Supporting Information

Variable Energy Transfer in One-Dimensional Chiral Mn/Cd-Based Halides and the Strong Stereo-Selective Fluorescence for Chiral Recognition

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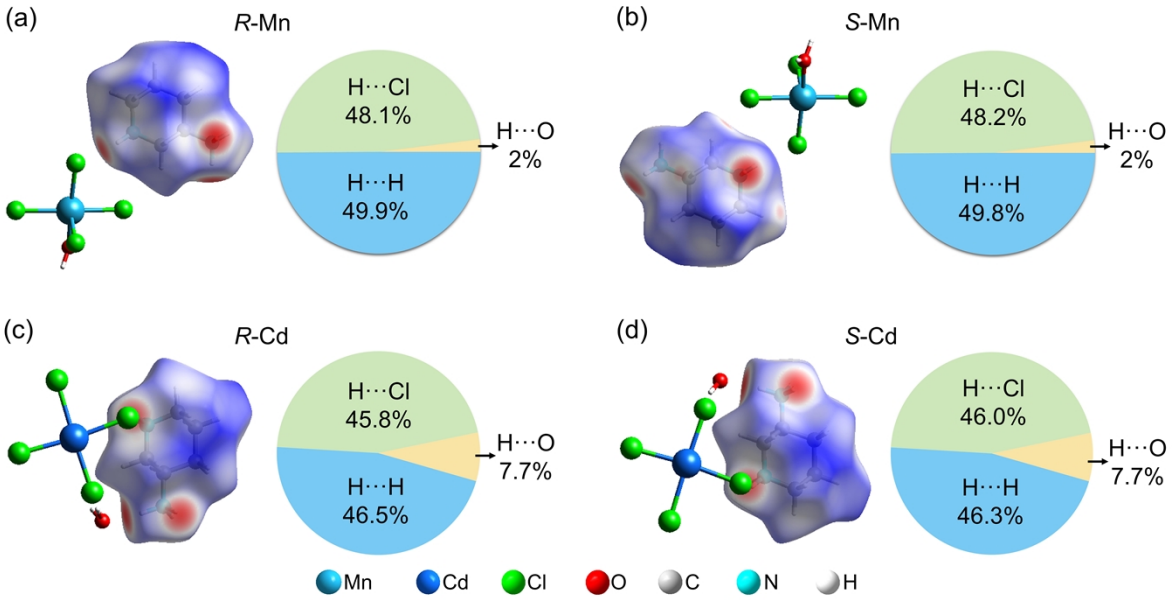

Fig. S1. The Hirshfeld surface analysis of organic cations and intermolecular interactions contribution diagram of *R*-Mn (a), *S*-Mn (b), *R*-Cd (c) and *S*-Cd (d) calculated by CrystalExplorer software.

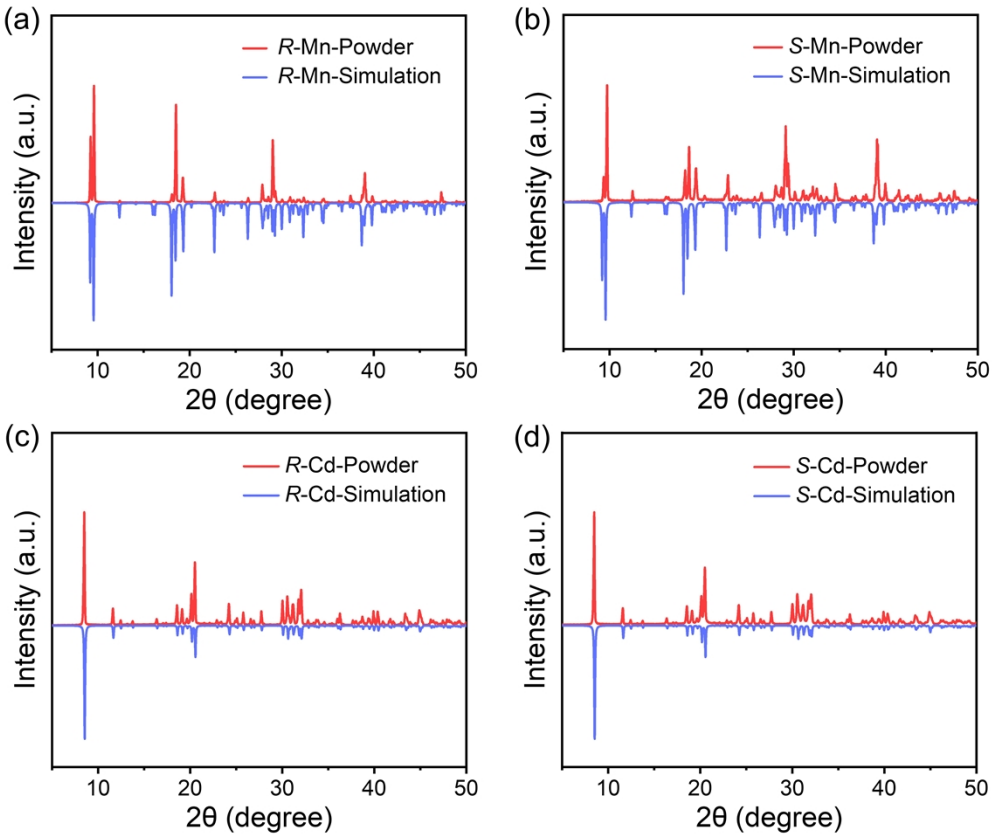

Fig. S2. Powder XRD of *R*-Mn (a), *S*-Mn (b), *R*-Cd (c) and *S*-Cd (d) compared with the simulated data from the single crystal structures.

