Supporting Information for

Oxidative Kinetic Resolution of Racemic Secondary Alcohols in Water with Chiral PNNP/Ir catalyst

Juanni Zhang, Xiangren Yang, Han Zhou, Yanyun Li,* Zhenrong Dong and Jingxing Gao*

National Engineering Laboratory for Green Chemical Productions of Alcohols, Ethers and Esters, State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China

yanyunli@xmu.edu.cn, jxgao@xmu.edu.cn

List of the Contents of the Supporting Information

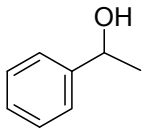
1. General methods

All experiments were carried out under nitrogen atmosphere with Schlenk techniques. All racemic alcohols were synthesized by $NaBH_4$ reduction in ethanol from their respective ketones. The conversion of the products was determined by GC. The ee of the products was determined by GC or HPLC.

2. A typical procedure for oxidative kinetic resolution of racemic secondary alcohols

An example is given by the oxidative kinetic resolution of racemic 1-phenylpropanol using chiral PNNP/Ir catalyst. Under nitrogen atmosphere, (*S*,*S*)-PNNP (0.005 mmol) and $[Ir(COD)Cl]_2$ (0.0025 mmol) were placed in a Schlenk tube equipped with a Teflon-coated magnetic stirring bar. Dichloromethane (0.5 mL) was then added and the mixture was stirred for a few minutes to generate catalyst *in situ*. Subsequently, acetone (2.2 mL), PPNCl (0.05 mmol), and water (8.0 mL) were successively introduced. After the mixture was stirred for 1 h, appropriate amount of KOH/^{i}PrOH solution was added. About 0.5 h, the racemic 1-phenylpropanol was added and the mixture was continually stirred at 28 °C for about 16 h. At the end of the reaction, the product was extracted with ethyl acetate and then passed through a short silica gel column. The conversion and the ee of the product were determined by GC.

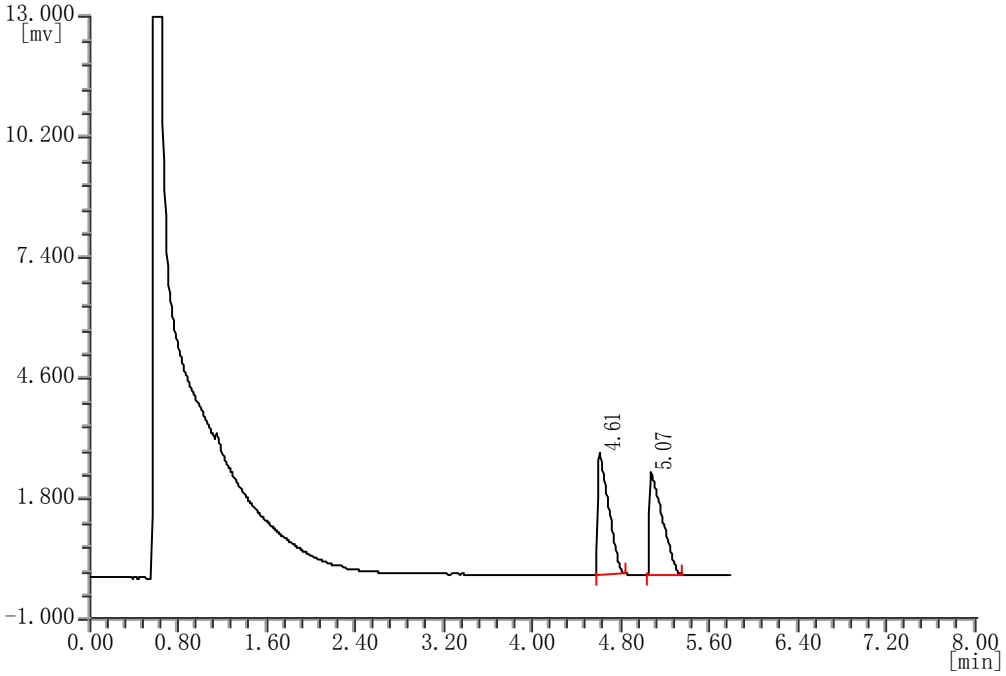
3. Chromatograph analytical data for chiral aromatic alcohols



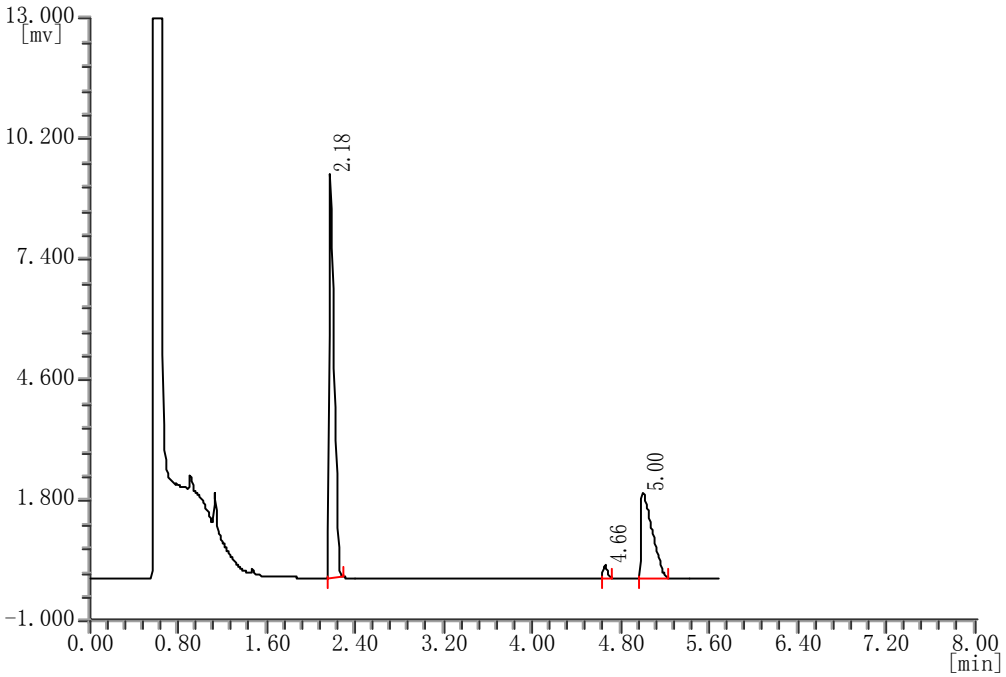
(**a**)

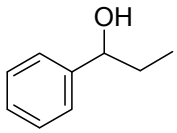
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 115 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **a**:



Resolved **a** (Table 4, Entry 1):

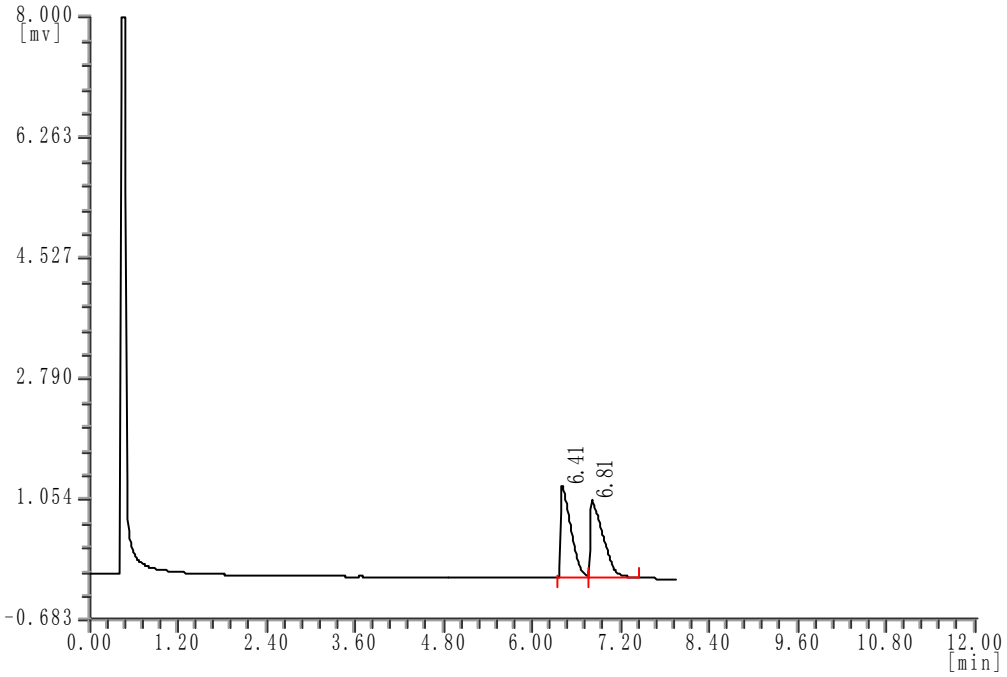




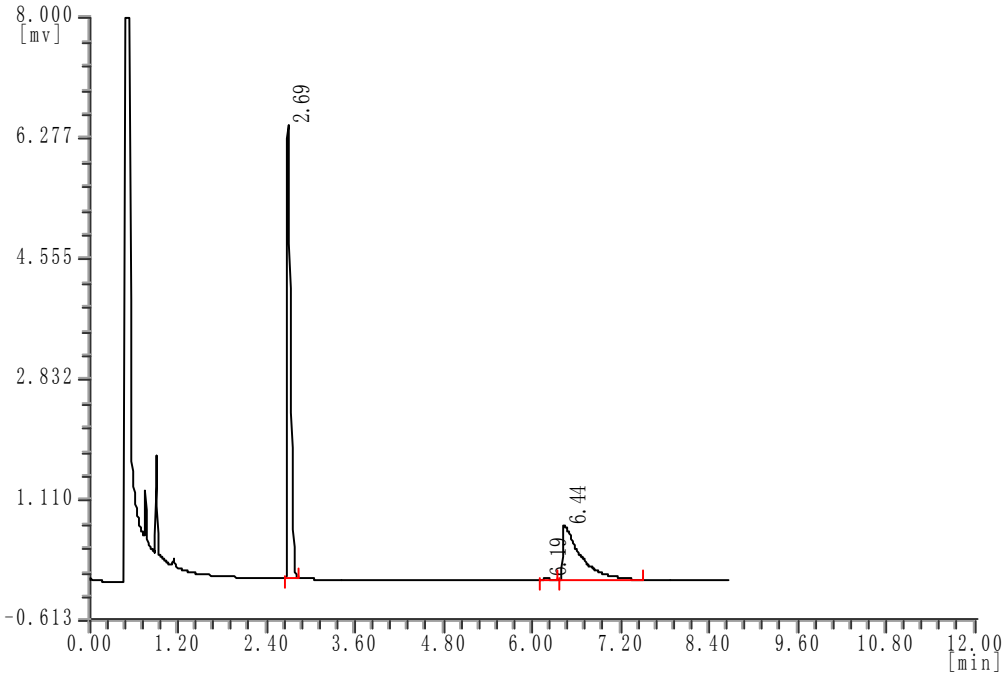
(**b**)

