

Advanced
**Synthesis &
Catalysis**

Supporting Information

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Non-racemic halohydrins via biocatalytic hydrogen transfer-reduction of halo-ketones and one-pot cascade-reaction to enantiopure epoxide

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Supporting information

Chiral GC-Analytics

GC analysis was performed on a Varian 3800 GC (FID) using a Chrompack Chirasil-DEX CB (25 m x 0.32 mm x 0.25 µm, 1.0 bar H₂) column.

Compound	Temperature program	t _{R1} [min]	t _{R2} [min]
1-Chloro-2-octanone 1a	100°C/0min-1.0°C/min-135°C/0min-15°C/min-170°C/1min	4.9	
1-Chloro-2-octanol 1b *	112°C/0min-0.5°C/min-116°C/0min-15°C/min-170°C/1min	4.8 (R)	5.6 (S)
1,2-Epoxyoctane 1c	40°C/2min-2°C/min-50°C/10min-2°C/min-80°C/10min-30°C/min-170°C/1min	19.2 (R)	19.6 (S)
? -Chloroacetophenone 2a	112°C/0min-0.5°C/min-122°C/0min-15°C/min-170°C/1min	7.7	
2-Chloro-1-phenylethanol 2b *	112°C/0min-0.5°C/min-116°C/0min-15°C/min-170°C/1min	7.8 (R)	8.6 (S)
3-Chloro-1-phenyl-2-propanol 3b *	112°C/0min-0.5°C/min-116°C/0min-15°C/min-170°C/1min	9.8 (R)	10.0 (S)
Isopropyl 4-chloro-3-hydroxybutanoic acid ester 4b	112°C/0min-0.5°C/min-116°C/0min-15°C/min-170°C/1min	5.3 (R)	5.5 (S)
3-Chloro-1-phenoxy-2-propanol 5b *	112°C/0min-0.5°C/min-116°C/0min-15°C/min-170°C/1min	11.4 (R)	11.6 (S)
1-Chloro-1-phenyl-2-propanone 6a	112°C/0min-0.4°C/min-122°C/0min-15°C/min-170°C/1min	8.5	8.7
		11.2(1R,2R)	11.3 (1S,2S)
1-Chloro-1-phenyl-2-propanol 6b	112°C/0min-0.4°C/min-122°C/0min-15°C/min-170°C/1min	13.6 (1R,2S)	14.6 (1S,2R)

*measured as its acetyl derivative

Table S1. GC-Data, chiral.

Derivatization (acetylation): After removal of the organic solvent of the sample under reduced pressure, acetic anhydride (100 µL) and 4-dimethylaminopyridine DMAP (5 mg) were added. The mixture was shaken at room temperature for 30 min at 150 rpm in Eppendorf tubes. After addition of water (0.5 mL) and extraction with ethyl acetate (3 x 200 µL), the combined organic phase was dried (Na₂SO₄) and analyzed.

Achiral GC-Analytics

GC analysis was performed on a Varian 3800 GC (FID). The following columns were used: J&W Scientific Agilent Technologies HP-1 (30 m x 0.25 mm x 0.25 μ m, 1.0 bar N₂) and CP 1301 (30 m x 0.25 mm x 0.25 μ m, 1.0 bar N₂).

Compound	Temperature program	Column	t _R [min]
1-Chloro-2-octanone 1a	100°C/0min-5°C/min-145°C/0min-30°C/min-270°C/0min	CP1301	5.9
1-Chloro-2-octanol 1b	100°C/0min-5°C/min-145°C/0min-30°C/min-270°C/0min	CP1301	6.2
? -Chloroacetophenone 2a	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	7.7
2-Chloro-1-phenylethanol 2b	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	7.6
3-Chloro-1-phenyl-2-propanone 3a	100°C/0min-15°C/min-270°C/2min	HP-1	10.1
3-Chloro-1-phenyl-2-propanol 3b	100°C/0min-15°C/min-270°C/2min	HP-1	11.1
Isopropyl 4-chloro-acetoacetat 4a	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	7.9
Isopropyl 4-chloro-3-hydroxybutanoic acid ester 4b	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	6.4
3-Chloro-1-phenoxy-2-propanone 5a	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	9.0
3-Chloro-1-phenoxy-2-propanol 5b	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	9.2
1-Chloro-1-phenyl-2-propanone 6a	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	7.3
1-Chloro-1-phenyl-2-propanol 6b	90°C/0min-5°C/min-120°C/0min-30°C/min-270°C/2min	CP1301	7.4

Table S2. GC-Data, achiral.