Supporting information for CrystEngComm

# In-situ ligand induced Ln-MOFs based on chromophore moiety: white light emission and turn-on detection of trace antibiotics

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## Contents:



### Section 1. Materials and physical measurements

Chemicals and solvents were used in this research without further purification. Ligand $H_3$tcptpy was synthesized according to our previous works [1]. The starting materials were provided by Henghua Chemical Technology (Jinan) Co., Ltd. Levofloxacin, nitrofurantoin, metronidazole, dimetridazole, oxacillin sodium, oxytetracycline were purchased from Anaiji Chemical Technology (Shanghai) Co., Ltd. Elemental analyses (C, H, N) were performed on a Vario EL III elemental analyzer. Infrared spectra were recorded on a VECTOR-22 spectrophotometer within 400–4000 $cm^{-1}$ using the samples prepared as pellets with KBr. The phase purity and crystallinity of each product were obtained by powder X-ray diffraction (PXRD). PXRD of compounds **1-4** were recorded at 298 K on a Bruker D8 Advance diffractometer (Cu-Kα, $\lambda$ = 1.54056 Å) operated at 40 kV and 30 mA, equipped with CuKa radiation and a graphite monochromator. Uv-Vis

absorption spectra measurements were carried out using a Hitachi UH 4150 UV-vis spectrophotometer. Thermogravimetric analysis (TGA) was performed using a SDT 2960 Simultaneous DSC-TGA instruments up to 800 °C, and the heating rate was 10°C $min^{-1}$ under an air follow of 100 mL $min^{-1}$. The photoluminescence spectra were measured with an Edinburgh FLS1000 fluorescence spectrophotometer. The corrected spectra were obtained via a calibration curve supplied with the instrument, taking, 300 W ozone free xenon arc lamp as detector, irradiation wavelength is from 300-800 nm. The emission measurements on Eu, Tb and Sm compounds are in the same range of 450-750 nm.

**Section 2. IR spectra.**

The IR spectra of complexes **1–4** closely resemble each other. The peaks around 3460 $cm^{-1}$ are ascribed to the O–H stretching vibration, suggesting the presence of water molecules in lattice. The pair bands in the ranges of 3070–3080 and 1480–1490 $cm^{-1}$ correspond to the C–H vibrations of the biphenyl group, while peaks in the ranges of 1610–1639 and 1396–1407 $cm^{-1}$ are related to the asymmetric and symmetric vibrations of carboxylate group, respectively [2, 3]

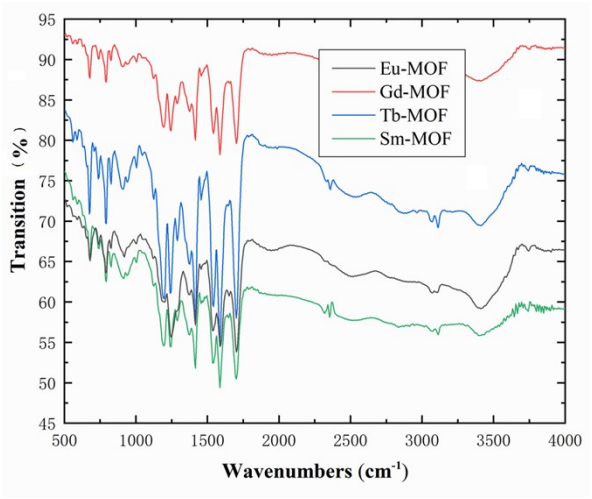
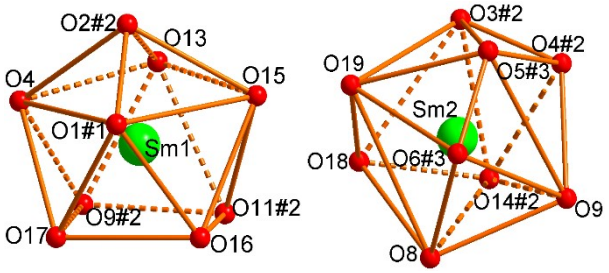



**Fig. S1** FT-IR spectra of compounds **1-4.**

The excellent luminescence properties and porous compounds **2** and **4** prompted us to choose it as a potential application for sensing organic molecules. Crystal compounds (2 mg) were grinded into powder samples and dispersed them in 3 mL of various solution. For **2**, the spectral intensity emitted by the ($^5D_0 \rightarrow {}^7F_2$) electric-dipole transition at 613 nm was selected to study its fluorescence response [1]. To be detection specific, 20 mg of MOFs samples **4** are mixed with DMF and water (20 mL), then these crystalline materials are put into suspension in ultrasound process

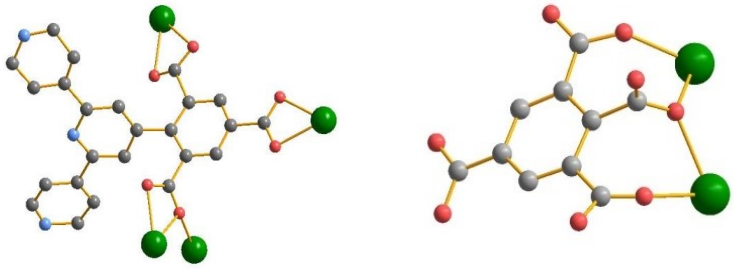
(100 w, 20 min) to form solvent, and then was added into various antibiotics solvent using micro sampler (2 or 5 μL) including furazolidone, metronidazole, oxytetracycline, levofloxacin, oxytetracycline, uric acid nitrofurantoin. Fluorometric titration of cation using Tb- MOF **2** to test the effect of $Cr_2O_7^{2+}$ and $Fe^{3+}$ on the fluorescence based on $Tb^{3+}$ ion, fluorometric titration were done by adding a few microliters of a working solution to 5 mL with a quartz cell. Exception for the special description case, 0.3M (mol/L) HAc–NaAc (pH=5.5) buffer solution was used to keep pH value stable.

