Supporting Information

Anomalous Near-infrared Emission and the Underlying "Structure-Luminescence" Correlation in the Multi-Peak Emission System of $KScF_4$: Yb^{3+}, Mn^{2+}

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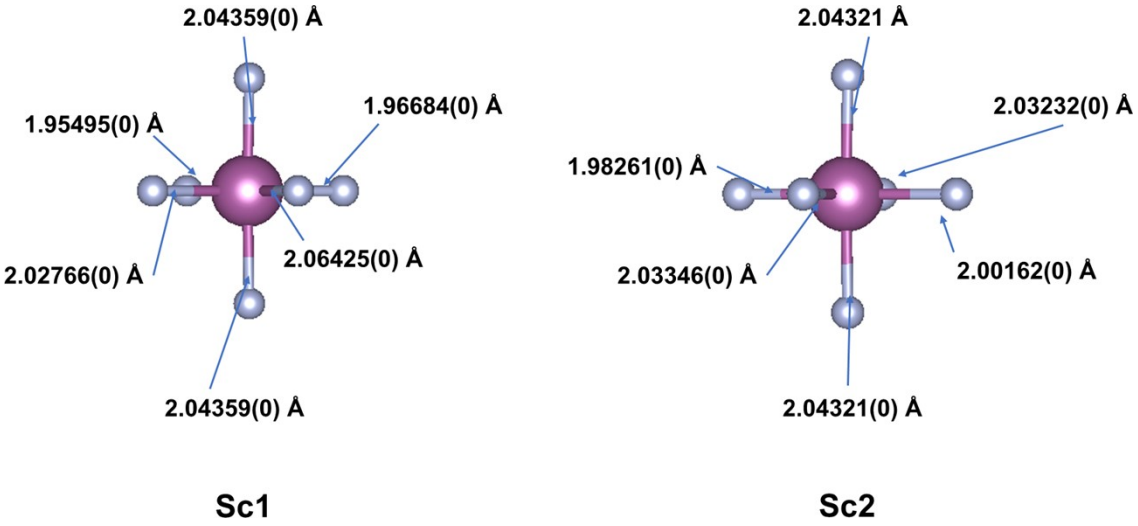

Fig. S1 The bond length of each Sc-F is in $[Sc1F_6]$ and $[Sc2F_6]$ octahedrons.

The average bond lengths of Sc-F in $[Sc1F_6]$ and $[Sc2F_6]$ octahedrons is 2.0168 Å and 2.0227 Å, respectively. In addition, the distortion indices of $[Sc1F_6]$ and $[Sc2F_6]$ octahedrons are calculated to be 0.01864 and 0.01021, respectively, according to the fomular $D_{dis} = \frac{1}{n}\sum_{i=1}^{n}\frac{|d_i - d_{av}|}{d_{av}}$.[1]

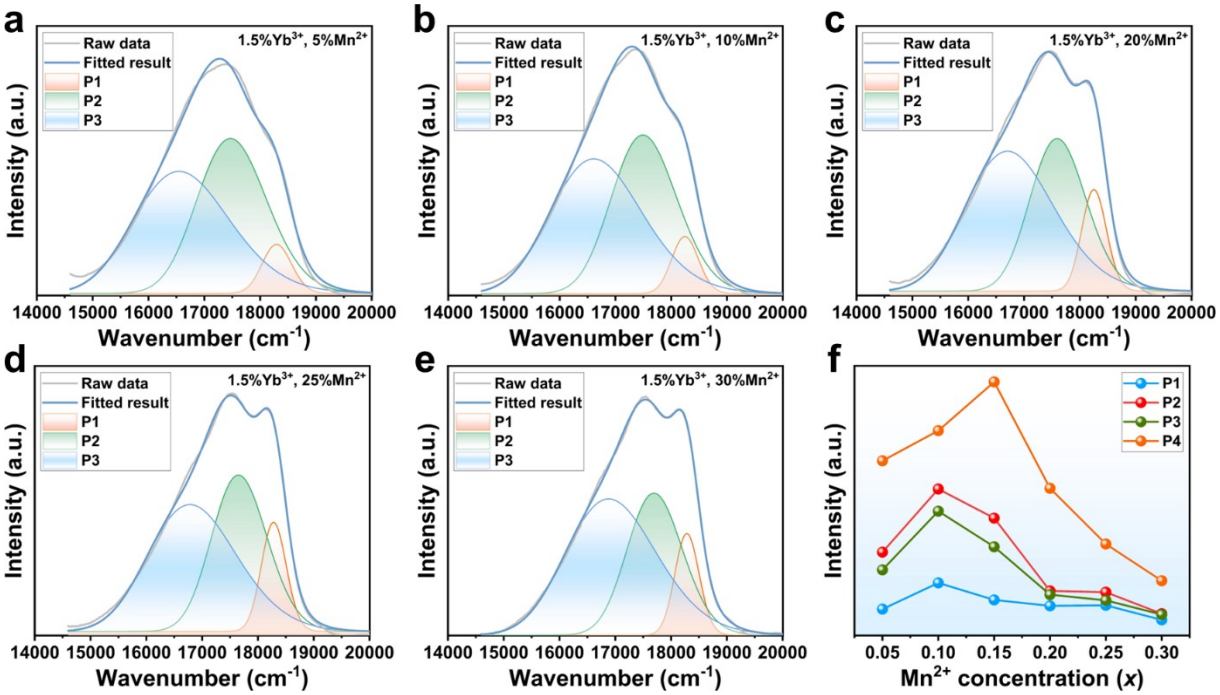

Fig. S2 (a-e) Gaussian decomposition of the emission peaks of $KScF_4$: 1.5%Yb^{3+}, $x$$Mn^{2+}$ (x = 5%-30%). (f) Variation trends of P1, P2, P3 and P4 emission intensities with Mn^{2+} concentration.