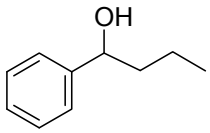
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 110 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **b**:



Resolved **b** (Table 4, Entry 2):

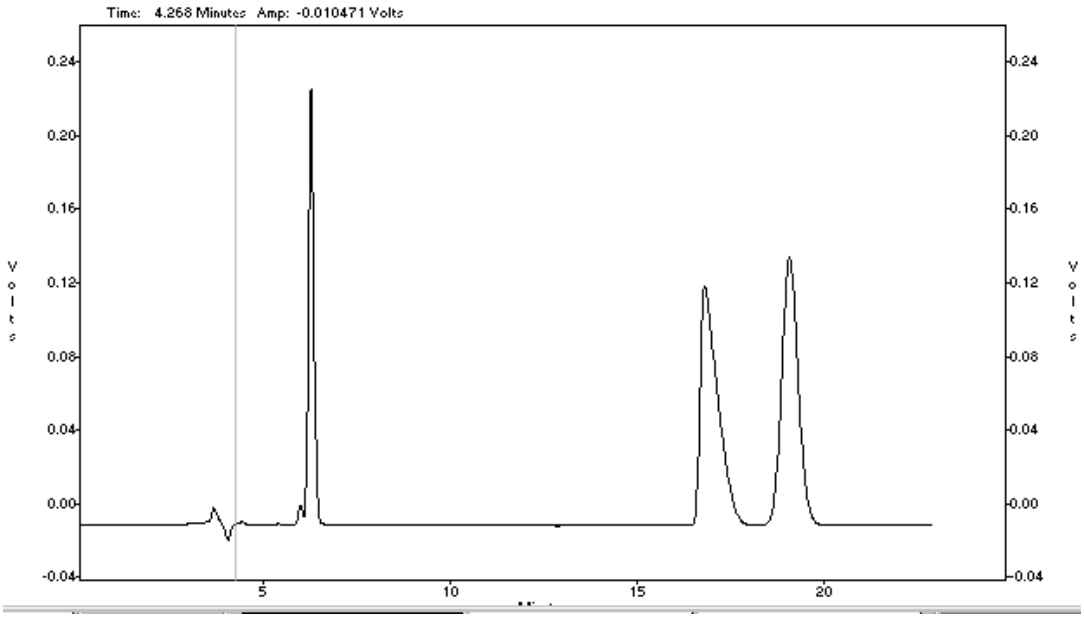




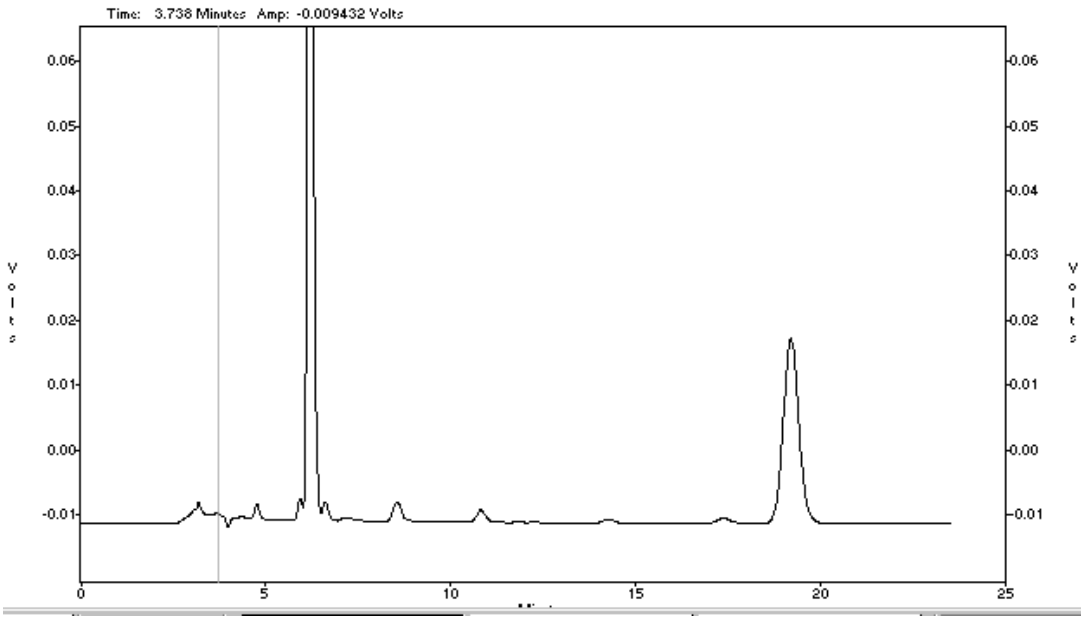
(**c**)

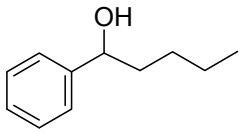
HPLC analysis: Daicel Chiralcel OD column, 4.6 mm i. d. × 250 mm; Eluent: *n*-hexane/*i*-PrOH = 98:2; flow rate = 0.9 mL/min; Temp., 25 °C; detection, 254 nm, (t_1 = 16.86 min, t_2 = 19.12 min)

Racemic **c**:



Resolved **c** (Table 4, Entry 3):

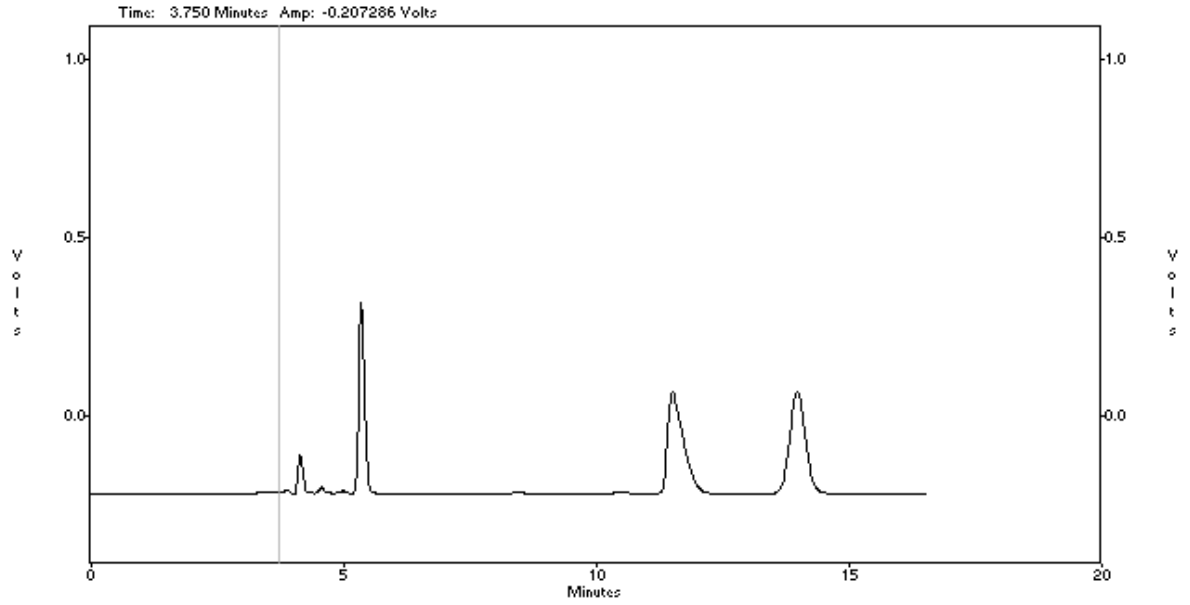




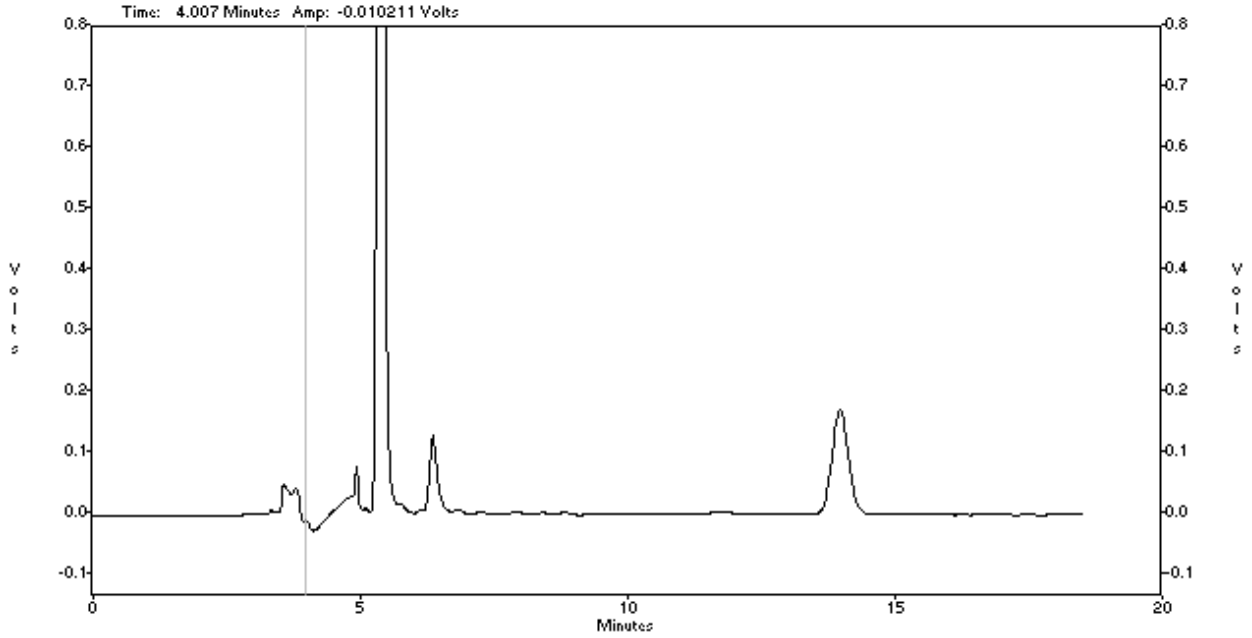
(**d**)

