Supplementary Information

Immobilization of *Burkholderia cepacia* on Pristine or Functionalized Multi-Walled Carbon Nanotubes and Application on Enzymatic Resolution of (*RS*)-1-Phenylethanol

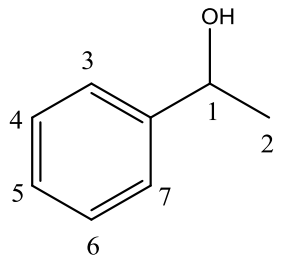
Michele R. G. Dias,[a] Alysson de Pauloveloso,[a] Lilian F. M. do Amaral,[a] Rhaísa T. Betim,[a] Maria G. Nascimento[b] and Cristiane Pilissão*[a]

[a]Departamento de Química e Biologia, Universidade Tecnológica Federal do Paraná, 81280-340 Curitiba-PR, Brazil

[b]Departamento de Química, Universidade Federal de Santa Catarina, 88040-900 Florianópolis-SC, Brazil

Chemical synthesis of racemic (RS)-1-phenylethanol

(*RS*)-1-Phenylethanol was obtained by the reduction of acetophenone using sodium borohydride and boric acid according to the methodology described by Cho *et al.*[1] A colorless liquid was obtained in 70% yield after purification by column chromatography on silica gel 60 (230-400 mesh) in *n*-hexane:ethyl acetate (7:3 v/v). This compound was also analyzed by ^{1}H NMR, FTIR and chiral GC.



^{1}H NMR (200 MHz, $CDCl_3$) δ 7.40-7.20 (m, 5H), 4.89 (q, 1H, ^3J 6.4 Hz), 2.01-1.94 (br s, 1H, –OH), 1.49 (d, 3H, ^3J 6.4 Hz); FTIR (ATR) ν / cm^{-1} 3343 (OH), 3030 (aromatic C–H), 2943 (methyl C–H), 1447 (C=C), 1073 (C–O); chiral GC-FID (N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature 230 °C, isotherm, 100 °C for 30 min), t_R 19.4 and 20.9 min.

