

Improving the emission quantum yield in dinuclear Eu(III) and Tb(III) complexes with 2-fluorobenzoate.

Ànnia Tubau, Laura Rodríguez, Ariadna Lázaro, Ramon Vicente and Mercè Font-Bardía.

SUPPLEMENTARY INFORMATION:

Crystal Data	Compound 1
Formula	C ₅₆ H ₃₈ Eu ₂ F ₈ O ₁₈
FW [g/mol]	1454.78
Crystal System	triclinic
Space Group	P-1
a [Å]	9.095(8)
b [Å]	11.378(10)
c [Å]	13.659(12)
α[deg]	110.68(3)
β [deg]	93.12(3)
γ [deg]	92.45(3)
V [Å ³]	1317.6(2)
Z	1
T(K)	100(2)
λ(Mo Kα) (Å)	0.71073
D _{calc} [g cm ⁻³]	1.833
μ(Mo Kα) [mm ⁻¹]	2.464
R	0.0199
wR ₂	0.0467
Table S1. Crystal data and single crystal X-Ray diffraction measurement details for compound 1 .	

Eu1-O1	2.586(13)	Eu1-O6 a	2.463(14)
Eu1-O2	2.430(13)	Eu1-O7	2.481(13)
Eu1-O3	2.354(13)	Eu1-O9	2.427(13)
Eu1-O4	2.356(13)	Eu1---Eu1	3.964(3)
Eu1-O5	2.638(13)	O1-Eu1-O2	51.69(4)
Eu1-O5_a	2.638(13)	Eu-O_a-Eu	105.19(5)
Table S2. Selected bond lengths (Å) and angles (°) for compound 1 . The symmetry transformation used to generate equivalent atoms is _a: -x+1,-y+1,-z+2			