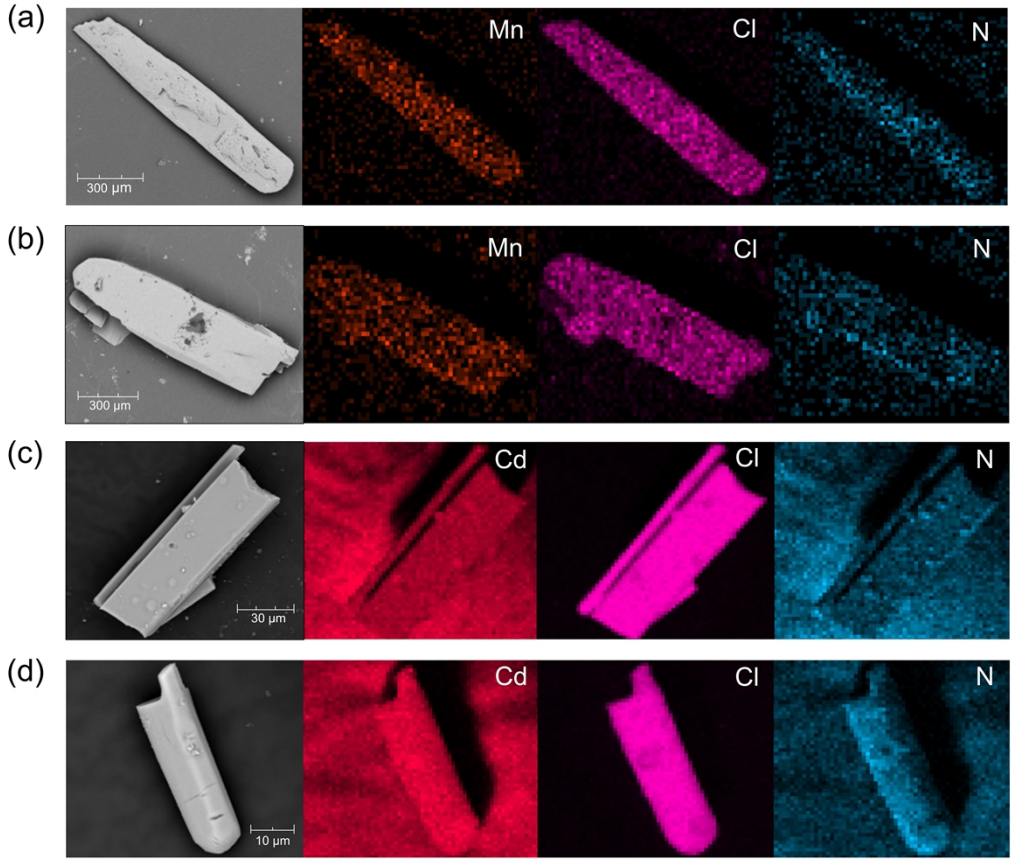

Fig. S3. SEM image and elemental mapping of Mn, Cl, and N of *R*-Mn (a) and *S*-Mn (b). SEM image and elemental mapping of Cd, Cl, and N of *R*-Cd (c) and *S*-Cd (d).

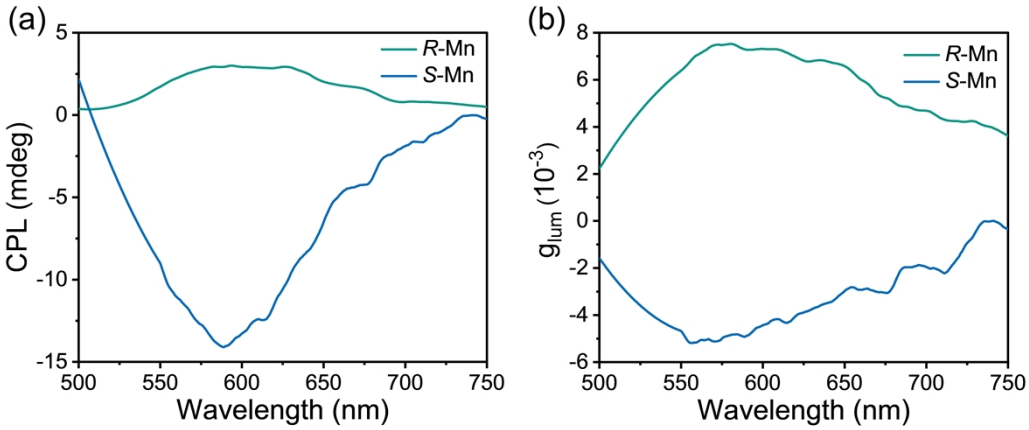

Fig. S4. (a) Circularly polarized luminescence (CPL) spectra of *R*/*S*-Mn. (b)The g_{lum} of *R*/*S*-Mn.

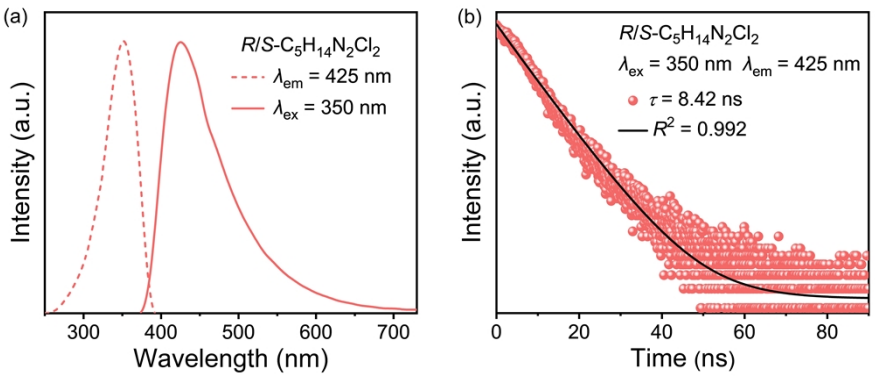

Fig. S5. (a) PLE and PL spectra of *R*/*S*-$C_5H_{14}N_2Cl_2$. (b) PL decay curve of *R*/*S*-$C_5H_{14}N_2Cl_2$.