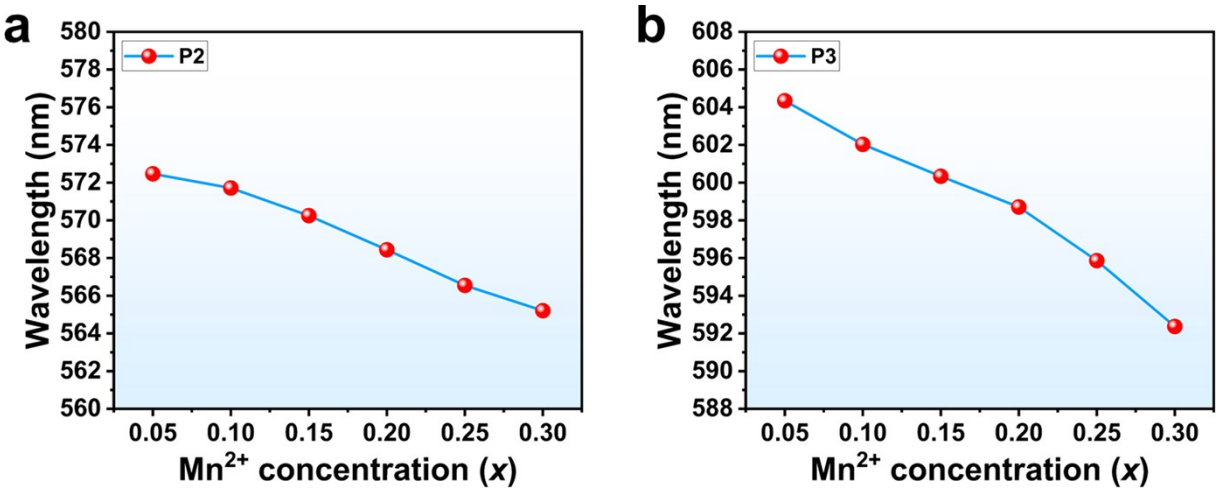

Fig. S3 Peak positions of (a) P2 and (b) P3 as a function of Mn^{2+} concentration.

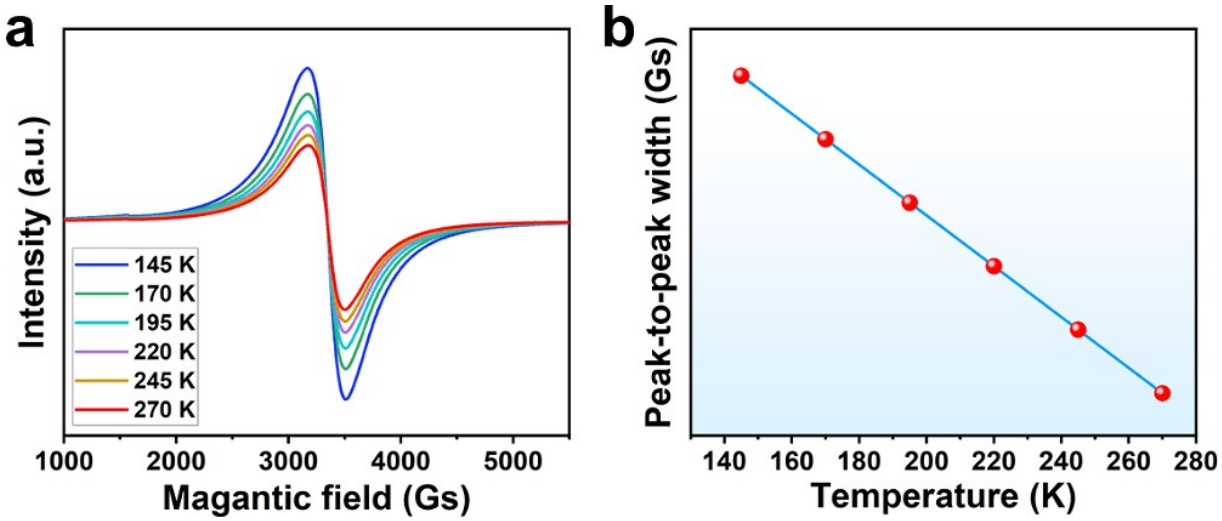

Fig. S4 (a) Variable Temperature ERP of $KScF_4$: 1.5%Yb^{3+}, 5%Mn^{2+}. (b) Peak-to-peak width with temperature in variable Temperature ERP of $KScF_4$: 1.5%Yb^{3+}, 5%Mn^{2+}.

