Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Dual Enzymatic Dynamic Kinetic Resolution by *Thermoanaerobacter ethanolicus* Secondary Alcohol Dehydrogenase and *Candida antarctica* Lipase B

Ibrahim Karume,[a] Musa M. Musa,*[,a] Odey Bsharat,[a] Masateru Takahashi,[b] Samir M. Hamdan,[b] and Bassam El Ali[a]

[a]*Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, 31261, KSA. Fax: +966-13-860-4277; Tel: +966-13-860-7343; E-mail: musam@kfupm.edu.sa*

[b]*Division of Biological and Environmental Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, KSA*

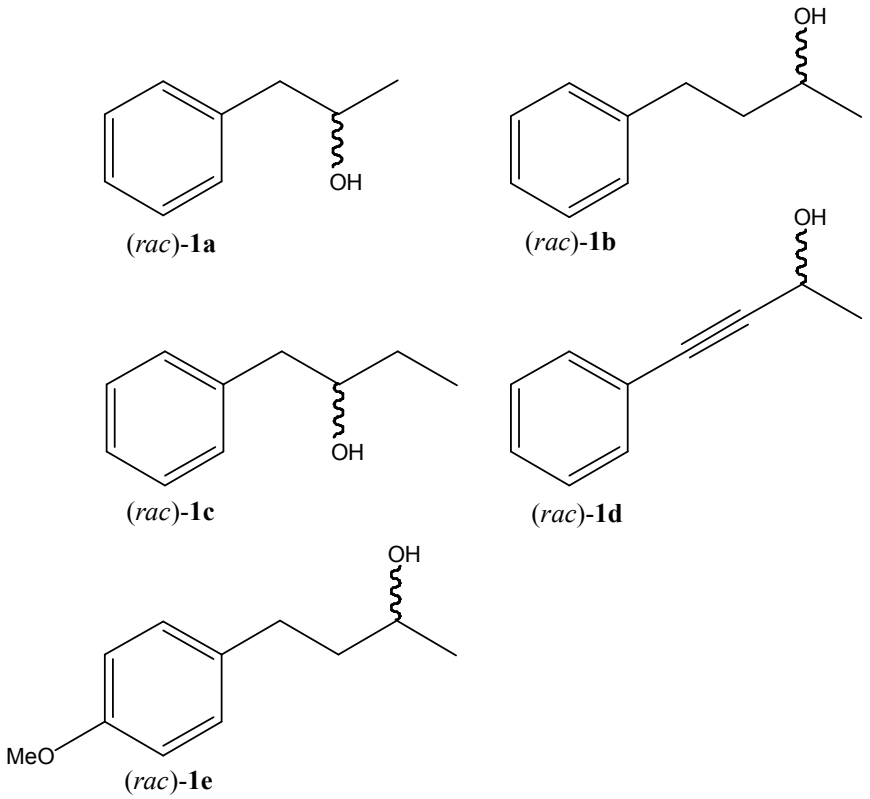

Figure S1. The structures of the alcohol substrates used in this study.

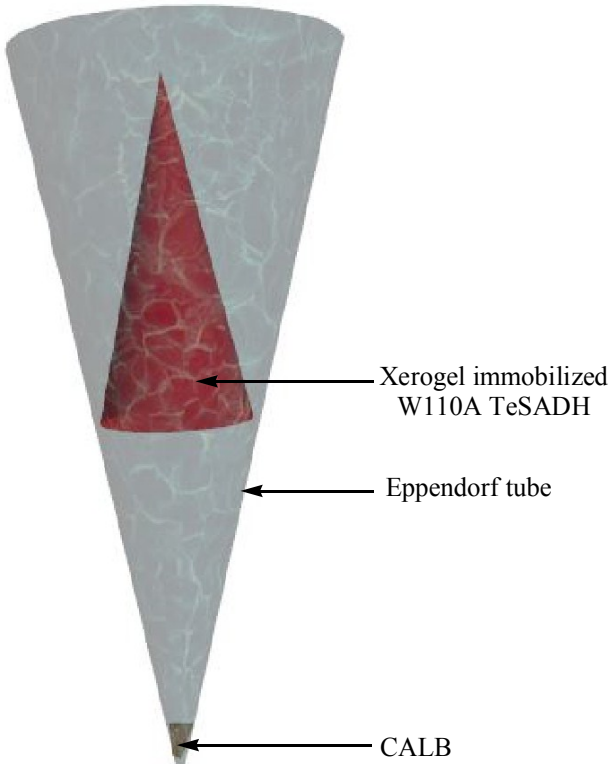

Figure S2. Reaction set-up for dual enzymatic DKR of phenyl-ring-containing secondary alcohols.

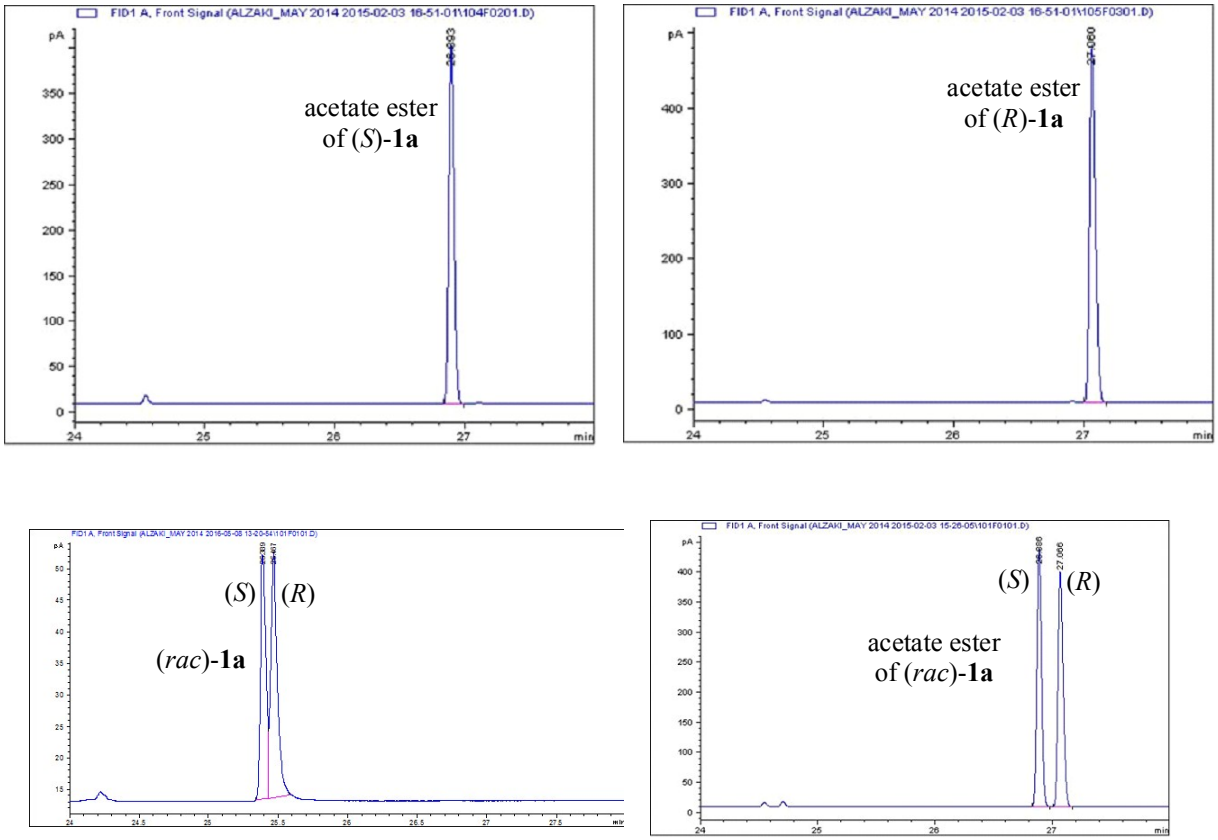

Figure S3. Gas chromatograms of the reference acetate ester of (*S*)-**1a**, (*R*)-**1a** and (*rac*)-**1a**.