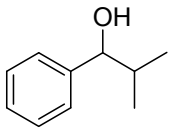
HPLC analysis: Daicel Chiralcel OD column, 4.6 mm i. d. × 250 mm; Eluent: *n*-hexane/*i*-PrOH = 98:2; flow rate = 0.9 mL/min; Temp., 25 °C; detection, 254 nm, (t_1 = 11.55 min, t_2 = 14.03 min)

Racemic **d**:



Resolved **d** (Table 4, Entry 4):

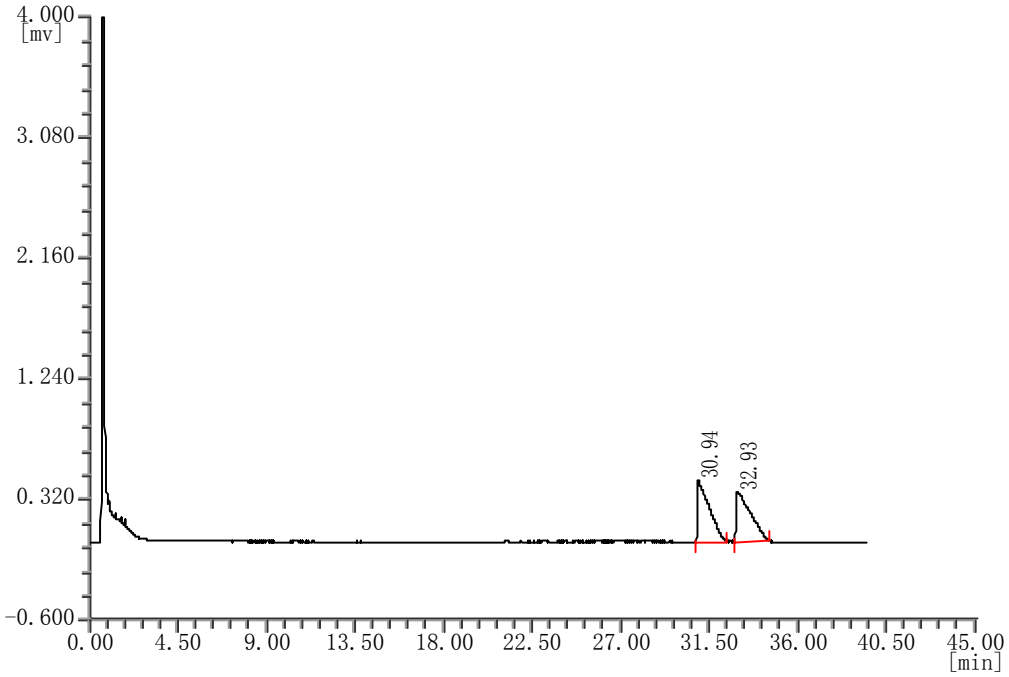




(**e**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 100 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **e**:



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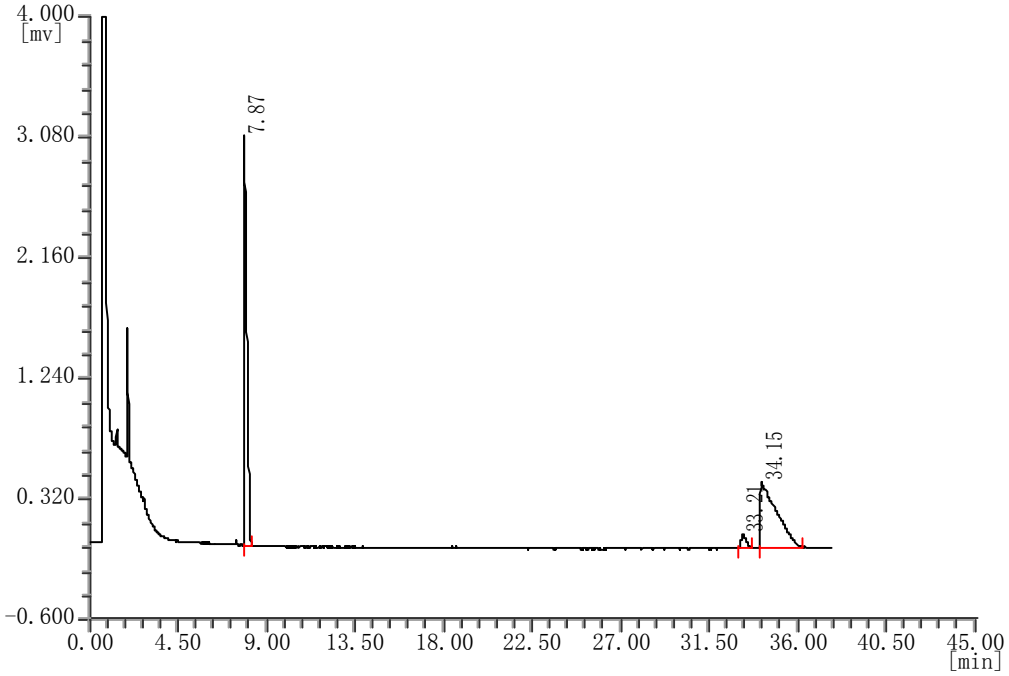
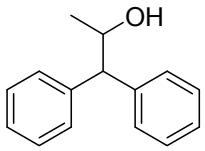
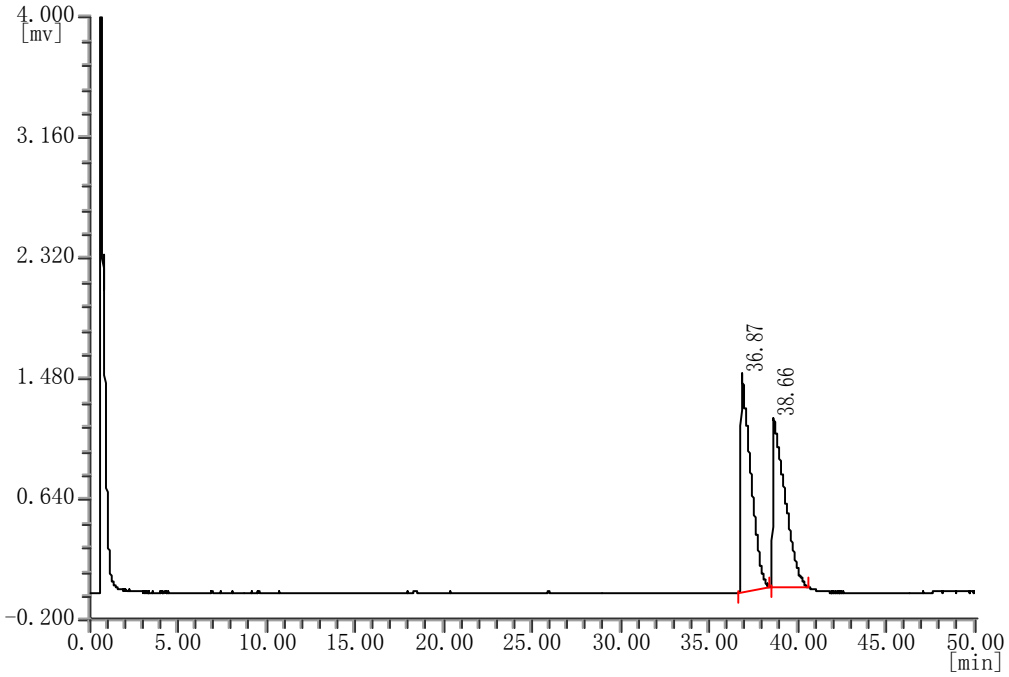




(**f**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 130 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **f**:



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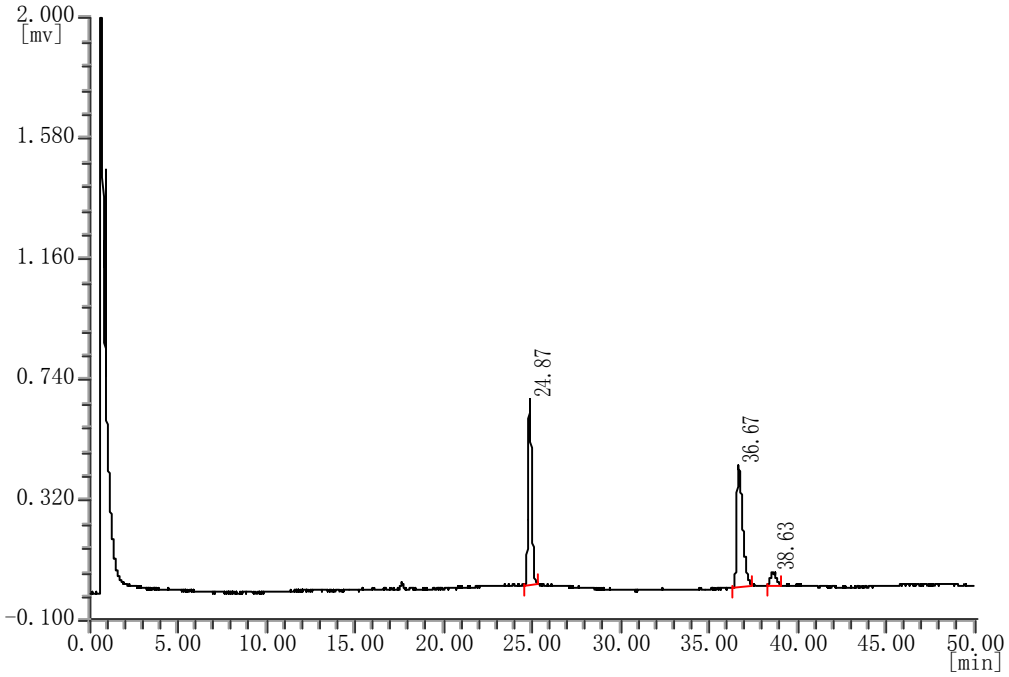
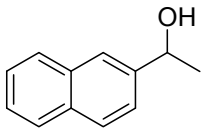
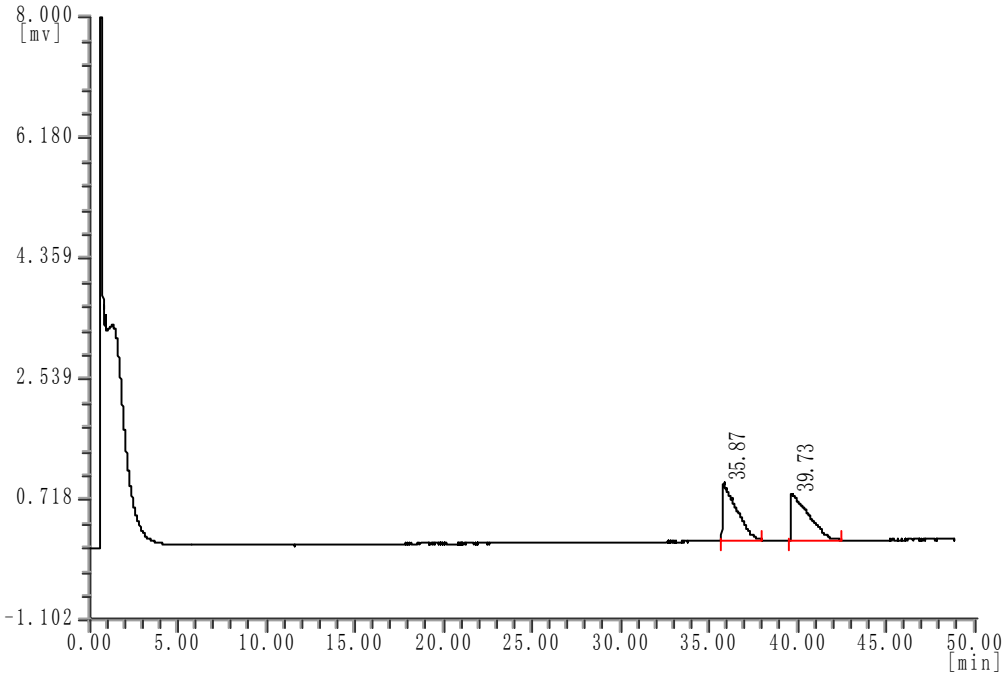




