Enhanced E/Z-Photoisomerization and Luminescence of Stilbene Derivative Co-coordinated in Di-β-Diketonate Lanthanide Complexes

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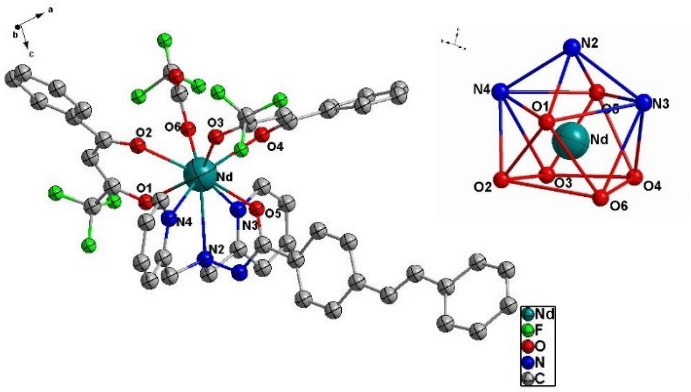


Figure S1. The Crystal structure and coordination polyhedron (inset) geometry of complex **2** ([Nd(tfd)$_2$(HL)(CF$_3$CO$_2$)]).

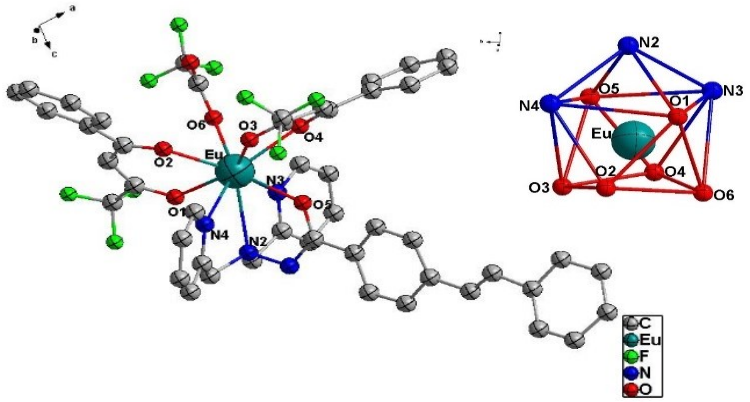


Figure S2. The Crystal structure and coordination polyhedron (inset) geometry of complex **3** ([Eu(tfd)$_2$(HL)(CF$_3$CO$_2$)]).

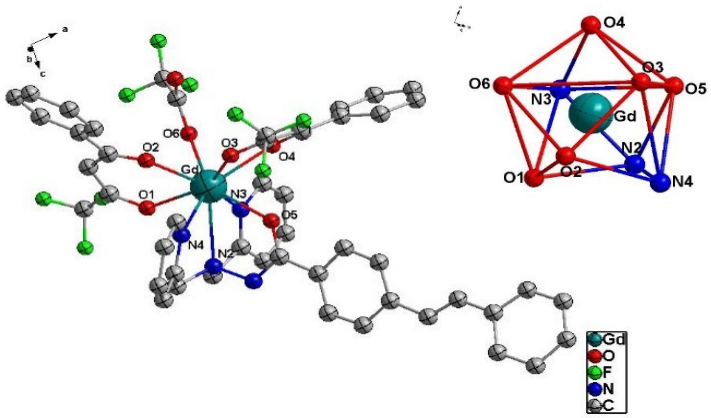


Figure S3. The Crystal structure and coordination polyhedron (inset) geometry of complex **4** ([Gd(tfd)$_2$(HL)(CF$_3$CO$_2$)]).

Table S1. Selected bond lengths (Å) of complexes 1–5.

$[La(tfd)_2HL(CF_3CO_2)]$		$[Nd(tfd)_2HL(CF_3CO_2)]$		$[Eu(tfd)_2HL(CF_3CO_2)]$		$[Gd(tfd)_2HL(CF_3CO_2)]$		$[Yb(tfd)_2L]$	
Bond lengths (Å)		Bond lengths (Å)		Bond lengths (Å)		Bond lengths (Å)		Bond lengths (Å)	
La01-O1	2.352(3)	Nd01-O1	2.414(4)	Eu01-O1	2.346(5)	Gd01-O1	2.365(76)	Yb01-O1	2.230(2)
La01-O2	2.373(3)	Nd01-O2	2.451(5)	Eu01-O2	2.372(4)	Gd01-O2	2.379(61)	Yb01-O2	2.332(2)
La01-O3	2.361(3)	Nd01-O3	2.414(5)	Eu01-O3	2.363(5)	Gd01-O3	2.369(81)	Yb01-O3	2.225(2)
La01-O4	2.423(4)	Nd01-O4	2.467(7)	Eu01-O4	2.396(5)	Gd01-O4	2.425(77)	Yb01-O4	2.296(2)
La01-O5	2.390(3)	Nd01-O5	2.434(5)	Eu01-O5	2.387(5)	Gd01-O5	2.382(70)	Yb01-O5	2.203(2)
La01-O6	2.380(4)	Nd01-O6	2.467(5)	Eu01-O6	2.339(5)	Gd01-O6	2.362(77)	Yb01-N2	2.504(3)
La01-N2	2.753(4)	Nd01-N2	2.818(7)	Eu01-N2	2.749(6)	Gd01-N2	2.758(103)	Yb01-N3	2.467(3)
La01-N3	2.624(4)	Nd01-N3	2.688(6)	Eu01-N3	2.631(6)	Gd01-N3	2.649(97)	Yb01-N4	2.546(3)
La01-N4	2.639(4)	Nd01-N4	2.692(6)	Eu01-N4	2.644(6)	Gd01-N3	2.631(106)	N1-N2	1.478(34)
N1-N2	1.425(45)	N1-N2	1.428(84)	N1-N2	1.407(85)	N1-N2	1.429(127)	C33-O5	1.291(4)
C33-O5	1.240(5)	C33-O5	1.230(9)	C33-O5	1.243(7)	C33-O5	1.246(12)	C33-N1	1.307(4)
C33-N1	1.334(6)	C33-N1	1.341(9)	C33-N1	1.322(9)	C33-N1	1.341(9)		

* O1,O2 and O3, O4 are from the two 4,4,4-Trifluoro-1-phenylbutane-1,3-dionates, O6 is from trifluoroacetate, O5 and N2 are from benzohydazide and N3, N4 are from pyridines of HL ligand.

Table S2. Selected angles(deg) of complexes **1**, **2** and **3**.

