

Supplementary Information for

**A multinuclear europium-based metal–organic framework as a high-performance X-ray  
scintillator**

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## Experimental Procedures

### Materials and Synthesis

**Materials.**  $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  (99.9%, Shanghai Macklin Biochemical Co., Ltd), 2,6-Naphthalenedicarboxylic acid (95%, Shanghai Adamas Reagent Co., Ltd.), 2-Fluorobenzoic acid (95%, Shanghai Adamas Reagent Co., Ltd.), and dimethylformamide (99.5%, Shanghai Macklin Biochemical Co., Ltd), hydrochloric acid (AR,  $\geq 99.5\%$ , Sinopharm Chemistry Reagent Co., Ltd) were used as received from commercial suppliers without further purification.

**Synthesis. Eu-ndc.** A mixture of  $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$  (2.23 mg), 2,6-Naphthalenedicarboxylic acid (1.08 mg, 5  $\mu\text{mol}$ ), 2-Fluorobenzoic acid (0.28 mg, 2  $\mu\text{mol}$ ), 60  $\mu\text{l}$  HCl and 940  $\mu\text{l}$  DMF was loaded into a 7 mL glass vial. The vial was sealed and heated at 120 °C for 72 h, then cooled to room temperature under ambient conditions. Transparent, rodlike single crystals of **Eu-ndc** were obtained, washed with DMF for 3 times, and then washed with ethanol, finally dried under ambient conditions.

### Characterizations

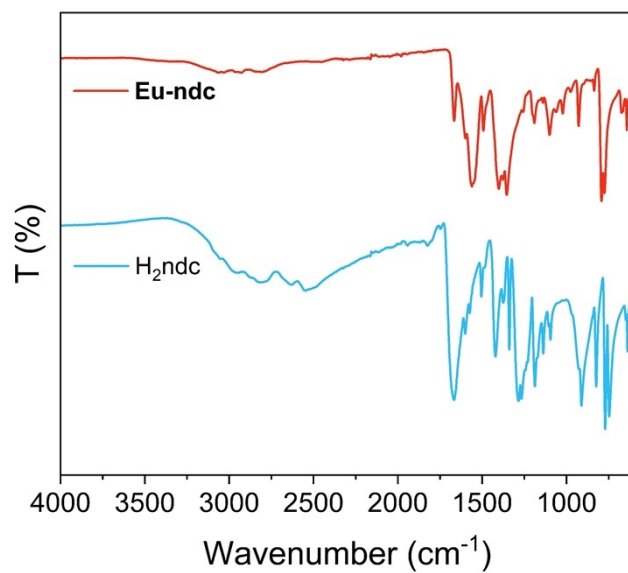
**General characterizations.** Single-crystal X-ray diffraction (SCXRD) analysis was performed on a Bruker D8 Venture diffractometer equipped with an I $\mu$ S 3.0 microfocus X-ray source (Mo K $\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$ ) and a CMOS detector at 298 K. Data collection and reduction were carried out using the APEX3 software package. The crystal structures were solved by intrinsic phasing using SHELXT and refined by full-matrix least-squares methods with SHELXL, as implemented in Olex2. PXRD patterns in steps of 0.02°. The simulated PXRD pattern of **Eu-ndc** was generated from their CIF using the Mercury. The thermal stabilities were investigated on a Waters SDT650 simultaneous thermal analyzer. The experiments were conducted in a dry N<sub>2</sub> atmosphere at a temperature range of 30-800 °C with a heating rate of 10 °C/min. The FTIR spectra were obtained via a Nicolet iS50 FTIR spectrometer, with measurements conducted at wavenumbers ranging from 600 to 4000 cm<sup>-1</sup>. The photoluminescence spectra, lifetimes, and PLQYs were measured using an Edinburgh FLS980 fluorescence spectrometer at room temperature. Phosphorescence measurements were measured at 77K on an Edinburgh Instruments FLS1000 fluorescence spectrometer.

**X-ray excitation luminescence spectroscopy.** The X-ray radiation was provided by a W K $\alpha$  radiation source (70 kV, 12W). The X-ray excitation luminescence spectra were collected on a NOVA cooled fiber optic spectrometer. The dose rate can be controlled by adjusting the current and voltage of the cathode ray tube.