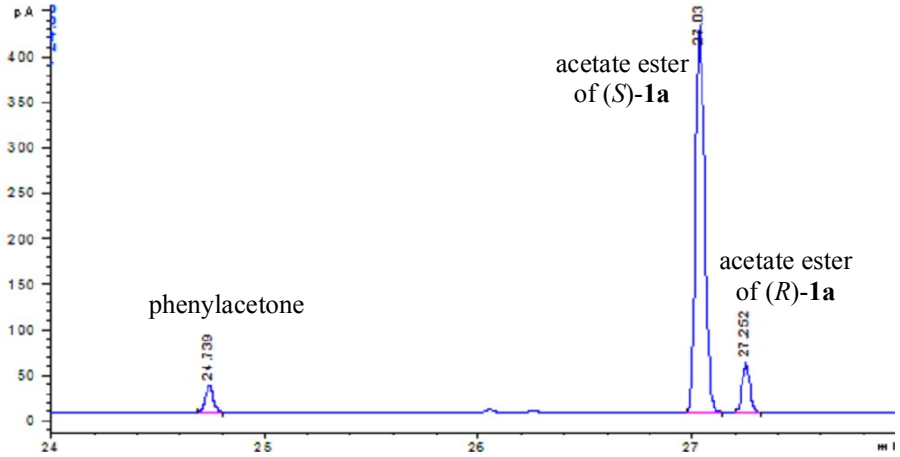

Figure S4. GC chromatogram of racemization of (*S*)-**1a** in hexane using xerogel-immobilized W110A TeSADH (see Table 1 in the main text, entry 7).

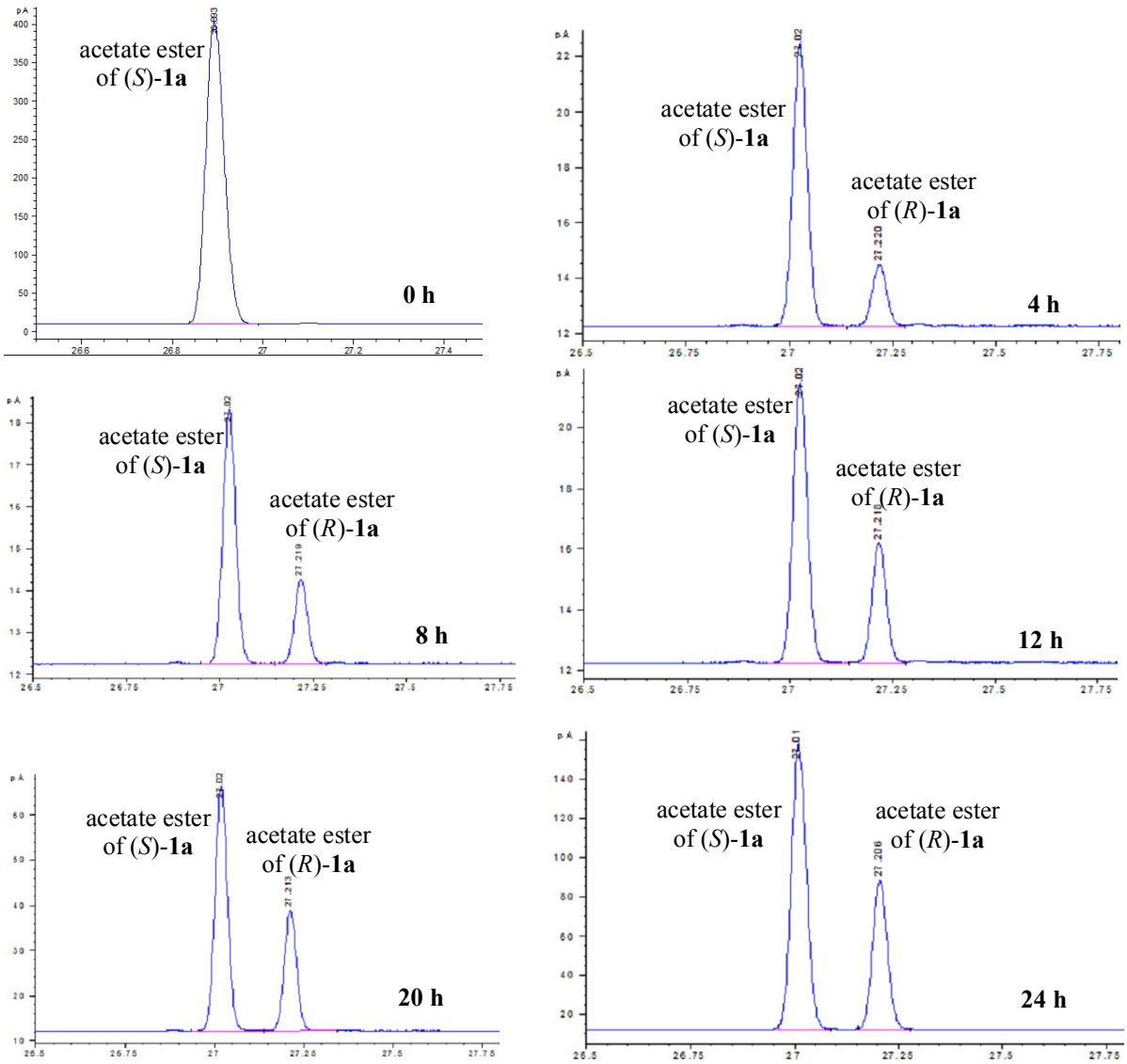

Figure S5. GC chromatogram of racemization of (*S*)-**1a** in biphasic medium-hexane/Tris-HCl at different time intervals (see Figure 1 in the main text).

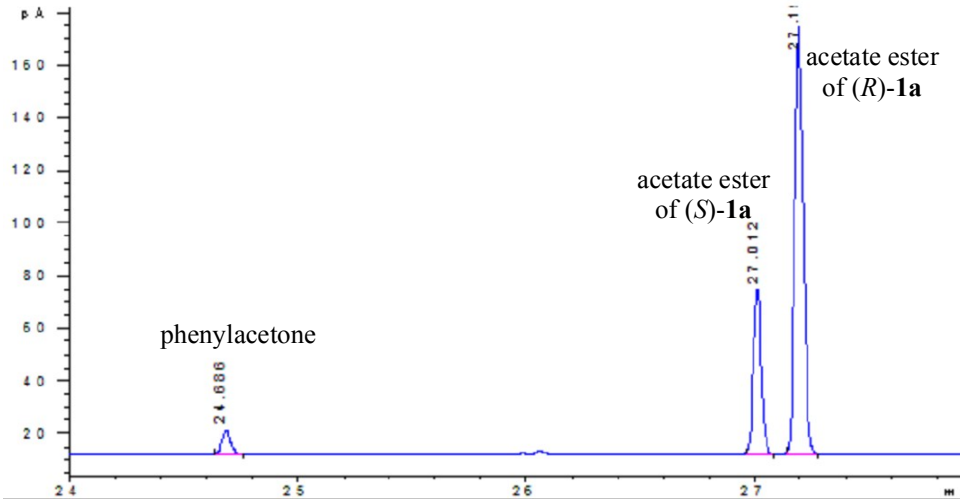

Figure S6. GC chromatogram of racemization of (*R*)-**1a** in hexane using xerogel-immobilized W110A TeSADH (see Table 2 in the main text, entry 2).

