Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Asymmetric Metal-Organic Frameworks with Double Helices for Enantioselective Recognition

Yang Li, Shumei Chen*, Zhong-Xuan Xu, Xin Wu*, Huabin Zhang, Jian Zhang

Powder X-ray Diffraction Studies

Powder X-ray diffraction (PXRD) data were collected with a Rigaku Mini Flex Ⅱ diffractometer with Cu-Kα radiation (λ = 1.54056 Å) with a step size of 5°/min under ambient conditions.

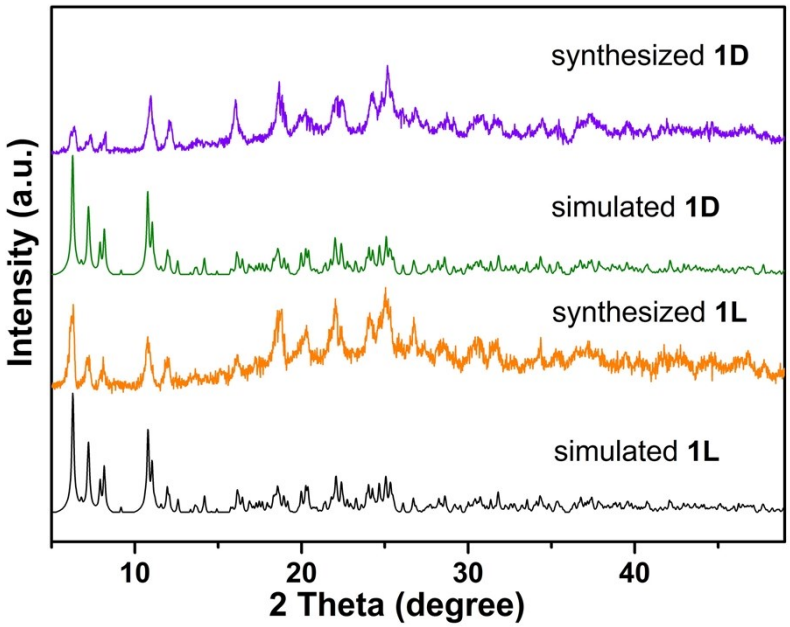


Fig. S1 The PXRD patterns of 1L and 1D.

Thermogravimetric Studies

Thermogravimetric analyses (TGA) were performed using a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10°C/min under a nitrogen atmosphere.

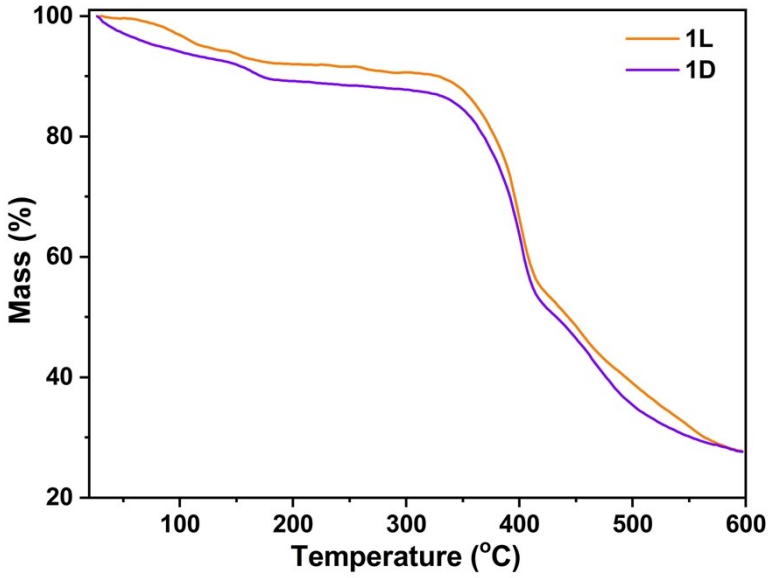


Fig. S2 The TG curves of 1L and 1D.

Circular Dichroism (CD) Spectra

The liguid-state CD spectra were recorded on a MOS-450 spectropolarimeter.

