Electronic Supplementary Material (ESI) for ChemComm.

Engineering a Homochiral Metal-Organic Framework Based on Amino Acid for Enantioselective Separation

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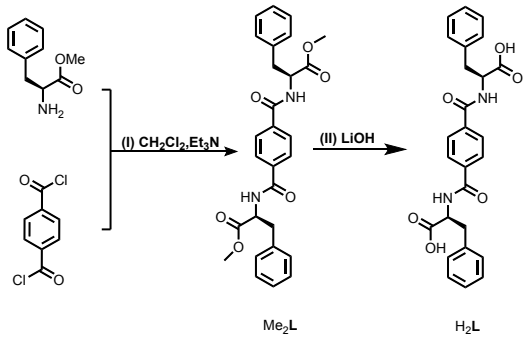
1. Materials and general procedures.

All of the chemicals are commercially available and used without any further purification. NMR date were collected on an Agilent VNMRS-600 spectrometer. The IR (KBr pellet) spectrum was recorded (400-4000 cm^{-1} region) on a Nicolet Magna 750 FTIR spectrometer. Electrospray ionization mass spectra (ES-MS) were recorded on a Finnigan LCQ mass spectrometer using MeOH as mobile phase. Single-crystal XRD data for (S)-**1** were collected several times at 100 K at NFPS (Shanghai) synchrotron radiation on BL17B beamline using λ = 0.65247 Å for several times, and the best dataset was chosen to be indexed, integrated and scaled using the APEX3 program. The structure of (S)-**1** was solved by the direct methods with SHELXS-2018 and refined with SHELXL-2018 using *OLEX 2-1.2*. All the hydrogen atoms attached to the ligand were placed in calculated positions and refined using a riding model. Contributions to scattering due to these highly disordered guest molecules in **1** were removed using the SQUEEZE subroutine of the PLATON software package. The structure was then refined again using the resulting new HKL file. **1** can be best formulated as $[(Zn_4O)_2(\mathbf{L})_6(bpy)_3]$, on the basis of single-crystal diffraction, IR spectra and thermogravimetric analyses (TGA). Crystal data and details of the data collection are given in Table S1, while the selected bond distances and angles are presented in Tables S2. CCDC number of **1** is 1968168, which contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif. Thermogravimetric analyses of **1** was carried out in a nitrogen atmosphere with a heating rate of 10 °C/min on a TGA-50 thermogravimetric analyzer. Powder X-ray diffraction (PXRD) data were collected on a DMAX2500 diffractometer using Cu Kα radiation. The simulated powder pattern was calculated using Mercury based on single crystal diffraction data of **1**. The circular dichroism (CD) spectra were recorded on a J-800 spectropolarimeter. The date of dye absorption experiment was recorded on an Agilent Technologies carry UV/Vis Spectrometer. Analytical high-performance liquid chromatography (HPLC) was performed on an Agilent Technologies 1260 Infinity II with UV detection. Analytical ChiralCel OD-H/OJ-H/AS-H column (4.6 mm×25 cm) from Daicel were used.

2. Synthesis

2.1 Synthesis of H_2**L**



2.1 Synthesis of Me_2**L**.

A mixture of Et_3N (16.8 mL, 120 mmol) and *L*-phenylalanine methyl ester (17.9 g, 100 mmol) in dry CH_2Cl_2 (80 mL) was stirred at 0 °C for 30 minutes, then a solution of terephthaloyl chloride 42.4 g (210 mmol) in 50 ml dry CH_2Cl_2 was added slowly. The resulting reaction mixture was stirred at 60 °C for 8 hours. After the reaction, the mixture was poured into water (100 mL) and washed by 2M HCl and saturated solution of $NaHCO_3$, respectively. The organic phase was dried over Na_2SO_4, and then concentrated under vacuum. The crude product was further purified by flash chromatography over silica gel, which afforded 46.3 g Me_2**L** with ca. 95% yield based on *L*-phenylalanine methyl ester.

2.2 Synthesis of H_2**L**.

Me_2**L** (20.0 g, 41.0 mmol) and $LiOH·H_2O$ (4.3 g, 102.5 mmol) were dissolved in a mixture solvent of THF (40 mL), MeOH (10 mL) and H_2O (10 mL). The reaction mixture was stirred at 100 °C for 8 h. After removal of the solvent in vacuo, the residue was diluted with H_2O and then acidified with 2M HCl. The precipitate was collected by filtration, washed with water, and dried in air to afford 16.3 g of white solid of H_2**L** in a ca. 98%.

2.3 Synthesis of (S)-**1** and (R)-**1**.

A mixture of $Zn(CH_3COO)_2·2H_2O$ (18.3 mg, 0.10 mmol), (S)-H_2**L** (23 mg, 0.05 mmol) and bipyridine (7.8 mg, 0.05 mmol) was placed in a glass vial containing DMA (5 mL), H_2O (5 mL) and EtOH (5 mL). The vial was sealed tightly and heated at 80°C for one day. Colorless triangular prism-like crystals of (S)-**1** were formed, washed with acetone, and dried in air. Yield: 23.6 mg, ~75% based on H_2**L**. The synthesis process of (R)-**1** is the same as that of (S)-**1**, except the ligand (R)-H_2**L** is instead by (S)-H_2**L**.

3. Table S1. Crystal data and structure refinement for 1.

Identification code	(S)-**1**
Empirical formula	$C_{93}H_{78}N_9O_{19}Zn_4$
Formula weight	1887.12
Temperature (K)	100
Wavelength (Å)	0.65247
Crystal system, space group	Trigonal, P321
Unit cell dimensions	a = 25.6587(8) Å alpha = 90 deg. b = 25.6587(8) Å beta = 90 deg. c = 10.1334(5) Å gamma = 120 deg.
Volume	5777.7(5) $Å^3$
Z, Calculated density	2, 1.085 mg/m^3
Absorption coefficient	0.697 mm^{-1}
F(000)	1942
θ range for data collection (º)	2.497 to 27.869
Limiting indices	-36<=h<=36, -36<=k<=36, -14<=l<=14
Reflections collected Independent reflections	103649 / 11693 [R(int) = 0.0872]
Completeness to theta Refinement method	98.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11693 / 58 / 412
Goodness-of-fit on F^2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0663, wR2 = 0.1837
R indices (all data)	R1 = 0.0739, wR2 = 0.1905
Absolute structure parameter	0.079(7)

4. Table S2. Selected Bond lengths [Å] and angles [º] for 1.

Zn(2)-O(7)	1.9481(1)
Zn(2)-O(6)#1	1.981(3)
Zn(2)-O(2)#2	2.209(3)
Zn(2)-O(5)#3	2.056(3)
Zn(2)-N(3)	2.077(4)
Zn(1)-O(7)	1.959(4)
Zn(1)-O(1)#4	1.974(3)
Zn(1)-O(1)#2	1.974(3)
Zn(1)-O(1)	1.974(3)

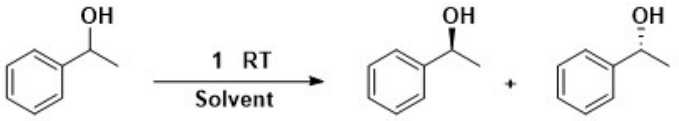
O(7)-Zn(2)-O(6)#1	111.77(1)
O(7)-Zn(2)-O(2)#2	88.70(1)
O(7)-Zn(2)-O(5)#3	101.69(1)
O(7)-Zn(2)-N(3)	151.30(1)
O(6)#1-Zn(2)-O(2)#2	93.20(1)
O(6)#1-Zn(2)-O(5)#3	102.24(2)
O(6)#1-Zn(2)-N(3)	94.37(1)
O(2)#2-Zn(2)-Zn(1)	62.49(9)
O(5)#3-Zn(2)-Zn(1)	114.87(1)
O(5)#3-Zn(2)-O(2)#2	156.43(2)
O(5)#3-Zn(2)-N(3)	83.29(1)
O(7)-Zn(1)-O(1)	106.89(1)
O(7)-Zn(1)-O(1)#2	106.88(1)
O(1)#4-Zn(1)-O(1)#2	111.93(9)
O(1)#4-Zn(1)-O(1)	111.93(9)
O(1)-Zn(1)-O(1)#2	111.93(9)
Zn(2)#4-O(7)-Zn(2)	112.78(1)
Zn(2)#4-O(7)-Zn(2)#2	112.78(1)
Zn(2)#2-O(7)-Zn(2)	112.78(1)
Zn(2)-O(7)-Zn(1)	105.92(1)
Zn(2)#4-O(7)-Zn(1)	105.92(1)
Zn(2)#2-O(7)-Zn(1)	105.92(1)

Symmetry transformations used to generate equivalent atoms:
#1 x-y+1,-y+1,-z+1 #2 -y+1,x-y+1,z
#3 -x,-x+y,-z+1 #4 -x+y,-x+1,z

5. Experimental procedure for chiral adsorption and separation.

5.1 General procedure for adsorption and separation: We have initially optimized separation condition including solvents and concentration by selecting 1-phenylethanol as a model substrate (Table S3). Then, solvent-exchanged sample of (S)-**1** (50 mg) was immersed in a solution of indicated racemic analyte in acetone for 8h at room temperature. After this, the solid sample was filtered, washed thoroughly with methanol to remove the analyte on the surface, and then soaked in acetone to extract the encapsulated guests. Optical purity of desorbed analytes was determined by HPLC with different Chiralcel column (4.6mm×25 cm). The results are sunmmrized in Table S3.

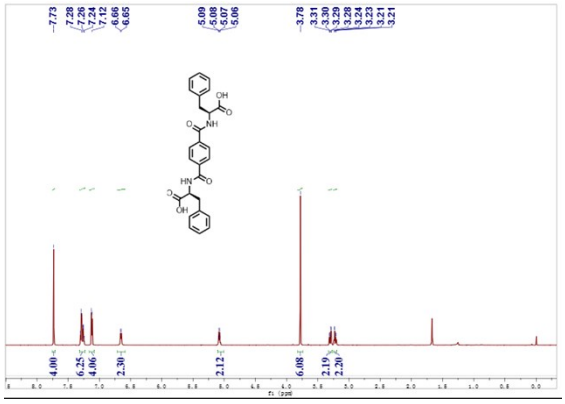
Table S3. Optimization of the separation conditions at room temperature.

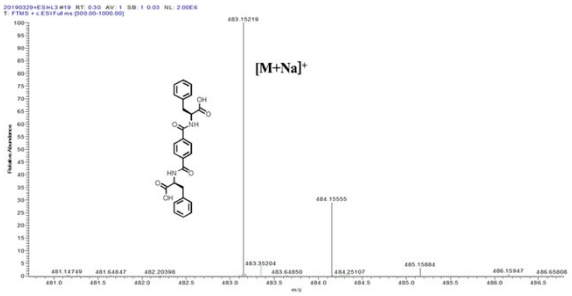


Entry	Solvent	Solvent volume (mL)	Substrate loading (mg)	ee (%)[b]
1	THF	5	15	36.0
2	EtOH	5	15	37.7
3	MeOH	5	15	39.5
4	CH_3CN	5	15	53.2
5	CH_2Cl_2	5	15	77.7
6	$(CH_3)_2CO$	5	15	94.2
7	$(CH_3)_2CO$	5	5	99.8
8	$(CH_3)_2CO$	5	10	99.8
9	$(CH_3)_2CO$	5	20	84.3
10	$(CH_3)_2CO$	5	25	76.7
11	$(CH_3)_2CO$	5	30	54.5

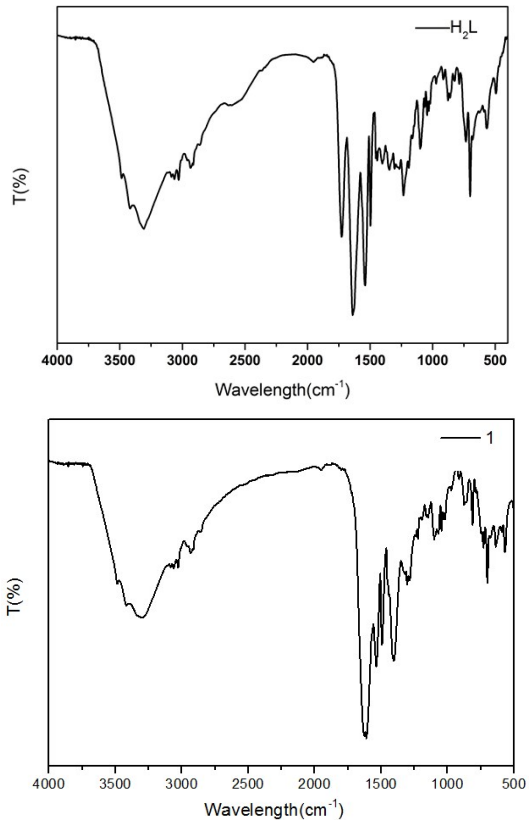
5.2 The procedure for the separation of (±)-ibuprofen: An empty glass column with an inner diameter of ca. 0.5 cm was packed with ca. 360 mg (S)-**1**. Then, racemic (±)-ibuprofen (6.3 mg, 30 μmol) was filled on the top of the packed material. After this, 80 mL acetone was served as eluent to run through the packed column. The resulting eluent at every 8 mL was collected separately and analyzed by HPLC. The experimental setup and HPLC results are shown in Fig S15.