$[La(tfd)_2HL(CF_3CO_2)]$ (1)		$[Nd(tfd)_2HL(CF_3CO_2)]$ (2)		$[Eu(tfd)_2HL(CF_3CO_2)]$ (3)	
Angles		Angles		Angles	
O2—La01—O5	135.41 (13)	O3—Nd01—O1	143.22 (16)	O6—Eu01—O1	74.60 (17)
O2—La01—O4	121.73 (12)	O3—Nd01—O2	73.36 (16)	O6—Eu01—O3	104.53 (17)
O2—La01—N4	143.99 (12)	O1—Nd01—O2	70.78 (16)	O1—Eu01—O3	142.42 (17)
O2—La01—O6	77.73 (12)	O3—Nd01—O5	73.21 (18)	O6—Eu01—O2	76.54 (17)
O2—La01—N3	69.67 (12)	O1—Nd01—O5	129.95 (17)	O1—Eu01—O2	71.39 (16)
O2—La01—N2	118.87 (12)	O2—Nd01—O5	134.70 (18)	O3—Eu01—O2	71.97 (17)
O1—La01—O2	71.37 (12)	O3—Nd01—O4	70.10 (17)	O6—Eu01—O5	140.20 (18)
O1—La01—O5	130.70 (12)	O1—Nd01—O4	138.87 (18)	O1—Eu01—O5	131.12 (16)
O1—La01—O4	138.37 (13)	O2—Nd01—O4	122.93 (17)	O3—Eu01—O5	73.56 (17)
O1—La01—O3	142.78 (12)	O5—Nd01—O4	71.24 (17)	O2—Eu01—O5	135.26 (17)
O1—La01—N4	76.68 (12)	O3—Nd01—O6	110.54 (18)	O6—Eu01—O4	71.69 (17)
O1—La01—O6	74.21 (12)	O1—Nd01—O6	72.08 (18)	O1—Eu01—O4	138.41 (17)
O1—La01—N3	84.01 (13)	O2—Nd01—O6	81.62 (18)	O3—Eu01—O4	70.81 (18)
O1—La01—N2	69.42 (12)	O5—Nd01—O6	139.15 (18)	O2—Eu01—O4	121.90 (17)
O5—La01—O4	70.79 (12)	O4—Nd01—O6	72.35 (17)	O5—Eu01—O4	70.32 (17)
O5—La01—N4	78.91 (13)	O3—Nd01—N3	139.71 (17)	O6—Eu01—N3	79.20 (18)
O5—La01—N3	74.79 (13)	O1—Nd01—N3	77.07 (16)	O1—Eu01—N3	76.51 (17)
O5—La01—N2	61.32 (12)	O2—Nd01—N3	144.99 (16)	O3—Eu01—N3	140.96 (18)
O4—La01—N4	73.91 (13)	O5—Nd01—N3	77.55 (18)	O2—Eu01—N3	143.78 (17)
O4—La01—N3	137.12 (13)	O4—Nd01—N3	74.65 (17)	O5—Eu01—N3	79.35 (18)
O4—La01—N2	118.88 (12)	O6—Nd01—N3	75.5 (2)	O4—Eu01—N3	73.90 (18)
O3—La01—O2	72.29 (12)	O3—Nd01—N4	75.61 (17)	O6—Eu01—N4	144.77 (17)
O3—La01—O5	73.78 (12)	O1—Nd01—N4	84.21 (17)	O1—Eu01—N4	84.21 (17)
O3—La01—O4	70.36 (13)	O2—Nd01—N4	69.11 (18)	O3—Eu01—N4	75.83 (18)
O3—La01—N4	140.42 (13)	O5—Nd01—N4	73.62 (18)	O2—Eu01—N4	70.09 (17)
O3—La01—O6	105.56 (13)	O4—Nd01—N4	136.35 (17)	O5—Eu01—N4	74.51 (17)
O3—La01—N3	76.12 (13)	O6—Nd01—N4	147.20 (18)	O4—Eu01—N4	136.79 (18)
O3—La01—N2	123.75 (12)	N3—Nd01—N4	121.52 (19)	N3—Eu01—N4	123.12 (19)
N4—La01—N2	62.00 (13)	O3—Nd01—N2	122.42 (18)	O6—Eu01—N2	131.76 (16)
O6—La01—O5	139.72 (13)	O1—Nd01—N2	69.43 (18)	O1—Eu01—N2	69.63 (16)
O6—La01—O4	71.34 (12)	O2—Nd01—N2	117.25 (17)	O3—Eu01—N2	123.57 (16)
O6—La01—N4	77.96 (14)	O5—Nd01—N2	60.56 (18)	O2—Eu01—N2	119.12 (17)
O6—La01—N3	145.23 (13)	O4—Nd01—N2	119.12 (18)	O5—Eu01—N2	61.52 (17)
O6—La01—N2	130.49 (12)	O6—Nd01—N2	126.71 (19)	O4—Eu01—N2	118.44 (17)
N3—La01—N4	123.33 (14)	N3—Nd01—N2	61.07 (18)	N3—Eu01—N2	61.94 (17)
N3—La01—N2	61.34 (13)	N4—Nd01—N2	60.46 (19)	N4—Eu01—N2	61.18 (16)

Table S3. Selected angles(deg) of complexes **4** and **5**.

$[Gd(tfd)_2HL(CF_3CO_2)]$ (4)		$[Yb(tfd)_2L]$ (5)	
Angles		Angles	
O1—Gd01—O5	131.3 (2)	O5—Yb01—O3	102.20 (8)
O1—Gd01—O3	142.8 (3)	O5—Yb01—O1	138.43 (8)
O1—Gd01—O2	71.7 (2)	O3—Yb01—O1	99.71 (8)
O1—Gd01—O4	137.7 (3)	O5—Yb01—O4	75.03 (8)
O1—Gd01—N3	76.4 (3)	O3—Yb01—O4	75.27 (8)
O1—Gd01—N4	84.6 (3)	O1—Yb01—O4	145.30 (8)
O1—Gd01—N2	69.6 (3)	O5—Yb01—O2	146.94 (8)
O5—Gd01—O4	71.1 (3)	O3—Yb01—O2	77.04 (8)
O5—Gd01—N3	79.8 (3)	O1—Yb01—O2	72.58 (8)
O5—Gd01—N4	74.6 (3)	O4—Yb01—O2	72.85 (8)
O5—Gd01—N2	61.7 (2)	O5—Yb01—N3	85.12 (8)
O3—Gd01—O5	73.8 (3)	O3—Yb01—N3	150.95 (8)
O3—Gd01—O2	71.8 (2)	O1—Yb01—N3	92.46 (8)
O3—Gd01—O4	70.3 (3)	O4—Yb01—N3	79.71 (8)
O3—Gd01—N3	140.6 (3)	O2—Yb01—N3	81.70 (8)
O3—Gd01—N4	76.3 (3)	O5—Yb01—N2	67.97 (8)
O3—Gd01—N2	124.4 (3)	O3—Yb01—N2	141.43 (8)
O6—Gd01—O1	73.7 (3)	O1—Yb01—N2	72.83 (8)
O6—Gd01—O5	140.4 (3)	O4—Yb01—N2	131.65 (8)
O6—Gd01—O3	104.6 (3)	O2—Yb01—N2	131.85 (8)
O6—Gd01—O2	77.2 (3)	N3—Yb01—N2	67.44 (9)
O6—Gd01—O4	71.3 (3)	O5—Yb01—N4	77.37 (8)
O6—Gd01—N3	78.1 (3)	O3—Yb01—N4	75.28 (8)
O6—Gd01—N4	144.6 (3)	O1—Yb01—N4	74.66 (8)
O6—Gd01—N2	130.8 (3)	O4—Yb01—N4	133.78 (8)
O2—Gd01—O5	134.8 (3)	O2—Yb01—N4	132.19 (8)
O2—Gd01—O4	121.4 (2)	N3—Yb01—N4	133.65 (9)
O2—Gd01—N3	143.9 (3)	N2—Yb00—N4	66.22 (9)
O2—Gd01—N4	69.5 (3)		
O2—Gd01—N2	119.0 (3)		
O4—Gd01—N3	73.8 (3)		
O4—Gd01—N4	137.3 (3)		
O4—Gd01—N2	119.1 (3)		
N3—Gd01—N2	62.3 (3)		
N4—Gd01—N3	123.9 (3)		
N4—Gd01—N2	61.6 (3)		

