Photophysical investigation of near infrared emitting lanthanoid complexes incorporating tris(2-naphthoyl)methane as a new antenna ligand

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SUPPLEMENTARY INFORMATION

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^{1}H- and ^{13}C-NMR spectra

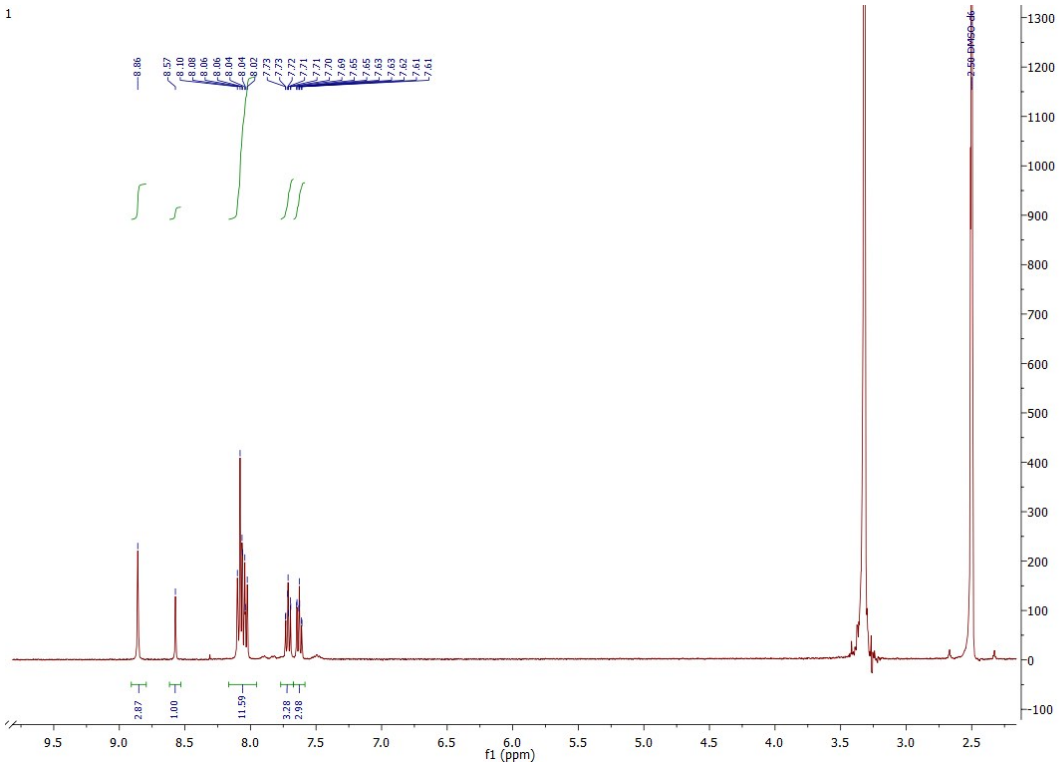

*Figure S1 ^{1}H NMR of the **tnm**H molecule in d-DMSO*

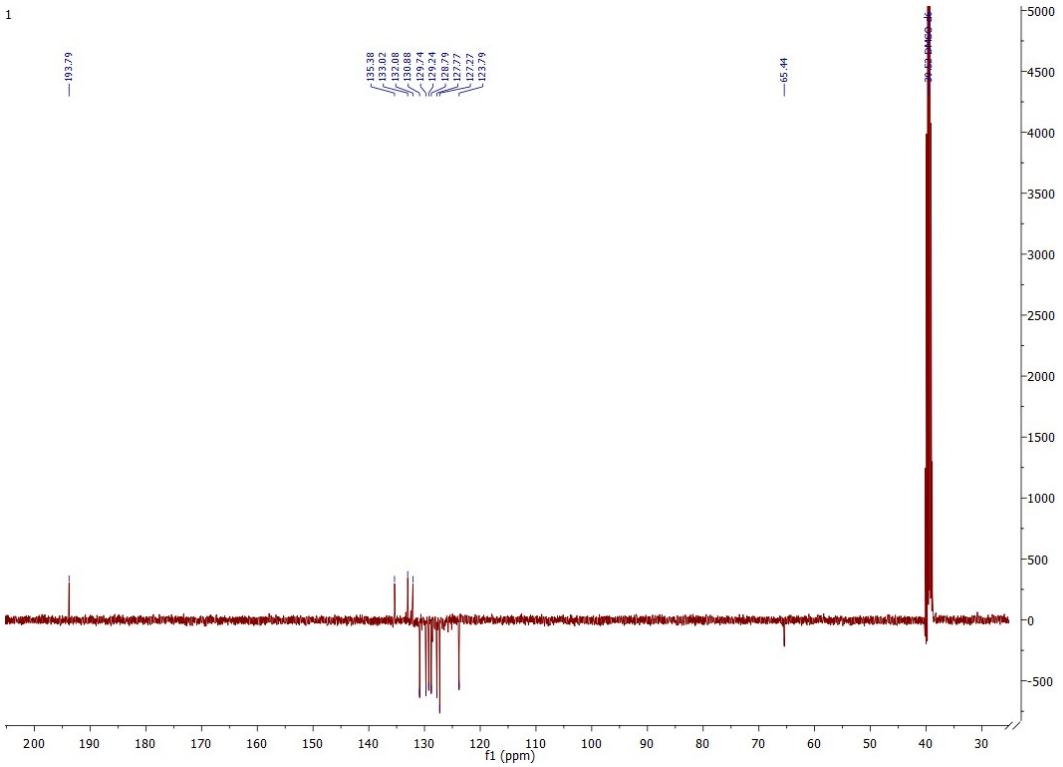

*Figure S2 ^{13}C NMR of the **tnm**H molecule in d-DMSO*

