

Supporting Information

A chiral emissive porous organic cage used for high-resolution gas chromatography separations

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1. Derivatization of amino acids

In order to overcome the problem of poor volatility of amino acids that cannot be directly analyzed in GC, it is necessary to derivatize them to prepare the lower boiling point amino acid derivatives to analyze. In this paper, all amino acids used for analysis in GC were had been derivatized and the process is as follows¹: Firstly, a certain quality of amino acid (about 50 mg) was added to the mixed solution of 1 mL isopropanol/acetyl chloride (volume ratio: 3:1), then transferred the mixture into a sealed Teflon reactor and placed it into the stainless steel reactor and heated to 110 °C for 0.5 h. The excess reagent was removed under a certain N₂ flow after the reaction was completed. Secondly, 5 mL THF was added to dissolved the above product and 1.0 mL TFAH was slowly added and then heated it again and kept it at 90°C for 0.5 h. After the reaction was cooled to room temperature, the mixture was dried in vacuum to remove the excess reagent. Finally, the residue was dissolved in DCM for further GC analysis.

2. Synthesis diagram of the chiral emissive porous organic cage of 3P-1

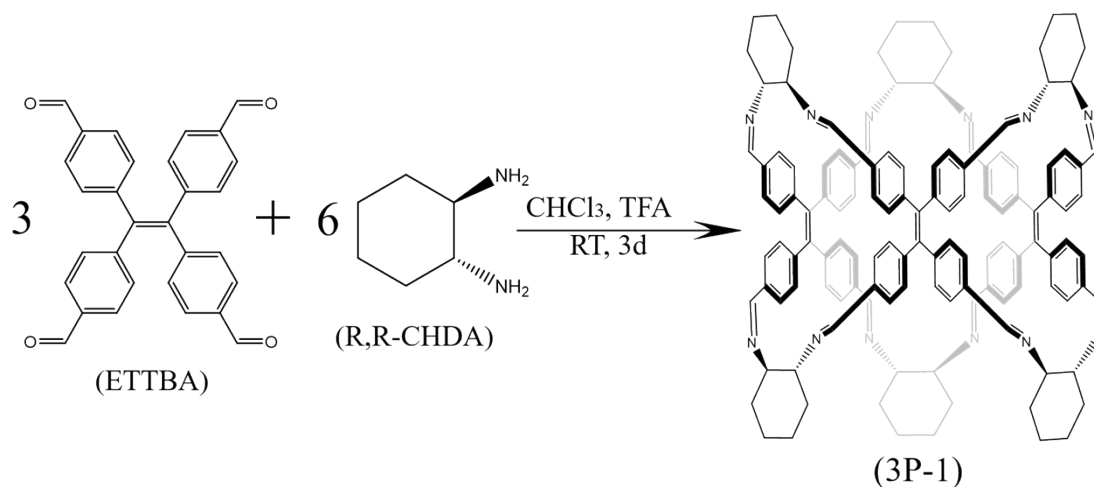


Fig. S1. Synthesis of 3P-1 by [3+6] cycloimination reaction.

3. The McReynolds constant of the 3P-1-coated column at 120°C

Table S1 McReynolds constant of the MCNs-coated column at 120°C

Benzene	Pyridine	1-Nitropropane	2-Pentanone	1-Butanol	Total	Ave
108	144	184	129	191	756	151

4. Separation of isomers on 3P-1-coated capillary column

Table S2 Chromatographic parameters of tested isomers on 3P-1-coated capillary column