(g)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 130 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **g**:



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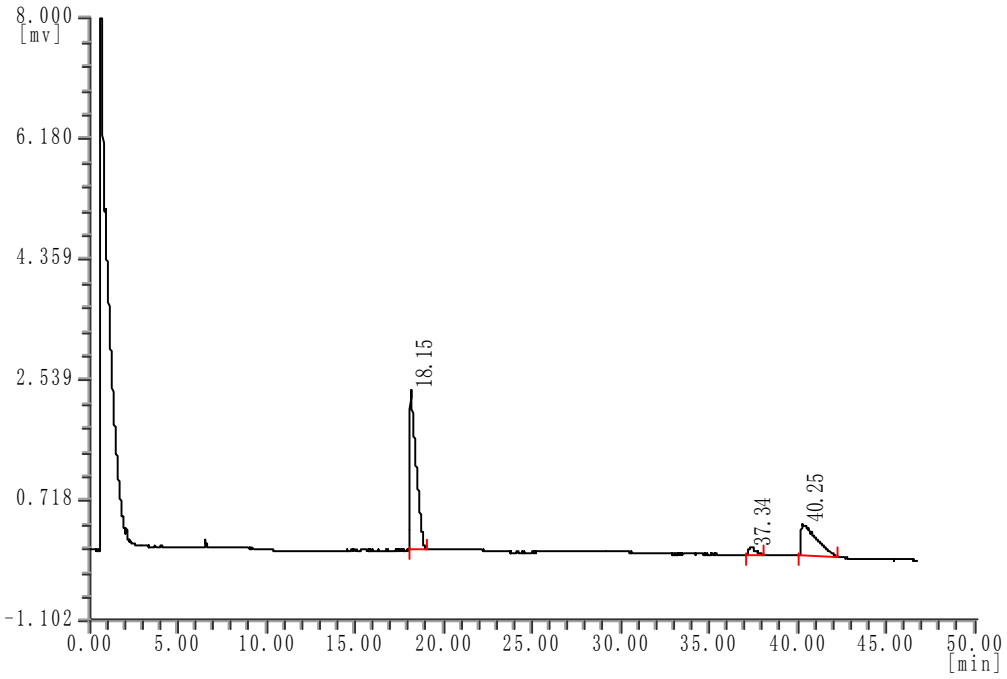
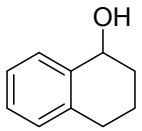
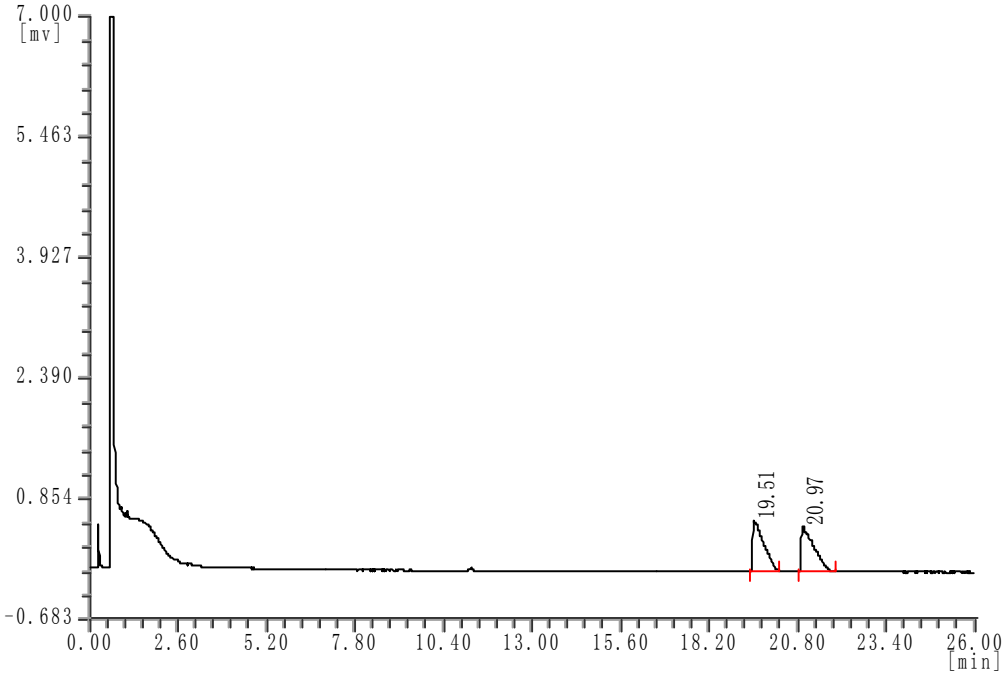




(**h**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **h**:



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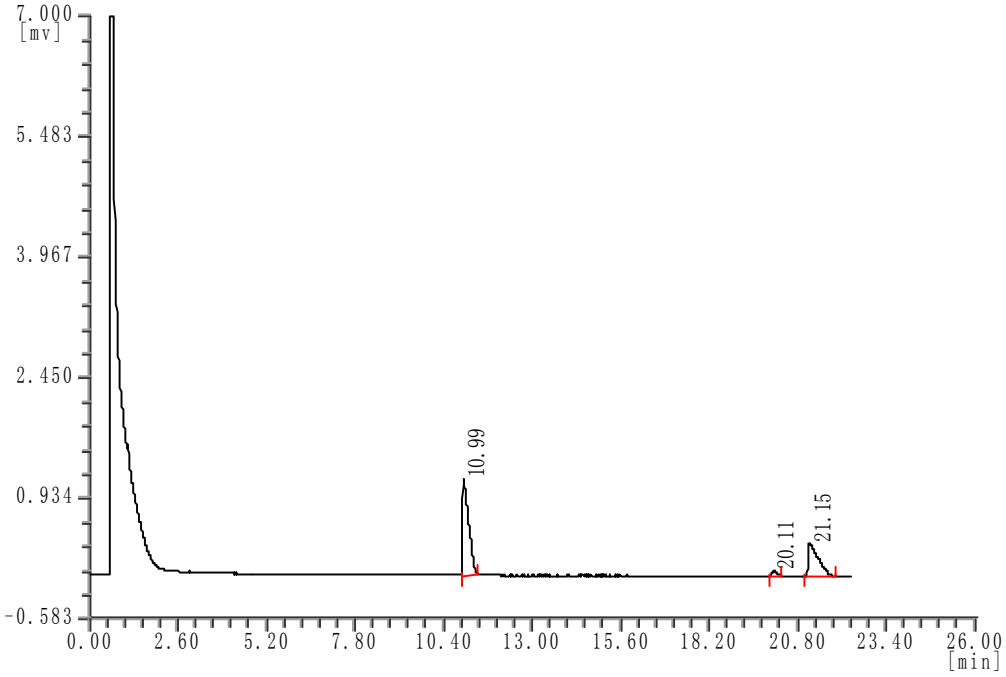
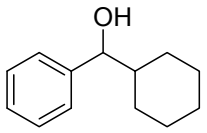
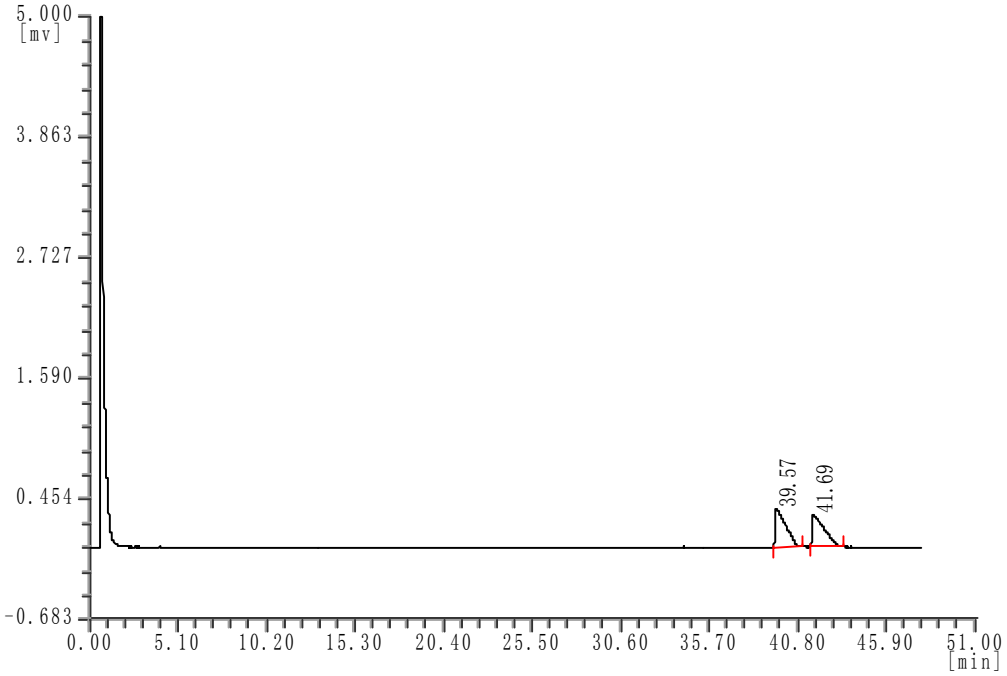