*e-mail: pilissao@utfpr.edu.br

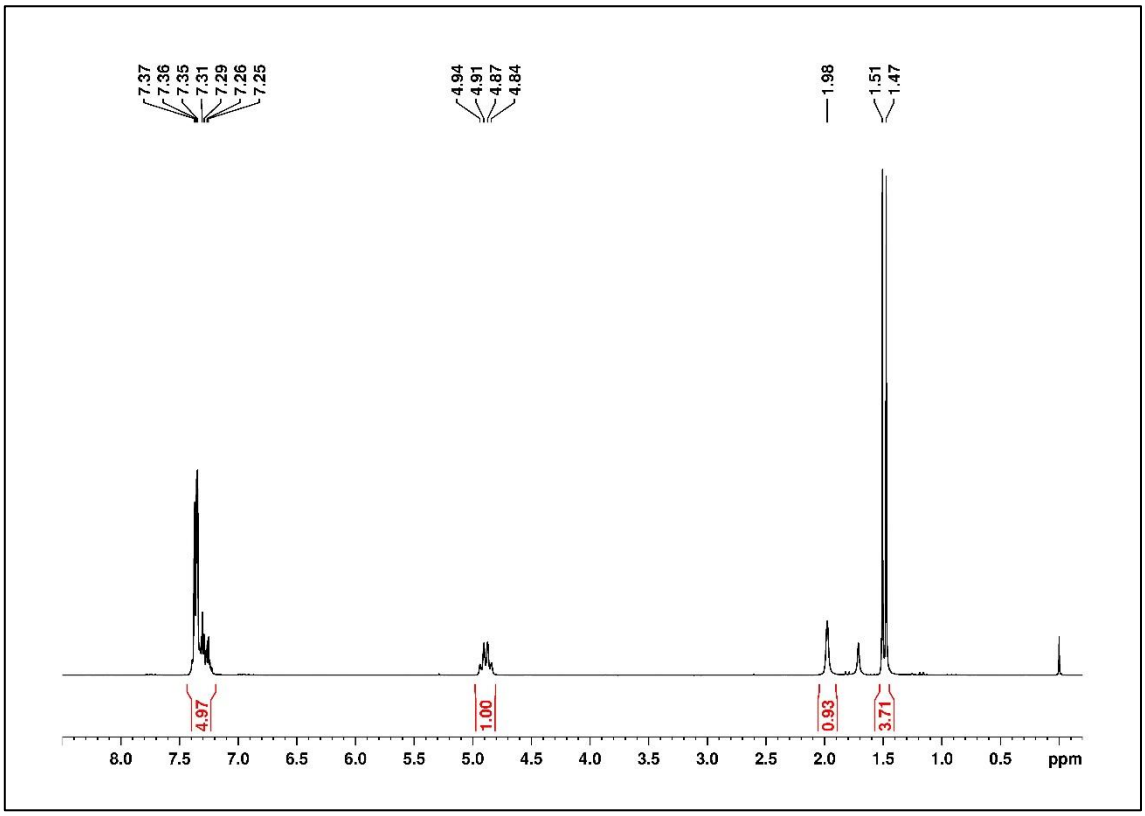


Figure S1. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of (*RS*)-1-phenylethanol.

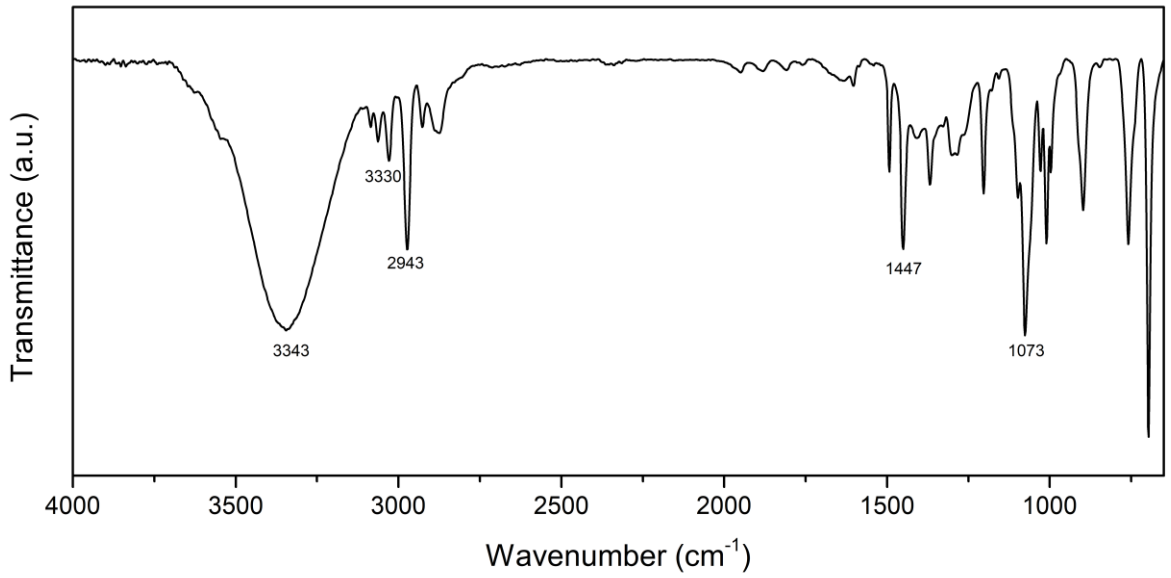


Figure S2. FTIR spectrum (ATR) of (*RS*)-1-phenylethanol.