6. Figure S1. NMR spectra and mass spectra of H_2L.

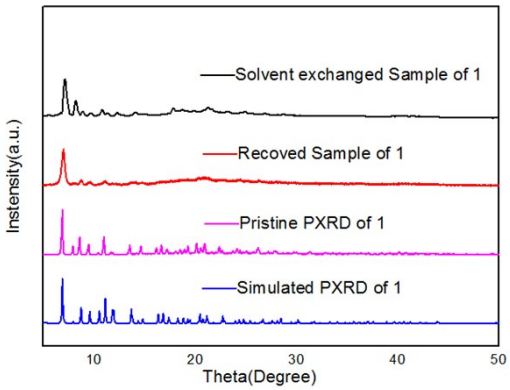




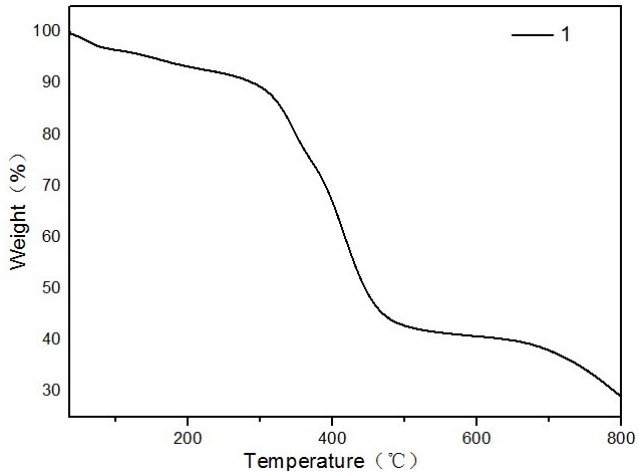
7. Figure S2. IR spectra of H_2L and 1.



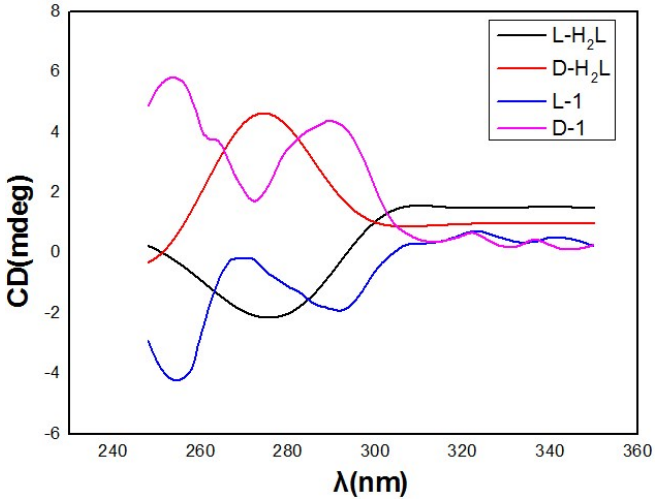
8. Figure S3. PXRD patterns of 1.



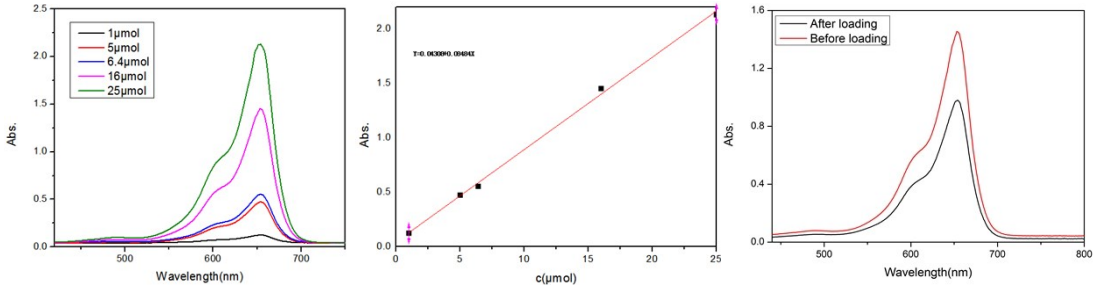
9. Figure S4. TGA curves of 1.



10. Figure S5. CD spectra of H_2L and 1.



11. Figure S6. The result of methylene blue adsorption by 1.



$n(MB)=V\times(c_{before}-c_{after})$ = 2 mL × 1.012×10^{-3} mol·L^{-1} = 2.024×10^{-6} mol;

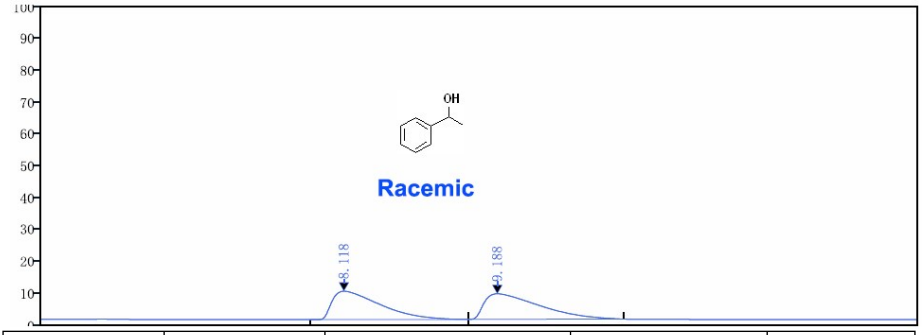
n((S)-**1**) = m/M= 5.4 mg/M = 2.86×10^{-6} mol;

n(MB): n((S)-**1**) =1.41

12. Figure S7. HPLC results of enantioseparation of secondary alcohols with (S)-1 as adsorbent.

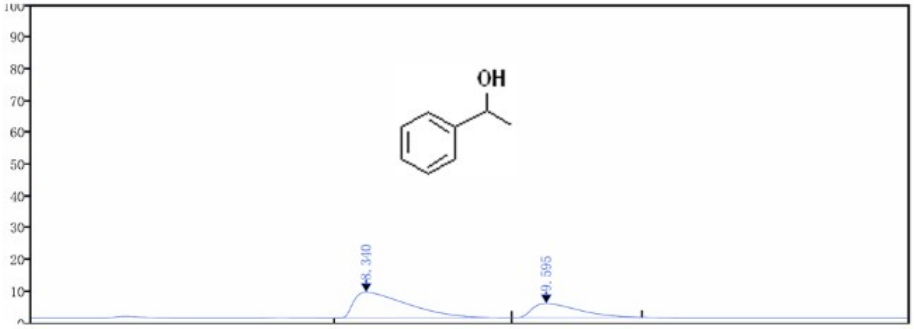
HPLC results of screening conditions for the separation of 1-phenylethanol with (S)-**1** (Table S3).

Racemic 1-phenylethanol: ChiralCel OJ-H column; hexane/i-PrOH =93/7, flow rate=1.0 mL/min, 220 nm; t_R=8.118 min, t_R =9.188 min.



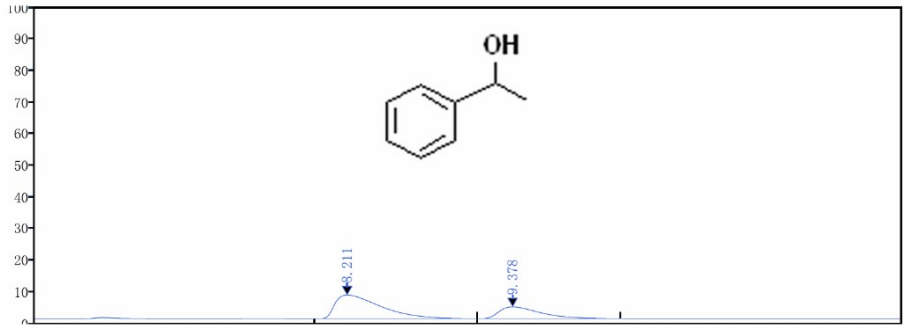
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	8.118	16401.06	49.19
2	MM	9.188	16938.35	50.81
The Total			3339.40	

1-phenylethanol (Entry 1 in Table S3):



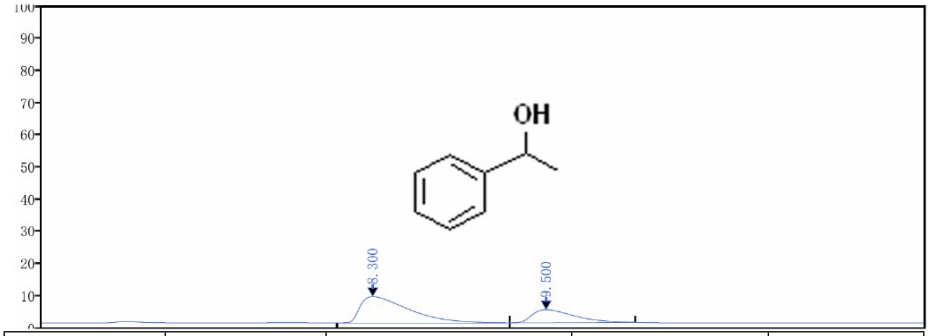
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.340	19067.70	68.01
2	MM	9.595	8967.50	31.99
The Total			28035.21	

1-phenylethanol (Entry 2 in Table S3):



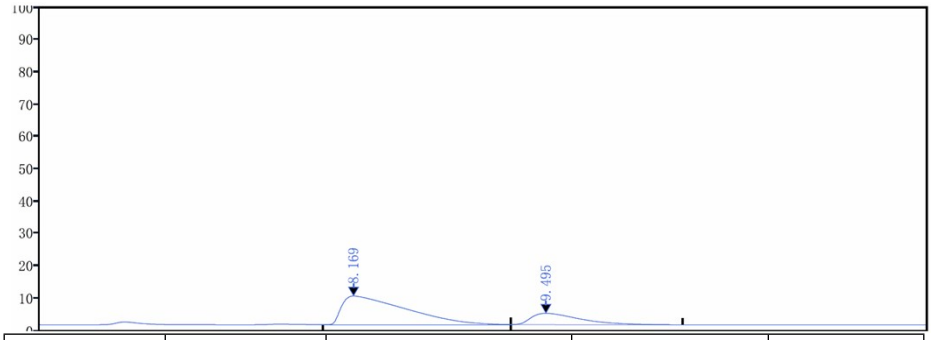
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.211	13629.89	68.83
2	MM	9.378	6172.39	31.17
The Total			19802.28	

1-phenylethanol (Entry 3 in Table S3):



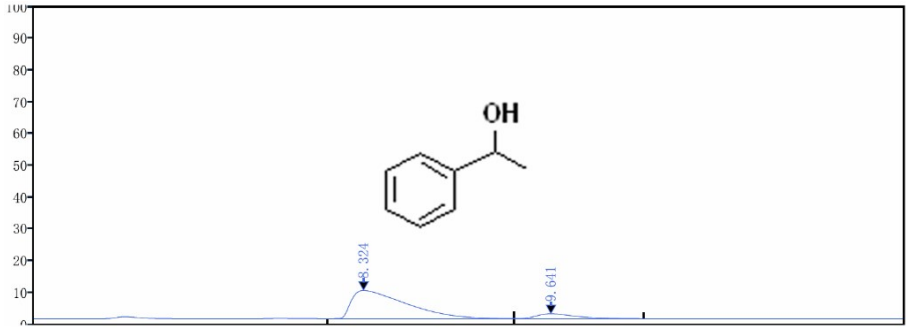
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MH	8.300	14532.98	69.71
2	HM	9.500	6314.31	30.29
The Total			20847.29	

1-phenylethanol (Entry 4 in Table S3):



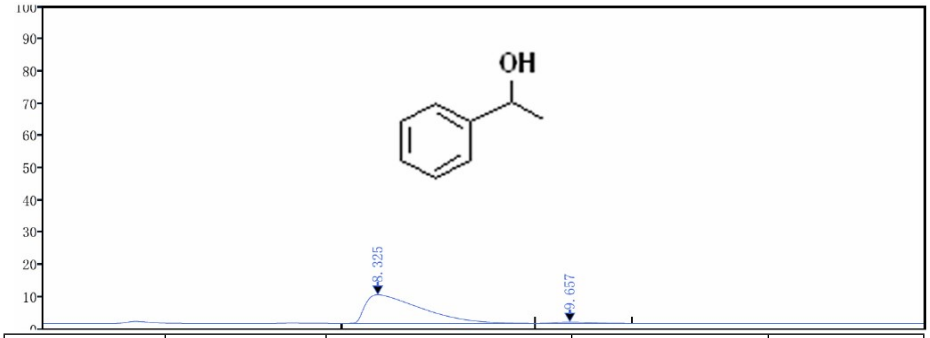
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.169	28431.16	76.60
2	MM	9.495	8684.39	23.40
The Total			37115.56	

1-phenylethanol (Entry 5 in Table S3):



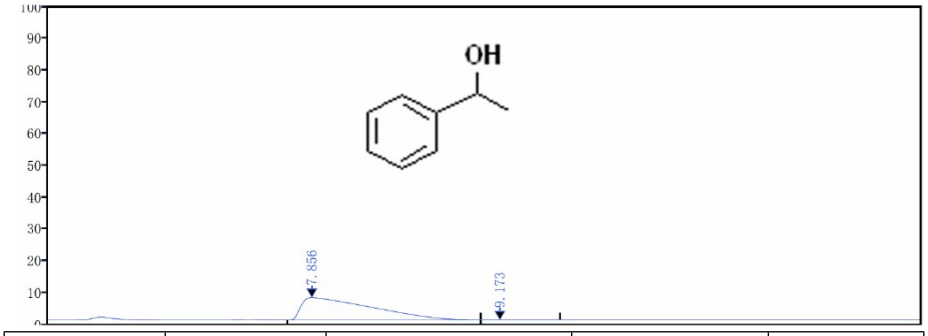
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HH	8.324	20428.79	88.89
2	HM	9.641	2553.59	11.11
The Total			22982.38	

1-phenylethanol (Entry 6 in Table S3):



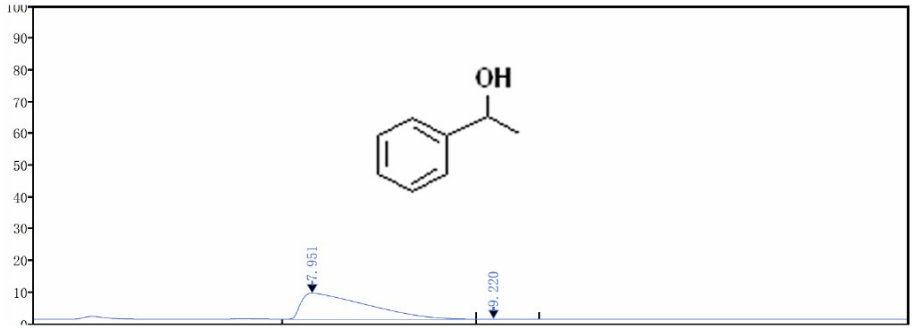
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	8.325	20372.04	97.10
2	MM	9.657	607.64	2.90
The Total			20979.68	

