

## Electronic Supplementary Information (ESI)

Ln(III) Complexes of bis(5-(pyridine-2-yl)-1,2,4-triazol-3-yl)methane ligand:  
synthes, structure and fluorescent properties.

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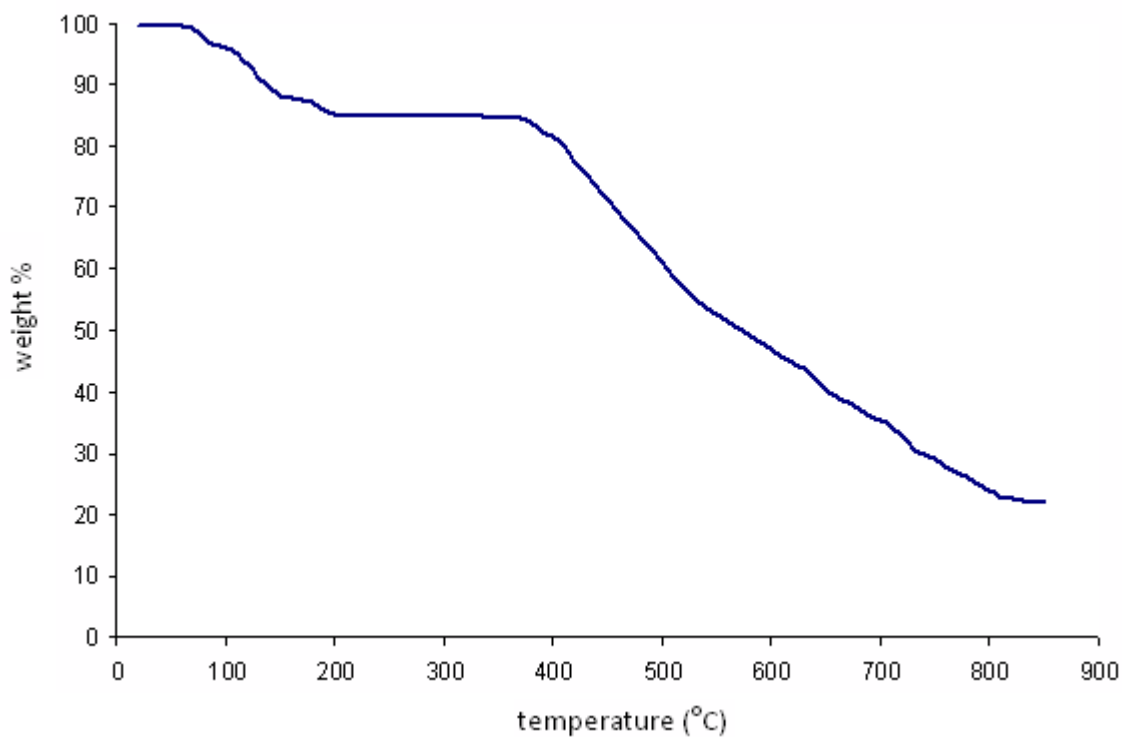


Figure S1a: TG curve of complex 2.