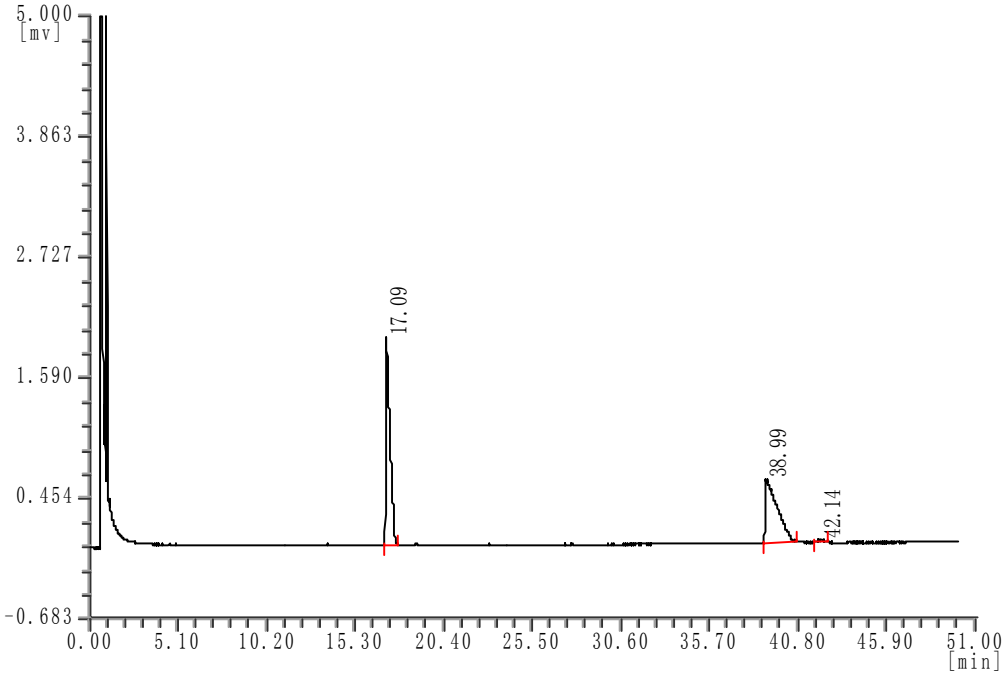
(i)

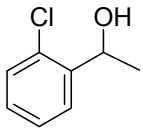
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 130 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **i**:



Resolved **i** (Table 4, Entry 9):

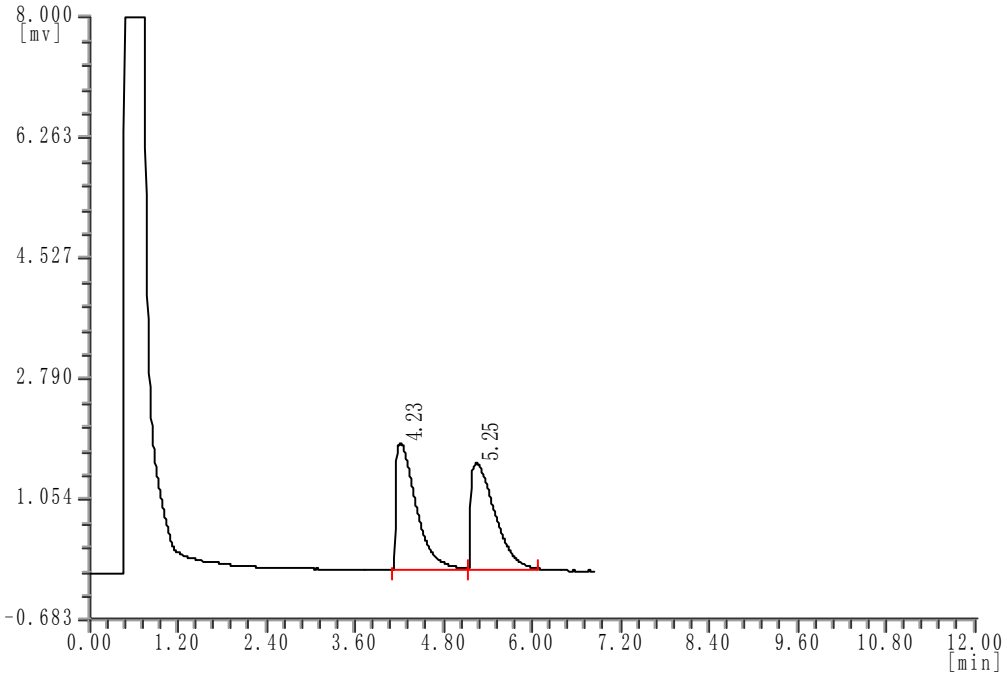




(**j**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 130 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **j**:



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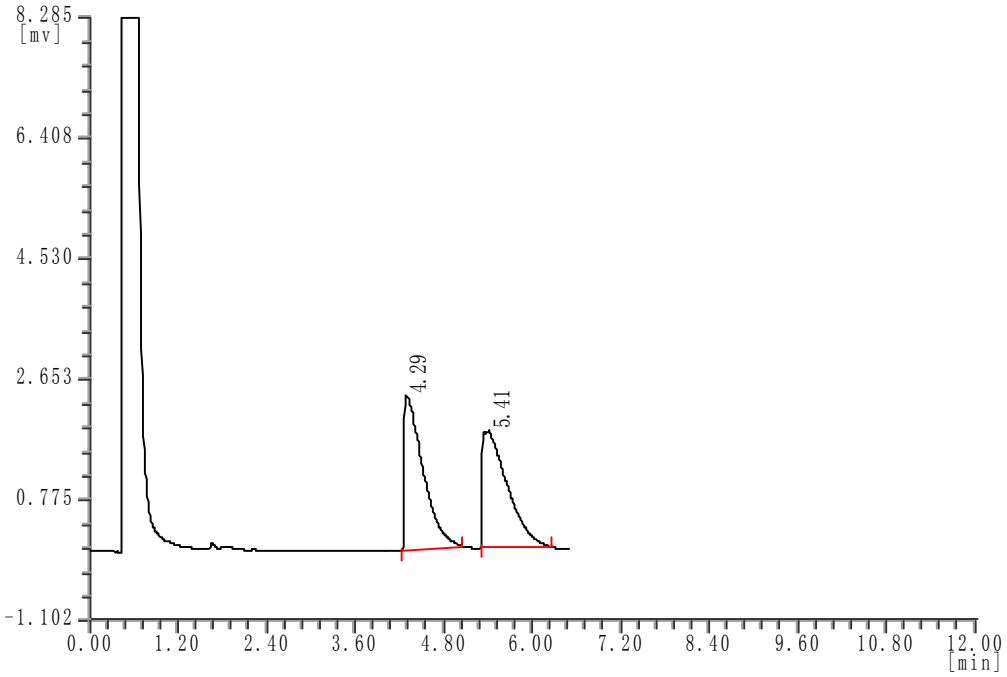
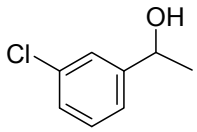
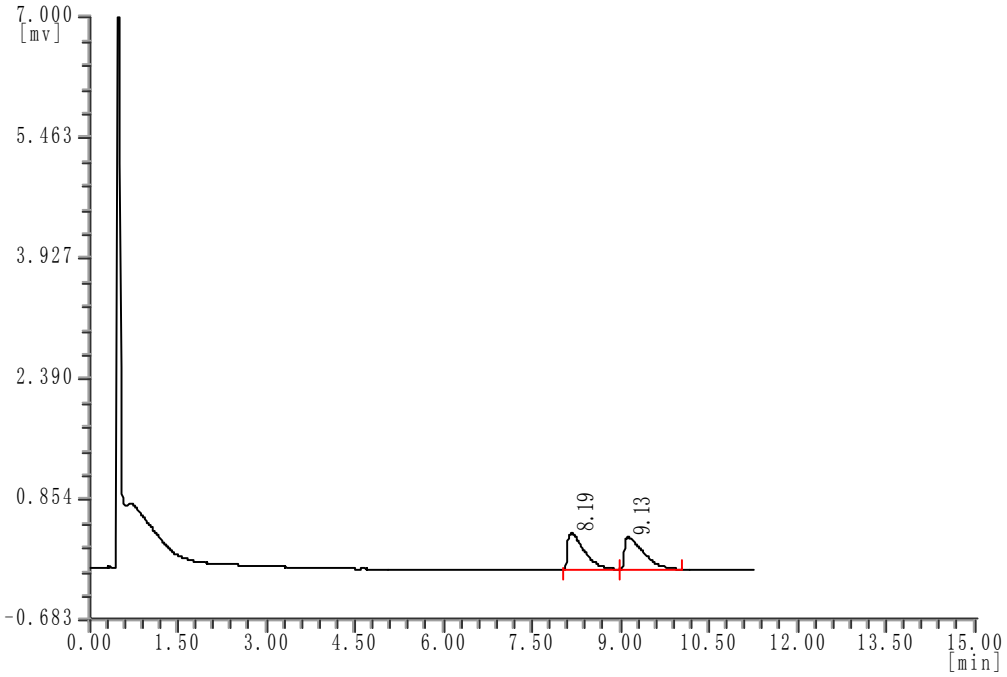




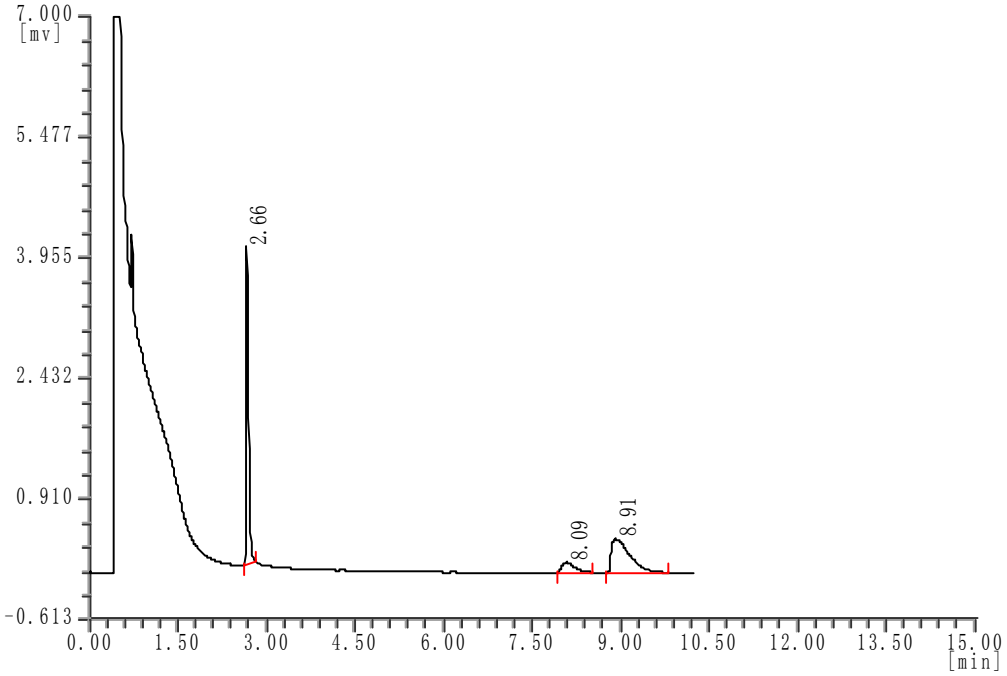
(**k**)

