Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


# Supporting Information

## Single Crystal Fluorescence Behavior of a New HOF Material: Potential Candidate for a New LED

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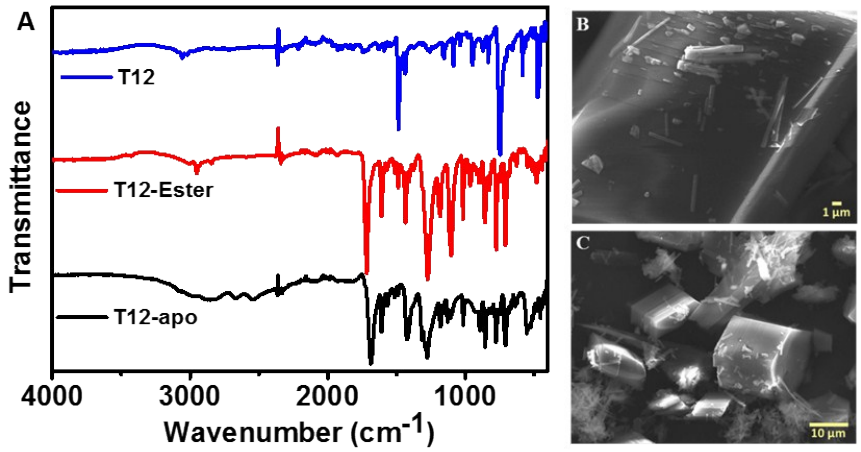


**Figure S1.** (A) Infrared spectra of T12, T12-ester and T12-apo in solid state. (B) and (C) SEM images of T12-apo in solid state.

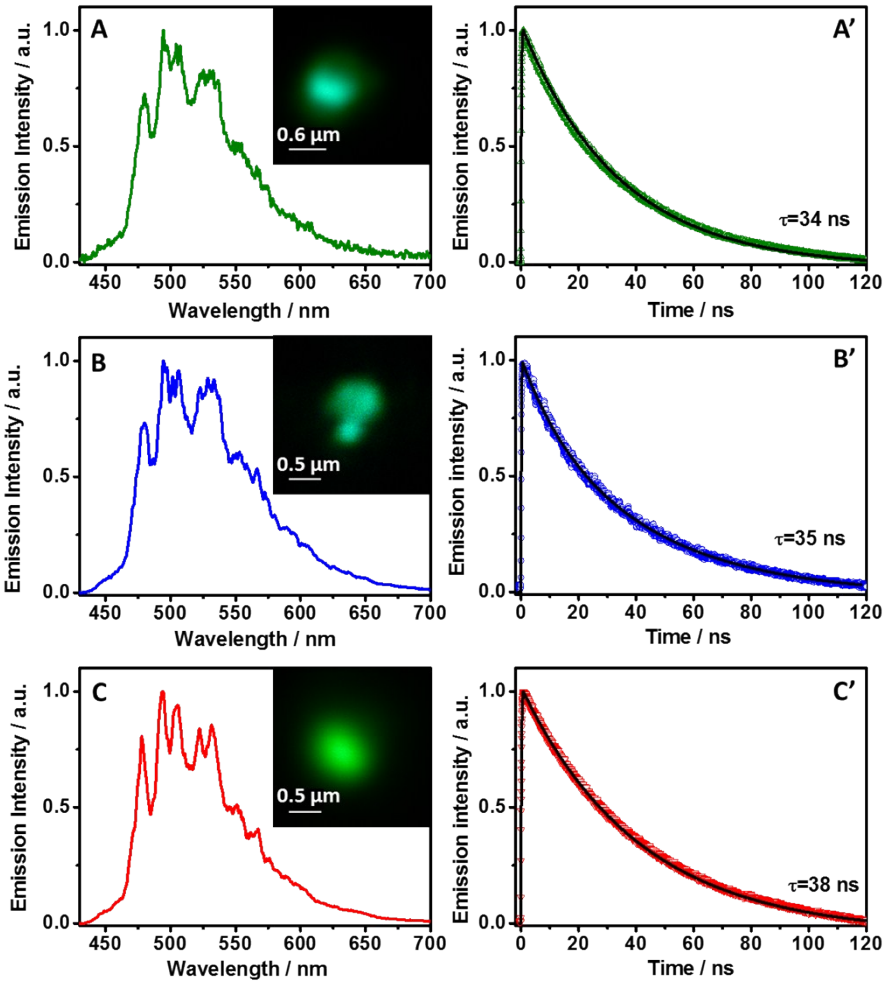


**Figure S2.** Emission (A-C) spectra and decays (A'-C') of small crystals of T12. The excitation wavelength was 390 nm, and the decays were recorded over the whole spectral range using a 430 nm long-pass filter. The solid lines are from the best-fit using a monoexponential function. The insets in (A-C) show the FLIM images of the crystals.