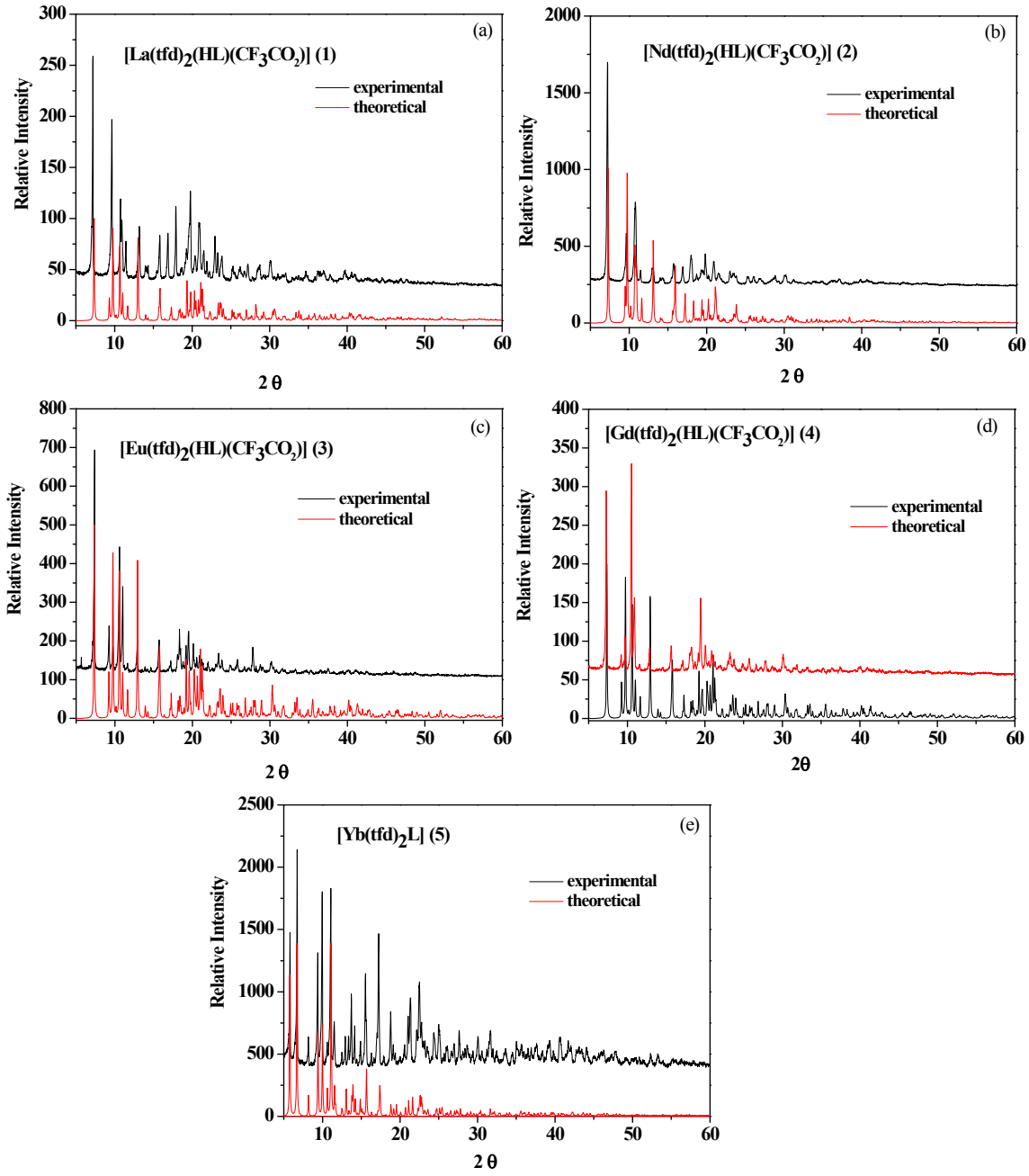


Figure S4. Observed (black) and calculated (red) X-ray powder diffraction patterns of complexes 1–5.

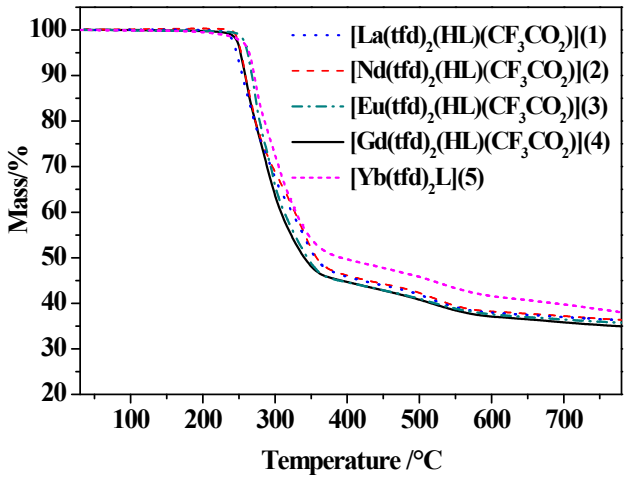


Figure S5. Thermogravimetric analysis (TGA) curves of complexes **1** (blue dot), **2** (red dash), **3** (dark cyan dash dot), **4** (balck solid) and **5** (magenta short dash).

Table S4. UV-vis absorption spectral data of Htfd， HL and complexes **1**–**5** in acetonitrile solutions.

Compounds	λ_{max}[nm]/ε_{max}[10^4 $Lmol^{-1}cm^{-1}$]	
Htfd	326/2.0	256/0.7
HL	317/5.1	263/1.8
1	325/2.0	257/3.4
2	324/4.9	257/2.8
3	327/2.1	257/3.0
4	324/5.0	257/2.7
5	320/19.3	263/7.1

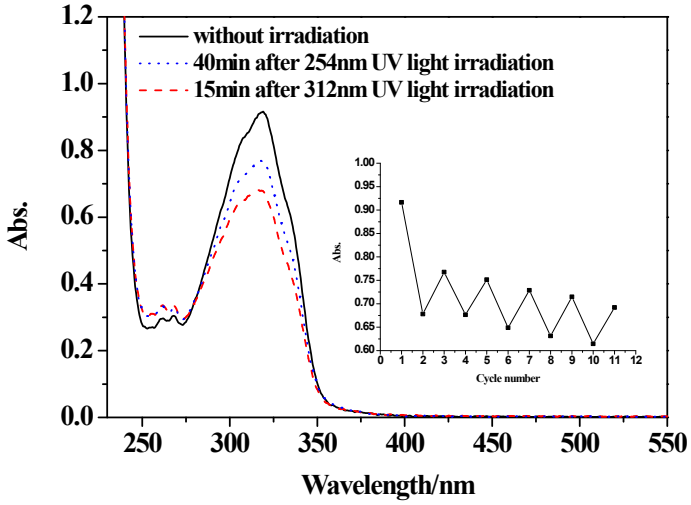


Figure S6. UV spectral changes of HL ligand in acetonitirle solution (2.0×10^{-5} mol/L) by the irradiation of UV light at 312 nm and 254 nm. Inset shows 5 cycles of the maximum absorption intensity at 317 nm alternatively modulated by the irradiation of UV light at 312 nm and 254 nm.