**Section 2. Additional structure descriptions**



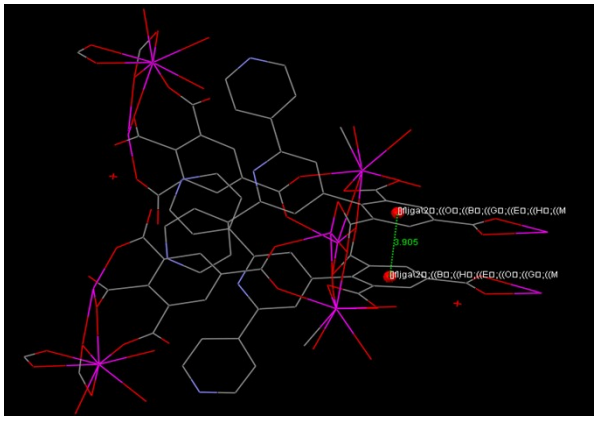

(a) (b)

**Fig.S2** Coordination geometry of Sm1 and Sm2 in **1.**

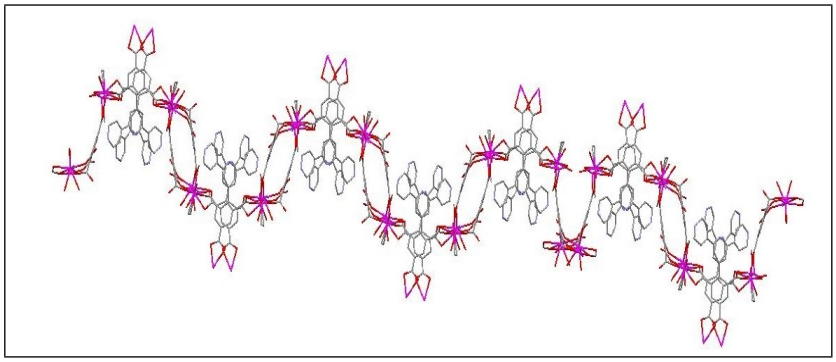


(a) (b)

**Fig. S3** Coordination patterns of the ligand$H_3$tcptpy (a) and $H_4$btca (b) in **1.**



(a)



(b)

**Fig.S4** (a) Illustration of π-π interaction **(**centroid-centroid separation of 3.9058Å). (b) One dimensional chain of dimer units attached to tricarboxyphenyl moieties.

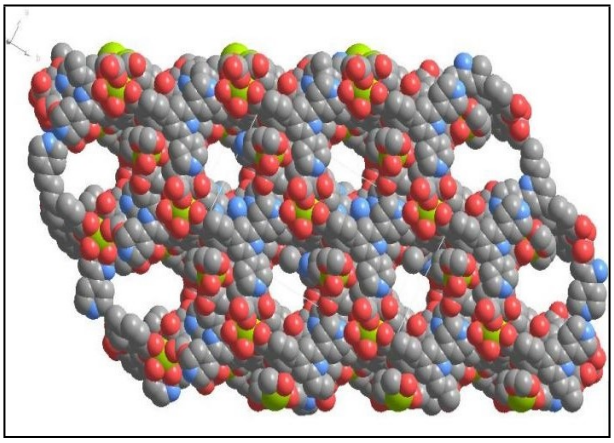
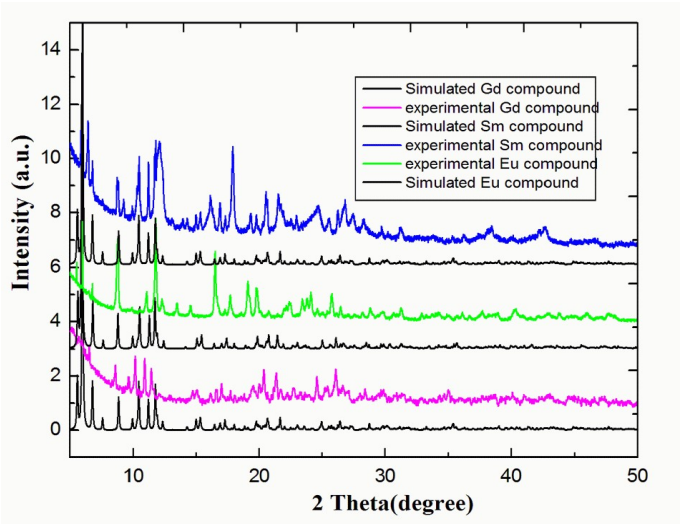
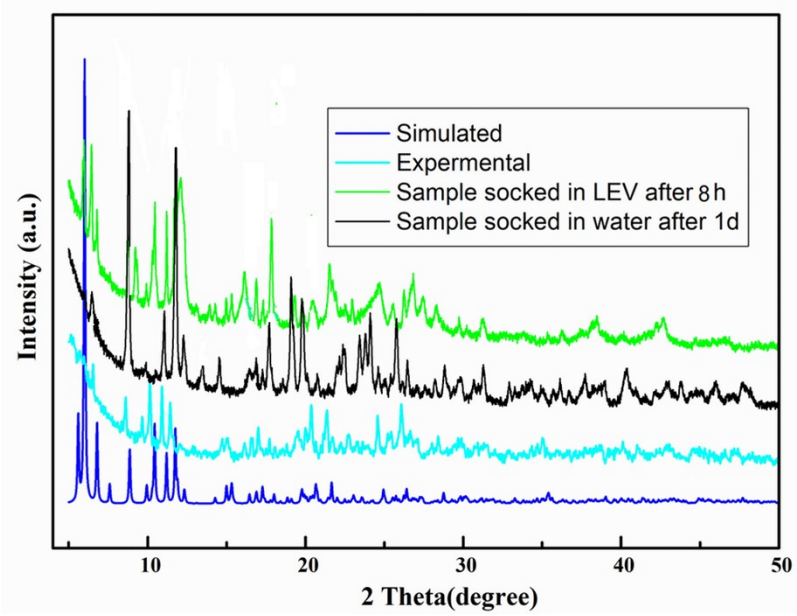


**Fig.S5** (a) Illustration of 3D porous structure with 1D tunnel along the *c* crystallographic axis in **1**.

## Section 3. Chemical and phase analysis of the compounds




(a)




(b)

**Fig.S6** (a) Comparison of powder XRD patterns of experimental with simulated of MOFs **1-3.** (b) Comparison of powder XRD patterns of experimental with simulated, and Tb-MOF immersed in water after 24h and immersed in LVE DMF solution for 8h. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