1-phenylethanol (Entry 7 in Table S3):



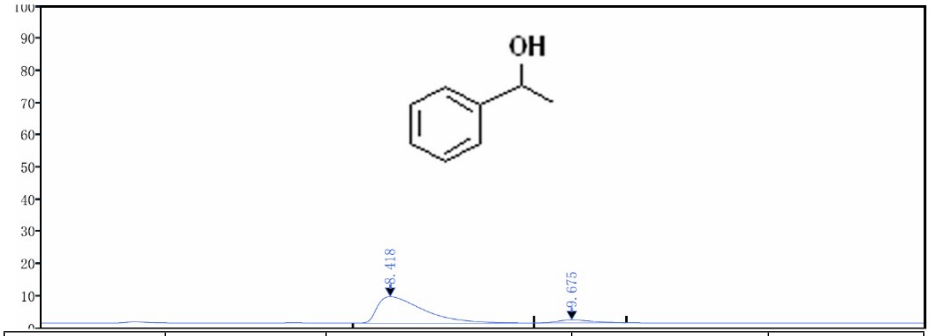
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.856	37824.18	99.91
2	MM	9.173	32.18	0.09
The Total			37856.37	

1-phenylethanol (Entry 8 in Table S3):



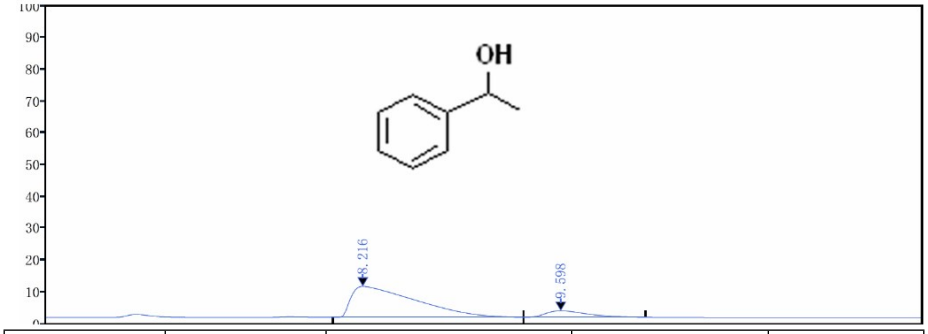
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.951	31854.63	99.91
2	MM	9.220	29.10	0.09
The Total			31883.72	

1-phenylethanol (Entry 9 in Table S3):



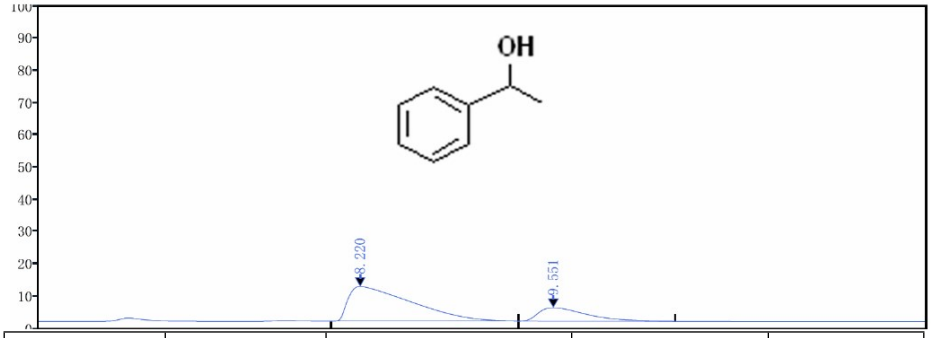
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MH	8.418	11512.08	92.19
2	HM	9.675	974.79	7.81
The Total			12486.87	

1-phenylethanol (Entry 10 in Table S3):



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.216	28894.43	88.32
2	MM	9.598	3821.68	11.68
The Total			32716.11	

1-phenylethanol (Entry 11 in Table S3):



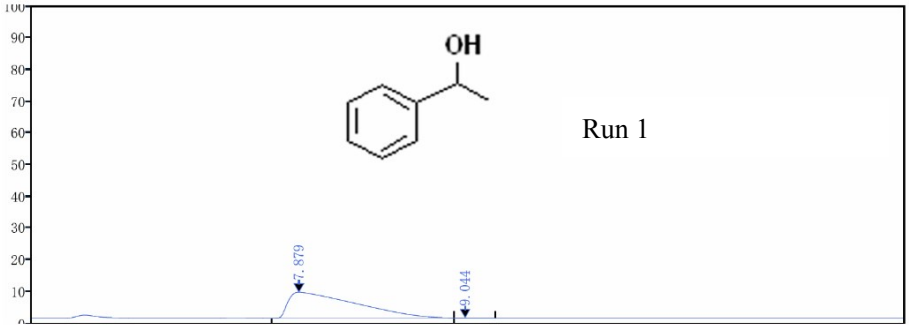
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.220	27274.26	77.29
2	MM	9.551	8012.48	22.71
The Total			35286.73	

The HPLC results of enantioseparation of 1-phenylethanol and its derivatives with (S)-**1**.

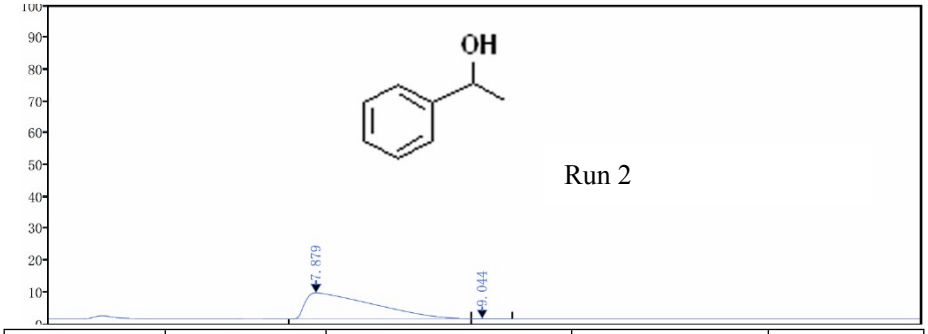
Racemic 1-phenylethanol: ChiralCel OJ-H column; hexane/i-PrOH =93/7, flow rate=1.0 mL/min, 220 nm; t_R=8.118 min, t_R =9.188 min.

Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	8.118	16401.06	49.19
2	MM	9.188	16938.35	50.81
The Total			3339.40	

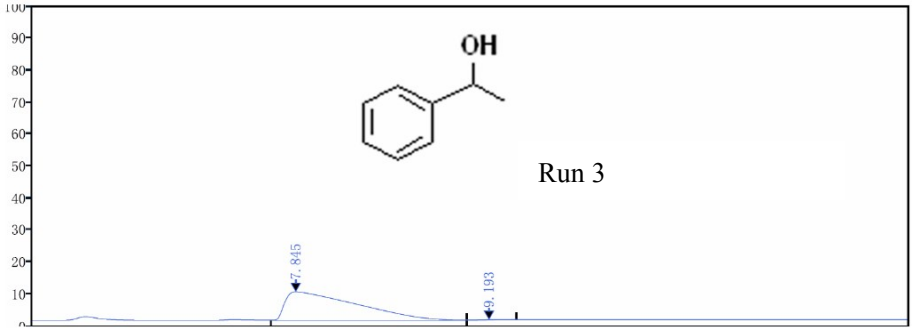
1-phenylethanol (**1a**' in Figure **2**):



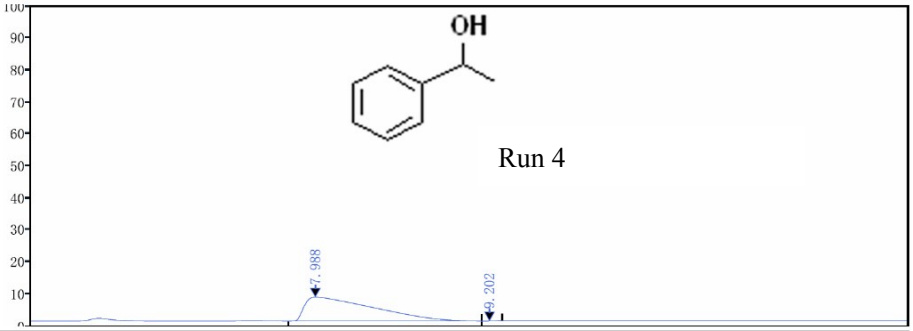
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.879	35279.46	99.91
2	MM	9.044	33.30	0.09
The Total			35312.76	



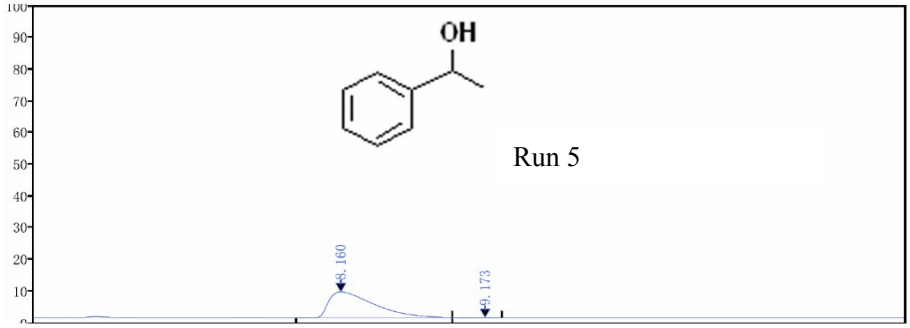
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.900	35888.87	99.66
2	MM	9.269	123.77	0.34
The Total			36012.64	



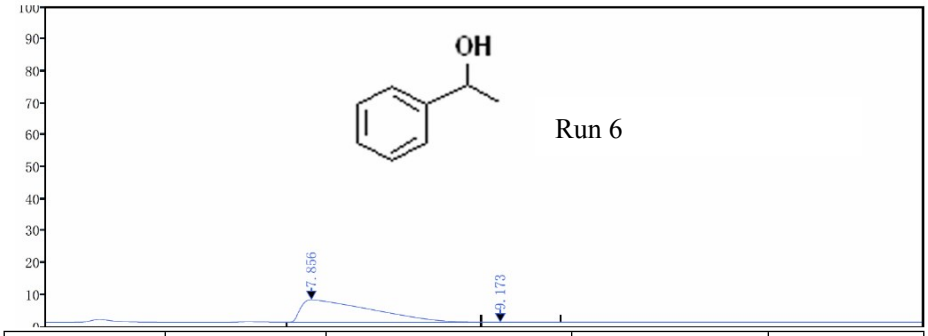
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.845	38377.58	99.74
2	MM	9.193	99.40	0.26
The Total			38476.99	



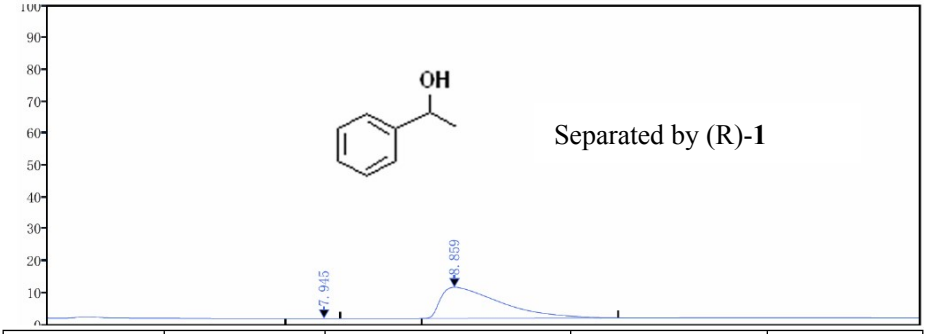
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.988	35302.30	99.96
2	MM	9.202	15.62	0.04
The Total			35317.93	



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.160	13609.18	99.73
2	MM	9.173	37.47	0.27
The Total			13646.65	

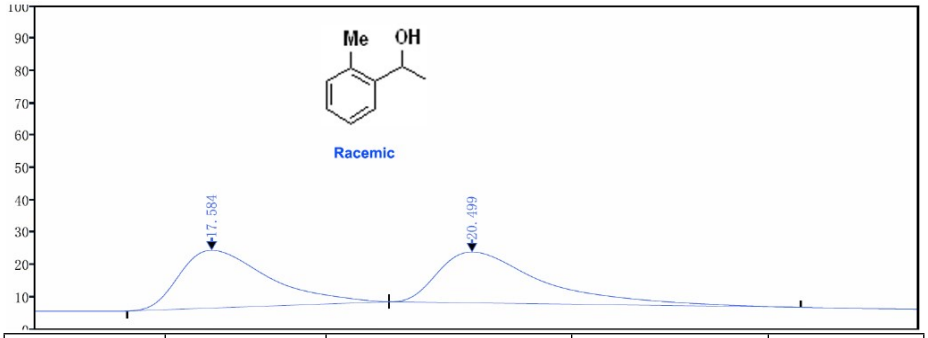


Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.856	37824.18	99.91
2	MM	9.173	32.18	0.09
The Total			37856.37	



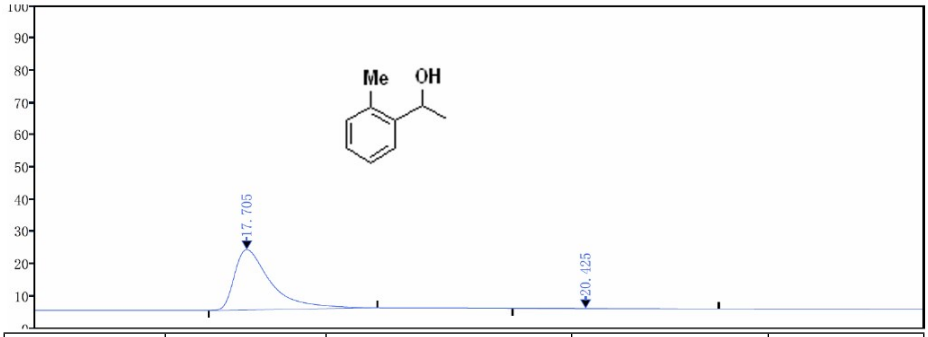
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.945	0.03	0.00
2	MM	8.859	17052.11	100.00
The Total			17052.13	

Racemic 1-(2-methylphenyl)ethanol: ChiralCel AD-H column; hexane/i-PrOH =99/1, flow rate=1.0 mL/min, 220 nm; t_R=17.584 min, t_R=20.499 min.