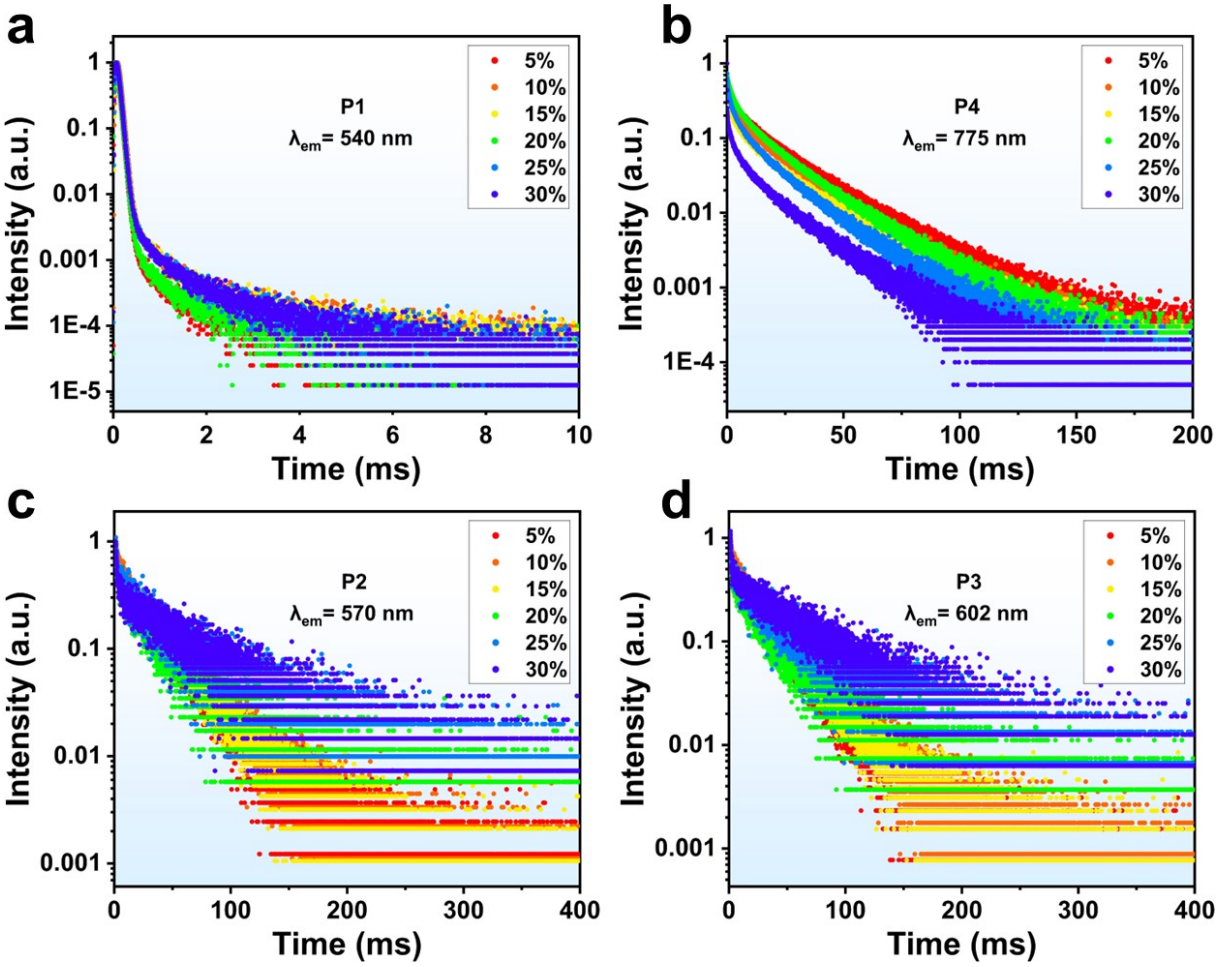

Fig. S5 Fluorescence decay curves of P1-P4 upon 396 nm excitation.

Table S1 Fluorescence lifetime of P1-P6.

Mn^{2+} concentration (x)	τ P1 (ms)	τ P2 (ms)	τ P3 (ms)	τ P4 (ms)	τ P5 (ms)	τ P6 (ms)
5%	0.07155	28.2841	28.1640	17.5457	1.7128	14.6435
10%	0.07073	27.0738	26.6328	15.0310	1.5637	13.3748
15%	0.06843	25.7021	25.9700	14.9756	1.3724	12.7804
20%	0.06612	24.6289	24.1434	13.8272	1.0401	12.2440
25%	0.06564	22.0052	22.3478	10.8412	0.9826	11.2419
30%	0.06464	20.3843	20.4329	7.28378	0.9714	10.8110