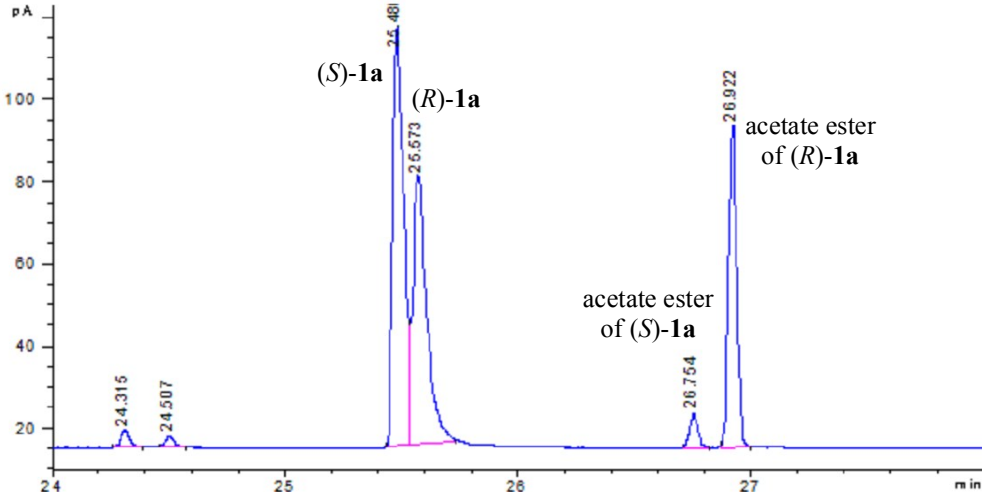

Figure S7. GC chromatogram of products of CALB-catalyzed KR of (*rac*)-**1a** using isopropenyl acetate after 3 h (see Table 3 in the main text, entry 1).

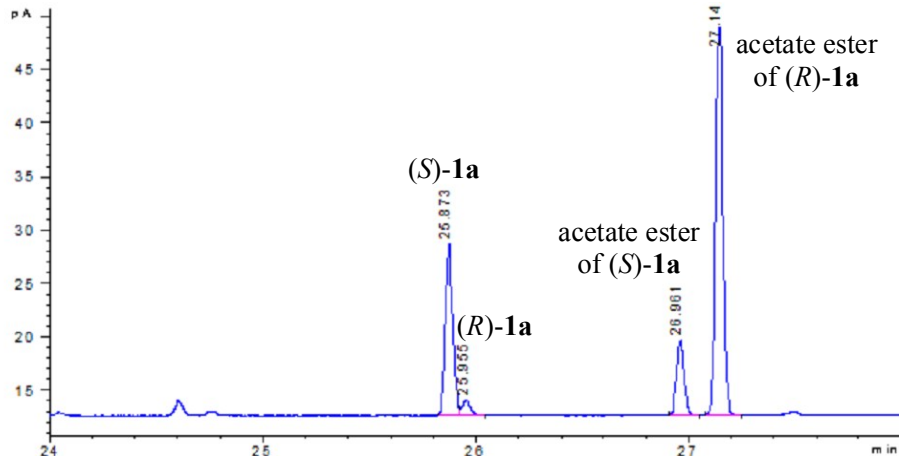

Figure S8. GC chromatogram of products of DKR of (*rac*)-**1a** using CALB-catalyzed KR and W110A TeSADH-catalyzed racemization (see Table 4 in the main text, entry 1).

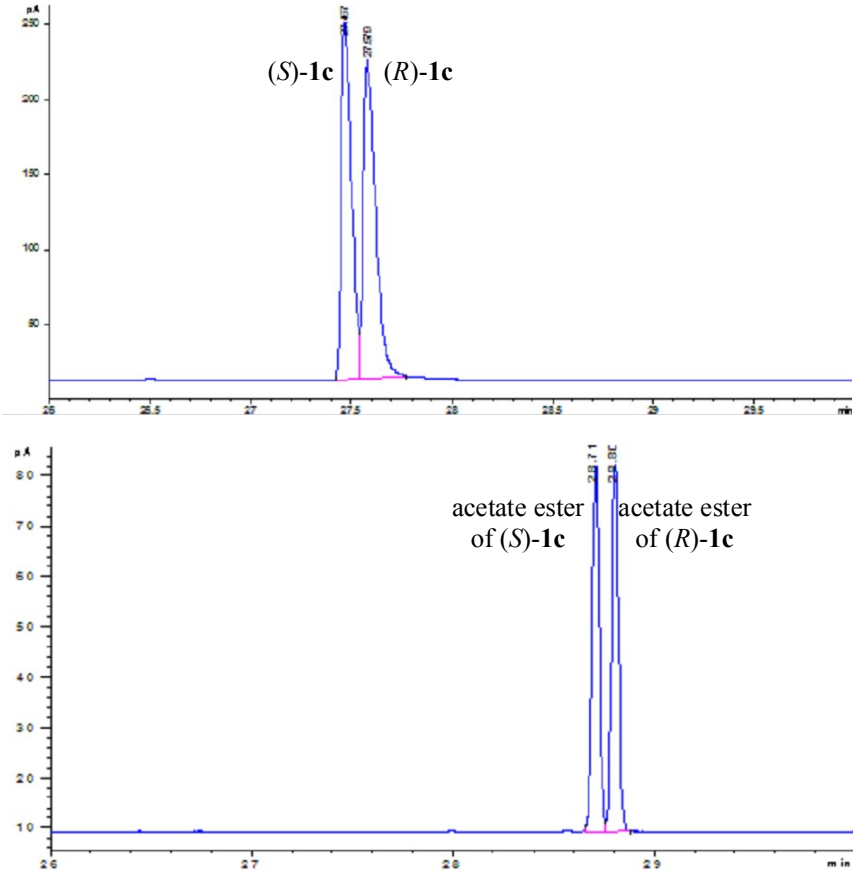

Figure S9. Gas chromatograms of the reference (*rac*)-**1c** and corresponding acetate ester derivative

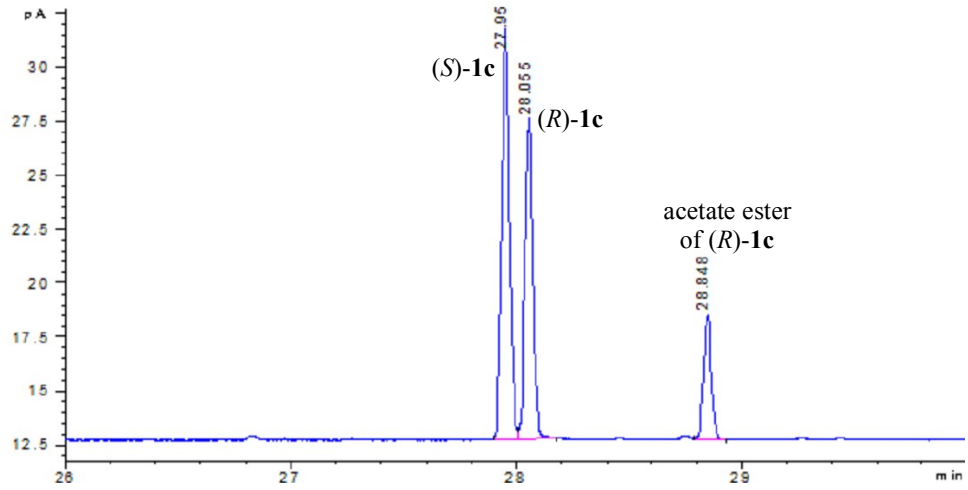

Figure S10. GC chromatogram of products of DKR of (*rac*)-**1c** using CALB-catalyzed KR and W110A TeSADH-catalyzed racemization (see Table 4 in the main text, entry 3).

