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Supporting Information

Lanthanide Complexes Efficacy in Promoting Fibroblast Migration and M2 Macrophage Polarization to Facilitate Wound Healing

Wajid Ali,[a] Fatemeh Jamshidi-Adegani[b], Zahra Mirsanei,[b,c] Juhaina Al-Kindi[b], Saeid Vakilian[b], Sulaiman Al-Hashmi[b], Mohammed Al-Broumi,[a] Jeremy M. Rawson,[d] Ahmed Al-Harrasi,[a*] M. Usman Anwar[a]*

[a]*Natural and Medical Sciences Research Centre, University of Nizwa, P O Box 33, PC 616, Birkat Almouz, Nizwa, Oman. E-mail: usman.anwar@unizwa.edu.om*

[b]Laboratory for Stem Cell & Regenerative Medicine, Natural and Medical Sciences Research Center, University of Nizwa, Nizwa, P. O. Box: 33, PC 616, Oman

[c]Department of Immunology, School of Medicine, Shahid Beheshti University of Medical Sciences, Tehran, Iran

[d]Department of Chemistry and Biochemistry, University of Windsor, 401 Sunset Ave, Windsor, ON, N9B3P4, Canada.

Contents

Table S 1: Crystal data for **1, 2, 4, 6 and 7**.

Compounds	**LH_3**	**1**	**2**	**4**	**6**	**7**
Chemical formula	$C_{11}H_{13}N_3O_4$	$Sm_4C_{68}H_{74}N_{18}O_{26}$	$Eu_4C_{68}H_{74}N_{18}O_{26}$	$Tb_4C_{68}H_{74}N_{18}O_{26}$	$Ho_4C_{68}H_{74}N_{18}O_{26}$	$Er_4C_{68}H_{74}N_{18}O_{26}$
Mr	251.24	2160.85	2165.27	2195.13	2219.17	2228.49
Crystal system, space group	Monoclinic, $P2_1/n$	Triclinic, P-1	Triclinic, P-1	Triclinic, P-1	Triclinic, P-1	Triclinic, P-1
Temperature (K)	296	173	150	173	150	170
a(Å)	9.7938(5)	11.393(2)	11.3839(4)	11.4008(14)	11.3425(5)	11.3514(4),
b(Å)	11.0121(7)	12.080(2)	12.0588(6)	12.1141(15)	12.0765(6)	12.0481(5)
c(Å)	11.4745(7)	14.473(3)	14.4588(7)	14.3980(18)	14.3119(7)	14.3157(5)
α (°)	90	85.37(3)	85.417(2)	85.328(4)	85.430(2)	85.452(2)
β (°)	104.533(2)	75.48(3)	75.454(2)	75.080(4)	74.914(2)	75.0480(10)
γ (°)	90	74.49(3)	74.695(2)	75.079(4)	75.428(2)	75.516(2)
V (Å^3)	1197.93(12)	1857.9(7)	1852.89(15)	1856.4(4)	1831.75(15)	1831.22(12)
Z	2	1	1	1	1	1
μ (mm^{-1})	0.108	3.209	3.434	19.175	4.369	4.632
Radiation type	MoK_α	MoK_α	MoK_α	CuKα	MoK_α	MoK_α
Absorption correction	Multi-scan, SADABS	Multi-scan, SADABS	Multi-scan, SADABS	Multi-scan, SADABS	Multi-scan, SADABS	Multi-scan, SADABS
T_{min}, T_{max}	0.7051, 0.7454	0.66, 0.91	0.6209, 0.7451	0.434, 0.748	0.5722, 0.754	0.5803, 0.7454
No. of measured, independent and observed [I > 2σ(I)] reflections	42527, 2456, 2109	30373, 6539, 4942	48079, 6305, 5157	9002, 2225, 1886	81415, 7475, 5931	34280, 6269, 5079
R_{int}	0.0250	0.0722	0.0418	0.0587	0.0636	0.0481
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.626	0.595	0.588	0.421	0.625	0.589
R[F^2 > 2σ(F^2)], wR(F^2), S	0.0409, 0.1109, 1.032	0.0470, 0.1261, 1.088	0.0610, 0.1955, 0.956	0.0444, 0.1023, 1.069	0.0372, 0.1181, 1.067	0.0367, 0.1069, 1.029
No. of reflections	2456	6539	6305	2225	7475	6269
No. of parameters	175	536	539	536	536	542
No. of restraints	3	567	550	519	1	4
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (eÅ^{-3})	0.250, -0.165	3.327, -1.360	4.787, -2.758	0.514, -0.435	4.232, -1.487	5.788, -1.340
CCDC	2285807	2285808	2285809	2285810	2285811	2285812

Table S 2: UV-Vis data for ligand (LH3) and complexes 1 – 7.