Absorption profiles

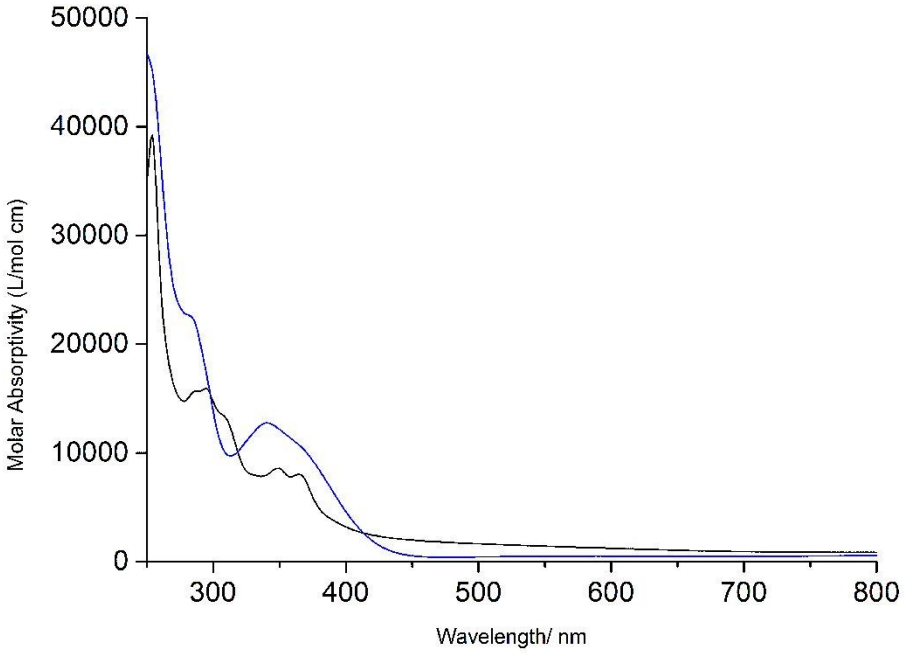

*Figure S3 Absorption profiles of **tnm**H (black trace) and **tnm** in excess of KOH (blue trace) from ca. 10^{-5}M solutions in EtOH*

Shape analysis studies

Determination of the geometrical parameters for the coordination sphere of the lanthanoid cations in the main assemblies. The analysis has been carried out considering the degree of distortion with respect to two ideal geometries: square antiprism and triangular dodecahedron.

