Electronic Supplementary Material (ESI) for RSC Advances.

New 10H perovskites $Ba_5Ln_{1-x}Mn_{4+y}O_{15-\delta}$ with spin glass behaviour

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Supporting Information

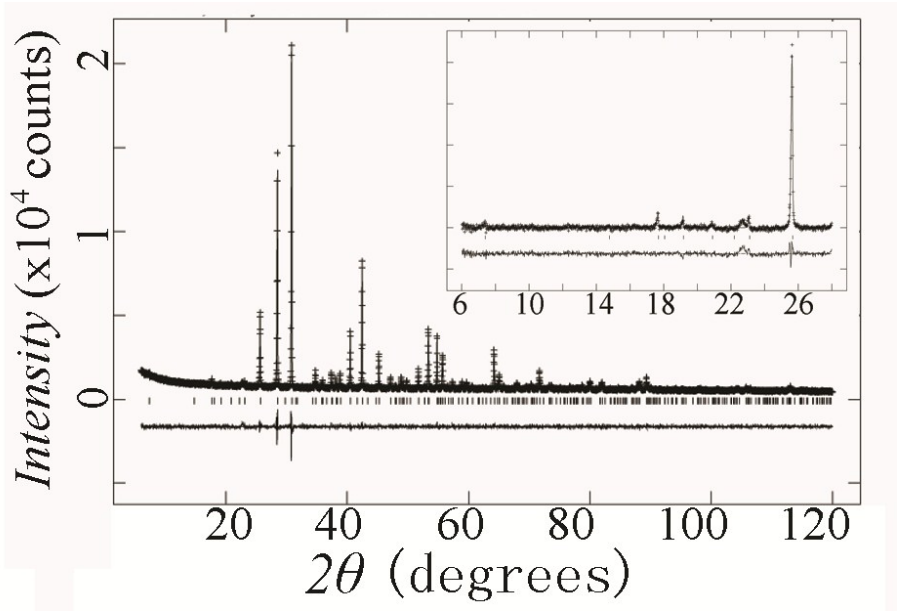

Figure S1. The fitted XRD plot of the $Ba_5Sm_{0.98}Mn_{4.01}O_{15-\delta}$ sample. The inset expands the low-angle regions

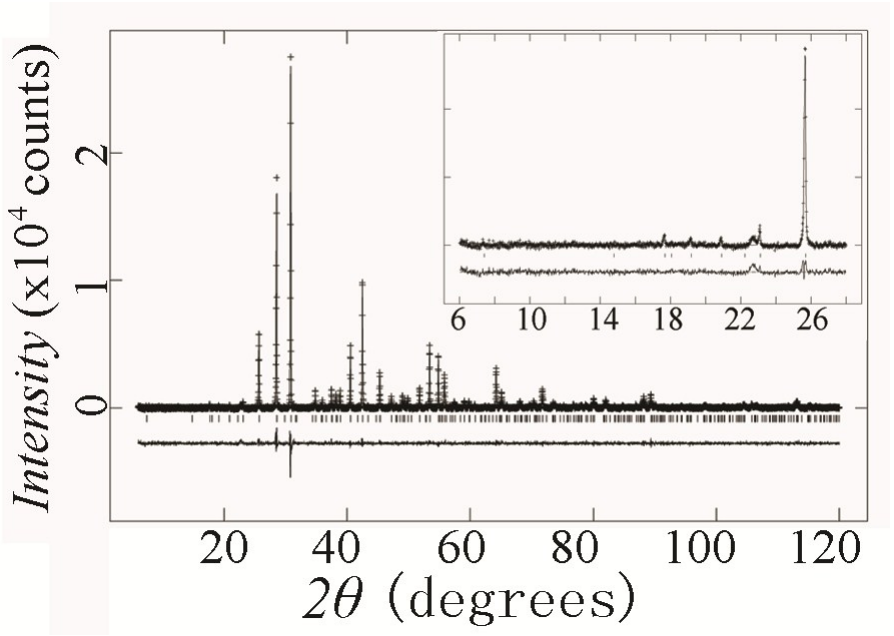

Figure S2. The fitted XRD plot of the $Ba_5Eu_{0.87}Mn_{4.02}O_{15-\delta}$ sample. The inset expands the low-angle regions