Isomers	T (°C)	V ^a	k			α		R _s	
			k ₁	k ₂	k ₃	α ₁	α ₂	R _{s1}	R _{s2}
<i>1,3,5-/1,2,4-/1,2,3</i> -trichlorobenzene	160	1.0	1.57	2.23	2.71	1.42	1.22	4.80	3.65
<i>o-,m-,p</i> -chlorotoluene	140	1.0	1.63	1.86	1.99	1.14	1.07	7.88	3.69
<i>o-, m-, p</i> -dibromobrnzene	160	1.0	4.07	4.43	4.71	1.09	1.06	1.92	1.26
<i>o-, m-, p</i> -cresol	160	1.0	2.26	2.86	2.96	1.26	1.03	1.96	0.34
<i>o-, m-, p</i> -chloroaniline	165	1.0	1.86	3.69	4.17	1.99	1.13	15.36	0.89
<i>o-, m-, p</i> -dimethylbenzene	135	1.0	0.58	0.61	0.64	1.04	1.06	0.52	0.59
α-, β-ionone	190	1.0	2.60	3.66			1.41		3.86

^a Flow rate of carrier gas (N₂), mL·min⁻¹.

5. Comparison of separation performance of nine racemates by 3P-1-coated GC columns and β-DEX 120 column

Table S3 Comparison of separation performance of nine racemates by 3P-1-coated GC columns, β-DEX 120 column, POC-1-coated column and [Fe₄L₆](ClO₄)₈ coated column

Racemates	3P-1-coated column				β-DEX 120 column ^{2,3}			POC-1-coated column ²			[Fe ₄ L ₆](ClO ₄) ₈ coated column ³		
	T (°C)	v ^a	α	R _s	T (°C)	α	R _s	T (°C)	α	R _s	T (°C)	α	R _s
Butyl glycidyl ether	110	1	1.07	1.85	100	1.01	0.70	- ^d	- ^d	- ^d	130	1.10	1.52
γ-Heptalactone	175	1	2.87	6.24	130	1.01	1.06	175	1.12	5.48	125	1.91	9.38
2-Hexanol	180	1	1.55	5.84	75	1.02	1.17	125	1.04	1.51	- ^d	- ^d	- ^d
DL-Threonine ^b	145	1	2.31	3.43	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d
DL-Isoleucine ^b	150	1	3.59	3.11	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d
3-Buten-2-ol	150	1	2.82	2.46	50	1.05	1.93	97	1.09	1.67	- ^d	- ^d	- ^d
2,3-Butanediol	105	1	1.12	0.51	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d	- ^d
Epichlorohydrin	85	1	1.05	0.38	65	1.00	- ^c	105	1.03	0.78	- ^d	- ^d	- ^d
Epibromohydrin	95	1	1.18	0.63	70	1.00	- ^c	120	1.02	0.91	- ^d	- ^d	- ^d

^a Flow rate of carrier gas (N₂), mL·min⁻¹.

^b Trifluoroacetyl isopropyl ester derivative.

^c Cannot be separated.

^d Not reported.