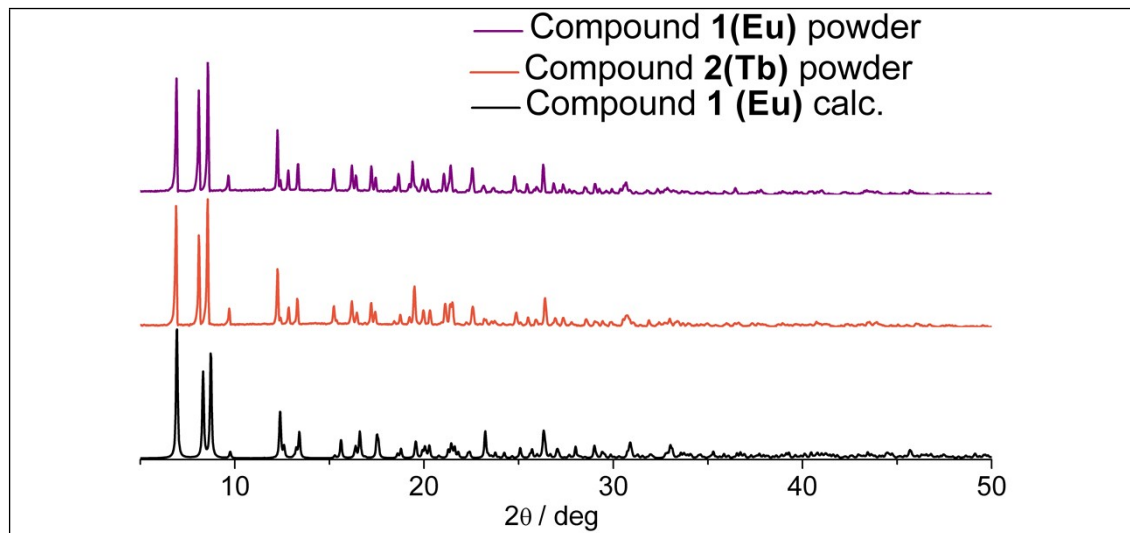