Table S1 Selected data from shape analysis of the coordination geometries for square antiprism (SAPR-8) and triangular dodecahedron (TDD-8) polyhedral.

Complex	**TTD-8**	**SAPR-8**
[Nd(**tnm**)$_3$(DMSO)$_2$]	0.636	1.963
[Sm(**tnm**)$_3$(DMSO)$_2$]	0.589	1.905
[Eu(**tnm**)$_3$(DMSO)$_2$]	0.563	1.923
[Gd(**tnm**)$_3$(DMSO)$_2$]	0.561	1.931
[Yb(**tnm**)$_3$(DMSO)$_2$]	0.497	1.872

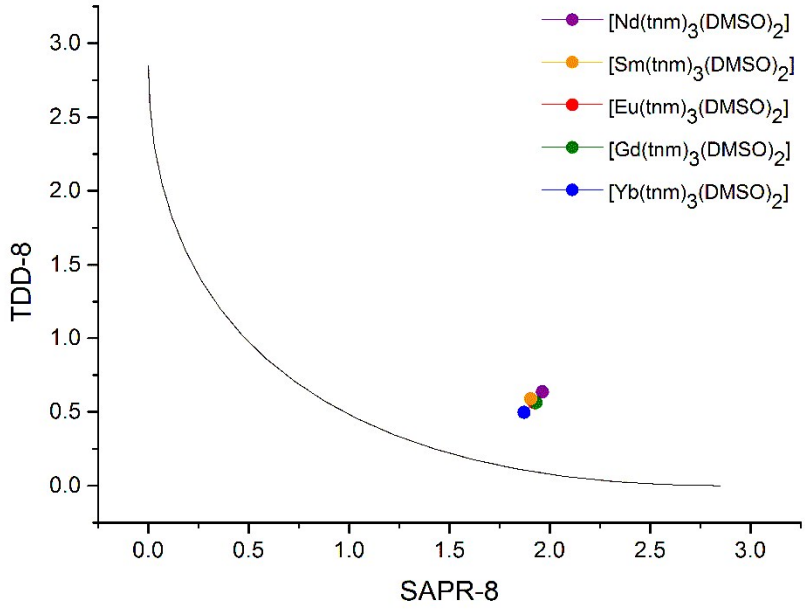

Figure S4. Shape analysis plot for square antiprism (SAPR-8) and triangular dodecahedron (TDD-8) polyhedral.

Emission plot of the $Gd(tnm)_3(DMSO)_2$ complex

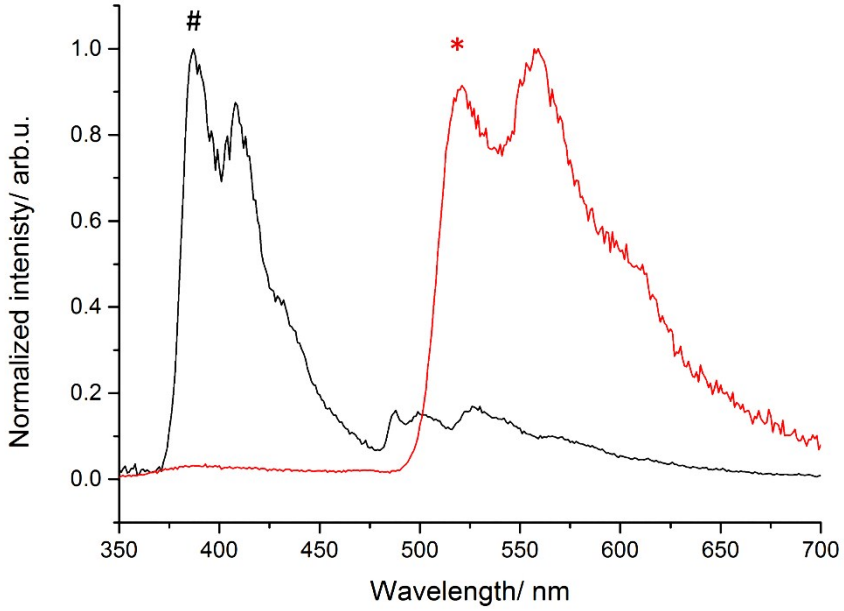

Figure S5. Emission of ligand tnm(black trace) and its Gd^{3+} complex (red trace) in an acetonitrile matrix at 77K. The asterisks denote the estimated position for the 0-phonon transition for the determination of the energy of the singlet state (black) and triplet state (red).