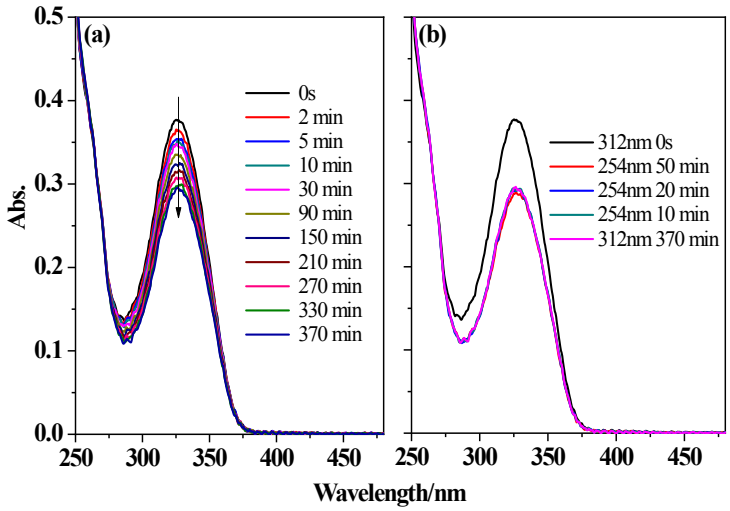


Figure S7. UV spectral changes of complex **1** in acetonitrile solution (2.0×10^{-5} mol/L) upon irradiation at UV 312 nm (a) and recoverable irradiation at UV 254 nm (b) as a function of time.

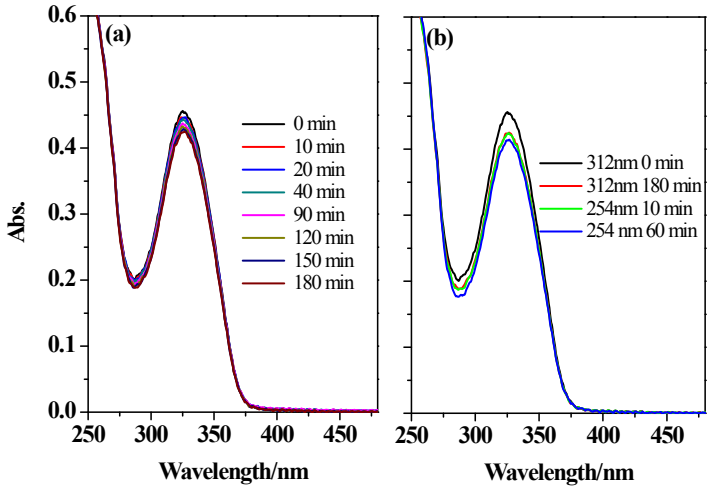


Figure S8. UV spectral changes of complex **3** in acetonitrile solutions (2.0×10^{-5} mol/L) upon irradiation at UV 312 nm (a) and recoverable irradiation at UV 254 nm (b) as a function of time.

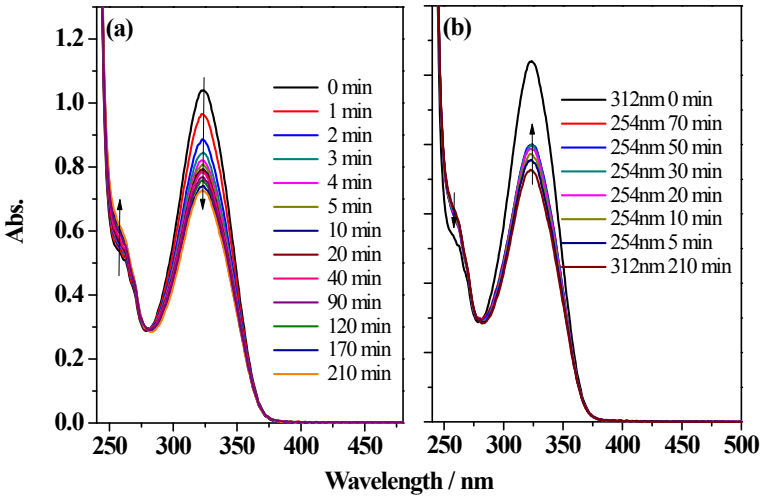


Figure S9. UV spectral changes of complex **4** in acetonitrile solutions (2.0×10^{-5} mol/L) upon irradiation at UV 312 nm (a) and recoverable irradiation at UV 254 nm (b) as a function of time.

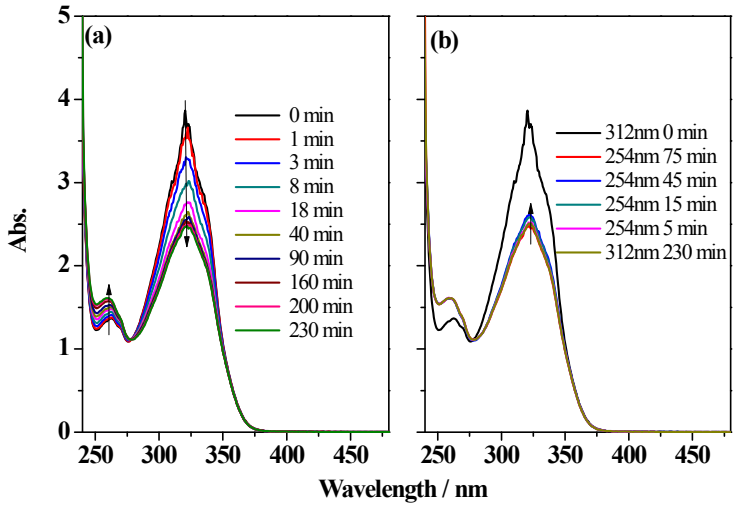


Figure S10. UV spectral changes of complex **5** in acetonitrile solutions (2.0×10^{-5} mol/L) upon irradiation at UV 312 nm (a) and recoverable irradiation at UV 254 nm (b) as a function of time.

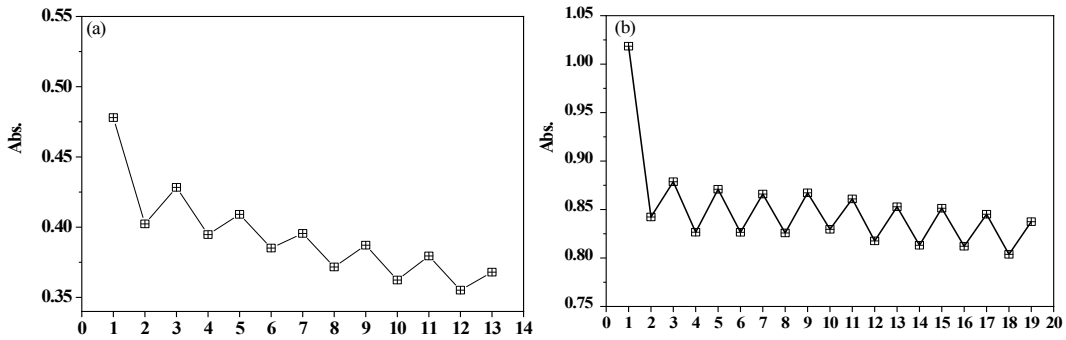


Figure S11. Cycles of the absorption intensity at 324 nm of complexes **1** (a) and **4** (b) in ethanol and acetonitrile solution (2.0×10^{-5} mol/L) alternatively modulated by the irradiation of UV light at 312 nm and 254 nm.