Compounds	Wavenumbers (ε)	Wavenumbers (nm), ε (M^{-1} cm^{-1})
Ligand LH_3	300 nm (9120 M^{-1} cm^{-1})	-
Complex 1	311 nm (144000 M^{-1} cm^{-1})	388 nm (54400 M^{-1} cm^{-1})
Complex 2	312 nm (113400 M^{-1} cm^{-1})	381 nm (37700 M^{-1} cm^{-1})
Complex 3	312 nm (146500 M^{-1} cm^{-1})	388 nm (56300 M^{-1} cm^{-1})
Complex 4	313 nm (125500 M^{-1} cm^{-1})	384 nm (44000 M^{-1} cm^{-1})
Complex 5	313 nm (94300 M^{-1} cm^{-1})	388 nm (35400 M^{-1} cm^{-1})
Complex 6	313 nm (92900 M−1cm−1)	383 nm (35900 M^{-1} cm^{-1})
Complex 7	313 nm (71300 M−1cm−1)	385 nm (30100 M^{-1} cm^{-1})

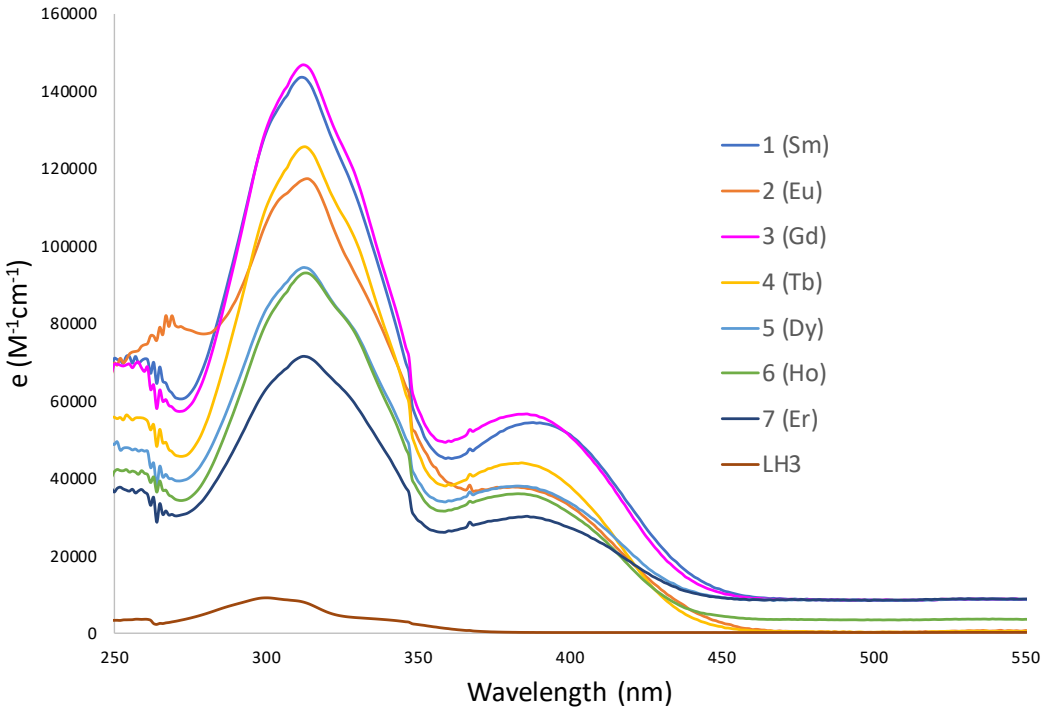

Figure S 1: UV–Vis solution spectra of complex **1** – **7** and free ligand **LH_3** (DMF, rt, concentration 10^{-5} –10^{-6} M).