Normalized excitation and emission plots

Yb(**tnm**)$_3$(DMSO)$_2$

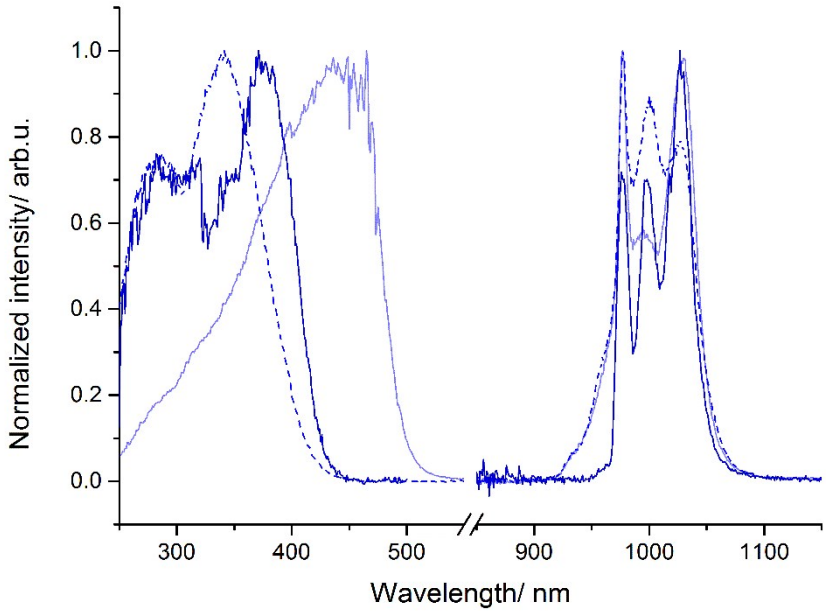

*Figure S6. Normalized emission plots for the Yb(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace),MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.*

Nd(**tnm**)$_3$(DMSO)$_2$

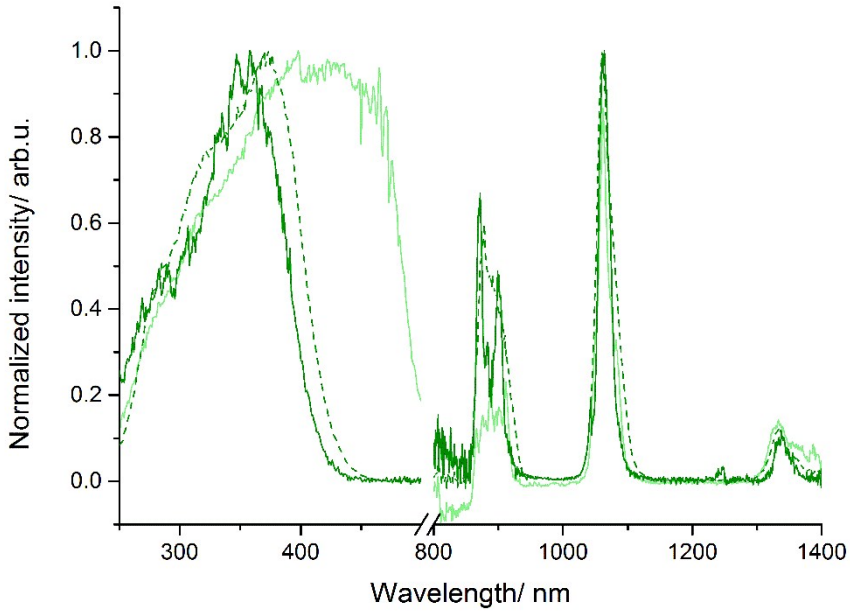

Figure S7. Normalized emission plots for the Nd(tnm)3(DMSO)2 in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