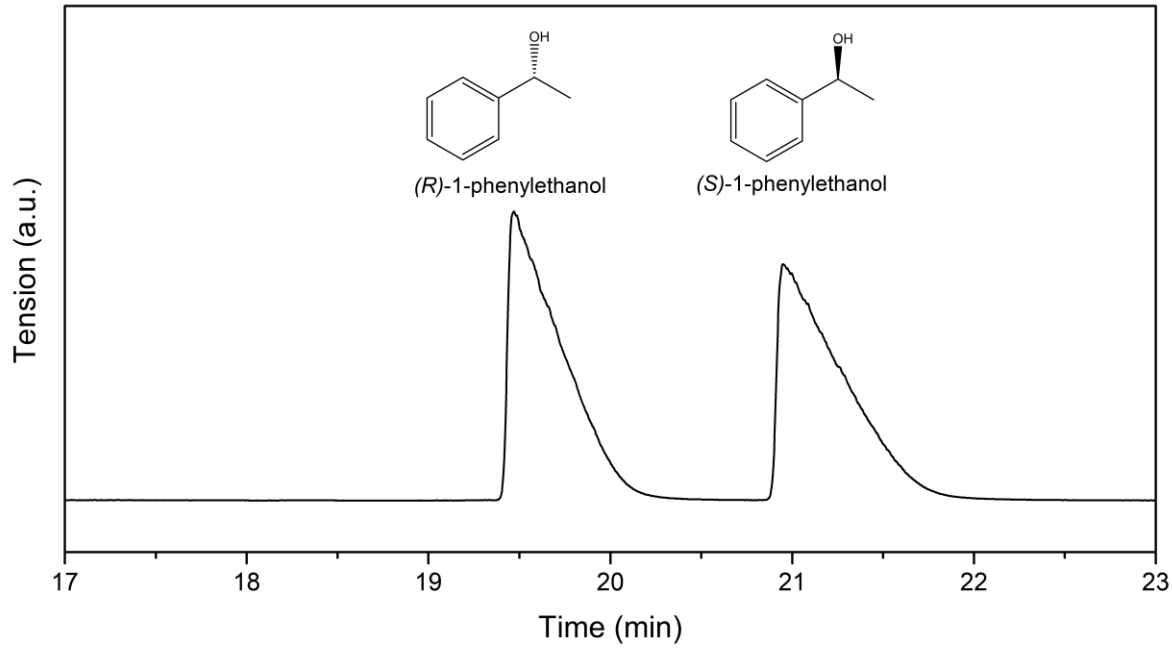


Figure S3. Chromatogram of the racemic mixture of (*RS*)-1-phenylethanol. Analysis conditions: N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature: 230 °C, programming: isotherm, 100 °C for 30 min. t_R = 19.4 and 20.9 min.

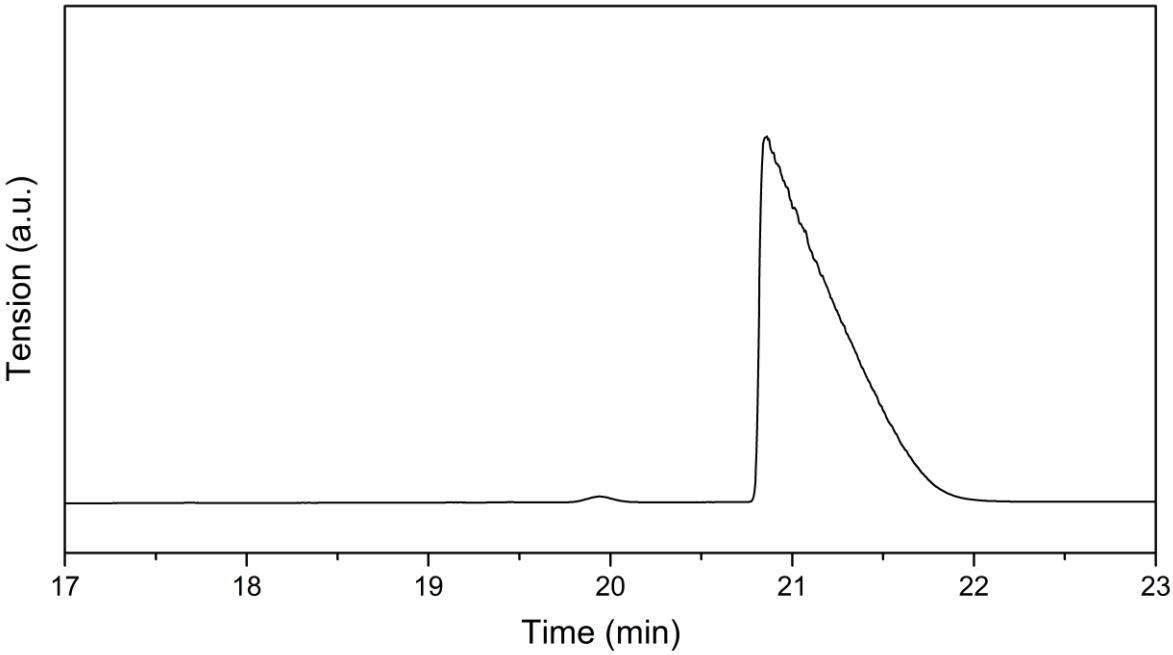
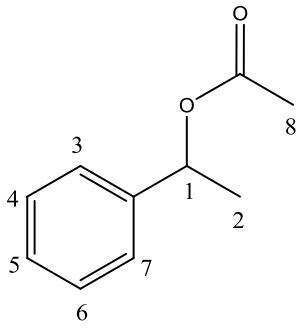


Figure S4. Chromatogram of (*S*)-1-phenylethanol (ee > 99%). Analysis conditions: N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature: 230 °C, programming: isotherm, 100 °C for 30 min. t_R = 20.9 min.