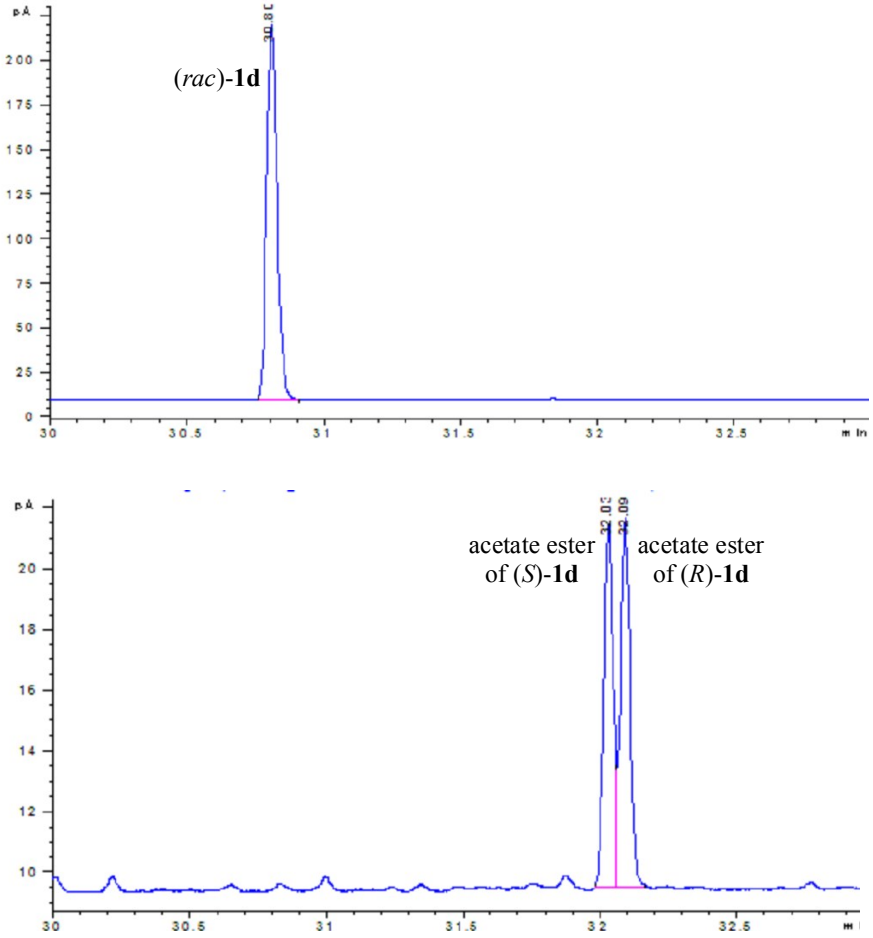

Figure S11. Gas chromatograms of the reference (*rac*)-**1d** and corresponding acetate ester derivative

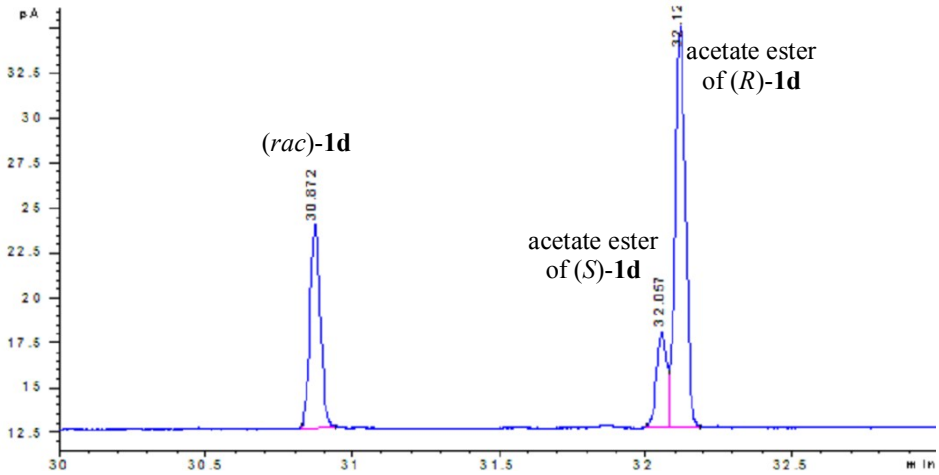

Figure S12. GC chromatogram of products of DKR of (*rac*)-**1d** using CALB-catalyzed KR and W110A TeSADH-catalyzed racemization (see Table 4 in the main text, entry 4).

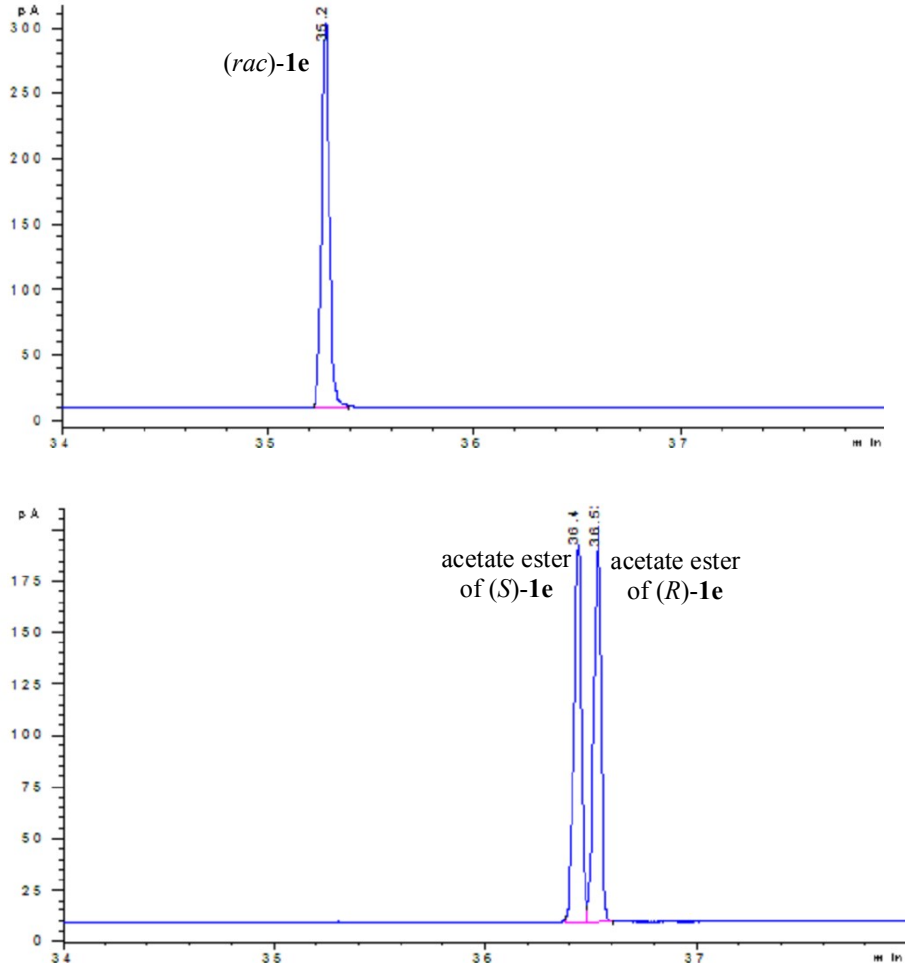

Figure S13. Gas chromatograms of the reference (*rac*)-**1e** and corresponding acetate ester derivative.

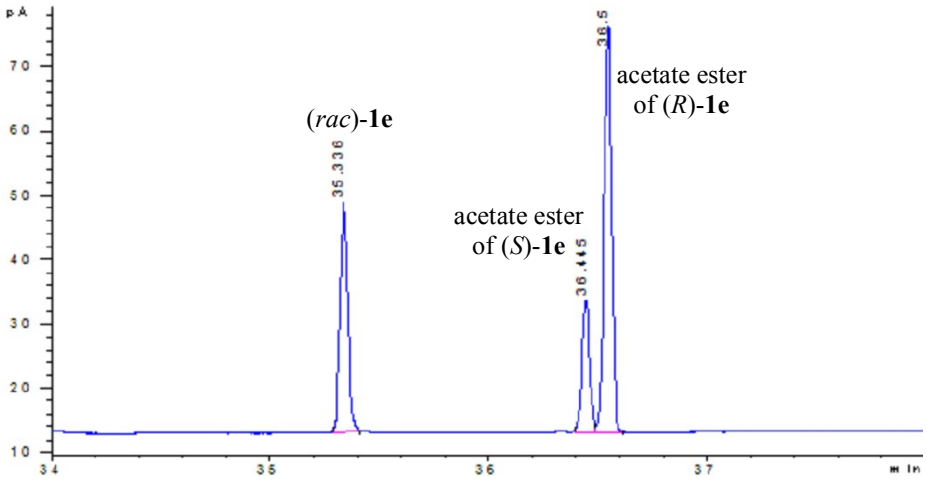

Figure S14. GC chromatogram of products of DKR of (*rac*)-**1e** using CALB-catalyzed KR and W110A TeSADH-catalyzed racemization (see Table 4 in the main text, entry 5).