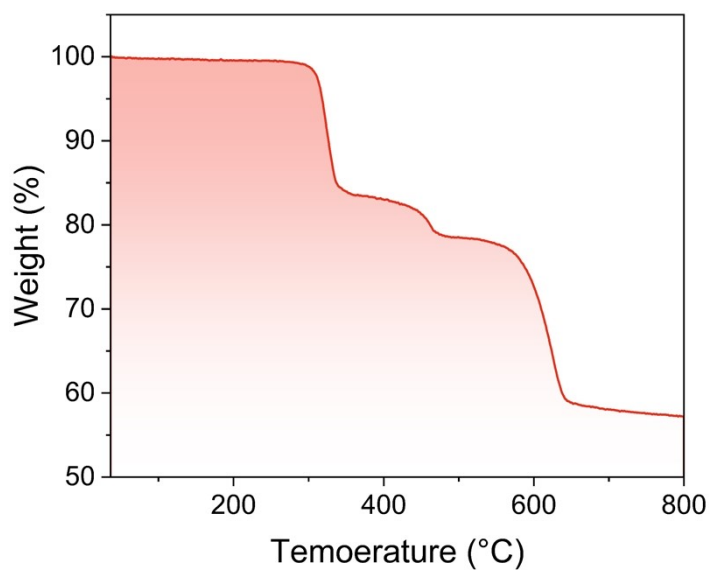
**Calculation of light yield.** Light yield was measured using a NOVA cooled fiber optic spectrometer. The X-ray tube was set to 40 kV and 100  $\mu\text{A}$ . The light yield of the **Eu-ndc** was calibrated using a commercial LYSO scintillator as a reference. From these radioluminescence spectra, corresponding photon counts (PC) were obtained. The emitted photons of the scintillators were normalized to the same X-ray attenuation according to the following equation:

$$\text{LY}_{[\text{Eu-ndc}]} = \text{LY}_{[\text{LYSO}]} * \text{PC}_{[\text{Eu-ndc}]} / \text{PC}_{[\text{LYSO}]}$$

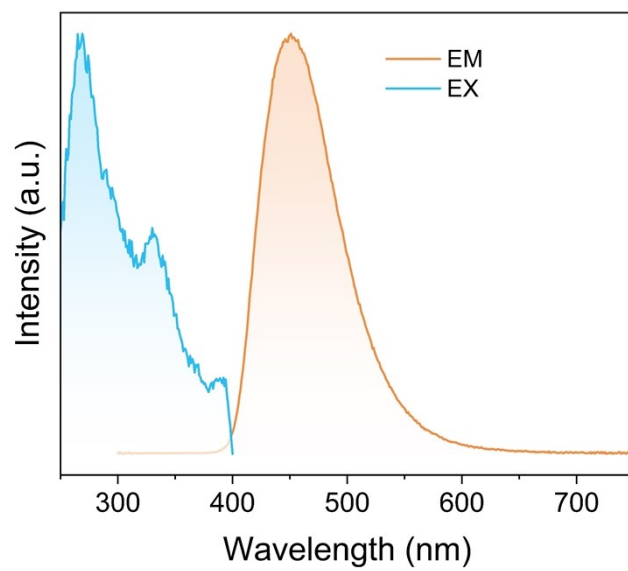
**Fabrication of the scintillation film.** The crystals of **Eu-ndc** were ground into fine powder. The fine powder was subsequently mixed with PDMS at a mass ratio of 1:9 (100 mg :900 mg), then add 90 mg of curing agent. Flexible scintillation films with a thickness of 250  $\mu\text{m}$  can be obtained via blade-coating and heating of the mixture at 100 °C for 60 min.



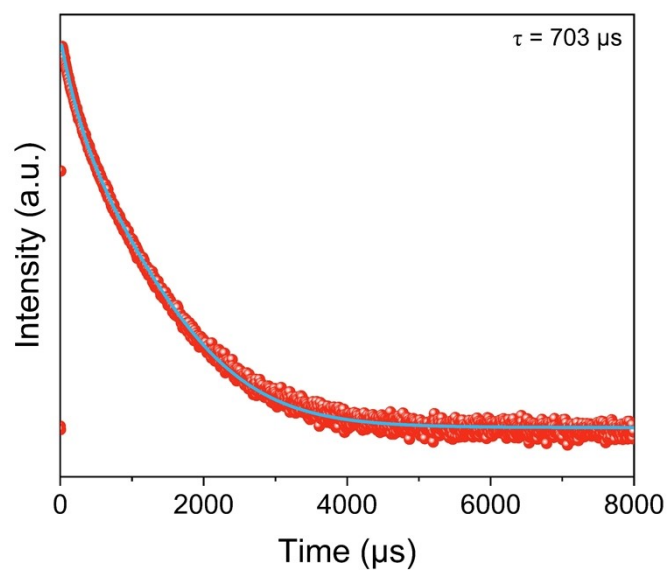
**Figure S1.** FTIR spectra of **Eu-ndc** and **H<sub>2</sub>ndc**.



