Supporting Information

Table S1. Selected hydrogen bond geometries for compounds **DFX**, **DFX-Ce** and **DFX-Eu.**

	D−H	A	d(D···A) / Å	d(H···A) / Å	<DHA / deg
DFX	O1-H1	O2 [-x+1, -y+1, -z-1]	2.673	1.855·	175.51
	O3-H3	N3 [x, -y+3/2, z-1/2]	2.800	2.007	162.78
	O4-H4	N2	2.690	1.970	146.09
DFX-Ce	O3-H3	N2	2.642	1.920	146.33
	O4-H4	N3	2.638	1.912	146.95
	O7-H7	N5	2.629	1.901	147.45
	O8-H8	N6	2.618	1.911	143.71
	O11-H11	N8	2.657	1.931	147.10
	O12-H12	N9	2.638	1.905	148.21
	O15-H15	N11	2.633	1.918	145.21
	O16-H16	N12	2.610	1.942	138.13
	O19-H19	N14	2.637	1.906	147.94
	O20-H20	N15	2.619	1.893	146.95
	O23-H23	N17	2.667	1.958	144.15
	O24-H24	N18	2.695	1.969	147.22
	O25-H25A	O17	2.745	2.263	117.41
	O25-H25B	O1 [-x+1, -y+1, -z+1]	2.824	2.429	112.12
DFX-Eu	O3-H3	N3	2.634	1.907	147.22
	O4-H4	N2	2.642	1.916	146.98
	O7-H7	N6	2.597	1.866	147.84
	O8-H8	N5	2.632	1.903	147.43
	O11-H11	N8	2.638	1.911	147.09
	O12-H12	N9	2.606	1.904	143.04
	O15-H15	N12	2.642	1.914	147.52
	O16-H16	N11	2.657	1.933	146.69
	O19-H19	O11 [-x+1, -y+1, -z]	2.878	2.485	110.69
	O19-H19	N14	2.651	1.922	147.48
	O20-H20	N15	2.612	1.884	147.31
	O23-H23	N17	2.663	1.946	145.50
	O24-H24	N18	2.689	1.965	146.71
	O25-H25B	O2	2.815	2.432	113.19

Table S2. Selected hydrogen bond geometries for compounds **DFX-Gd** and **DFX-Tb.**

	D−H	A	d(D···A) / Å	d(H···A) / Å	<DHA / deg
DFX-Gd	O3-H3	O15 [x, y-1, z]	2.802	2.394	111.63
	O3-H3	N2	2.672	1.967	143.66
	O4-H4	N3	2.686	1.971	145.34
	O7-H7	O11 [x, y, z-1]	2.872	2.450	112.99
	O7-H7	N5	2.656	1.932	146.83
	O8-H8	N6	2.612	1.893	145.86
	O11-H11	N8	2.637	1.918	145.85
	O12-H12	N9	2.599	1.858	149.57
	O15-H15	N11	2.654	1.935	145.87
	O16-H16	N12	2.646	1.930	145.44
	O19-H19	N14	2.627	1.899	147.41
	O20-H20	N15	2.587	1.852	148.65
	O23-H23	O23 [-x+1, -y+2, -z+1]	2.901	2.489	112.37
	O23-H23	N17	2.640	1.926	145.03
	O24-H24	N18	2.628	1.903	146.79
	O25-H25B	O6	2.764	2.225	126.96
DFX-Tb	O3-H3	N21	2.666	1.940	147.10
	O4-H4	N19	2.708	1.981	147.46
	O7-H7	N2	2.646	1.920	147.02
	O8-H8	N3	2.609	1.878	147.86
	O11-H11	N23	2.626	1.895	147.75
	O12-H12	N22	2.628	1.889	149.36
	O15-H15	N6	2.664	1.934	147.84
	O16-H16	N5	2.650	1.925	146.87
	O19-H19	N28	2.617	1.891	147.08
	O20-H20	N30	2.616	1.880	148.73
	O23-H23	N7	2.634	1.905	147.59
	O24-H24	N9	2.602	1.877	146.89
	O27-H27	N11	2.635	1.906	147.58
	O28-H28	N12	2.659	1.930	147.67
	O31-H31	N34	2.663	1.936	147.28
	O32-H32	N35	2.666	1.944	146.46
	O35-H35	N15	2.634	1.901	148.38
	O36-H36	N14	2.607	1.875	148.05
	O39-H39	N32	2.627	1.901	146.98
	O40-H40	N33	2.628	1.887	149.67
	O43-H43	N17	2.639	1.919	145.97
	O44-H44	N18	2.656	1.925	147.93
	O47-H47	N25	2.637	1.905	148.14
	O48-H48	N26	2.639	1.904	148.71
	O51-H51A	O38 [-x+1, -y+1, -z+1]	2.750	2.062	137.57
	O51-H51B	O42 [-x+1, -y+1, -z+1]	3.023	2.278	146.43