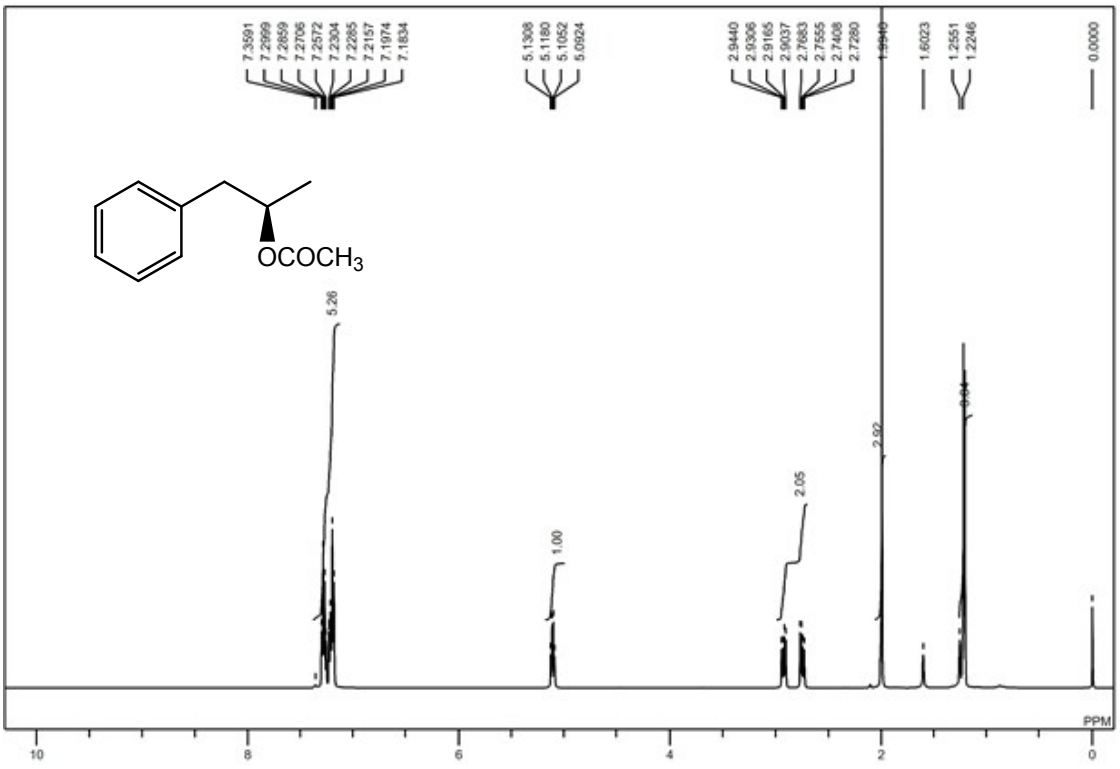

Figure S15. ^{1}H NMR spectrum of (*R*)-**2a** produced by DKR of (*rac*)-**1a**.

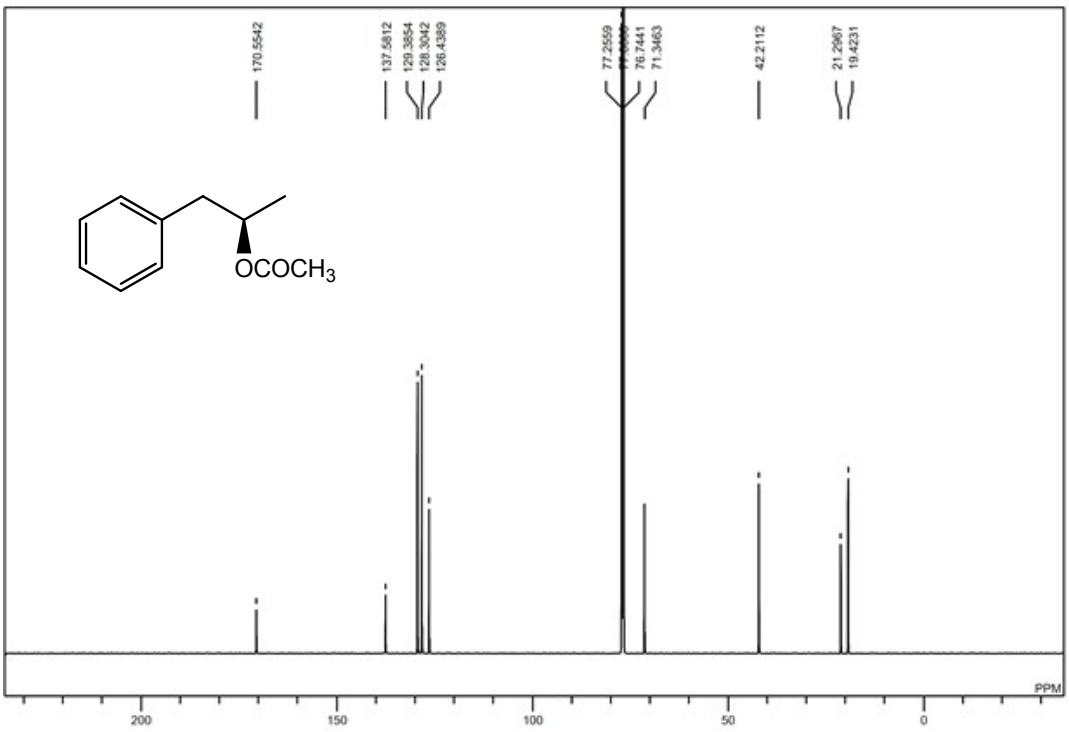

Figure S16. ^{13}C NMR spectrum of (*R*)-**2a** produced by DKR of (*rac*)-**1a**.

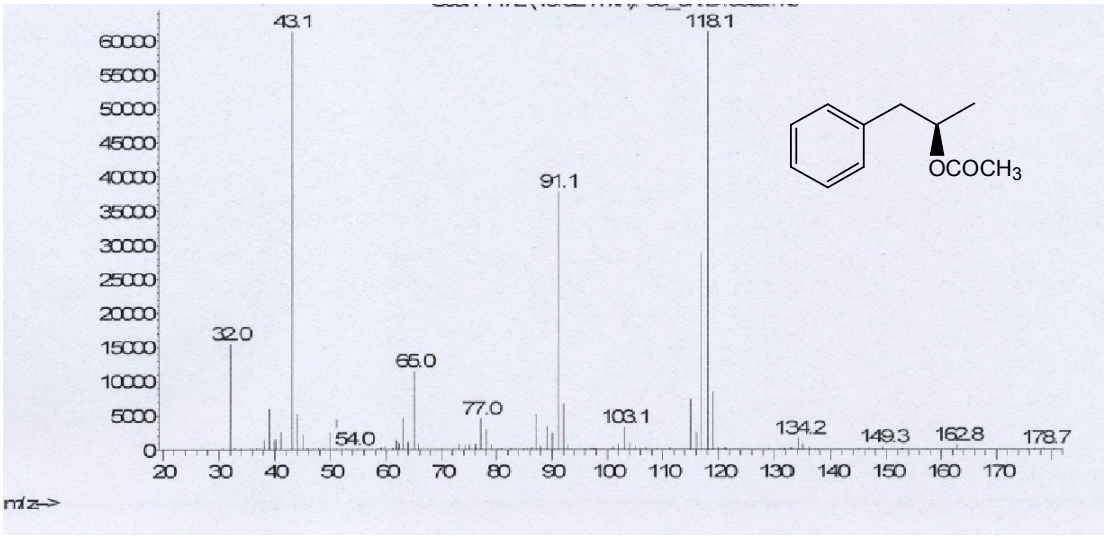

Figure S17. MS spectrum of (*R*)-**2a** produced by DKR of (*rac*)-**1a**.