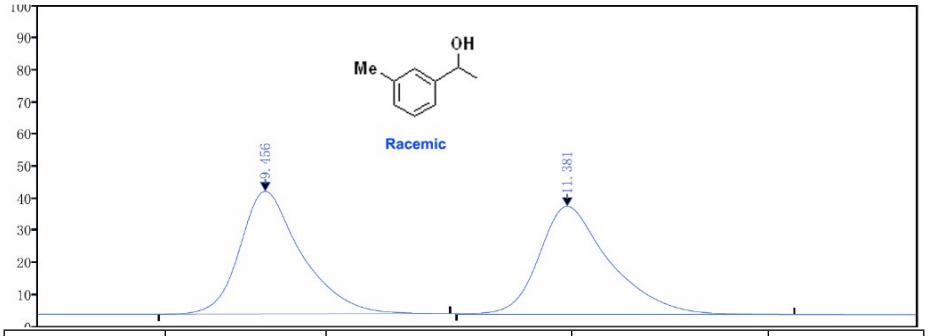
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	17.584	99770.23	49.18
2	MM	20.499	103083.03	50.82
The Total			202853.26	

1-(2-methylphenyl)ethanol (**1b**' in Figure **2**):



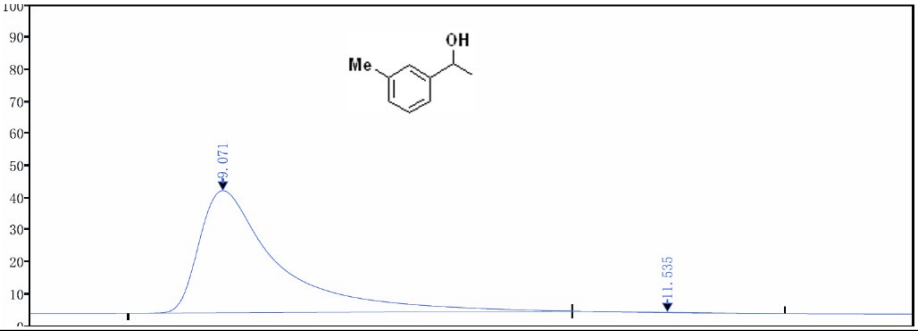
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	17.705	17604.39	99.84
2	MM	20.425	29.09	0.16
The Total			17633.49	

Racemic 1-(3-methylphenyl)ethanol: ChiralCel OD-H column; hexane/i-PrOH =95/5, flow rate = 0.8 mL/min, 220 nm; t_R=9.456 min, t_R=11.381 min.



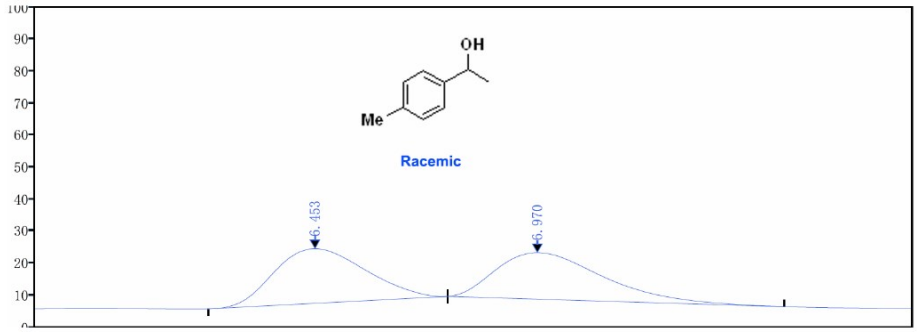
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HH	9.456	9441.98	49.68
2	HM	11.381	9563.45	50.32
The Total			19005.43	

1-(3-methylphenyl)ethanol (**1c**' in Figure **2**):



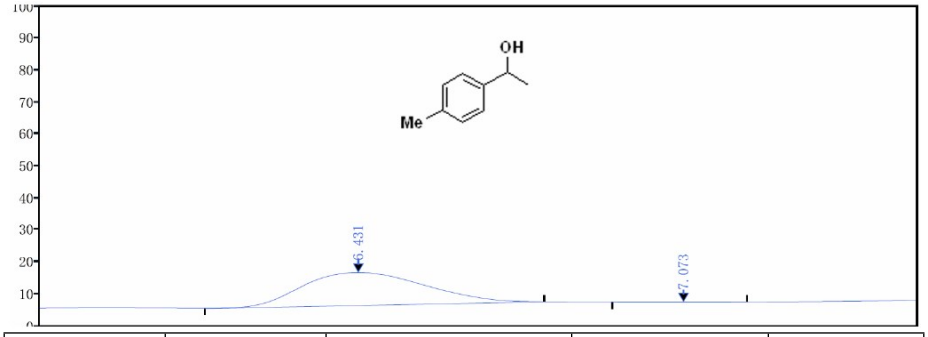
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	9.071	27597.88	99.57
2	MM	11.535	119.35	0.43
The Total			27717.23	

Racemic 1-(4-methylphenyl)ethanol: ChiralCel AD-H column; hexane/i-PrOH =95/5, flow rate = 1.0 mL/min, 220 nm; t_R= 6.453min, t_R=6.970 min.



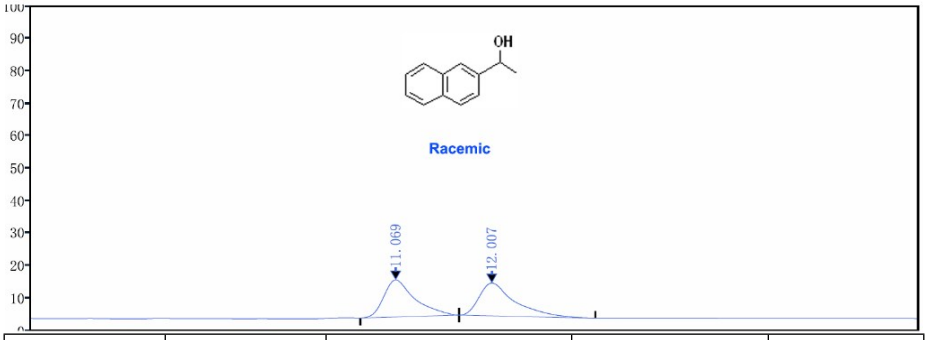
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	6.453	8934.80	49.97
2	MM	6.970	8946.49	50.03
The Total			17881.29	

1-(4-methylphenyl)ethanol (**1d**' in Figure **2**):



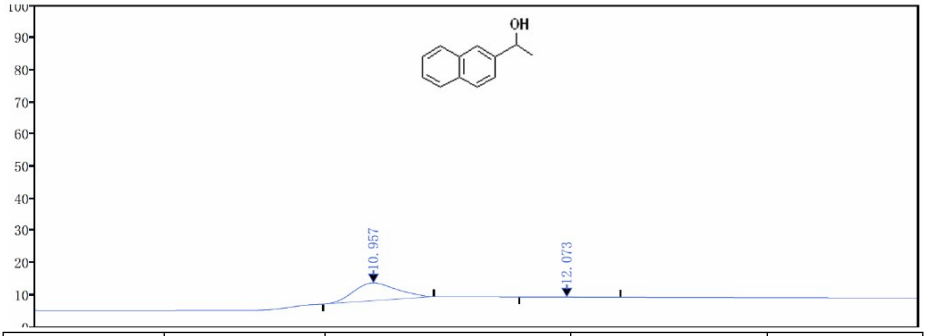
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	6.431	4482.47	99.70
2	MM	7.073	13.42	0.30
The Total			4495.89	

Racemic 2-naphthalenemethano: ChiralCel OJ-H column; hexane/i-PrOH =97/3, flow rate = 1mL/min, 220 nm; tR=11.069 min, tR=12.007 min.



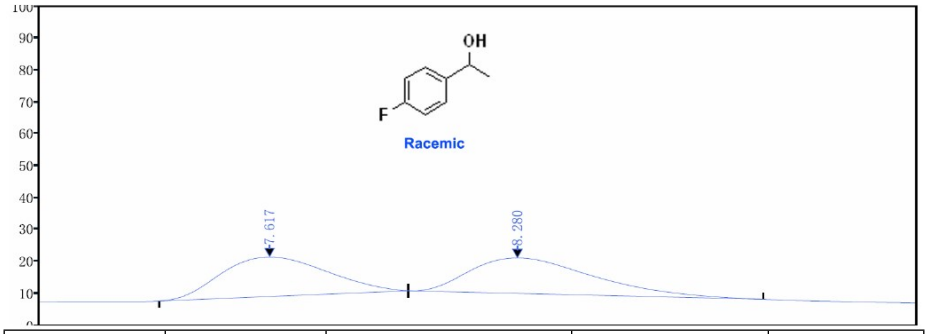
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	11.069	684.94	49.56
2	MM	12.007	697.06	50.44
The Total			1382.00	

2-naphthalenemethano (**1e**' in Figure **2**):



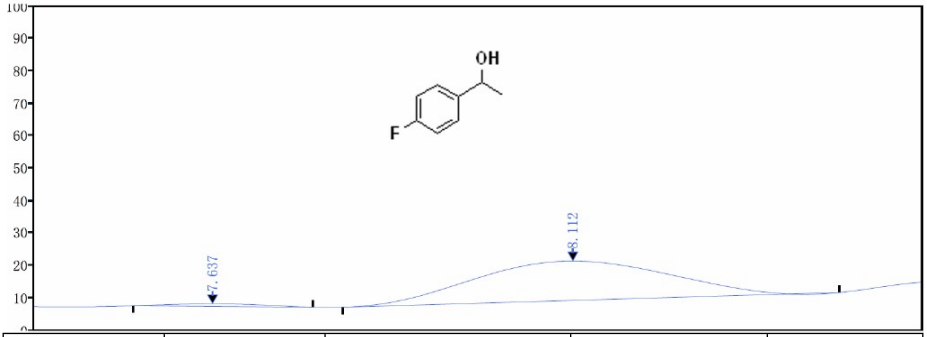
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	10.957	177.59	100.00
2	MM	12.073	0.00	0.00
The Total			177.59	

Racemic 1-(4-fluorophenyl)ethanol: ChiralCel OD-H column; hexane/i-PrOH =95/5, flow rate = 1.0 mL/min, 220 nm; t_R=7.617 min, t_R=8.280 min.



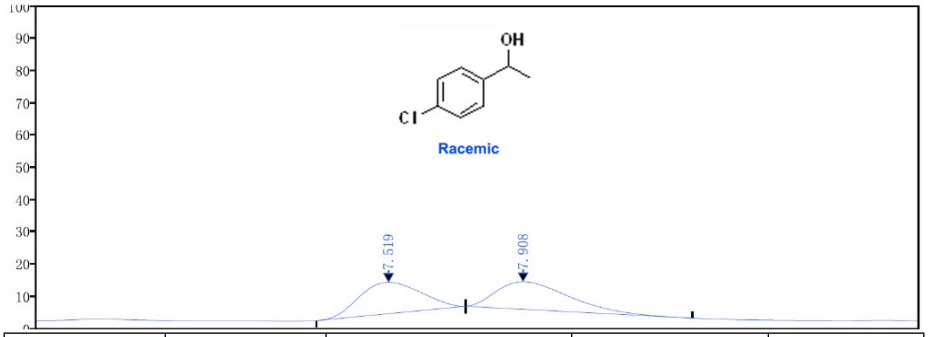
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.617	153.23	48.75
2	MM	8.280	161.09	51.25
The Total			314.32	

1-(4-fluorophenyl)ethanol (**1f**' in Figure **2**):



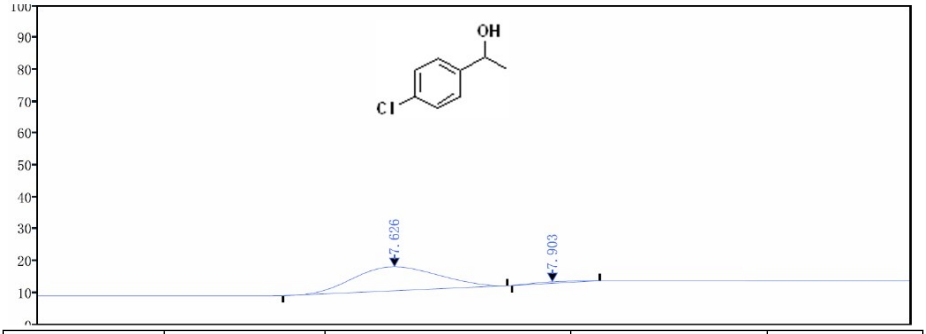
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.637	6.93	3.05
2	MM	8.112	220.74	96.95
The Total			227.67	

Racemic 1-(4-chlorophenyl)ethanol: ChiralCel AS-H column; hexane/i-PrOH =95/5, flow rate = 1.0 mL/min, 230 nm; t_R=7.519min, t_R =7.908min.



