

Supporting Information

Non-Salen Coumarin Schiff Base Chiral Fluorescent Probe Turn on Circularly Polarized Luminescence by Mg²⁺ and Zn²⁺

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Contents

Computational Studies.	S2
¹ H and ¹³ C Spectra of Compounds	S2–S6
LC-MS spectrum of the compound L	S6
photophysical properties of the probe	S7-S9
IR spectra and DFT Optimized structure calculated	S9
Chiral enantiomer recognition FL Spectra of L1 and L2	S10-S11

Computational Studies. The DFT calculations were performed by using the Gaussian 09 program⁴ at the B3LYP 6-311(g) level.

¹H and ¹³C Spectra of Compounds

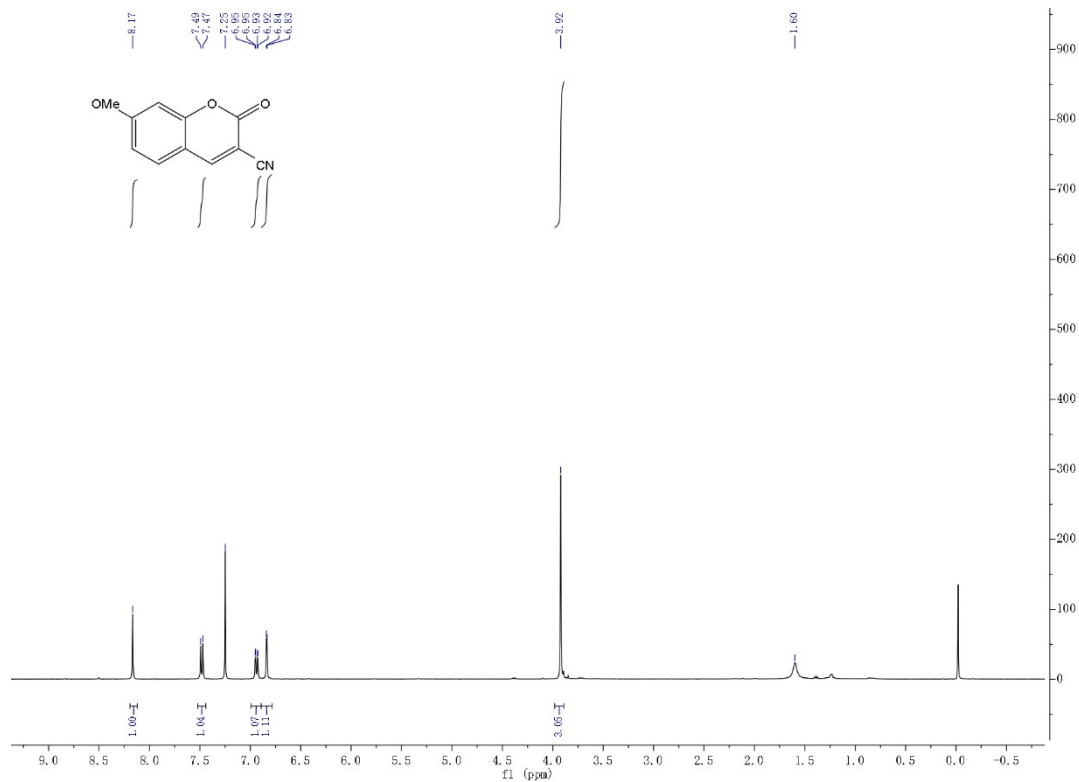


Figure S1. ¹H NMR spectrum of the compound 2a

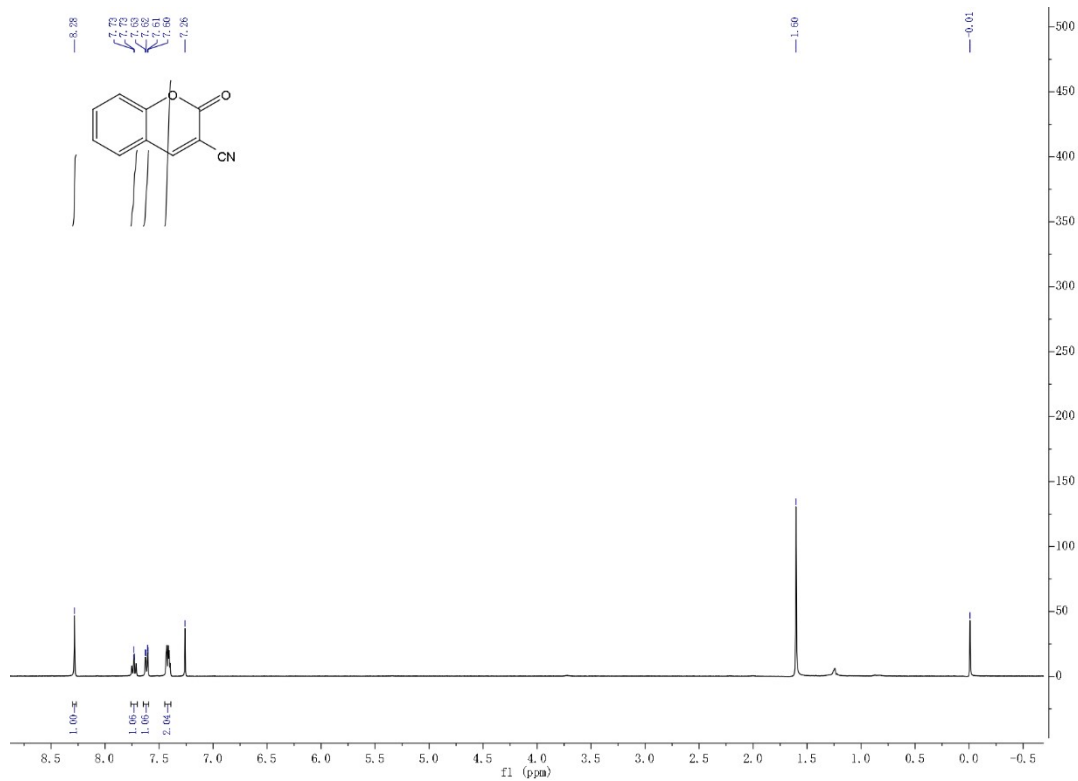