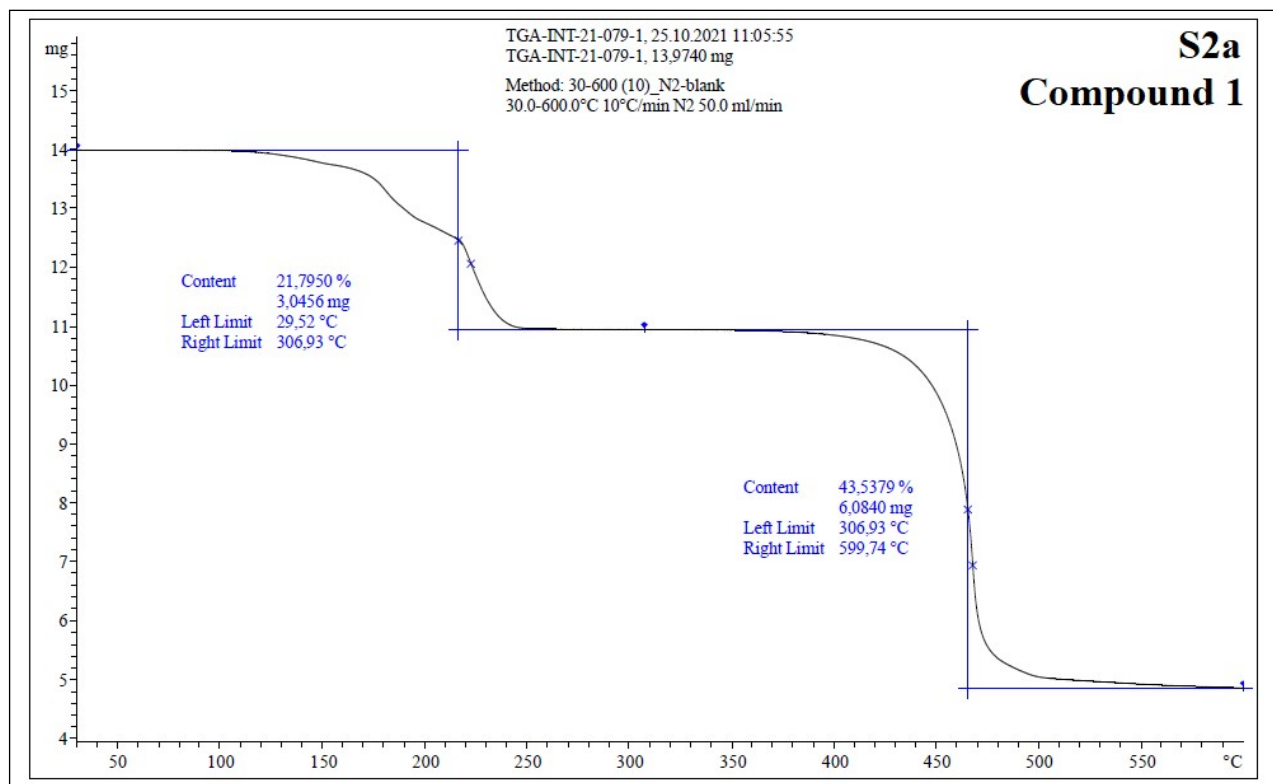
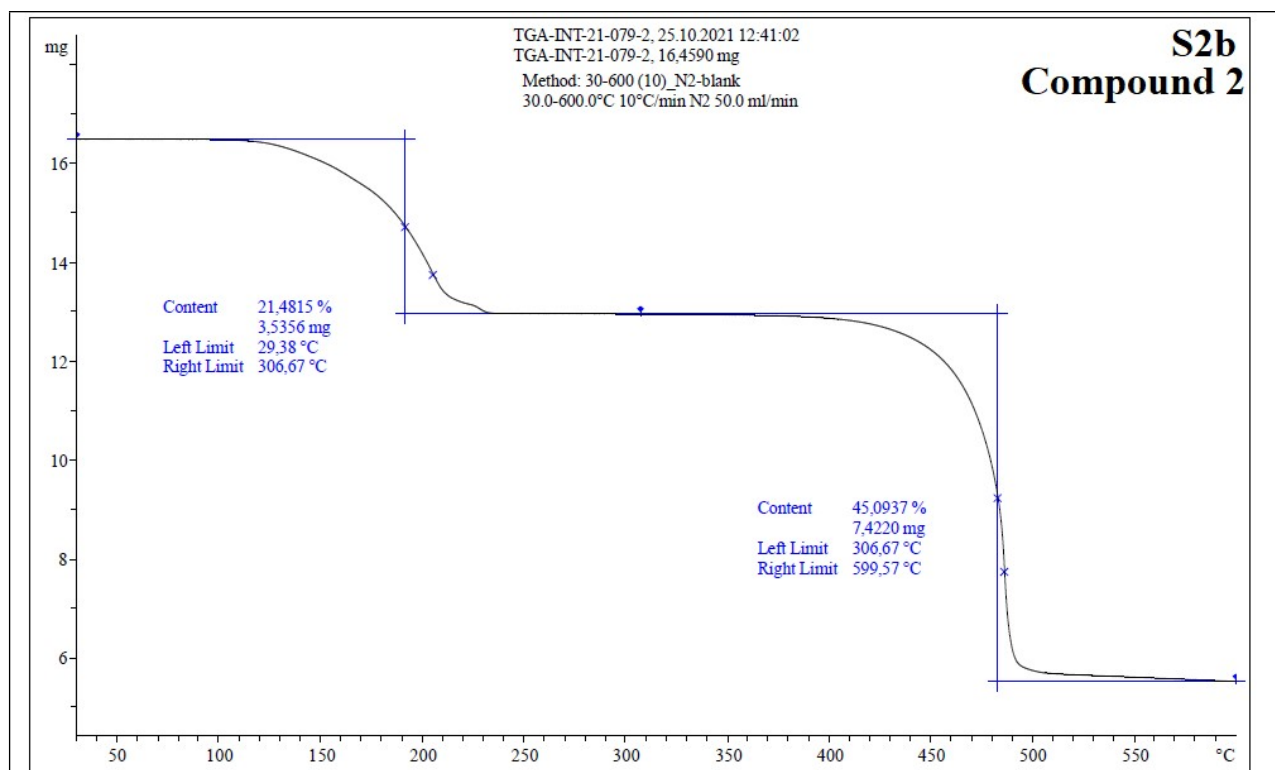