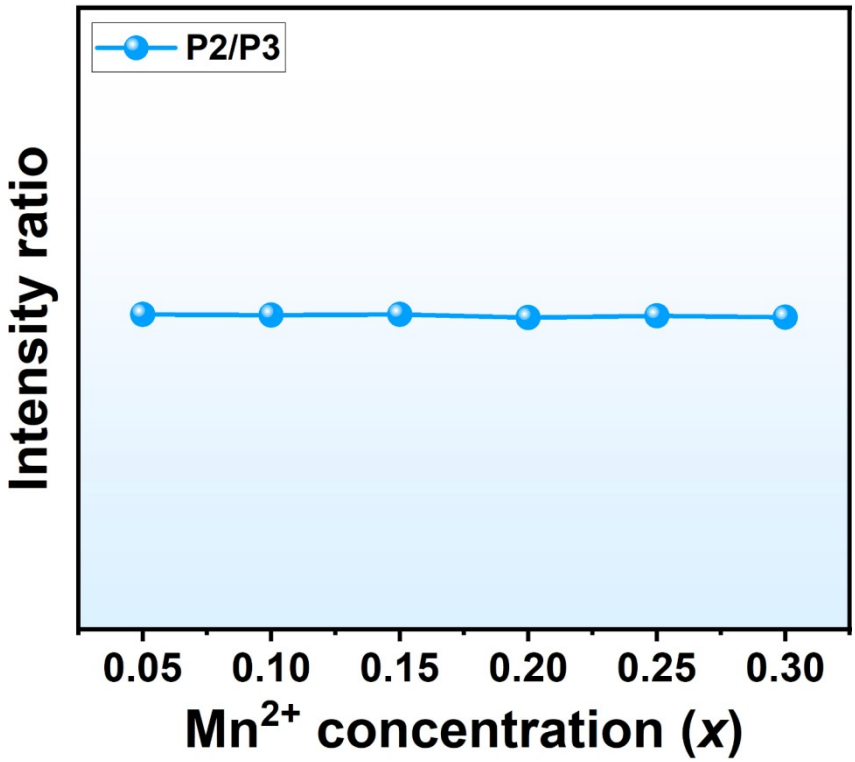

Fig. S6 The emission intensity ratio of P2 to P3 with changing Mn^{2+} concentration.

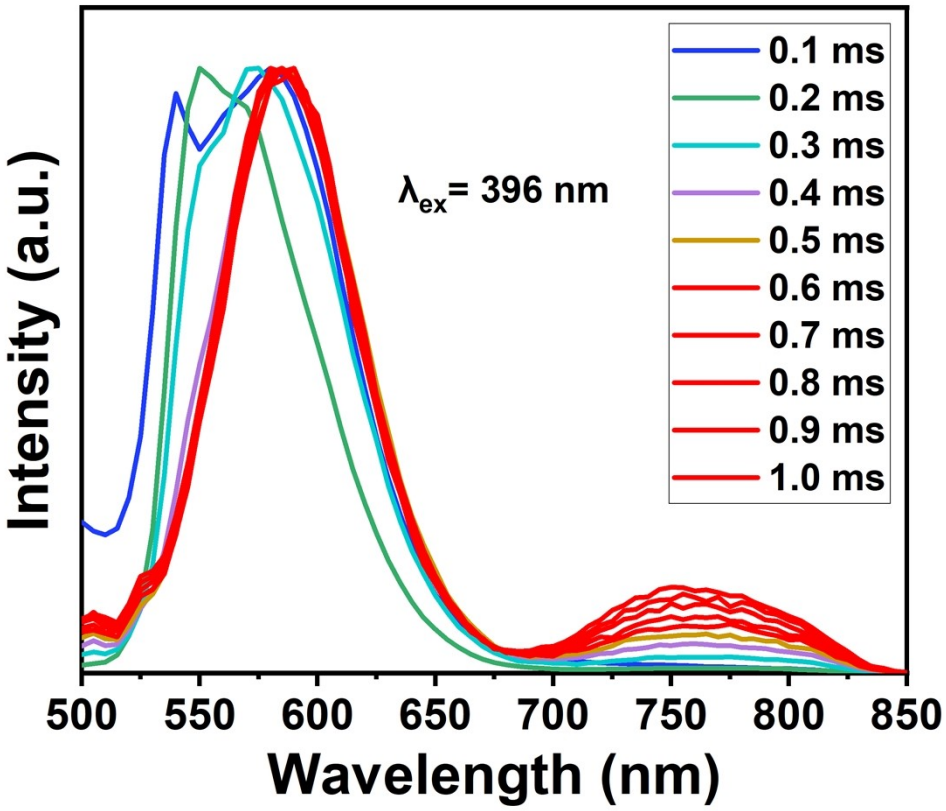

Fig. S7 The time-resolved spectrum of $KScF_4$: 1.5%Yb^{3+}, 20%Mn^{2+} excited by 396 nm light. (The difference between the spectra which were shown in the original manuscript lies in the difference between the measurement and calibration of the instrument.).