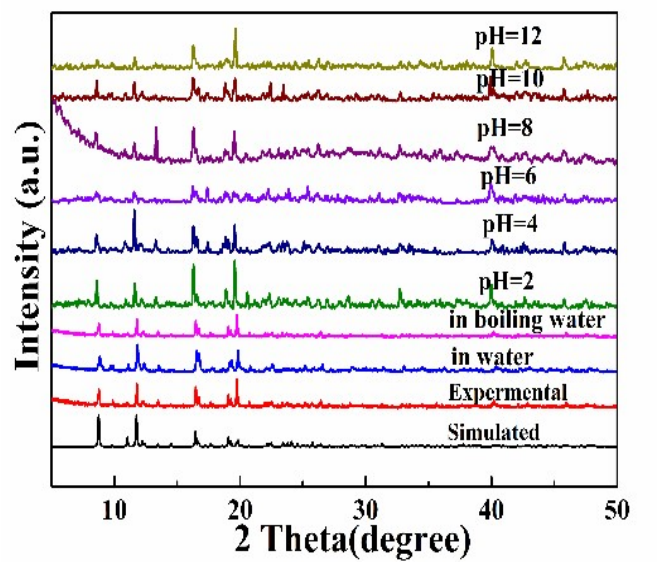



**Fig. S7** Comparison the experiment and simulated PXRD patternsfor MOF-**4** (Tb) soaked in water, boiling water and in different pH solutions.

**Section 4. Additional details on characterization of series compounds**

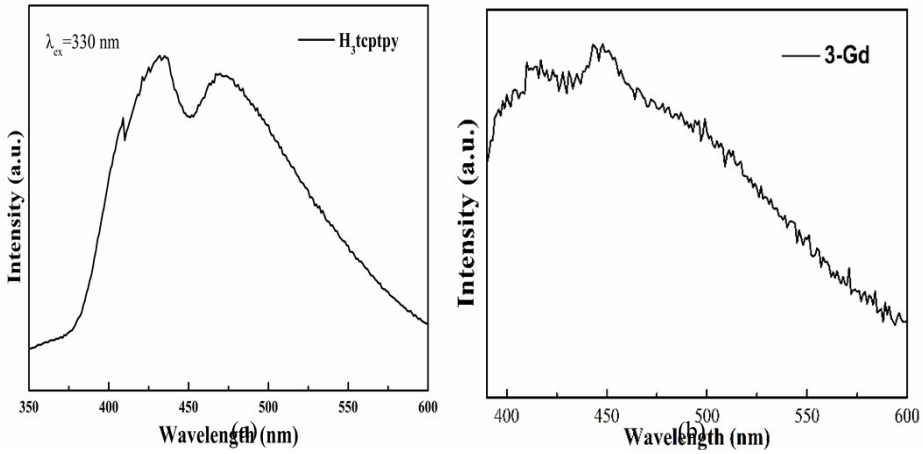



**Fig. S8** (a) Emission fluorescence spectrum of $H_3$tcptp ligand; (b) Phosphorescence spectrum of compound **3** (Gd) measured at 77 K.

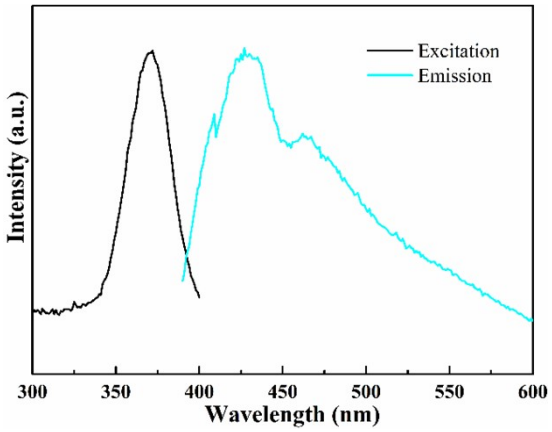



**Fig.S9** Solid state excitation and emission spectra of **3** at room temperature.

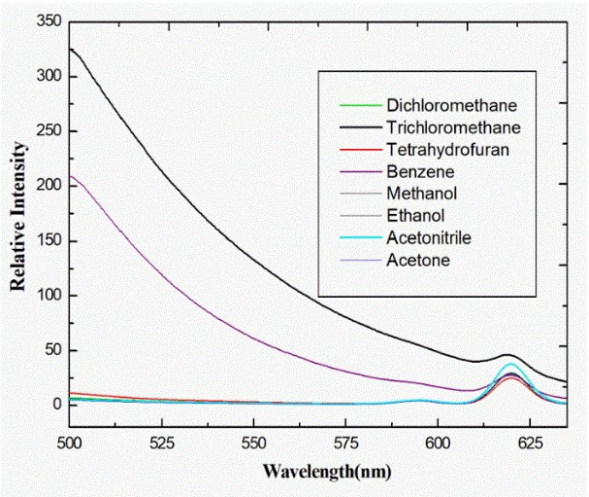
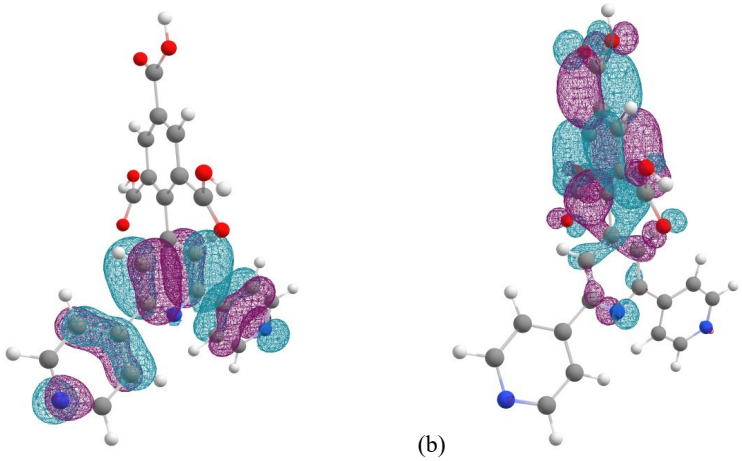
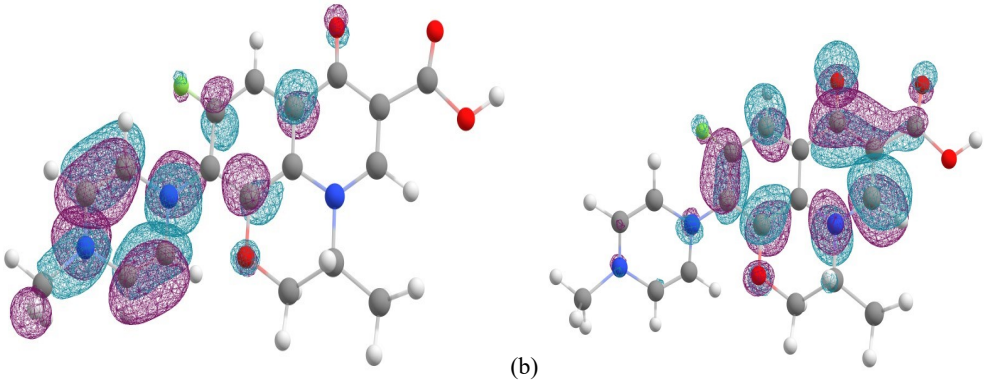