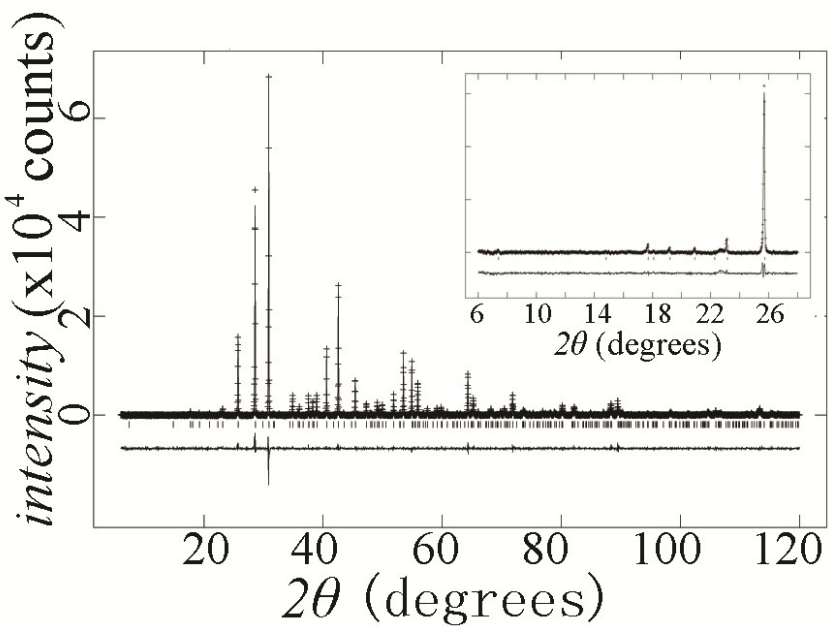

Figure S3. The fitted XRD plot of the $Ba_5Gd_{0.82}Mn_{4.17}O_{15-\delta}$ sample. The inset expands the low-angle regions

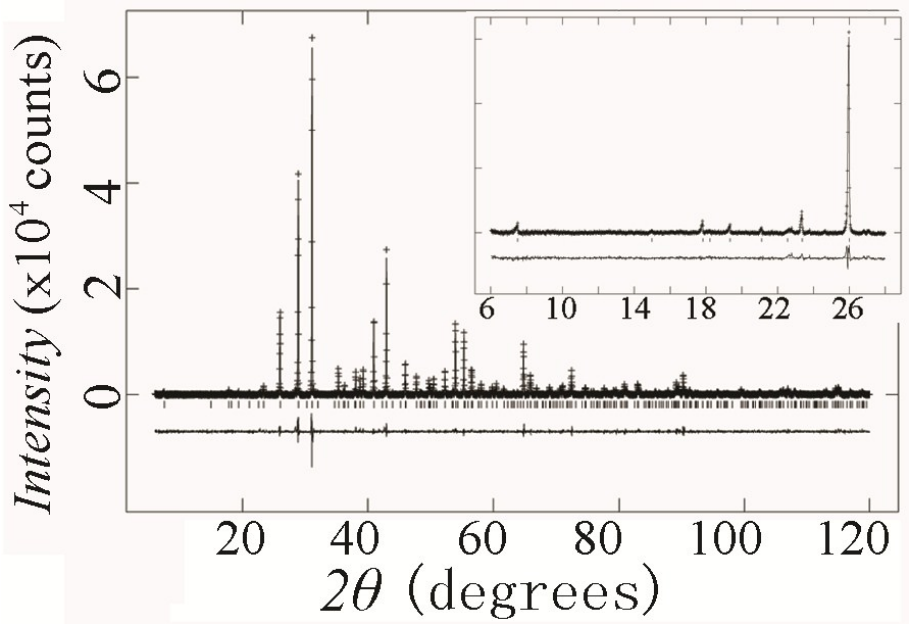

Figure S4. The fitted XRD plot of the $Ba_5Tb_{0.85}Mn_{4.15}O_{15-\delta}$ sample. The inset expands the low-angle regions