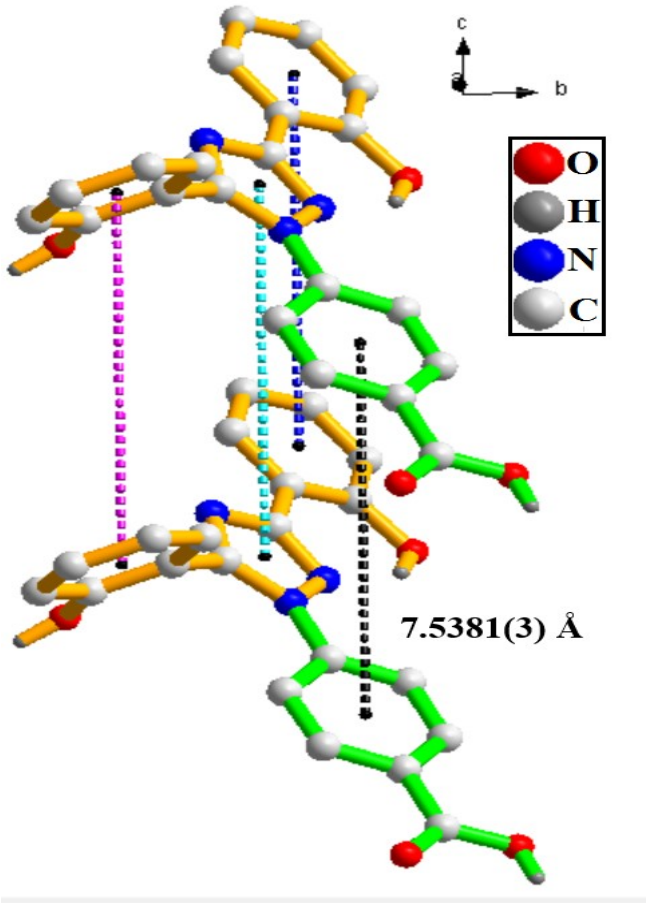

Figure S1. Perspective view of a slip-stack orientation in **DFX** stabilized by some π···π packing interactions between two adjacent phenyl rings or triazole rings with the distance of 7.5381 (3) Å.

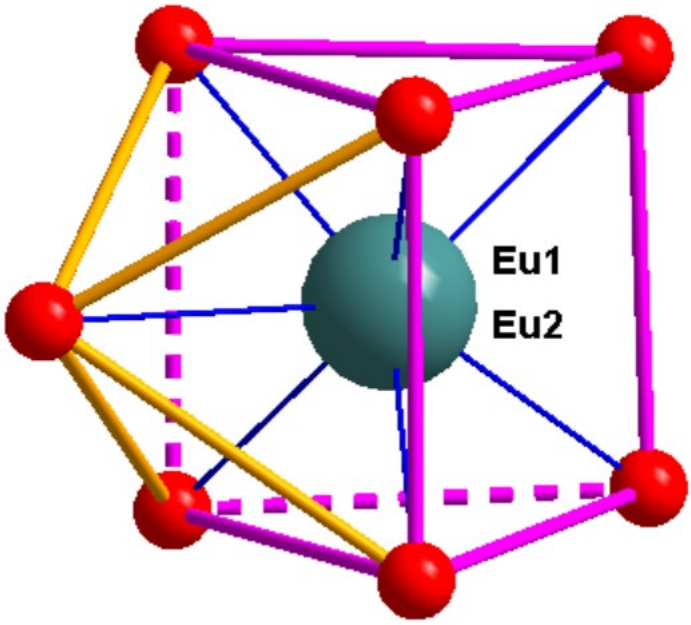

Figure S2. The distorted monocaped trigonal-prismatic coordination polyhedron in **DFX-Eu**.

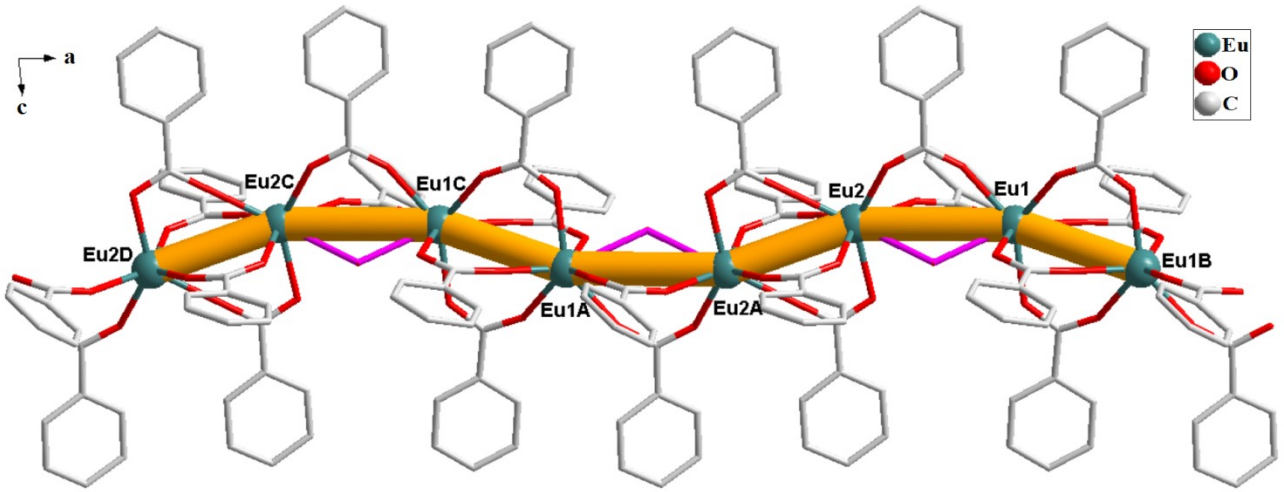

Figure S3. Formation of the cruciform-like 1D coordination polymer chain running along the *a* axis in **DFX-Eu**. Eu-Eu vectors are highlighted in yellow for emphasising the undulation direction of the chain. Symmetry codes: A (1-x, 1-y, 1-z), B (2-x, 1-y, 1-z) , C (-1+x, y, z) , D (-x, 1-y,1- z).