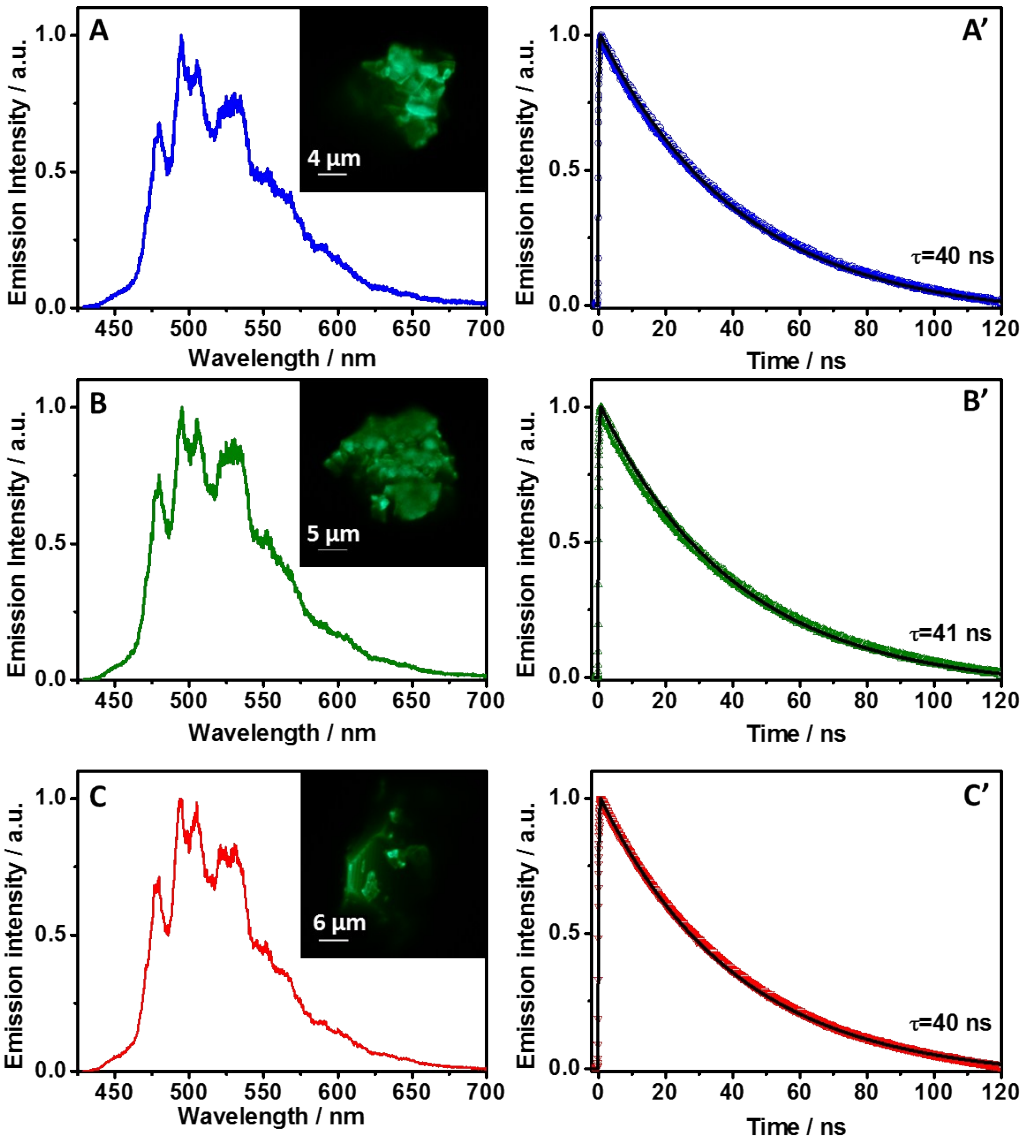


**Figure S3.** Emission (A-C) spectra and decays (A'-C') of large crystals of T12. The excitation wavelength was 390 nm, and the decays were recorded over the whole spectral range using a 430 nm long-pass filter. The solid lines are from the best-fit using a monoexponential function. The insets in (A-C) show the FLIM images of the crystals.