Figure S2 . ¹H NMR spectrum of the compound 2b

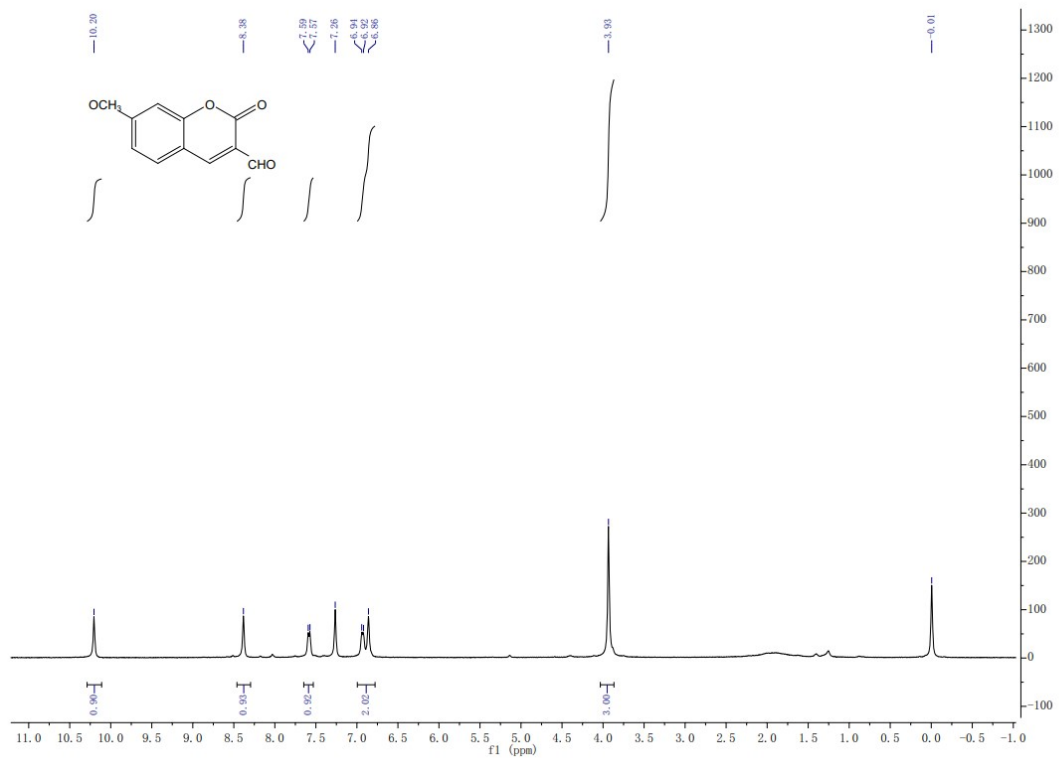


Figure S3 . ¹H NMR spectrum of the compound 3a

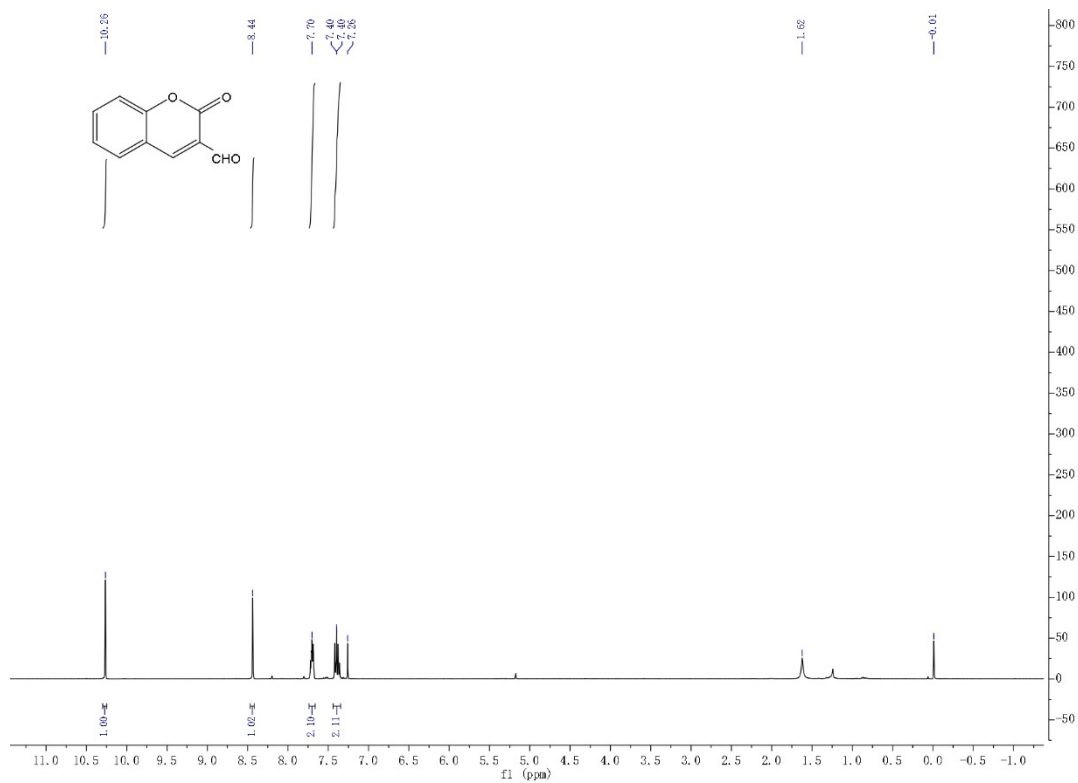


Figure S4 . $^1\text{H NMR}$ spectrum of the compound 3b

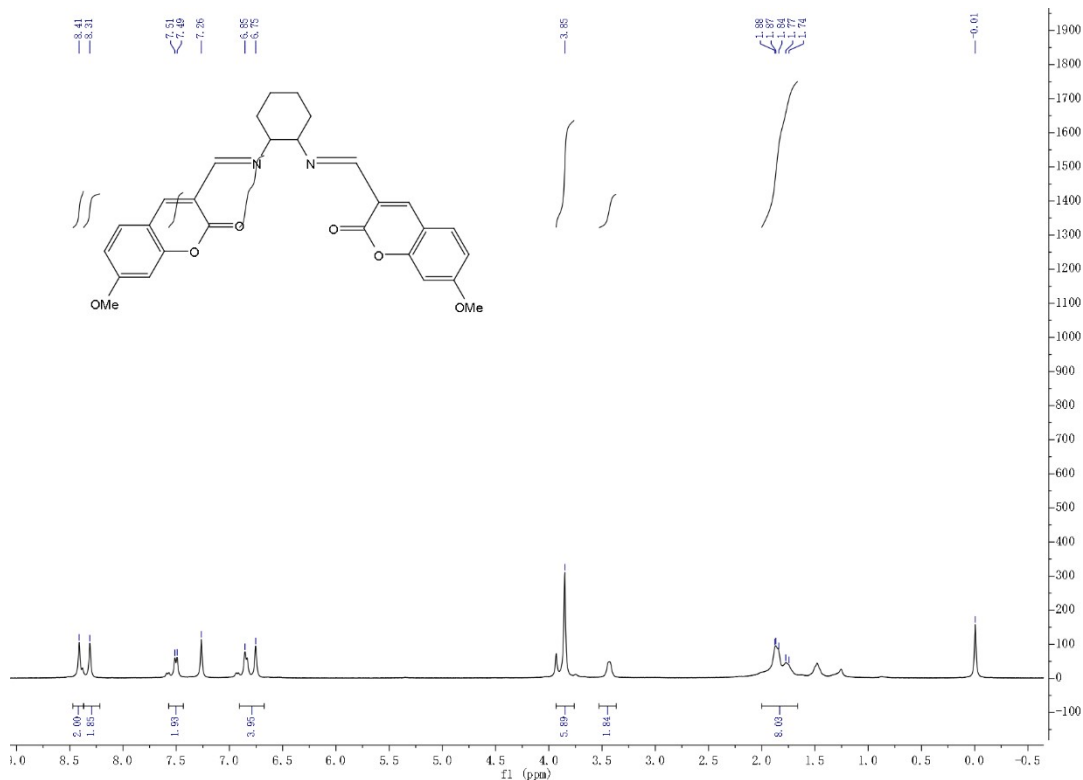


Figure S5 . $^1\text{H NMR}$ spectrum of the compound L1