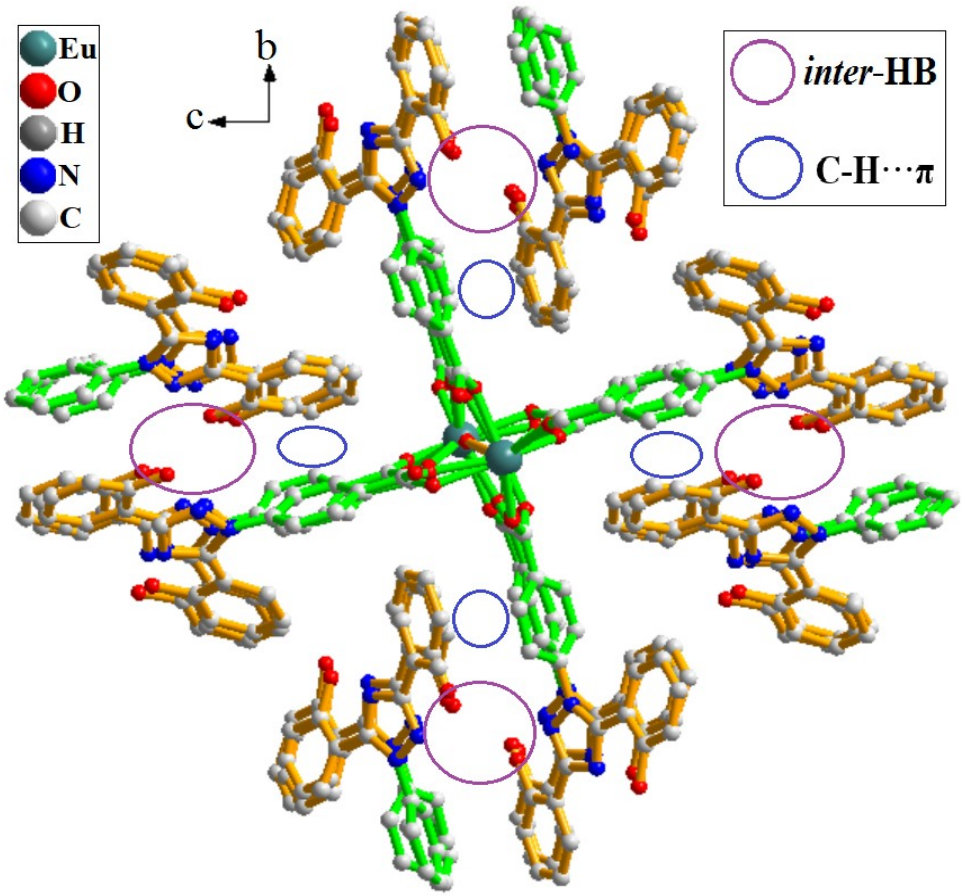

Figure S4. The local magnification diagram for the 3D supramolecular architecture of **DFX-Eu.**

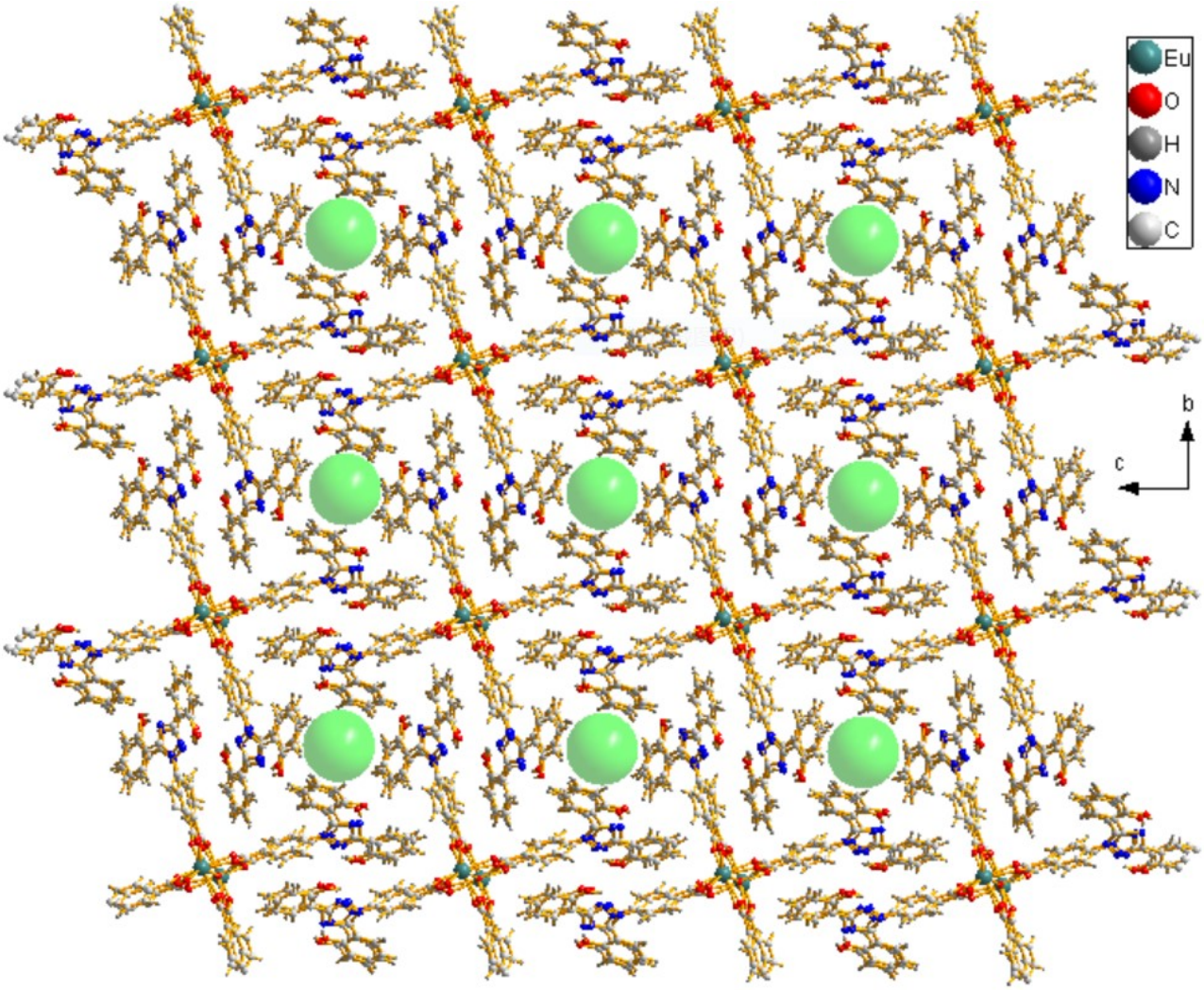

Figure S5. The 3D supramolecular architecture with tube and labyrinth-like micro-voids for **DFX-Eu** (tubular shaped-voids are highlighted with the pale green spheres).