**Fig. S10** PL spectra of the $^5D_4 \rightarrow {}^7F_2$ transition intensities of compound **2** dispersed in different solvents ($\lambda_{ex}$ = 352 nm).



(a) (b)

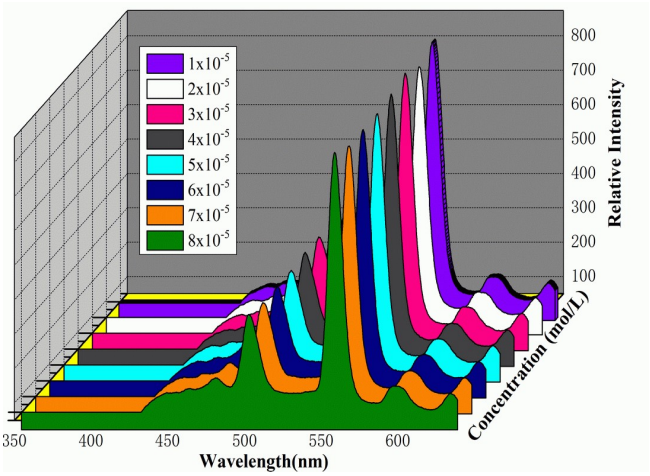
**Fig. S11** The diagram and plots of selected molecular orbitals for $H_3$tcptp ligand (a) HOMO (b) LUMO, $\Delta E(S_0 \rightarrow S_1)$=3.97eV (320 nm)



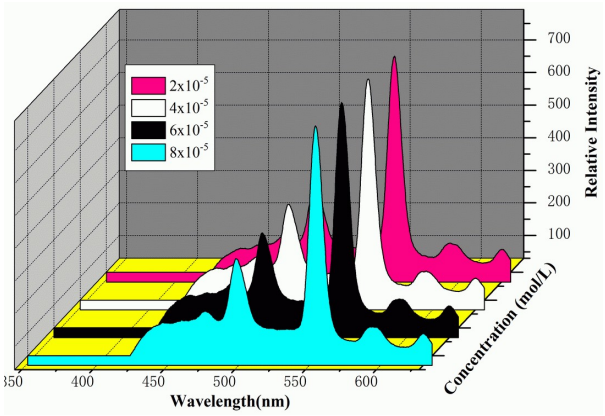
(a) (b)

**Fig. S12** The diagram and plots of selected molecular orbitals for levofloxacin (a) HOMO (b) LUMO.

**Fig. S13** UV-vis absorption spectrum of $H_3$tcptp in methanol.



(a)




(b)

**Fig. S14** Fluorescence spectra of the Tb(tcptp)- MOF in the presence of different gentamicin concentrations (a); different cephalexin concentrations (b).