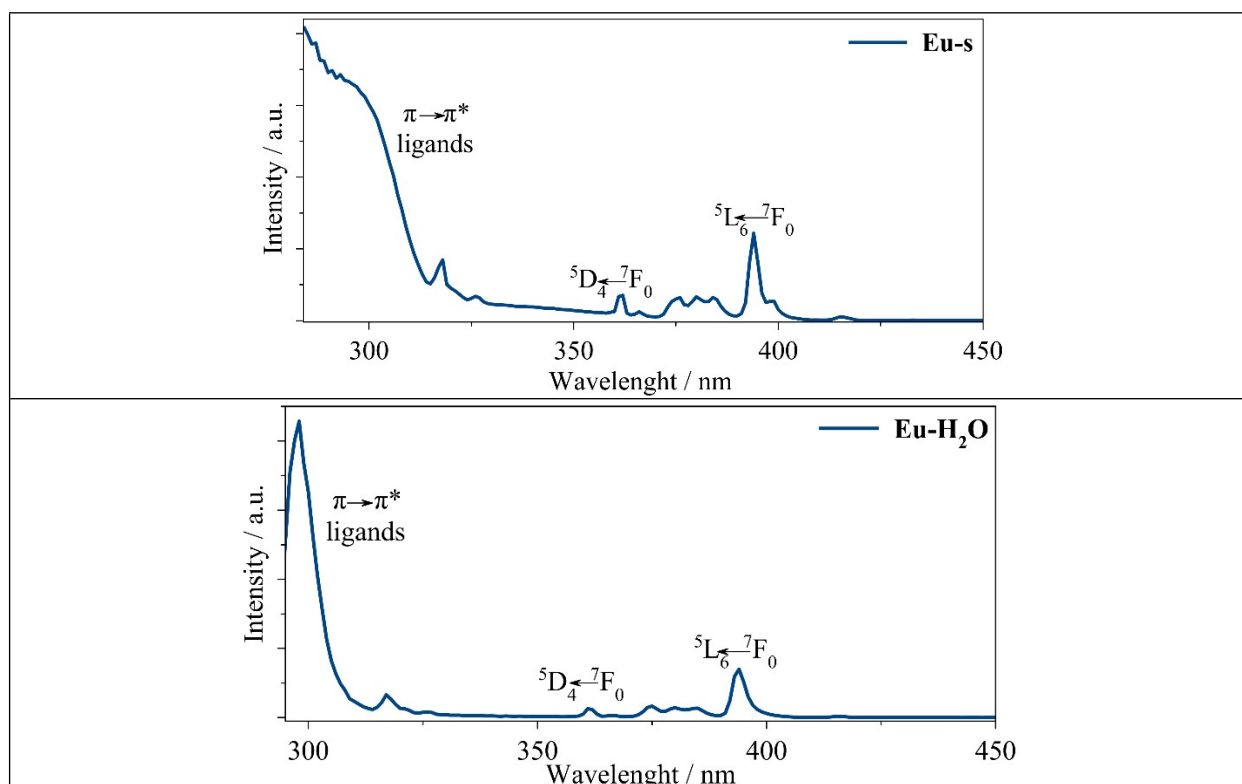