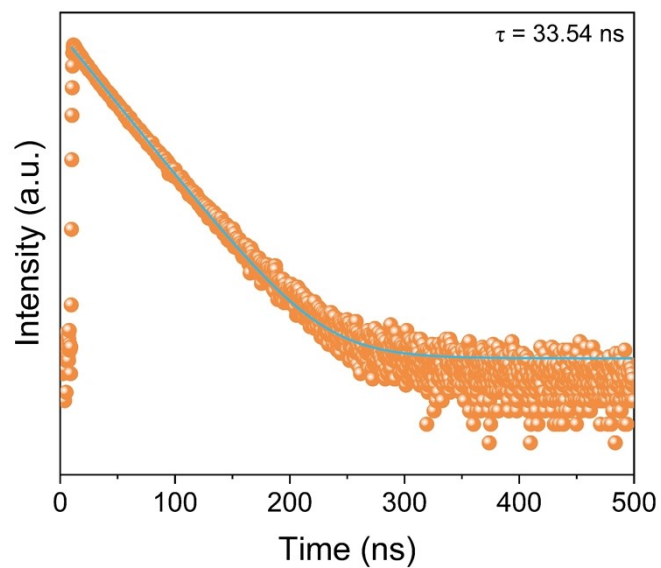
**Figure S2.** Thermogravimetric analysis (TGA) curve of **Eu-ndc**.



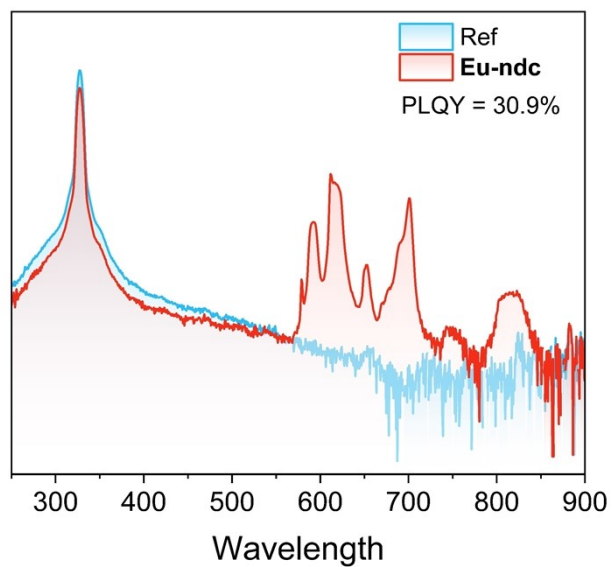
**Figure S3.** Excitation and emission spectra of H<sub>2</sub>ndc.



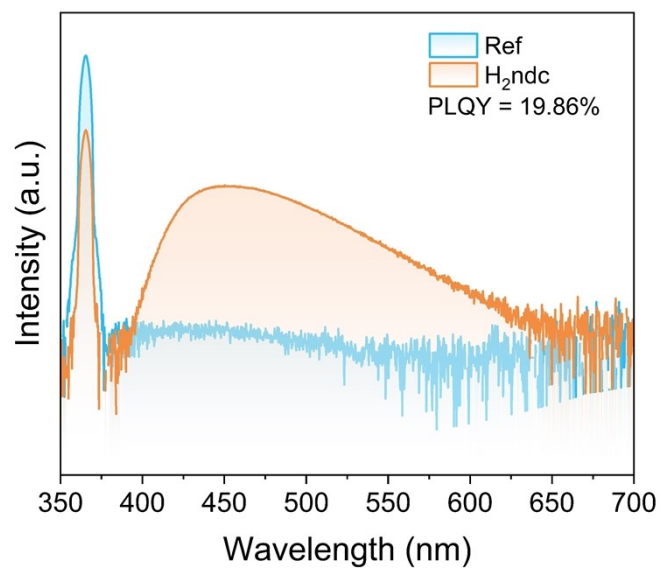
**Figure S4.** Time-resolved photoluminescence decay profile of Eu-ndc.