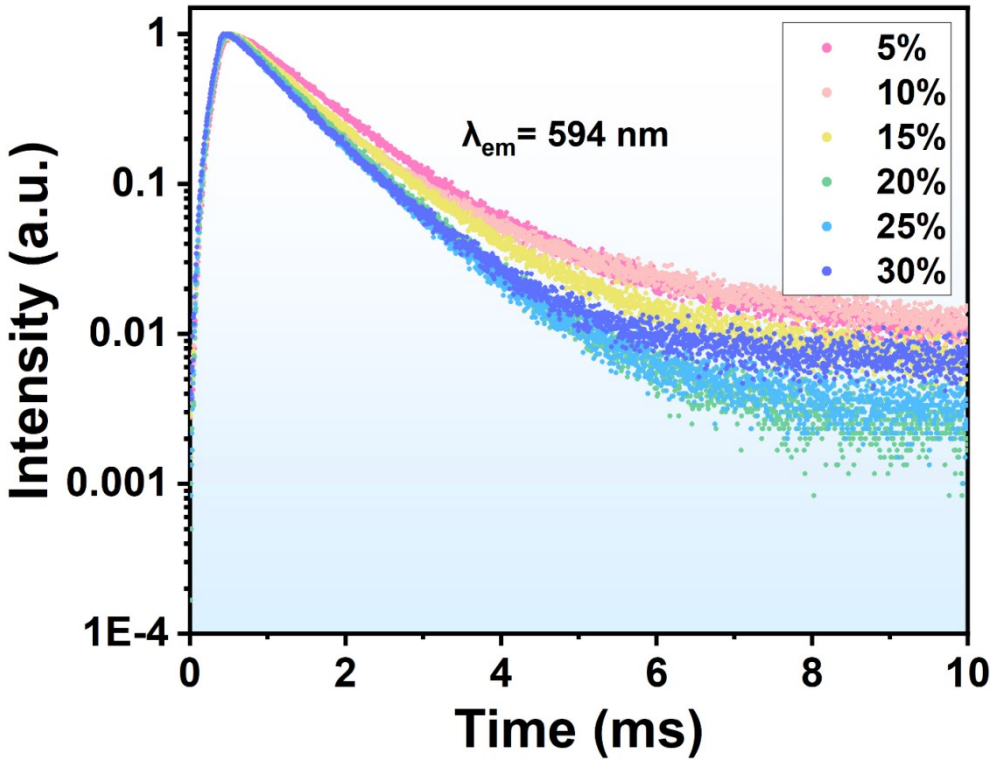

Fig. S8 The initial 10 s of the UC decay curves of P5.

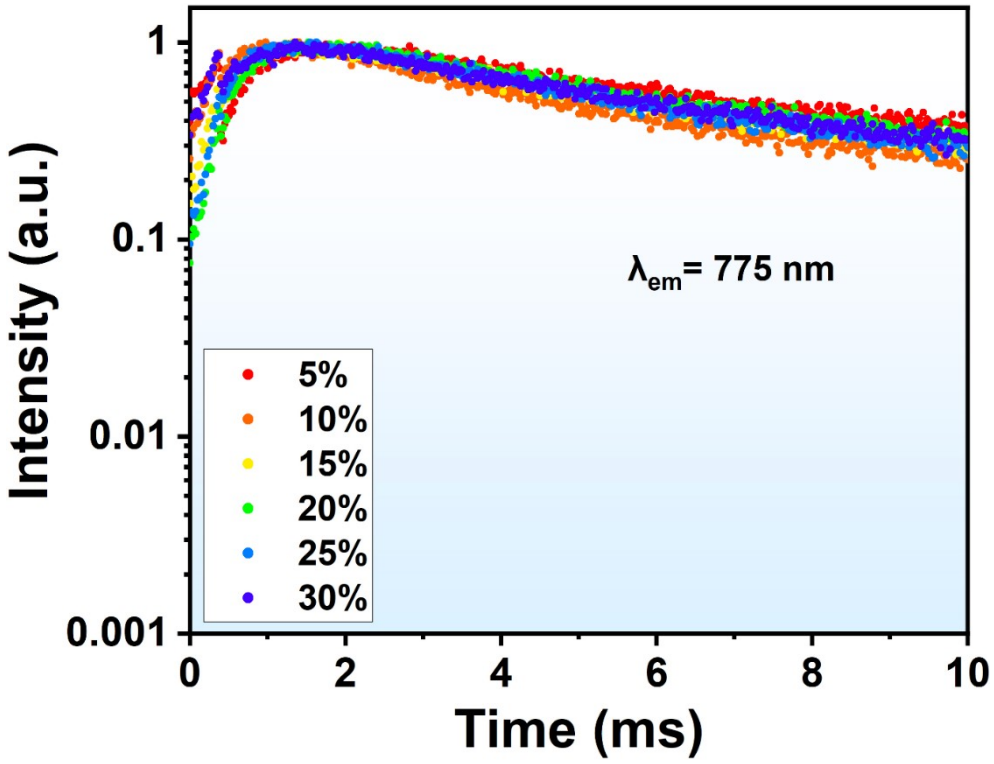

Fig. S9 The initial 10 s of the UC decay curves of P6.

