

# Electronic Supplementary Information on the New Journal of Chemistry Publication Entitled

## **Chiral Covalent Triazine Framework CC-DMP**

### **CCTF@SiO<sub>2</sub> Core-Shell Microspheres Used for HPLC**

#### **Enantioseparation**

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## 1 Chemicals

(2S,5S)-2,5-dimethylpiperazine (DMP, 98%) was acquired from Wuxi LabNetwork (Wuhan) Chemical Technology (Hubei, China). Cyanuric chloride (CC, 98%) was acquired from Shanghai Adamas-beta Reagent (Shanghai, China). 1, 4-Dioxane (99%) was acquired from Shanghai Aladdin Biochemical Technology (Shanghai, China). Bare silica microspheres (UniSil 5-120, particle size: 5 $\mu$ m, pore size: 120 Å) were acquired from Nano-micro Technology (Suzhou, China). Hydrochloric acid and acetone were acquired from Yunnan Yanglin Industrial Development Zone Shandian Pharmaceutical (Yunnan, China). Anhydrous ethanol, isopropanol, and n-hexane were acquired from Guangdong Guanghua Technology (Guangdong, China). Anhydrous K<sub>2</sub>CO<sub>3</sub> (99%) was purchased from Tianjin Shengao Chemical Reagent (Tianjin, China). The chiral compounds utilized to estimate the chromatographic column's separation performance were obtained from Sigma-Aldrich (Missouri, USA), Adamas-beta (Shanghai, China), and TCI (Tokyo, Japan).

## 2 Instrumentations

A high-pressure column packing system (Shenzhen Zhengda Fluid Mechanical and Electrical Equipment, China) was utilized to prepare the CC-DMP CCTF@SiO<sub>2</sub> packed column. ELGA LabWater water purification equipment (London, UK) was utilized to create deionized water. The chromatographic separation of chiral compounds was performed on a 230 II high performance liquid chromatograph installed with an EC 2006 chromatographic workstation (Dalian Yilite Analytical Instrument, China). D/Max-3B powder X-ray diffraction (PXRD, Rigaku, Japan), S-3000N scanning electron microscope (SEM, Hitachi Science Systems, Japan), Fourier transform infrared spectroscopy (FTIR, WI, USA), and focused ion beam scanning electron microscopy (FIB-SEM, Helios G5) were utilized to characterize the prepared materials. The surface area and pore size of SiO<sub>2</sub> and CC-DMP CCTF@SiO<sub>2</sub> were examined by nitrogen adsorption-desorption isotherms at 77 K using the Micromeritics ASAP 2460 (BET, USA) instrument. The particle size distribution of CC-DMP CCTF@SiO<sub>2</sub> was obtained on the laser particle analyzer (Malvern

Mastersizer 2000, UK). The Chiralpak AD-H column (25 cm length  $\times$  4.6 mm i.d.) was obtained from Daicel Chiral Technologies (Shanghai, China). The stainless steel empty liquid chromatographic column (25 cm length  $\times$  2.1 mm i.d.) was obtained from Dalian Ripley Technology Instruments (Dalian, China).

### 3 Calculation of the thermodynamic parameters

The retention factors ( $k'$ ), separation factors ( $\alpha$ ), and resolution values ( $R_S$ ) were calculated from Eqs. (1), (2) and (3), respectively.

$$k' = \frac{t_R - t_0}{t_0} \quad (1)$$

$$\alpha = \frac{t_2 - t_0}{t_1 - t_0} \quad (2)$$

$$R_S = \frac{t_2 - t_1}{W_{1/2(1)} + W_{1/2(2)}} \quad (3)$$

where  $t_0$  is the column void time which was determined by 1,3,5-tri-tert-butylbenzene,  $t_1$  is the retention time for the faster moving analytes and  $t_2$  for the slower, meanwhile  $W_{1/2(1)}$  and  $W_{1/2(2)}$  is the corresponding peak width at half height.

The temperature dependence of the retention factor  $k'$  can be described by the van' t Hoff equation [Eq. (4)], and the Gibbs free energy change ( $\Delta G$ ) was calculated using Eq. (5).

$$\ln k' = -\frac{\Delta H}{RT} + \frac{\Delta S}{R} + \ln \Phi \quad (4)$$

$$\Delta G = \Delta H - T \Delta S \quad (5)$$

Here  $\Delta H$  is the enthalpy change and  $\Delta S$  is the entropy change for the transfer of solutes from the mobile phase to the stationary phase,  $R$  is the gas constant,  $T$  is the absolute temperature, and  $\Phi$  represents the column phase ratio which was calculated according to Eq. (6):

