

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

Laura Abad Galán,^{[a],[b]} Satoshi Wada,^[c] Lee Cameron^[a], Alexandre N. Sobolev,^[d] Yasuchika Hasegawa,^[e] Eli Zysman-Colman,^{*[b]} Mark I. Ogden,^{*[a]} and Massimiliano Massi^{*[a]}

^{a.} School of Molecular and Life Sciences and Curtin Institute for Functional Molecules and Interfaces, Curtin University, Kent Street, Bentley 6102 WA, Australia.

^{b.} Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St. Andrews, St. Andrews, Fife, KY16 9ST, United Kingdom

^{c.} Graduate School of Chemical Sciences and Engineering, Hokkaido University, Kita-13 Jo, Nishi-8 Chome, Kita-ku, Sapporo, Hokkaido, 060-8628 Japan

^{d.} School of Molecular Sciences and CMCA, M310, University of Western Australia, Crawley 6009 WA, Australia.

^{e.} Faculty of Engineering, Hokkaido University, Kita-13 Jo, Nishi-8 Chome, Kita-ku, Sapporo, Hokkaido, 060-8628 Japan

SUPPLEMENTARY INFORMATION

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

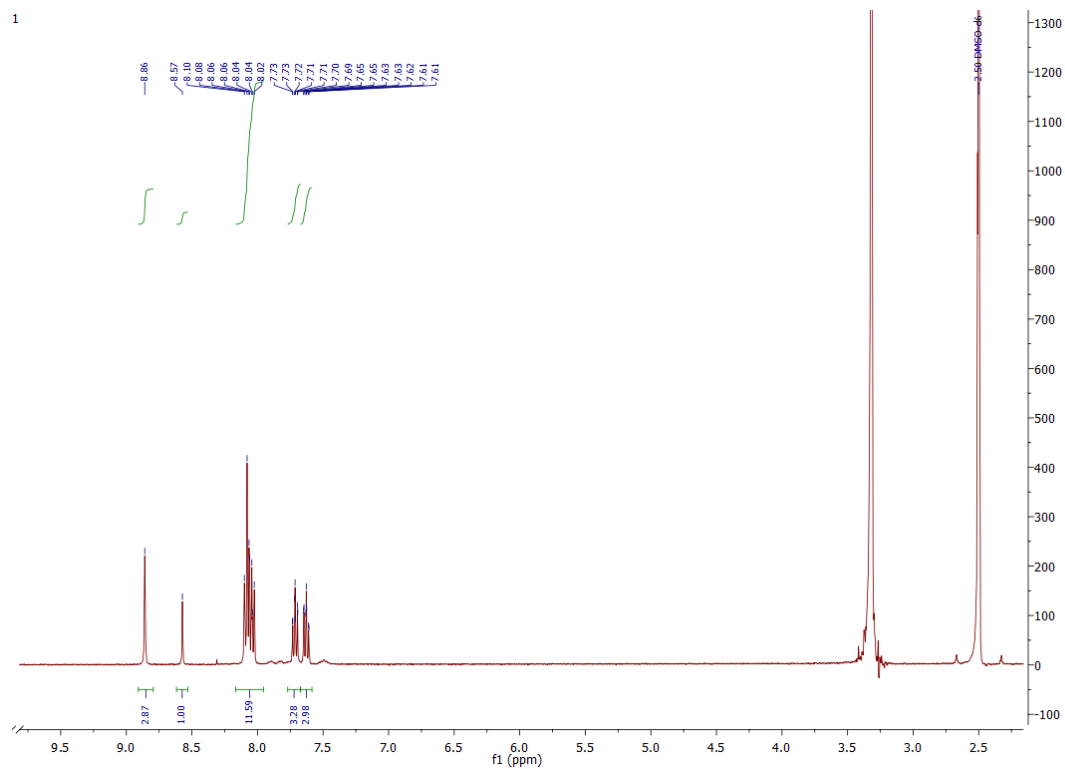