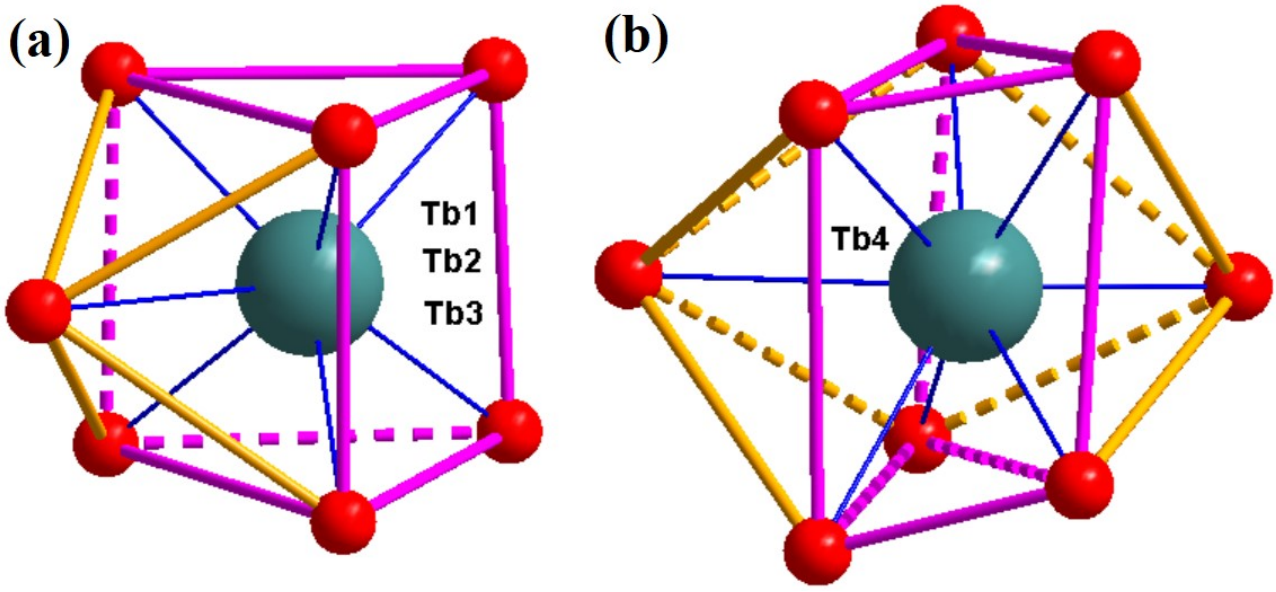

Figure S6. (a) The distorted monocaped trigonal-prismatic coordination polyhedron in **DFX-Tb**; (b) the distorted bicaped trigonal-prismatic coordination polyhedron in **DFX-Tb**.

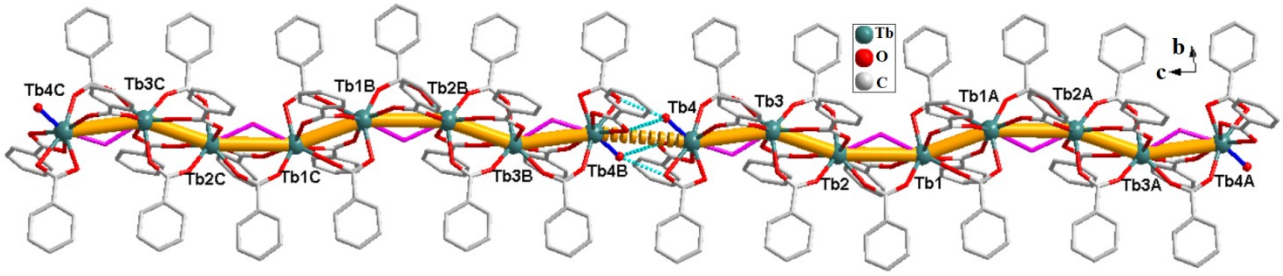

Figure S7. The local magnification diagram for the cruciform-like 1D coordination polymer chain self-healed by intrachain hydrogen bonds along the *a* axis in **DFX-Tb**. Tb-Tb vectors are highlighted in yellow for emphasising the undulation direction of the chain. Symmetry codes: A (1-x, 1-y, 1-z), B (1-x, 1-y, -z) , C (x, y, 1+z) .