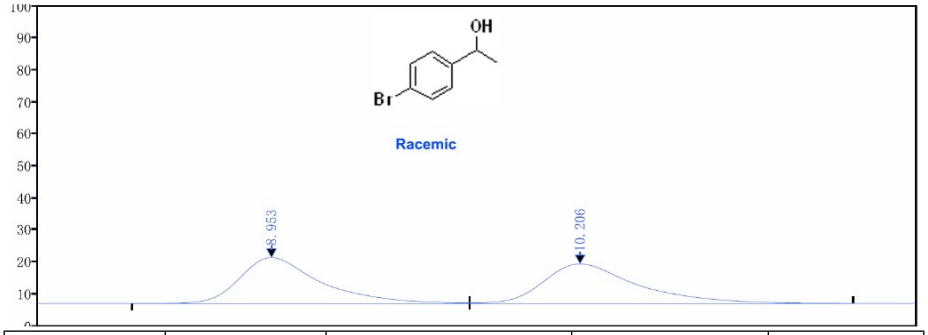
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.519	2874.70	48.93
2	MM	7.908	3000.30	51.07
The Total			5875.00	

1-(4-chlorophenyl)ethanol (**1g**' in Figure **2**):



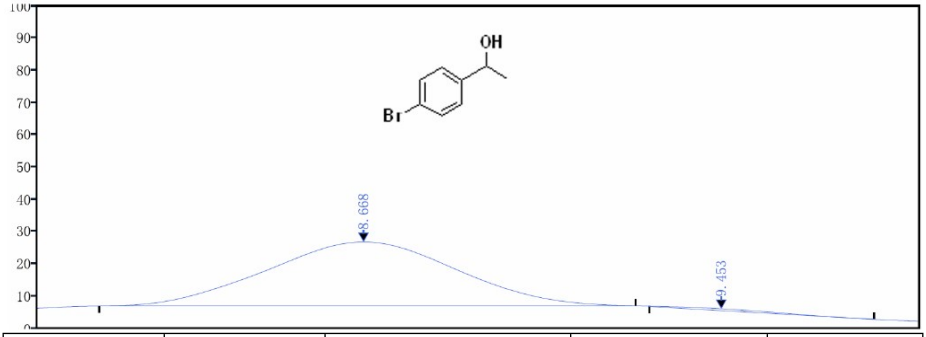
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.626	217.05	96.77
2	MM	7.903	7.25	3.23
The Total			224.31	

Racemic 1-(4-bromophenyl)ethanol: ChiralCel OD-H column; hexane/i-PrOH =95/5, flow rate = 1.0 mL/min, 220 nm; t_R=8.953 min, t_R=10.206 min.



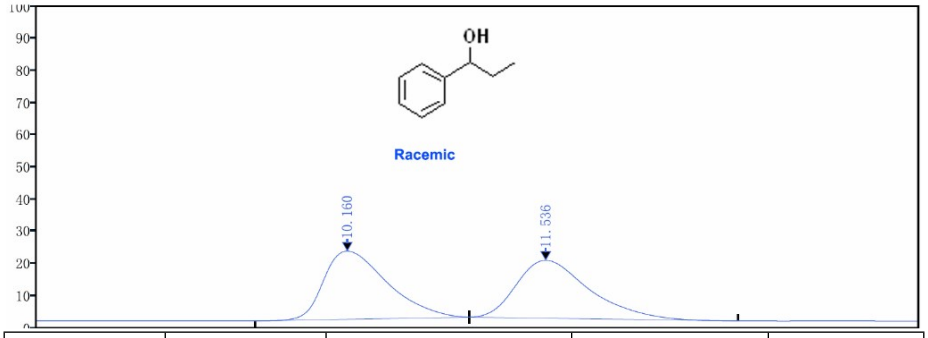
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	BM	8.953	34175.07	50.03
2	MM	10.206	34133.93	49.97
The Total			68309.00	

1-(4-bromophenyl)ethanol (**1h**' in Figure **2**):



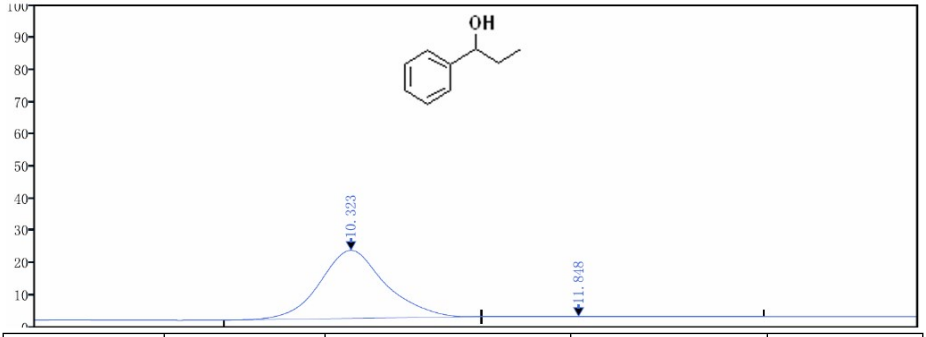
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.668	959.65	98.42
2	MM	9.453	15.39	1.58
The Total			975.05	

Racemic 1-phenylpropanol: ChiralCel AS-H column; hexane/i-PrOH =97/3, flow rate = 1.0 mL/min, 254 nm; t_R=10.160 min, t_R=11.536 min.



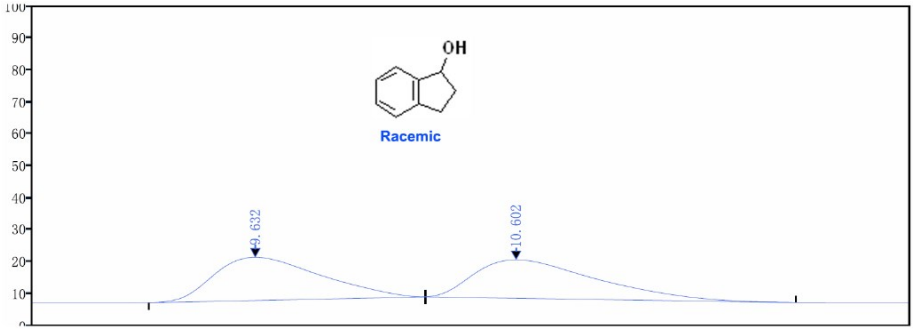
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	10.160	5191.84	50.48
2	MM	11.536	5093.52	49.52
The Total			10285.35	

1-phenylpropanol (**1i**' in Figure **2**):



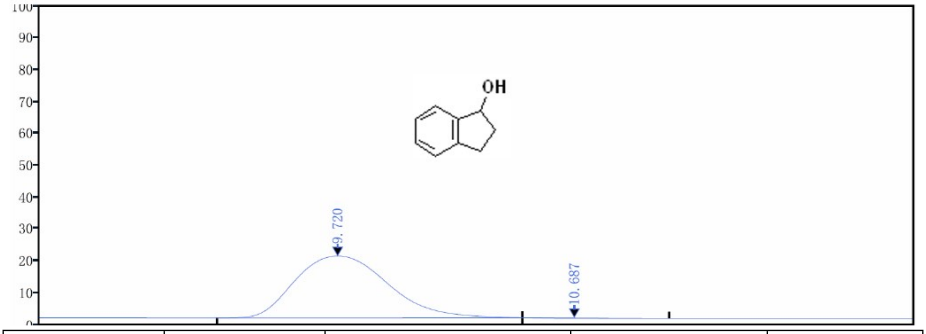
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	10.323	544.20	99.76
2	MM	11.848	1.29	0.24
The Total			545.49	

Racemic 2,3-dihydro-1H-inden-1-ol: ChiralCel OD-H column; hexane/i-PrOH =95/5, flow rate = 1.0 mL/min, 220 nm; tR = 9.632 min, tR =10.602 min.



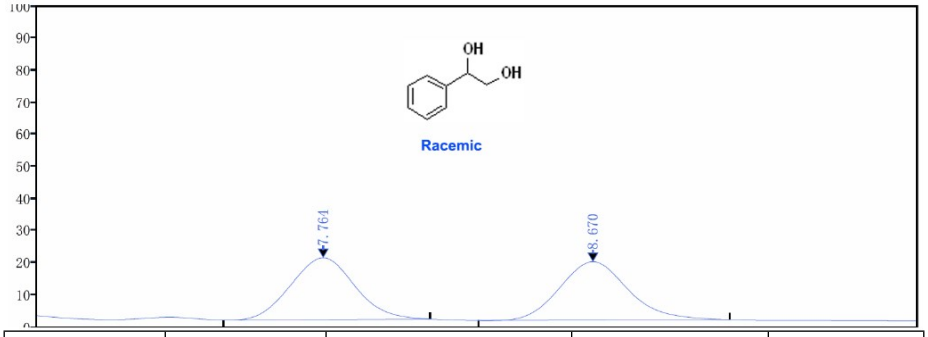
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	9.632	22554.42	49.49
2	MM	10.602	23022.83	50.51
The Total			45577.26	

2,3-dihydro-1H-inden-1-ol (**1j**' in Figure **2**):



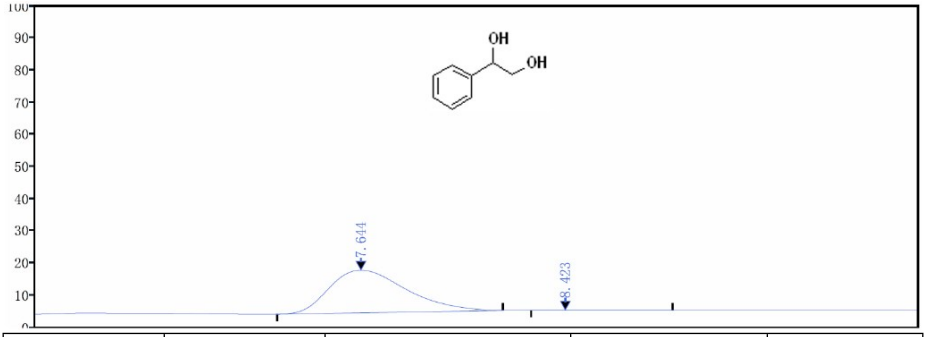
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	9.720	2011.29	99.61
2	MM	10.687	7.93	0.39
The Total			2019.21	

Racemic 1-phenylethane-1,2-diol: ChiralCel OJ-H column; hexane/i-PrOH =90/10, flow rate = 1.0 mL/min, 220 nm; tR= 7.764 min, tR=8.670 min.



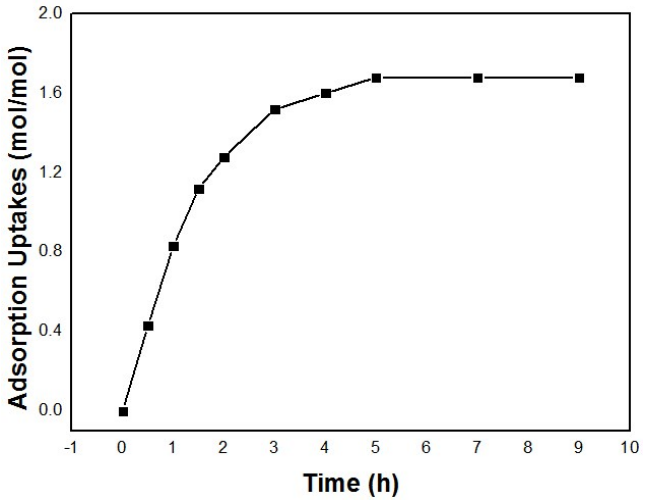
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.767	170.14	49.79
2	MM	8.670	171.58	50.21
The Total			341.71	

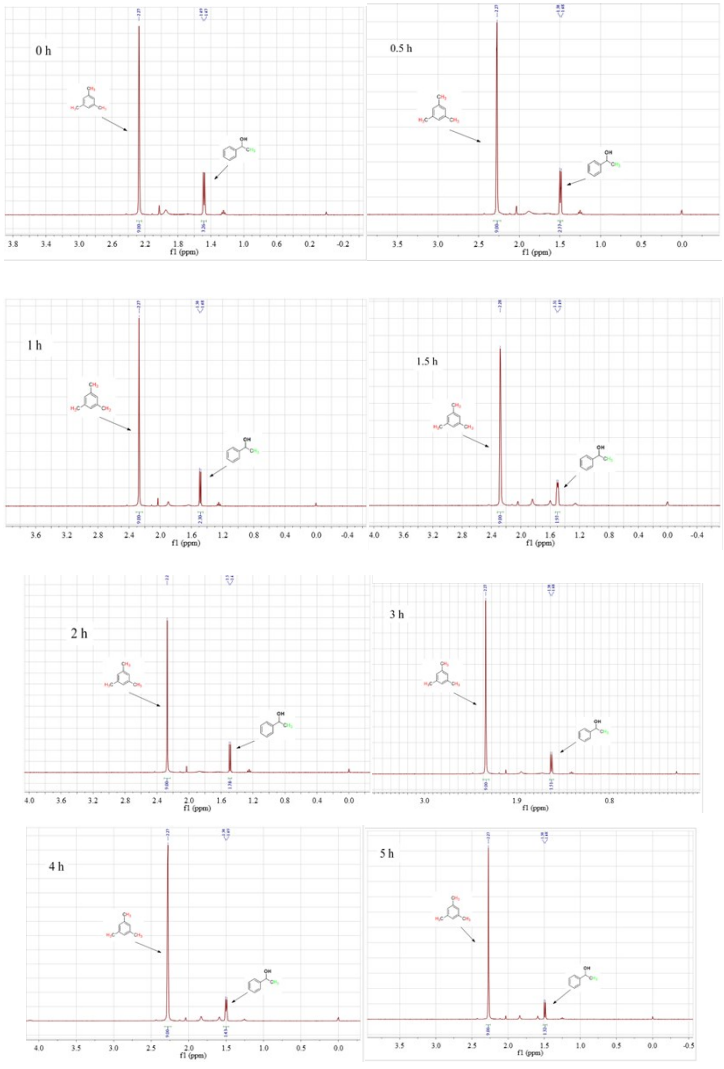
1-phenylethane-1,2-diol (**1k**' in Figure **2**):

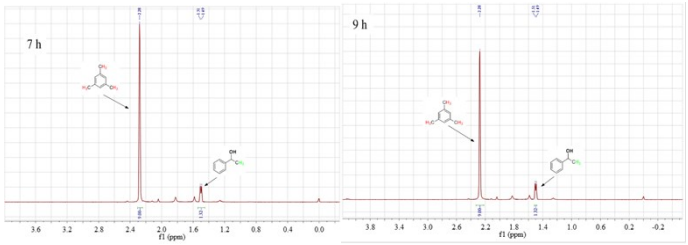


Serial Number	Type	Retention Time [min]	Peak area	Area %
1	BH	7.644	1355.76	99.98
2	MM	8.423	0.31	0.02
The Total			1356.07	

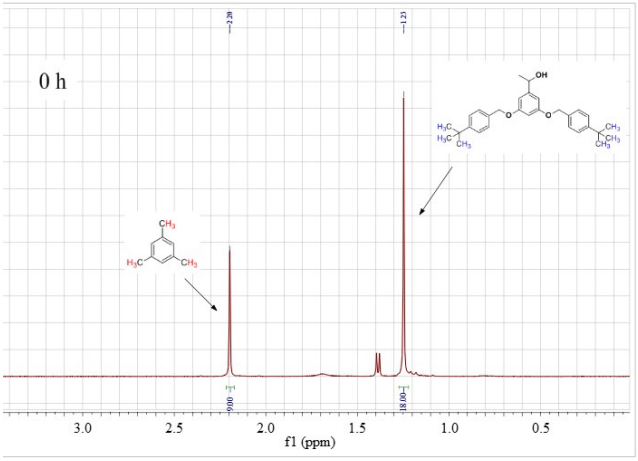
13. Figure S8. Adsorption kinetic profile of 1 toward 1-phenylethanol.