Chemical synthesis of racemic (*RS*)-1-Phenylethyl acetate

The racemic (*RS*)-1-phenylethyl acetate was prepared by chemical acetylation of the precursor alcohol (*RS*)-**1** (0.6 mL, 5 mmol) employing acetic anhydride (2.3 mL, 25 mmol) in dichloromethane (30 mL) and acid acetic (1%) as

described in the literature.[2] A colorless oil was obtained in 70% yield after purification by column chromatography on silica gel using a mixture of *n*-hexane and ethyl acetate (7:3 v/v) as the eluent. This compound was used as a standard in the chiral gas chromatography analysis and was also analyzed by ^{1}H NMR and FTIR.



^{1}H NMR (200 MHz, $CDCl_3$) δ 7.40-7.20 (m, 5H), 5.92 (q, 1H, *J* 6.6 Hz), 1.59 (d, 3H, *J* 6.6 Hz), 2.12 (s, 3H); FTIR (ATR) ν / cm^{-1} 3030 (aromatic C–H), 2986 (methyl C–H), 1738 (C=O), 1235 (C–O); chiral GC-FID (N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature 230 °C, isotherm, 100 °C for 30 min), t_R 17.6 and 19.2 min.

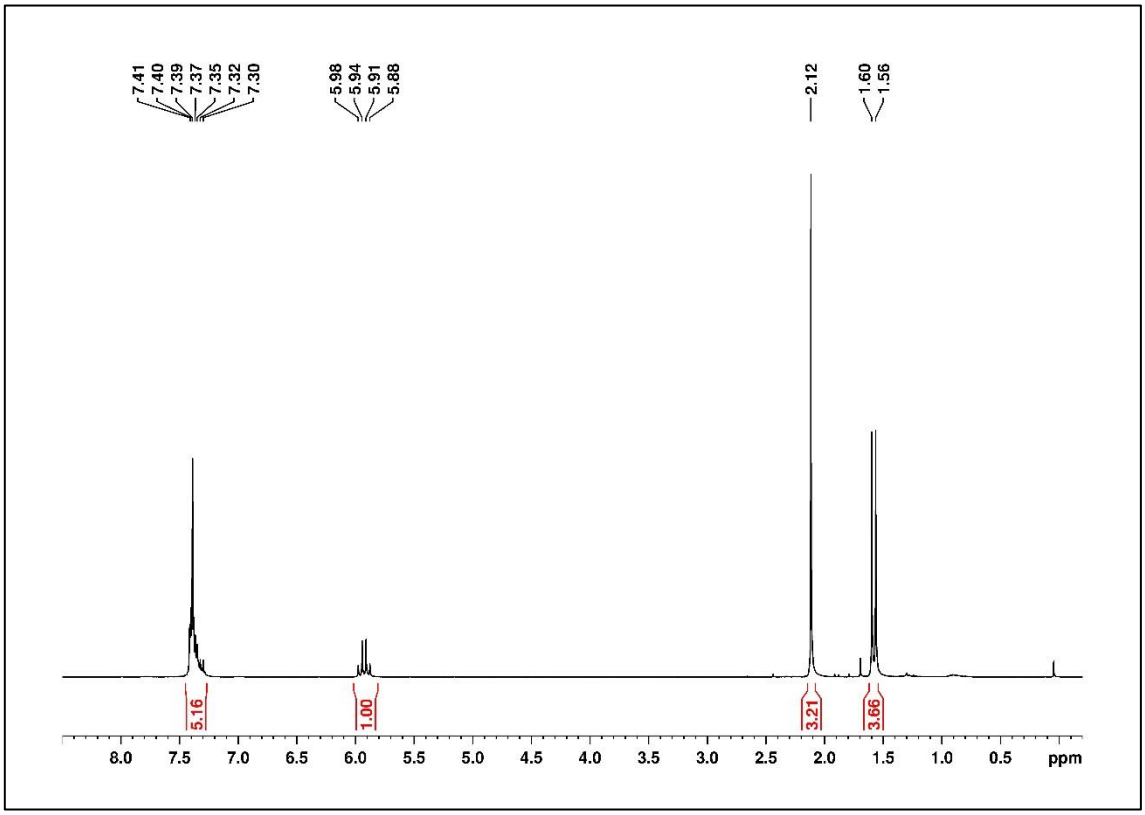


Figure S5. ^{1}H NMR spectrum (200 MHz, $CDCl_3$) of (*RS*)-1-phenylethyl acetate.