6. The separation chromatograms on the commercial β -DEX 120 column

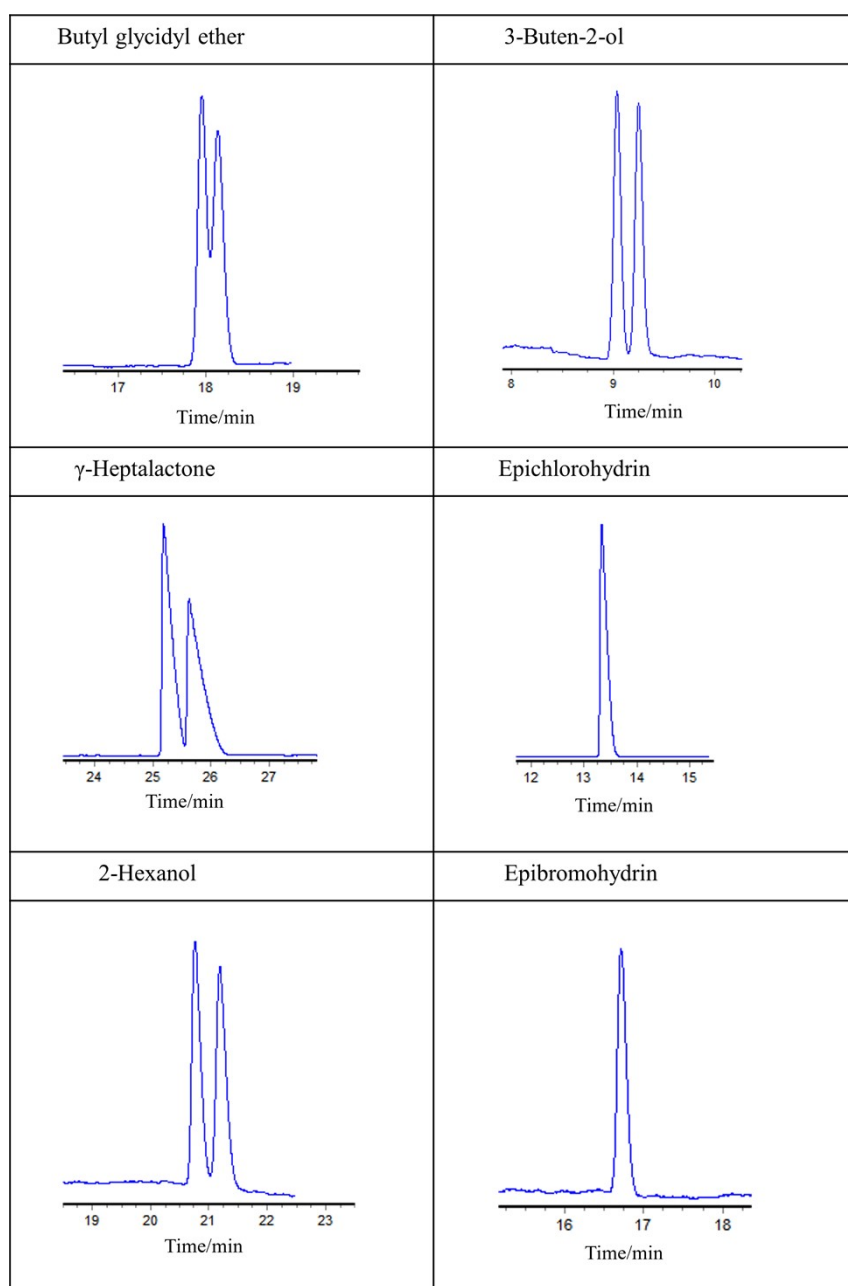


Fig. S2. GC chromatograms on the commercial β -DEX 120 column

7. The structure of separated racemates and isomers