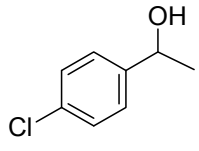
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **k**:



Resolved **k** (Table 4, Entry 11)

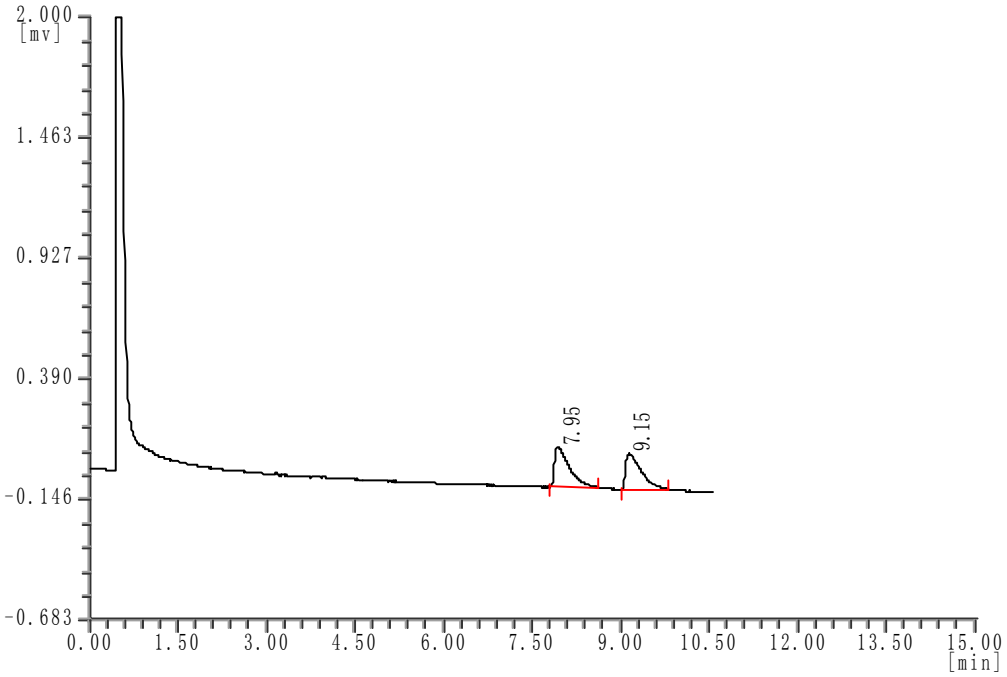




(**l**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **l**:



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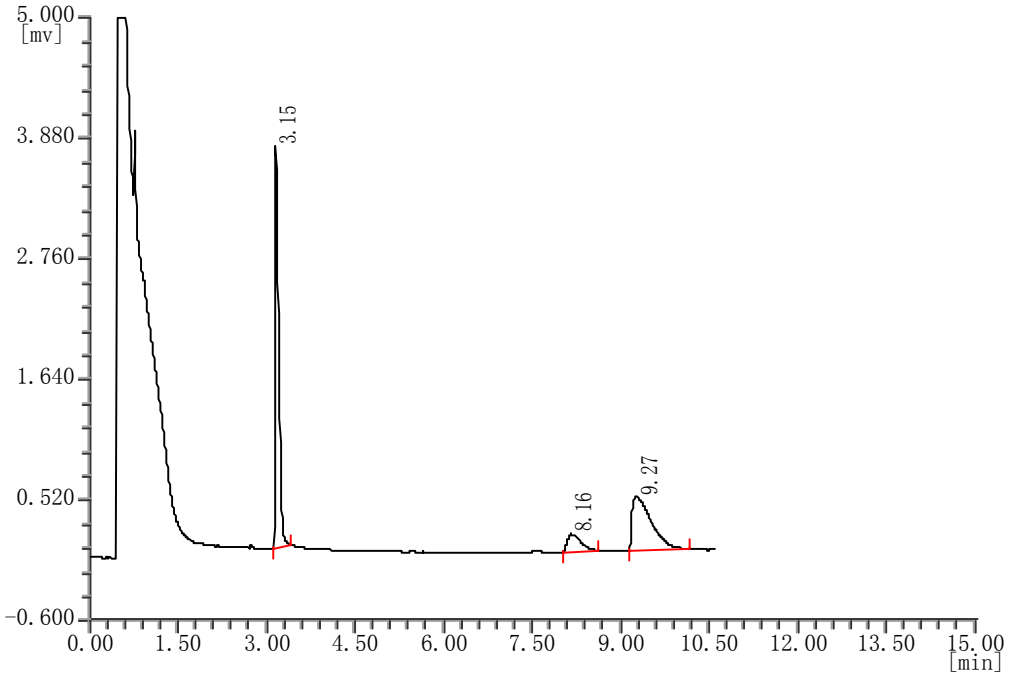
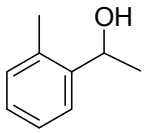
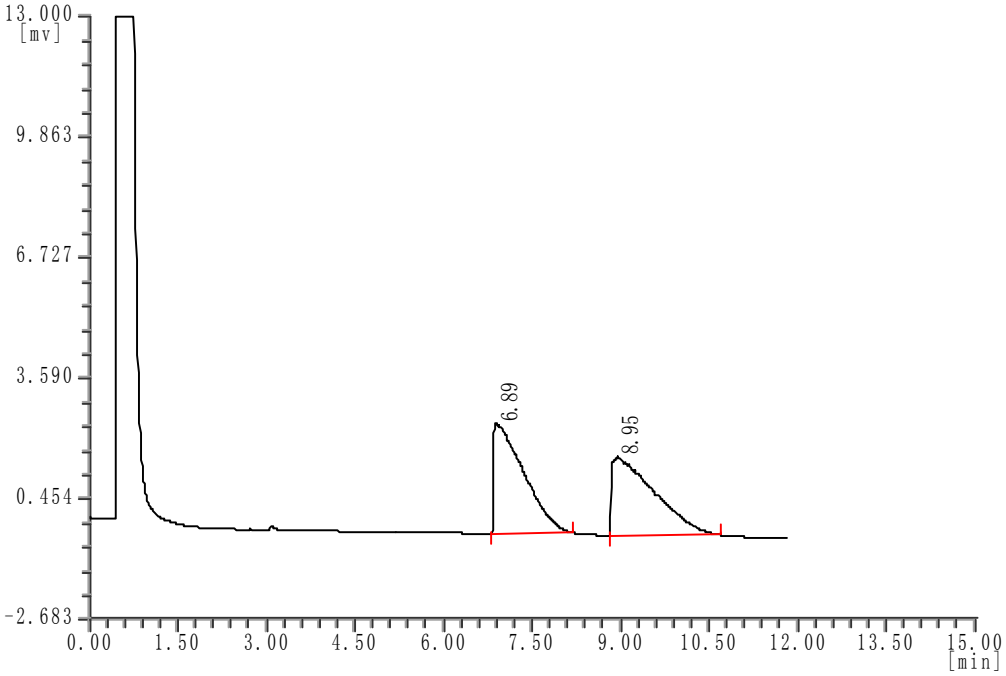




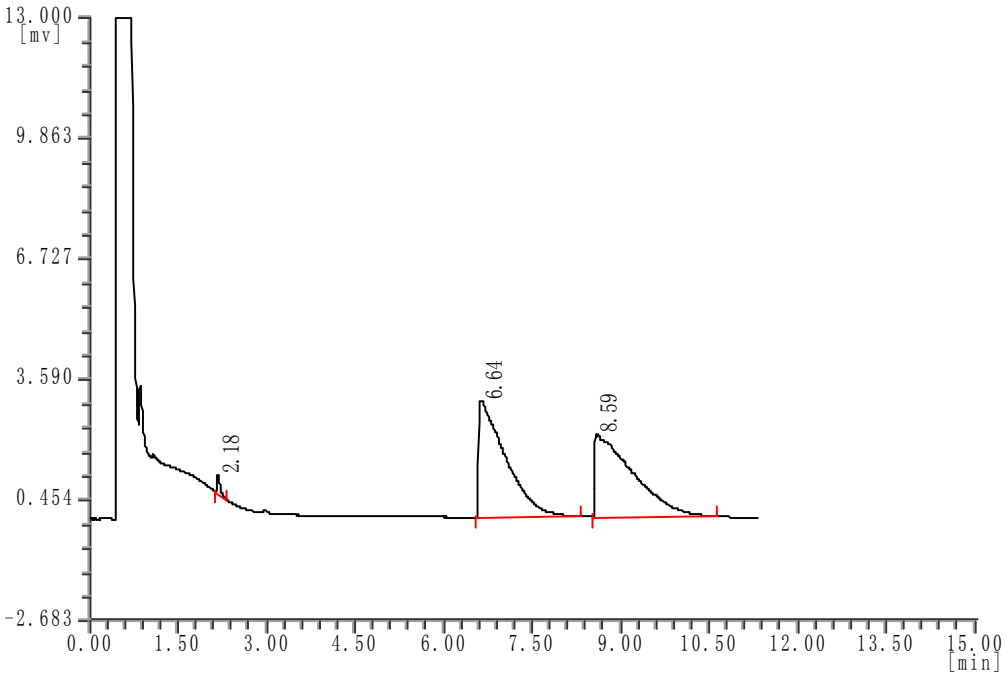
(**m**)

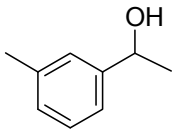
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 110 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **m**:



Resolved **m** (Table 4, Entry 13):