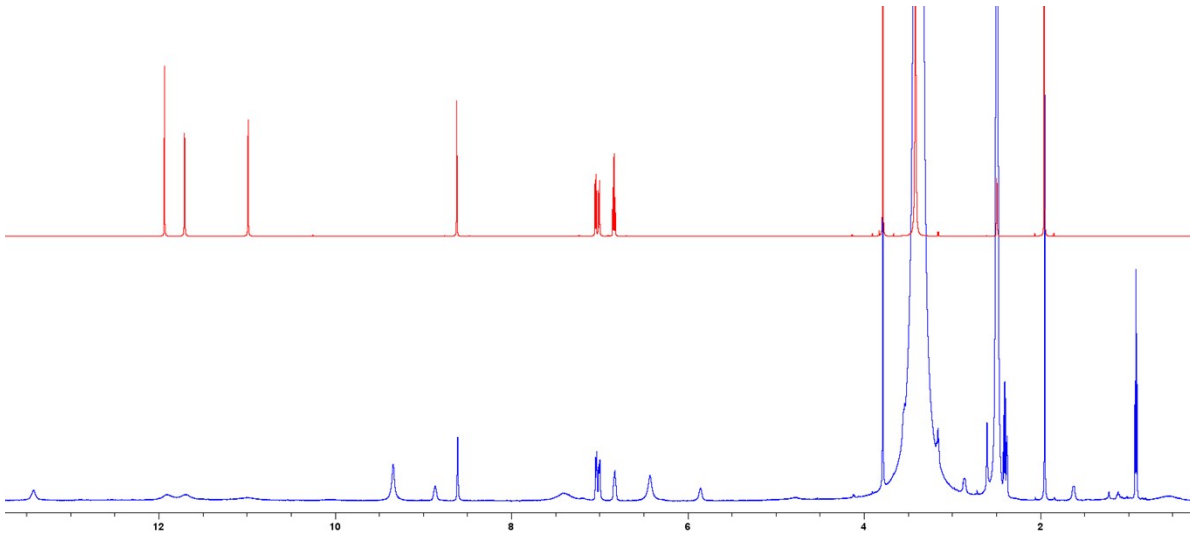

Figure S 2: ^{1}H NMR of ligand **LH_3** (top) and complex **2**(Eu) in DMSO-d_6

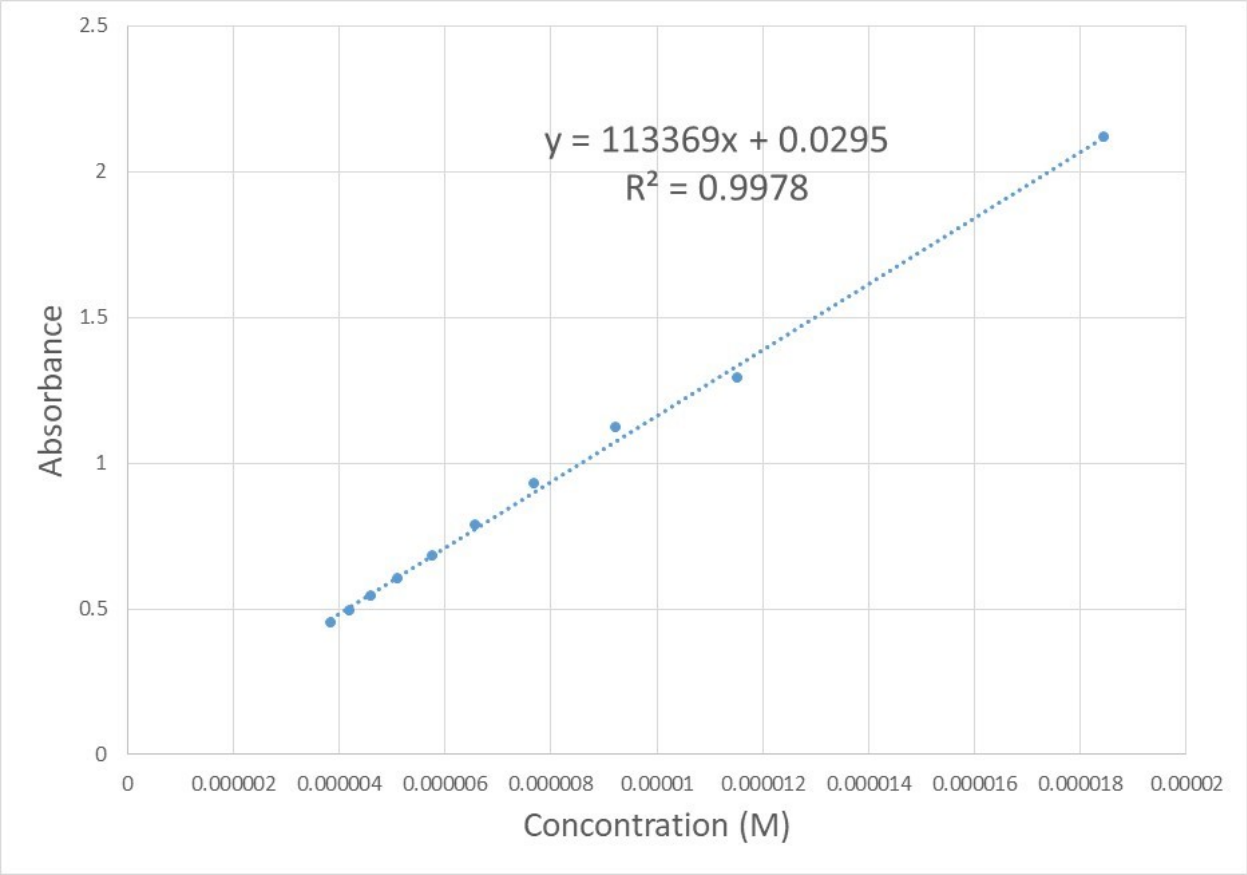