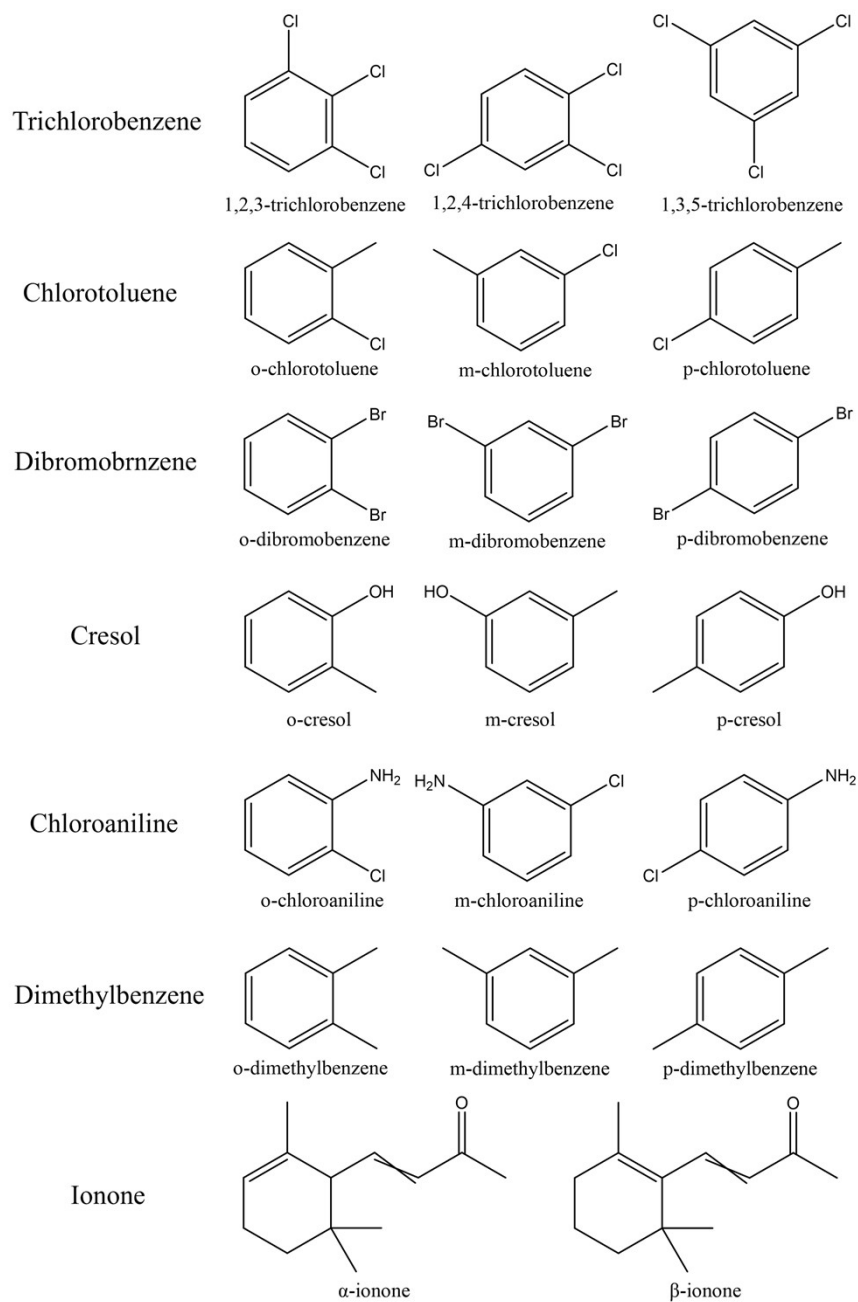


Fig. S3. Molecular structures of separated isomers.

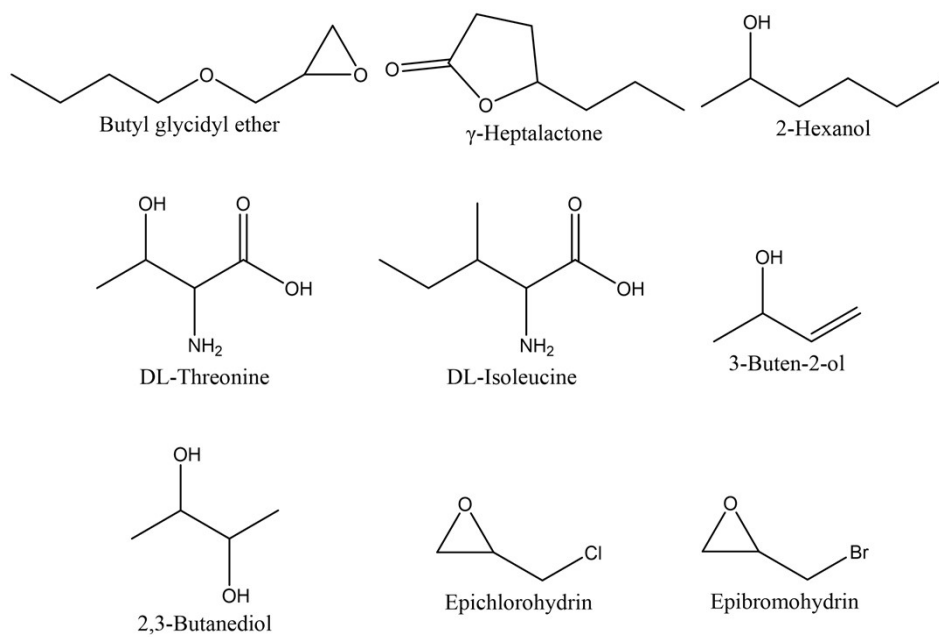


Fig. S4. Molecular structures of separated racemates.