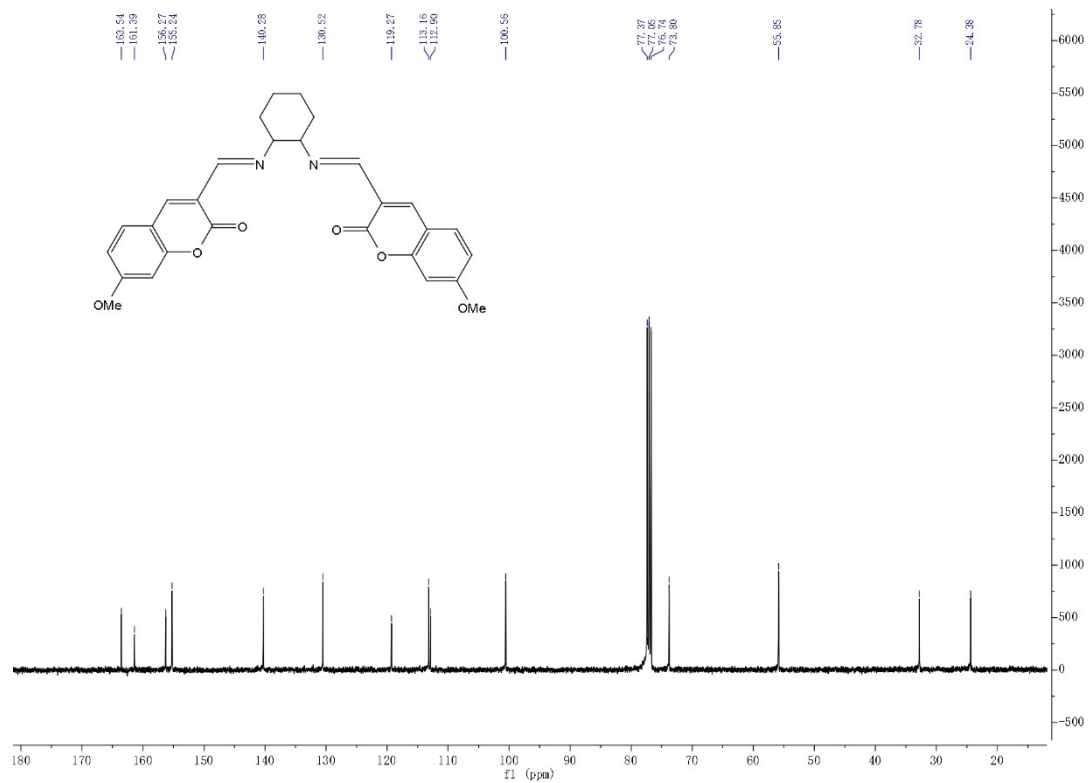


Figure S6 . ^{13}C NMR spectrum of the compound L1

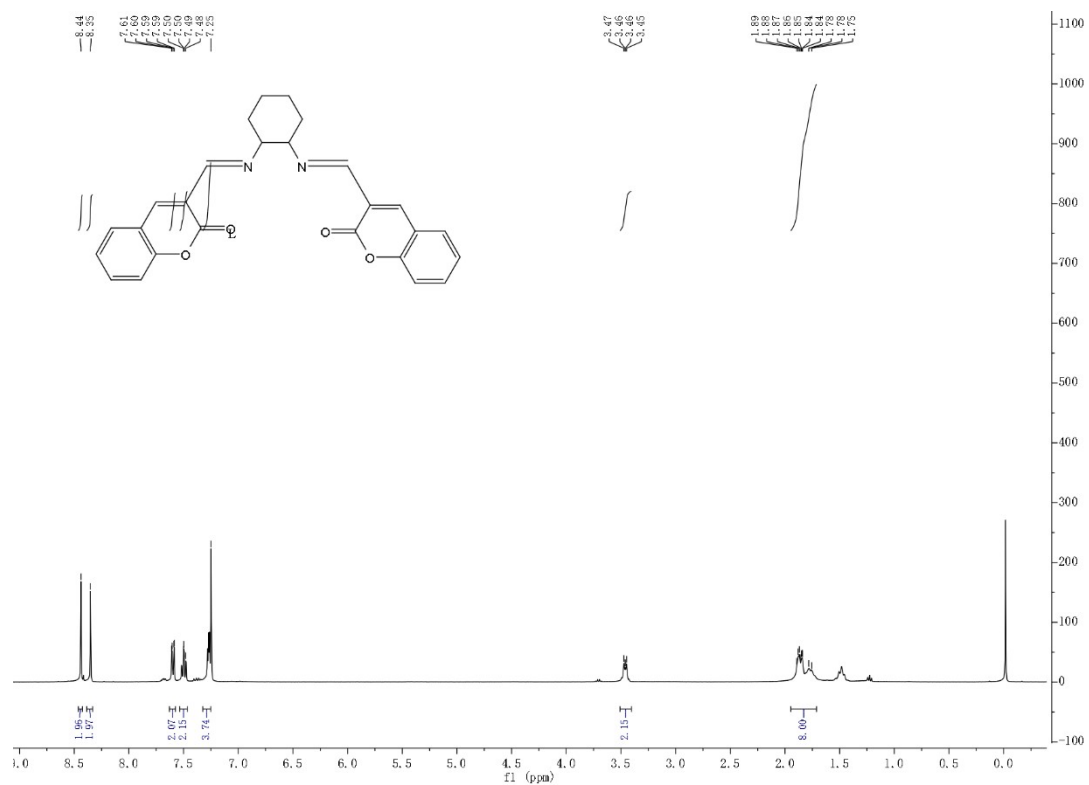


Figure S7 . ^1H NMR spectrum of the compound L2

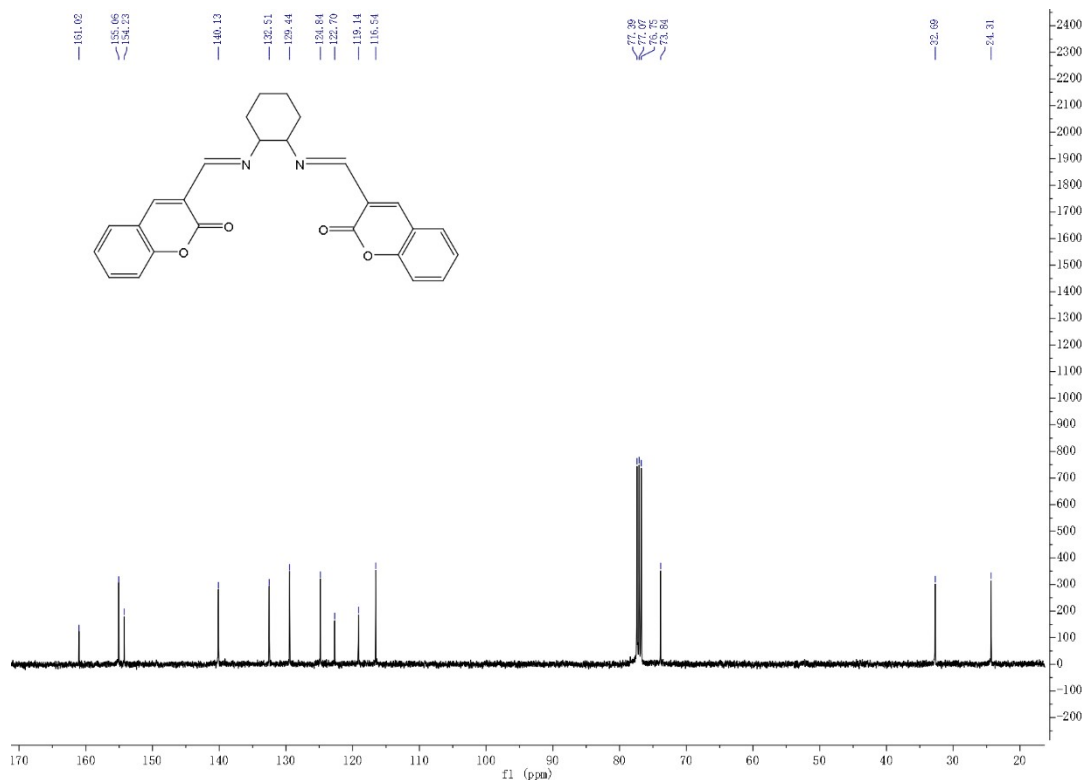


Figure S8. ^{13}C NMR spectrum of the compound L2

LC-MS spectrum of the compound L

Sample Spectra

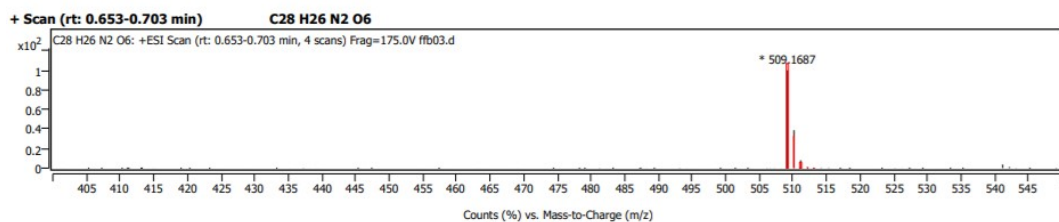