Figure S1 ^1H NMR of the *tnmH* molecule in *d*-DMSO

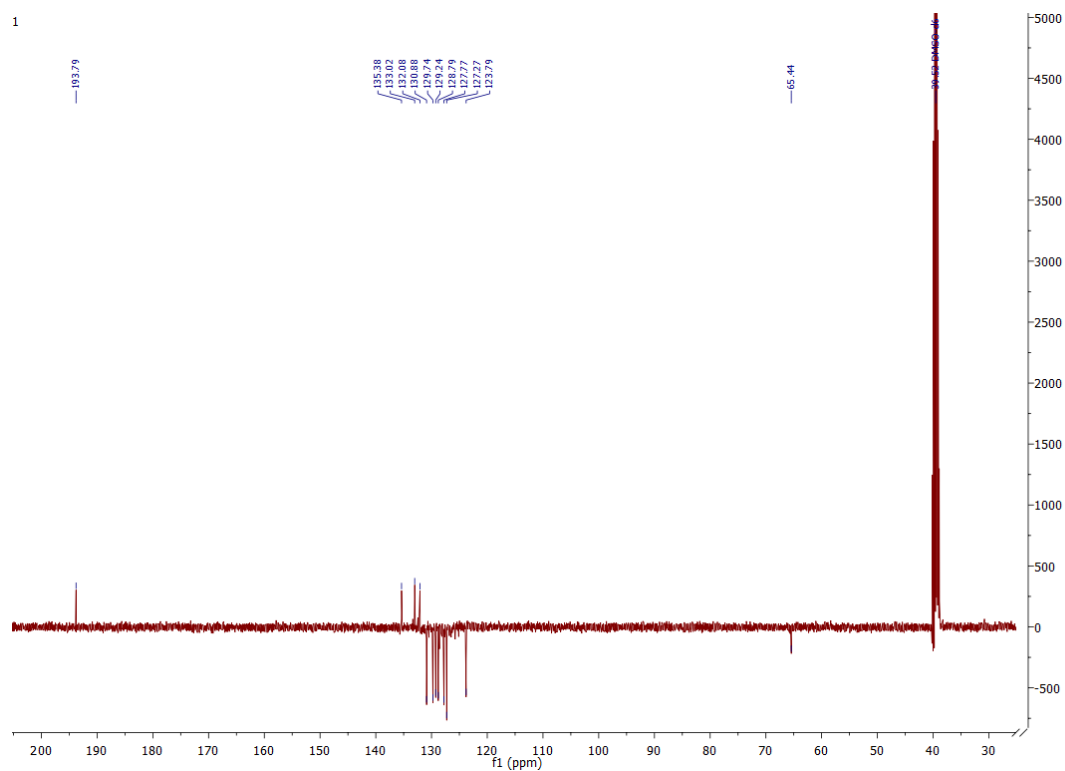


Figure S2 ^{13}C NMR of the *tnmH* molecule in *d*-DMSO

Absorption profiles

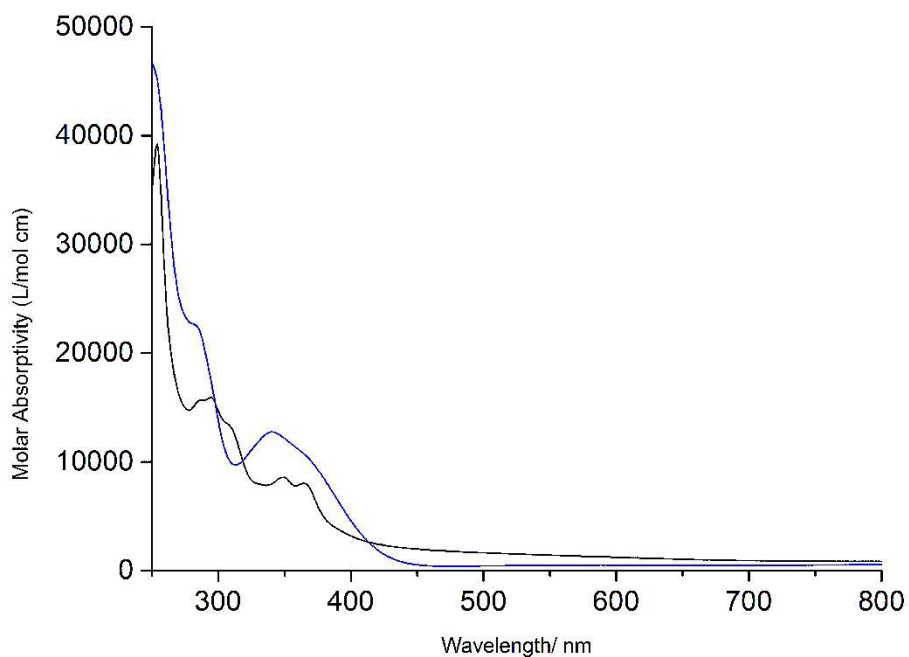


Figure S3 Absorption profiles of **tnmH** (black trace) and **tnm** in excess of KOH (blue trace) from ca. 10^{-5} M solutions in EtOH

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

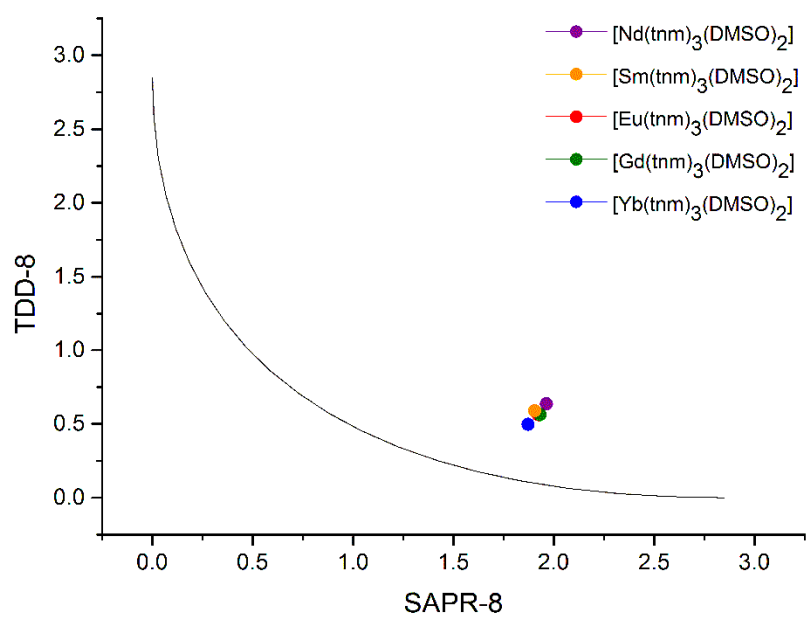


Figure S4. Shape analysis plot for square antiprism (SAPR-8) and triangular dodecahedron (TDD-8) polyhedral.