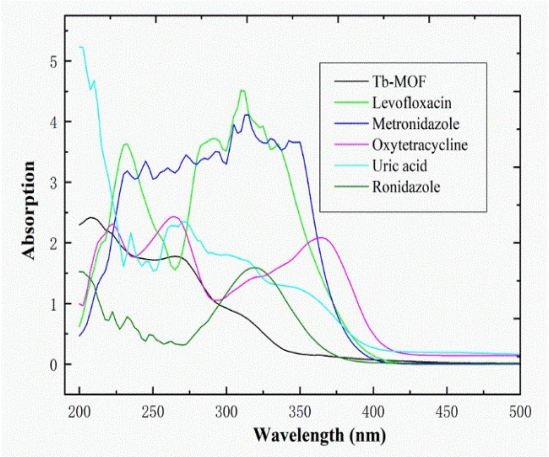



**Fig. S15** The UV/vis absorption spectra of series of antibiotics in aqueous solution.

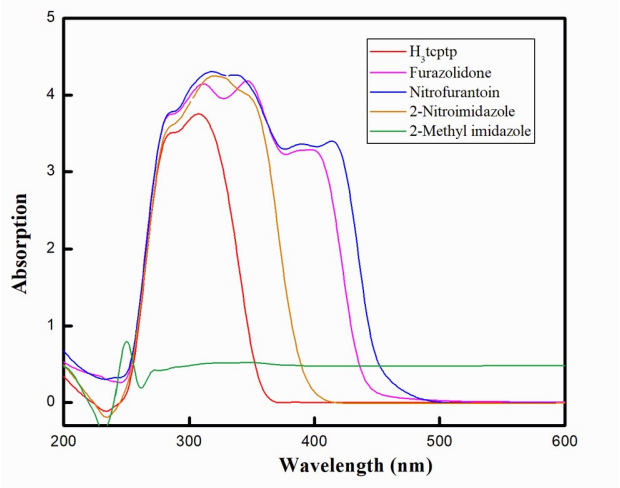



**Fig. S16** The UV/vis absorption spectra of $H_3$tcptp and imidazole antibiotics in solution.

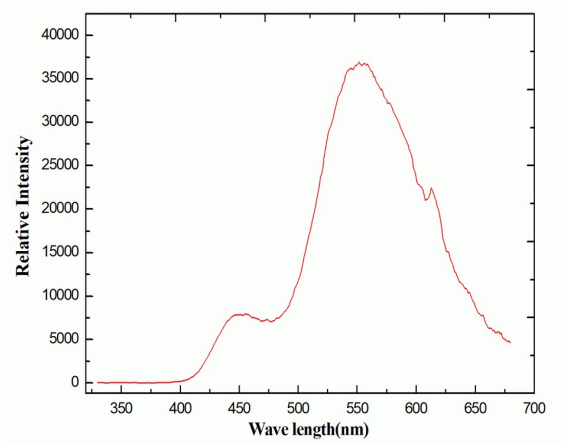



**Fig. S17** Phosphorescence spectrum of Glevofloxacin complex measured at 77 K.

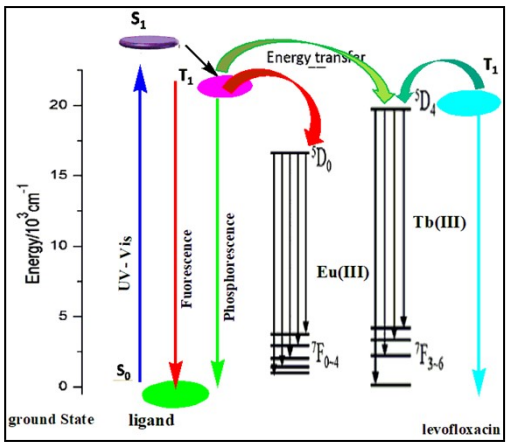



**Fig. S18** (a) Schematic illustration of the photophysical processes for Ln-based complexes, and leading to levofloxacin sensitization on $Tb^{3+}$ luminescence.

## Section 5. Additional figures

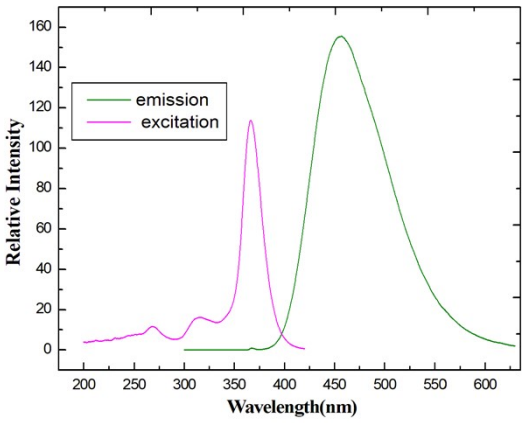



**Fig. S19** The excitation and emission spectrum of levofloxacin in DMF solution

**Fig. S20** UV/vis absorption spectra MOF-**4** (Tb) adding of levofloxacin antibiotic

in aqueous solution.

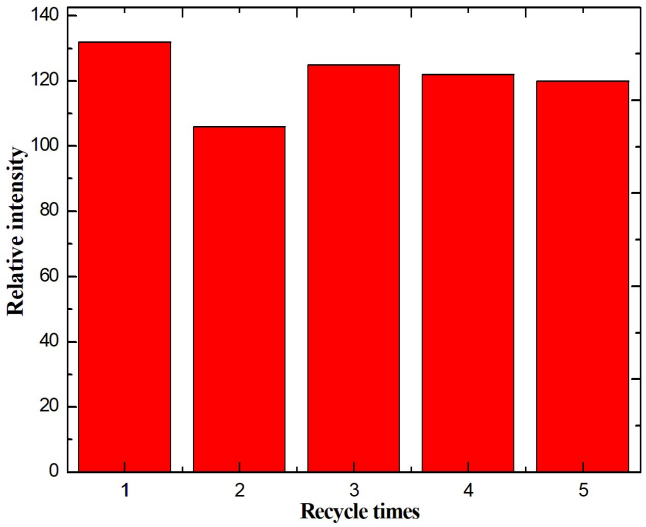



**Fig. S21** Luminescence intensity of MOF-**4** (Tb) at 546 nm after repeat experiments of sensing for levofloxacin in aqueous state ($\lambda_{ex}$ = 294 nm).

## Section 6. Additional tables

Table S1 Selectedbond length (Å) and bond angle (°) of complexes **1-4**

| Compound **1** | | | | | |
|---|---|---|---|---|---|
| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
| Sm1-O1$^{1}$ | 2.440(2) | Sm1-O15 | 2.476(4) | Sm2-O6$^{3}$ | 2.598(2) |
| Sm1-O2$^{1}$ | 2.563(2) | Sm1-O16 | 2.535(6) | Sm2-O8 | 2.366(2) |
| Sm1-O4 | 2.447(2) | Sm1-O17 | 2.472(6) | Sm2-O9 | 2.418(3) |
| Sm1-O9$^{2}$ | 2.513(2) | Sm2-O3$^{2}$ | 2.532(2) | Sm2-O14$^{2}$ | 2.410(2) |
| Sm1-O11$^{2}$ | 2.386(3) | Sm2-O4$^{2}$ | 2.548(2) | Sm2-O18 | 2.425(3) |
| Sm1-O13 | 2.352(3) | Sm2-O5$^{3}$ | 2.482(2) | Sm2-O19 | 2.452(3) |
| Angle | Degree (°) | Angle | Degree (°) | Angle | Degree (°) |
| O1$^{1}$-Sm1-O2$^{1}$ | 51.54(8) | O1$^{1}$-Sm1-O4 | 87.25(9) | O1$^{1}$-Sm1-O17 | 71.52(16) |
| O1$^{1}$-Sm1-O15 | 82.95(15) | O1$^{1}$-Sm1-O16 | 69.50(14) | O4-Sm1-O15 | 139.41(15) |
| O4-Sm1-O2$^{1}$ | 73.52(8) | O4-Sm1-O9$^{2}$ | 67.00(8) | O9$^{2}$-Sm1-O2$^{1}$ | 136.81(8) |
| O4-Sm1-O16 | 139.09(18) | O4-Sm1-O17 | 71.3(2) | O11$^{2}$-Sm1-O2$^{1}$ | 140.53(9) |
| O9$^{2}$-Sm1-O16 | 109.43(17) | O11$^{2}$-Sm1-O1$^{1}$ | 133.52(10) | O11$^{2}$-Sm1-O15 | 72.60(12) |
| O11$^{2}$-Sm1-O4 | 136.11(8) | O11$^{2}$-Sm1-O9$^{2}$ | 70.19(8) | O13-Sm1-O4 | 78.00(8) |
| O11$^{2}$-Sm1-O16 | 65.69(15) | O11$^{2}$-Sm1-O17 | 102.9(2) | O13-Sm1-O15 | 78.88(18) |
| O13-Sm1-O11 | 72.9(3) | O13-Sm1-O2$^{1}$ | 78.88(8) | O15-Sm1-O9$^{2}$ | 137.20(13) |
| O15-Sm1-O16 | 107.4(5) | O16-Sm1-O2$^{1}$ | 111.72(16) | O8-Sm2-O3$^{2}$ | 160.61(8) |
| O17-Sm1-O9$^{2}$ | 72.4(3) | O17-Sm1-O15 | 139.6(3) | O8-Sm2-O6$^{3}$ | 71.81(8) |
| O3$^{2}$-Sm2-O6$^{3}$ | 142.1(3) | O5$^{3}$-Sm2-O6$^{3}$ | 51.01(7) | O9-Sm2-O4$^{2}$ | 66.86(8) |