Figure S9. LC-MS spectrum of the compound L1

Sample Spectra

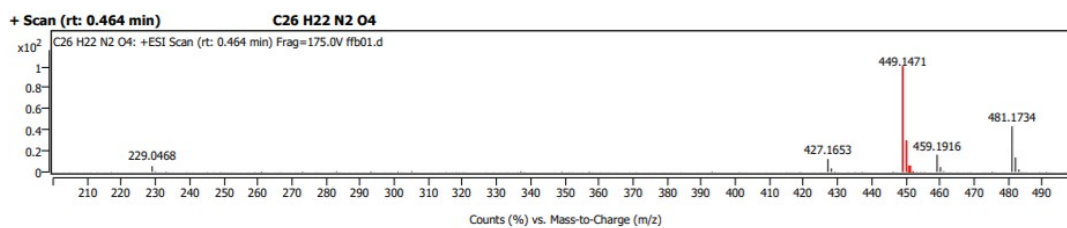


Figure S10. LC-MS spectrum of the compound L2

photophysical properties of the probe

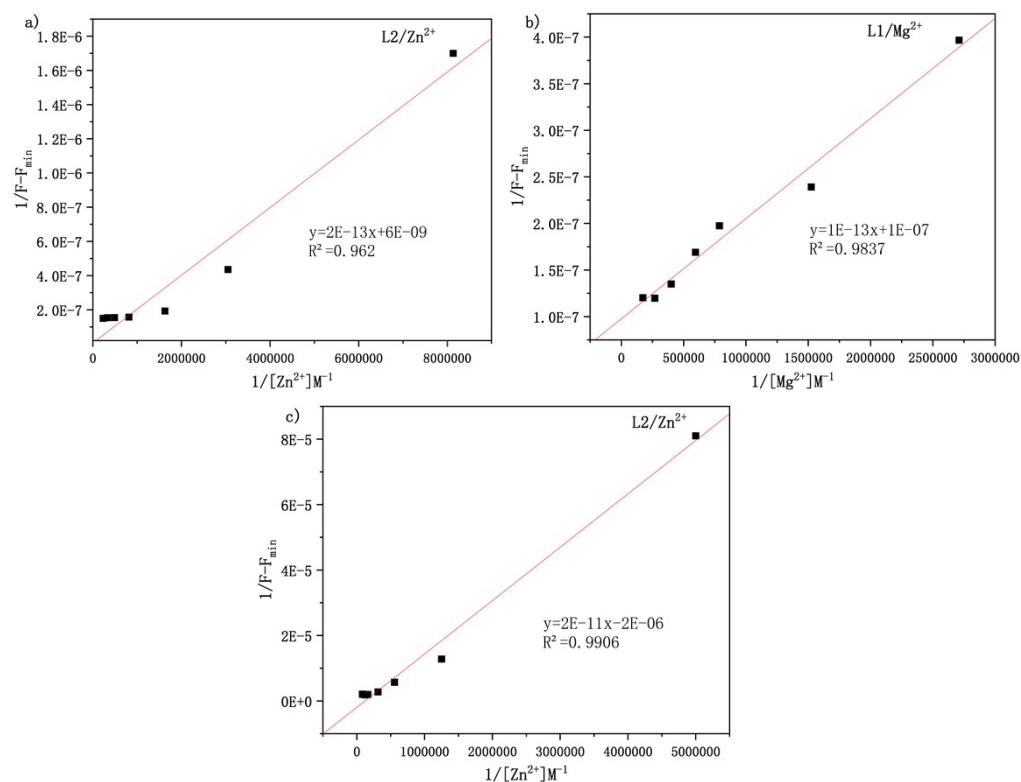


Figure S11. Benesi-Hildebrand curve of the emission changes for the complexation (a) L1/ Zn^{2+} , (b) L1/ Mg^{2+} and (c) L2/ Zn^{2+} .