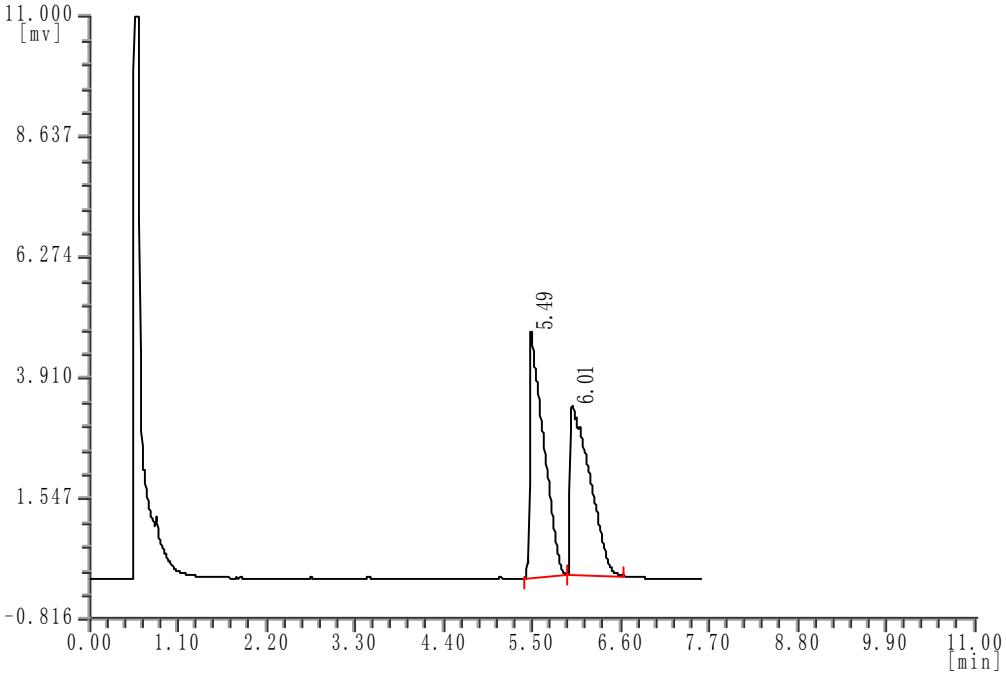




(**n**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **n**



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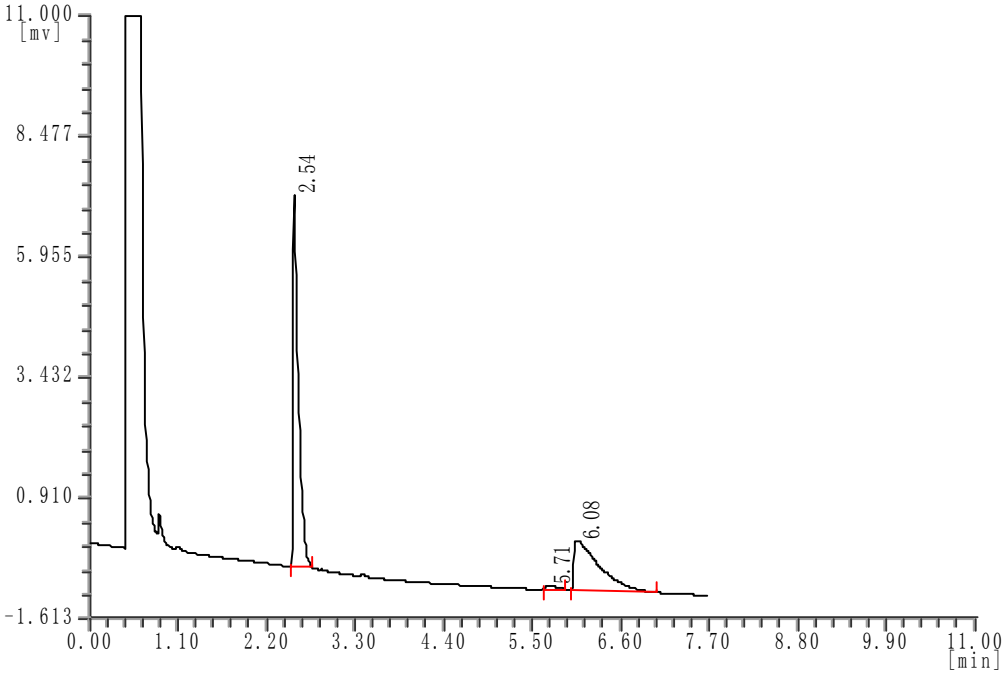
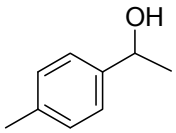
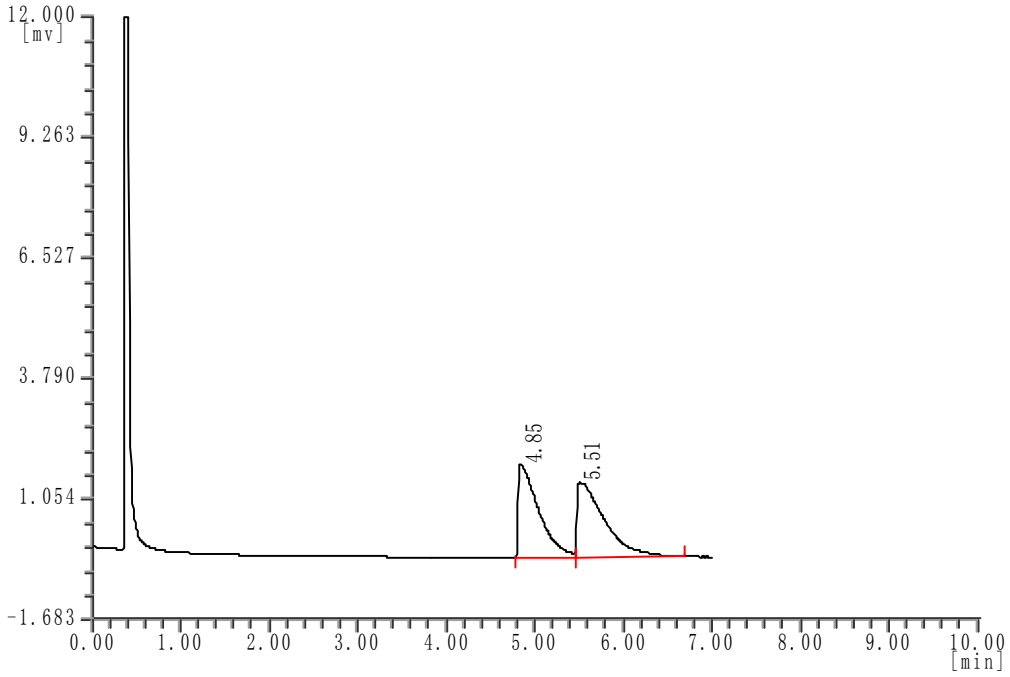




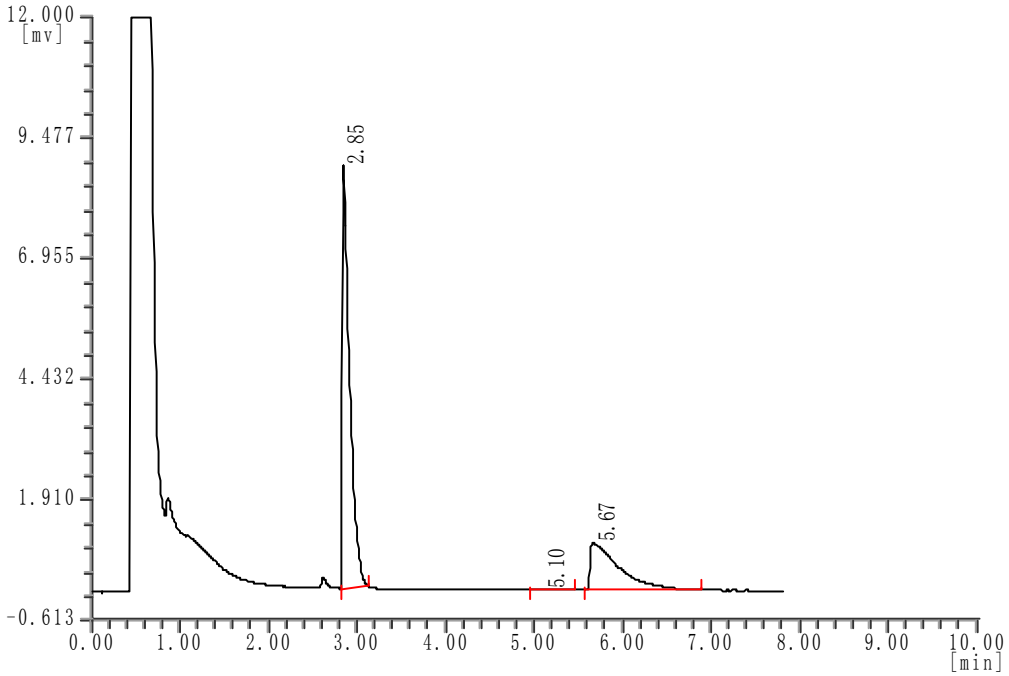
(**o**)

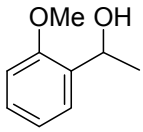
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **o**:



Resolved **o** (Table 4, Entry 15):

