Electronic Supplementary Information

Mutated variant of *Candida antarctica* lipase B in (*S*)-selective dynamic kinetic resolution of secondary alcohols

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Experimental section

Unless otherwise mentioned, all chemicals, were purchased from commercial sources. All reactions were performed in dry glassware under an argon atmosphere. ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz respectively using a Bruker Avance II spectrometer. Enantiomeric excess was determined by chiral gas chromatography using a CP-Chirasil-DEX CB column (25 m Ø * 0.32 mm).

Isopropenyl acetate was dried over $CaCl_2$, distilled and stored over molecular sieves. 1-Phenylheptanol was prepared by $NaBH_4$-reduction of the corresponding ketone. Ruthenium catalyst **4** was prepared according to a literature procedure.[1] CalB W104A was prepared as previously described, and the enzyme load on the resin was 0.26 %.[2] The enzyme load of the commercially available CalB (Novozym 435) is approximately 3 %.

Kinetic resolution of 1-phenylpropanol

1a (30 mg, 0.25 mmol) and immobilized CalB W104A (5 mg) were dissolved in toluene (0.5 mL). Once heated to the desired temperature, isopropenyl acetate (83 μL, 0.75 mmol) was added.

Kinetic resolution of 1-phenylheptanol

1a (96 mg, 0.5 mmol) and immobilized CalB W104A (20 mg) were dissolved in toluene (1 mL). Once heated to the desired temperature, isopropenyl acetate (83 μL, 0.75 mmol) was added.

General procedure for dynamic kinetic resolution of 1a and 1b

Ru-catalyst **4** (16 mg, 0.025 mmol), CalB W104A (30 mg) and Na_2CO_3 (53 mg, 0.5 mmol) were dissolved in dry toluene (0.5 mL) in a Schlenk-tube. ^{t}BuOK (0.025 mmol, 100 μL of a 0.5 M solution in dry THF) was added. After 6 minutes of stirring, alcohol **1** (0.5 mmol in 0.5 mL toluene) was added, and after additional 4 minutes isopropenyl acetate (83 μL, 0.75 mmol) was added. When the reaction was finished, the reaction mixture was filtered through a plug of silica and concentrated. Purification by flash column chromatography (Pentane/EtOAc 4:1) yielded the pure acetate **2**.

References

[1] B. Martín-Matute, M. Edin, K. Bogár, F. B. Kaynak and J.-E. Bäckvall, *J. Am. Chem. Soc.*, 2005, **127**, 8817-8825.
[2] M. Vallin, P.-O. Syrén and K. Hult, *ChemBioChem*, 2010, **11**, 411-416.