Table S1. The g_{abs} value of L1/ Zn^{2+} , L1/ Mg^{2+}

Substance	Corresponding peak(nm)	g_{abs} value
(S,S)-L1		1.1129E-03
(R,R)-L1	368	-1.1124E-03
(S,S)-L1/ Zn^{2+}		9.7168E-04
(R,R)-L1/ Zn^{2+}	382	-9.4900E-04
(S,S)-L1/ Mg^{2+}		1.1810E-03
(R,R)-L1/ Mg^{2+}	377	-1.2202E-03
(S,S)-L2		2.0230E-03
(R,R)-L2	345	-2.1840E-03
(S,S)-L2/ Zn^{2+}		2.4360E-03
(R,R)-L2/ Zn^{2+}	345	-2.4740E-03

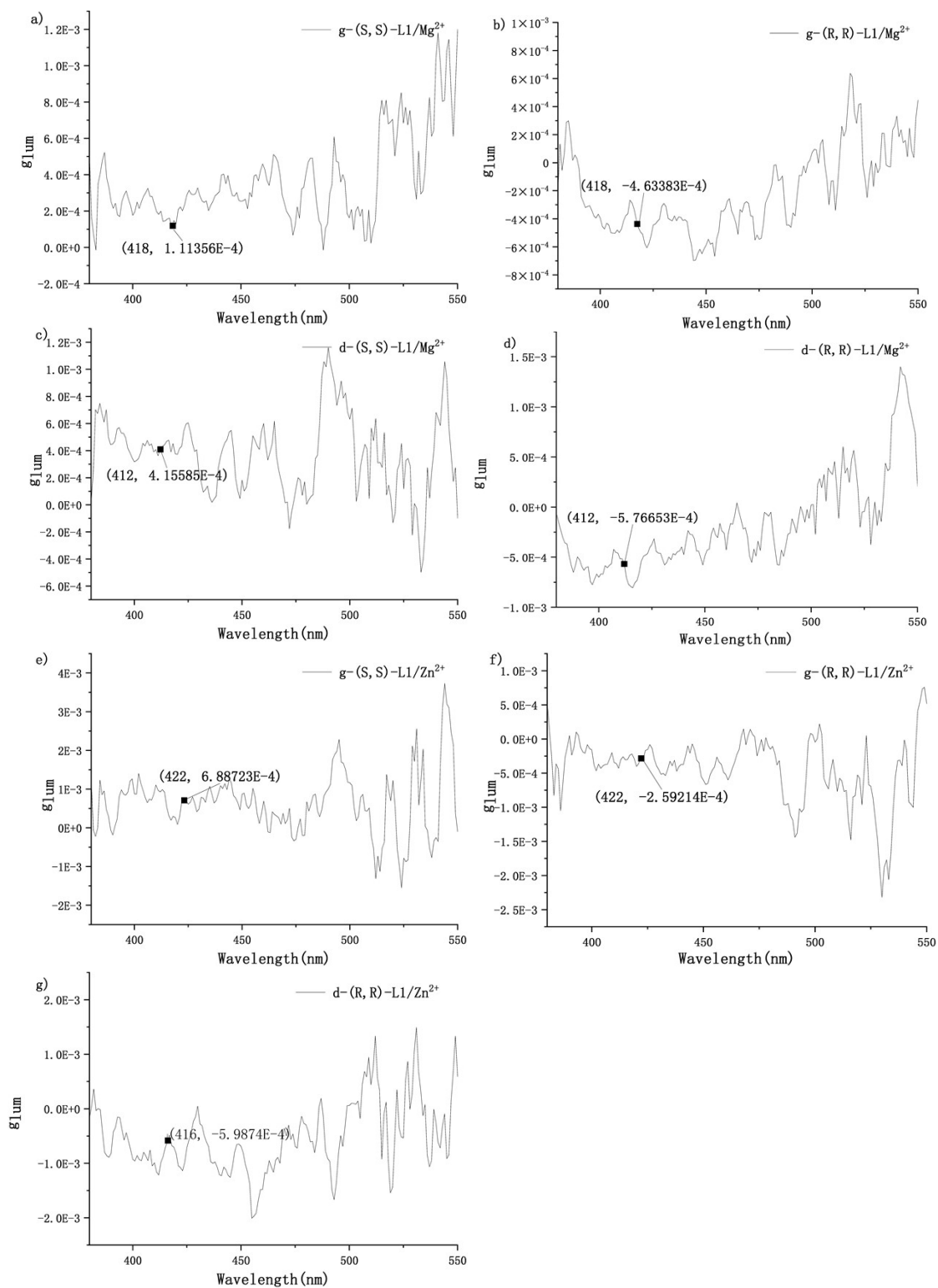


Figure S12. g_{lum} spectra of (a-d) (S,S)/(R,R)-L1/ Mg^{2+} and (e-f) (S,S)/(R,R)-L1/ Zn^{2+} at two order of magnitude concentration states of 10^{-5} and 10^{-4} . “g” indicates concentration of 3×10^{-4} M, “d” indicates concentration of 2×10^{-5} M, $Ex_{(CPL)}=318$ nm .

Table S2. The g_{lum} value of L1/ Zn^{2+} , L1/ Mg^{2+}

Substance	the highest peak in synchronization (nm)	g_{lum} value
(a)g-(S,S)-L1/Mg ²⁺	418	1.11356×10^{-4}
(b)g-(R,R)-L1/Mg ²⁺		-4.63661×10^{-4}
(c)d-(S,S)-L1/Mg ²⁺		4.15585×10^{-4}
(d)d-(R,R)-L1/Mg ²⁺	412	-5.76653×10^{-4}
(e)g-(S,S)-L1/Zn ²⁺		6.88723×10^{-4}
(f)g-(R,R)-L1/Zn ²⁺	422	-2.59214×10^{-4}
d-(S,S)-L1/Zn ²⁺		-
(g)d-(R,R)-L1/Zn ²⁺		-5.9874×10^{-4}