Figure S1. Calculated powder pattern of the single crystal (black line) compared with the experimental powder X-ray diffraction of the phase pure compounds (orange and purple lines). Single crystal X-Ray diffraction was measured at 100 K and Powder X-Ray diffraction was measured at room temperature.





Figures S2a and S2b. Thermogravimetry measurements for compounds 1 (Sa1) and 2 (Sa2). The measurement is performed in the 30–600 °C temperature range and under N₂ atmosphere, with a heating rate of 10 °C min⁻¹



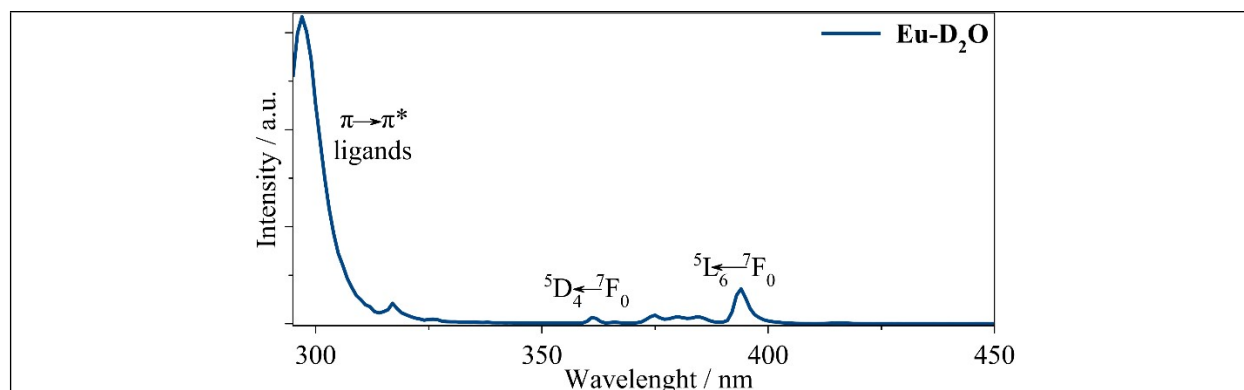


Figure S3. Excitation spectra of compound **1** in the microcrystalline sample (Eu-s), dissolved in water (Eu-H₂O) and in deuterium oxide (Eu-D₂O). Excitation spectra were recorded at λ_{em} of 617 nm ($^5D_0 \rightarrow ^7F_2$).