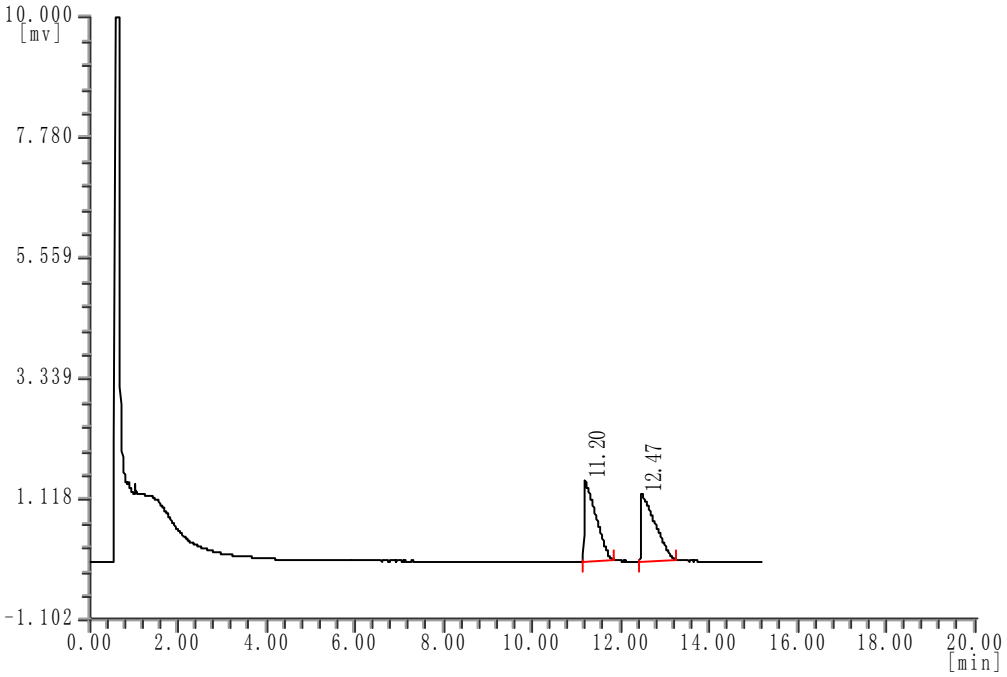




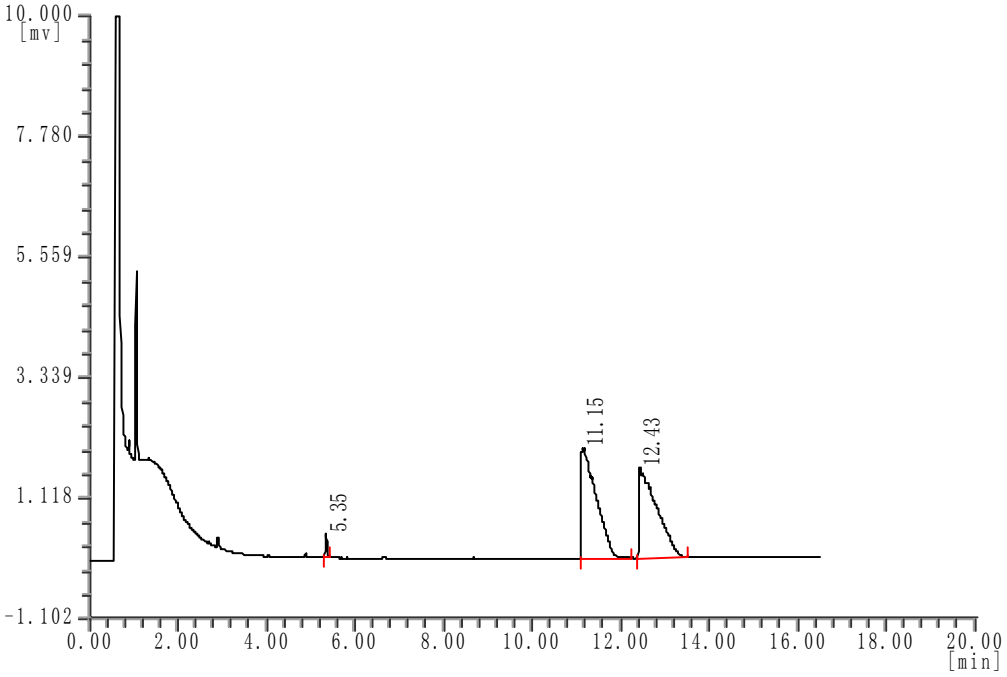
(**p**)

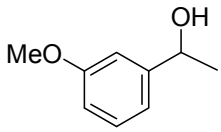
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **p**:



Resolved **p** (Table 4, Entry 16)

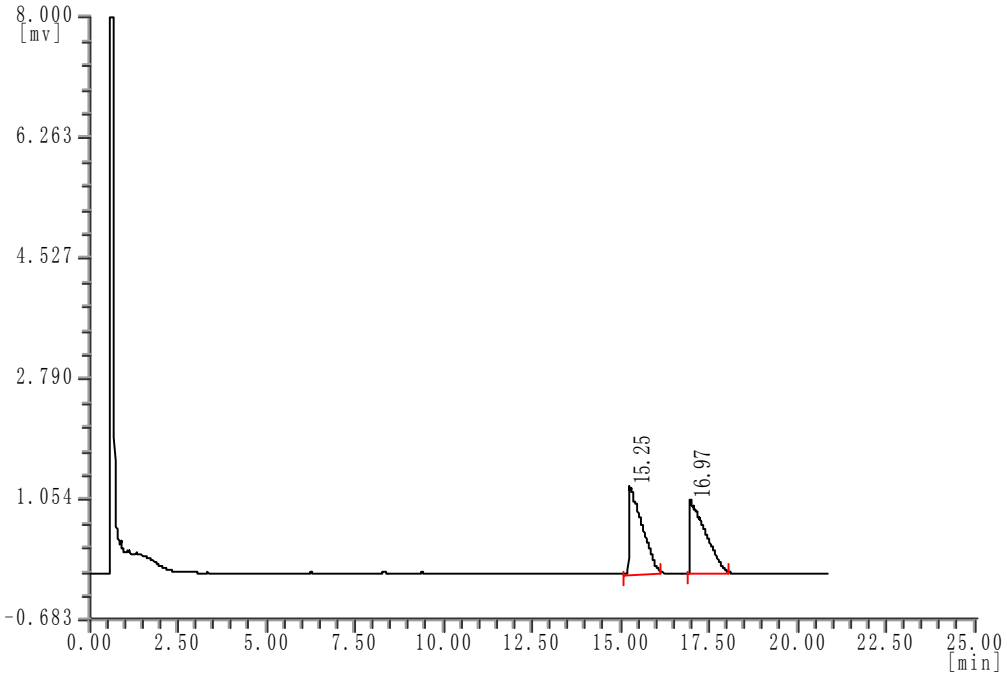




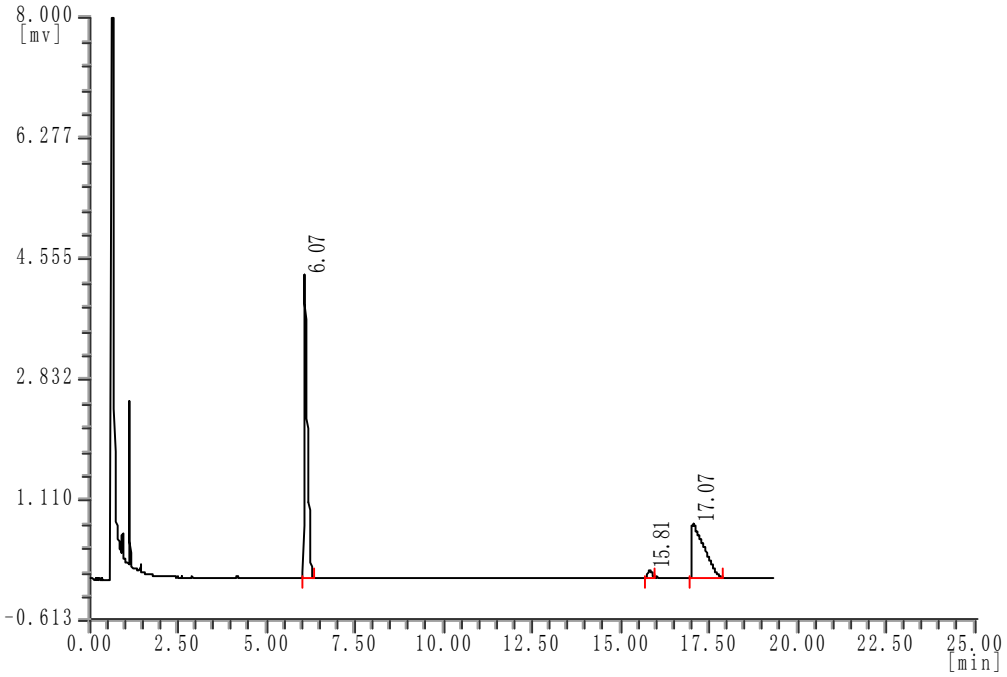
(**q**)

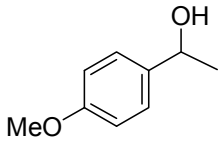
GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **q**:



Resolved **q** (Table 4, Entry 17)

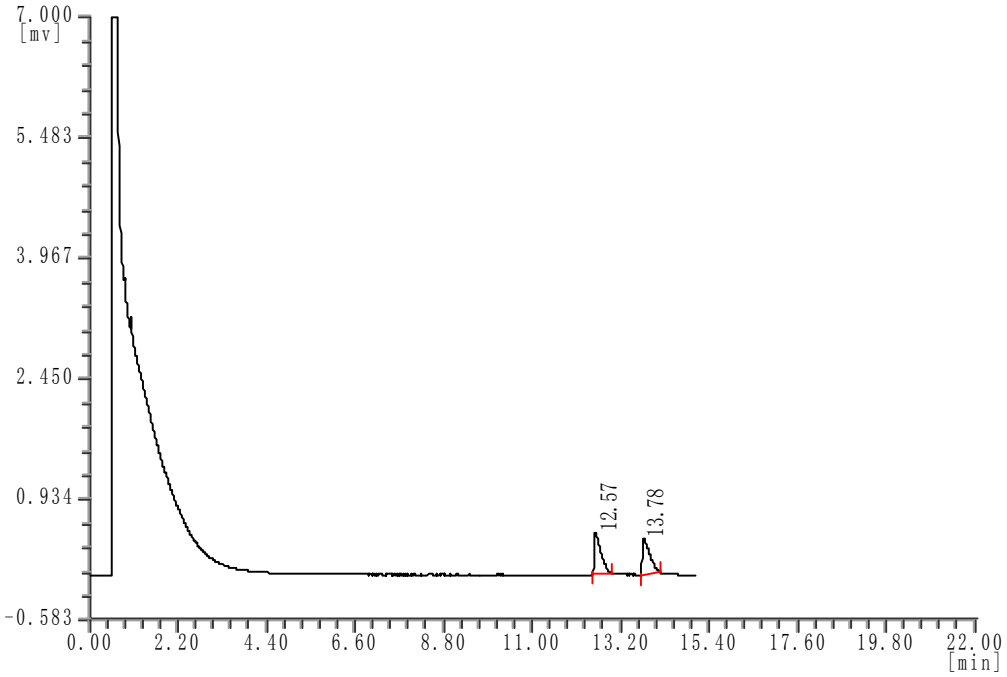




(**r**)

GC analysis: Chiral CP-Chirasil-Dex CB column, 0.25 mm × 25 m, column temperature = 120 °C (isothermal), inject temperature = 250 °C, detector temperature = 250 °C, inlet pressure = 0.12 MPa.

Racemic **r**:



Resolved **r** (Table 4, Entry 18)