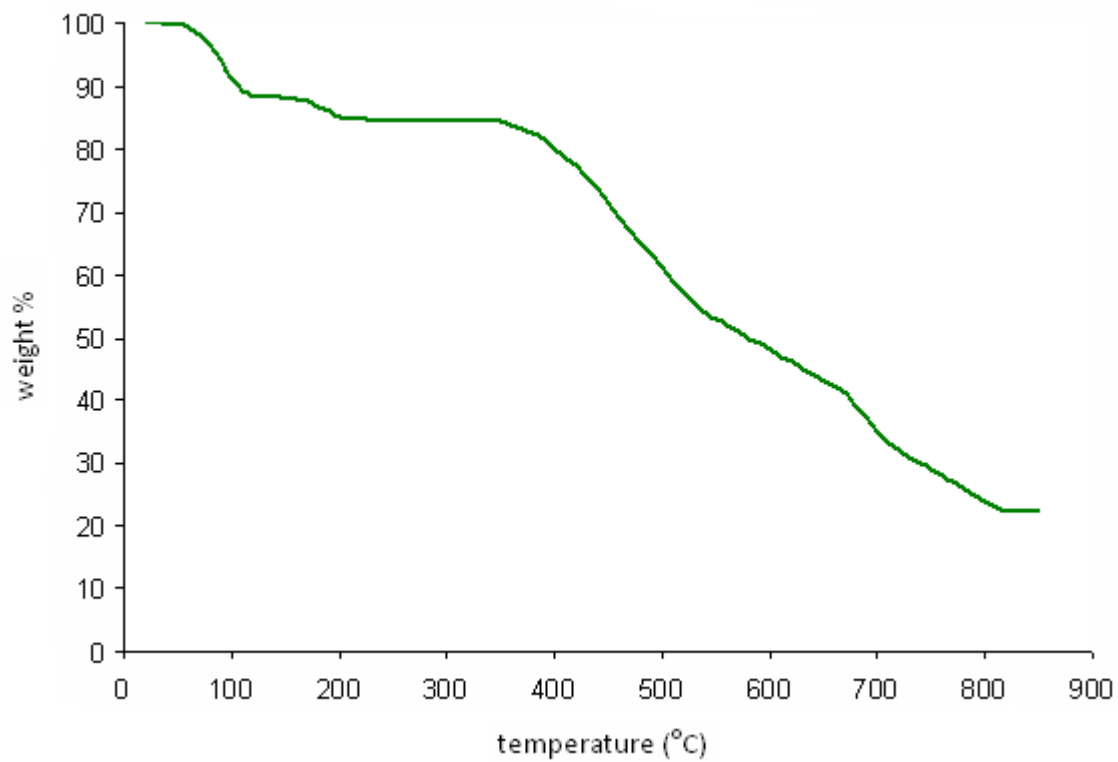


Figure S1b: TG curve of complex 4.

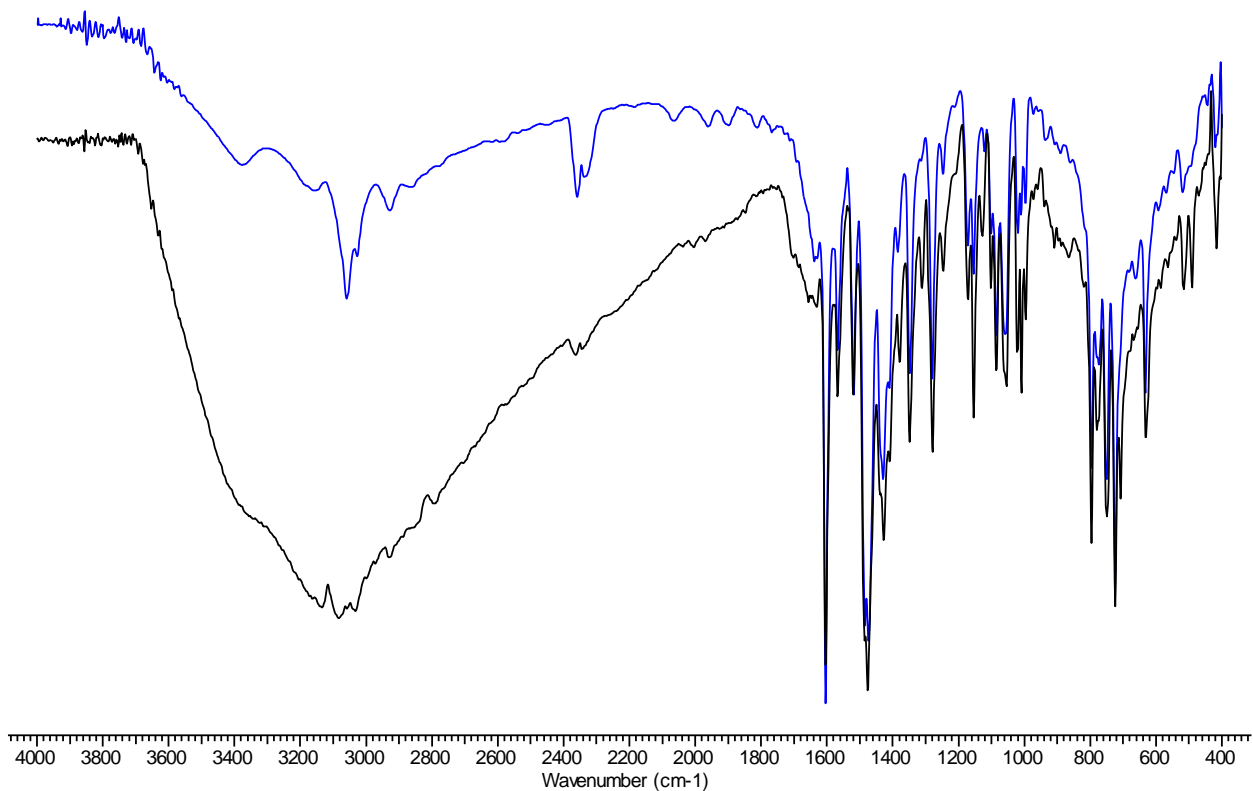


Figure S2: IR-spectra of complex 3 (Black line – complex 1 (hydrate), blue line complex 1 (anhydrous sample)).