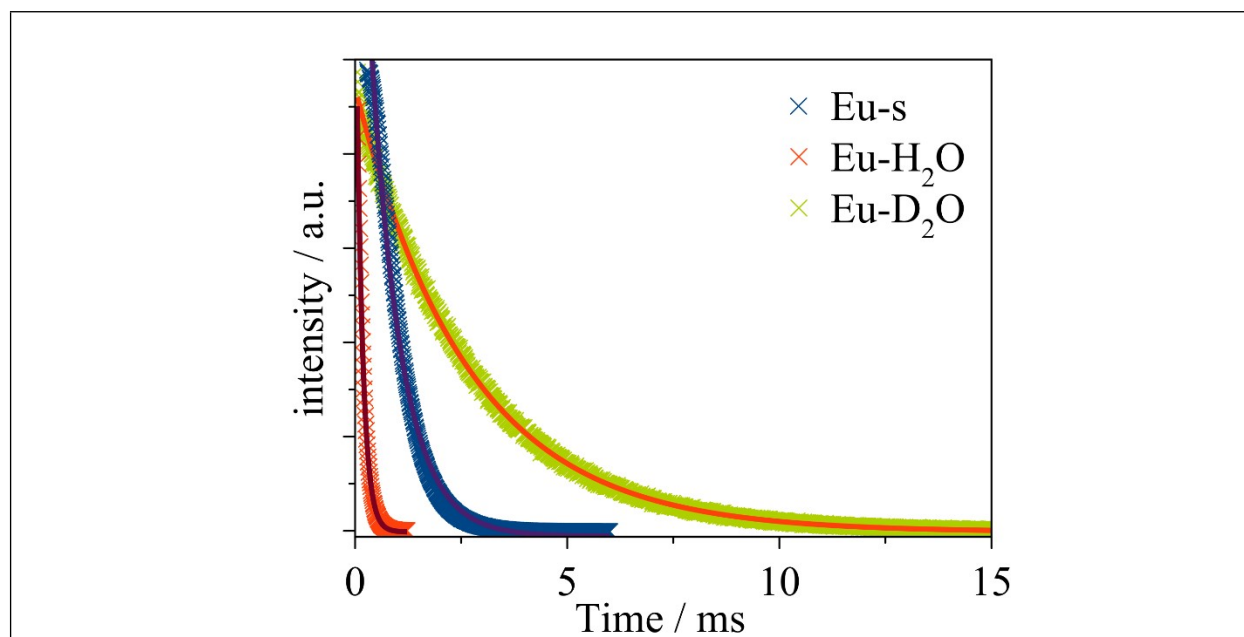
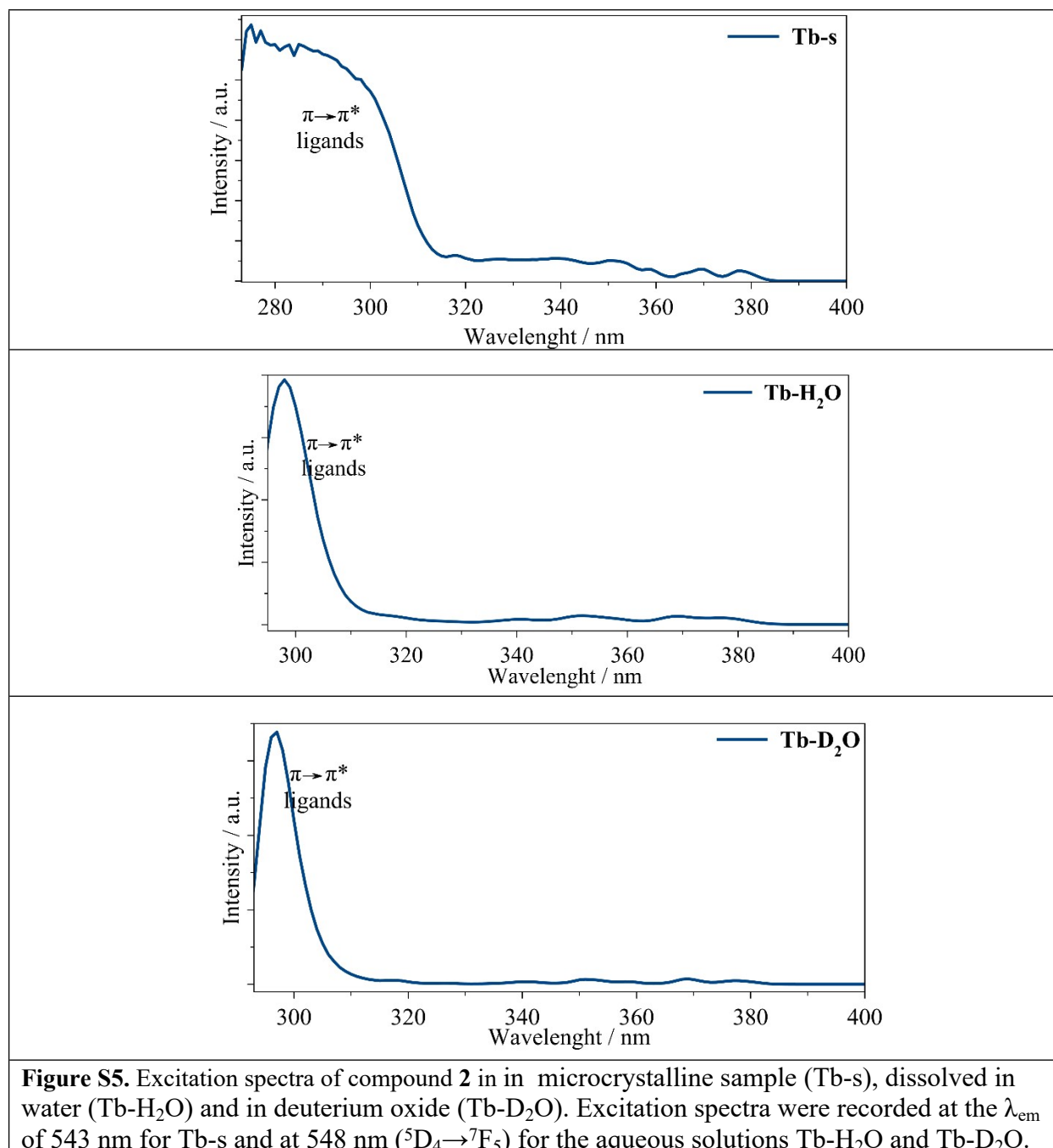