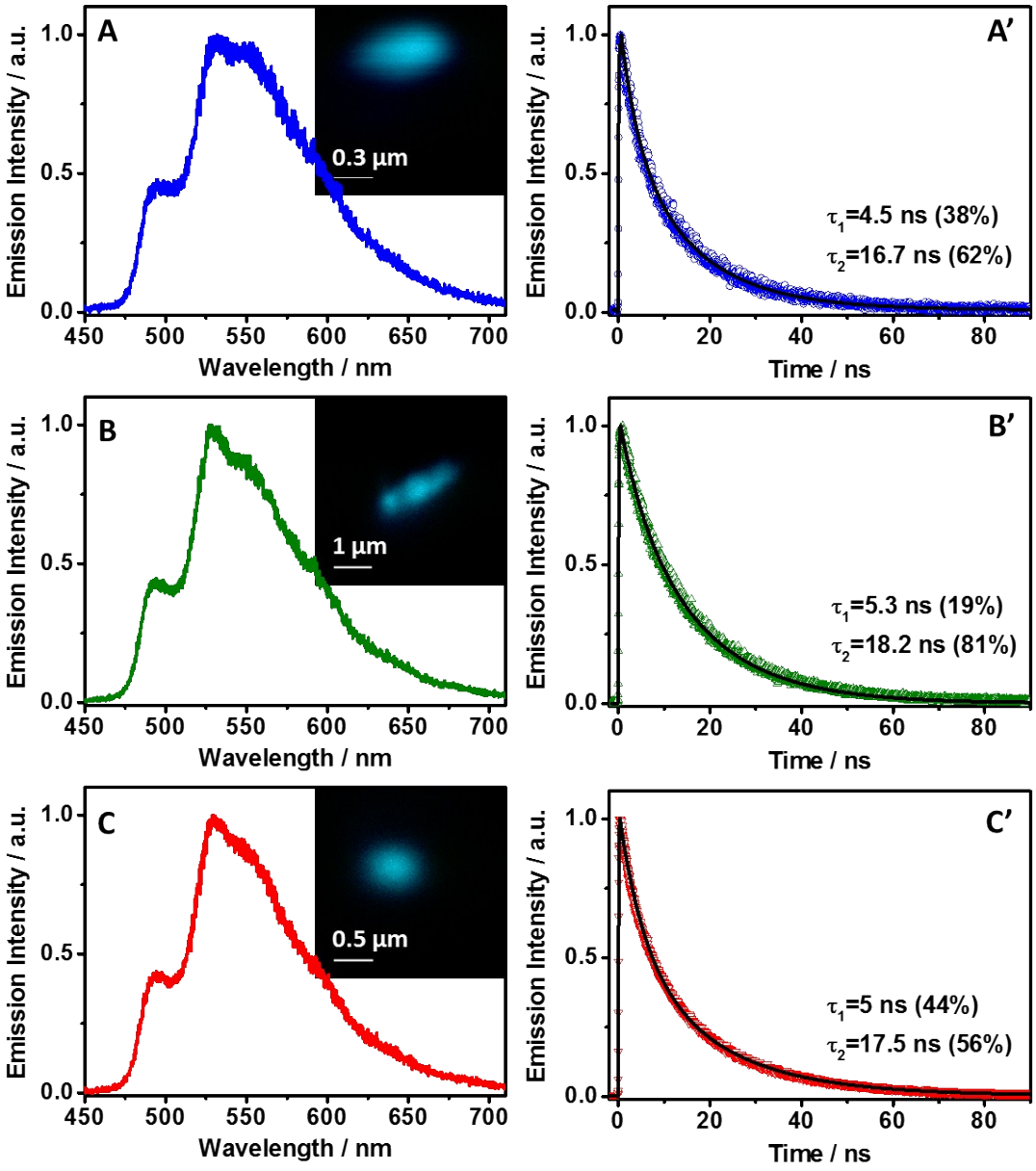


**Figure S4.** Emission (A-C) spectra and decays (A'-C') of small crystals of T12-Ester. The excitation wavelength was 390 nm, and the decays were recorded over the whole spectral range using a 430 nm long-pass filter. The solid lines are from the best-fit using a monoexponential function. The insets in (A-C) show the FLIM images of the crystals.