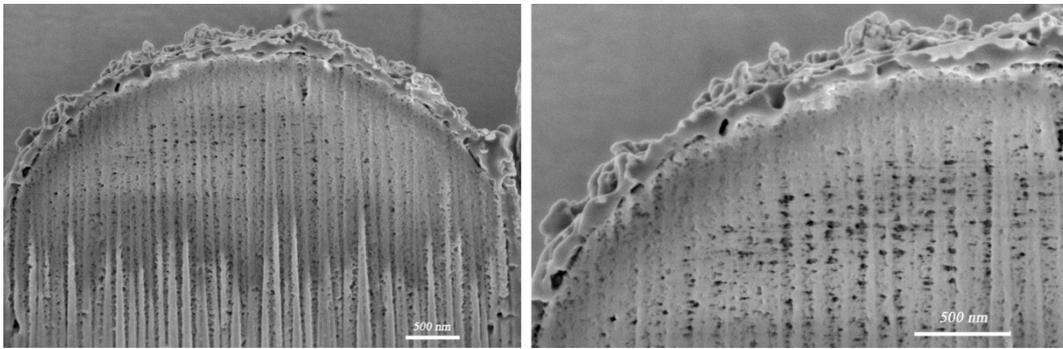
$$\Phi = \frac{V_S}{V_0} \quad (6)$$

in which the volume of the stationary phase in the column ( $V_S$ ) was obtained from Eq.(7) and the void volume of the column ( $V_0$ ) was evaluated based on Eq. (8):

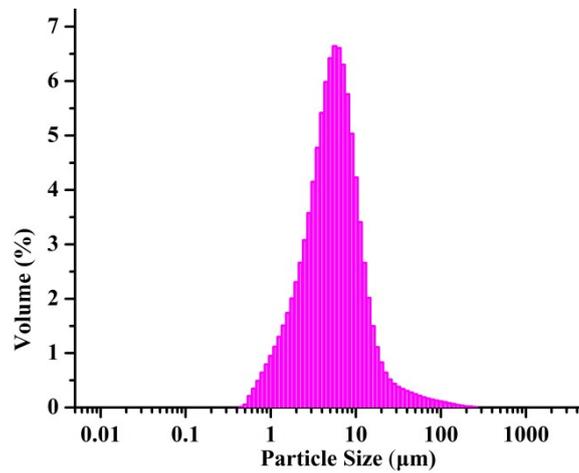
$$V_S = V_{col} - V_0 \quad (7)$$

$$V_0 = t_0 \times t_F \quad (8)$$

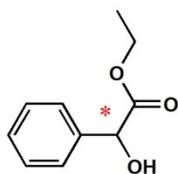
$V_{col}$  in Eq. (7) is the geometric volume of the column and  $F$  in Eq.(8) is the flow rate of the mobile phase.



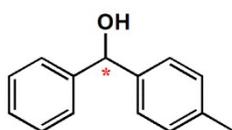
**Fig S1** FIB-SEM image of the CC-DMP CCTF@SiO<sub>2</sub>



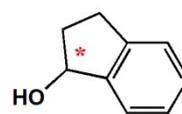
**Fig. S2** Size distribution of the CC-DMP CCTF@SiO<sub>2</sub>



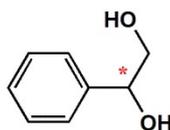
ethyl mandelate



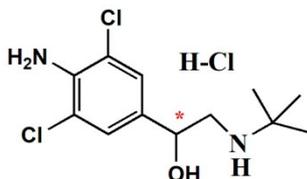
4-methylbenzhydrol



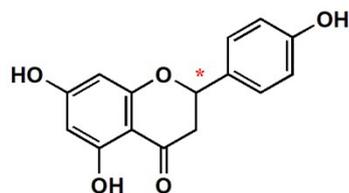
2,3-dihydro-1H-inden-1-ol



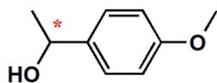
1-phenyl-1,2-ethanediol



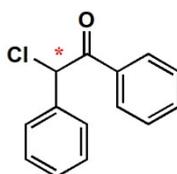
clenbuterol hydrochloride



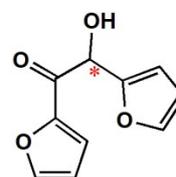
naringenin



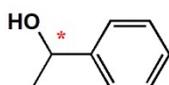
1-(4-methoxyphenyl) ethanol



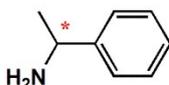
2-chloro-2-phenylacetophenone



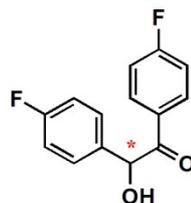
2,2'-furoin



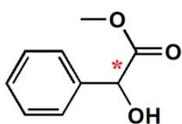
1-phenyl ethanol



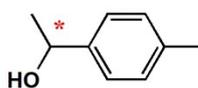
1-phenylethylamine



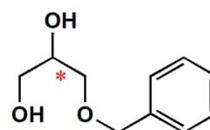
1,2-bis(4-fluorophenyl)-2-hydroxyethanone