Eu(**tnm**)$_3$(DMSO)$_2$

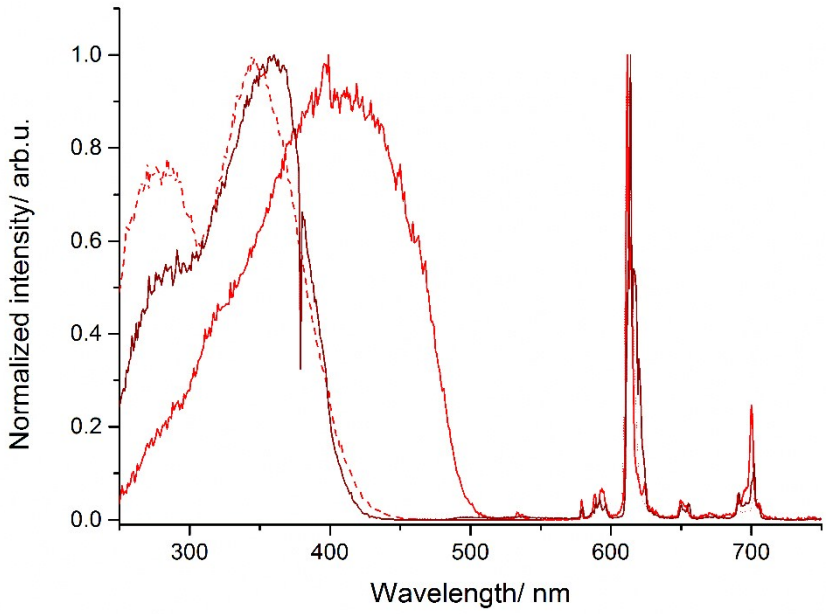

*Figure S8. Normalized emission plots for the Eu(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace) and MeCN at RT (dash trace) and 77K (dark red trace) with excitation wavelength at 350 nm.*

Sm(**tnm**)$_3$(DMSO)$_2$

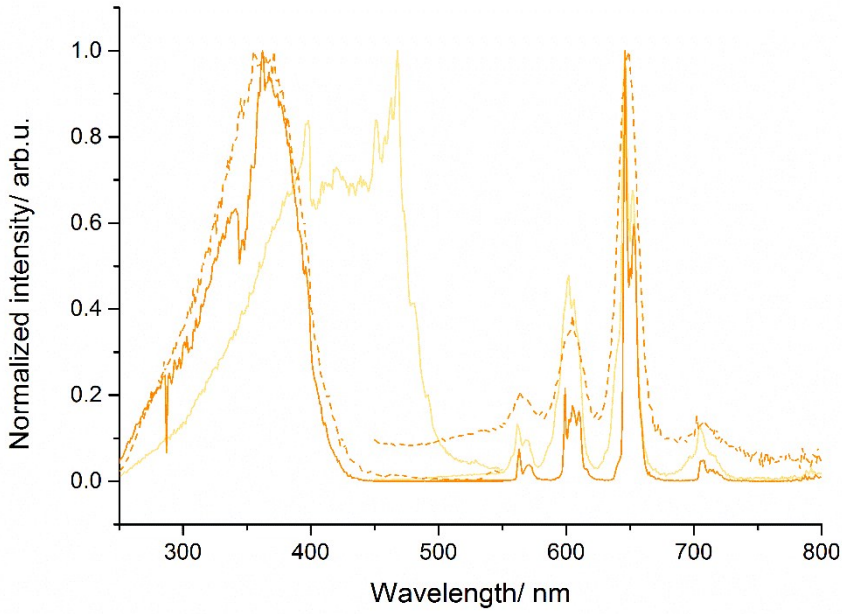

*Figure S9. Normalized emission plots for the Sm(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.*