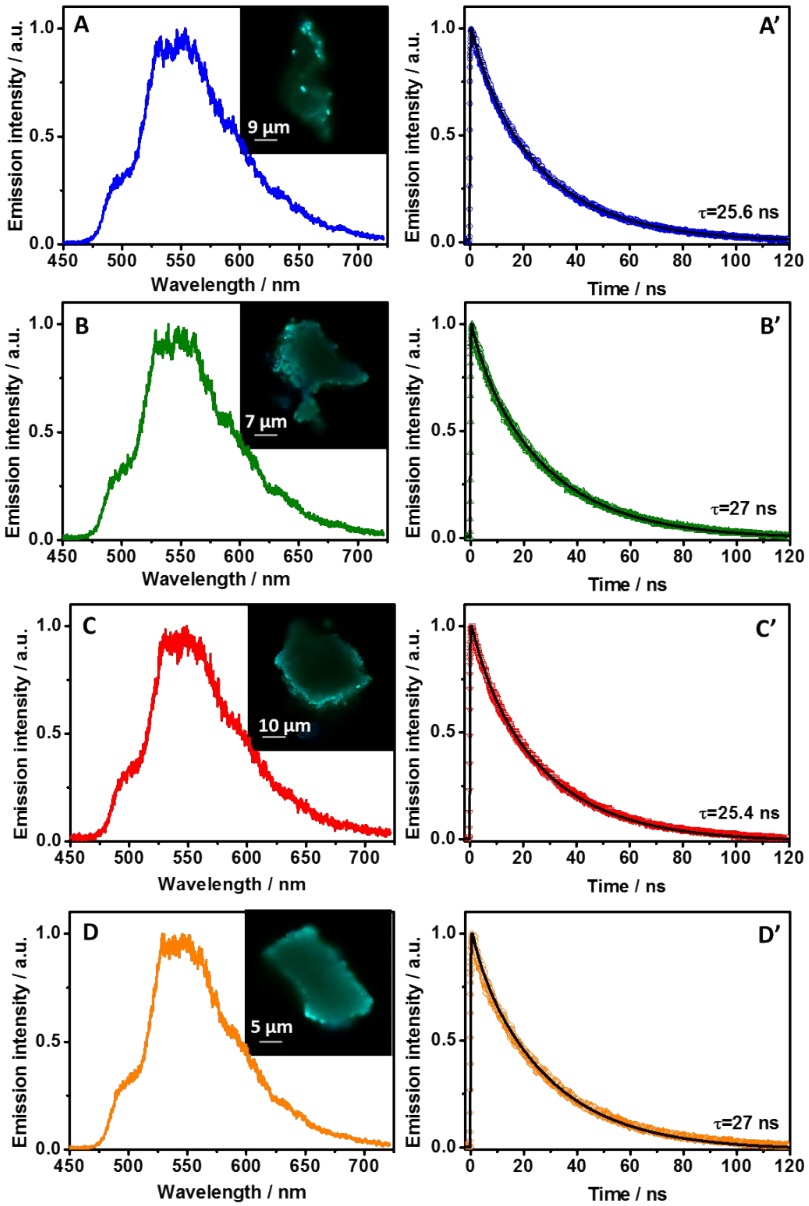


**Figure S5.** Emission (A-D) spectra and decays (A'-D') of large crystals of T12-Ester. The excitation wavelength was 390 nm, and the decays were recorded over the whole spectral range using a 430 nm long-pass filter. The solid lines are from the best-fit using a monoexponential function. The insets in (A-D) show the FLIM images of the crystals.