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

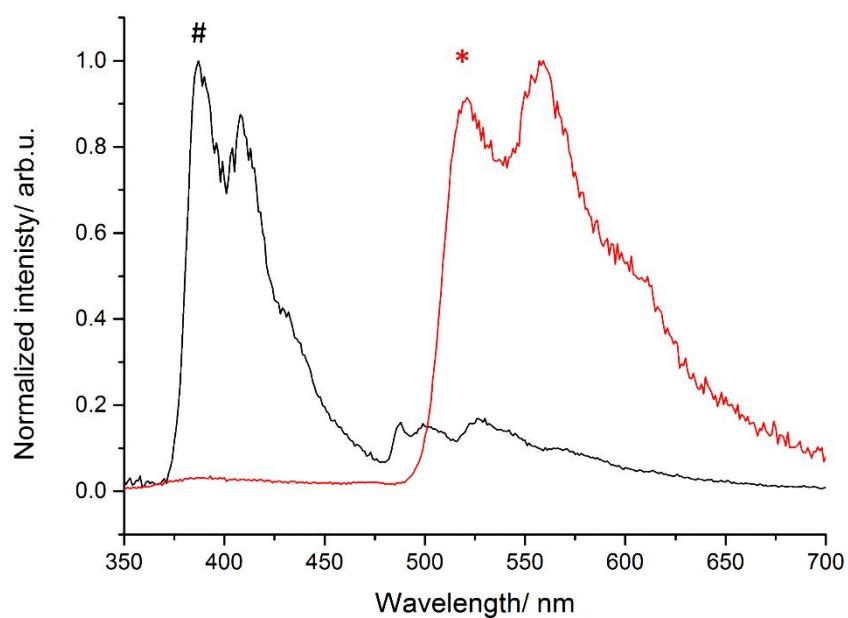


Figure S5. Emission of ligand tnm (black trace) and its Gd^{3+} complex (red trace) in an acetonitrile matrix at 77K. The asterisks denote the estimated position for the 0-phonon transition for the determination of the energy of the singlet state (black) and triplet state (red).

Normalized excitation and emission plots

$\text{Yb}(\text{tnm})_3(\text{DMSO})_2$

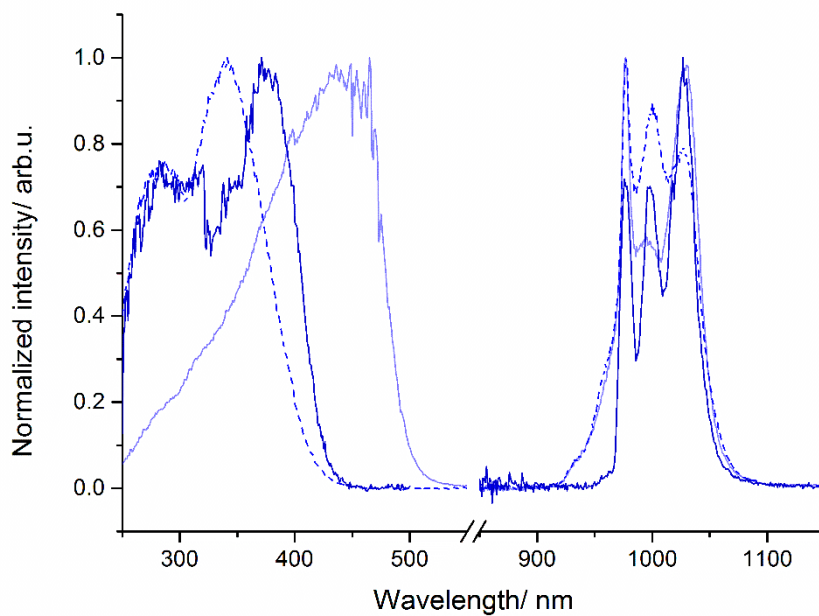


Figure S6. Normalized emission plots for the $\text{Yb}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

$\text{Nd}(\text{tnm})_3(\text{DMSO})_2$

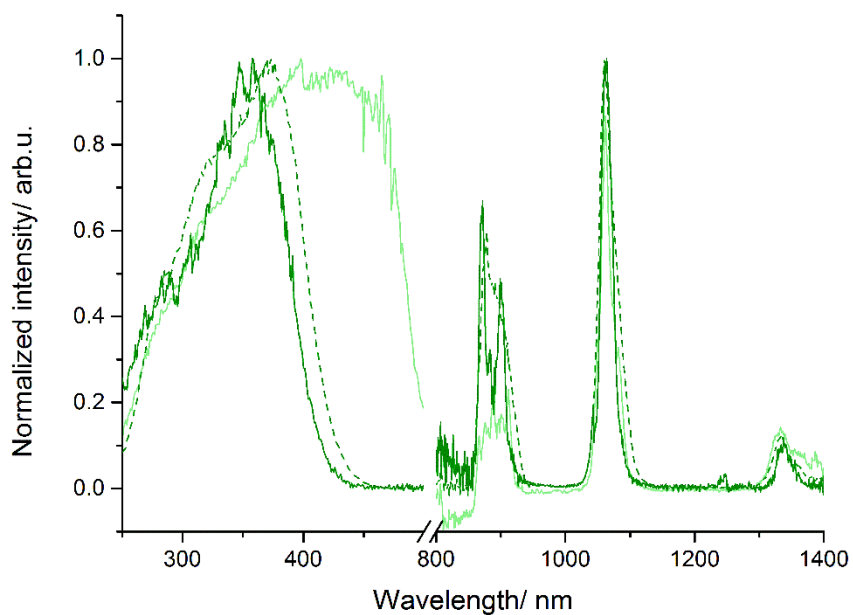


Figure S7. Normalized emission plots for the $\text{Nd}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

