Supplementary Information for

Terbium(III)-based coordination polymer with millimeter single-crystal size, high selectivity and sensitivity for folic acid

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Table S1 Crystal data and structure refinement parameters for the complex

Complex	**[Tb(Hpda)(pda)(H_2O)$_2$]·4H_2O**
Empirical formula	$C_{14}H_{19}N_2O_{14}Tb$
Crystal system	Monoclinic
Formula weight	598.23
Temperature (K)	273.15
Space group	$P2_1/c$
a (Å)	14.0209(8)
b (Å)	11.2186(7)
c (Å)	12.8497(7)
α (°)	90
β (°)	102.327(2)

γ (°)	90
Volume ($Å^3$)	1974.6(2)
Z	4
ρ_{calc} (mg/cm^3)	2.012
μ (mm^{-1})	3.660
F(000)	1176.0
θ range for collection (°)	2.974 to 30.594
Index ranges	-17≤ h ≤20, -14≤ k ≤16, -18≤ l ≤18
Reflections collected/unique	33196 / 5681 [R(int) = 0.0211]
Data/restraints/parameters	5681/2/299
Goodness-of-fit on F^2	1.117
Final R indices［I>2sigma(I)］	R_1 = 0.0211, wR_2 = 0.0551
R indices (all data)	R_1 = 0.0244, wR_2 = 0.0562

Table S2 Selected bond lengths (Å) and angles (°) of the complex

[Tb(Hpda)(pda)(H_2O)$_2$]·4H_2O			
Tb(1)-O(6)#1	2.5149(16)	Tb(1)-O(8)#1	2.4704(17)
Tb(1)-O(1)	2.5194(18)	Tb(1)-O(4)	2.4397(18)
Tb(1)-O(5)	2.4494(16)	Tb(1)-N(2)#1	2.5729(18)
Tb(1)-O(10)	2.4041(18)	Tb(1)-N(1)	2.572(2)
Tb(1)-O(9)	2.4460(17)		
O(6)#1-Tb(1)-O(1)	83.81(6)	O(6)#1-Tb(1)-N(2)#1	62.12(5)
O(6)#1-Tb(1)-N(1)	71.90(6)	O(1)-Tb(1)-N(2)#1	65.40(6)
O(1)-Tb(1)-N(1)	62.25(6)	O(5)-Tb(1)-O(6)#1	136.85(6)

O(5)-Tb(1)-O(1)	139.17(6)	O(5)-Tb(1)-O(8)#1	77.31(6)
O(5)-Tb(1)-N(2)#1	129.30(6)	O(5)-Tb(1)-N(1)	118.66(6)
O(10)-Tb(1)-O(6)#1	73.10(6)	O(10)-Tb(1)-O(1)	140.40(6)
O(10)-Tb(1)-O(5)	71.85(6)	O(10) -Tb(1)-O(8)#1	85.78(7)
O(10)-Tb(1)-O(4)	80.12(7)	O(10)-Tb(1)-N(2)#1	75.36(6)
O(10)-Tb(1)-N(1)	134.06(7)	O(10)-Tb(1)-O(9)	141.37(6)
O(8)#1-Tb(1)-O(6)#1	124.07(5)	O(8)#1-Tb(1)-O(1)	81.06(6)
O(8)#1-Tb(1)-N(2)#1	62.59(6)	O(8)#1-Tb(1)-N(1)	139.06(7)
O(4) -Tb(1)-O(6)#1	75.34(6)	O(4)-Tb(1)-O(1)	124.96(6)
O(4)-Tb(1)-O(5)	74.58(6)	O(4)-Tb(1)-O(8)#1	151.29(6)
O(4)-Tb(1)-N(2)#1	135.34(6)	O(4)-Tb(1)-N(1)	62.93(6)
N(1)-Tb(1)-N(2)#1	111.98(6)	O(9)-Tb(1)-O(6)#1	144.00(6)
O(9)-Tb(1)-O(1)	71.60(7)	O(9)-Tb(1)-O(5)	70.38(6)
O(9) -Tb(1)-O(8)#1	78.40(7)	O(9)-Tb(1)-O(4)	97.35(7)
O(9)-Tb(1)-N(2)#1	124.83(7)	O(9)-Tb(1)-N(1)	73.45(7)

Symmetry Codes: #1 = 1+x, 3/2-y, 1/2+z

Table S3 Distances (Å) and angles (°) of hydrogen bonds for the complex.