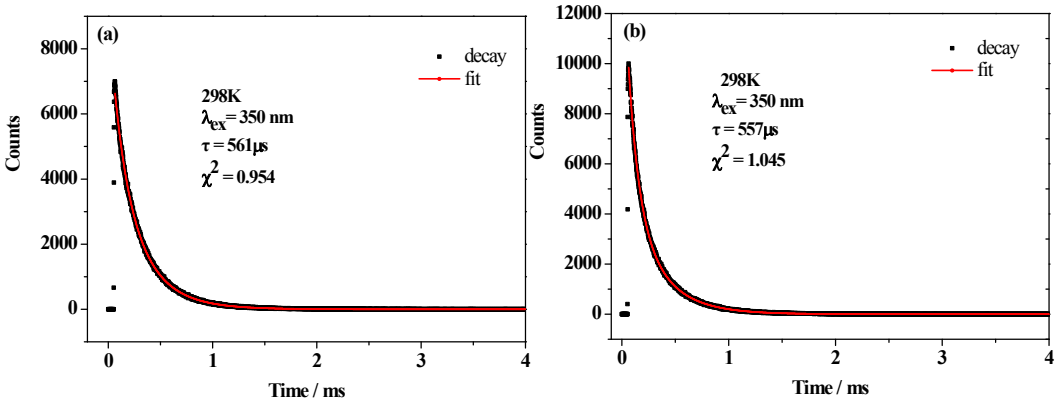


Figure S12. Luminescence decay curves of complex 3 in acetonitrile solution (a) and in solid (b)

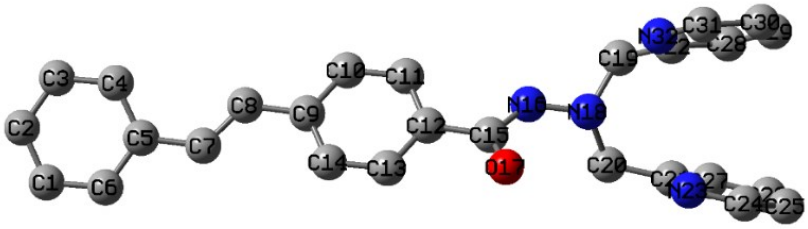


Figure S13. Structure diagram of ligand HL after optimization by CAM-B3LYP.

Table S5. Bond lengths(Å) and angles(º) of HL optimized by three methods

Bond	Bond lengths (Å)			Bond	Bond angle (º)		
	CAM-B3LYP	B3LYP	PBE0		CAM-B3LYP	B3LYP	PBE0
C_7-C_8	1.340	1.350	1.361	C_5-C_7-C_8	126.73	127.00	126.98
C_{15}-N_{16}	1.367	1.370	1.383	N_{16}-N_{18}-C_{19}	110.80	110.75	109.74
C_{15}-O_{17}	1.223	1.220	1.239	C_{15}-N_{16}-N_{18}	120.29	120.42	119.89
N_{16}-N_{18}	1.395	1.402	1.407	O_{17}-C_{15}-N_{16}	123.36	123.38	123.27
C_4-C_5	1.402	1.410	1.418	C_{19}-C_{22}-N_{32}	116.28	116.31	116.10
N_{18}-C_{19}	1.466	1.476	1.479	C_{20}-C_{21}-N_{23}	116.81	116.69	116.65
C_{19}-N_{32}	1.338	1.345	1.353	C_7-C_8-C_9	126.44	126.67	126.69

Table S6. Selected bond lengths(Å) and angles(º) of complex **1** determined by X-ray diffraction and optimized by three different functional

Bond	Bond length (nm)				Bond	Bond angles (º)			
	measured	CAM-B3LYP	B3LYP	PBE0		measured	CAM-B3LYP	B3LYP	PBE0
La-O_1	2.352	2.484	2.507	2.501	O_1-La-O_2	71.37	68.19	68.51	69.00
La-O_2	2.373	2.480	2.490	2.483	O_1-La-O_5	130.70	123.86	123.78	123.77
La-O_6	2.380	2.445	2.453	2.437	O_1-La-O_6	74.21	79.15	78.78	78.97
La-O_3	2.361	2.451	2.474	2.469	O_1-La-N_2	69.42	65.11	65.41	64.66
La-O_4	2.422	2.527	2.537	2.527	O_5-La-O_4	70.79	72.40	73.33	72.94
La-O_5	2.390	2.566	2.583	2.573	O_5-La-N_2	61.32	58.82	58.45	59.23
La-N_2	2.752	2.955	2.988	2.963	O_4-La-N_2	118.88	121.41	122.28	121.91
La-N_3	2.643	2.829	2.864	2.848	N_4-La-N_2	62.00	59.24	58.91	59.11
La-N_4	2.640	2.775	2.809	2.793	O_6-La-O_5	139.72	136.22	136.68	137.16
C_{40}-C_{41}	1.201	1.340	1.351	1.362	O_6-La-N_2	130.49	124.20	124.19	124.01
C_{41}-C_{42}	1.410	1.468	1.466	1.464	N_3-La-N_4	123.33	117.48	116.93	117.29
C_{40}-C_{37}	1.509	1.467	1.464	1.462	C_{40}-C_{41}-C_{42}	125.70	126.73	127.05	127.06
					C_{41}-C_{40}-C_{37}	129.40	126.19	126.52	126.49

Table S7. Selected bond lengths(Å) and angles(º) for complex 3 determined by X-ray diffraction and optimized by three different functional

Bond lengths (nm)					Bond angles (º)				
Bond	measured	CAM-B3LYP	B3LYP	PBE0	Bond	measured	CAM-B3LYP	B3LYP	PBE0
Eu-O_1	2.346	2.361	2.375	2.372	O_6-Eu-O_1	74.60	76.37	76.62	76.56
Eu-O_2	2.372	2.376	2.392	2.387	O_1-Eu-O_2	71.39	71.18	71.62	71.88
Eu-O_3	2.363	2.341	2.380	2.400	O_1-Eu-O_5	131.12	125.84	126.06	126.49
Eu-O_4	2.396	2.422	2.425	2.409	O_5-Eu-O_4	70.32	72.89	73.70	73.82
Eu-O_5	2.387	2.444	2.466	2.468	O_5-Eu-O_6	140.20	137.86	139.17	139.76
Eu-O_6	2.339	2.346	2.339	2.330	O_1-Eu-N_2	69.63	65.12	65.62	65.30
Eu-N_2	2.749	2.870	2.905	2.884	O_4-Eu-N_2	118.44	121.37	123.51	124.55
Eu-N_3	2.631	2.713	2.780	2.784	O_5-Eu-N_2	61.52	60.77	60.44	61.20
Eu-N_4	2.644	2.702	2.703	2.692	O_6-Eu-N_2	131.76	123.24	126.56	126.64
C_{40}-C_{41}	1.168	1.340	1.351	1.362	N_4-Eu-N_2	61.18	60.55	60.48	60.65
C_{41}-C_{42}	1.465	1.468	1.466	1.464	N_3-Eu-N_2	61.94	60.36	59.72	59.78
C_{40}-C_{37}	1.507	1.467	1.464	1.462	C_{40}-C_{41}-C_{42}	126.00	126.71	127.04	127.03
					C_{41}-C_{40}-C_{37}	129.30	126.21	126.40	126.53

