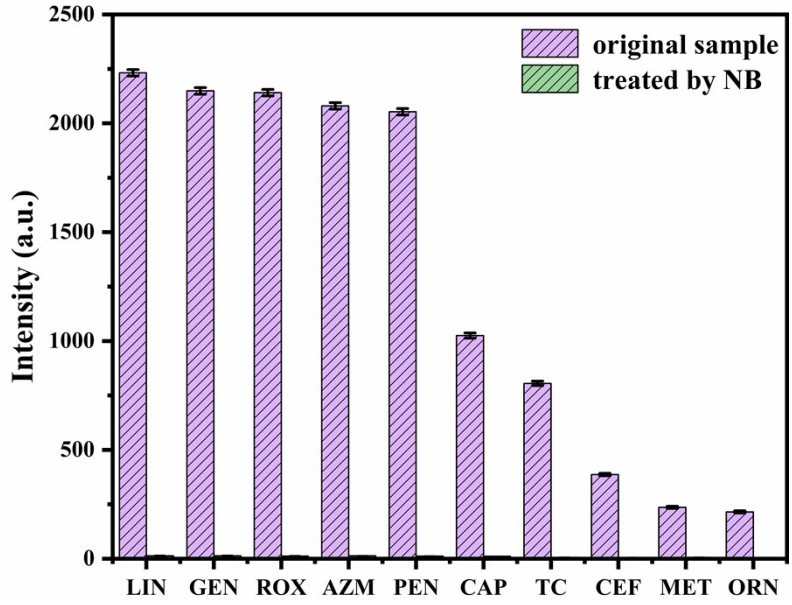

Fig S11. Fluorescence intensity of stable supernatant when antibiotic molecules are present and after addition of nitrobenzene.

The cartesian coordinates of all the optimized structures

1. Cartesian coordinates for structural optimization of Cd-HCIA-1in S_0

Cd	-4.44212100	-0.18147600	0.14589100
O	-2.93931300	-1.60747900	-0.94488900
O	-4.08628000	-7.83268200	-0.07836100
O	0.95833900	-4.97570700	-1.37611900
O	-3.76970600	-0.37898500	2.38707900
H	-4.19051200	-5.31375400	-0.45006000
H	-0.35819600	-7.11975000	-1.19147500
H	-0.74838600	-2.84054300	-1.10137900
H	1.23005700	-3.08778000	-2.20168100
H	1.43594700	-3.18856600	-0.43593300
H	-1.62360300	-0.60642000	0.95503100
H	-1.13416300	-1.41578000	5.14935400
H	3.01161000	-3.57698400	-3.68925600
H	-4.20778000	-0.17351700	-3.06058100
N	-5.77264200	0.02808200	-1.72696000
N	-6.67178800	0.03089600	0.85892100
C	-3.34973400	-2.73003600	-0.48179500
C	-2.55517400	-3.95857400	-0.79139300
C	-3.14080200	-5.21848100	-0.68644100
C	-2.35054500	-6.36453200	-0.83710700
C	-0.98556100	-6.24397600	-1.09627000
C	-0.39718300	-4.97746000	-1.18990600
C	-1.18203800	-3.82733800	-1.05863100
C	-2.94184100	-7.72122500	-0.64961000
C	1.62141400	-3.69611700	-1.38532300
C	3.08729000	-3.94911400	-1.57401600
C	-1.54469600	-0.99823600	3.07163900
C	3.64558800	-3.83812100	-2.85143800
C	-2.98393300	-0.73110200	3.28575600
C	-5.27904600	-0.02637200	-2.97162700
C	-7.09872700	0.20262700	-1.52518800
C	-7.58574700	0.23450700	-0.11879100
O	-4.36114900	2.26574800	0.44997700
C	-7.05396500	0.04504500	2.14519400
C	3.90971100	-4.29579900	-0.49238400
C	-0.98745700	-0.86479300	1.79027200
C	-0.71781600	-1.32245200	4.15701700
C	5.00327100	-4.04402200	-3.05121600
O	-3.37694100	-0.87247300	4.54470900
C	-6.08788200	0.09455700	-4.09769100
C	-7.96281900	0.33875800	-2.61444200
C	-8.93525900	0.44991900	0.19545500
C	-3.21681500	2.37717000	-0.12100600
C	-8.37971800	0.24876000	2.52217100
H	-6.27705600	-0.11408200	2.88461000
H	3.48541400	-4.38196300	0.50004200
C	5.27291100	-4.50168100	-0.68447200
C	0.37574600	-1.07066800	1.59818800
C	0.63987000	-1.52834400	3.95724000
C	5.83013900	-4.36828500	-1.96584600