Donor-H···acceptor	**d(D-H)/Å**	**d(H···A)/Å**	**d(D···A)/Å**	**Angle/°**
O10-H10A···O12#1	0.85	1.92	2.724(3)	156.7
O10-H10B···O11	0.85	1.89	2.740(3)	177.6
O12-H12A···O7	0.85	1.84	2.689(3)	173.5
O11-H11A···O7#2	0.85	2.04	2.891(3)	176.4
O9-H9B···O3#3	0.85	1.89	2.732(3)	168.4
O14-H14B···O2	0.85	1.65	2.482(4)	166.6

O14-H14C···O3#4	0.90(7)	1.74(7)	2.632(4)	177(6)

Symmetry Codes: #1 = 2-x, 2-y, 1-z; #2 = 2-x, -1/2+y, 3/2-z; #3 = 1-x, -1/2+y, 3/2-z; #4 = +x, -1+y, +z

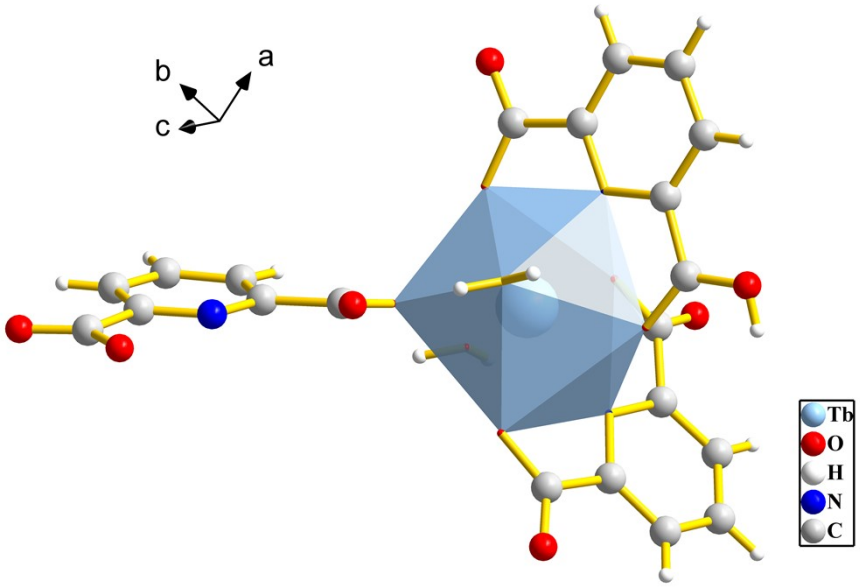

Fig. S1. The coordination environment of Tb^{III} with surrounding oxygen atoms.

Table S4. The *CShM* values calculated by *SHAPE* 2.1[3, 4] of Tb^{III} ion in the complex.

Coordination Geometry	Tb1
Johnson triangular cupola J3 (C3v)	14.613
Capped cube J8 (C4v)	9.172
Spherical-relaxed capped cube (C4v)	7.618
Capped square antiprism J10 (C4v)	1.907
Spherical capped square antiprism (C4v)	1.107
Tricapped trigonal prism J51 (D3h)	2.303
Spherical tricapped trigonal prism (D3h)	1.079
Tridiminished icosahedron J63 (C3v)	11.044
Hula-hoop (C2v)	10.605
Muffin (Cs)	1.146