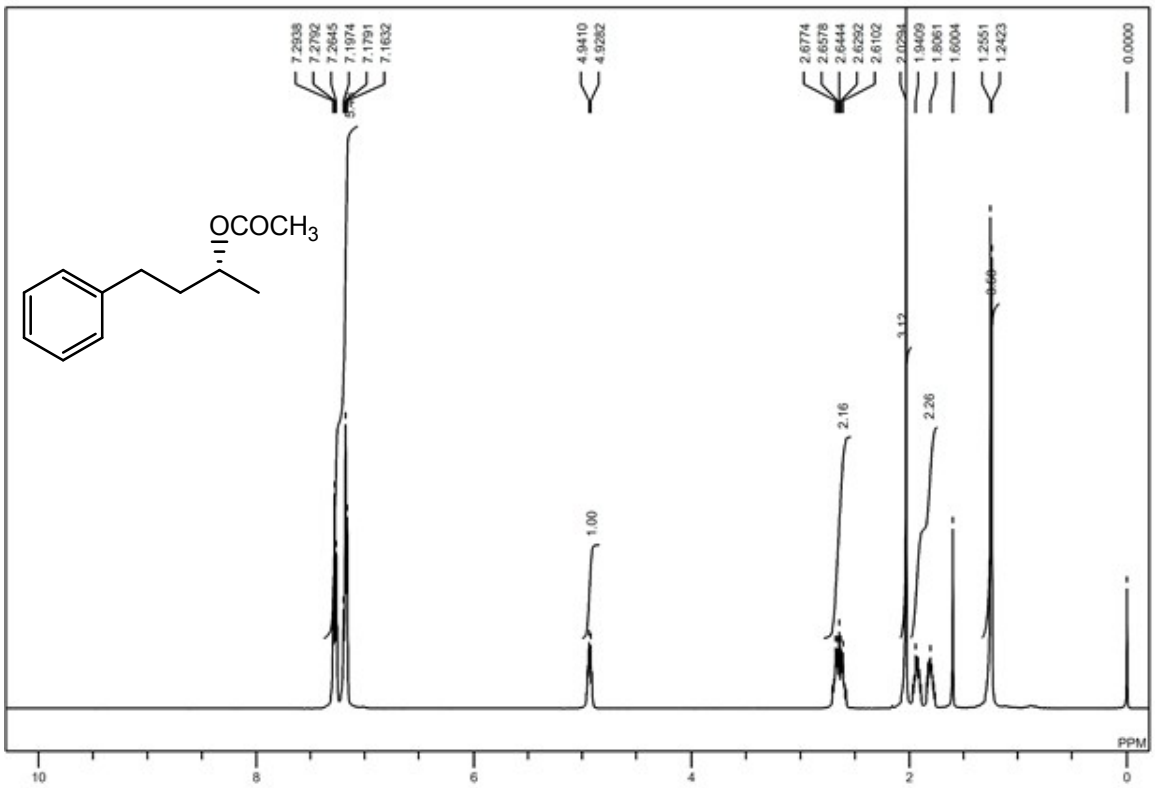

Figure S18. ^{1}H NMR spectrum of (*R*)-**2b** produced by DKR of (*rac*)-**1b**.

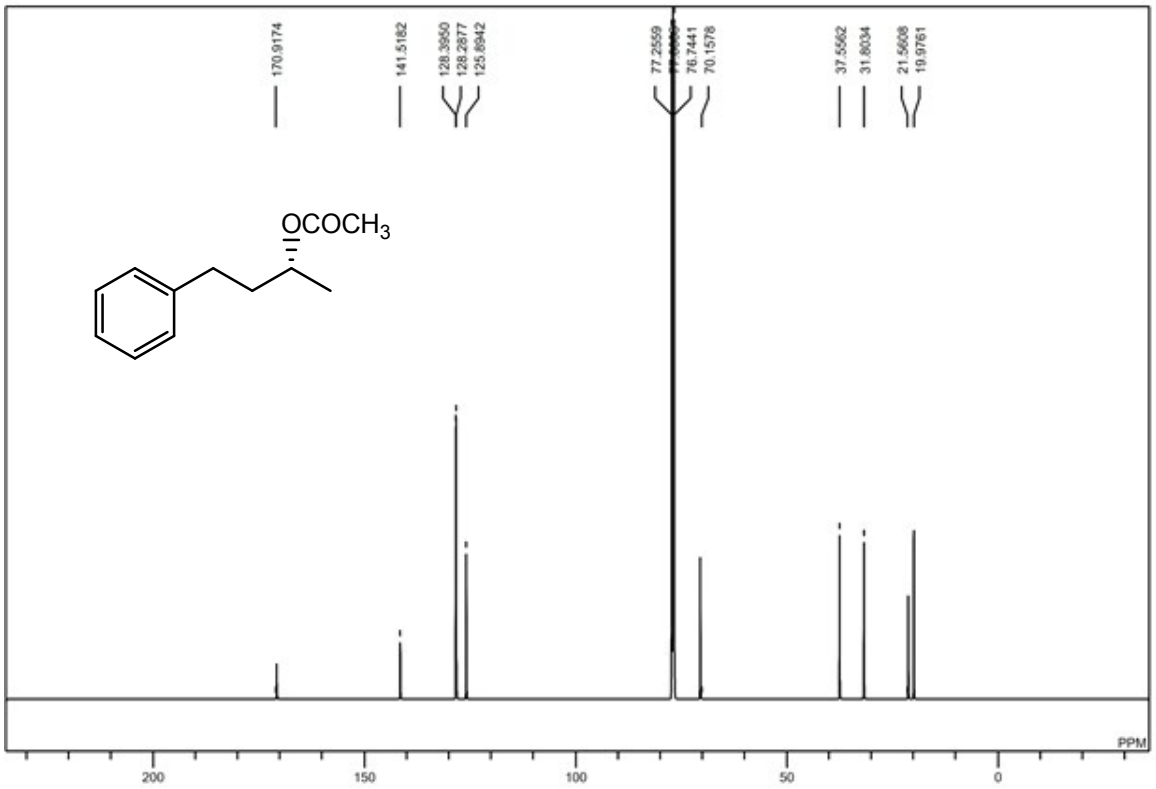

Figure S19. ^{13}C NMR spectrum of (*R*)-**2b** produced by DKR of (*rac*)-**1b**.

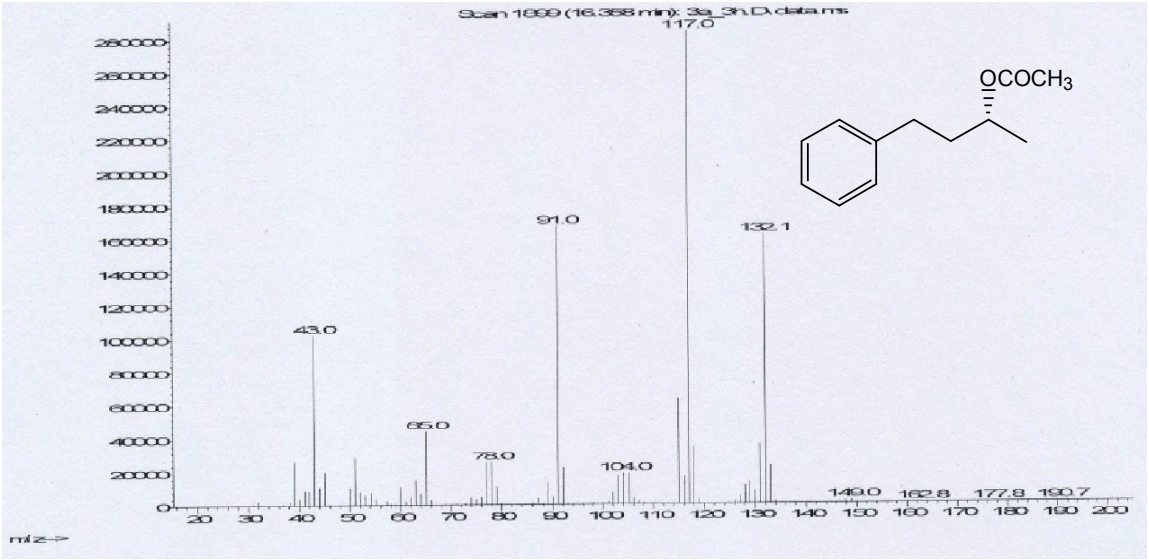

Figure S20. MS spectrum of (*R*)-**2b** produced by DKR of (*rac*)-**1b**.