| | | | | | |
|---|---|---|---|---|---|
| O5$^{3}$-Sm2-O4$^{2}$ | 124.41(8) | O8-Sm2-O5$^{3}$ | 122.68(8) | O9-Sm2-O18 | 133.01(9) |
| O8-Sm2-O4$^{2}$ | 68.06(8) | O8-Sm2-O14$^{2}$ | 86.42(8) | O14$^{2}$-Sm2-O4$^{2}$ | 74.72(8) |
| O9-Sm2-O5$^{3}$ | 97.04(9) | O14$^{2}$-Sm2-O3$^{2}$ | 81.60(8) | O18-Sm2-O6$^{3}$ | 124.83(9) |
| O9-Sm2-O19 | 89.76(9) | O14$^{2}$-Sm2-O6$^{3}$ | 150.05(9) | O19-Sm2-O4$^{2}$ | 122.49(9) |
| O14$^{2}$-Sm2-O5$^{3}$ | 150.19(9) | O14$^{2}$-Sm2-O19 | 132.63(10) | Sm1-O4-Sm2$^{2}$ | 110.76(8) |
| O14$^{2}$-Sm2-O18 | 142.78(8) | O18-Sm2-O5$^{3}$ | 137.17(10) | Sm2-O9-Sm1$^{2}$ | 112.93(9) |
| O18-Sm2-O4$^{2}$ | 66.59(9) | O19-Sm2-O3$^{2}$ | 80.29(9) | O18-Sm2-O19 | 124.73(9) |

Compound **2**

| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
|---|---|---|---|---|---|
| Eu1-Eu2 | 4.1021(14) | Eu1-O15 | 2.52(2) | Eu2-O8$^{1}$ | 2.308(13) |
| Eu1-O5$^{2}$ | 2.348(10) | Eu1-O16 | 2.403(17) | Eu2-O12 | 2.450(11) |
| Eu1-O6$^{2}$ | 2.575(11) | Eu2-O1$^{1}$ | 2.506(11) | Eu2-O13 | 2.351(10) |
| Eu1-O7 | 2.384(12) | Eu2-O21 | 2.548(11) | Eu2-O17 | 2.428(14) |
| Eu1-O10$^{1}$ | 2.513(10) | Eu2-O3$^{3}$ | 2.366(12) | Eu2-O18 | 2.441(15) |
| Eu1-O12$^{1}$ | 2.512(11) | Eu2-O43 | 2.609(12) | O1-Eu2$^{1}$ | O1-Eu2$^{1}$ |
| O1-Eu2$^{1}$ | 2.510(11) | O2-Eu2$^{1}$ | 2.548(11) | O3-Eu2$^{4}$ | 2.447(13) |
| O5-Eu1$^{2}$ | 2.453(12) | O6-Eu1$^{2}$ | 2.575(11) | O8-Eu2$^{1}$ | 2.388(13) |
| O10-Eu1$^{1}$ | 2.510(11) | | | | |

| Angle | Degree (°) | Angle | Degree (°) | Angle | Degree (°) |
|---|---|---|---|---|---|
| O2-Eu1-Eu2$^{1}$ | 35.7(3) | O121-Eu1-O1$^{5}$ | 108.8(7) | O12-Eu2-Eu1$^{1}$ | 34.5(2) |
| O2-Eu1-O6$^{2}$ | 72.6(4) | O15-Eu1-Eu2$^{1}$ | 135.2(8) | O12-Eu2-O1$^{1}$ | 118.3(4) |
| O2-Eu1-O12$^{1}$ | 67.3(4) | O15-Eu1-O62 | 112.4(6) | O12-Eu2-O2$^{1}$ | 67.4(4) |
| O2-Eu1-O15 | 137.5(8) | O16-Eu1-Eu2$^{1}$ | 148.1(6) | O12-Eu2-O3$^{3}$ | 89.5(5) |
| O52-Eu1-Eu2$^{1}$ | 121.2(4) | O16-Eu1-O2 | 139.9(5) | O12-Eu2-O4$^{3}$ | 77.4(4) |
| O52-Eu1-O2 | 87.7(4) | O16-Eu1-O5$^{2}$ | 80.5(6) | O12-Eu2-O17 | 135.0(5) |
| O52-Eu1-O6$^{2}$ | 51.6(4) | O16-Eu1-O6$^{2}$ | 70.0(5) | O12-Eu2-O18 | 149.2(5) |
| O52-Eu1-O12$^{1}$ | 139.7(5) | O16-Eu1-O12$^{1}$ | 138.7(5) | O13-Eu2-Eu1$^{1}$ | 105.7(3) |
| O52-Eu1-O15 | 68.5(5) | O16-Eu1-O15 | 72.2(10) | O13-Eu2-O11 | 161.3(4) |
| O62-Eu1-Eu2$^{1}$ | 103.7(3) | O11-Eu2-Eu11 | 84.1(3) | O13-Eu2-O2$^{1}$ | 140.0(4) |
| O7-Eu1-Eu2$^{1}$ | 67.7(3) | O11-Eu2-O21 | 51.2(4) | O13-Eu2-O3$^{3}$ | 122.1(4) |
| O7-Eu1-O2 | 78.8(4) | O11-Eu2-O4$^{3}$ | 122.6(4) | O13-Eu2-O4$^{3}$ | 72.3(4) |
| O7-Eu1-O5$^{2}$ | 130.7(4) | O21-Eu2-Eu1$^{1}$ | 34.3(2) | O13-Eu2-O8$^{1}$ | 86.1(4) |
| O7-Eu1-O6$^{2}$ | 79.2(4) | O21-Eu2-O4$^{3}$ | 107.3(4) | O13-Eu2-O12 | 73.8(4) |
| O7-Eu1-O10$^{1}$ | 82.6(4) | O33-Eu2-Eu1$^{1}$ | 83.6(4) | O13-Eu2-O17 | 78.8(5) |
| O7-Eu1-O12$^{1}$ | 76.6(4) | O33-Eu2-O11 | 74.1(4) | O13-Eu2-O18 | 94.5(5) |
| O7-Eu1-O15 | 143.3(8) | O33-Eu2-O2$^{1}$ | 67.9(4) | O17-Eu2-Eu1$^{1}$ | 131.7(4) |
| O7-Eu1-O16 | 80.4(7) | O33-Eu2-O4$^{3}$ | 49.9(4) | O17-Eu2-O11 | 82.8(5) |
| O10$^{1}$-Eu1-Eu2$^{1}$ | 101.0(3) | O43-Eu2-Eu1$^{1}$ | 99.3(3) | O17-Eu2-O21 | 123.4(5) |
| O10$^{1}$-Eu1-O2 | 136.7(4) | O8$^{1}$-Eu2-Eu1$^{1}$ | 65.7(3) | O17-Eu2-O3$^{3}$ | 135.5(5) |
| O10$^{1}$-Eu1-O5$^{2}$ | 132.6(5) | O8$^{1}$-Eu2-O11 | 83.6(4) | O17-Eu2-O4$^{3}$ | 126.6(5) |