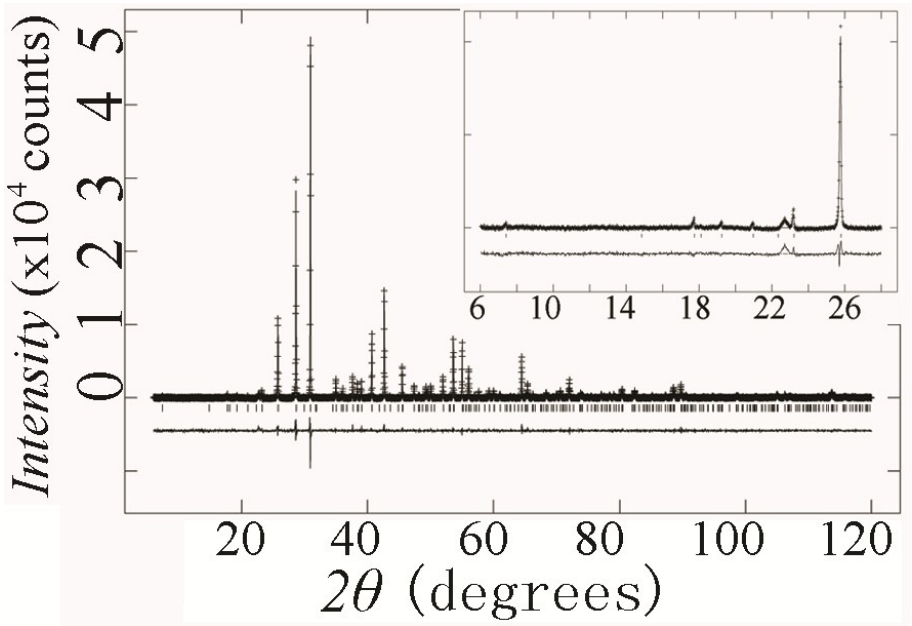

Figure S5. The fitted XRD plot of the $Ba_5Dy_{0.86}Mn_{4.12}O_{15-\delta}$ sample.The inset expands the low-angle regions

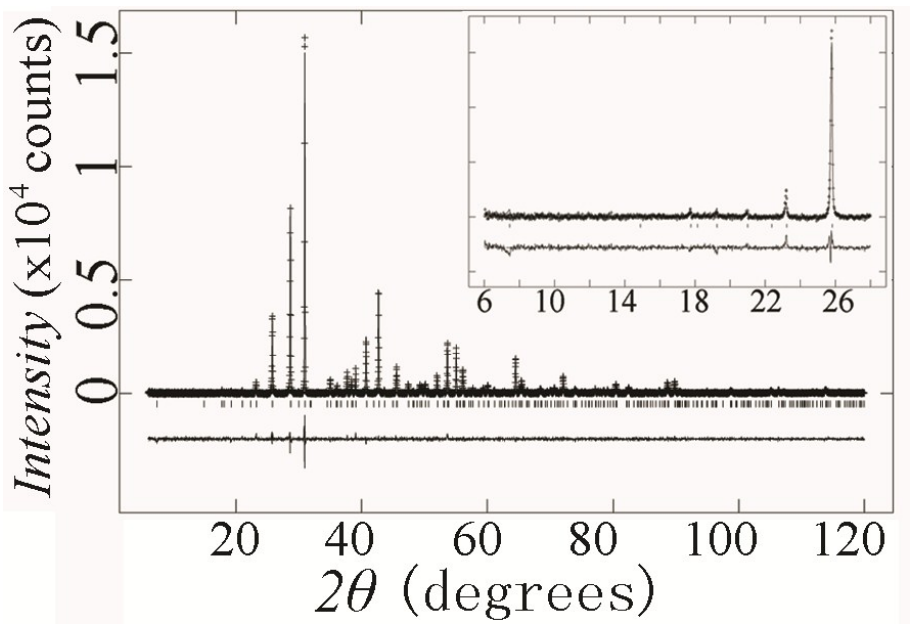

Figure S6. The fitted XRD plot of the $Ba_5Ho_{0.86}Mn_{4.12}O_{15-\delta}$ sample. The inset expands the low-angle regions