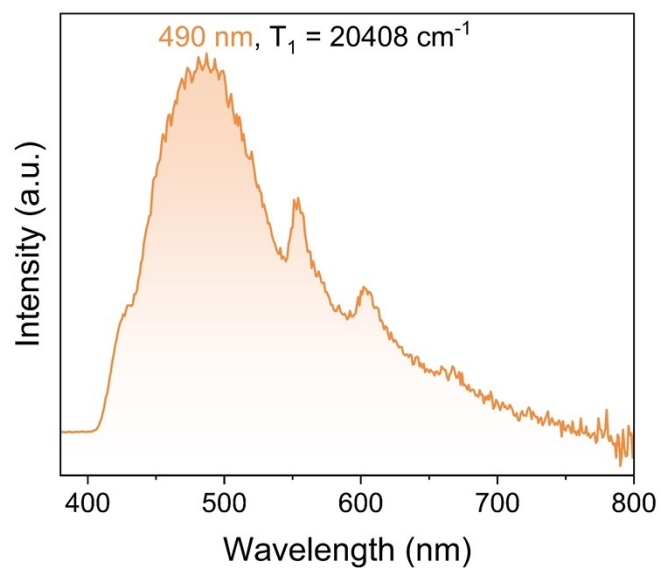
**Figure S5.** Time-resolved photoluminescence decay profile of H<sub>2</sub>ndc.



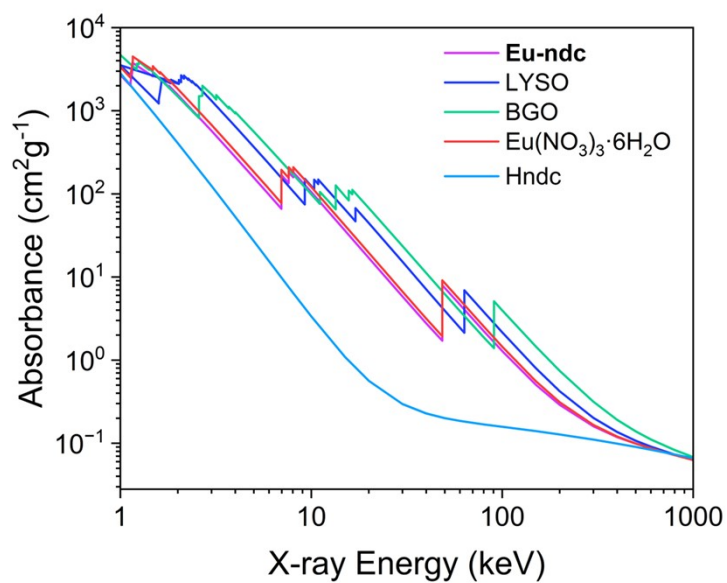
**Figure S6.** Photoluminescence quantum yield of Eu-ndc.



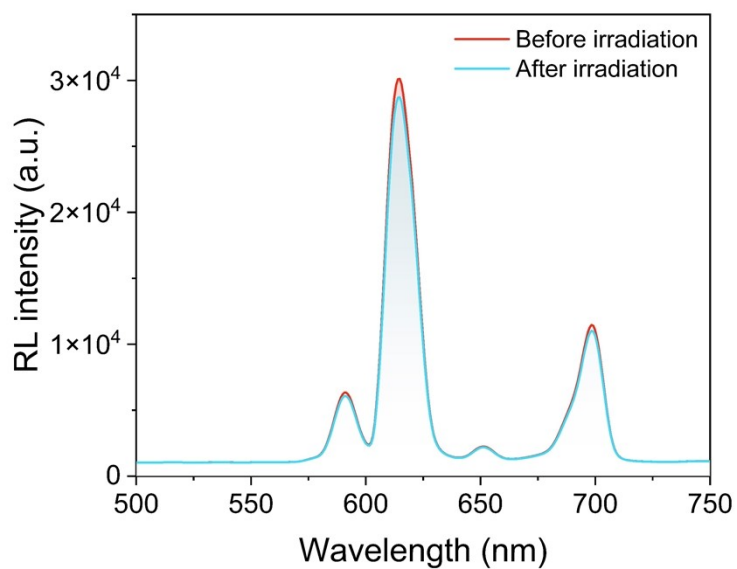
**Figure S7.** Photoluminescence quantum yield of H<sub>2</sub>ndc.



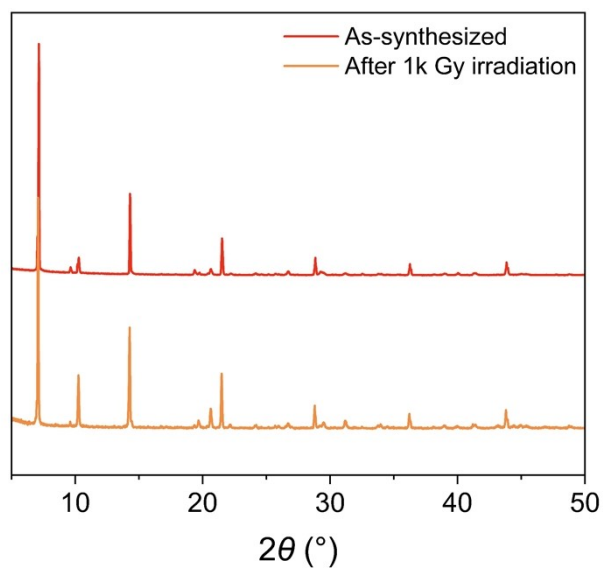
**Figure S8.** 77 K phosphorescence spectroscopy of H<sub>2</sub>ndc.