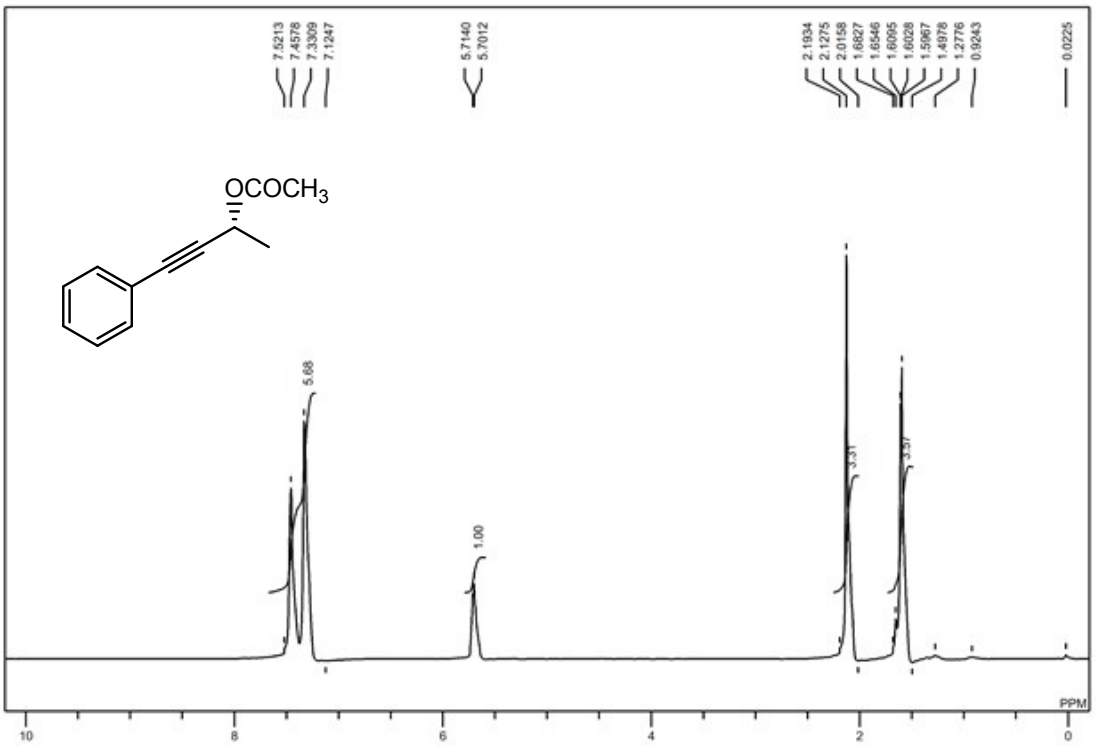

Figure S21. ^{1}H NMR spectrum of (*R*)-**2d** produce by DKR of (*rac*)-**1d**.

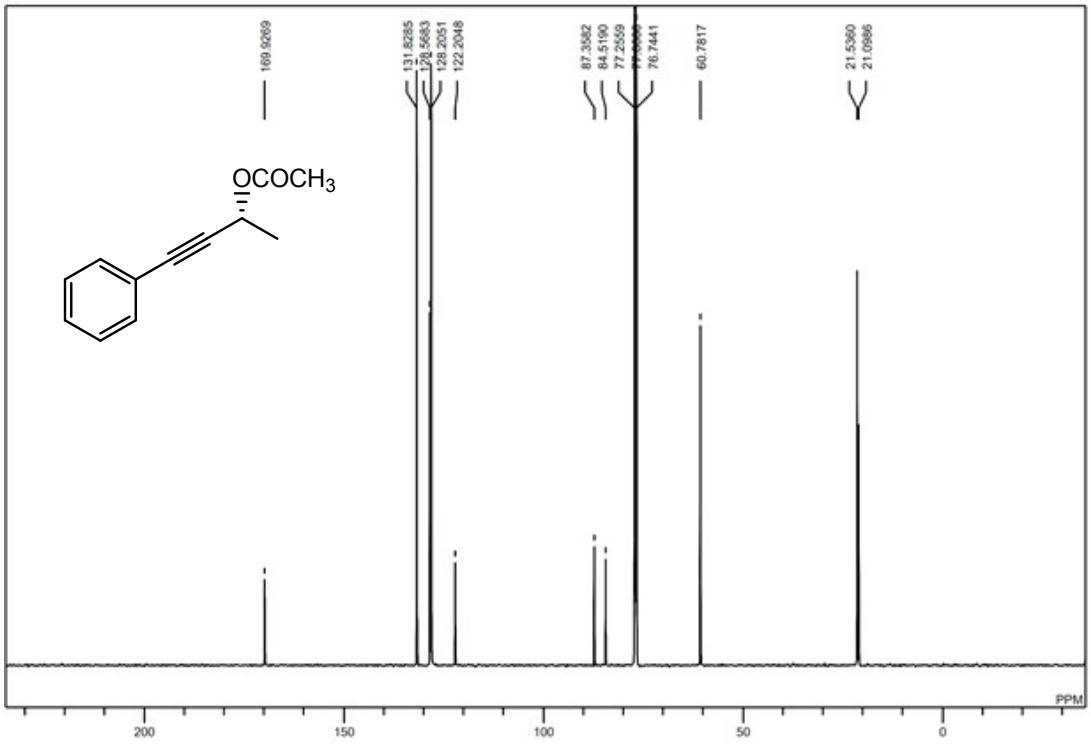

Figure S22. ^{13}C NMR spectrum of (*R*)-**2d** produce by DKR of (*rac*)-**1d**.

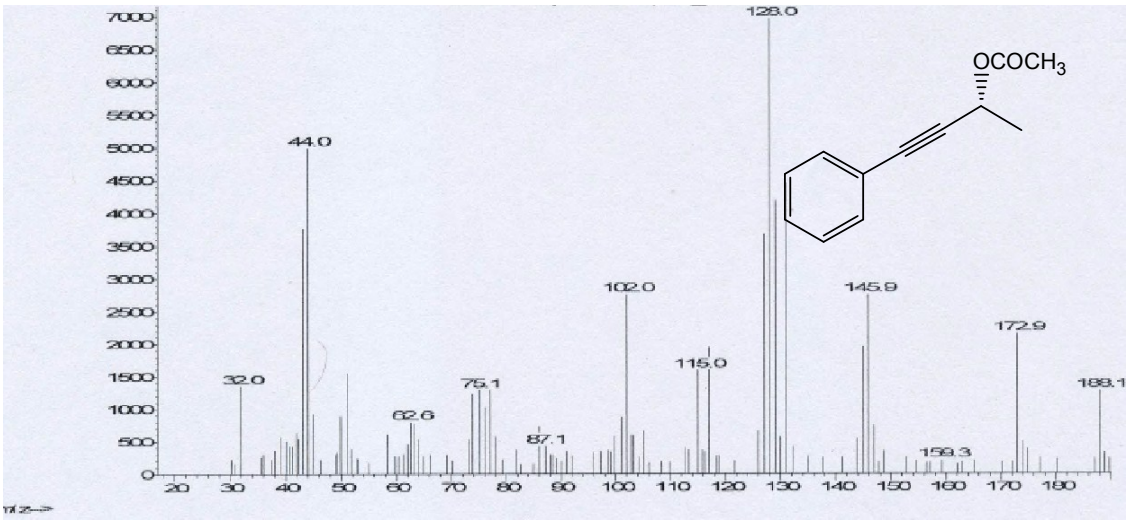

Figure S23. MS spectrum of (*R*)-**2d** produce by DKR of (*rac*)-**1d**.