Table S8. Selected bond lengths(Å) and angles(º) of the complex 2 determined by X-ray diffraction and optimized by UCAM-B3LYP

Bond lengths (nm)			Bond angle (º)		
Bond	measured	UCAM-B3LYP	Bond	measured	UCAM-B3LYP
Nd-O_1	2.414	2.425	O_6-Nd-O_1	72.08	78.22
Nd-O_2	2.451	2.417	O_1-Nd-O_2	70.78	70.05
Nd-O_3	2.414	2.380	O_1-Nd-O_5	129.95	125.24
Nd-O_4	2.467	2.483	O_5-Nd-O_4	71.24	72.16
Nd-O_5	2.434	2.498	O_5-Nd-O_6	139.15	138.79
Nd-O_6	2.467	2.356	O_1-Nd-N_2	69.43	65.39
Nd-N_2	2.818	2.906	O_4-Nd-N_2	119.12	120.13
Nd-N_3	2.688	2.748	O_5-Nd-N_2	60.56	59.87
Nd-N_4	2.692	2.714	O_6-Nd-N_2	126.71	127.44
C_{40}-C_{41}	1.261	1.340	N_4-Nd-N_2	60.46	60.33
C_{41}-C_{42}	1.477	1.468	N_3-Nd-N_2	61.07	59.62
C_{40}-C_{37}	1.466	1.467	C_{40}-C_{41}-C_{42}	126.00	126.78
			C_{41}-C_{40}-C_{37}	126.70	126.14

Table S9. Selected bond lengths(Å) and angles(º) of the complex **4** determined by X-ray diffraction and optimized by UCAM-B3LYP

Bond lengths (nm)			Bond angle (º)		
Bond	**measured**	**UCAM-B3LYP**	**Bond**	**measured**	**UCAM-B3LYP**
$Gd\text{-}O_1$	2.365	2.353	$O_6\text{-}Gd\text{-}O_1$	73.70	76.48
$Gd\text{-}O_2$	2.379	2.367	$O_1\text{-}Gd\text{-}O_2$	71.70	70.23
$Gd\text{-}O_3$	2.369	2.325	$O_1\text{-}Gd\text{-}O_5$	131.30	126.13
$Gd\text{-}O_4$	2.425	2.448	$O_5\text{-}Gd\text{-}O_4$	71.10	73.10
$Gd\text{-}O_5$	2.381	2.437	$O_5\text{-}Gd\text{-}O_6$	140.40	135.13
$Gd\text{-}O_6$	2.362	2.326	$O_1\text{-}Gd\text{-}N_2$	69.60	64.92
$Gd\text{-}N_2$	2.758	2.855	$O_4\text{-}Gd\text{-}N_2$	119.00	123.82
$Gd\text{-}N_3$	2.649	2.665	$O_5\text{-}Gd\text{-}N_2$	61.70	61.22
$Gd\text{-}N_4$	2.631	2.743	$O_6\text{-}Gd\text{-}N_2$	130.80	121.97
$C_{40}\text{-}C_{41}$	1.230	1.340	$N_4\text{-}Gd\text{-}N_2$	61.60	59.90
$C_{41}\text{-}C_{42}$	1.430	1.468	$N_3\text{-}Gd\text{-}N_2$	62.30	60.70
$C_{40}\text{-}C_{37}$	1.480	1.467	$C_{40}\text{-}C_{41}\text{-}C_{42}$	133.00	126.76
			$C_{41}\text{-}C_{40}\text{-}C_{37}$	130.00	126.05

Table S10. Selected bond lengths(Å) and angles(º) of the complex **5** determined by X-ray diffraction and optimized by UCAM-B3LYP

Bond lengths (nm)			Bond angle (º)		
Bond	**measured**	**UCAM-B3LYP**	**Bond**	**measured**	**UCAM-B3LYP**
$Yb\text{-}O_1$	2.230	2.425	$O_1\text{-}Yb\text{-}O_2$	72.58	71.99
$Yb\text{-}O_2$	2.332	2.417	$O_1\text{-}Yb\text{-}O_5$	138.43	138.83
$Yb\text{-}O_3$	2.225	2.380	$O_5\text{-}Yb\text{-}O_4$	75.03	74.94
$Yb\text{-}O_4$	2.296	2.483	$O_1\text{-}Yb\text{-}N_2$	72.83	73.33
$Yb\text{-}O_5$	2.203	2.498	$O_4\text{-}Yb\text{-}N_2$	131.65	133.08
$Yb\text{-}N_2$	2.504	2.356	$O_5\text{-}Yb\text{-}N_2$	67.97	66.78
$Yb\text{-}N_3$	2.467	2.906	$N_4\text{-}Yb\text{-}N_2$	66.22	66.25
$Yb\text{-}N_4$	2.546	2.748	$N_3\text{-}Yb\text{-}N_2$	133.65	66.47
$C_{40}\text{-}C_{41}$	1.334	1.340	$C_{40}\text{-}C_{41}\text{-}C_{42}$	126.60	126.74
$C_{41}\text{-}C_{42}$	1.467	1.469	$C_{41}\text{-}C_{40}\text{-}C_{37}$	126.40	126.60
$C_{40}\text{-}C_{37}$	1.471	1.468			

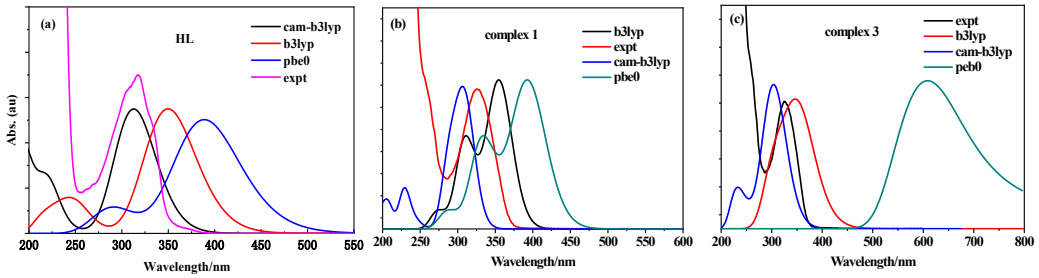


Figure S14. Overlay of calculated and experimental absorption spectra of HL(a), complexes **1**(b) and **3**(c) in acetonitrile solution.