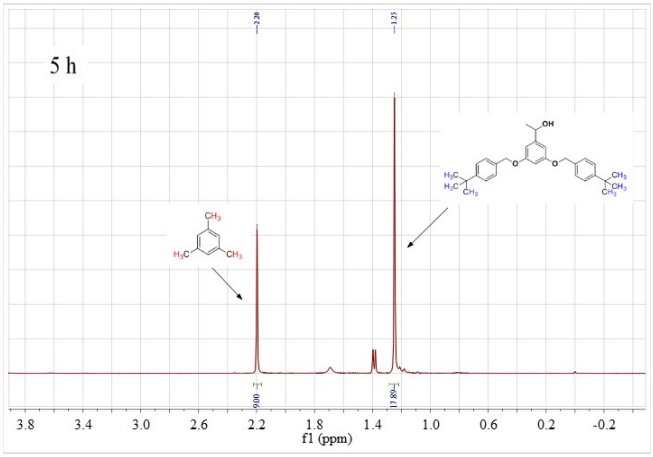






14. Figure S9. The 1H NMR result of bulky substrate (1l in table 1) adsorption by 1.





15. Figure S10-13. The result of the theory calculation on the adsorption of 1-phenylethanol with 1.

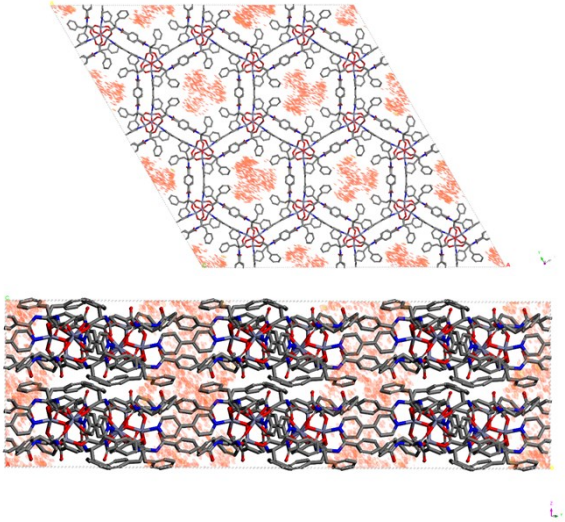


Figure S10. Adsorption location of (R)-1-phenylethanol within the MOF 1 (The colored area indicates adsorption location of guests).

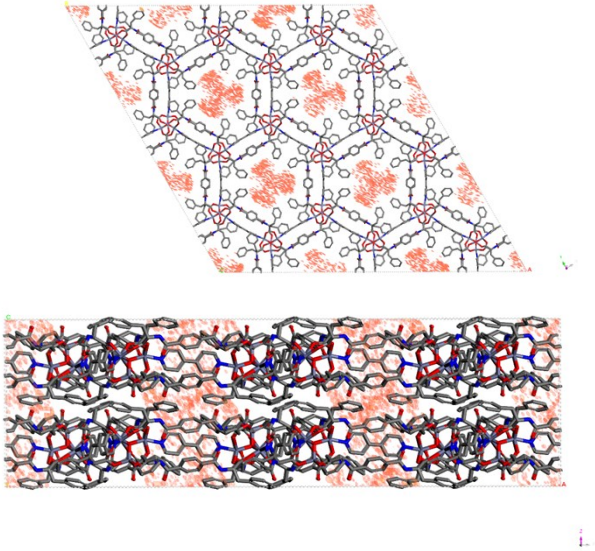


Figure S11. Adsorption location of (S)-1-phenylethanol within the MOF 1 (The colored area indicates adsorption location of guests).

The adsorption location of 1-phenylethanol molecules was calculated by Adsorption Locator Tools of Material Studio. The energy distribution of adsorption location was calculated through simulated annealing. (R)- or (S)-1-phenylethanol in a 3X3X2 supercell was selected as the adsorbate with a loading number of 16 and a fraction of 1.00. Monte Carlo options are set as the default values. The calculation was performed with 10 cycles and 15000 steps per cycles.

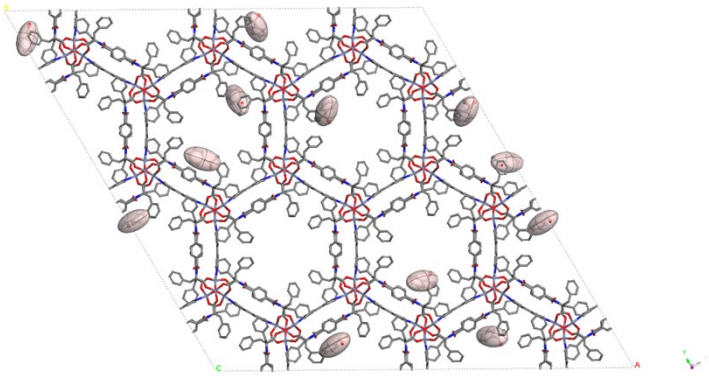


Figure 12. Most stable adsorption sites of (S)-1-phenylethanol with a total energy of -102.65 kcal/mol.

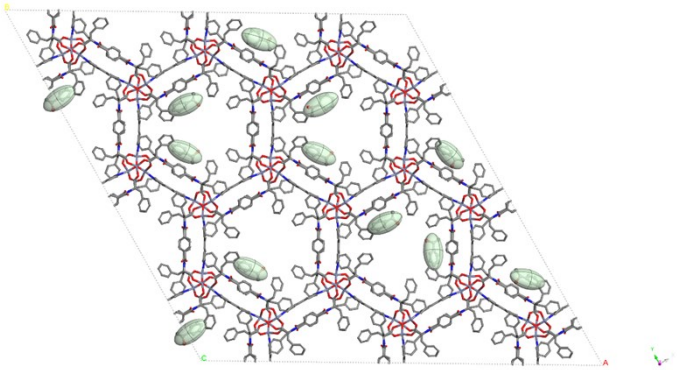
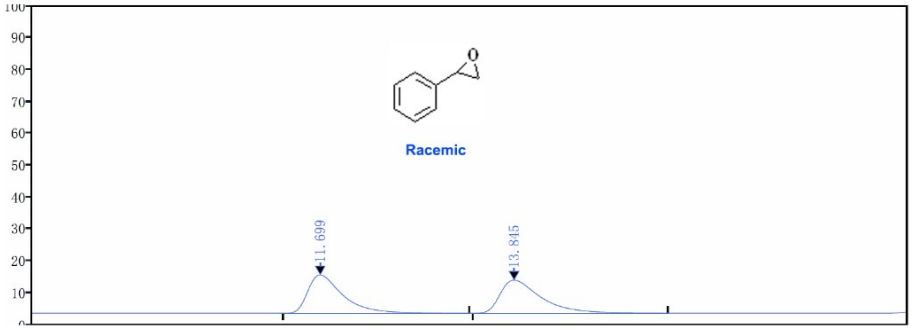


Figure 13. Most stable adsorption sites of (R)-1-phenylethanol with a total energy of -99.54 kcal/mol.

The exact location of guest molecules absorbed in the framework was calculated by the Sorption module of Material Studio. A Metropolis method was applied and an ultra-fine quality was selected for calculation. 12 (R)- or (S)-1-phenylethanol molecules with a fraction of 1.00 were loaded in a lattice cell. A universal forcefield was selected to calculate energy. Ewald & Group method was selected for electrostatic interaction, while Atom based method was chosen for van der Waals interaction.

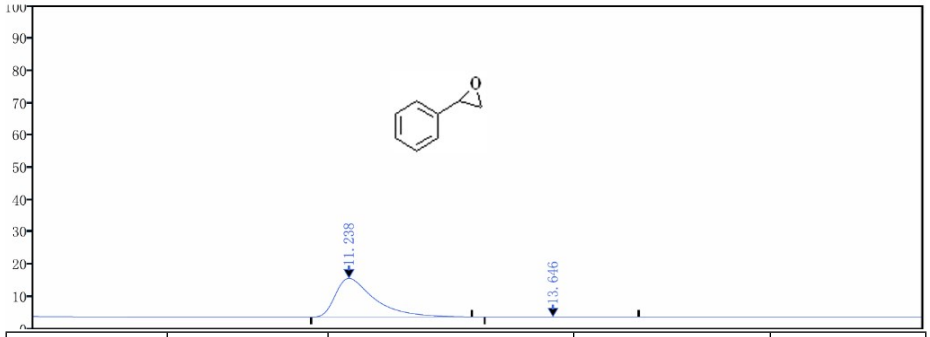
15. Figure S14. HPLC results of enantioseparation of epoxides with (S)-1 as chiral adsorbent.

Racemic styrene oxide: ChiralCel AS-H column; hexane/i-PrOH =99.5/0.5, flow rate=0.6 mL/min, 230 nm; tR=11.699 min, tR =13.845 min.



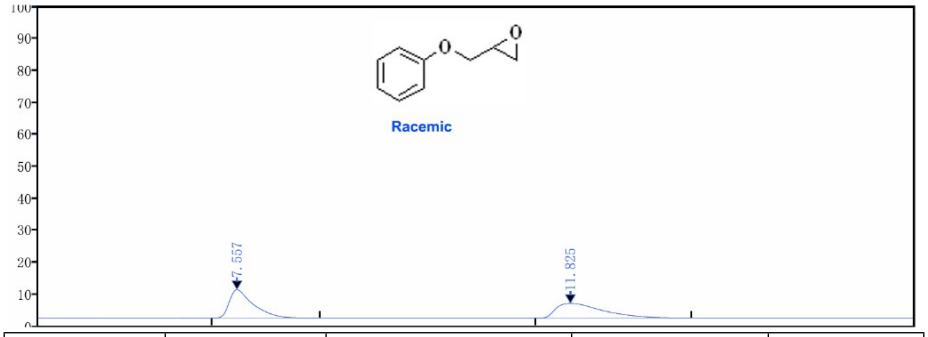
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HH	11.699	2054.99	49.88
2	HM	13.845	2065.14	50.12
The Total			4120.12	

Styrene oxide (**2a**' in Figure 3):



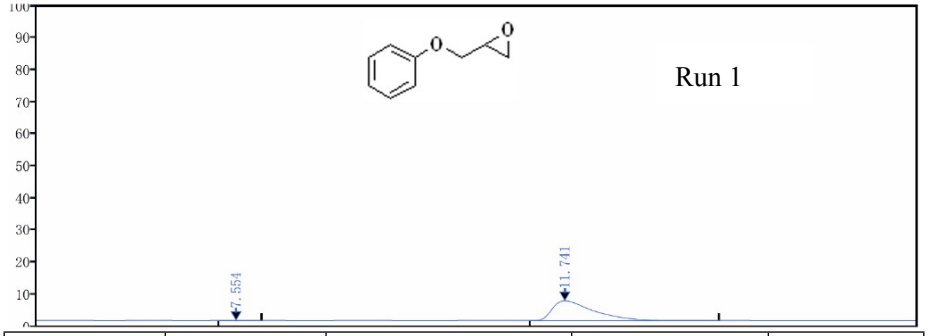
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HH	11.238	713.06	99.96
2	MM	13.646	0.27	0.04
The Total			713.33	

Racemic phenyl glycidyl ether: ChiralCel OD-H column; hexane/i-PrOH =90/10, flow rate=1.0 mL/min, 254 nm; tR=7.326 min, tR=11.733 min.