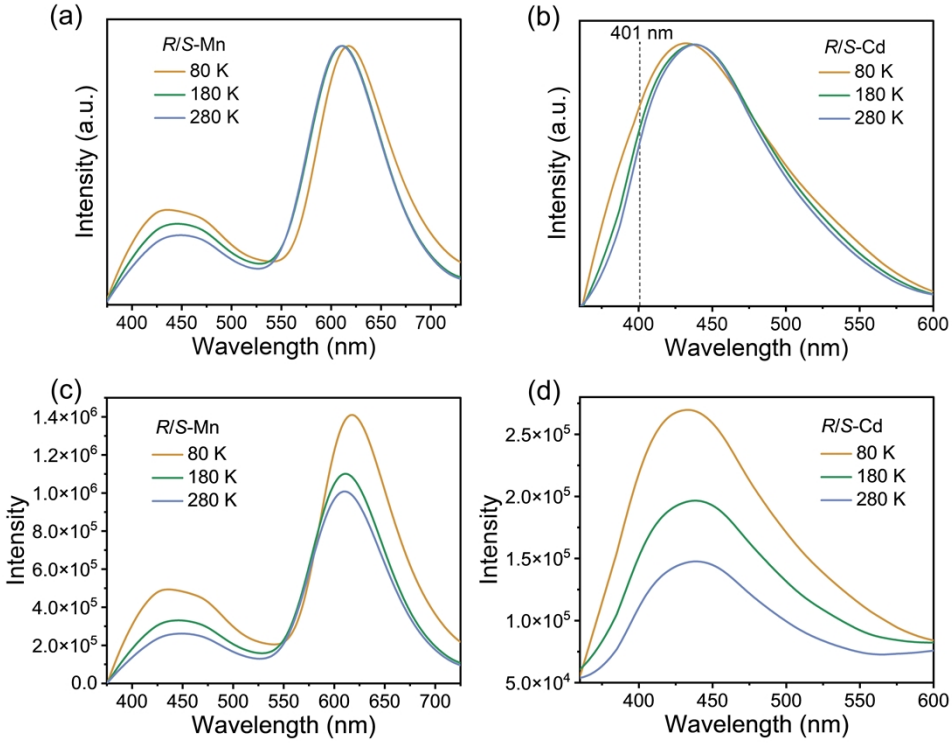

Fig. S6. (a) Normalized PL spectra of *R*/*S*-Mn at 80 k, 180 k and 280 k. (b) Normalized PL spectra of *R*/*S*-Cd at 80 k, 180 k and 280 k. (c) PL spectra of *R*/*S*-Mn at 80 k, 180 k and 280 k. (d) PL spectra of *R*/*S*-Cd at 80 k, 180 k and 280 k.

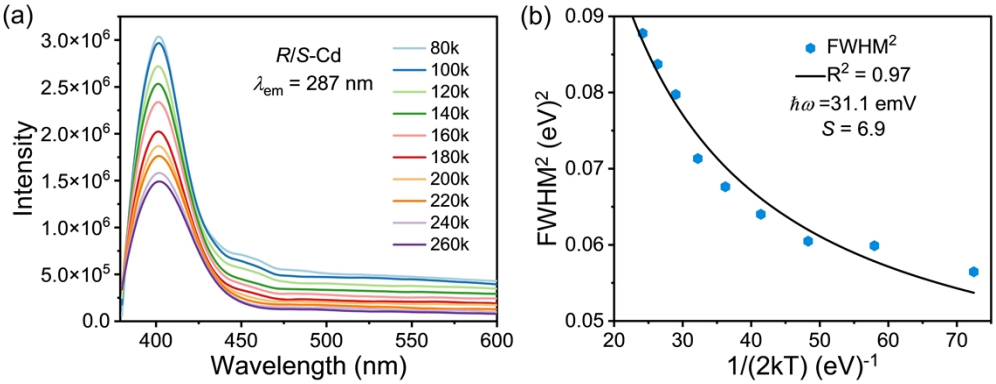

Fig. S7. (a) Temperature-dependent PL spectra of *R*/*S*-Cd at 287 nm excitation. (b) The $FWHM^2$ fitting curve of *R*/*S*-Cd as a function of 1/(2kT).

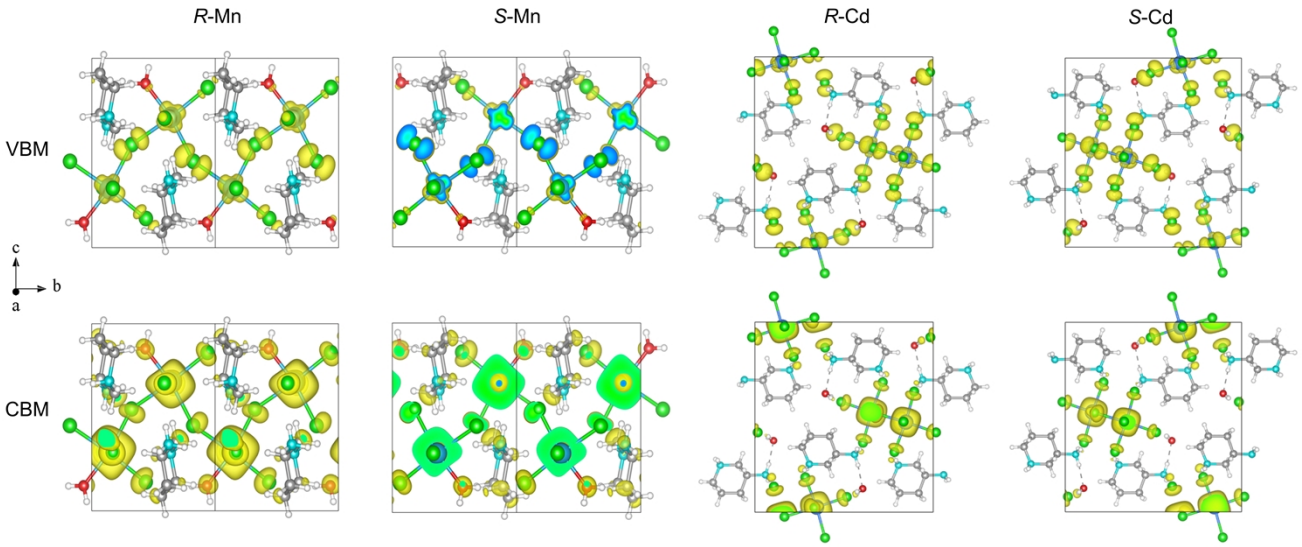

Fig. S8. The calculated charge densities of *R*-Mn, *S*-Mn, *R*-Cd and *S*-Cd.