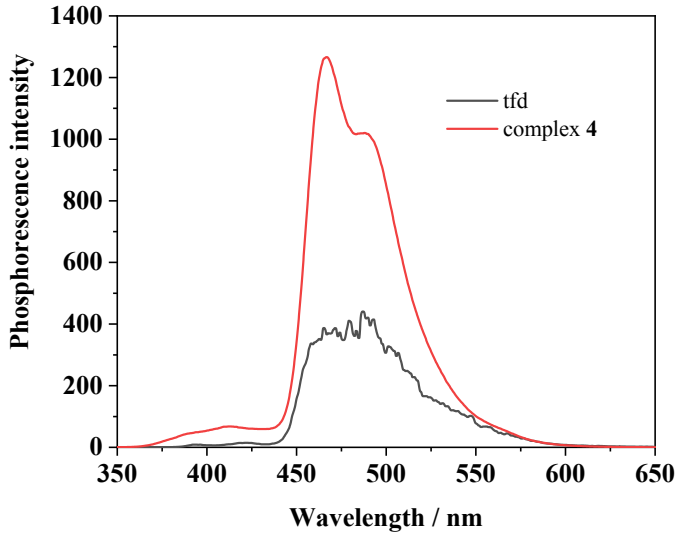


Figure S15. Phosphorescence spectra of tfd (black line) and complexes **4** (red line) in acetonitrile solutions at 77K.

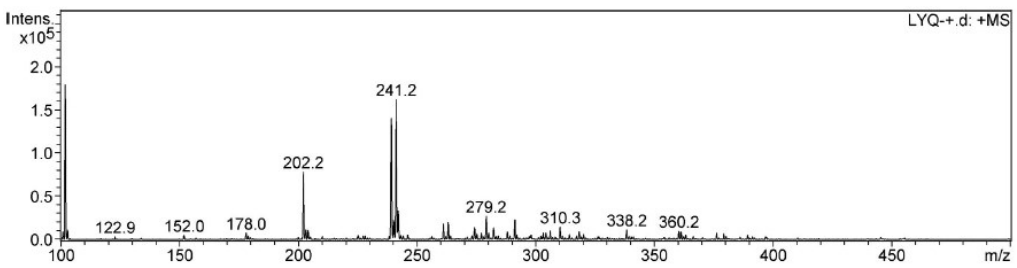


Figure S16. ESI mass spectrum of L1 in methanol solution.

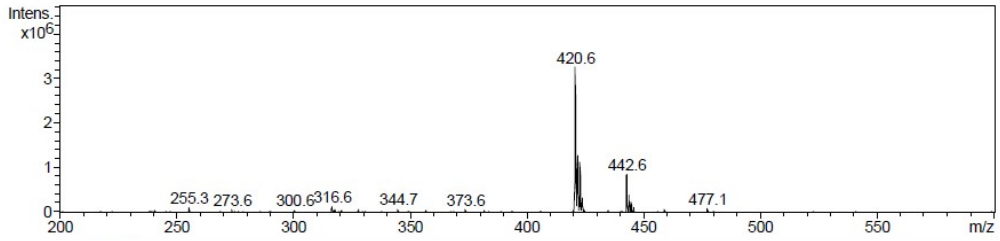


Figure S17. ESI mass spectrum of HL in methanol solution.

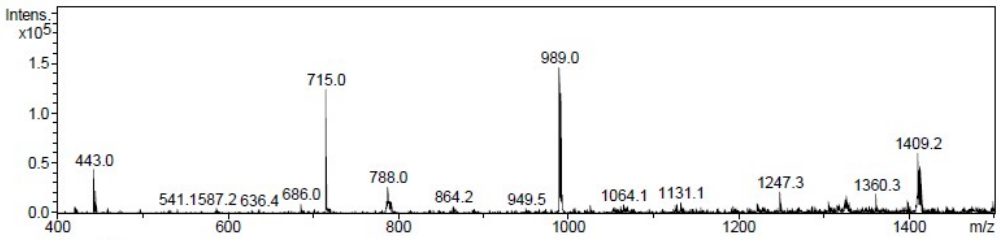


Figure S18. ESI mass spectrum of complex 1 in methanol solution.

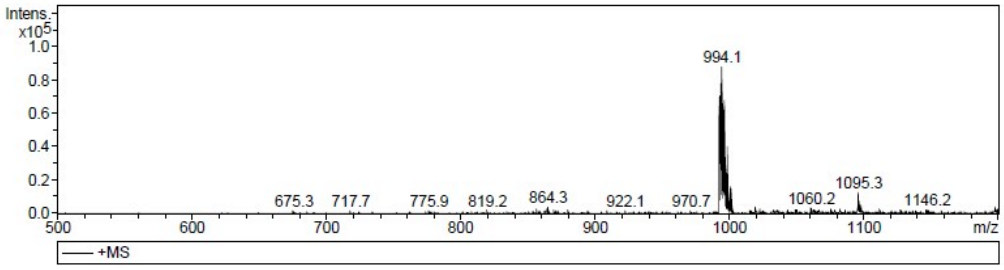


Figure S19. ESI mass spectrum of complex 2 in methanol solution.

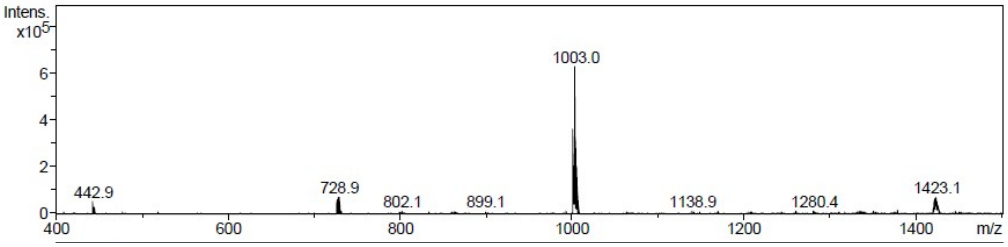


Figure S20. ESI mass spectrum of complex **3** in methanol solution.

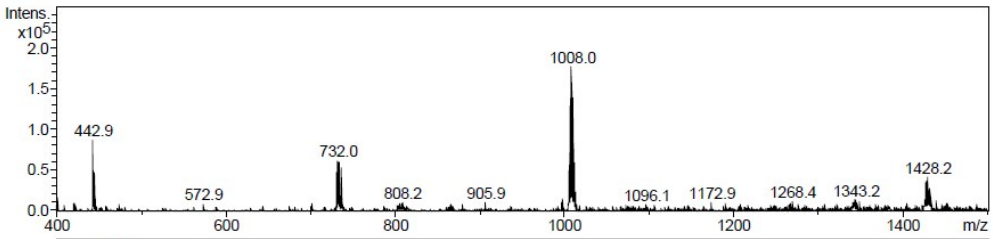


Figure S21. ESI mass spectrum of complex **4** in methanol solution.