Table S1. Crystal data and experimental details for complex 4.

Parameter	<b>1</b>
Formula	[NdL(HL)H <sub>2</sub> O]·6H <sub>2</sub> O
M	843.67
T, K	173
Crystal system	Monoclinic
Space group	C 2/c
Unit cell parameters	
a, Å	11.5441(3)
b, Å	23.7400(6)
c, Å	27.0161(6)
V, Å <sup>3</sup>	7386.2(3)
β °	93.9660(10)
Z	8
D <sub>calc.</sub> g·cm <sup>-3</sup>	1.563
μ <sub>Mo.</sub> mm <sup>-1</sup>	1.473
F(000)	3488
θ <sub>max.</sub> deg	1.72 – 29.00
Index ranges	-15 ≤ h ≤ 15, -28 ≤ k ≤ 32, -35 ≤ l ≤ 36
Reflections measured/ reflections independent	9766 / 8235
Parameters	526
GOOF	1.016
R(I > 2σ(I))	R <sub>1</sub> = 0.0434; wR <sub>2</sub> = 0.1296
Residual electron density (max/min), e/Å <sup>3</sup>	-0.796 / 1.425

Table S2. The most relevant bonds and angles of complex 4.

Bond	<i>d</i> /Å	Angle	<i>ω</i> /degree
Nd1 O1	2.451(3)	O1 Nd1 N5	74.85(10)
Nd1 N5	2.510(3)	O1 Nd1 N2	114.63(10)
Nd1 N2	2.522(4)	N5 Nd1 N2	69.35(11)
Nd1 N13	2.549(3)	O1 Nd1 N13	78.06(10)
Nd1 N10	2.582(4)	N5 Nd1 N13	152.62(11)
Nd1 N16	2.693(4)	N2 Nd1 N13	127.32(10)
Nd1 N1	2.695(4)	O1 Nd1 N10	121.13(10)
Nd1 N8	2.722(4)	N5 Nd1 N10	123.64(10)
Nd1 N9	2.746(3)	N2 Nd1 N10	124.23(10)
		N13 Nd1 N10	68.43(10)
		O1 Nd1 N16	70.45(10)
		N5 Nd1 N16	109.94(10)
		N2 Nd1 N16	73.08(11)
		N13 Nd1 N16	63.58(10)
		N10 Nd1 N16	126.42(10)
		O1 Nd1 N1	140.42(10)
		N5 Nd1 N1	130.27(10)
		N2 Nd1 N1	63.85(10)
		N13 Nd1 N1	74.92(10)
		N10 Nd1 N1	74.10(10)
		O1 Nd1 N8	69.92(10)
		N5 Nd1 N8	64.00(10)
		N2 Nd1 N8	129.84(10)
		N1 Nd1 N16	71.80(10)
		N13 Nd1 N8	102.79(9)
		N10 Nd1 N8	72.22(10)
		N16 Nd1 N8	140.01(10)
		N1 Nd1 N8	144.34(10)
		O1 Nd1 N9	145.08(9)
		N5 Nd1 N9	76.39(10)
		N2 Nd1 N9	72.11(10)
		N13 Nd1 N9	126.95(10)
		N10 Nd1 N9	62.15(10)
		N16 Nd1 N9	139.26(10)
		N1 Nd1 N9	74.28(10)
		N8 Nd1 N9	79.92(10)