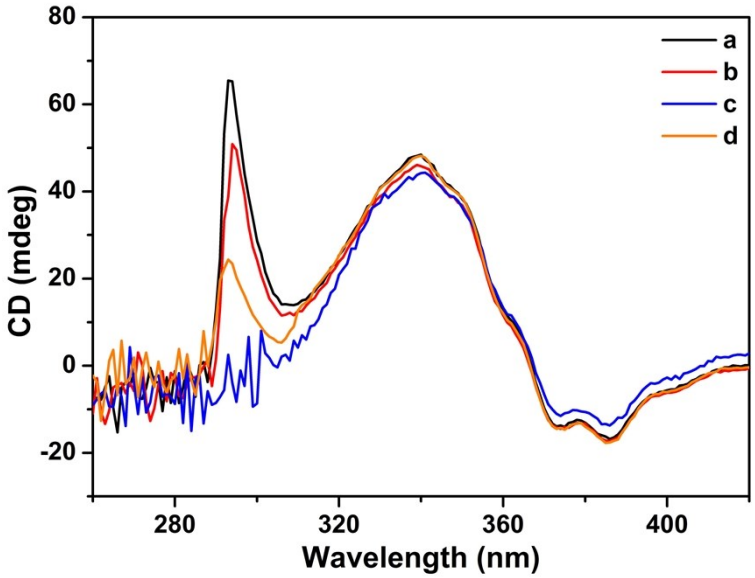


Fig. S3 (a) The CD signals of L-carvone solution without compound 1L. (b-d) The CD signals of L-carvone solution with different amount of compound 1L (b. 100 mg, c. 200 mg, d. 300 mg).

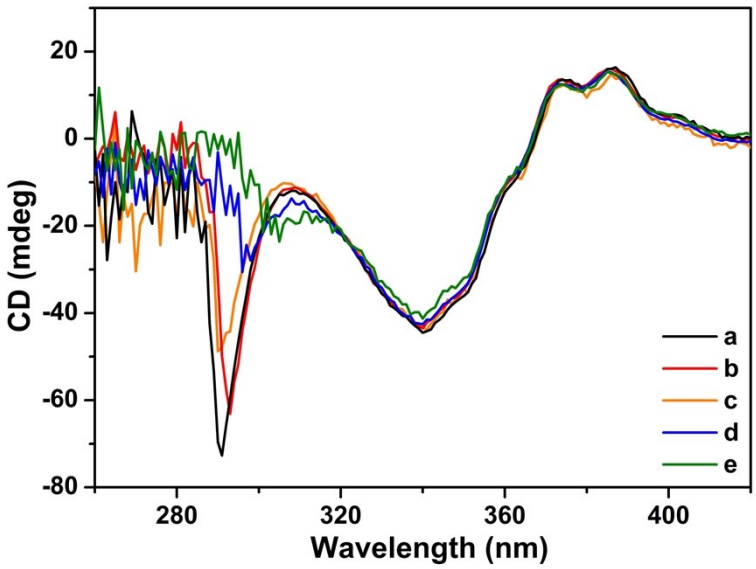
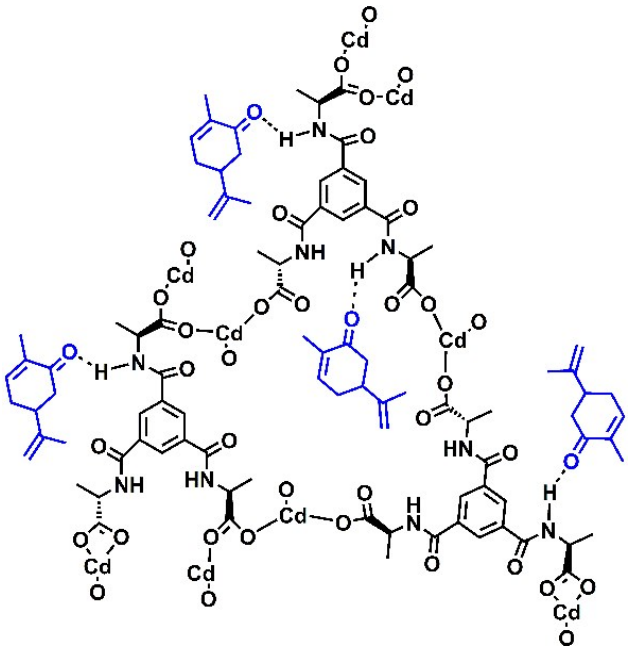


Fig. S4 (a) The CD signals of D-carvone solution without compound 1L. (b-e) The CD signals of D-carvone solution with different amount of compound 1L (b. 100 mg, c. 200 mg, d. 300 mg, e. 400 mg).



Scheme S1. Schematic illustration of the interaction between 1L and carvone.