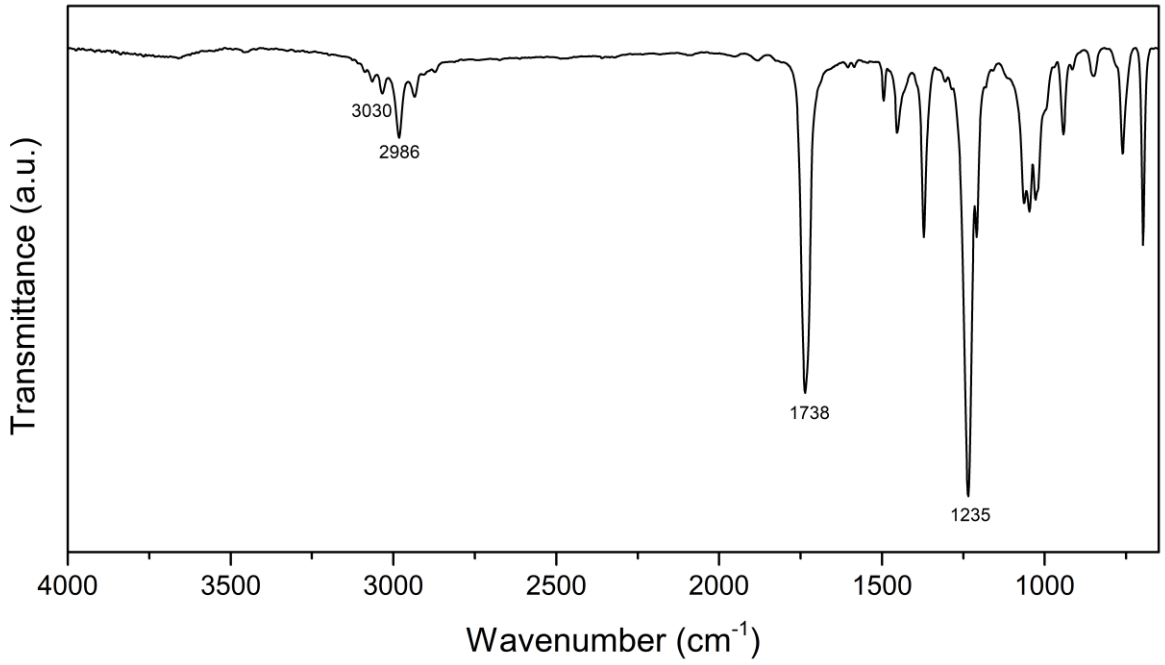


Figure S6. FTIR spectrum (ATR) of (*RS*)-1-phenylethyl acetate.