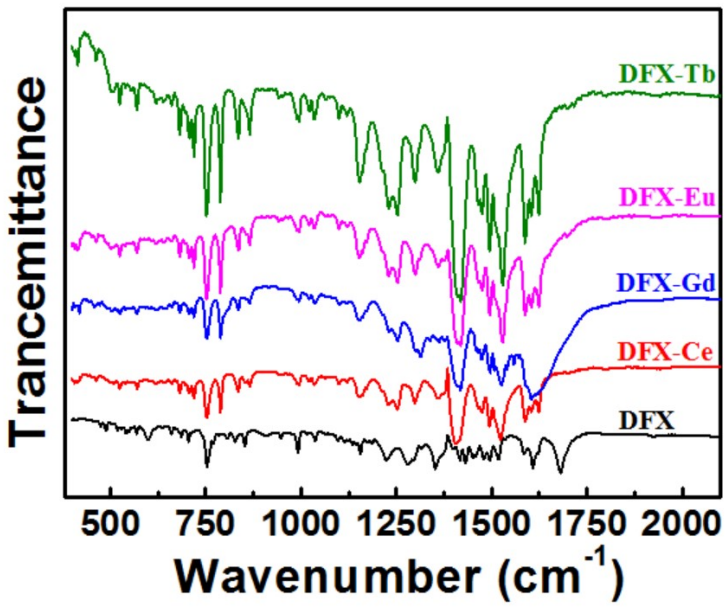

Figure S8. FT-IR spectra for **DFX**, **DFX-Ce**, **DFX-Gd** , **DFX-Eu** and **DFX-Tb.**

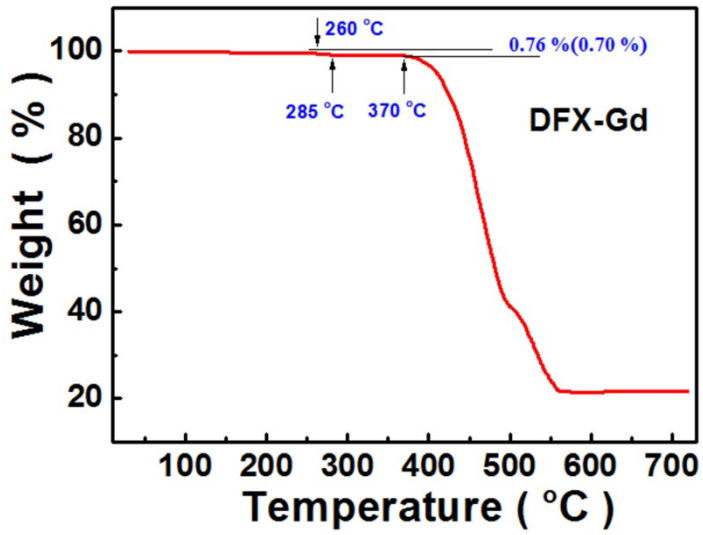

Figure S9. TG curve of compound **DFX-Gd.**

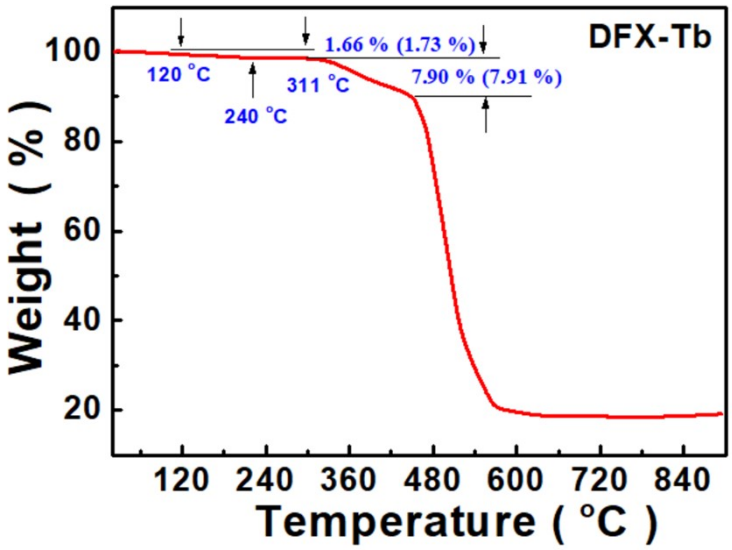

Figure S10. TG curve of compound **DFX-Tb.**

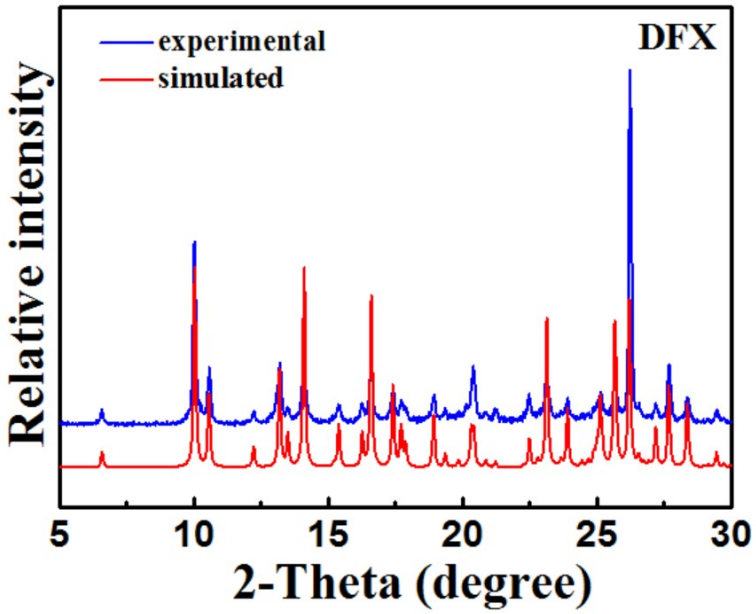

Figure S11. The experimental and simulated PXRD patterns for **DFX**. The top is the experimental pattern, and the bottom is the simulated one.