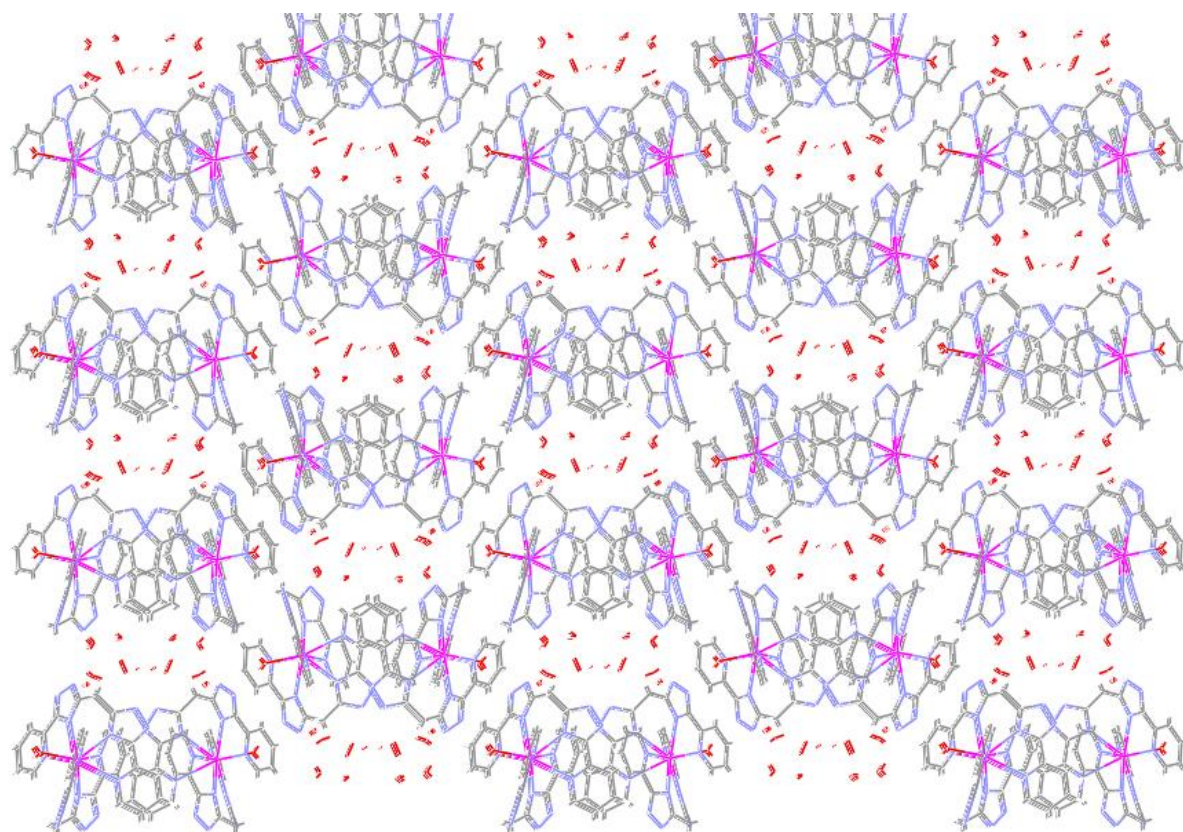


Figure S3. Packing diagram of complex 4 along axis *a*.