mandelic acid methyl ester



1-(4-methylphenyl) ethanol



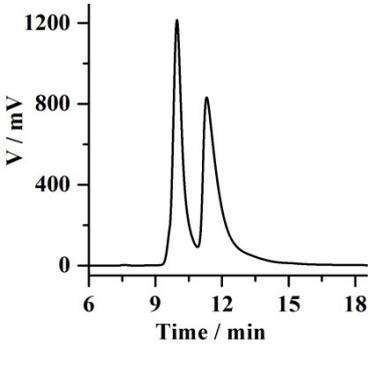
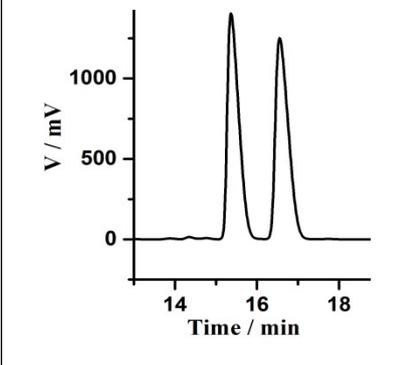
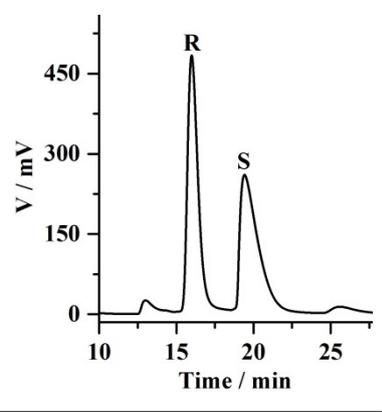
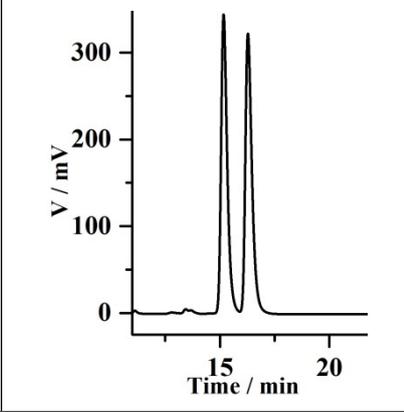
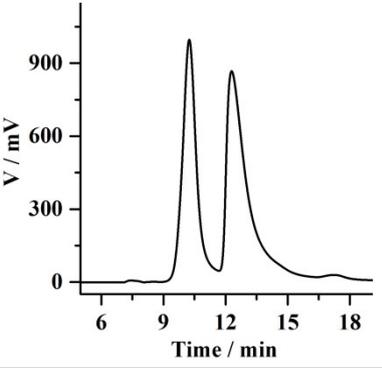
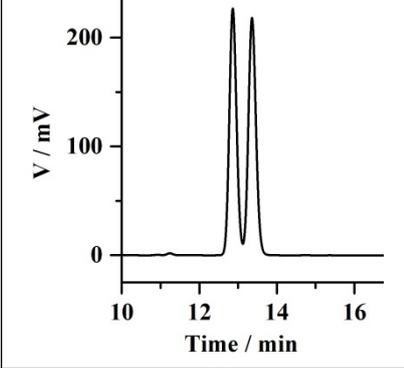
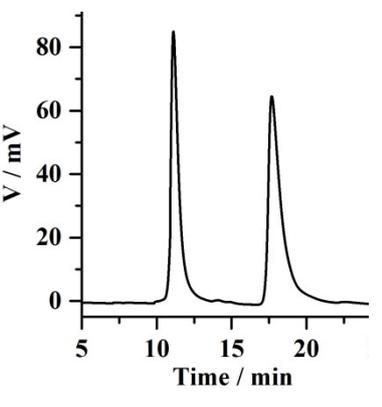
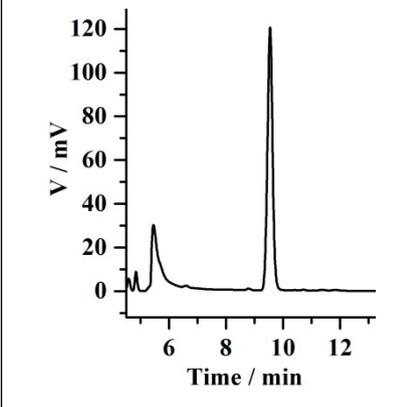
3-benzyloxy-1,2-propanediol