$\text{Eu}(\text{tnm})_3(\text{DMSO})_2$

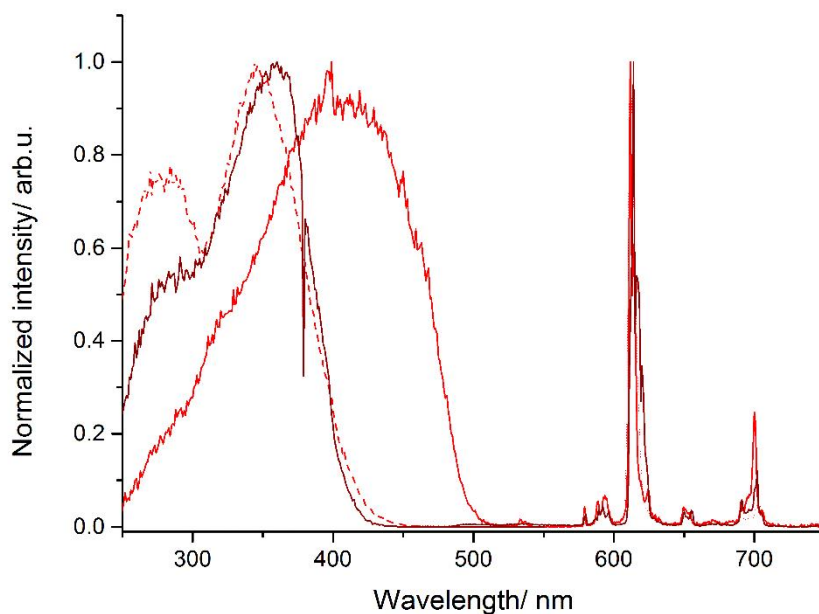


Figure S8. Normalized emission plots for the $\text{Eu}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace) and MeCN at RT (dash trace) and 77K (dark red trace) with excitation wavelength at 350 nm.

$\text{Sm}(\text{tnm})_3(\text{DMSO})_2$

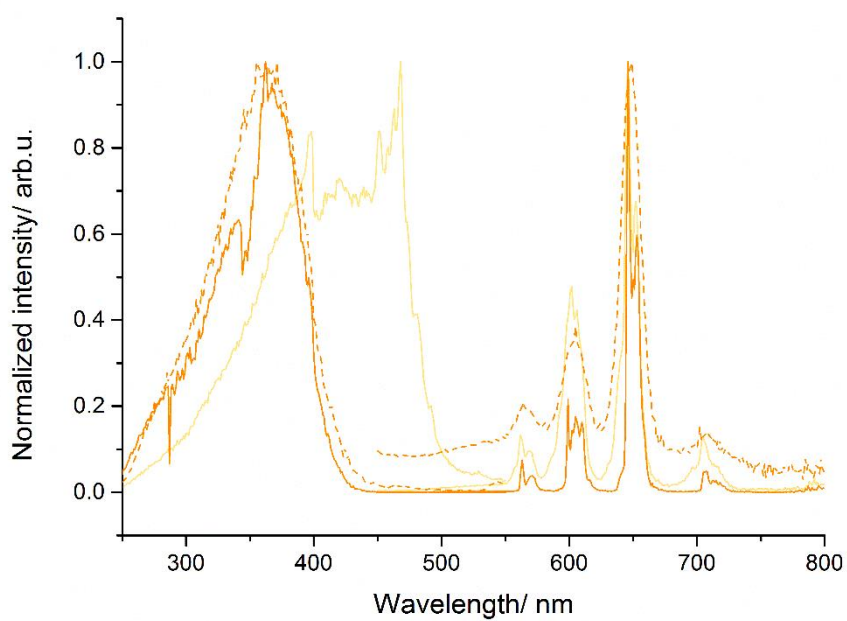


Figure S9. Normalized emission plots for the $\text{Sm}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