Figure S 3 Variable concentration UV-Vis studies of complex **2** (Eu).

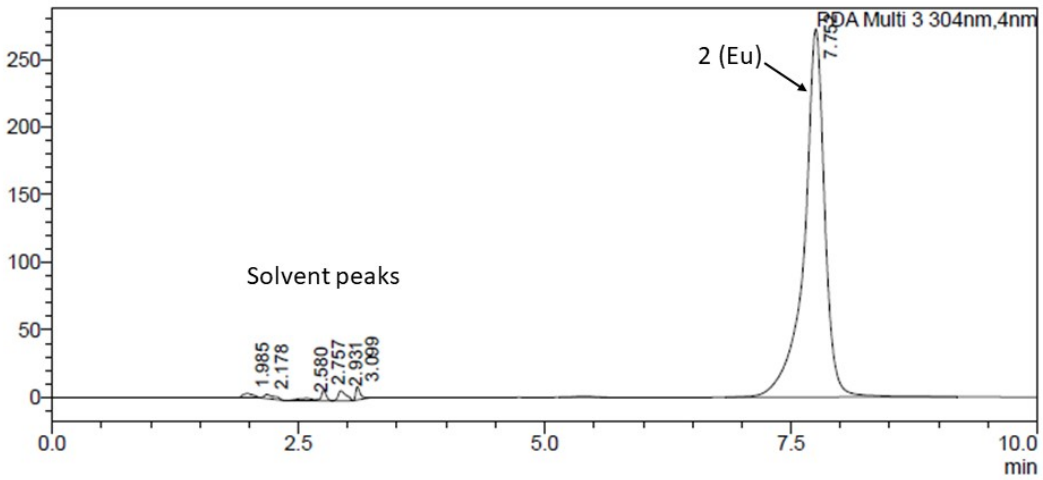

Figure S 4: HPLC chromatogram of **2 (Eu)** incubated in DMSO for 0 – 72 hours.