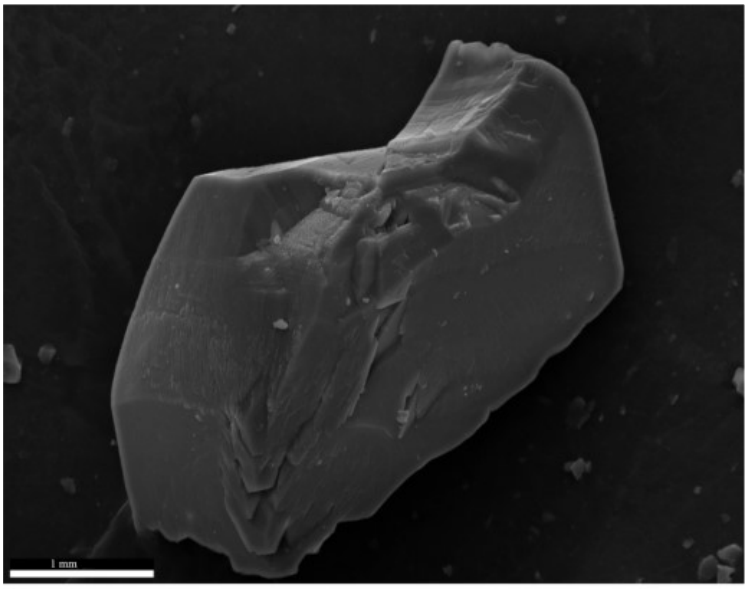

Fig. S2. Scanning electron microscope (SEM) photographs of the single crystal.

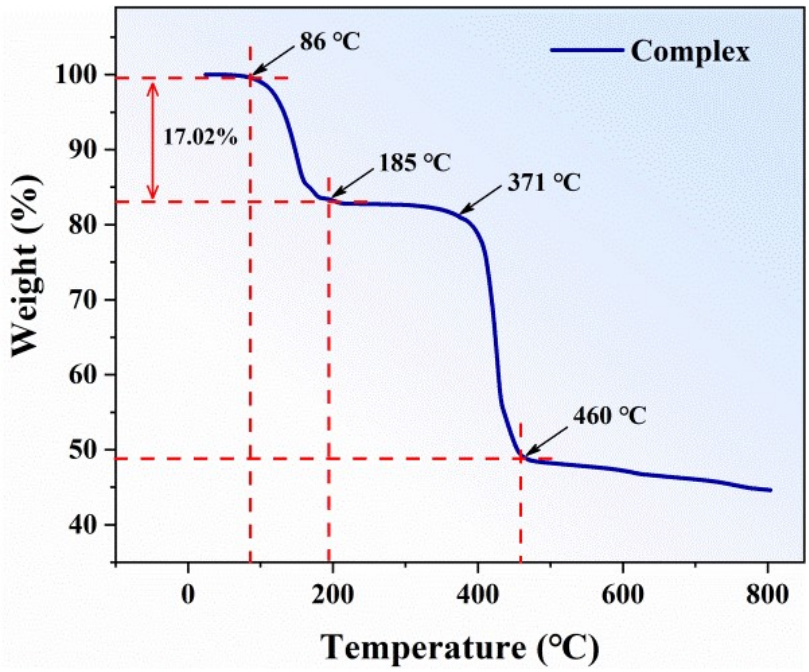

Fig. S3. The thermal gravimetric (TGA) curve of the complex.

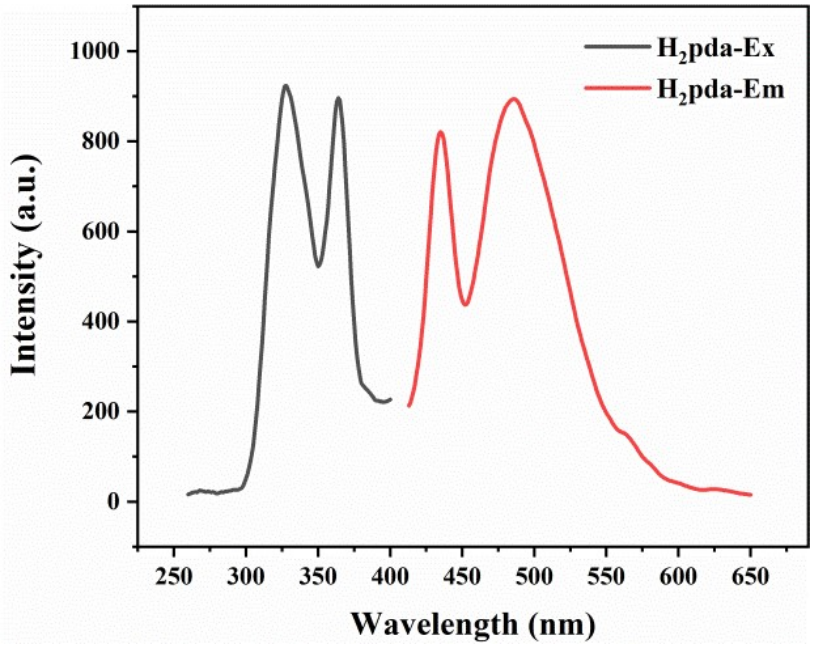

Fig. S4. Room-temperature excitation and emission spectra for H_2pda ligand.