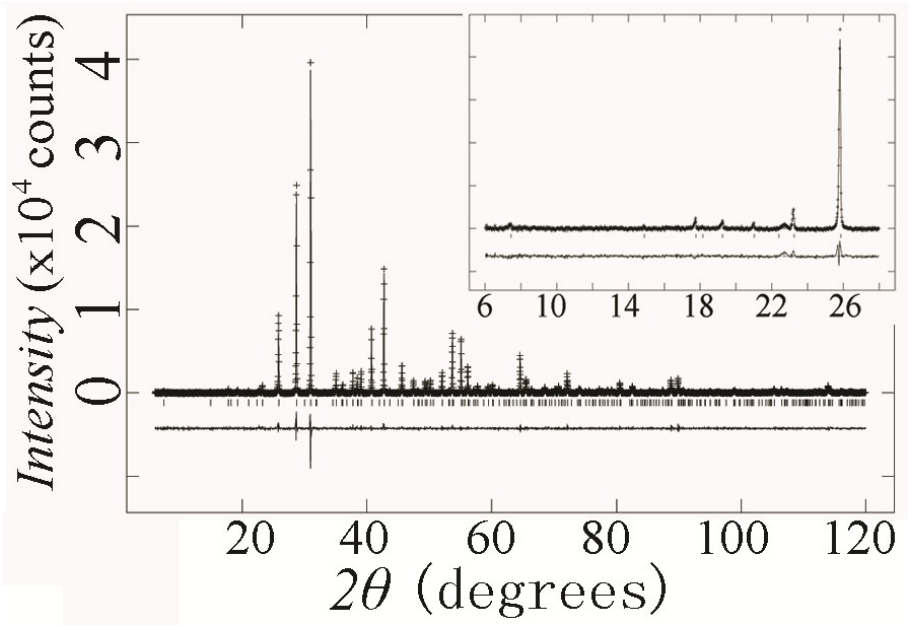

Figure S7. The fitted XRD plot of the $Ba_5Er_{0.82}Mn_{4.17}O_{15-\delta}$ sample. The inset expands the low-angle regions

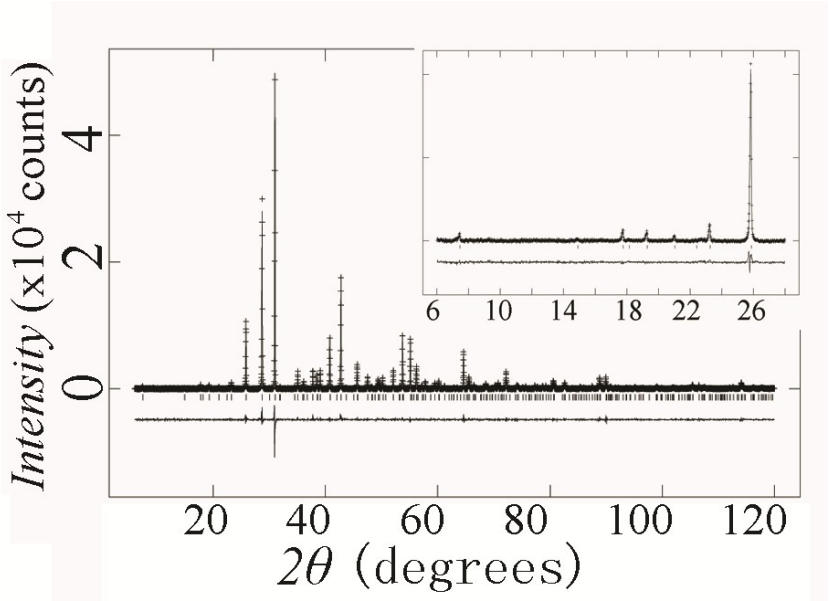

Figure S8. The fitted XRD plot of the $Ba_5Tm_{0.80}Mn_{4.14}O_{15-\delta}$ sample. The inset expands the low-angle regions