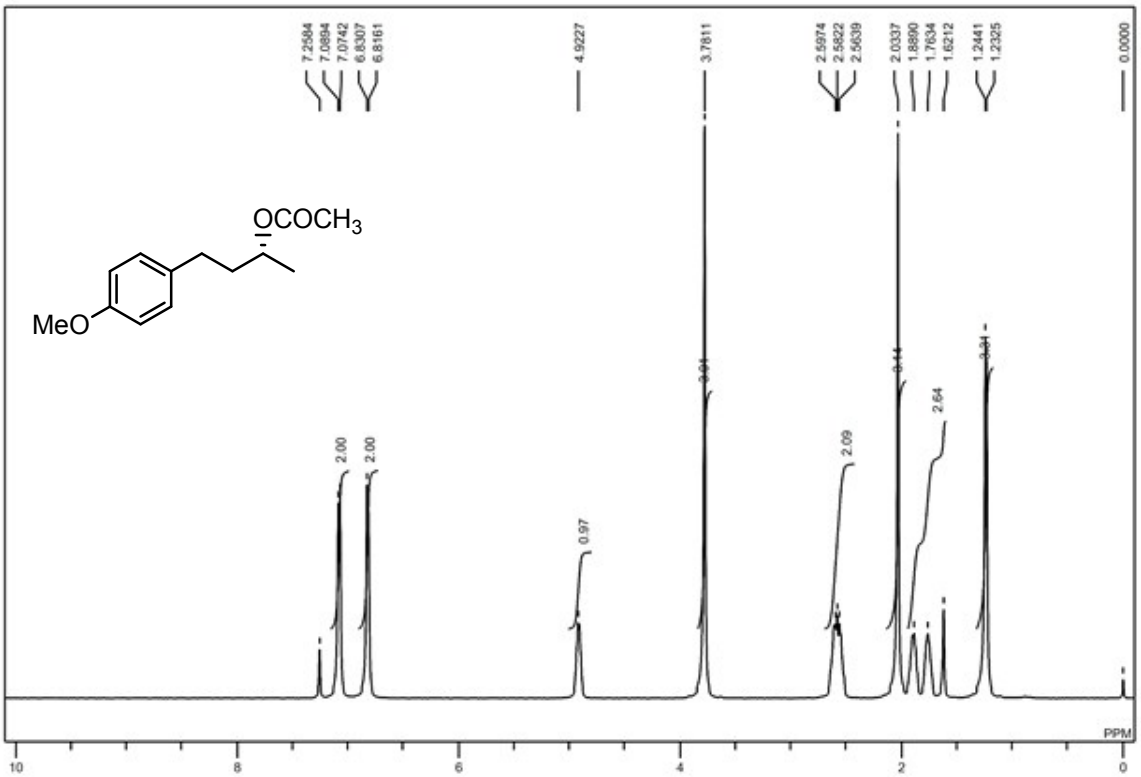

Figure S24. ^{1}H NMR spectrum of (*R*)-**2e** produced by DKR of (*rac*)-**1e**.

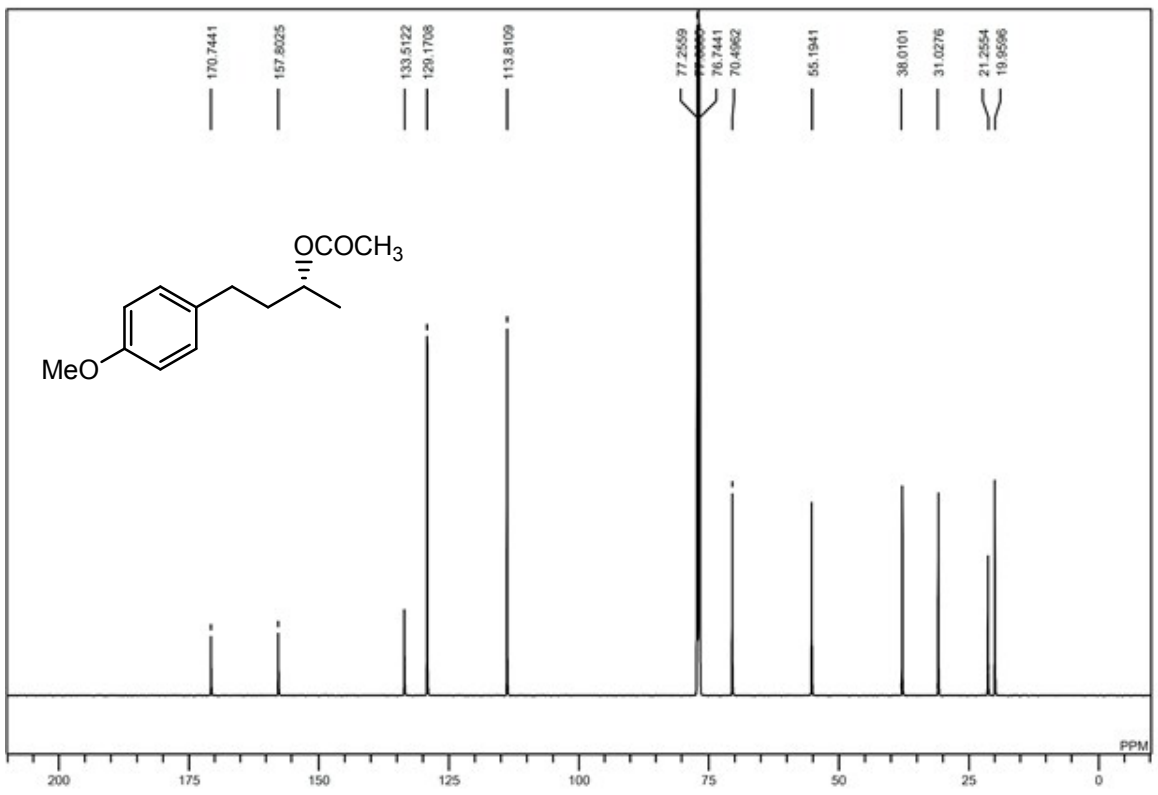

Figure S25. ^{13}C NMR spectrum of (*R*)-**2e** produced by DKR of (*rac*)-**1e**.

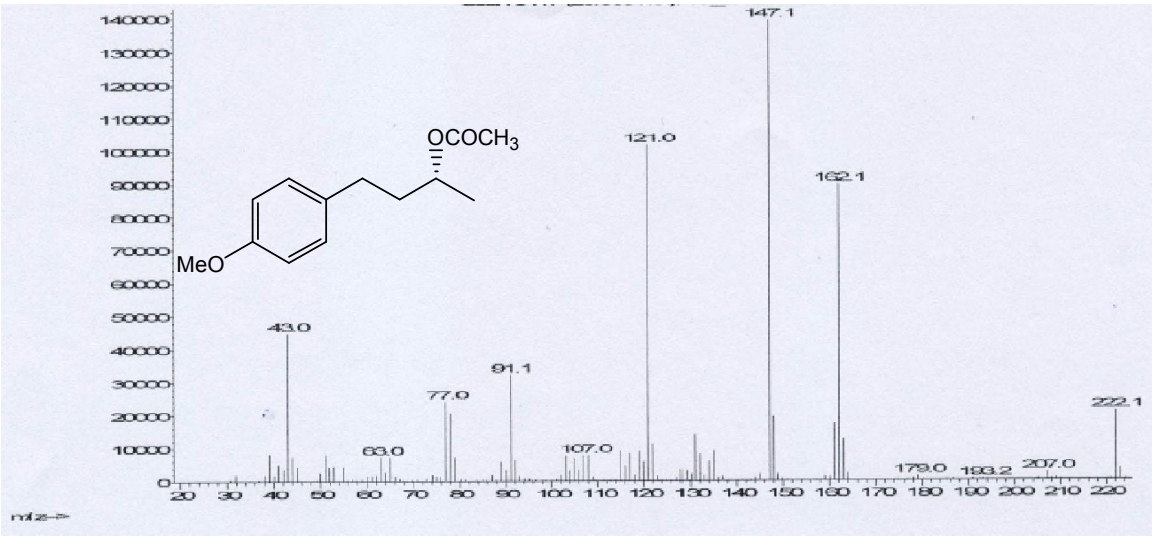

Figure S26. MS spectrum of (*R*)-**2e** produced by DKR of (*rac*)-**1e**.