Excited state lifetime decay plots

$\text{Yb}(\text{tnm})_3(\text{DMSO})_2$

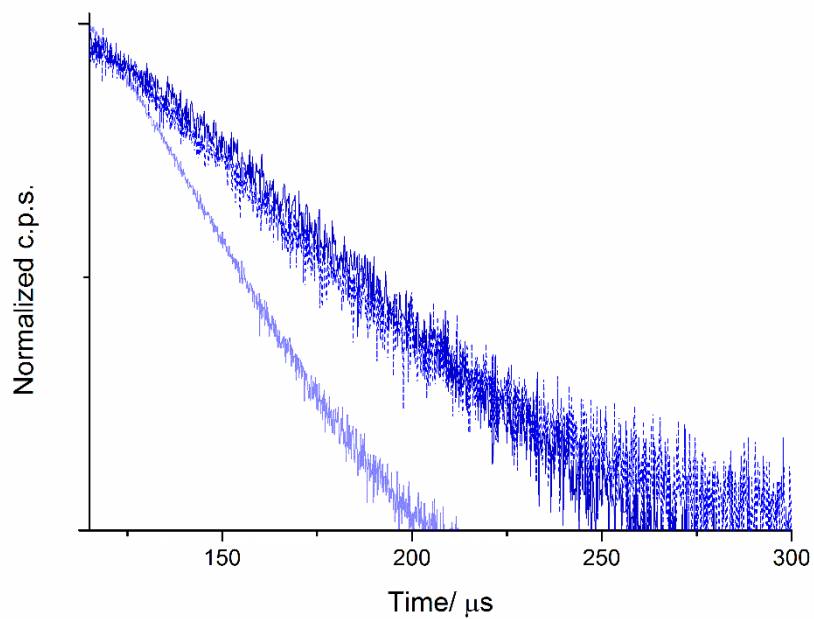


Figure S10. Lifetime decay at 980nm for $\text{Yb}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

$\text{Nd}(\text{tnm})_3(\text{DMSO})_2$

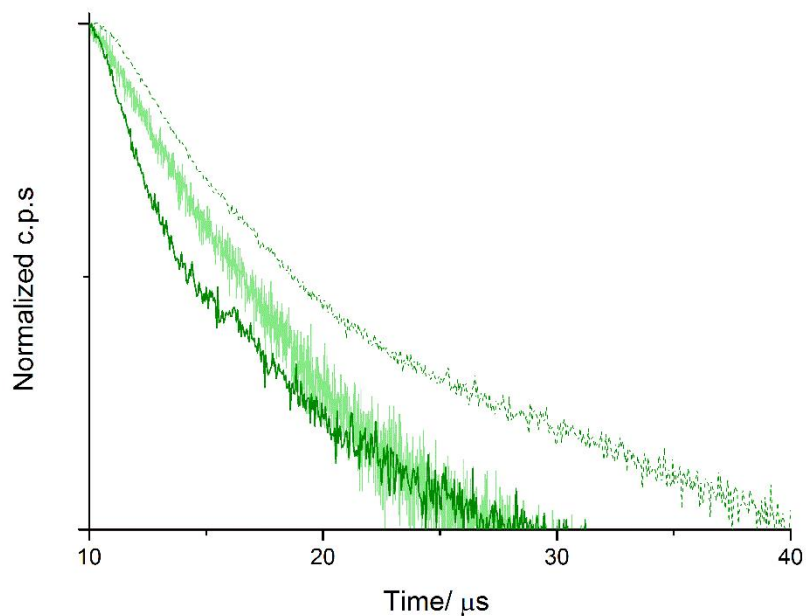


Figure S11. Lifetime decay at 1060nm for $\text{Nd}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.