H	5.41975700	-3.95055800	-4.04349600
H	-4.32783400	-0.67569000	4.61108900
C	-7.45282800	0.28268700	-3.90846600
H	-5.64422900	0.04959100	-5.08386800
H	-9.02476500	0.47760500	-2.47199700
H	-9.66977400	0.61615400	-0.57915500
C	-9.33626500	0.45086700	1.52955500
C	-2.62580900	3.73392700	-0.30987100
H	-8.63827900	0.25602600	3.57345600
H	5.90996900	-4.75415700	0.15164300
H	0.79965100	-0.98324400	0.60574400
C	1.19816500	-1.41735600	2.67981600
H	1.27343200	-1.78934800	4.79527800
C	7.26980300	-4.63449900	-2.17997700
H	-8.12516700	0.38224200	-4.75264500
H	-10.37698000	0.61985200	1.77936600
C	-3.41579600	4.87998300	-0.15816500
C	-1.26055500	3.85448500	-0.56797600
C	2.66404200	-1.67034900	2.49112500
O	7.66238700	-4.49404000	-3.43891500
O	8.05468300	-4.98864900	-1.28124400
H	-4.46729200	4.78660600	0.06859800
C	-2.83014200	6.13988800	-0.26309600
H	-0.60253000	2.99732400	-0.63785500
C	-0.67220900	5.12100200	-0.66175100
H	2.84903500	-2.17837900	1.54194100
H	3.05470100	-2.27886100	3.30756600
O	3.32711700	-0.39076200	2.48191600
H	8.61119300	-4.69617800	-3.50379100
C	-3.62478900	7.36863000	0.04627300
C	-1.45706500	6.27112200	-0.53049000
O	0.68330400	5.12275400	-0.84803700
C	4.68264000	-0.38900900	2.29571700
O	-4.64493200	7.28134600	0.80798200
H	-1.02046900	7.25608700	-0.58926800
C	1.34638400	6.40234500	-0.85720600
C	5.46750000	-1.53913100	2.16445000
C	5.27101800	0.87750600	2.20208100
H	0.95603000	7.00967500	-1.67467900
H	1.15947200	6.90891100	0.09146800
C	2.81226100	6.14934700	-1.04589700
H	5.03606000	-2.52649300	2.21135700
C	6.84058000	-1.40789900	1.89706700
H	4.64986000	1.75740500	2.29318000
C	6.63600200	0.99806100	1.94291900
C	3.37055800	6.26034100	-2.32332100
C	3.63468100	5.80266200	0.03573300
C	7.63520800	-2.63663500	1.58761300
C	7.42626600	-0.14798700	1.79226100
C	7.22729700	2.35475500	1.75540800
H	2.73666500	6.52135000	-3.16125300
C	4.72824100	6.05443800	-2.52310000
H	3.20882600	5.70988200	1.02676700
C	4.99788200	5.59678100	-0.15635500
O	7.22481000	-3.75898700	2.05075600
H	8.47742700	-0.05668500	1.55733400
O	6.60448700	3.39142200	2.15062200

C	5.55511000	5.73017600	-1.43772900
H	5.14471800	6.14760600	-3.51541100
H	5.63250200	5.32739000	0.67688900
C	6.99477300	5.46396200	-1.65186000
O	7.38735700	5.60442100	-2.91079800
O	7.77965300	5.10981300	-0.75312800
H	8.33627700	5.40278000	-2.97563700
O	8.64119300	-2.55056600	0.83650900
H	9.03600200	-3.42900800	0.68333600
O	8.34897600	2.46399700	1.19552100
H	8.59540300	3.40295900	1.11009100
O	-3.22182700	8.47062700	-0.40844200
H	-3.77643700	9.20471000	-0.08814800
O	-2.32583900	-8.74656000	-1.04050100
H	-2.82619000	-9.55193300	-0.81778400
O	-4.35540700	-2.81563500	0.26958300
O	-2.60003500	1.35184200	-0.51201000

2. Cartesian coordinates for structural optimization of Cd-HCIA-1 in S_1

Cd	-4.45303700	-0.19076600	0.14359000
O	-2.94759400	-1.61434800	-0.94671900
O	-4.08389900	-7.84138200	-0.07930000
O	0.95595700	-4.97588800	-1.37678300
O	-3.78062000	-0.38672600	2.38491300
H	-4.19294300	-5.31848900	-0.45513800
H	-0.35706000	-7.12212600	-1.19440800
H	-0.75806600	-2.84288000	-1.11458000
H	1.22526600	-3.08703600	-2.20246700
H	1.43020400	-3.18684400	-0.43734800
H	-1.63424100	-0.61286600	0.95284100
H	-1.14348200	-1.41872100	5.14787100
H	3.00714500	-3.57369300	-3.68974200
H	-4.22062400	-0.18251400	-3.05282300
N	-5.78363500	0.01616600	-1.72949900
N	-6.68317700	0.01786300	0.85624600
C	-3.35613800	-2.73753500	-0.48349500
C	-2.55940300	-3.96474700	-0.79276300
C	-3.14286200	-5.22564900	-0.68768400
C	-2.35059700	-6.37035500	-0.83803400
C	-0.98578400	-6.24747700	-1.09701100
C	-0.39958900	-4.97995900	-1.19077500
C	-1.18645600	-3.83117700	-1.05981500
C	-2.93956800	-7.72803800	-0.65039400
C	1.61681400	-3.69515200	-1.38610500
C	3.08315500	-3.94564000	-1.57453300
C	-1.55464400	-1.00200200	3.06991600
C	3.64145300	-3.83389700	-2.85189000
C	-2.99437400	-0.73732700	3.28376900
C	-5.28975600	-0.03764500	-2.97408100
C	-7.11005100	0.18844600	-1.52795700
C	-7.59733900	0.21972200	-0.12163900
O	-4.37635300	2.25664700	0.44726900
C	-7.06557300	0.03156900	2.14245800
C	3.90601200	-4.29071400	-0.49271700
C	-0.99744300	-0.86781200	1.78861000
C	-0.72736800	-1.32459900	4.15547400