| | | | | | |
|---|---|---|---|---|---|
| O10[1]-Eu1-O6[2] | 140.8(5) | O8[1]-Eu2-O2[1] | 75.9(4) | O17-Eu2-O18 | 66.7(5) |
| O10[1]-Eu1-O12[1] | 70.5(4) | O8[1]-Eu2-O3[3] | 143.8(4) | O18-Eu2-Eu1[1] | 154.6(4) |
| O10[1]-Eu1-O15 | 66.4(6) | O8[1]-Eu2-O4[3] | 149.6(4) | O18-Eu2-O11 | 81.2(5) |
| O10[1]-Eu1-O16 | 72.8(5) | O8[1]-Eu2-O12 | 76.2(4) | O18-Eu2-O21 | 124.1(4) |
| O12[1]-Eu1-Eu2[1] | 33.0(3) | O8[1]-Eu2-O17 | 66.8(5) | O18-Eu2-O3[3] | 72.4(5) |
| O12[1]-Eu1-O6[2] | 136.3(4) | O8[1]-Eu2-O18 | 132.4(5) | O18-Eu2-O4[3] | 71.9(5) |

Compound **3**

| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
|---|---|---|---|---|---|
| Gd1-O2 | 2.408(6) | Gd1-O15 | 2.365(9) | Gd2-O4[3] | 2.606(6) |
| Gd1-O5[2] | 2.546(6) | Gd1-O16 | 2.594(18) | Gd2-O8[1] | 2.382(6) |
| Gd1-O6[2] | 2.426(6) | Gd1-O17 | 2.410(8) | Gd2-O12 | 2.395(7) |
| Gd1-O7 | 2.319(6) | Gd2-O1[1] | 2.506(6) | Gd2-O13 | 2.340(6) |
| Gd1-O10[1] | 2.372(7) | Gd2-O2[1] | 2.532(5) | Gd2-O18 | 2.426(6) |
| Gd1-O12[1] | 2.490(5) | Gd2-O3[3] | 2.464(6) | Gd2-O19 | 2.436(6) |
| Angle | Degree (°) | Angle | Degree (°) | Angle | Degree (°) |
| O2-Gd1-Gd2[1] | 35.43(13) | O10[1]-Gd1-O5[2] | 141.7(2) | O8[1]-Gd2-O1[1] | 82.9(2) |
| O2-Gd1-O5[2] | 73.67(19) | O10[1]-Gd1-O6[2] | 131.5(3) | O8[1]-Gd2-O2[1] | 75.5(2) |
| O2-Gd1-O17 | 142.3(3) | O10[1]-Gd1-C9[2] | 143.5(2) | O8[1]-Gd2-O18 | 67.2(2) |
| O5[2]-Gd1-Gd2[1] | 104.63(14) | O12[1]-Gd1-Gd2[1] | 32.76(15) | O8[1]-Gd2-O19 | 132.3(2) |
| O5[2]-Gd1-O16 | 112.0(5) | O12[1]-Gd1-O5[2] | 137.0(2) | O12-Gd2-Gd1[1] | 34.23(13) |
| O6[2]-Gd1--Gd2[1] | 120.4(2) | O12[1]-Gd1-O16 | 108.7(5) | O12-Gd2-O1[1] | 117.82(19) |
| O6[2]-Gd1-O16 | 69.3(4) | O15-Gd1-O5[2] | 117.7(3) | O12-Gd2-O4[3] | 77.6(2) |
| O7-Gd1-Gd2[1] | 68.12(15) | O15-Gd1-O6[2] | 71.2(3) | O12-Gd2-O18 | 135.2(3) |
| O7-Gd1-O2 | 78.7(2) | O15-Gd1-O10[1] | 93.7(4) | O12-Gd2-O19 | 149.5(2) |
| O7-Gd1-O12[1] | 77.4(2) | O16-Gd1-Gd2[1] | 135.7(5) | O13-Gd2-O3[3] | 122.5(2) |
| O7-Gd1-O15 | 148.3(3) | O17-Gd1-Gd2[1] | 150.5(3) | O13-Gd2-O4[3] | 71.6(2) |
| O7-Gd1-O16 | 141.7(5) | O17-Gd1-O5[2] | 71.0(3) | O13-Gd2-O8[1] | 85.9(2) |
| O10[1]-Gd1-Gd2[1] | 101.25(15) | O17-Gd1-O12[1] | 139.3(3) | O13-Gd2-O18 | 77.3(3) |
| O3[3]-Gd2-O2[1] | 68.6(2) | O1[1]-Gd2-O2[1] | 51.86(19) | O18-Gd2-O2[1] | 124.7(2) |
| O3[3]-Gd2-O4[3] | 50.9(2) | O1[1]-Gd2-O4[3] | 124.1(2) | O18-Gd2-O3[3] | 135.3(3) |
| O4[3]-Gd2-Gd1[1] | 100.11(15) | O2[1]-Gd2-Gd1[1] | 33.47(14) | O18-Gd2-O4[3] | 124.7(2) |
| O8[1]-Gd2-Gd1[1] | 65.74(15) | O2[1]-Gd2-O4[3] | 108.3(2) | O18-Gd2-O19 | 66.6(2) |