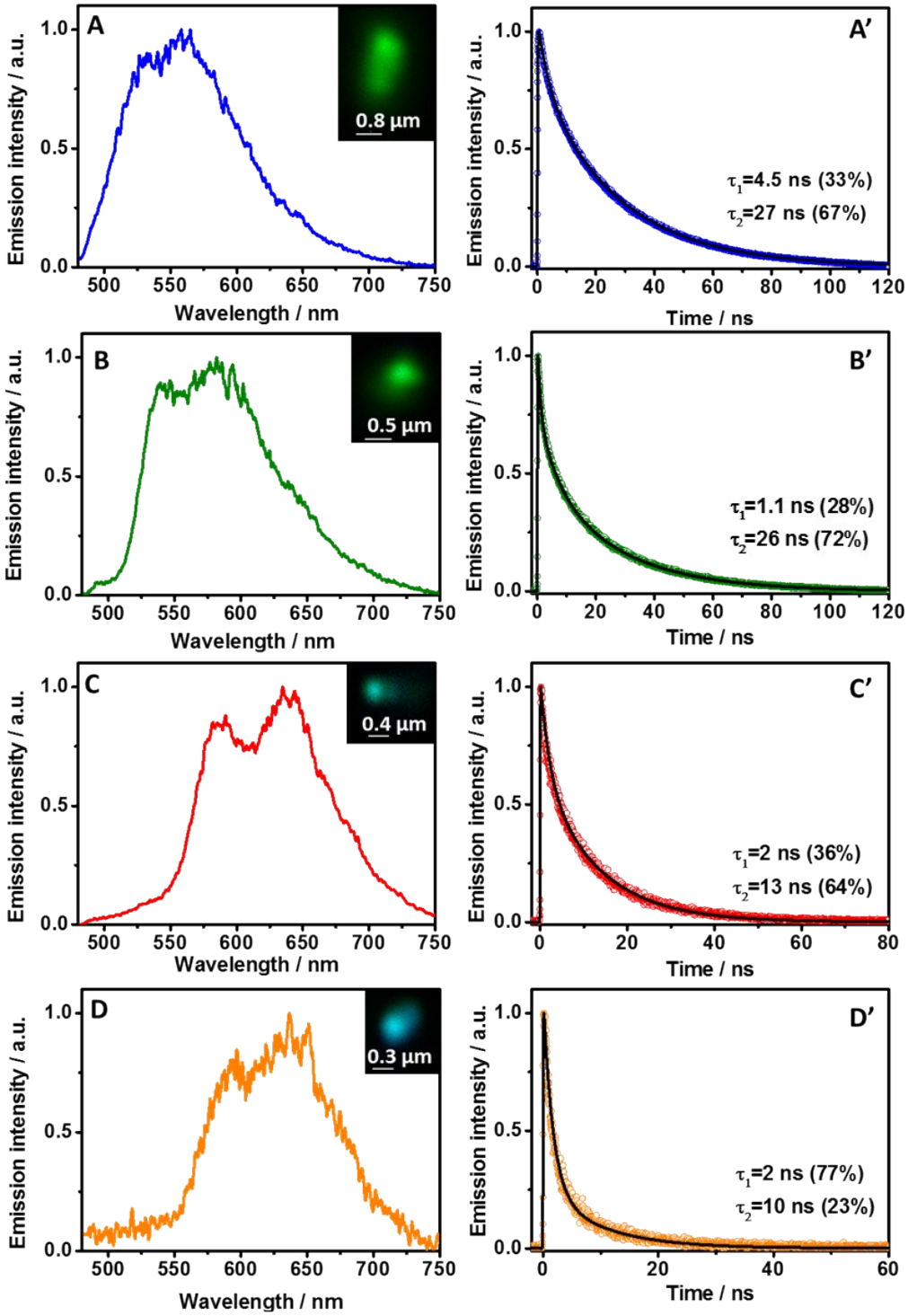


**Figure S6.** Emission (A-D) spectra and decays (A'-D') of small crystals of T12-apo. The excitation wavelength was 390 nm, and the decays were recorded over the whole spectral range using a 430 nm long-pass filter. The solid lines are from the best-fit using a monoexponential function. The insets in (A-D) show the FLIM images of the crystals.