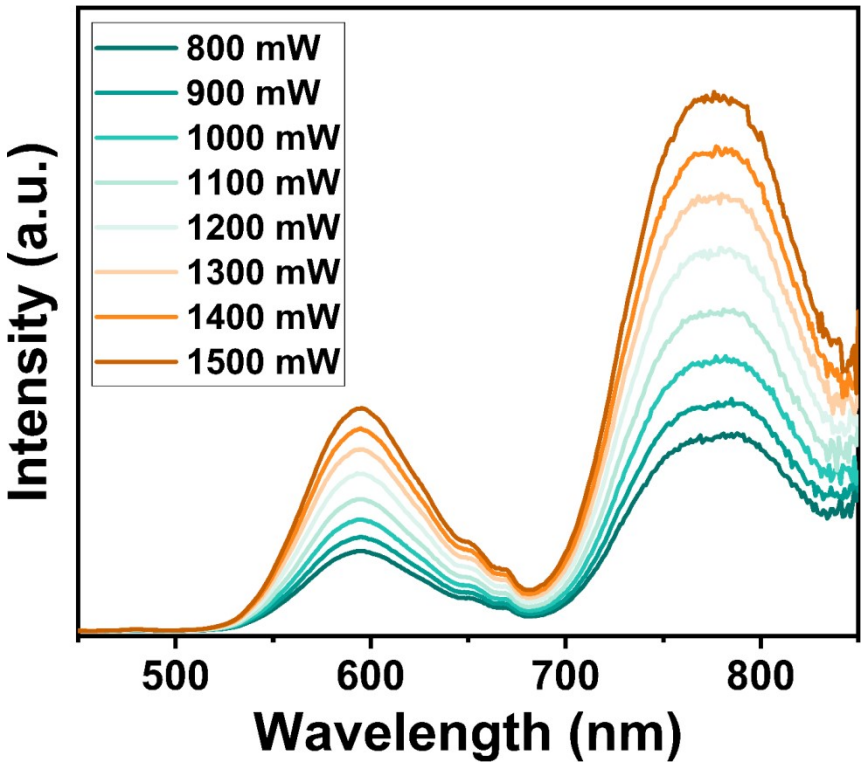

Fig. S10 Pump power-dependent UC emission spectra of $KScF_4$: 1.5%Yb^{3+}, 20%Mn^{2+}.

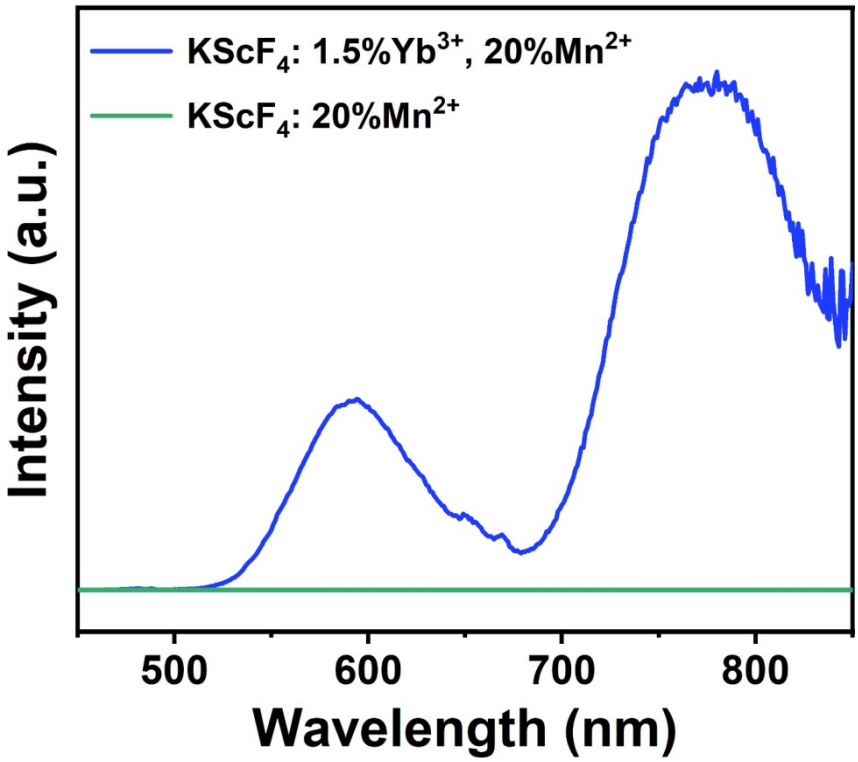

Fig. S11 UC emission spectra of $KScF_4$: 1.5%Yb^{3+}, 20%Mn^{2+} and $KScF_4$: 20%Mn^{2+}.