IR spectra and DFT Optimized structure calculated

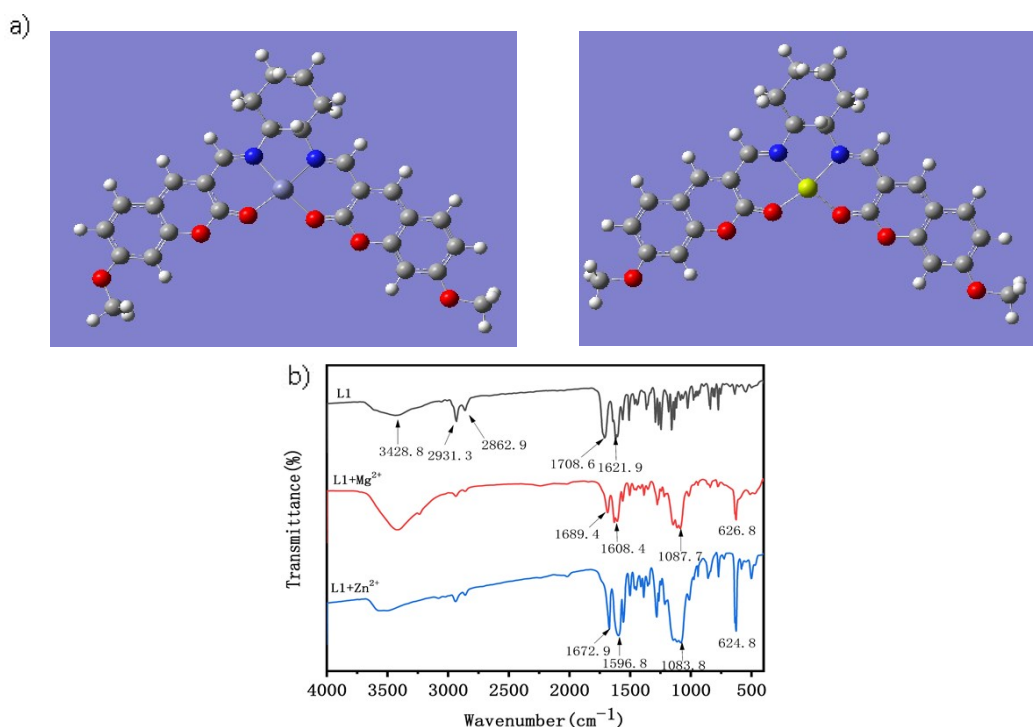


Figure S13. (a) optimized structure calculated at the DFT-B3LYP 6-311g for L1/Zn²⁺ (left) and L1/Mg²⁺ (right);

(b) IR spectra of L1, L1/Zn²⁺ and L1/Mg²⁺.