Compound **4**

| Bond | Length (Å) | Bond | Length (Å) | Bond | Length (Å) |
|---|---|---|---|---|---|
| Tb1-O1 | 2.399(7) | Tb1-O15 | 2.387(11) | Tb2-O6[4] | 2.481(7) |
| Tb1-O2 | 2.517(8) | Tb1-O16 | 2.362(17) | Tb2-O8 | 2.317(7) |
| Tb1-O5[1] | 2.382(7) | Tb2-O3[3] | 2.571(7) | Tb2-O9 | 2.393(7) |
| Tb1-O9[2] | 2.466(7) | Tb2-O4[3] | 2.457(6) | Tb2-O13[2] | 2.376(7) |
| Tb1-O11[2] | 2.344(8) | Tb2-O5[4] | 2.533(7) | Tb2-O17 | 2.401(6) |
| Tb1-O14 | 2.299(6) | Tb2-O18 | 2.409(7) | Tb2-O19 | 2.466(7) |

| Angle | Degree (°) | Angle | Degree (°) | Angle | Degree (°) |
|---|---|---|---|---|---|
| O1-Tb1-O9[1] | 138.0(3) | O14-Tb1-O2 | 79.4(2) | O16-Tb1-O15 | 134.1(12) |
| O5[2]-Tb1-O1 | 87.5(3) | O14-Tb1-O5[2] | 79.5(2) | O4[3]-Tb2-O3[3] | 51.5(2) |
| O5[2]-Tb1-O2 | 73.7(2) | O14-Tb1-O9[1] | 78.2(2) | O4[3]-Tb2-O5[4] | 68.4(2) |
| O5[2]-Tb1-O15 | 142.1(4) | O14-Tb1-O15 | 80.8(4) | O5[4]-Tb2-O3[3] | 108.2(2) |
| O9[1]-Tb1-O2 | 138.1(2) | O14-Tb1-O16 | 144.6(12) | O6[4]-Tb2-O3[3] | 124.4(2) |
| O11[1]-Tb1-O9[1] | 70.9(2) | O16-Tb1-O1 | 70.0(12) | O8-Tb2-O5[4] | 139.1(2) |
| O11[1]-Tb1-O15 | 71.7(4) | O16-Tb1-O2 | 113.4(13) | O8-Tb2-O6[4] | 160.5(2) |
| O8-Tb2-O13[1] | 84.8(2) | O9-Tb2-O4[3] | 89.8(2) | O13[1]-Tb2-O3[3] | 148.5(3) |
| O8-Tb2-O18 | 95.1(3) | O9-Tb2-O64 | 117.8(2) | O131-Tb2-O5[4] | 76.1(2) |
| O9-Tb2-O3[3] | 77.1(2) | O9-Tb2-O17 | 135.8(2) | O13[1]-Tb2-O6[4] | 83.5(2) |
| O9-Tb2-O18 | 148.5(2) | O13[1]-Tb2-O9 | 76.5(2) | O13[1]-Tb2-O17 | 66.9(2) |
| O13[1]-Tb2-O18 | 133.0(2) | O17-Tb2-O4[3] | 134.3(3) | O17-Tb2-O6[4] | 82.4(3) |
| O17-Tb2-O3[3] | 125.7(3) | O17-Tb2-O5[4] | 123.7(3) | O17-Tb2-O18 | 67.1(2) |
| O18-Tb2-O3[3] | 71.5(2) | O18-Tb2-O4[3] | 71.1(2) | O18-Tb2-O5[4] | 124.3(3) |

Symmetry codes **1**: [1]1-x, +y, 3/2-z; [2]3/2-x, 3/2-y,1-z; [3]1/2+x,1/2+y,+Z; [4]-1/2+x,-1/2+y,+z; **2**: [1] 3/2-X, 1/2-Y, 1-Z; [2]1-X,+Y, 3/2-Z; [3] 1/2+X,-1/2+Y,+Z; [4]-1/2+X, 1/2+Y,+Z; **3**: [1]1-x,+y,1/2-z; [2] 1/2-x,3/2-y,1-z; [3]1/2-x,1/2+y,1/2-z; [4]-1/2+x, 3/2-y,1/2+z; [5]1/2-x,-1/2+y, 1/2-z; [6]1/2+x,3/2-y,-1/2+z; **4**:[1]1/2-x,3/2-y,1-z; [2]1-x,+y,1/2-z;[3]1/2-x, 1/2+y,1/2-z; [4]-1/2+x,3/2-y,1/2+z; [5]1/2-x,-1/2+y,1/2-z; [6] 1/2+x,3/2-y,-1/2+z.

Table S2 Quenching yield of antibiotic analytes taking Tb -MOF **4** as indicator

| Analytes | Initial intensity | Final intensity | Quench yield (%) |
|---|---|---|---|
| Ornidazole | 2509 | 274.1 | 89.07533 |
| Dimetridazole | 3367 | 1147 | 65.93407 |
| Nitrofurantoin | 3114 | 1882 | 39.56326 |
| Nitrofurazone | 2334 | 406.7 | 82.57498 |
| Furazolidone | 2298 | 1098 | 52.21932 |
| Sulfadiazine | 2747 | 1824 | 33.60029 |
| Metronidazole | 2959 | 1189 | 59.81751 |
| Nitrofuran | 3236 | 801.9 | 75.21941 |
| Ronidazole | 2708 | 442.3 | 83.66691 |

Under concentration of analytes of $1x10^{-3}$ mol/L.

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