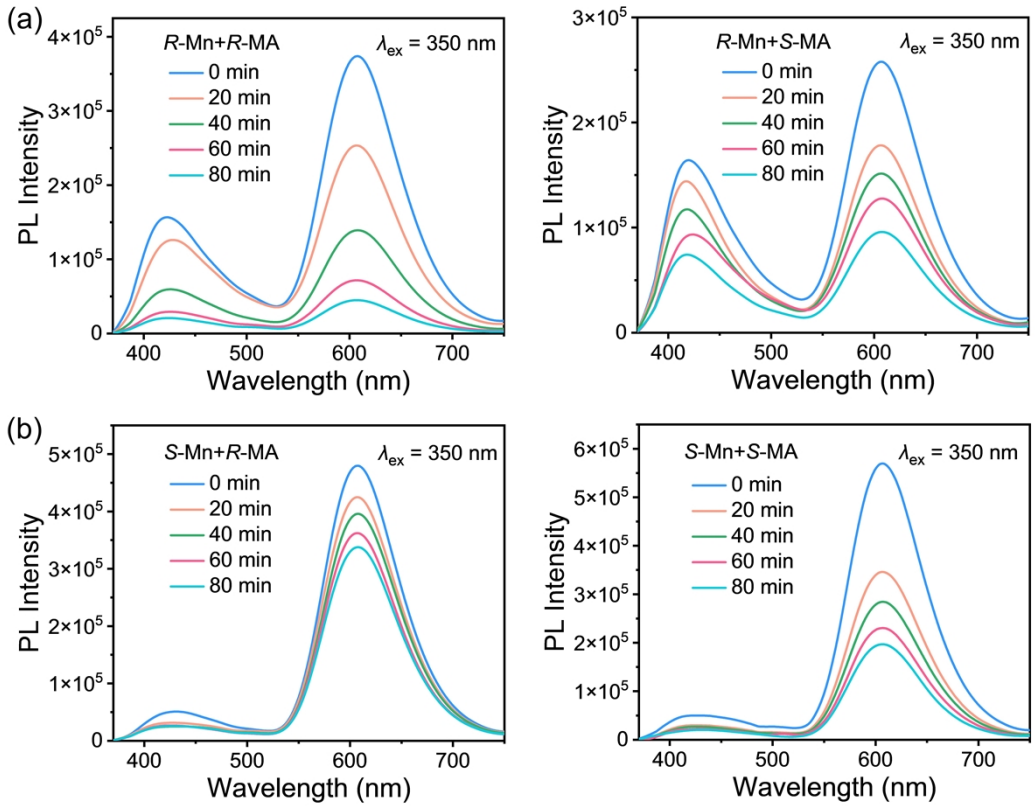

Fig. S9. PL intensity of *R*-Mn (a) and *S*-Mn (b) in the presence of *R* or *S*-MA over time. λ_{ex} = 350 nm, slit = 1.7/1.7 nm.

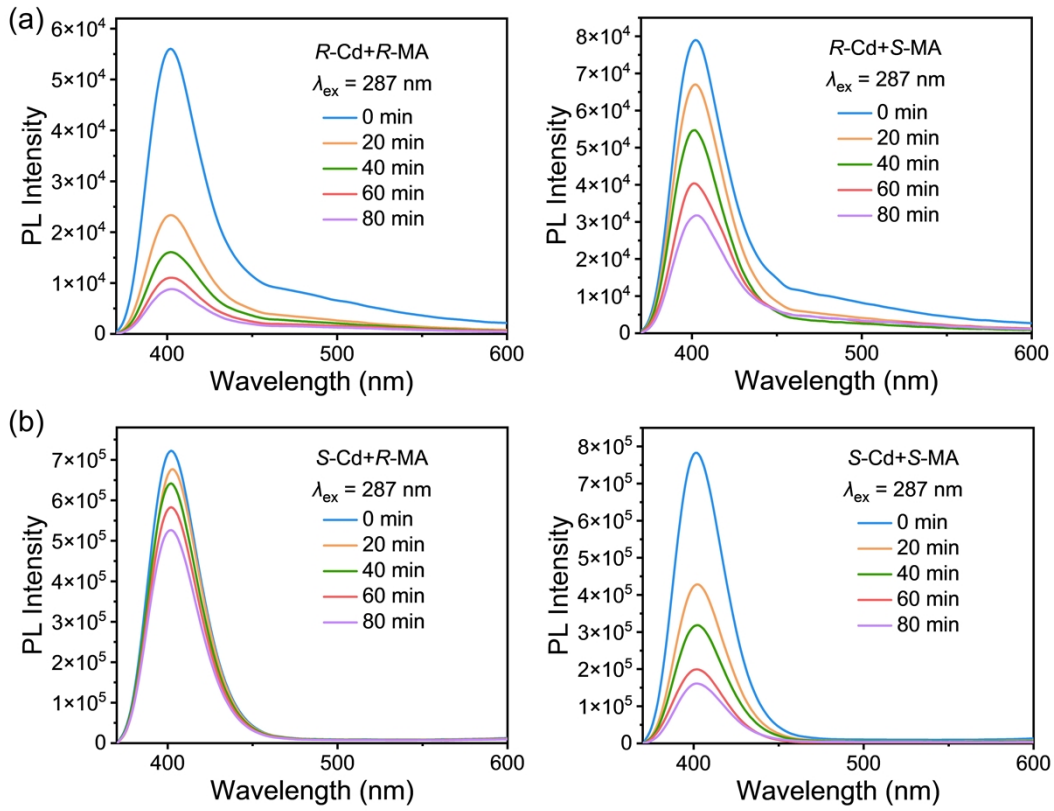

Fig. S10. PL intensity of *R*-Cd (a) and *S*-Cd (b) in the presence of *R* or *S*-MA over time. λ_{ex} = 287 nm, slit = 1.5/1.5 nm.