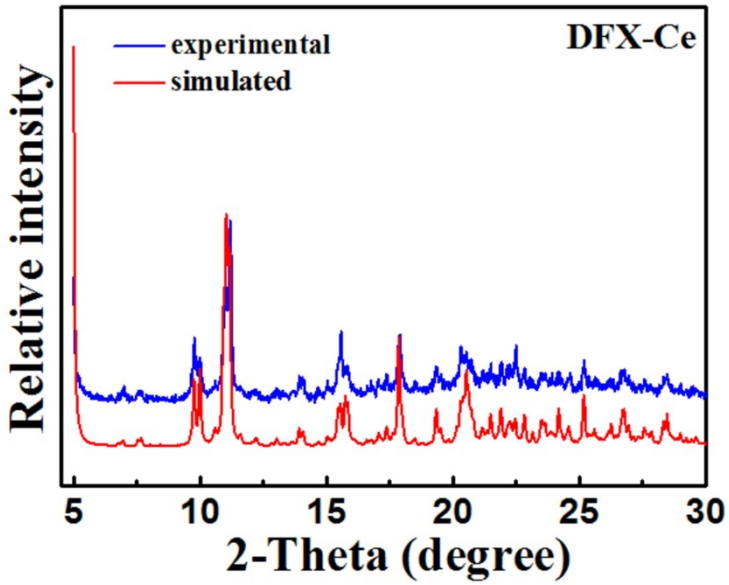

Figure S12. The experimental and simulated PXRD patterns for **DFX-Ce**. The top is the experimental pattern, and the bottom is the simulated one.

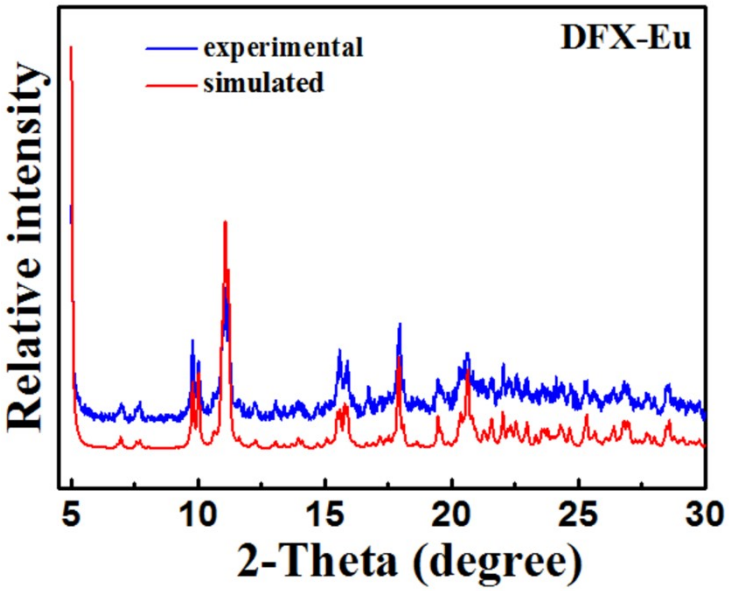

Figure S13. The experimental and simulated PXRD patterns for **DFX-Eu**. The top is the experimental pattern, and the bottom is the simulated one.

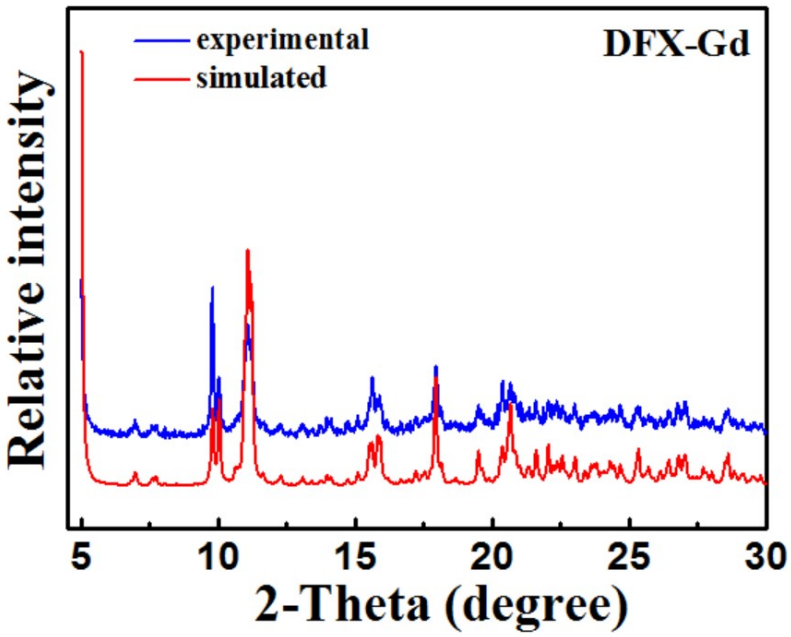

Figure S14. The experimental and simulated PXRD patterns for **DFX-Gd**. The top is the experimental pattern, and the bottom is the simulated one.

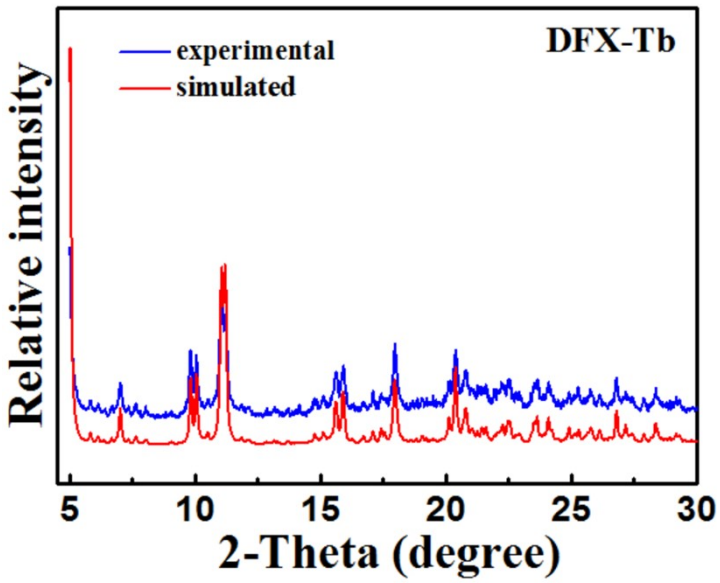

Figure S15. The experimental and simulated PXRD patterns for **DFX-Tb**. The top is the experimental pattern, and the bottom is the simulated one.