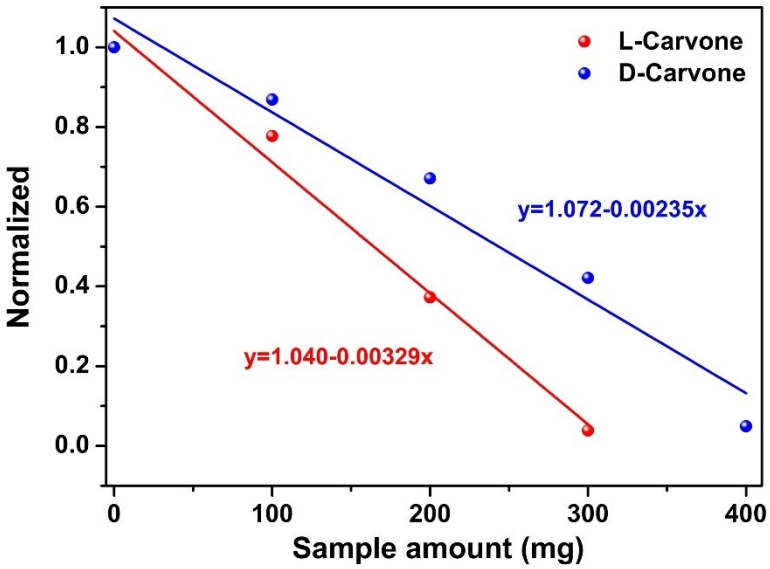


Fig. S5 The linear fits of CD signals based on Fig. 4.

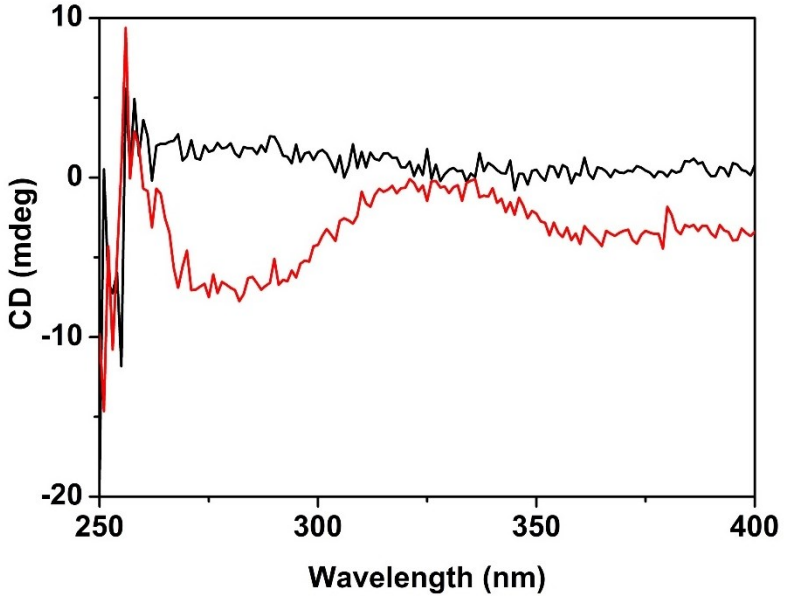


Fig. S6 Enantioselective separation of racemic mixtures of carvone in ethanol solutions by 1L.

Table S1. Distance (Å) and angles (°) of hydrogen bonding for 1L.

D-H···A	d (D-H)	d (H···A)	d (D···A)	∠(DHA)
N(1)-H(1A) ···O(23)	0.86	2.39	3.198(9)	158
N(2)-H(2B) ···O(6)	0.86	2.29	2.648(7)	105
N(3)-H(3A) ···O(8)	0.86	2.27	2.643(8)	107
N(4)-H(4B)···O(31)	0.86	2.27	3.053(10)	152
N(5)-H(5A)···O(34)	0.86	2.35	3.159(9)	157
N(7)-H(7A)···O(7)	0.86	2.23	3.041(9)	158
N(10)-H(10A)···O(29)	0.86	2.26	2.617(7)	105
N(11)-H(11A)···O(32)	0.86	2.29	2.630(9)	104
N(12)-H(12B)···O(35)	0.86	2.27	2.632(8)	106

Table S2. Summary of representative chiral sensors

Sample	Probe molecules	Enantioselectivity (K_S/K_R)	Measurement	Ref.
1L	carvone	1.36	CD	In this work
Zn-MOF-C-Tb	Cinchonine/Cinchonidine	1.4	Fluorescence	*Nat. Commun.* 2019, **10**, 5117.
1	amino alcohols	1.17-1.39	Fluorescence	*J. Am. Chem. Soc.* 2012, **134**, 9050-9053.
MIL-101@c-PANI	carvone	1.638	UV–vis absorbance spectra	*ACS Appl. Mater. Interfaces* 2018, **10**, 26365–26371
chirMOF 1	1-phenylethylamine	1.6	QCM sensor	*Angew. Chem. Int. Ed.* 2021, **60**, 3566-3571.
(S)-6	2-Amino-1-propanol	1.8	Fluorescence	*Chem. Sci.* 2016, **7**, 3614-3620.
MOF1	phenylalaminol	1.43	Fluorescence	*J. Am. Chem. Soc.* 2019, **141**, 17685–17695
1.XB	BINOL-PO_4	1.51	^{1}H NMR titration	*Chem. Commun.*, 2016, **52**, 5527-5530