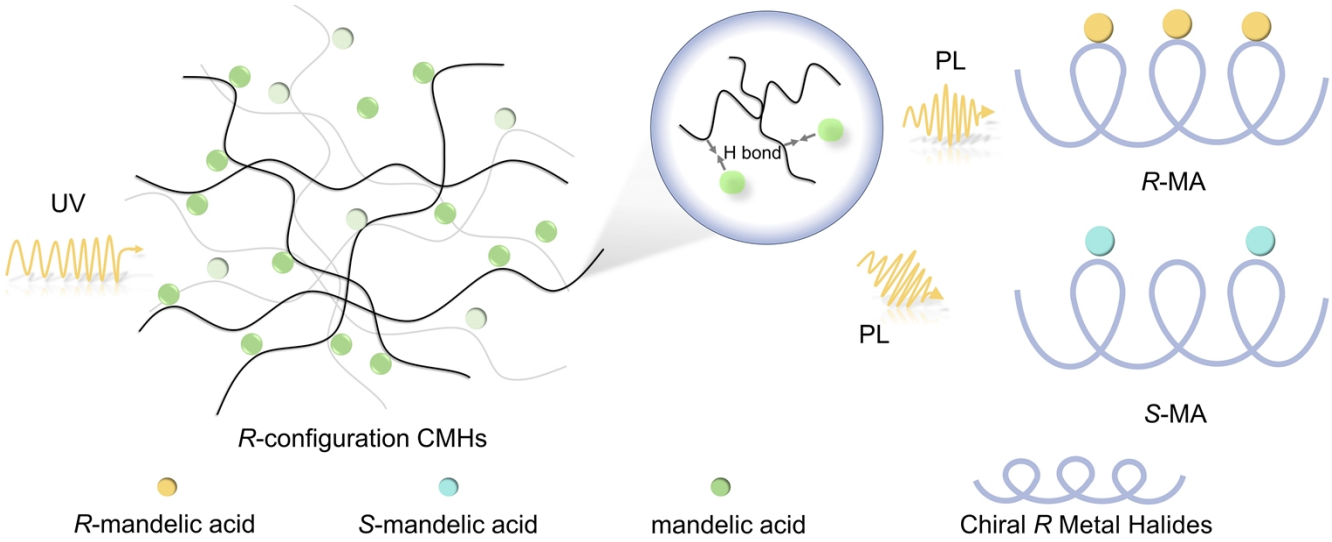

Fig. S11. Schematic diagram of identifying MA based on differences in PL quenching of *R*-configuration CMHs.

Table S1. Crystal data and structure refinement for *R*-Mn, *S*-Mn, *R*-Cd and *S*-Cd.

	R-Mn	*S*-Mn	*R*-Cd	*S*-Cd
Empirical formula	(*R*-$C_5H_{14}N_2$)$MnCl_4$·H_2O	(*S*-$C_5H_{14}N_2$)$MnCl_4$·H_2O	(*R*-$C_5H_{14}N_2$)$CdCl_4$·H_2O	(*S*-$C_5H_{14}N_2$)$CdCl_4$·H_2O
Formula weight	316.94	316.94	374.4	374.4
Temperature/K	293(2)	293(2)	293(2)	293(2)
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic
Space group	$P2_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$
a/Å	9.3137(10)	9.3099(10)	5.8315(4)	5.8283(4)
b/Å	6.7659(10)	6.7679(10)	14.1609(11)	14.1608(10)
c/Å	9.6874(10)	9.6863(10)	15.1674(10)	15.1852(12)
α/°	90	90	90	90
β/°	97.631(10)	97.620(10)	90	90
γ/°	90	90	90	90
Volume/Å^3	605.051(13)	604.929(13)	1252.51(15)	1253.29(16)
Z	2	2	4	4
ρ_{calc} /g·cm^{-3}	1.740	1.740	1.985	1.984
μ/mm^{-1}	16.749	16.752	2.565	2.563
F(000)	322	322	736	736
θ range/°	6.194 to 76.352	4.606 to 76.074	2.686 to 27.155	2.683 to 26.689
Index ranges	-11 ≤ *h* ≤ 11, -8 ≤ *k* ≤ 8, -12 ≤ *l* ≤ 11	-11 ≤ *h* ≤ 11, -8 ≤ *k* ≤ 8, -12 ≤ *l* ≤ 12	-7 ≤ *h* ≤ 7, -18 ≤ *k* ≤ 18, -19 ≤ *l* ≤ 15	-7 ≤ *h* ≤ 7, -17 ≤ *k* ≤ 17, -19 ≤ *l* ≤ 19
Reflections collected	10009	10652	17943	17682
Independent Reflections	2443 (R_{int} = 0.0435)	2472 (R_{int} = 0.0272)	2891 (R_{int} = 0.0462)	2652 (R_{int} = 0.0627)
Goodness-of-fit	1.049	1.107	1.027	1.055
Final *R* indexes	R_1=0.0387, wR_2=0.1006	R_1=0.0234, wR_2=0.0632	R_1=0.0282, wR_2=0.0424	R_1=0.0282, wR_2=0.0668
$\Delta\rho_{max}$(e/Å^3)	0.92	0.23	0.31	0.33
$\Delta\rho_{min}$(e/Å^3)	-0.69	-0.34	-0.46	-1.28
Flack parameter	0.010(7)	-0.004(5)	-0.024(17)	-0.004(18)