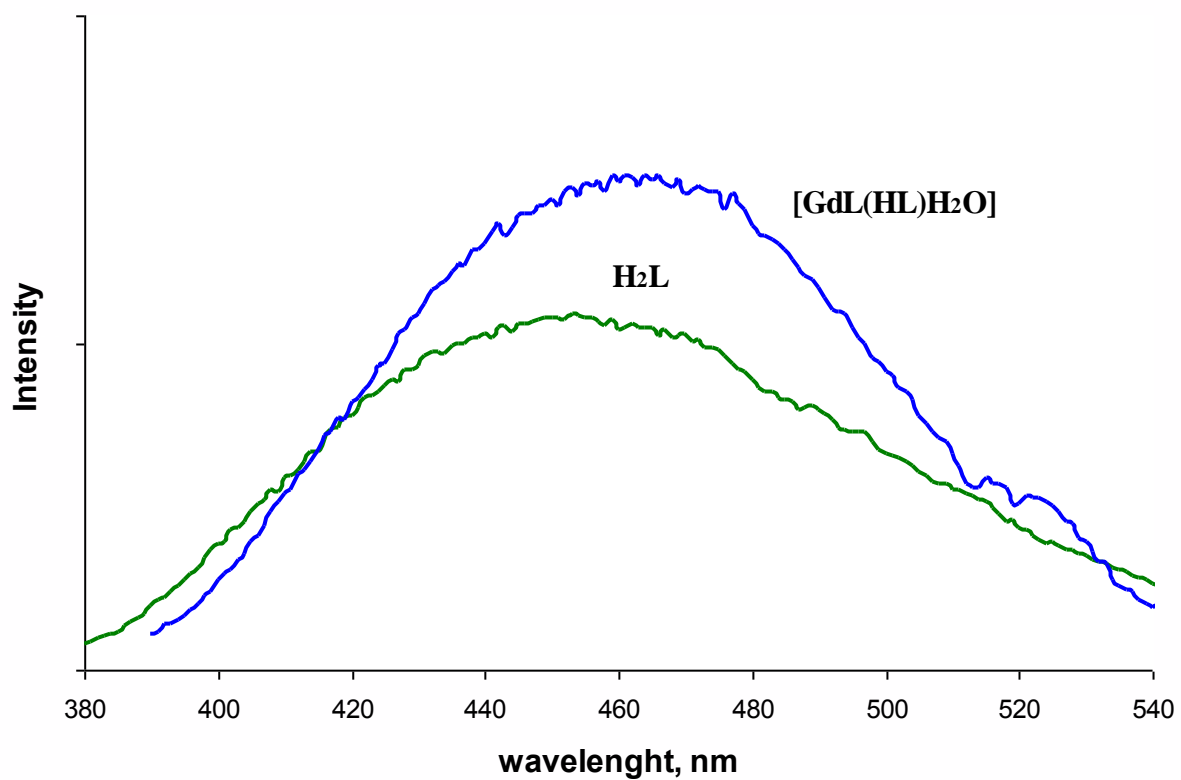


Figure S4. Luminescence spectra of solid samples of H<sub>2</sub>L and Gd complex 298 K excited at 330 nm.