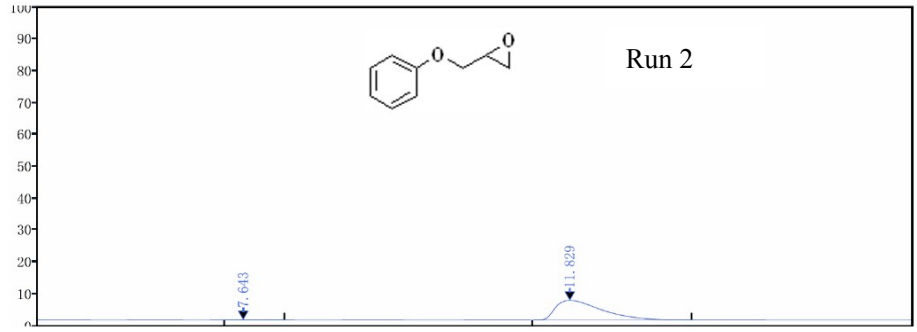


Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.557	10386.15	49.67
2	HM	11.825	10524.22	50.33
The Total			20910.37	

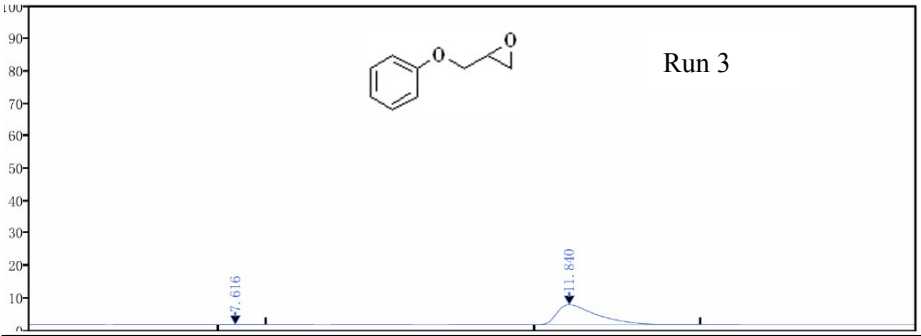
Phenyl glycidyl ether (**2b**' in Figure 3):



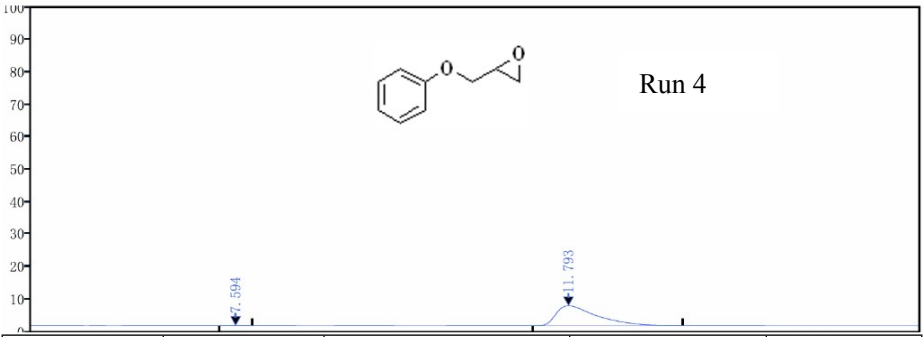
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.554	13.16	0.24
2	HM	11.741	5447.22	99.76
The Total			5460.38	



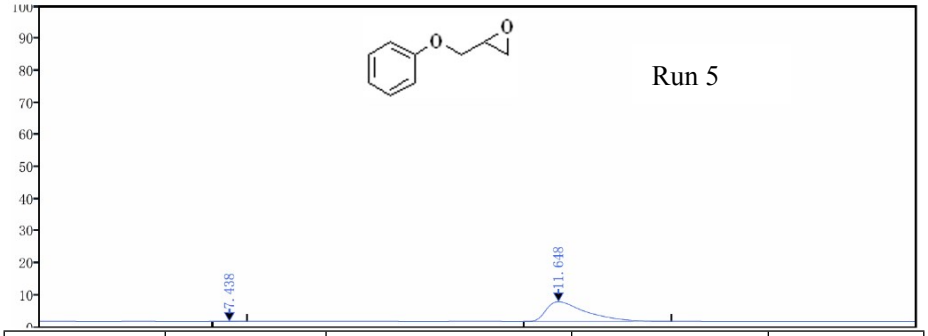
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.643	34.65	0.32
2	HM	11.829	10642.71	99.68
The Total			10677.36	



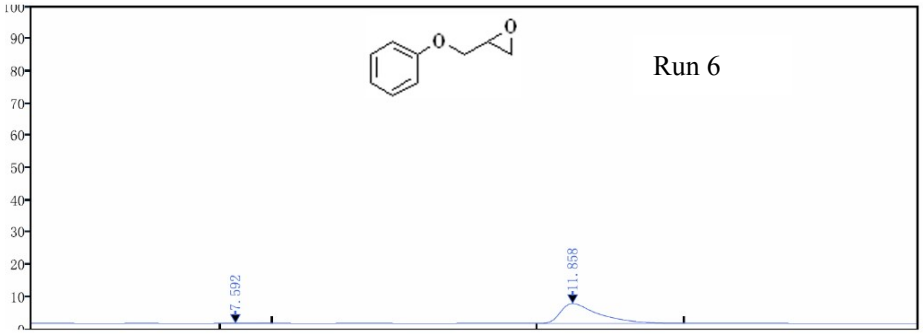
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.616	14.58	0.29
2	HM	11.840	5032.77	99.71
The Total			5047.36	



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.594	11.84	0.22
2	HM	11.793	5440.43	99.78
The Total			5452.27	

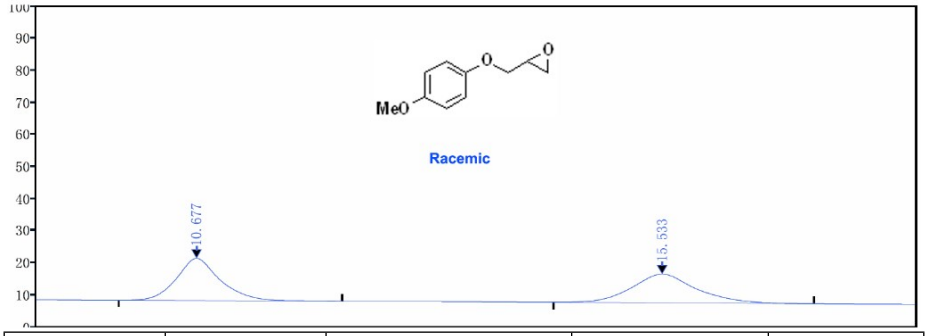


Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.438	9.12	0.2
2	HM	11.648	4566.89	99.80
The Total			4576.01	



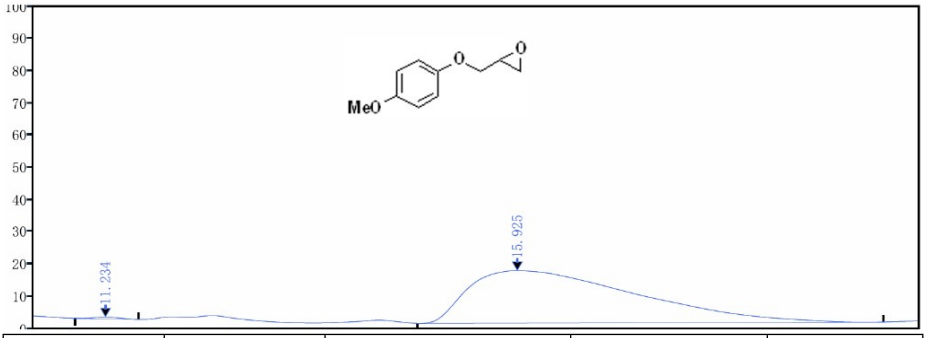
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HM	7.592	9.47	0.31
2	HM	11.858	3043.12	99.69
The Total			3052.59	

Racemic 4-methoxyphenyl glycidyl ether: ChiralCel OD-H column; hexane/i-PrOH=90/10, flow rate=1.0 mL/min, 254 nm; tR=10.677 min, tR=15.533 min.



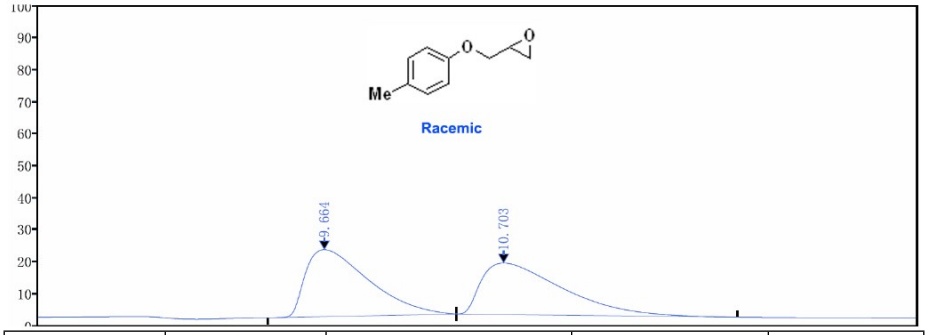
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	BM	10.677	810.33	50.33
2	BM	15.533	799.81	49.67
The Total			1610.14	

4-Methoxyphenyl glycidyl ether (**2c**' in Figure 3):



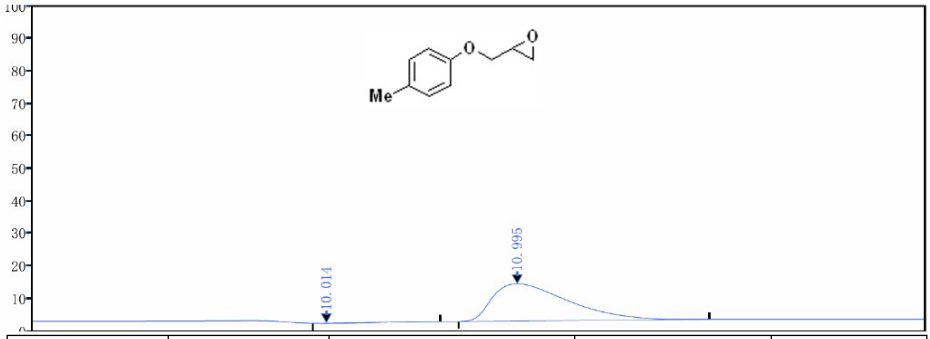
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	11.234	10.47	0.52
2	MM	15.925	2022.07	99.48
The Total			2032.54	

Racemic 4-methylphenyl glycidyl ether: ChiralCel AS-H column; hexane/i-PrOH =95/5, flow rate=1.0 mL/min, 254nm; tR=9.664 min, tR =10.703 min.



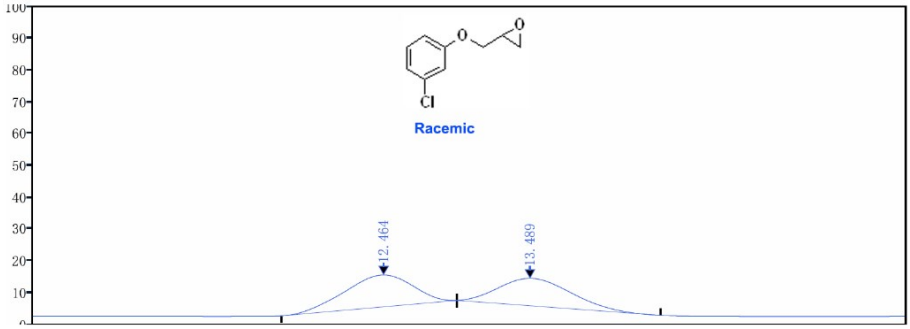
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	9.664	713.58	50.19
2	MM	10.703	708.29	49.81
The Total			1421.87	

4-Methylphenyl glycidyl ether (**2d**' in Figure 3):



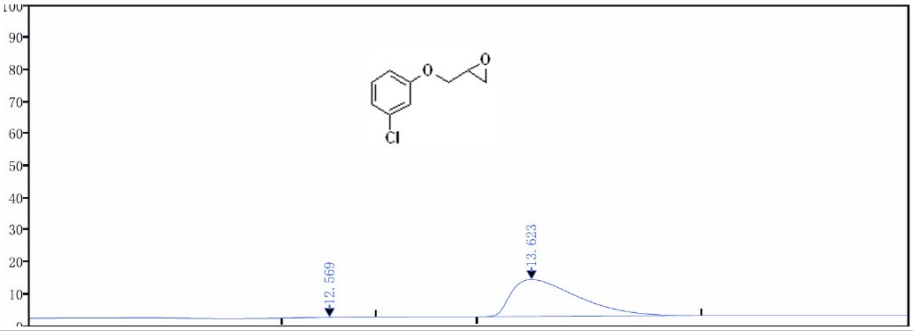
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	10.014	0.66	0.15
2	MM	10.995	432.87	99.85
The Total			433.53	

Racemic 3-chlorophenyl glycidyl ether: ChiralCel OD-H column; hexane/i-PrOH=98/2, flow rate=0.8 mL/min, 254nm; tR=12.464 min, tR=13.489 min.



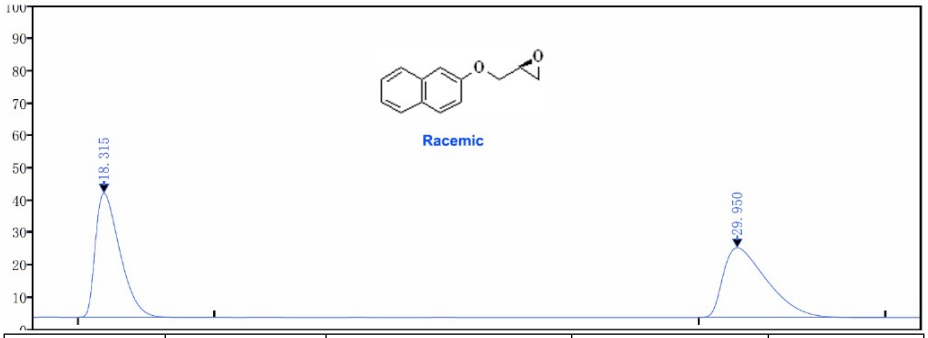
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	12.464	5702.15	52.17
2	MM	13.489	5227.33	47.83
The Total			10929.48	

3-Chlorophenyl glycidyl ether (**2e**' in Figure 3):



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	12.569	2.39	0.47
2	MM	13.623	504.61	99.53
The Total			507.00	

Racemic 2-naphthol glycidyl ether: ChiralCel OJ-H column; hexane/i-PrOH =70/30, flow rate=1.5 mL/min, 254 nm; tR=18.315 min, tR=29.950 min; ee=99.8%.