Excited state lifetime decay plots

Yb(**tnm**)$_3$(DMSO)$_2$

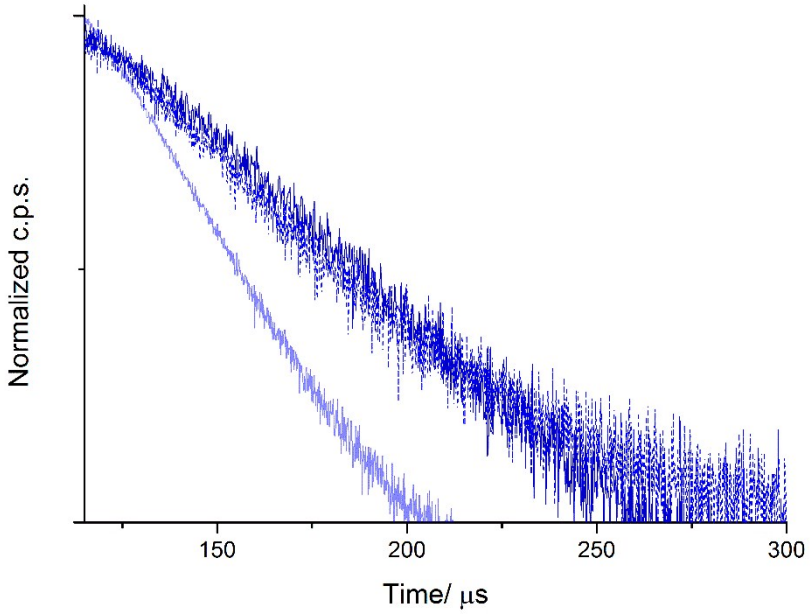

*Figure S10. Lifetime decay at 980nm for Yb(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace),MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.*

Nd(**tnm**)$_3$(DMSO)$_2$

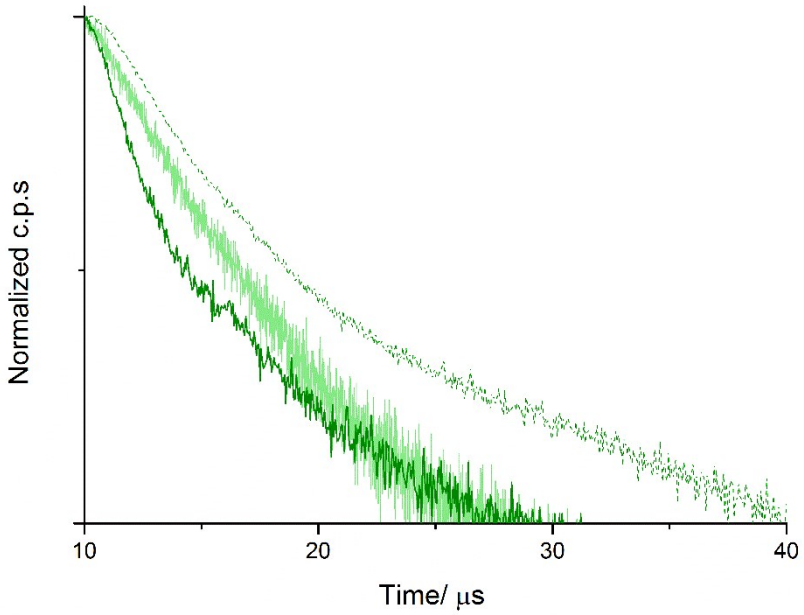

Figure S11. Lifetime decay at 1060nm for Nd(tnm)3(DMSO)2 in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