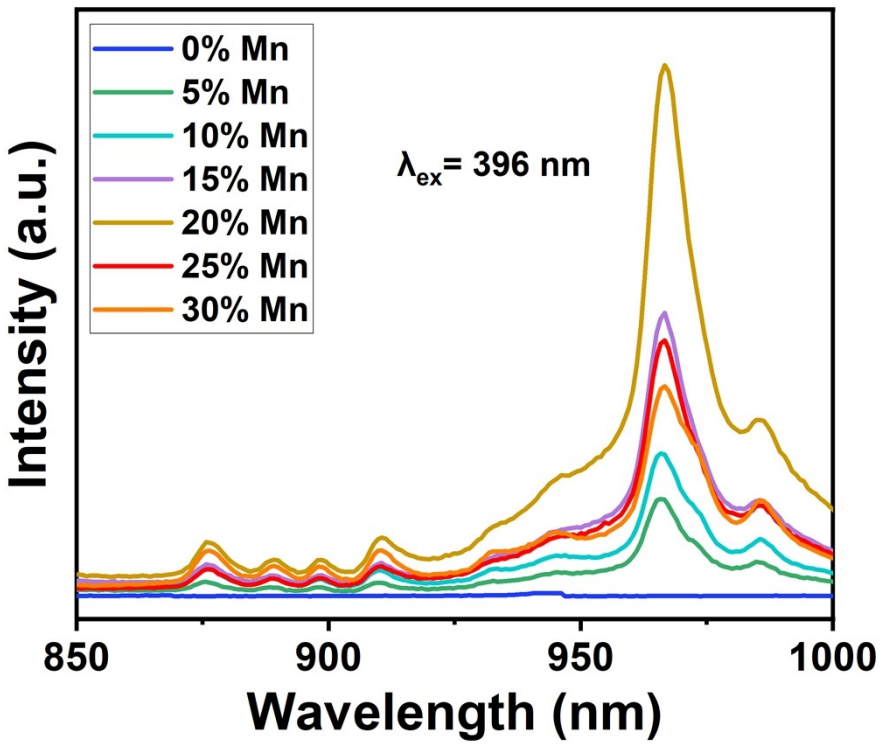

Fig. S12 The Stokes emission spectra of $KScF_4$: 1.5%Yb^{3+}, xMn^{2+} (x = 0%-30%) excited by 396 nm light.

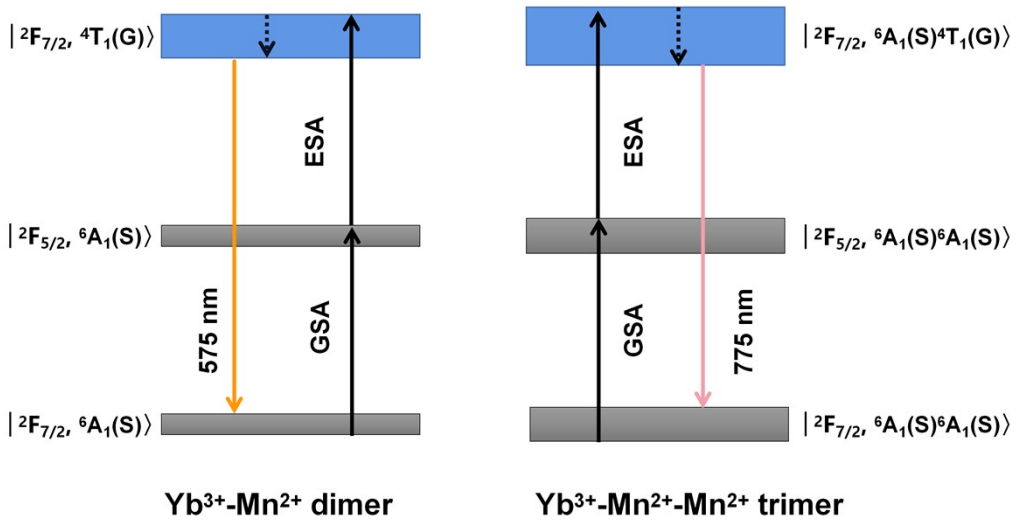

Fig. S13 UC luminescence mechanism diagram in $KScF_4$: 1.5%Yb^{3+}, xMn^{2+} (x = 0%-30%).

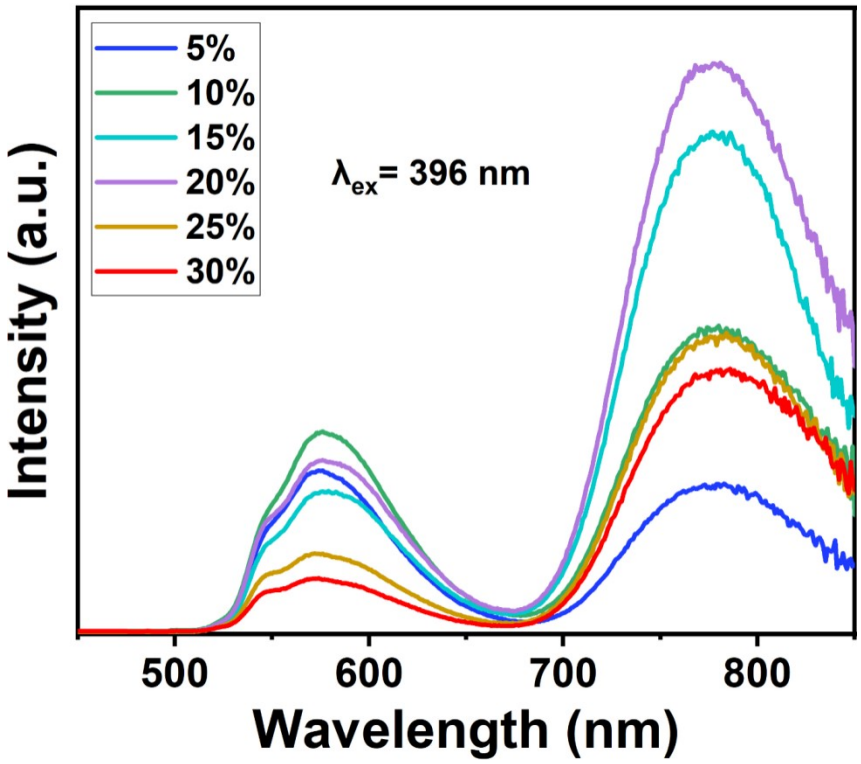

Fig. S14 The emission spectra of $KScF_4$: $x$$Mn^{2+}$ (x = 5%-30%) excited by 396 nm light.