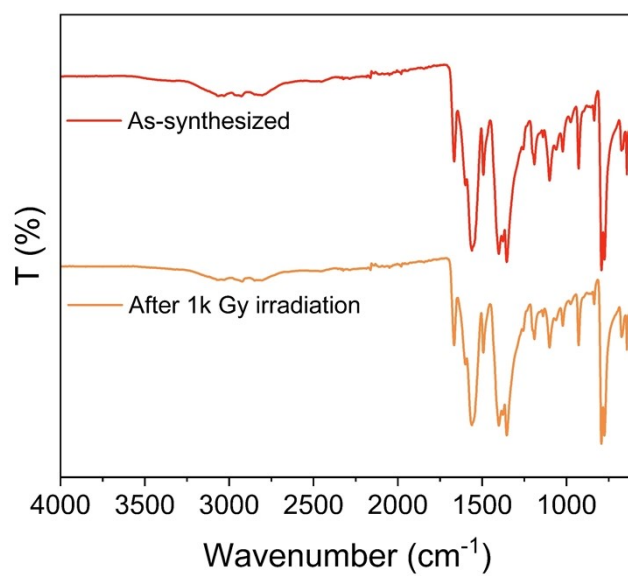
**Figure S9.** X-ray absorption coefficients of **Eu-ndc**, LYSO, BGO,  $\text{Eu}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ , and  $\text{H}_2\text{ndc}$ .



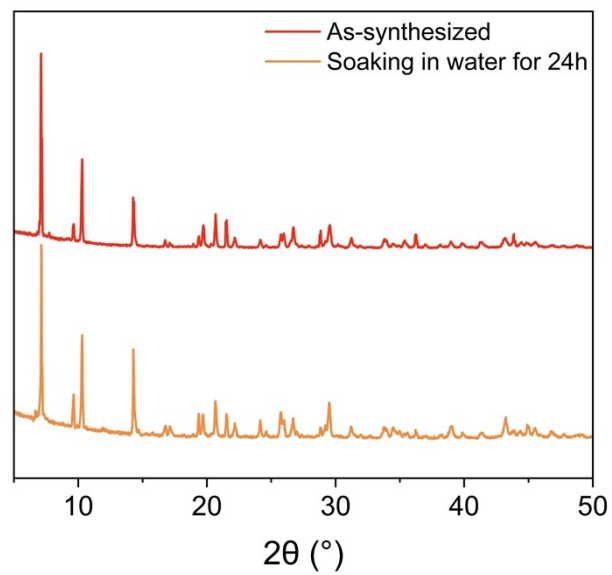
**Figure S10.** XEL of **Eu-ndc** before and after irradiation.



**Figure S11.** PXRD patterns of **Eu-ndc** before and after 1 kGy X-ray irradiation.



**Figure S12.** FTIR spectra of **Eu-ndc** before and after 1 kGy X-ray irradiation.



**Figure S13.** PXRD patterns of **Eu-ndc** before and after immersion in water for 24h.

**Table S1** Crystallographic data for **Eu-ndc**.

<b>Compound</b>	<b>Eu-ndc</b>
CCDC	2543588
Formula	C <sub>19.5</sub> H <sub>10.5</sub> Eu <sub>1.5</sub> O <sub>9.5</sub>
Formula weight	624.72
$\rho_{calc.}$ (g cm <sup>-3</sup> )	1.725
$\mu$ (mm <sup>-1</sup> )	3.931
Colour	Colorless
Habit	Hexagonal
Space group	$P\bar{3}$
a (Å)	10.5876(4)
b (Å)	10.5876(4)
c (Å)	24.7779(15)
$\alpha$ (deg)	90
$\beta$ (deg)	90
$\gamma$ (deg)	120
$V$ (Å <sup>3</sup> )	2405.4(2)
$Z$	4
$T$ (K)	298
$\lambda$ (Å)	0.711
$\Theta_{max}$ (deg)	29.135
$R_1$	0.1106
$\omega R_2$	0.2149
$R_{int}$	0.1547
$Goof$	1.108