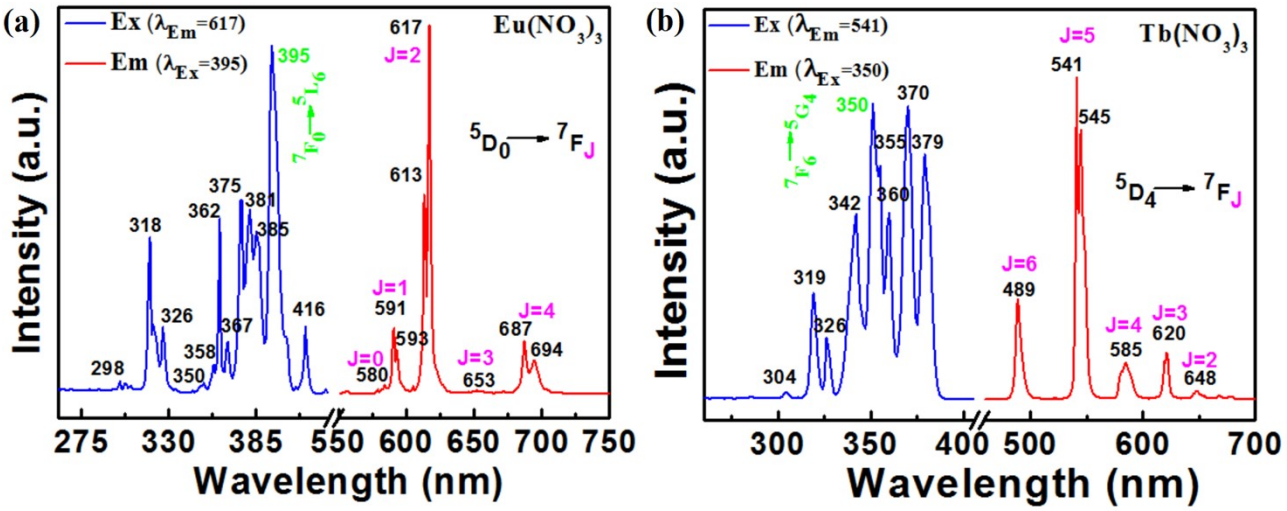

Figure S16. (a) The excitation (left, λ_{em} = 617 nm) and emission (right, λ_{ex} = 395 nm) spectra for $Eu(NO_3)_3 \cdot 6H_2O$; (b) The excitation (left, λ_{em} = 514 nm) and emission (right, λ_{ex} = 350 nm) spectra for $Tb(NO_3)_3 \cdot 6H_2O$.