Eu(**tnm**)$_3$(DMSO)$_2$

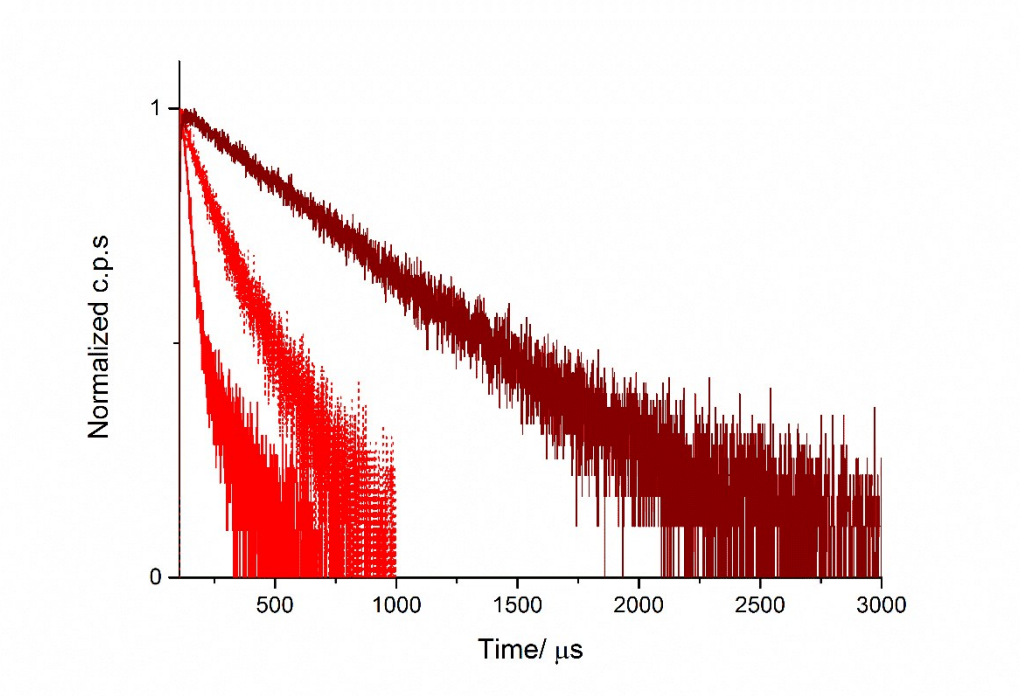

*Figure S12. Lifetime decay at 612nm for Eu(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace) and MeCN at RT (dash trace) and 77K (dark red trace) with excitation wavelength at 350 nm.*

Sm(**tnm**)$_3$(DMSO)$_2$

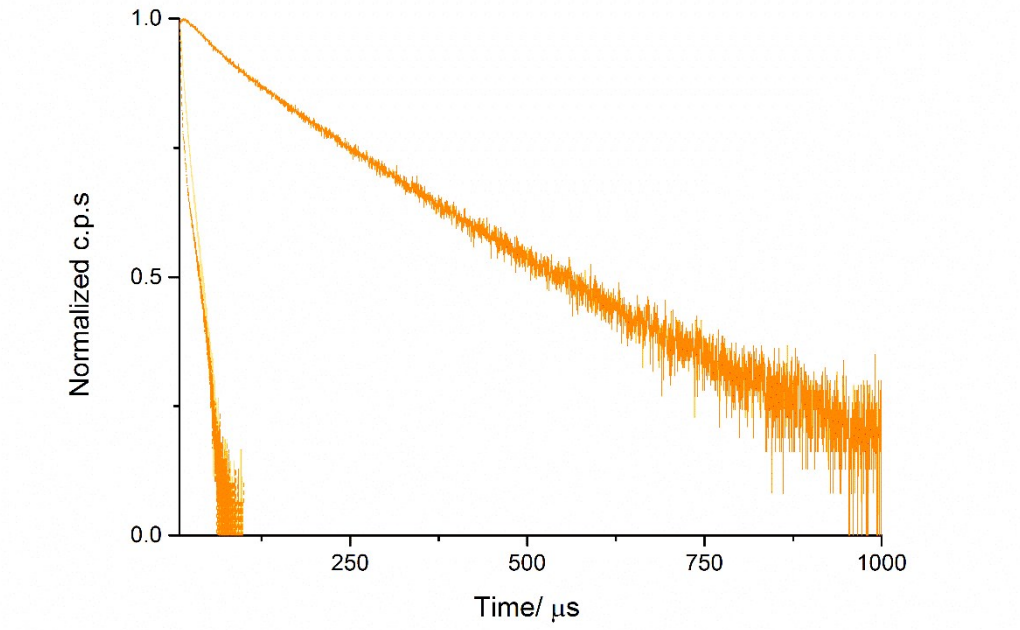

*Figure S13. Lifetime decay at 654 nm for Sm(**tnm**)$_3$(DMSO)$_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.*