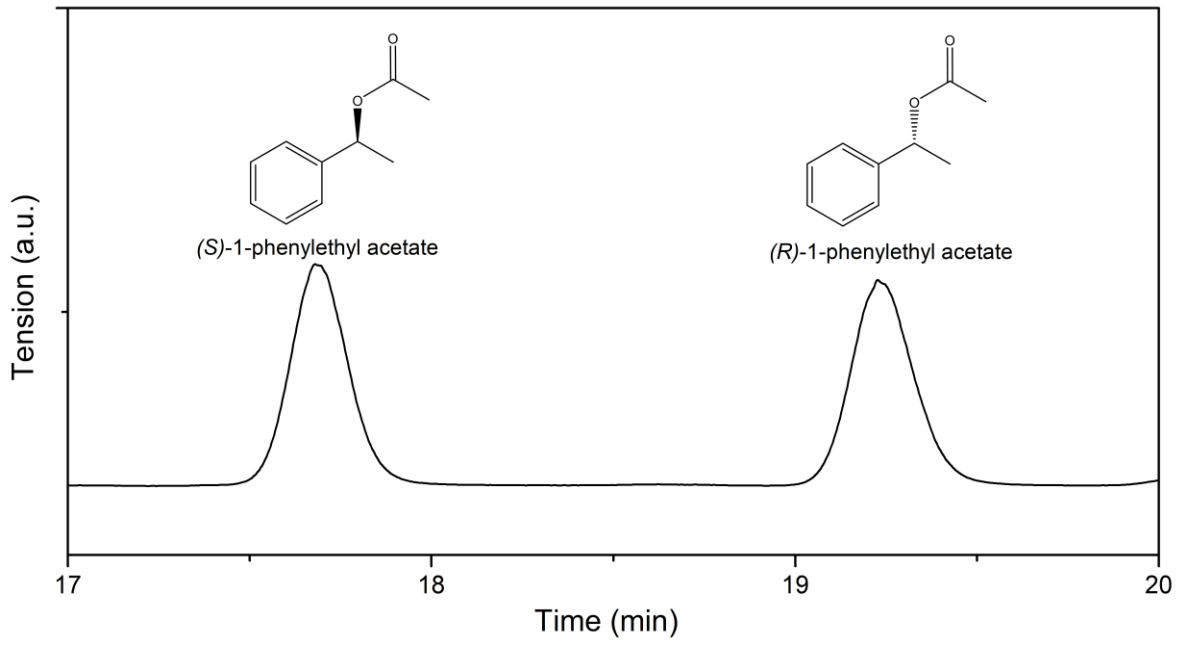


Figure S7. Chromatogram of the racemic mixture of (*RS*)-1-phenylethyl acetate. Analysis conditions: N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature: 230 °C, programming: isotherm, 100 °C for 30 min. t_R = 17.6 and 19.2 min.

Enzymatic resolution of (*RS*)-**1**

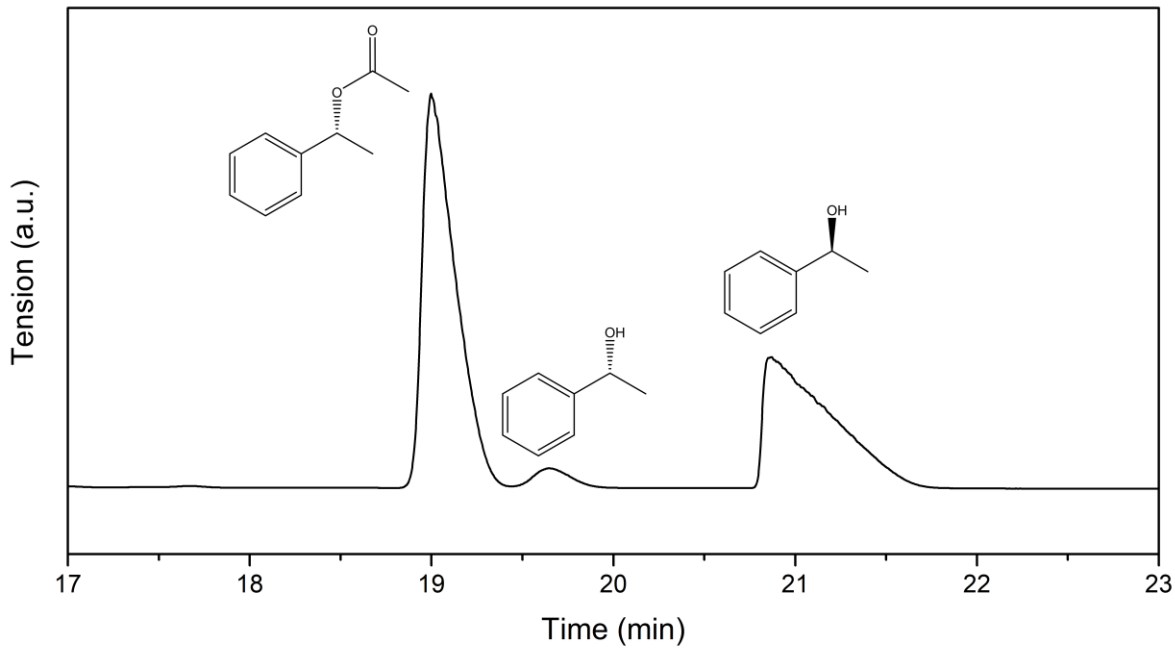


Figure S8. Chromatogram of (*RS*)-1-phenylethanol resolution catalyzed by BCL immobilized on MWCNTs-A. Analysis conditions: N_2, 120 kPa, split 1:60, β-ciclodex column, injector and detector temperature: 230 °C, programming: isotherm, 100 °C for 30 min. (*R*)-**3**: t_R = 19.2 min; (*R*)-**1**: t_R = 19.6 min; (*S*)-**1**: t_R = 20.9 min.

References

1. Cho, B. T.; Kang, S. K.; Kim, M. S.; Ryu, S. R.; Na, D. K.; *Tetrahedron* **2006**, *62*, 8164.
2. Chojnacka, A.; Obara, R.; Wawrzenczyk, C.; *Tetrahedron: Asymmetry* **2007**, *18*, 101.