C	4.99952200	-4.03747800	-3.05142700
O	-3.38732800	-0.87916400	4.54268700
C	-6.09863000	0.08168900	-4.10028900
C	-7.97421200	0.32289300	-2.61736500
C	-8.94727000	0.43284800	0.19236600
C	-3.23212700	2.36995500	-0.12356000
C	-8.39173400	0.23305000	2.51920000
H	-6.28311900	-0.12845700	2.87195000
H	3.48158700	-4.37722200	0.49962100
C	5.26959600	-4.49426500	-0.68456400
C	0.36614400	-1.07135700	1.59676800
C	0.63070300	-1.52817100	3.95593800
C	5.82678600	-4.36012200	-1.96587600
H	5.41608000	-3.94329800	-4.04362000
H	-4.33849600	-0.68441600	4.60846900
C	-7.46392900	0.26748500	-3.91130200
H	-5.66387900	0.03072800	-5.08826700
H	-9.03434100	0.46105300	-2.47502300
H	-9.68037200	0.59650700	-0.58157900
C	-9.34847900	0.43332900	1.52640500
C	-2.64344500	3.72770200	-0.31256700
H	-8.65887800	0.23129800	3.56647800
H	5.90705000	-4.74536300	0.15167500
H	0.78974100	-0.98320200	0.60431000
C	1.18899900	-1.41643400	2.67858000
H	1.26456500	-1.78807900	4.79412600
C	7.26694200	-4.62387700	-2.17974400
H	-8.12990700	0.36656100	-4.75778800
H	-10.38717500	0.59307600	1.78134800
C	-3.43544100	4.87241300	-0.16117700
C	-1.27836300	3.85058200	-0.57048600
C	2.65534100	-1.66691700	2.49015400
O	7.65947200	-4.48295200	-3.43864600
O	8.05229800	-4.97651200	-1.28083100
H	-4.48563500	4.77742900	0.06999700
C	-2.85195600	6.13331300	-0.26623500
H	-0.65614000	2.97184200	-0.66643400
C	-0.69219900	5.11810100	-0.66438900
H	2.84140600	-2.17477200	1.54112200
H	3.04707300	-2.27451900	3.30679800
O	3.1619800	-0.38618500	2.48082600
H	8.60866300	-4.68329300	-3.50329300
C	-3.64877900	7.36072900	0.04280400
C	-1.47906800	6.26688200	-0.53344300
O	0.66333700	5.12217100	-0.85047000
C	4.67174400	-0.38211400	2.29483200
O	-4.66888400	7.27180600	0.80437300
H	-1.04452900	7.25286800	-0.59180000
C	1.32419900	6.40290800	-0.85975700
C	5.45861700	-1.53089600	2.16388100
C	5.25794000	0.88540300	2.20106900
H	0.93323400	7.01030300	-1.67704900
H	1.13673900	6.91001300	0.08865600
C	2.79054100	6.15242000	-1.04818300
H	5.02881800	-2.51897500	2.21067200
C	6.83150800	-1.39732900	1.89668300
H	4.63510600	1.76418800	2.29155300

C	6.62275200	1.00828000	1.94209300
C	3.34883800	6.26416300	-2.32554200
C	3.61339700	5.80734500	0.03363100
C	7.62831100	-2.62473900	1.58756000
C	7.41502500	-0.13642200	1.79175000
C	7.21172300	2.36596500	1.75443900
H	2.71453100	6.52365600	-3.16362900
C	4.70690700	6.06058000	-2.52508000
H	3.18740500	5.71362000	1.02451300
C	4.97698200	5.60379500	-0.15821600
O	7.21978900	-3.74772100	2.05083300
H	8.46603500	-0.04333200	1.55683200
O	6.58705700	3.40161800	2.14938200
C	5.53417200	5.73793700	-1.43952800
H	5.12340900	6.15405300	-3.51736400
H	5.61189800	5.33522900	0.67507400
C	6.97432700	5.47418200	-1.65339600
O	7.36685700	5.61510700	-2.91229800
O	7.75968300	5.12154800	-0.75448400
H	8.31598700	5.41448100	-2.97704000
O	8.63426000	-2.53705400	0.83659300
H	9.03025100	-3.41493800	0.68331200
O	8.33329600	2.47705600	1.19470300
H	8.57777400	3.41644900	1.10853900
O	-3.24765900	8.46334500	-0.41203900
H	-3.80289200	9.19660200	-0.09129800
O	-2.32173100	-8.75237100	-1.04101700
H	-2.82076500	-9.55842700	-0.81830700
O	-4.36177500	-2.82474900	0.26774500
O	-2.61351200	1.34563100	-0.51429500

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