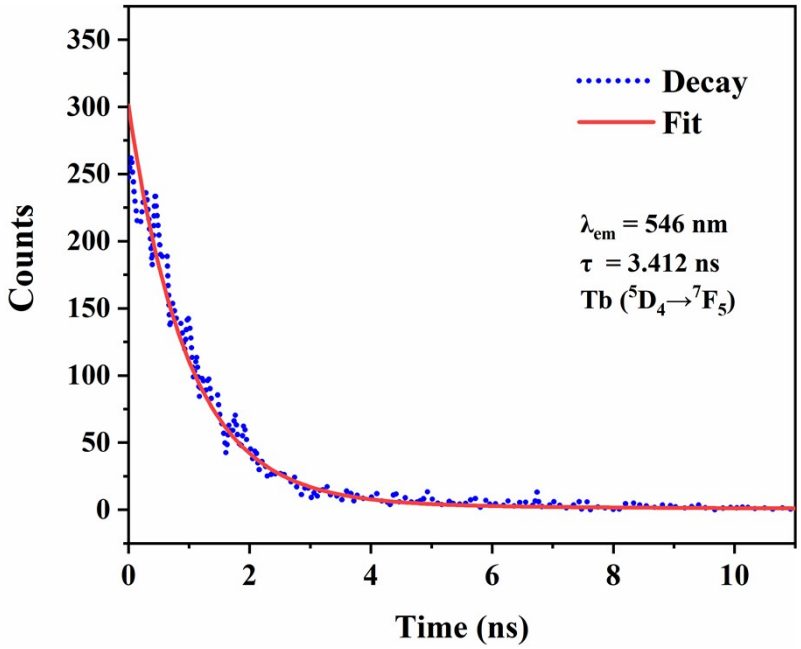

Fig. S5. The fluorescence decay and fit profiles of the complex (λ_{em} = 546 nm).

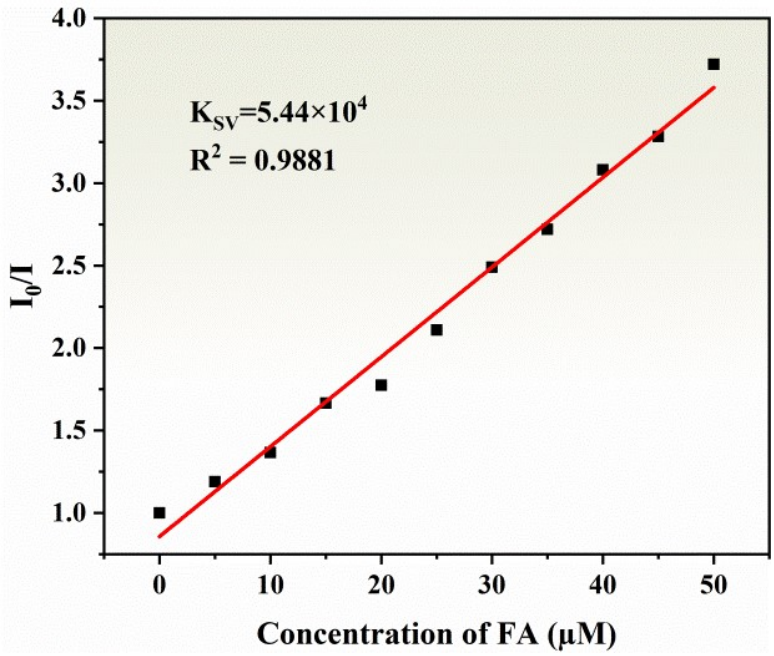

Fig. S6. Linear relationships between the fluorescence intensity (I/I_0) and concentration of FA

Table S5 Comparison of the present work with other reported sensors for FA detection