Table S2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	*U*iso*/*U*eq
		R-Mn		
Mn1	0.53173(7)	0.64105(9)	0.68789(7)	0.0186(2)
Cl1	0.25625(10)	0.67041(17)	0.68708(11)	0.0268(3)
Cl2	0.52719(10)	0.82289(12)	0.45575(10)	0.0234(2)
Cl3	0.57962(11)	0.93822(16)	0.84621(10)	0.0272(3)
Cl4	0.79855(10)	0.58974(16)	0.68266(11)	0.0261(3)
N1	1.2020(4)	0.6240(6)	0.3554(4)	0.0264(8)
H1A	1.213435	0.601502	0.446673	0.032
H1B	1.217014	0.751559	0.339834	0.032
H1C	1.265326	0.551681	0.315996	0.032
N2	0.7956(4)	0.6397(6)	0.3066(4)	0.0295(8)
H2A	0.733855	0.709765	0.349519	0.035
H2B	0.778624	0.512209	0.320369	0.035
O1	0.5496(4)	0.4349(5)	0.8661(3)	0.0304(7)
H1F	0.533710	0.459332	0.950281	0.046
H1G	0.574113	0.311749	0.867379	0.046
C1	0.9464(4)	0.6879(7)	0.3685(4)	0.0234(8)
H1D	0.960026	0.655892	0.466945	0.028
H1E	0.964342	0.828065	0.358555	0.028
C2	1.0515(4)	0.5692(6)	0.2942(4)	0.0208(8)
H2	1.036412	0.428085	0.309882	0.025
C3	1.0308(5)	0.6094(8)	0.1389(4)	0.0299(10)
H3A	1.096097	0.526974	0.093812	0.036
H3B	1.053002	0.746587	0.121778	0.036
C4	0.8748(5)	0.5648(8)	0.0791(5)	0.0328(10)
H4A	0.860171	0.596710	-0.019367	0.039
H4B	0.855959	0.424865	0.088896	0.039
C5	0.7698(5)	0.6831(8)	0.1532(5)	0.0336
H5A	0.783269	0.823147	0.137622	0.040
H5B	0.671112	0.648696	0.116161	0.040
		S-Mn		
Mn1	0.46824(5)	0.35979(7)	0.31214(5)	0.02247(13)
Cl1	0.20120(8)	0.41115(12)	0.31729(8)	0.02997(18)
Cl2	0.47280(8)	0.17801(10)	0.54410(7)	0.02706(17)
Cl3	0.42044(8)	0.06287(12)	0.15384(8)	0.03117(19)
Cl4	0.74349(8)	0.33041(13)	0.31253(8)	0.03071(17)
N1	-0.2023(3)	0.3772(4)	0.6444(3)	0.0307(6)
H1C	-0.265280	0.452548	0.681758	0.037
H1D	-0.218412	0.250773	0.662364	0.037

H1E	-0.212823	0.395906	0.552616	0.037
N2	0.2047(3)	0.3615(5)	0.6940(3)	0.0321(6)
H2A	0.221794	0.488973	0.680413	0.039
H2B	0.266731	0.291501	0.651356	0.039
O1	0.4506(3)	0.5667(4)	0.1336(2)	0.0349(5)
H1F	0.422261	0.687394	0.131465	0.052
H1G	0.470406	0.544087	0.051066	0.052
C1	0.0537(3)	0.3133(5)	0.6315(3)	0.0280(6)
H1D	0.035828	0.173107	0.641272	0.034
H1E	0.040564	0.345375	0.533058	0.034
C2	-0.0516(3)	0.4315(5)	0.7053(3)	0.0240(6)
H2	-0.036462	0.572567	0.689617	0.029
C3	-0.0310(3)	0.3915(6)	0.8609(3)	0.0341(8)
H3A	-0.053502	0.254446	0.877986	0.041
H3B	-0.096221	0.474167	0.905802	0.041
C4	0.1251(4)	0.4355(6)	0.9211(3)	0.0357(8)
H4A	0.144214	0.575382	0.911715	0.043
H4B	0.139521	0.403013	1.019462	0.043
C5	0.2297(4)	0.3180(6)	0.8473(4)	0.0375(8)
H5A	0.328466	0.352176	0.884596	0.045
H5B	0.216187	0.177969	0.862598	0.045
		R-Cd		
Cd1	0.20074(6)	0.65371(2)	0.52647(2)	0.03537(10)
Cl1	0.19802(18)	0.83413(6)	0.47633(6)	0.0285(2)
Cl2	0.1926(2)	0.60643(7)	0.36534(6)	0.0301(2)
Cl3	0.2141(2)	0.48433(8)	0.58014(8)	0.0429(3)
Cl4	0.19117(19)	0.71711(7)	0.68355(6)	0.0273(2)
N1	0.6884(7)	0.6945(2)	0.7528(2)	0.0291(8)
H1A	0.821499	0.708750	0.727360	0.035
H1B	0.577361	0.721299	0.721286	0.035
N2	0.8078(6)	0.4412(2)	0.8035(2)	0.0272(8)
H2A	0.797555	0.422156	0.747735	0.033
H2B	0.679404	0.426268	0.832017	0.033
H2C	0.926382	0.412827	0.829298	0.033
O1	0.7275(6)	0.3953(2)	0.6235(2)	0.0461(9)
H1E	0.610866	0.427147	0.607870	0.069
H1F	0.840816	0.425170	0.602028	0.069
C1	0.6573(8)	0.5908(3)	0.7513(3)	0.0281(11)
H1C	0.666078	0.568066	0.691032	0.034
H1D	0.507465	0.574676	0.774606	0.034
C2	0.8413(7)	0.5450(3)	0.8061(2)	0.0225(10)