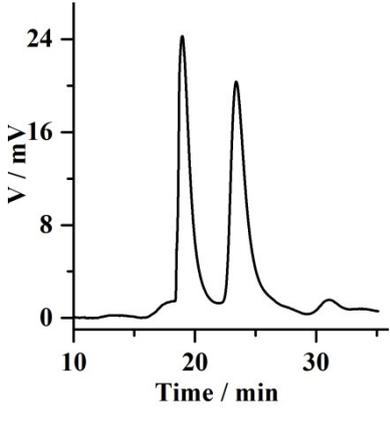
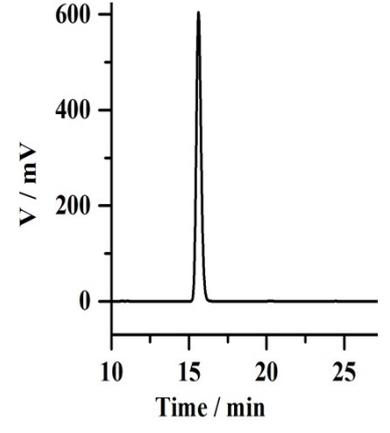
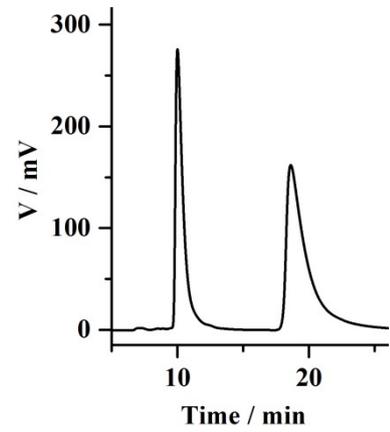
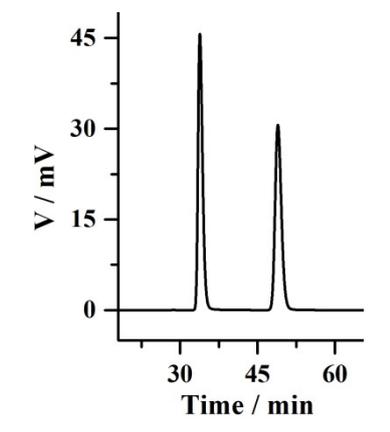
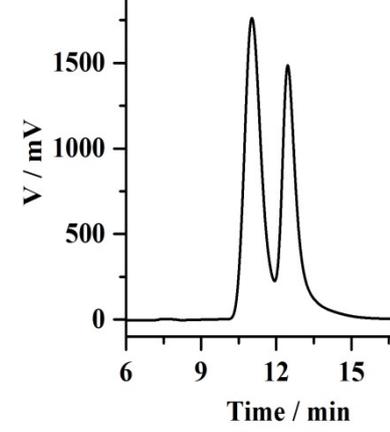
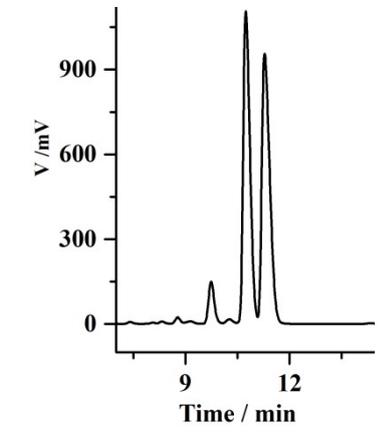


2,2,2-trifluoro-1-(9-anthryl)ethanol

**Fig. S3** Structures of the chiral compounds separated on the CC-DMP CCTF@SiO<sub>2</sub> packed column.

**Table S1** HPLC chromatograms for the separation of 16 chiral compounds on the CC-DMP CCTF@SiO<sub>2</sub> and Chiralpak AD-H columns (separation conditions as shown in Table 1).

Chiral compounds	CC-DMP CCTF@SiO <sub>2</sub> -packed column	Chiralpak AD-H
ethyl mandelate		
4-methylbenzhydrol		
2,3-dihydro-1H-inden-1-ol		
1-phenyl-1,2-ethanediol		

<p style="text-align: center;"><b>clenbuterol hydrochloride</b></p>		
<p style="text-align: center;"><b>naringenin</b></p>		
<p style="text-align: center;"><b>1-(4-methoxyphenyl) ethanol</b></p>		
<p style="text-align: center;"><b>2-chloro-2- phenylacetophenone</b></p>	