Chiral enantiomer recognition FL Spectra of L1 and L2

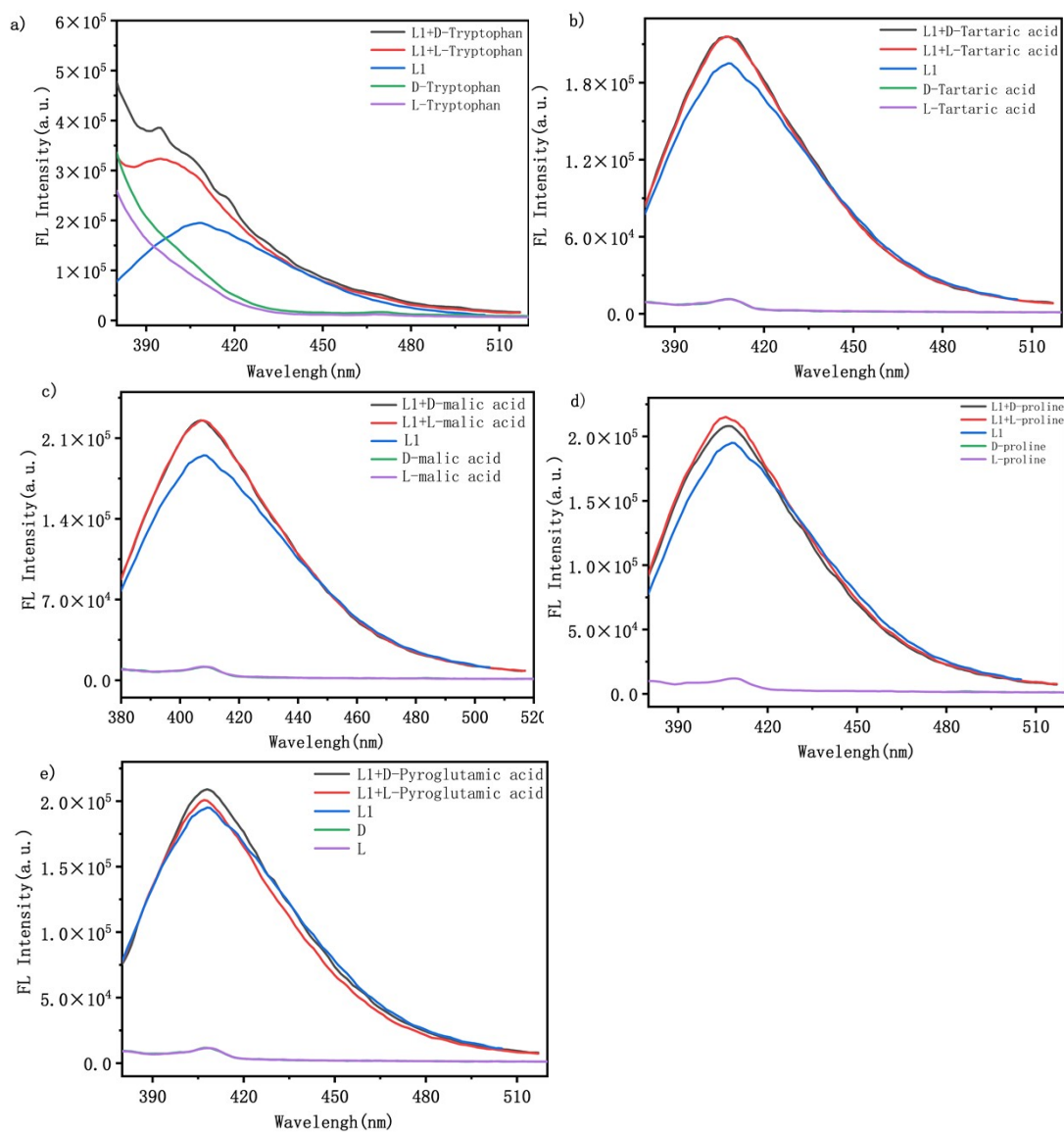


Figure S14. Fluorescence emission spectra of seven chiral enantiomers added to the probe L1 separately ($\lambda_{\text{exc}}=365\text{nm}, \lambda_{\text{em}}=408\text{ nm}$; Slit width: EX=5 nm, EM=5 nm). (a): (D)- and (L)-tryptophan; (b): (D)- and (L)-tartaric acid; (c): (D)- and (L)-malic acid; (d): (D)- and (L)-proline; (e): (D)- and (L)-pyroglutamic acid.

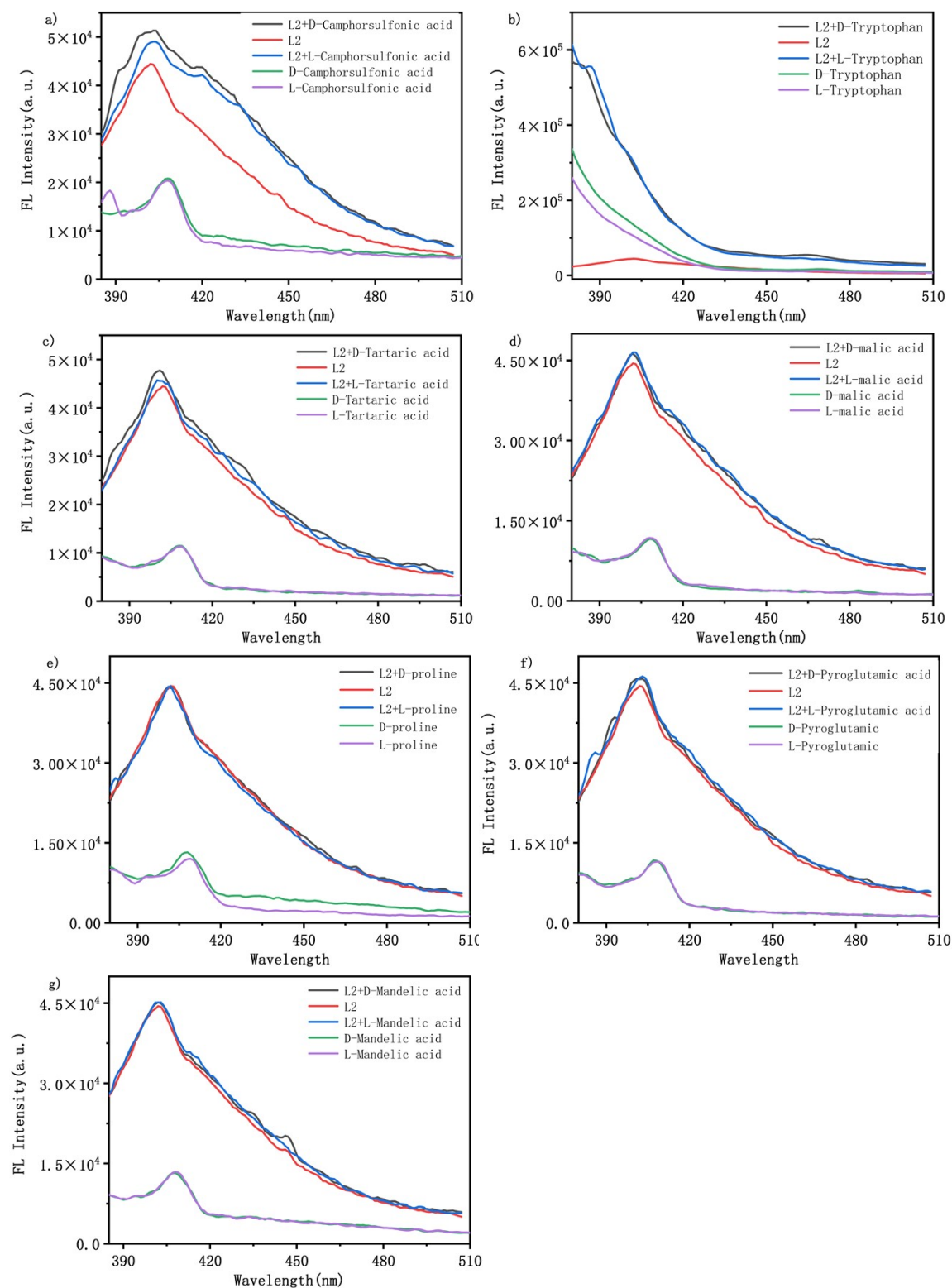


Figure S15. Fluorescence emission spectra of seven chiral enantiomers added to the probe L2 separately ($\lambda_{\text{ex}}=365\text{nm}$, $\lambda_{\text{em}}=408\text{ nm}$; Slit width: EX=5 nm, EM=5 nm). (a): (D)- and (L)-camphorsulfonic acid; (b): (D)- and (L)-tryptophan; (c): (D)- and (L)-tartaric acid; (d): (D)- and (L)-malic acid; (e): (D)- and (L)-proline; (f): (D)- and (L)-pyroglutamic acid; (g): (D)- and (L)-mandelic acid.