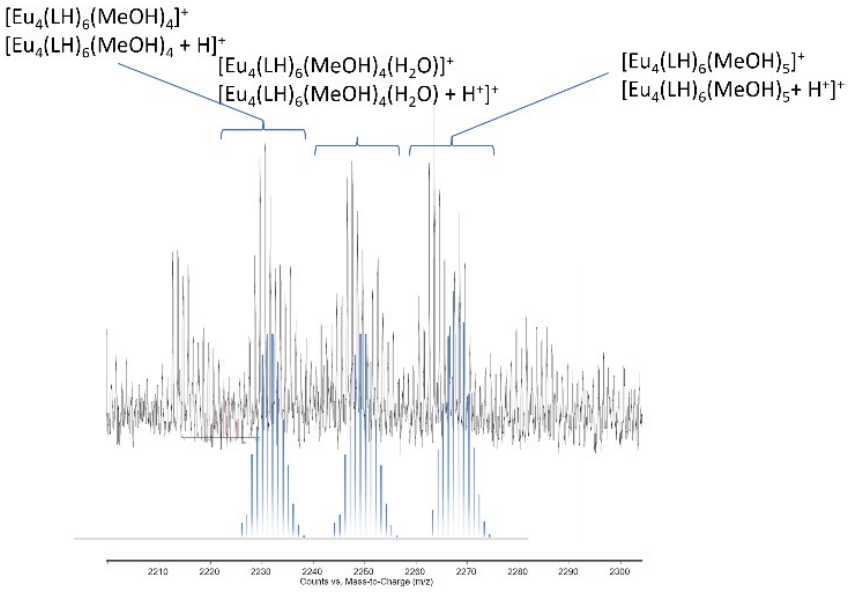

Figure S 5: Mass spectrum (ESI$^+$) for **2(Eu)** (black) revealing the complexity of isotopomers. The blue lines represent the sum of the six molecular ions labelled, as a marker for where the distributions of isotopomers are expected.

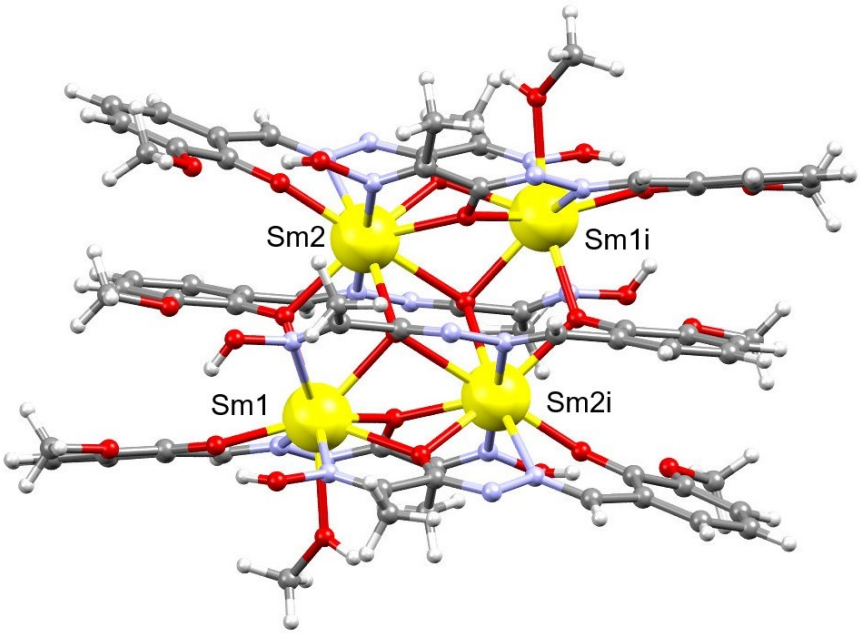

Figure S 6: Molecular structure of **$Sm_4(C_{11}H_{11}N_3O_4)_6(CH_3OH)_2$ (1)**. Color codes: Grey = Carbon; blue = Nitrogen; Red = oxygen.

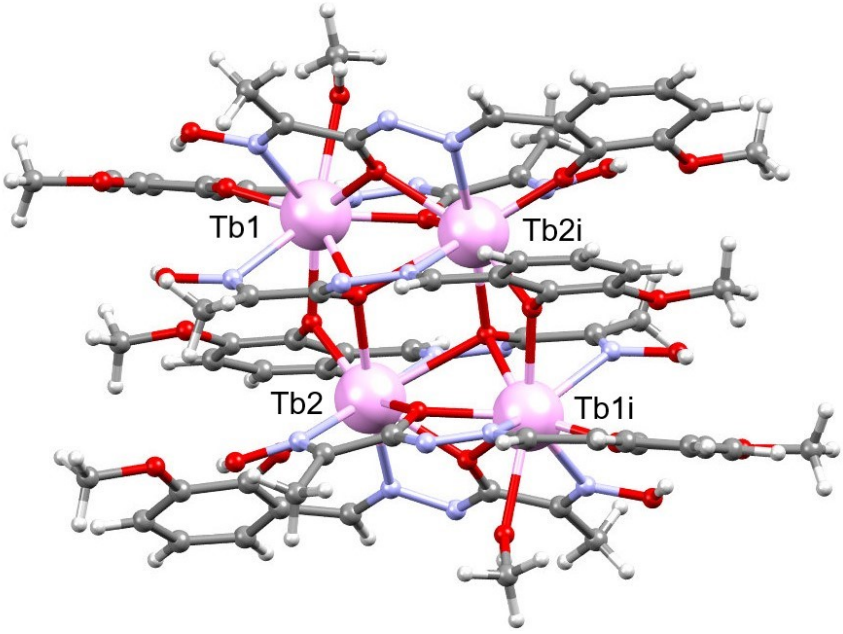

Figure S 7: Molecular structure of **$Tb_4(C_{11}H_{11}N_3O_4)_6(CH_3OH)_2$ (4).** Color codes: Grey = Carbon; blue = Nitrogen; Red = oxygen.