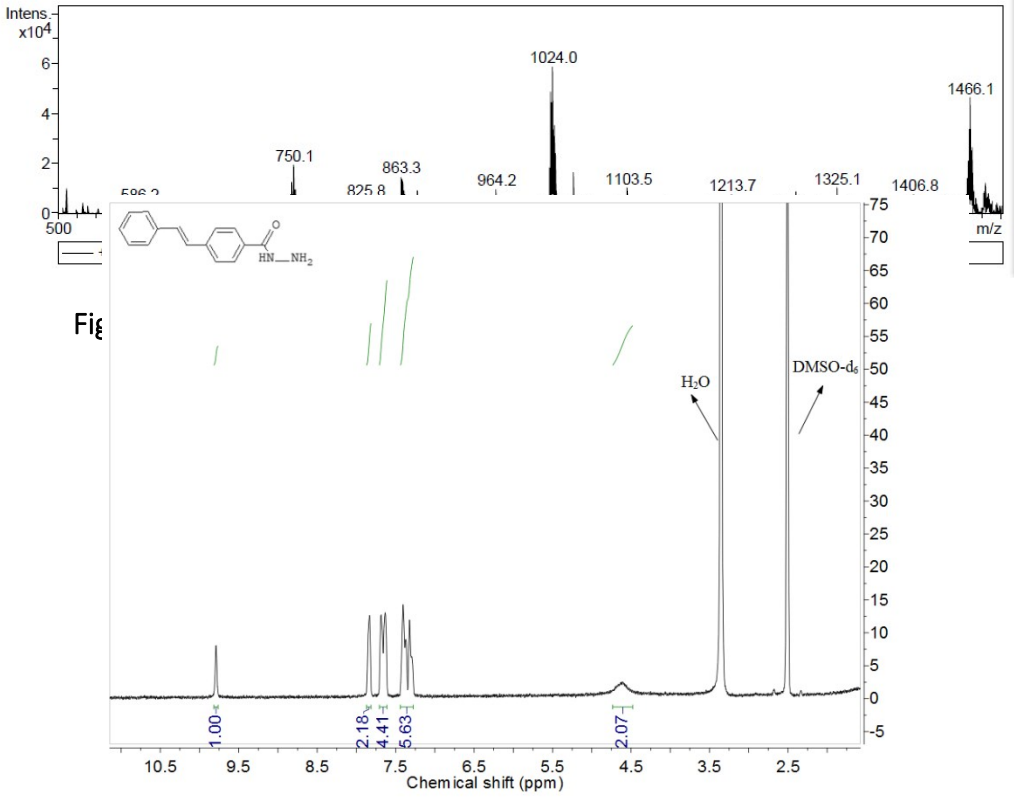
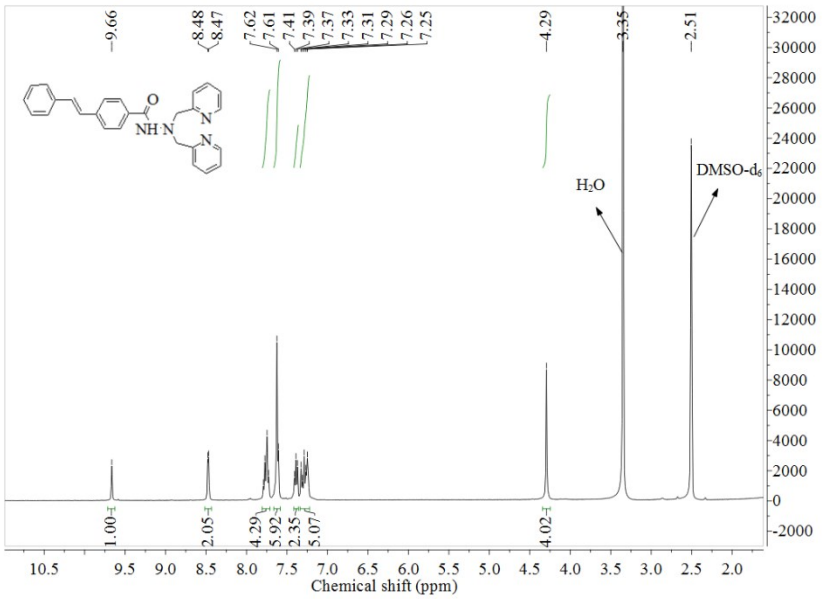
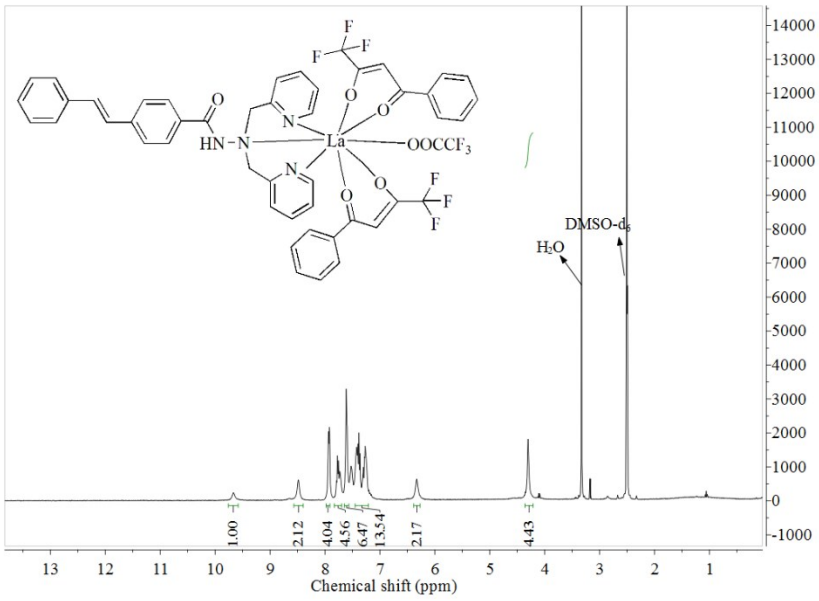


Figure S22. ^{1}H NMR spectrum of L1 in DMSO-d_6.





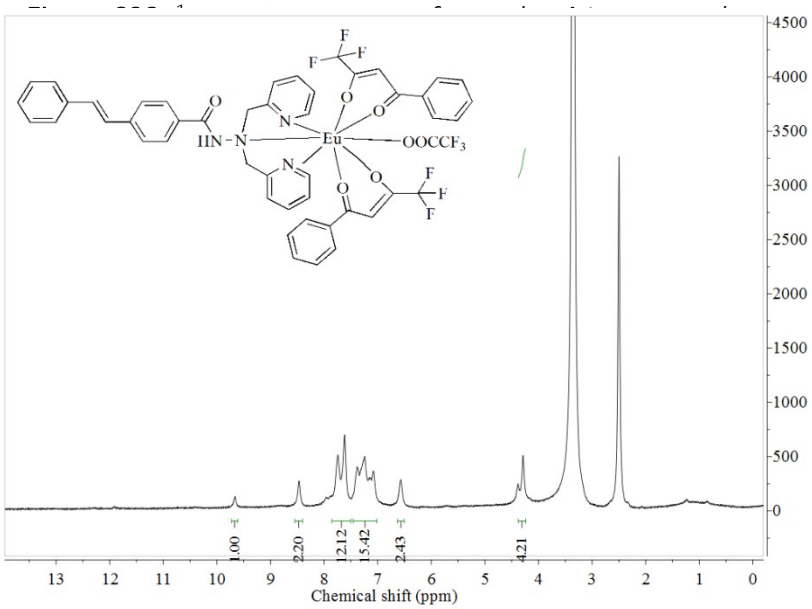


Figure S24. ^{1}H NMR spectrum of complex **3** in DMSO-d_6.