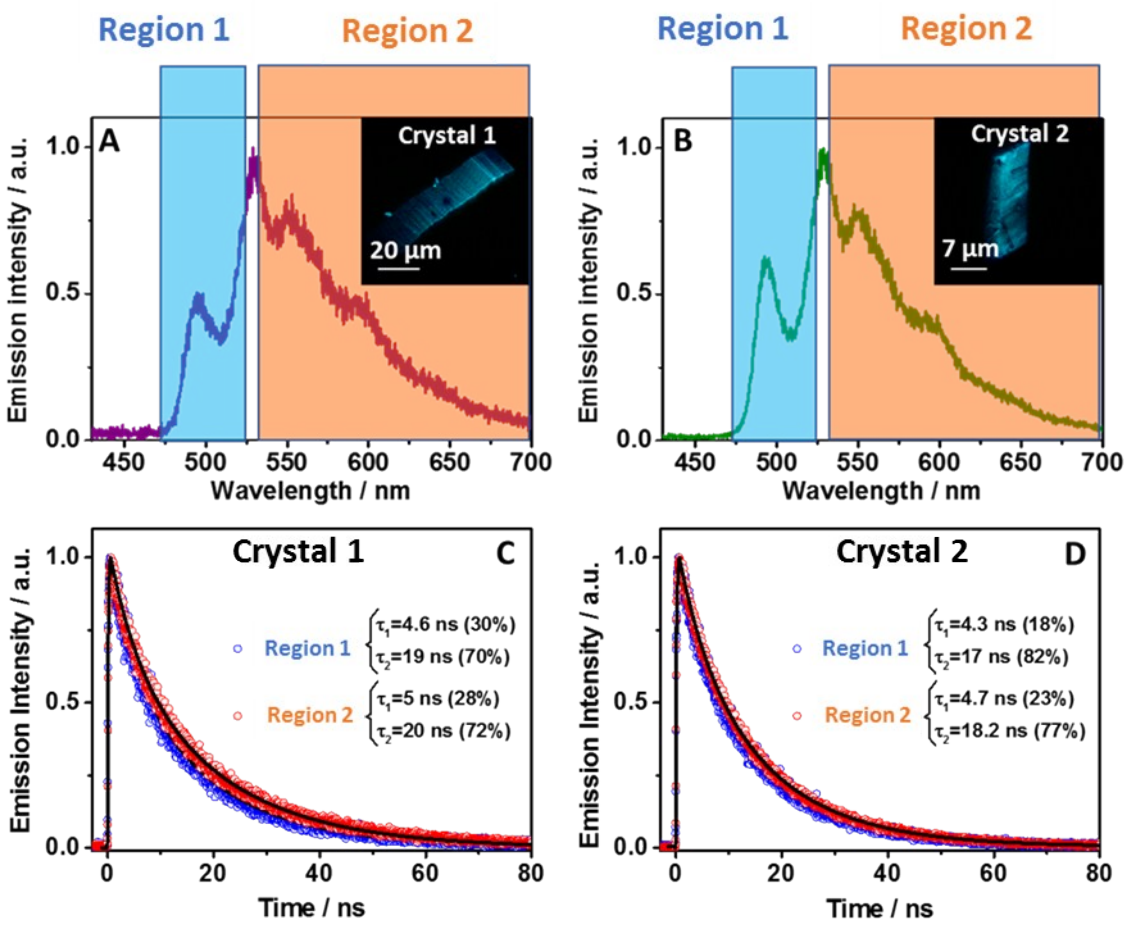


**Figure S7.** Emission (A-B) spectra and (C-D) decays of large crystals of T12-apo. The excitation wavelength was 390 nm and the decays are measured at selected spectral range using two different filters. For region 1, we used a FF01-503/40 Chroma filter, and for region 2 we used a 530 nm long-pass filter (HQ530LP, Chroma). The solid lines are from the best-fit using a multiexponential function. The insets of (A) and (B) show the FLIM images of the large crystals.