H2	0.990549	0.559660	0.779686	0.027
C3	0.8402(8)	0.5807(3)	0.8994(3)	0.0336(12)
H3A	0.965446	0.552317	0.932067	0.04
H3B	0.697476	0.563360	0.927918	0.040
C4	0.8662(9)	0.6877(3)	0.8994(3)	0.0418(14)
H4A	0.853824	0.710968	0.959341	0.050
H4B	1.017140	0.704231	0.877366	0.050
C5	0.6854(9)	0.7347(3)	0.8428(3)	0.0422(12)
H5A	0.535421	0.725205	0.868956	0.051
H5B	0.714497	0.802030	0.839969	0.051
		S-Cd		
Cd1	0.79950(7)	0.34617(2)	0.47350(2)	0.03402(13)
Cl1	0.80216(19)	0.16595(6)	0.52358(7)	0.0271(2)
Cl2	0.80743(19)	0.39346(7)	0.63471(7)	0.0287(2)
Cl3	0.7862(2)	0.51560(8)	0.41992(10)	0.0418(3)
Cl4	0.80896(19)	0.28293(7)	0.31624(7)	0.0261(2)
N1	0.3112(7)	0.3054(2)	0.2470(2)	0.0281(8)
H1A	0.422267	0.278474	0.278385	0.034
H1B	0.177959	0.291118	0.272364	0.034
N2	0.1926(7)	0.5587(2)	0.1967(3)	0.0257(8)
H2A	0.320005	0.573409	0.167488	0.031
H2B	0.205338	0.577608	0.252388	0.031
H2C	0.073191	0.587321	0.171730	0.031
O1	0.2725(6)	0.6045(3)	0.3759(2)	0.0439(9)
H1E	0.380528	0.573704	0.400150	0.066
H1F	0.150568	0.579229	0.395618	0.066
C1	0.3427(7)	0.4096(3)	0.2486(3)	0.0256(10)
H1C	0.492150	0.425873	0.224997	0.031
H1D	0.334339	0.432411	0.308784	0.031
C2	0.1576(6)	0.4545(3)	0.1942(3)	0.0196(9)
H2	0.008434	0.439786	0.220657	0.024
C3	0.1592(9)	0.4197(3)	0.1011(3)	0.0337(12)
H3A	0.301923	0.437544	0.072746	0.040
H3B	0.033679	0.448132	0.068612	0.040
C4	0.1341(10)	0.3117(3)	0.1004(3)	0.0415(13)
H4A	-0.016922	0.294574	0.122024	0.050
H4B	0.148138	0.288633	0.040524	0.050
C5	0.3141(9)	0.2659(3)	0.1571(3)	0.0402(12)
H5A	0.286531	0.198385	0.159707	0.048
H5B	0.464134	0.275839	0.130990	0.048

Table S3. The main bond lengths of *R*-Mn and *S*-Mn.

R-Mn		*S*-Mn	
Atom–Atom	Length/Å	Atom–Atom	Length/Å
Mn1–Cl1	2.5724(11)	Mn1–Cl1	2.5697(8)
Mn1–Cl2	2.5824(10)	Mn1–Cl2	2.5838(8)
Mn1–Cl2	2.5588(12)	Mn1–Cl2	2.5570(8)
Mn1–Cl3	2.5322(11)	Mn1–Cl3	2.5311(9)
Mn1–Cl4	2.5163(11)	Mn1–Cl4	2.5174(8)
Mn1–O1	2.209(3)	Mn1–O1	2.214(2)
N1–C2	1.495(5)	N1–C2	1.493(5)
N2–C1	1.488(5)	N2–C1	1.491(4)
N2–C5	1.503(6)	N2–C5	1.501(5)
C1–C2	1.519(5)	C1–C2	1.516(4)
C2–C3	1.516(6)	C2–C3	1.518(4)
C3–C4	1.521(6)	C3–C4	1.522(5)
C4–C5	1.516(7)	C4–C5	1.509(5)

Table S4. The main bond angles of *R*-Mn and *S*-Mn.

R-Mn		*S*-Mn	
Atom–Atom–Atom	Angles/°	Atom–Atom–Atom	Angles/°
Cl1–Mn1–Cl2	85.54(4)	Cl1–Mn1–Cl2	85.60(3)
Cl1–Mn1–Cl2	93.44(4)	Cl1–Mn1–Cl2	93.50(3)
Cl1–Mn1–Cl3	92.06(4)	Cl1–Mn1–Cl3	91.98(3)
Cl1–Mn1–Cl4	176.26(5)	Cl1–Mn1–Cl4	176.30(4)
Cl2–Mn1–Cl2	87.12(2)	Cl2–Mn1–Cl2	87.13(2)
Cl2–Mn1–Cl3	97.56(4)	Cl2–Mn1–Cl3	97.55(3)
Cl2–Mn1–Cl3	174.87(3)	Cl2–Mn1–Cl3	174.86(3)
Cl2–Mn1–Cl4	87.12(4)	Cl2–Mn1–Cl4	87.16(3)
Cl2–Mn1–Cl4	90.80(4)	Cl2–Mn1–Cl4	90.80(3)
Cl3–Mn1–Cl4	91.53(6)	Cl3–Mn1–Cl4	91.54(3)
O1–Mn1–Cl1	91.30(9)	O1–Mn1–Cl1	91.19(7)
O1–Mn1–Cl2	83.30(9)	O1–Mn1–Cl2	83.24(7)
O1–Mn1–Cl2	168.94(10)	O1–Mn1–Cl2	168.93(7)
O1–Mn1–Cl3	92.24(9)	O1–Mn1–Cl3	92.29(7)
O1–Mn1–Cl4	87.51(9)	O1–Mn1–Cl4	87.53(7)
Mn1–Cl2–Mn1	148.42(4)	Mn1–Cl2–Mn1	148.45(2)
C1–N2–C5	111.9(3)	C1–N2–C5	111.9(2)
C1–C2–C3	111.8(3)	C1–C2–C3	111.7(3)
C2–C3–C4	109.3(4)	C2–C3–C4	109.5(3)
C3–C4–C5	111.0(4)	C3–C4–C5	111.1(3)
N1–C2–C1	108.1(3)	N1–C2–C1	108.4(2)
N1–C2–C3	109.7(4)	N1–C2–C3	109.7(3)
N2–C1–C2	109.1(3)	N2–C1–C2	109.1(2)
N2–C5–C4	109.7(4)	N2–C5–C4	109.9(3)

Table S5. Hydrogen-bonds data of *R*-Mn and *S*-Mn.

