Supporting Information

Synthesis of homochiral zeolitic imidazolate frameworks via solvent-assisted linker exchange for enantioselective sensing and separation

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Materials and methods

All materials were commercially available in analytical grade and used without further purification.

$^1$H NMR spectra were recorded with an AVANCE III (400 MHz) spectrometer. IR spectra were recorded with a VERTEX70 FT-IR spectrophotometer. UV-Vis spectra were recorded with a Lambda 950 spectrophotometer. Powder X-ray diffractograms (PXRDs) were recorded on a MiniFlex II powder X-ray diffractometer. The elemental analysis results were obtained by a vario MICRO elemental analyser. Thermogravimetric analyses (TGA) (N$_2$ atmosphere, heating rate of 10 °C/min) were carried out with a NETZSCH STA 449F3 TGA apparatus. The liquid and solid-state CD spectra were recorded using Biologic Science Instruments at 25 °C.

Preparation of S(R)-OH-bim

S(R)-OH-bim was synthesized according to previous report.$^1$

Preparation of ZIF-78

Crystal sample of ZIF-78 was synthesized according to previous report.$^2$

Preparation of S(R)-ZIF-78h through SALE

1.62 g (10 mmol) S-OH-bim was dissolved in 40 mL n-butyl alcohol to obtain 0.25 M stock solution. And 100 mg as-synthesized ZIF-78 was placed in a 13 mL sealed glass bottle along with 5 mL stock solution above. Then it was allowed to reaction at 120 °C for 7 days, but the solution need to be replaced with fresh stock solution every 24 hours. The solid sample was washed and collected as S-ZIF-78h in approximately 80% yield. R-ZIF-78h was prepared in the same way except for R-OH-bim replacing S-OH-bim.

CD measurement of D(L)-proline with S-ZIF-78h

D(L)-proline standard aqueous solutions were prepared in concentration of 0.07M. Then they were mixed in a volume ratio of 4:1, 3:1, 2:1, 1:1, 1:2, 1:3 and 1:4. Once the CD signals of those mixed samples were recorded, 0.1mg S-ZIF-78h was added into 2mL of them each, following by another measurement in 10 seconds. All the quantities used here were according to condition optimization.
Elemental analysis

**ZIF-78** structure formula: Zn(2-nim)(5-nbim), molecule formula: ZnC_{10}H_{6}N_{6}O_{4}, calculated: C 35.37%, H 1.78%, N 24.75%, found: 34.23%, H 2.21%, N 23.52%.

**S-ZIF-78h** Structure formula: Zn(2-nim)(5-nbim)$_{0.743}$(S-OH-bim)$_{0.257}$, molecule formula: ZnC$_{10.514}$H$_{7.285}$N$_{5.743}$O$_{3.743}$, calculated: C 37.21%, H 2.16%, N 23.70%, found: C 37.57%, H 2.68%, N 22.26%.

![Fig. S1](image_url)  
**Fig. S1** $^1$H NMR spectra (d-TFA) of 5-nbim in n-butanol solution and solutions replaced at different day.
Fig. S2 \( ^1 \text{H} \) NMR spectra (d-TFA) of S-ZIF-78h in detail.

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\begin{align*}
\text{Exchange Ratio} & = \frac{1.04}{3} \\
& = \frac{1}{1 + \frac{1.04}{3}} \\
& \approx 0.388
\end{align*}
\]

$100\% = 25.7\%$
Fig. S3 \textsuperscript{1}H NMR spectra (d-TFA) of R-ZIF-78h in detail.

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\frac{0.90}{3} = \frac{1 + \frac{0.90}{3}}{}
\]

Exchange Ratio = \( \frac{1 + \frac{0.90}{3}}{} \) * 100% = 23.1%

Fig. S4 Photos of (a) ZIF-78, S-ZIF-78h (b) before and (c) after immersed in 0.07M D-proline for 8 hours.
Fig. S5 UV absorption spectra of S(R)-OH-bim in aqueous solution.

Fig. S6 IR spectra of S-OH-bim, S-ZIF-78h and ZIF-78.

After SALE, S-ZIF-78h shows an extra weak absorption peak at 2975 cm\(^{-1}\), corresponding to C-H stretching vibration of CH\(_3\) which can only be observed in S-OH-bim. It indicated that 5-NO\(_2\)-bim
did be replaced by S-OH-bim in a certain ratio.

**Fig. S7** TGA analysis of S(R)-ZIF-78, S-ZIF-78h after BET measurement and as-synthesized ZIF-78.

After SALE, S(R)-OH-bim becomes less stable than ZIF-78, whose framework collapses at about 330 °C. The same weight-loss pattern indicates the same framework between S(R)-ZIF-78h and ZIF-78. So is S-ZIF-78h after BET measurement.
**Fig. S8** The powder XRD patterns of S-ZIF-78h, S-ZIF-78h after BET measurement and S-ZIF-78h in 0.07M D-proline for 8 hours.
**Fig. S9** linear fits of CD signals at 214nm in different ee%.

![Graph](image)

**Fig. S10** Absolute value changes of CD signals in different ee% according to linear fits.