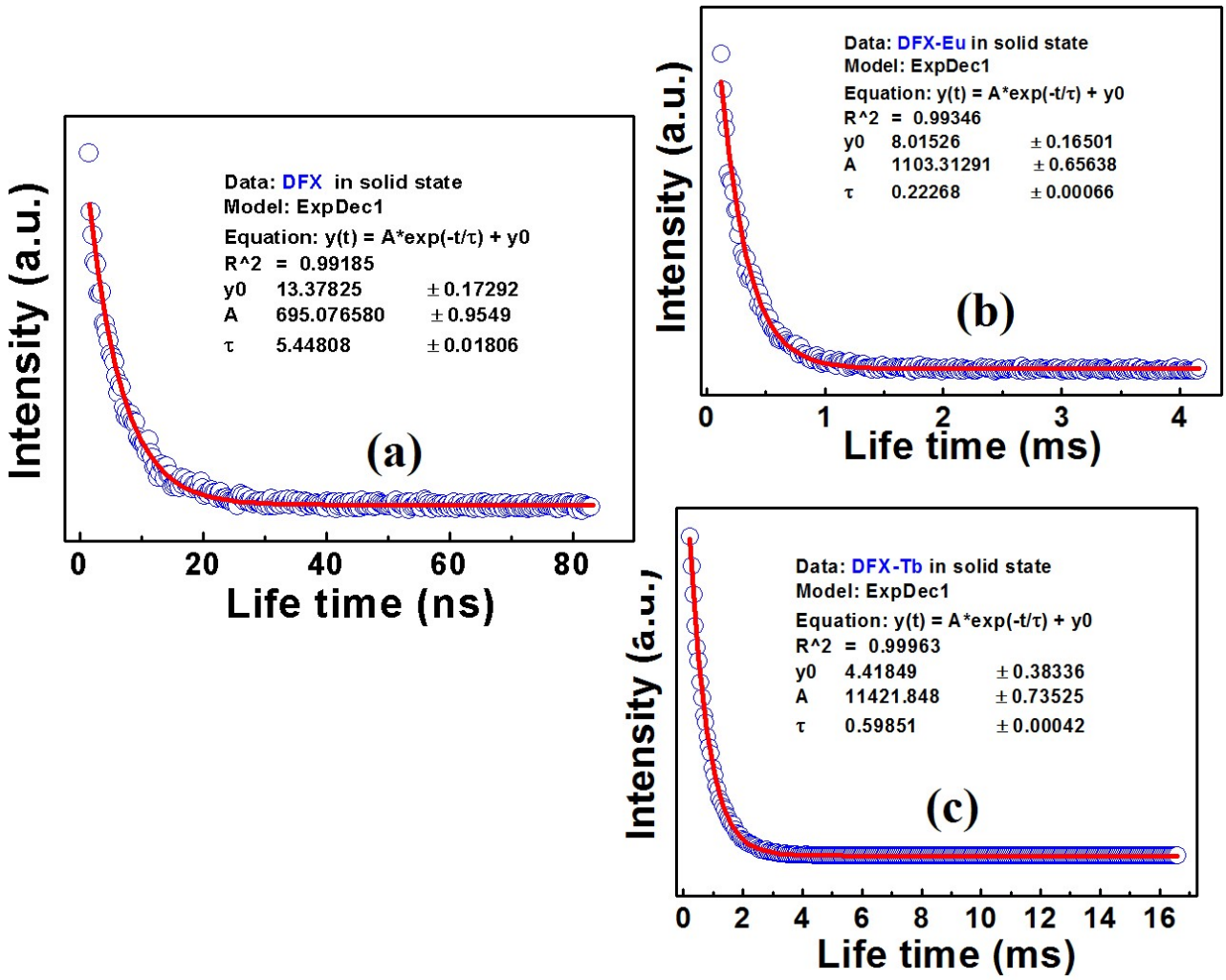

Figure S17. Emission decay curves by monitoring the transitions (a) π*→π (588 nm) of the intraligand for **DFX**, (b) $^5D_0 \rightarrow {}^7F_2$ (616 nm) of the Eu^{3+} ion for **DFX-Eu** and (c) $^5D_4 \rightarrow {}^7F_5$ (540 nm) of the Tb^{3+} ion for **DFX-Tb**.The excitations were done at 343, 394 and 356 nm for the ligand, Eu^{3+} and Tb^{3+} ion. [O: experimental data; —: fitted according to equation $y(t) = A \exp(-t/\tau) + y_0$].

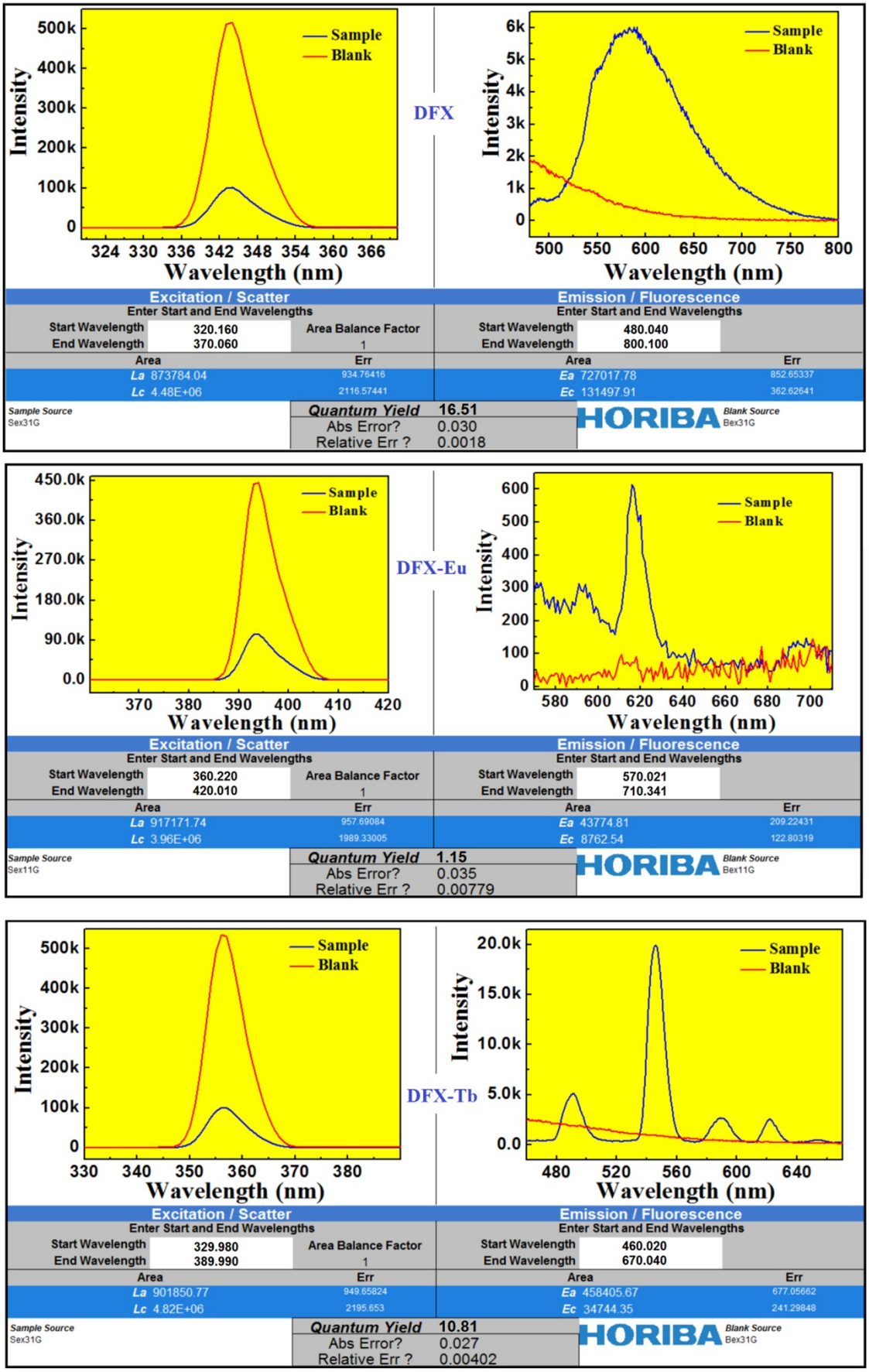

Figure S18. The measurement details of solid state fluorescence quantum yield for **DFX** (top), **DFX-Eu** (middle) and **DFX-Tb** (down).