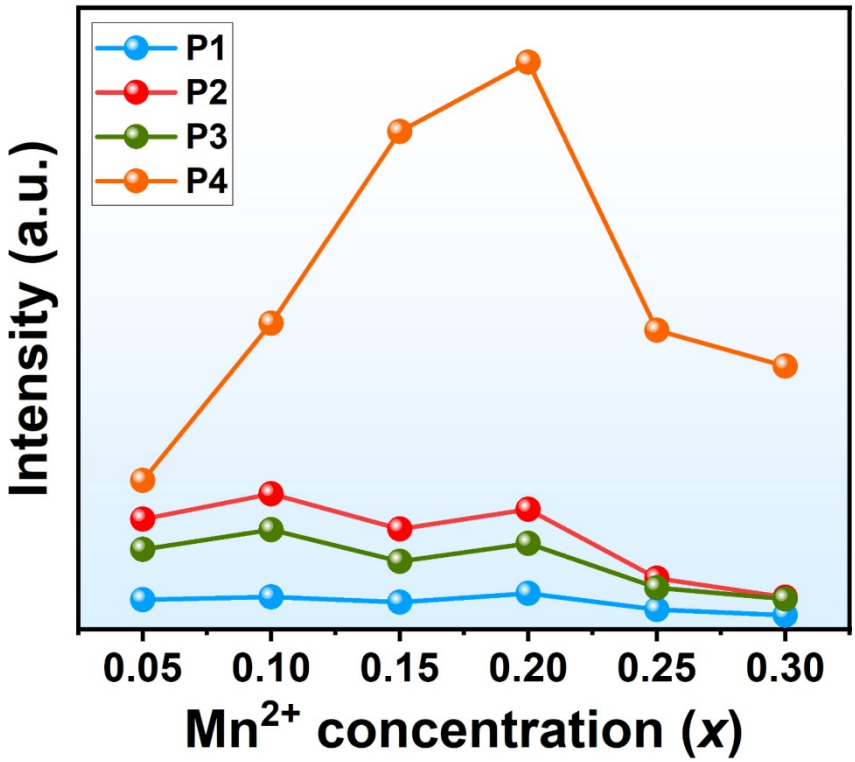

Fig. S15 Variation trends of P1, P2, P3 and P4 emission intensities with Mn^{2+} concentration.

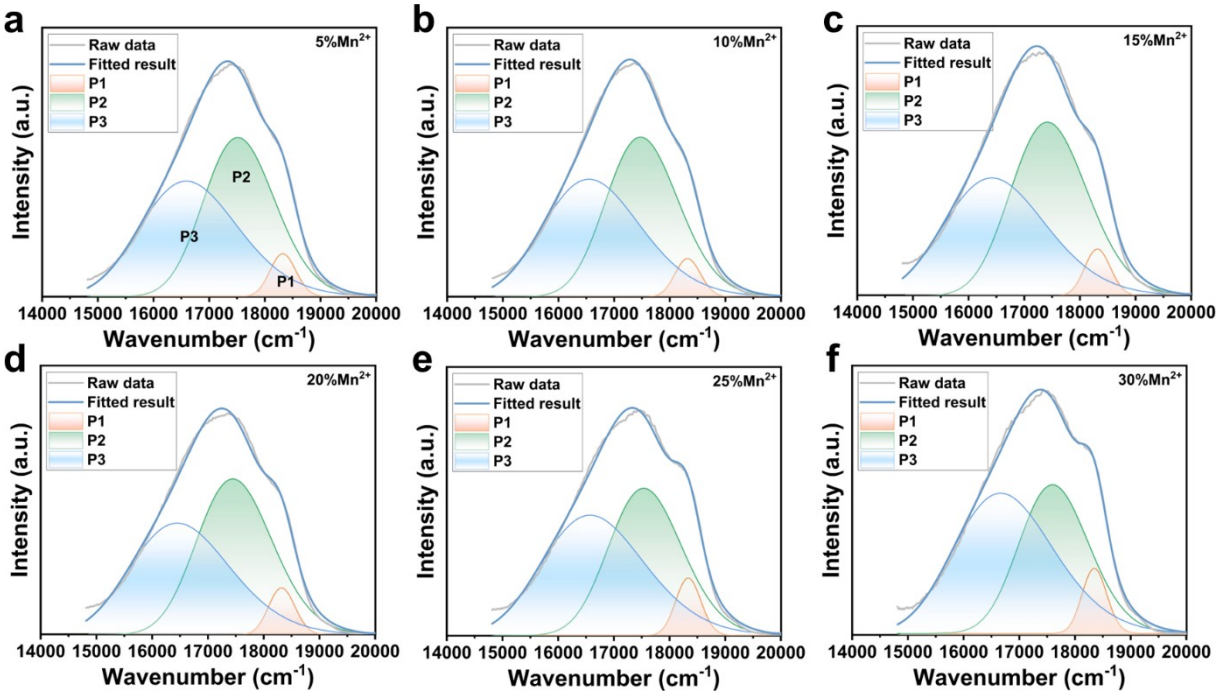

Fig. S16 Gaussian decomposition of the emission peaks of $KScF_4$: $x$$Mn^{2+}$ (x = 5%-30%).

Reference

[1] W. Zhou, Y. Ou, L. Huang, E. Song, F. Ma, Z. Xia, H. Liang, Q. Zhang, *Adv. Mater.* **2022**, *34*, 2206287.