Figure S4. Time decay curves at r.t. for compound **1** in the microcrystalline sample (Eu-s), dissolved in water (Eu-H₂O) and in deuterium oxide (Eu-D₂O). Thick and continuous lines represent the monoexponential fittings of the curves. ($I(t) = I_0 \exp(-t/\tau_{obs})$)



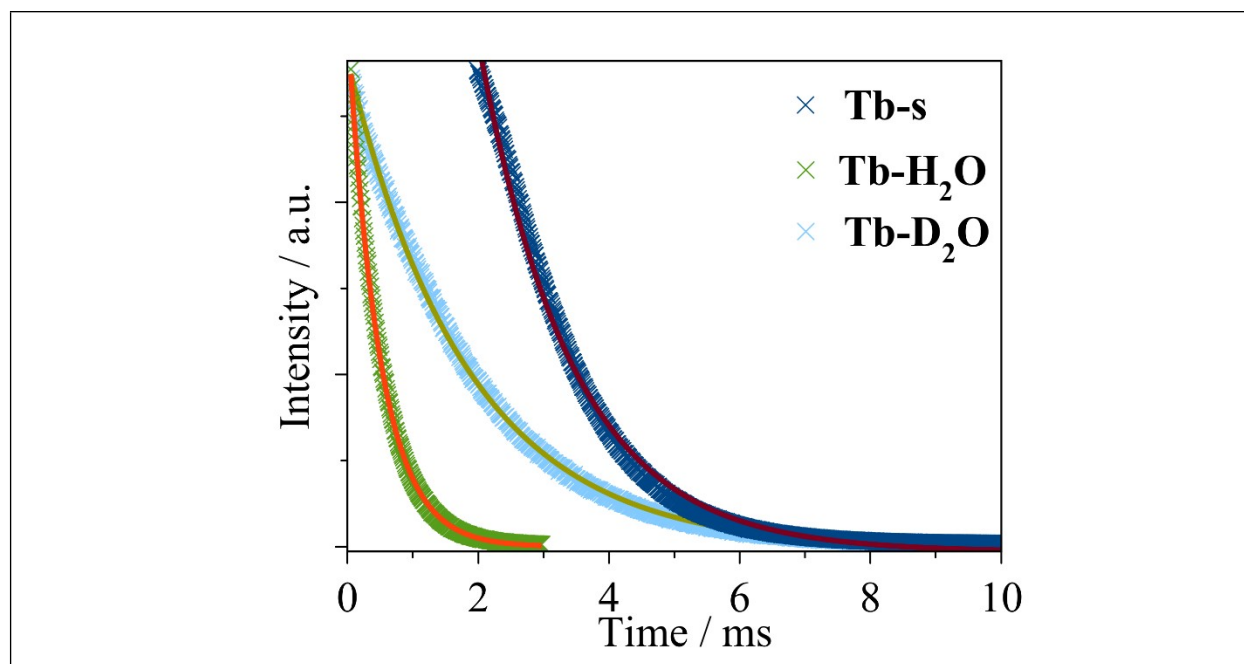


Figure S6. Time decay curves at r.t. for compound **2** in microcrystalline sample (Tb-s), dissolved in water (Tb-H₂O) and in deuterium oxide (Tb-D₂O). Thick and continuous lines represent the monoexponential fittings of the curves. ($I(t) = I_0 \exp(-t/\tau_{\text{obs}})$)

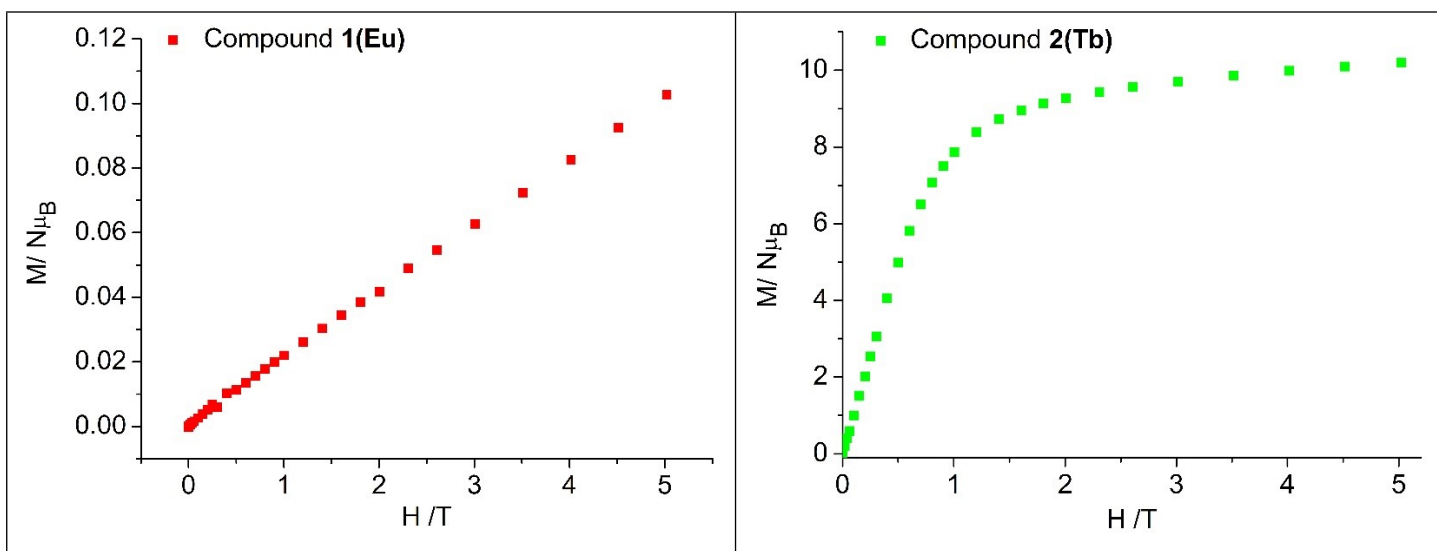


Figure S7. Magnetization dependency in front of the dc magnetic field at 2K for compounds **1**(red) and **2**(green)