8. The NMR spectra of 3P-1

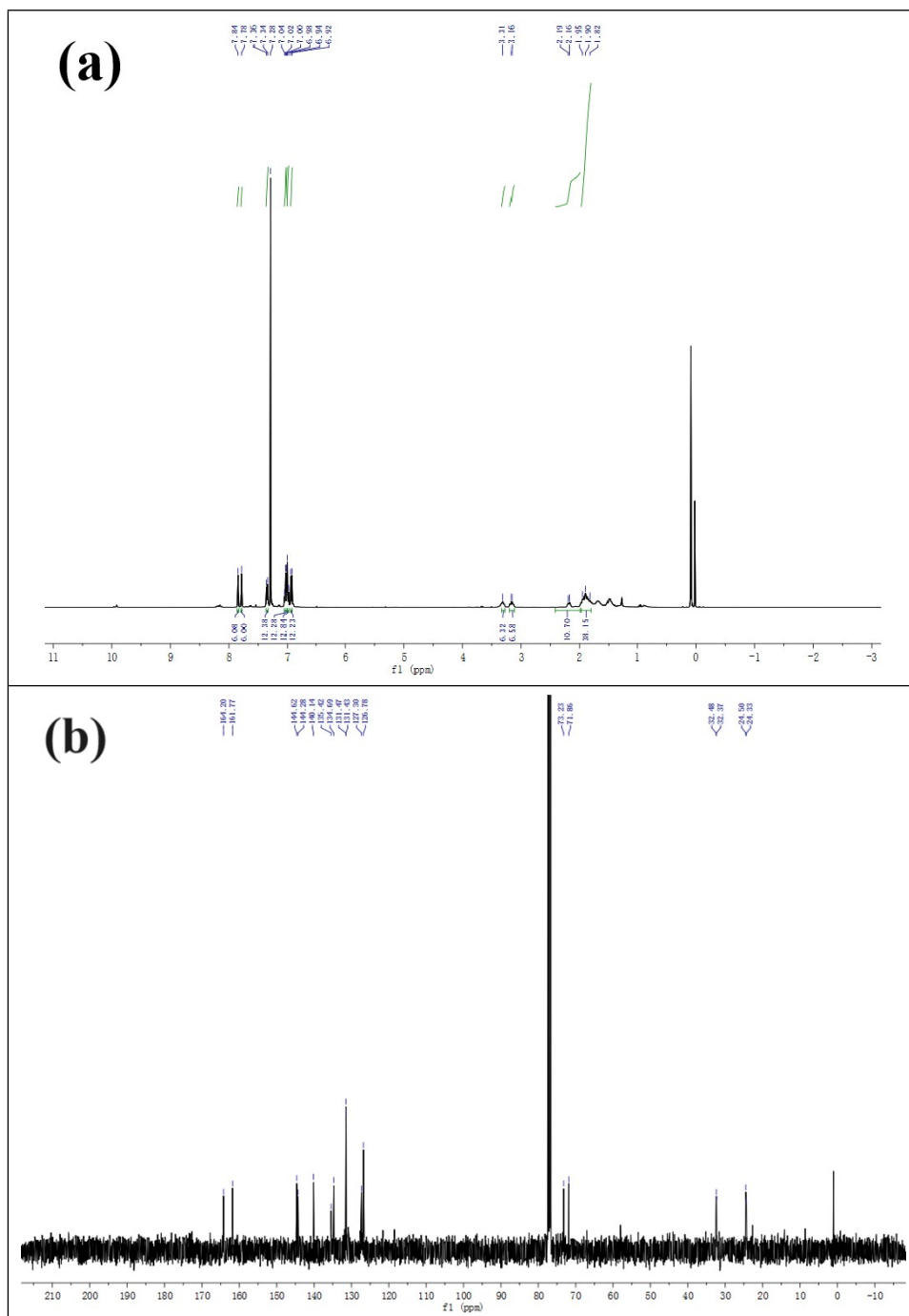


Fig. S5. ^1H NMR (400 MHz, CDCl_3), (b) ^{13}C NMR spectra of 3P-1.