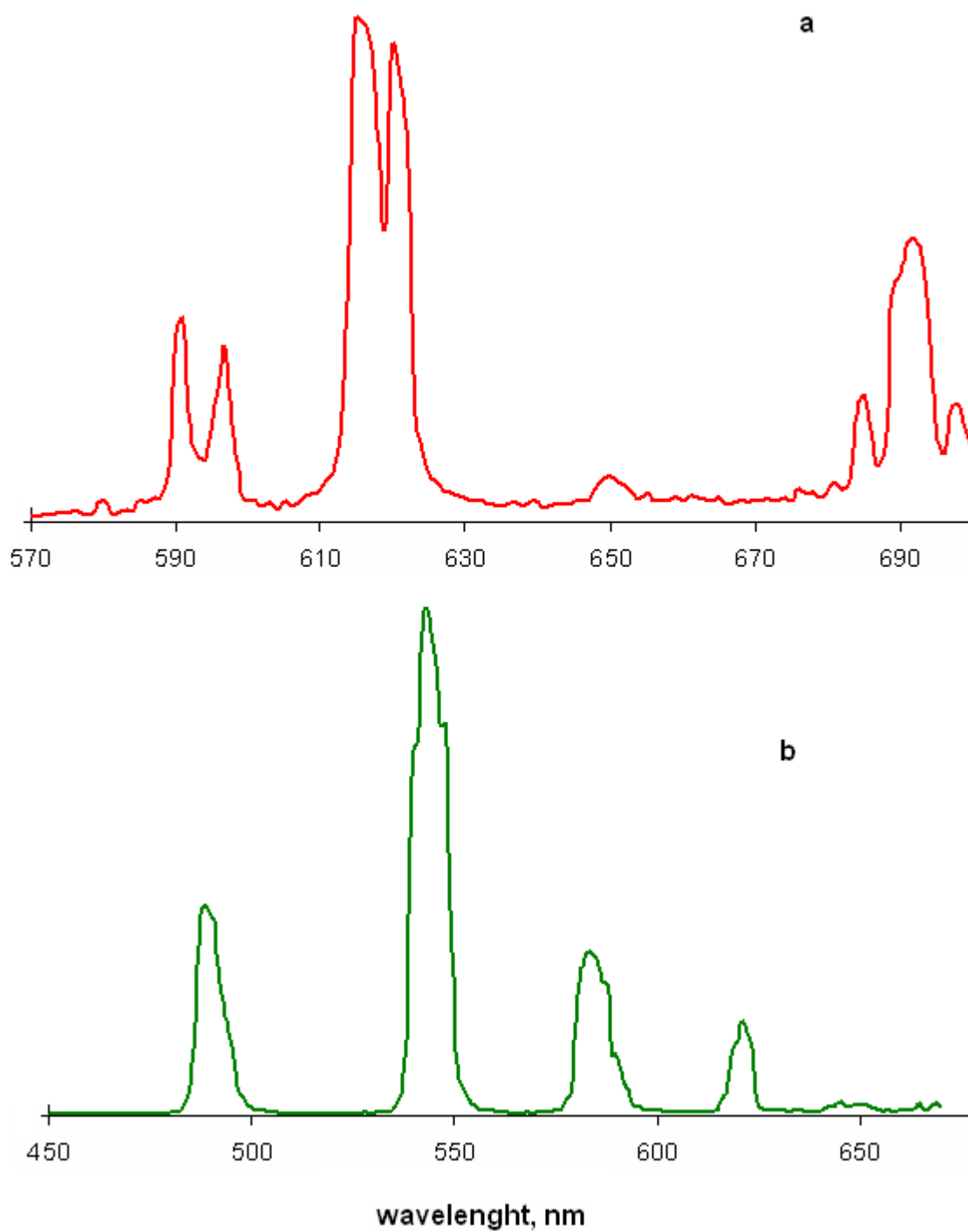


Figure S5. Emission spectra of Eu(III) (a) and Tb(III) (b) complexes in the water solution at 298 K.



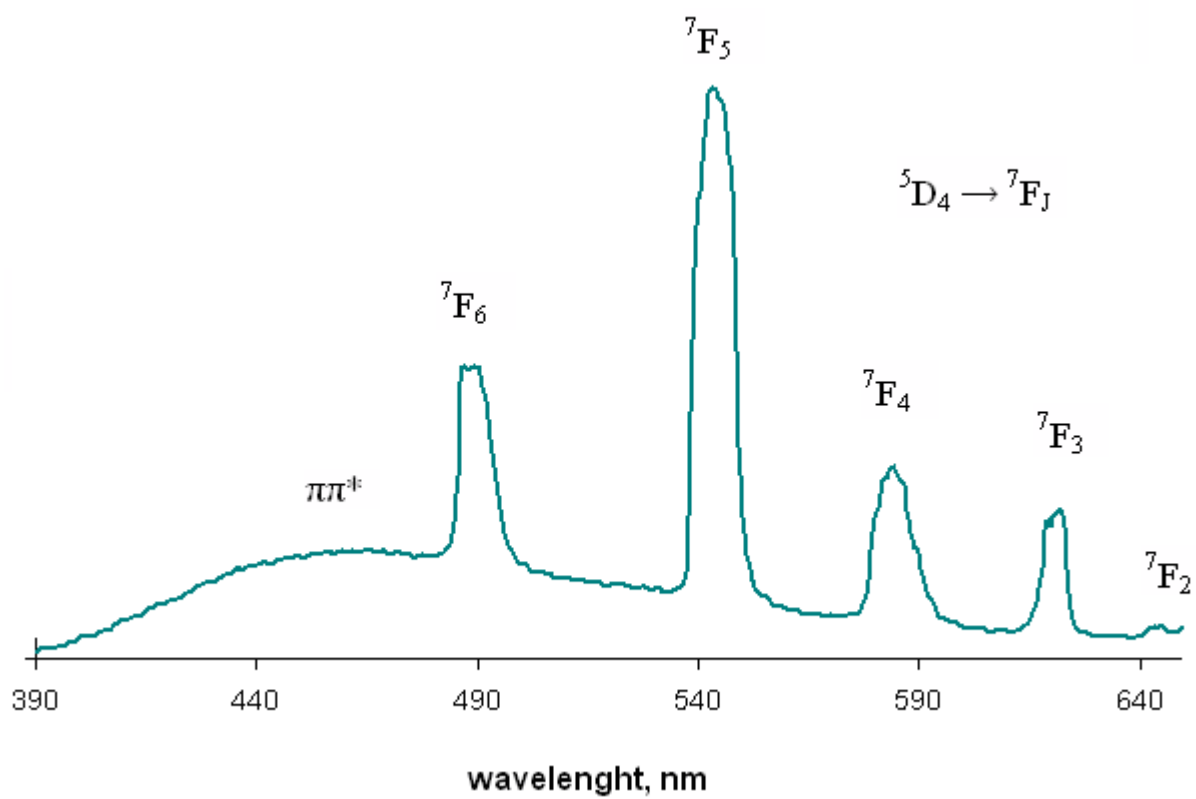


Figure S6. Emission spectra of Tb(III) complex solution at pH = 6.