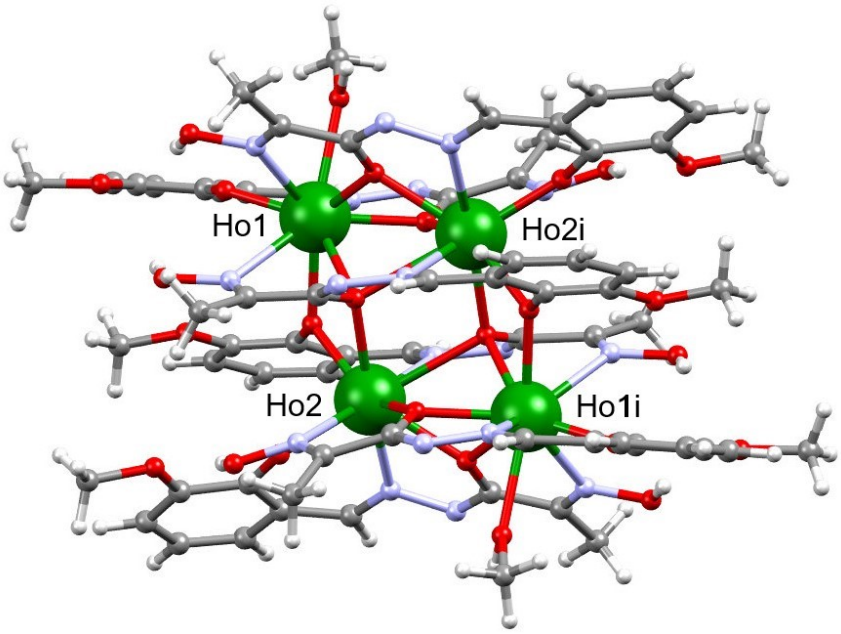

Figure S 8: Molecular structure of **$Ho_4(C_{11}H_{11}N_3O_4)_6(CH_3OH)_2$ (6).** Color codes: Grey = Carbon; blue = Nitrogen; Red = oxygen.

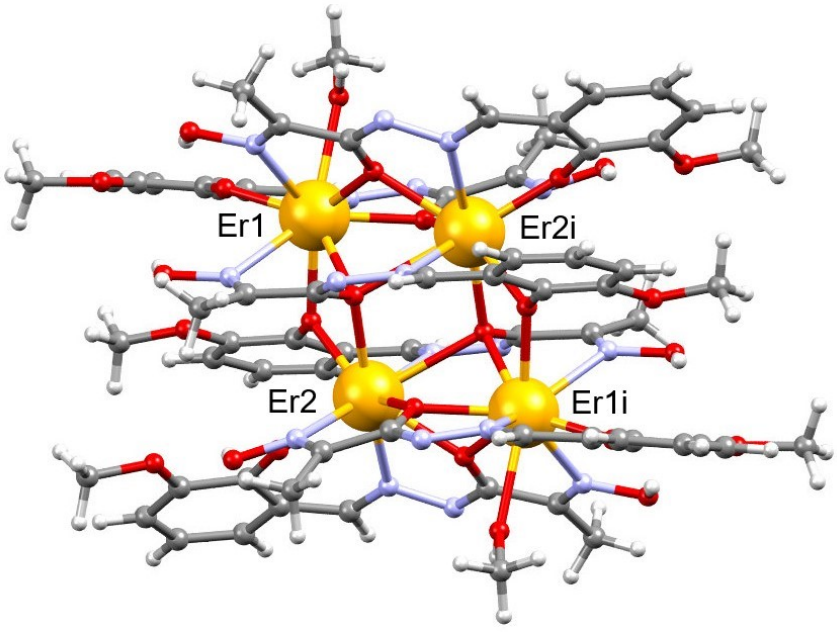

Figure S 9: Molecular structure of **$Er_4(C_{11}H_{11}N_3O_4)_6(CH_3OH)_2$ (7).** Color codes: Grey = Carbon; blue = Nitrogen; Red = oxygen.