9. The baseline of 3P-1-coated capillary column

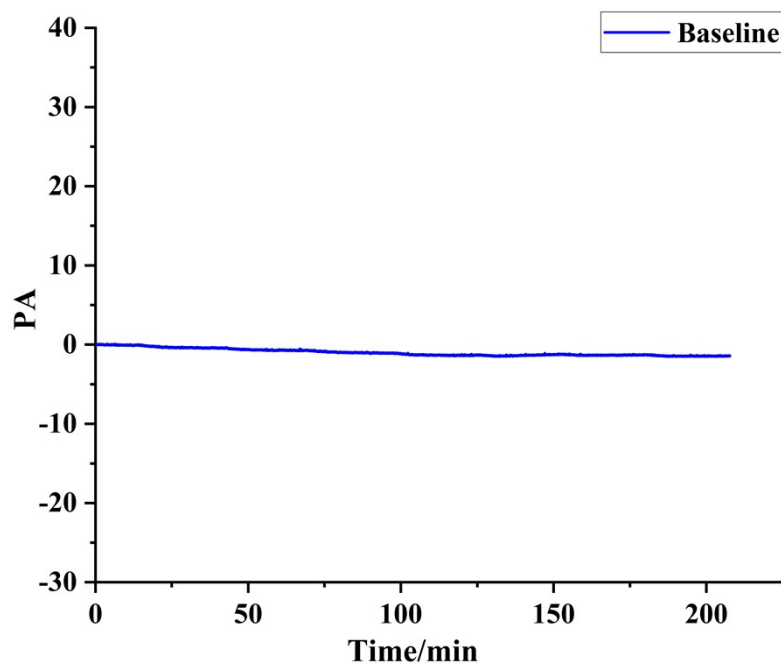


Fig. S6. The baseline of 3P-1-coated capillary column at 200 °C for about 200 min.

10. The long-term stability experiments of 3P-1-coated capillary column

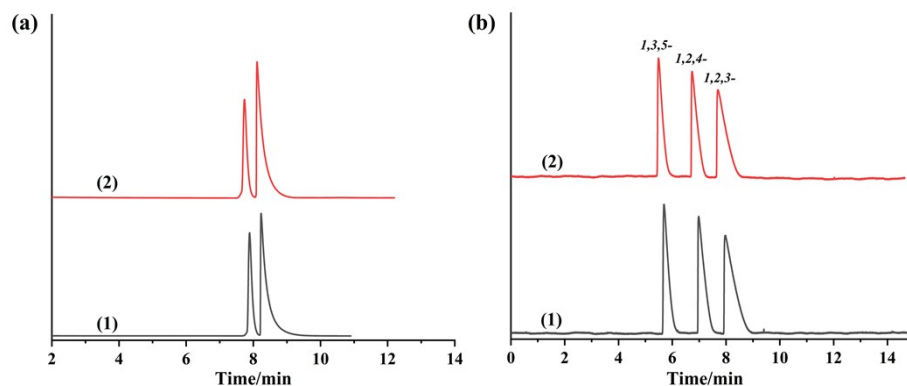


Fig. S7. The long-term stability of the 3P-1-coated column was characterized by GC separation of butyl glycidyl ether at 110 °C (a) and 1,3,5-/1,2,4-/1,2,3-trichlorobenzene at 160 °C (b). N_2 flow rate of $1.0 \text{ mL} \cdot \text{min}^{-1}$ for (a) and (b). (1)-just used; (2)-after four months of storage.

Reference:

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- 2 H. X. Li, T. P. Xie, K. Q. Yan, S. M. Xie, B. J. Wang, J. H. Zhang and L. M. Yuan, *Microchim. Acta*, 2020, **187**, 269.
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