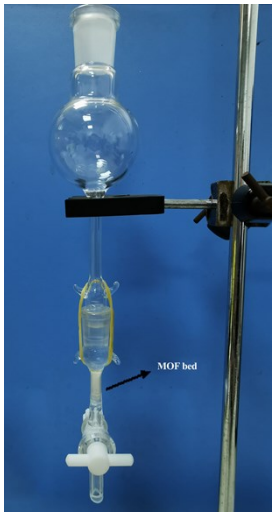


Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HB	18.315	4377.47	49.95
2	HB	29.950	4385.87	50.05
The Total			8763.34	

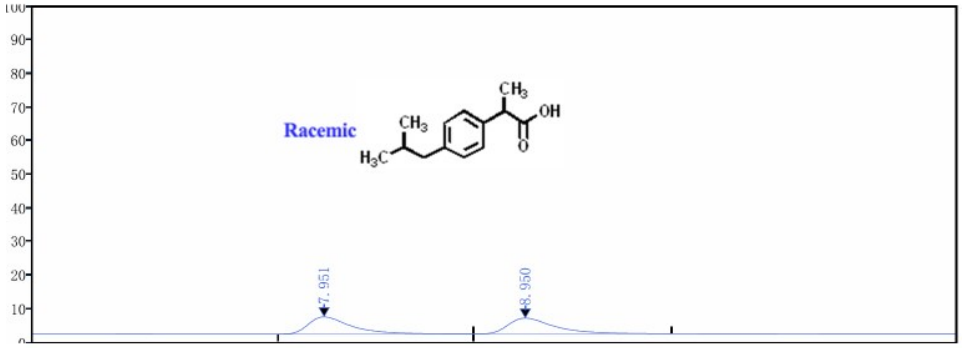
2-Naphthol glycidyl ether (**2f**' in Figure 3):

Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	18.549	2.42	0.11
2	HH	30.079	2233.18	99.89
The Total			2235.60	

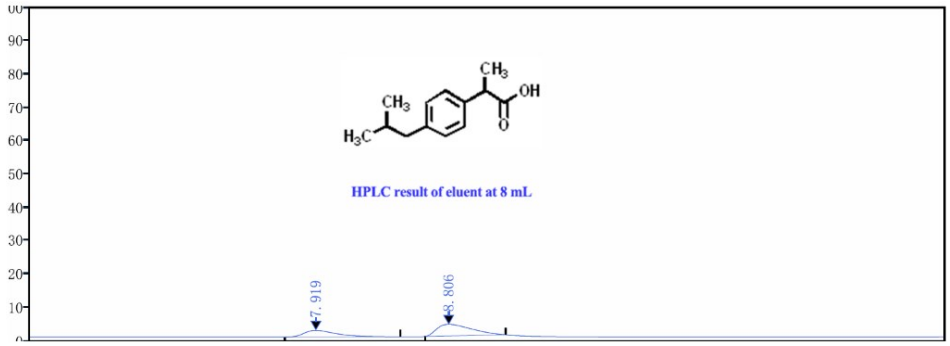
16. Figure S15. Enantioseparation of racemic ibuprofen by (S)-1 packing column (Experimental setup and HPLC results).



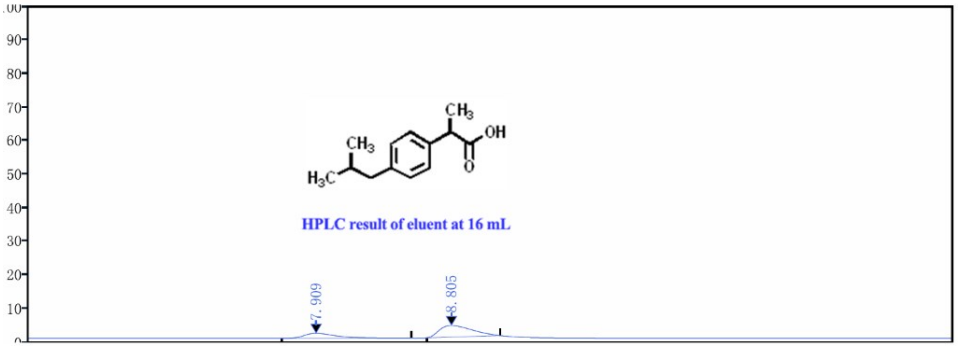
Racemic Ibuprofen: ChiralCel AS-H column; hexane/i-PrOH=99.5/0.5, flow rate=0.47 mL/min, 230nm; t_R=7.951min, t_R=8.950min.



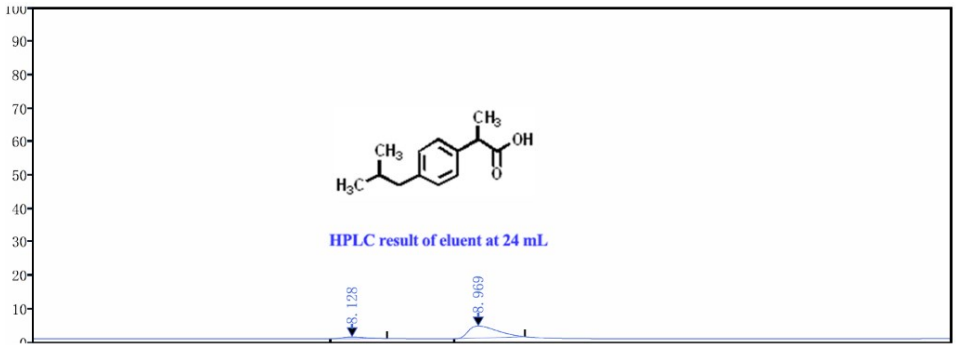
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	HH	7.951	446.45	50.14
2	HM	8.950	444.02	49.86
The Total			890.47	



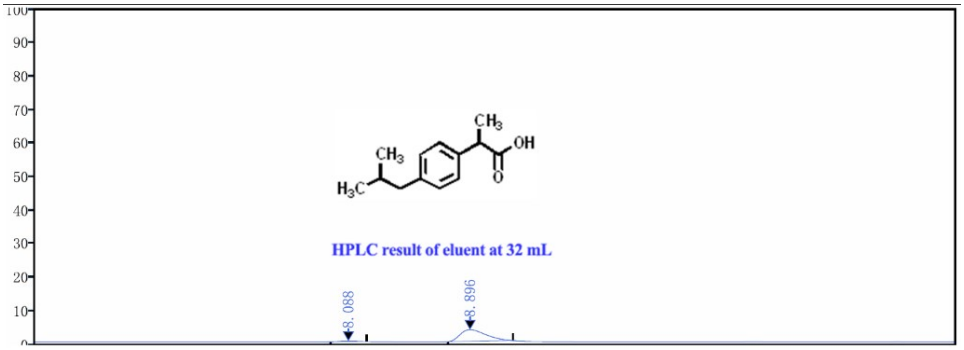
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.919	2090.23	34.44
2	MM	8.806	3979.24	65.56
The Total			6069.47	



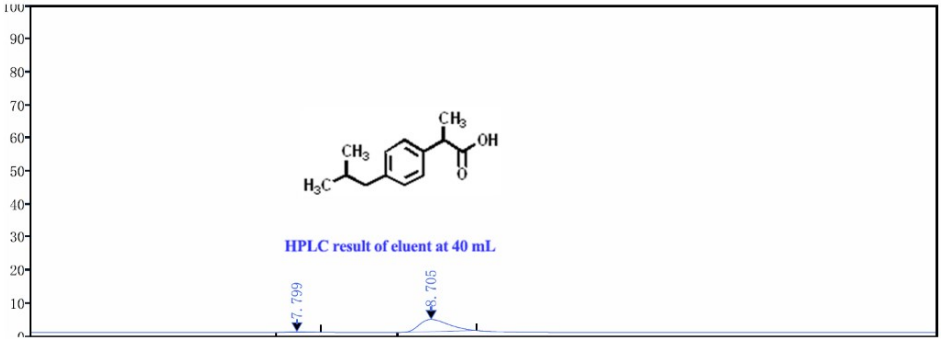
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.909	1268.32	29.74
2	MM	8.805	2996.35	70.26
The Total			4264.67	



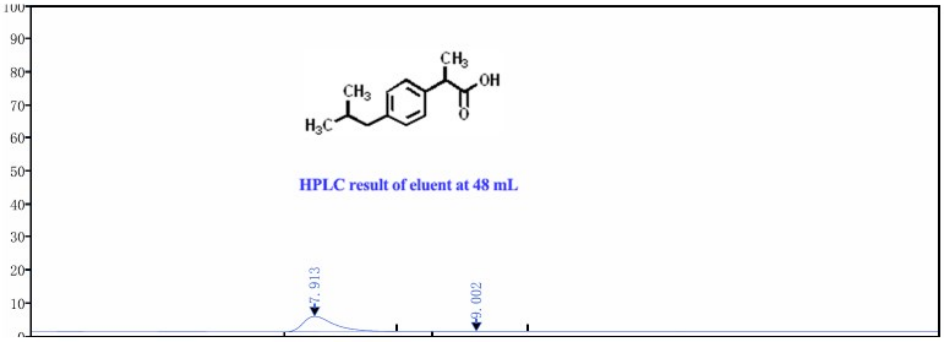
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.128	317.12	9.72
2	MM	8.969	2946.66	90.28
The Total			3263.67	



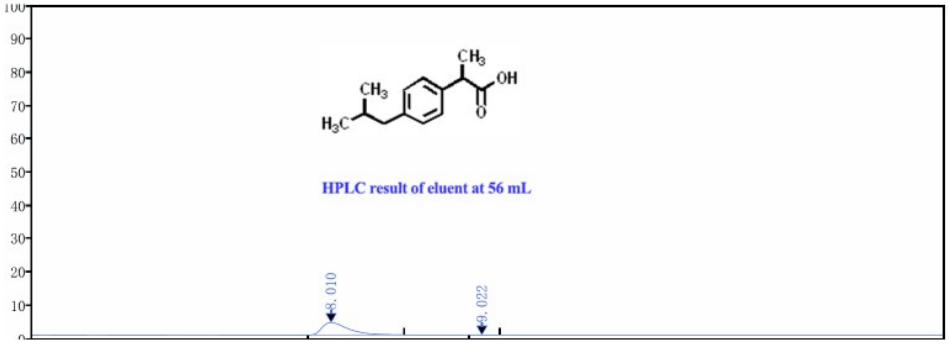
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.088	50.48	3.98
2	MM	8.896	1219.22	96.02
The Total			1269.7	



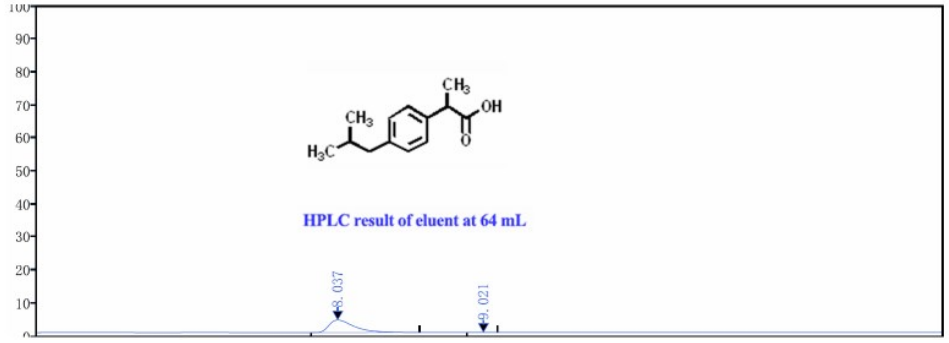
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.799	39.39	3.05
2	MM	8.705	1251.65	96.95
The Total			1291.04	



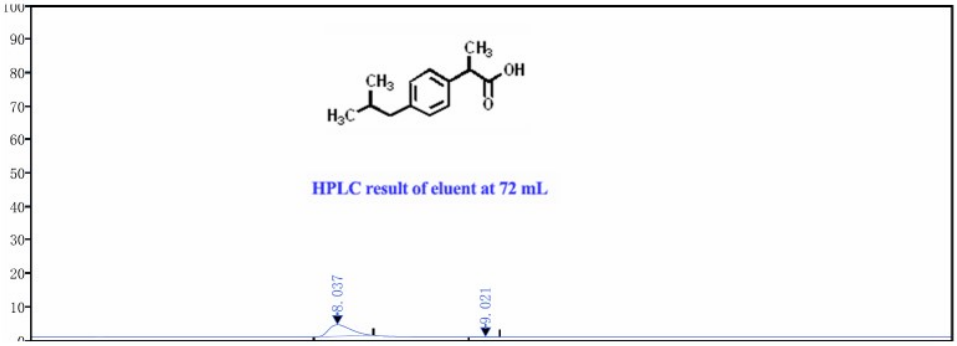
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.913	839.44	99.97
2	MM	9.002	0.22	0.03
The Total			839.66	



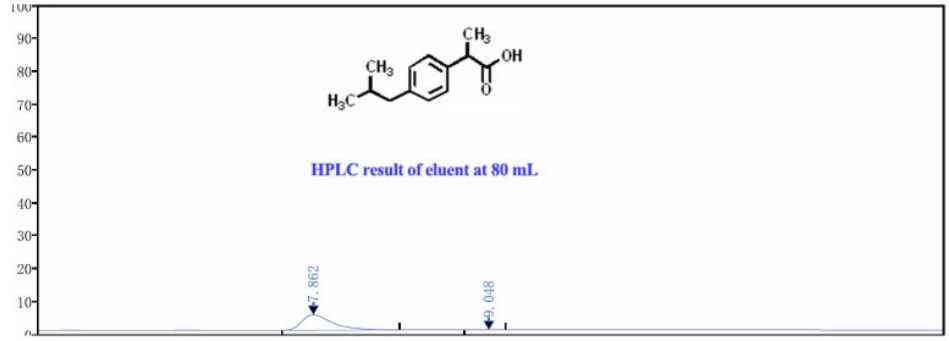
Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.010	2802.66	100.00
2	MM	9.022	0.02	0.00
The Total			2802.68	



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.037	2404.60	100.00
2	MM	9.021	0.00	0.00
The Total			2404.60	



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	8.037	1978.36	100.00
2	MM	9.021	0.00	0.00
The Total			1978.36	



Serial Number	Type	Retention Time [min]	Peak area	Area %
1	MM	7.862	537.22	100.00
2	MM	9.048	0.02	0.00
The Total			537.24	