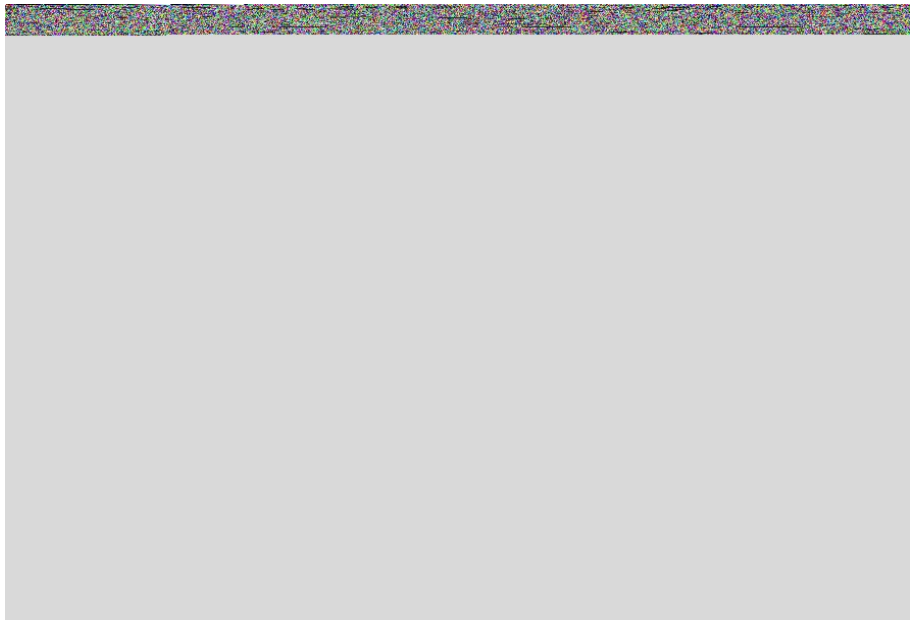

Figure S9. The fitted XRD plot of the $Ba_5Yb_{0.83}Mn_{4.17}O_{15-\delta}$ sample. The inset expands the low-angle regions

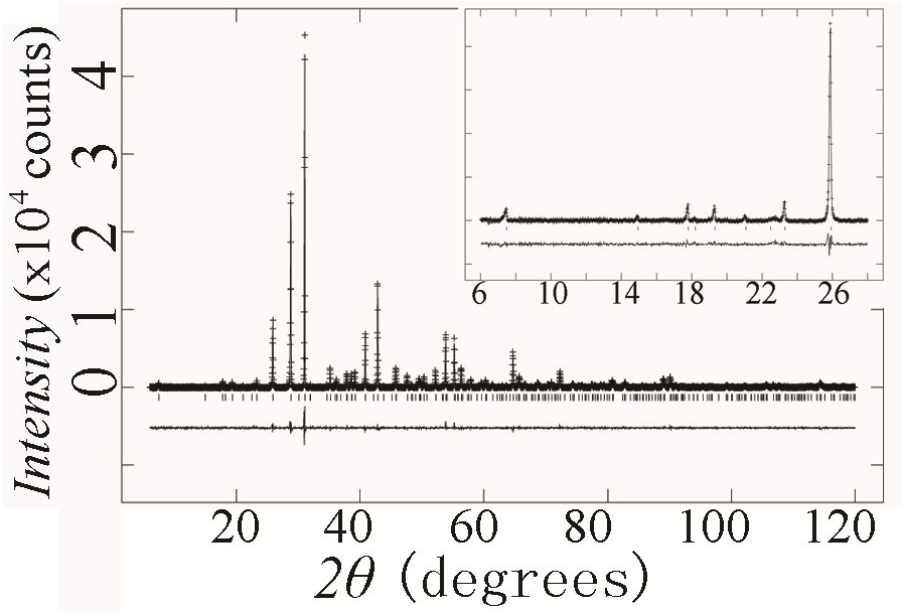

Figure S10. The fitted XRD plot of the $Ba_5Lu_{0.78}Mn_{4.21}O_{15-\delta}$ sample. The inset expands the low-angle regions

TABLE S1. The structural parameters for $Ba_5Ln_{1-x}Mn_{4+y}O_{15-\delta}$ from fits to x-ray diffraction profiles, showing lattice parameters, atomic coordinates, isotropic temperature (*U*) factors for the cation sites (oxygen atom values were fixed to be 0.025 Å), and M-O and Mn-Mn distances. The structure has space group $P6_3/mmc$. Sites: Ba1: 2d (⅔ ⅓ ¼); Ba2: 4f (⅔ ⅓ z_1); Ba3: 4e (0 0 z_2); Ln: 2a(0 0 ½); Mn1: 4f (⅓ ⅔ z_3); Mn2: 4f (⅓ ⅔ z_4); O1: 6h(x_1 –x_1 ¼); O2: 12k (x_2 –x_2 z_5); O3: 12k (x_3 –x_3 z_6)