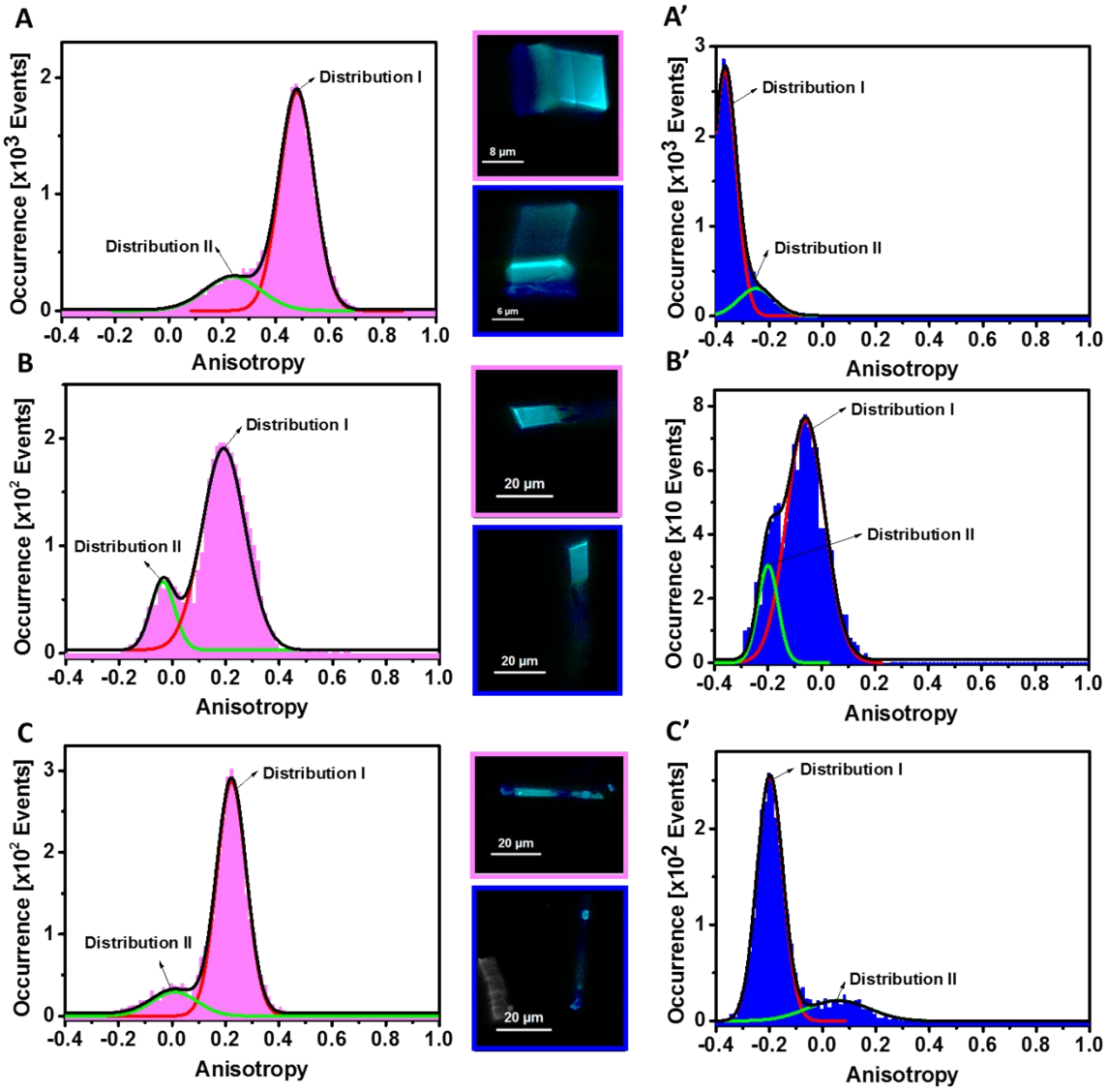


**Figure S8.** Histograms of the emission anisotropy for (A-C) 1 and (A'-C') 2 positions of T12-apo crystal. The solids lines are from the Gaussian distribution fits, showing two different populations of the emitters. The related data are given in table S1. The images show the 1 and 2 positions of the crystals. The excitation wavelength was 390 nm and the anisotropy was measured over the whole spectral range using a 430 nm long-pass filter.

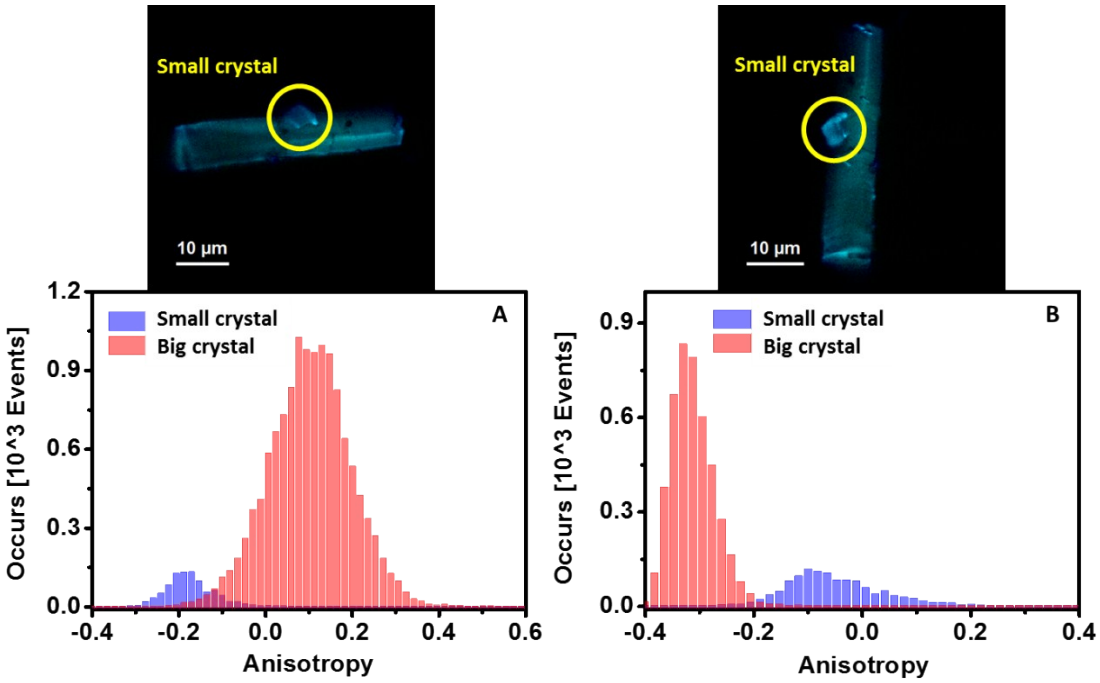


**Figure S9.** Histograms of the emission anisotropy for (A) 1 and (B) 2 positions of T12-apo crystal with respect to the plane of observation. The images show the 1 and 2 positions of the crystals. The excitation wavelength was 390 nm and the anisotropy was measured over the whole spectral range using a 430 nm long-pass filter.