D–H···A	d(D–H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
		R-Mn		
N1–H1A···Cl1	0.89	2.36	3.201(4)	159
N1–H1B···Cl4	0.89	2.30	3.173(4)	166
N1–H1C···Cl3	0.89	2.40	3.254(4)	162
N2–H2A···Cl2	0.89	2.42	3.291(4)	165
N2–H2B···Cl1	0.89	2.34	3.214(4)	169
		S-Mn		
N1–H1C···Cl3	0.89	2.41	3.252(3)	159
N1–H1D···Cl4	0.89	2.31	3.176(2)	164
N1–H1E···Cl1	0.89	2.35	3.203(3)	161
N2–H2A···Cl1	0.89	2.33	3.212(3)	169
N2–H2B···Cl2	0.89	2.42	3.293(3)	165

Table S6. The main bond lengths of *R*-Cd and *S*-Cd.

R-Cd		*S*-Cd	
Atom–Atom	Length/Å	Atom–Atom	Length/Å
Cd1–Cl1	2.6658(10)	Cd1–Cl1	2.6629(10)
Cd1–Cl1	2.9053(11)	Cd1–Cl1	2.9040(11)
Cd1–Cl2	2.5344(10)	Cd1–Cl2	2.5385(10)
Cd1–Cl3	2.5342(11)	Cd1–Cl3	2.5347(11)
Cd1–Cl4	2.5466(10)	Cd1–Cl4	2.5510(10)
N1–C1	1.480(5)	N1–C1	1.487(5)
N1–C5	1.478(5)	N1–C5	1.476(6)
N2–C2	1.483(5)	N2–C2	1.490(5)
C1–C2	1.505(5)	C1–C2	1.501(5)
C2–C3	1.504(5)	C2–C3	1.498(6)
C3–C4	1.522(6)	C3–C4	1.537(6)
C4–C5	1.513(6)	C4–C5	1.503(7)

Table S7. The main bond angles of *R*-Cd and *S*-Cd.

R-Cd		*S*-Cd	
Atom–Atom–Atom	Angles/°	Atom–Atom–Atom	Angles/°
Cl1–Cd1–Cl1	86.20(3)	Cl1–Cd1–Cl1	86.21(3)
Cl1–Cd1–Cl2	88.74(3)	Cl1–Cd1–Cl2	88.70(3)
Cl1–Cd1–Cl2	89.02(3)	Cl1–Cd1–Cl2	89.01(3)
Cl1–Cd1–Cl3	177.41(4)	Cl1–Cd1–Cl3	177.43(4)
Cl1–Cd1–Cl3	95.22(4)	Cl1–Cd1–Cl3	95.21(4)
Cl1–Cd1–Cl4	85.92(3)	Cl1–Cd1–Cl4	86.03(3)
Cl1–Cd1–Cl4	88.34(3)	Cl1–Cd1–Cl4	88.40(3)
Cl2–Cd1–Cl3	93.45(4)	Cl2–Cd1–Cl3	93.46(4)
Cl2–Cd1–Cl4	177.41(4)	Cl2–Cd1–Cl4	174.27(3)
Cl3–Cd1–Cl4	91.94(4)	Cl3–Cd1–Cl4	91.86(4)
Cd1–Cl1–Cd1	93.84(3)	Cd1–Cl1–Cd1	93.83(3)
C1–N1–C5	113.3(3)	C1–N1–C5	113.0(3)
C1–C2–C3	111.8(4)	C1–C2–C3	112.1(3)
C2–C3–C4	109.6(3)	C2–C3–C4	109.5(4)
C3–C4–C5	111.6(4)	C3–C4–C5	111.1(4)
N1–C1–C2	109.4(4)	N1–C1–C2	108.8(4)
N1–C5–C4	110.3(4)	N1–C5–C4	110.9(4)
N2–C2–C1	108.6(3)	N2–C2–C1	107.9(3)
N2–C2–C3	111.0(3)	N2–C2–C3	111.4(3)

Table S8. Hydrogen-bonds data of *R*-Cd and *S*-Cd.

D–H···A	d(D–H)/Å	d(H···A)/Å	d(D···A)/Å	∠D–H···A/°
		R-Cd		
N1–H1A···Cl4	0.89	2.26	3.131(4)	166
N1–H1B···Cl4	0.89	2.32	3.101(4)	146
N2–H2A···O1	0.89	1.97	2.845(4)	170
N2–H2B···Cl2	0.89	2.28	3.139(3)	163
N2–H2C···Cl2	0.89	2.30	3.134(3)	155
O1–H1E···Cl3	0.85	2.49	3.314(3)	165
O1–H1F···Cl3	0.85	2.36	3.173(3)	162
		S-Cd		
N1–H1A···Cl4	0.89	2.33	3.102(4)	146
N1–H1B···Cl4	0.89	2.25	3.127(4)	166
N2–H2A···Cl2	0.89	2.28	3.136(4)	162
N2–H2C···Cl2	0.89	2.30	3.137(4)	156
N2–H2B···O1	0.89	1.95	2.836(5)	171
O1–H1E···Cl3	0.85	2.52	3.316(4)	156
O1–H1F···Cl3	0.85	2.34	3.173(3)	168