Ln	*a*/Å	*c*/Å	*V*/Å^3	*Ba1: 100xU /Å^2*	*Ba2: z_1*	*Ba2: 100xU,/Å^2*	*Ba3:z_2*	*Ba3: 100xU /Å^2*	*Ln: 100xU /Å^2*	*Mn1: z_3*	*Mn1: 100xU, /Å^2*	*Mn2: z_4*	*Mn2: 100xU /Å^2*	*O1: x_1*	*O2: x2*	*O2: z5*	*O3: x_3*	*O3: z_6*	*d_{Ln-O} / Å*	*$d^{[a]}_{Mn1-O}$ / Å*	*$d^{[a]}_{Mn2-O}$ / Å*	*$d_{Mn1-Mn2}$ / Å*	*$d_{Mn2-Mn2}$ / Å*
Sm	5.7978(1)	24.0387(4)	699.79(2)	1.0(2)	0.4392(1)	1.1(1)	0.3419(1)	0.8(1)	2.1(2)	0.4040(3)	0.3(3)	0.2995(3)	2.4(3)	0.179(2)	0.177(1)	0.4445(7)	0.488(1)	0.3505(6)	2.22(1)	1.93(1)	1.97(1)	2.52(1)	2.37(1)
Eu	5.7957(1)	23.9851(3)	697.72(2)	1.5(2)	0.4396(1)	1.7(1)	0.3422(1)	1.4(1)	2.2 (2)	0.4042(3)	1.4(3)	0.2996(3)	2.8(3)	0.186(2)	0.176(2)	0.4456(7)	0.485(1)	0.3510(5)	2.20(1)	1.93(1)	1.93(1)	2.51(1)	2.38(1)
Gd	5.7898(1)	23.9556(3)	695.44(1)	1.3(1)	0.4400(1)	1.7(1)	0.3423(1)	1.5(1)	1.7(1)	0.4042(2)	1.9(2)	0.300 (3)	2.7(2)	0.183(2)	0.175(1)	0.4471(6)	0.484(1)	0.3511(5)	2.17(1)	1.93(1)	1.93(1)	2.49(1)	2.41(1)
Tb	5.7508(1)	23.6530(3)	677.44(1)	1.7(1)	0.4417(1)	1.6(1)	0.3441(1)	1.3(1)	2.6(1)	0.4060(3)	1.7(2)	0.3013(3)	2.2(2)	0.181(2)	0.172(1)	0.4490(6)	0.484(1)	0.3524(5)	2.10(1)	1.93(1)	1.94(1)	2.48(1)	2.43(1)
Dy	5.7772(2)	23.8843(6)	690.36(5)	1.3 (1)	0.4408(1)	1.6(1)	0.3427(1)	1.5(1)	2.8(1)	0.4044(3)	1.5 (3)	0.3003(3)	2.7(2)	0.181(2)	0.177(1)	0.4466(6)	0.485(1)	0.3512(5)	2.18(1)	1.92(1)	1.94(1)	2.49(1)	2.40(1)
Ho	5.7736(1)	23.8554(4)	688.66(2)	1.7(2)	0.4417(1)	1.7(1)	0.3431(1)	1.4 (1)	4.0(2)	0.4041(3)	0.4(2)	0.2993(3)	2.6(3)	0.187(2)	0.175(2)	0.4442(7)	0.480(1)	0.3502(6)	2.20(1)	1.90(1)	1.89(1)	2.50(1)	2.35(1)
Er	5.7695(1)	23.8303(3)	686.96(2)	1.4 (1)	0.4415(1)	1.6(1)	0.3432(1)	1.6(1)	2.7 (1)	0.4048(3)	1.7 (2)	0.3002(3)	2.5(2)	0.184(2)	0.175(1)	0.4473(6)	0.484(1)	0.3515(5)	2.15(1)	1.92(1)	1.93(1)	2.49(1)	2.39(1)
T m	5.7658(1)	23.8029(3)	685.31(1)	1.5(1)	0.4417(1)	1.7(1)	0.3434(1)	1.6(1)	2.0(1)	0.4057(2)	2.2(2)	0.3005(3)	2.4(2)	0.184(2)	0.173(1)	0.4480(5)	0.485(1)	0.3511(5)	2.13(1)	1.94(1)	1.92(1)	2.50(1)	2.40(1)
Yb	5.7639(2)	23.766 (1)	683.80(7)	1.0 (2)	0.4424(1)	1.3 (1)	0.3440(1)	0.9(1)	1.7(2)	0.4054(3)	0.7(3)	0.2996(4)	2.5(3)	0.183(2)	0.174(2)	0.4474(9)	0.488(2)	0.3508(7)	2.14(1)	1.95(1)	1.94(1)	2.52(1)	2.36(1)
Lu	5.7573(1)	23.7459(3)	681.63(2)	2.7 (1)	0.4423(1)	2.8(1)	0.3440(1)	2.5(1)	2.6(1)	0.4062(2)	2.9(2)	0.3010(2)	3.3(2)	0.188(1)	0.172(1)	0.4490(4)	0.485(1)	0.3508(4)	2.10(1)	1.95(1)	1.90(1)	2.50(1)	2.42(1)