Sensing materials	Linear range	Detection limit	Reference
CQDs	1.14-47.57 μM	0.38 μM	42
OVA-CuNCs	0.5-200 μM	0.18 μM	43
Ag@Cu-MOFs	0.5-73 μM	0.27 μM	44
C_{60} FNP	0-80 μM	0.24 μM	45
Paper-based sensor	1-300 μM	0.28 μM	46
Bis-TPE-1	0-100 μM	0.63 μM	47
$[Tb(Hpda)(pda)(H_2O)_2]\cdot4H_2O$	0-100 μM	0.22 μM	**This work**

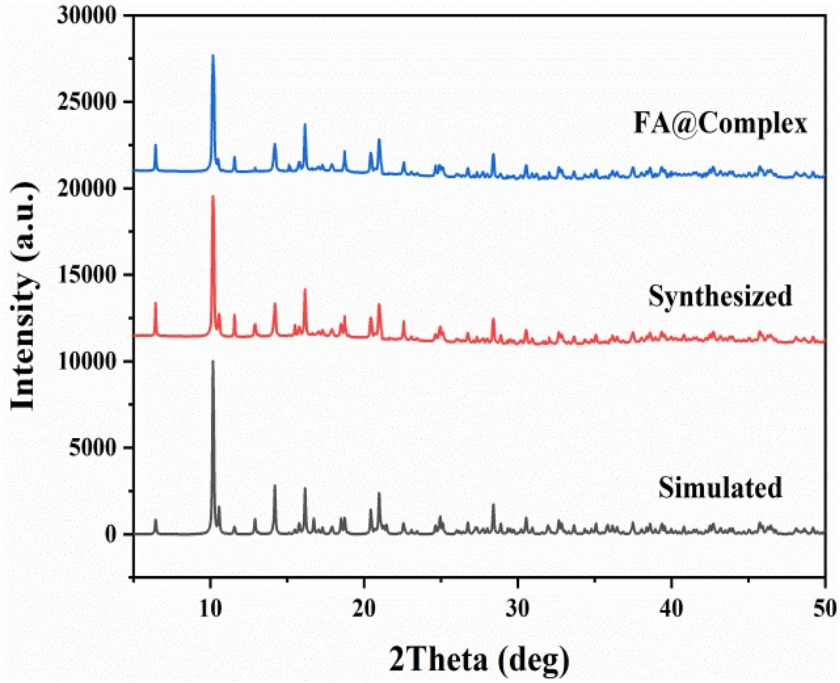

Fig. S7. The PXRD patterns of FA@Complex.

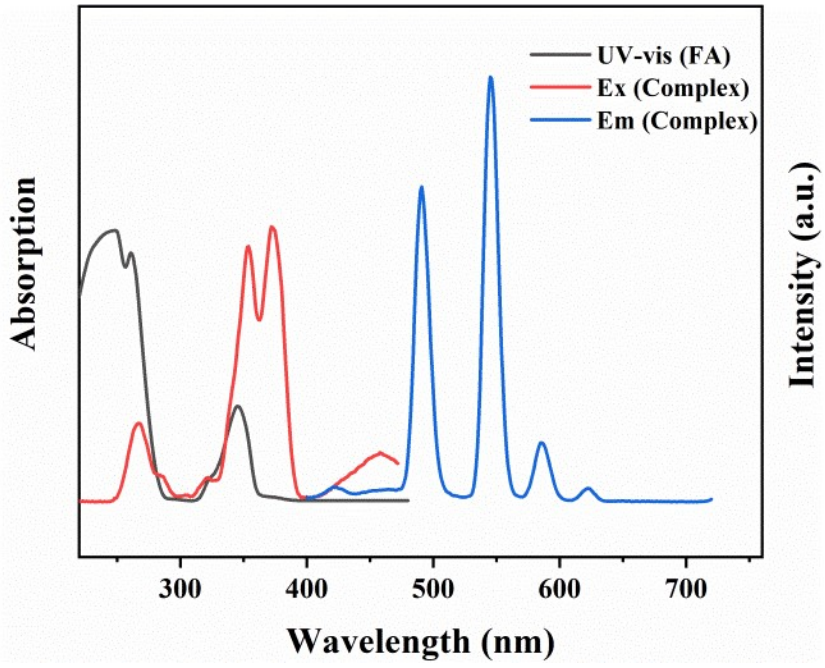

Fig. S8. The UV-Vis absorption spectra of FA and the fluorescence spectrum of the complex.