$\text{Eu}(\text{tnm})_3(\text{DMSO})_2$

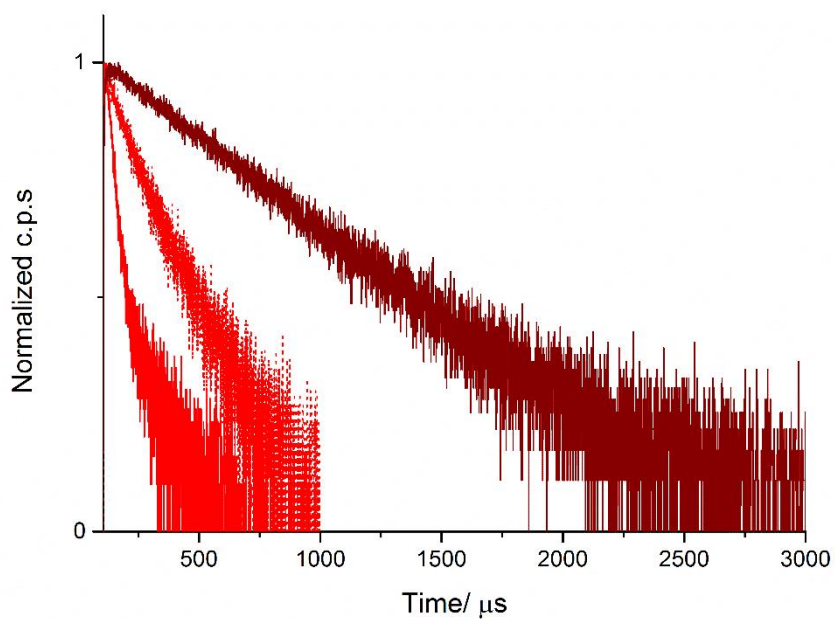


Figure S12. Lifetime decay at 612nm for $\text{Eu}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace) and MeCN at RT (dash trace) and 77K (dark red trace) with excitation wavelength at 350 nm.

$\text{Sm}(\text{tnm})_3(\text{DMSO})_2$

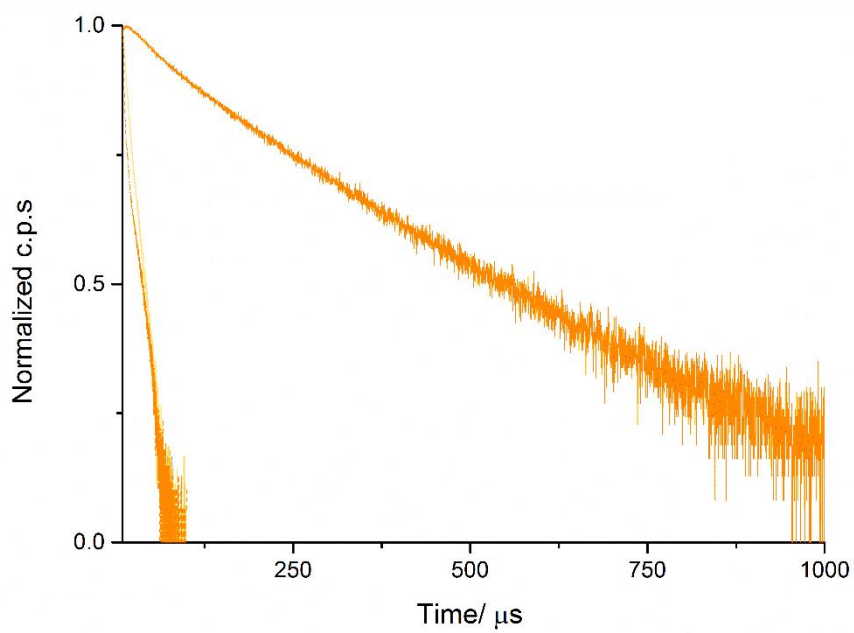


Figure S63. Lifetime decay at 654 nm for $\text{Sm}(\text{tnm})_3(\text{DMSO})_2$ in the solid state (solid trace), MeCN at RT (dash trace) and frozen matrix (dark trace) with excitation wavelength at 350 nm.