[a] the average bond length

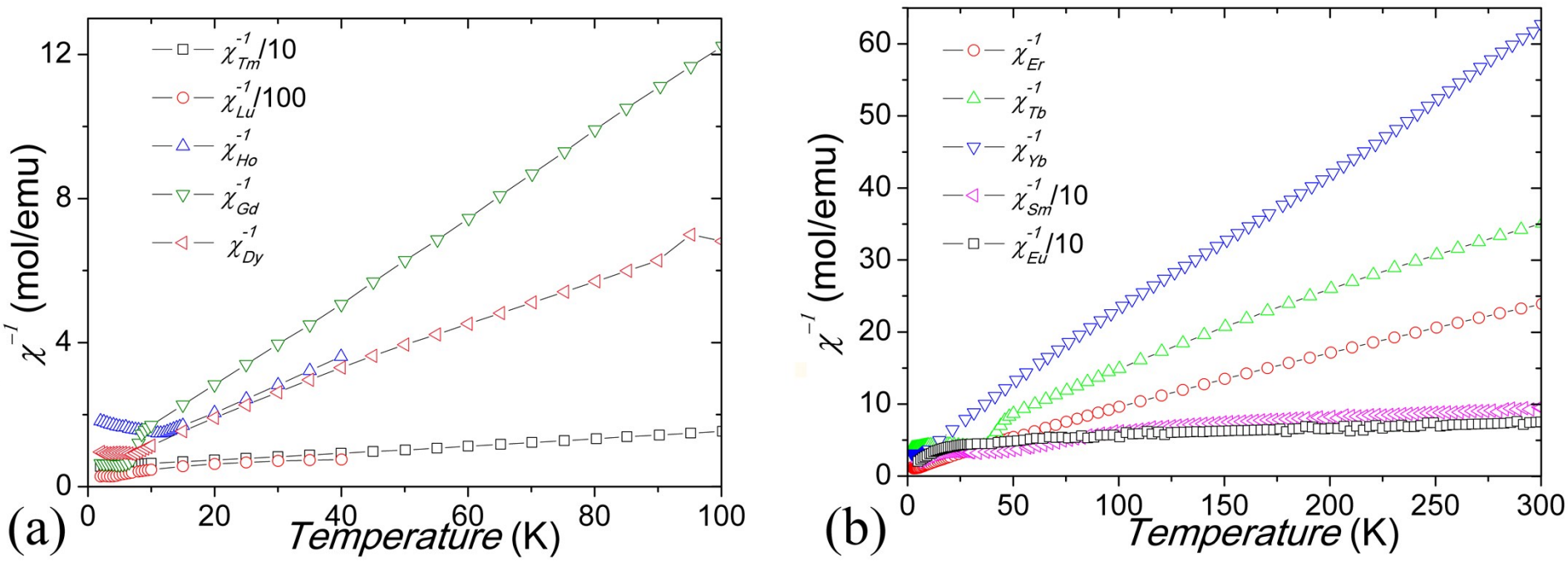

Figure S11. inverse susceptibility χ^{-1} vs. temperature for $Ba_5Ln_{1-x}Mn_{4+y}O_{15-\delta}$ (a) *Ln*=Tm, Lu, Ho, Gd and Dy at 20 Oe; (b) *Ln* = Er, Tb, Yb, Eu and Sm at 1000 Oe. For clarity, χ^{-1} are scaled by 0.1 for the Sm, Eu and Tm samples, and by 0.01 for the Lu sample.