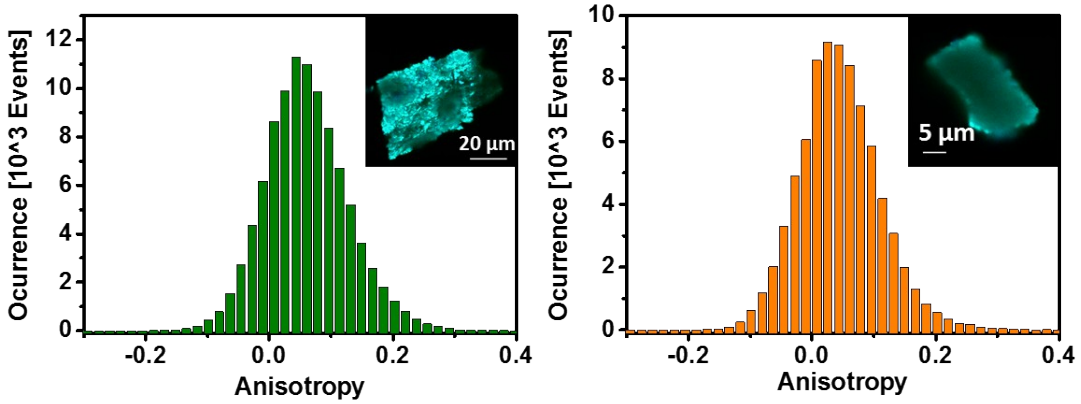


**Figure S10.** Histograms of the emission anisotropy value using two crystals of T12-Ester crystals. The excitation wavelength was 390 nm and the anisotropy was measured over the whole spectral range using a 430 nm long-pass filter. Insets: Images of the explored crystals.

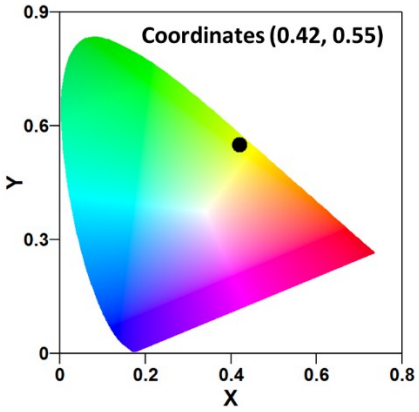


**Figure S11.** Commission International De I'Eclairage coordinates of T12-apo.

| Crystal in | Orientation of the crystal | Distribution | Anisotropy Maximum | Contribution | FWHM |
|---|---|---|---|---|---|
| **Figure 6A** | **1** | I | 0.19 | 86 | 0.22 |
| | | II | -0.13 | 14 | 0.17 |
| **Figure 6A'** | **2** | I | -0.32 | 85 | 0.12 |
| | | II | -0.05 | 15 | 0.30 |
| **Figure 6B** | **1** | I | 0.26 | 81 | 0.16 |
| | | II | 0.13 | 19 | 0.13 |
| **Figure 6B'** | **2** | I | -0.35 | 84 | 0.12 |
| | | II | -0.12 | 16 | 0.34 |
| **Figure S8A** | **1** | I | 0.48 | 81 | 0.15 |
| | | II | 0.24 | 19 | 0.24 |
| **Figure S8A'** | **2** | I | -0.36 | 86 | 0.10 |
| | | II | -0.24 | 14 | 0.15 |
| **Figure S8B** | **1** | I | 0.19 | 84 | 0.19 |
| | | II | -0.03 | 16 | 0.10 |
| **Figure S8B'** | **2** | I | -0.05 | 83 | 0.16 |
| | | II | -0.19 | 17 | 0.08 |
| **Figure S8C** | **1** | I | 0.22 | 87 | 0.13 |
| | | II | 0.01 | 13 | 0.19 |
| **Figure S8C'** | **2** | I | -0.19 | 83 | 0.11 |
| | | II | 0.05 | 17 | 0.27 |

**Table S1.** Obtained values from the deconvolution of the histogram of the emission anisotropy for the 1 and 2 orientations of the crystals, shown in Figures 6 and S8. The excitation wavelength was 390 nm and the anisotropy was measured over the whole spectral range using a 430 nm long-pass filter.