

Lipase catalyzed kinetic resolution of racemic 1,2-diols containing a chiral quaternary center

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Supporting Information

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1. HPLC Analyses

For the determination of the enantiomeric excesses of compounds (*R*)-**1-6c** and (*S*)-**1-6d** (Table S1), the following columns were employed: column A: Chiralcel OD (0.46 cm x 25 cm) and column B: Chiralpak AD-H (0.46 cm x 25 cm), both from Daicel. The optical purity of the chiral 1,2-diols **1-6c** is determined after acetylation to the acetates **1-6d**.

Table S1. Determination of enantiomeric excesses of acetates **1-6d** by HPLC.

Compounds	Column	Flow rate (mL min ⁻¹)	T (°C)	Eluent ^a	Retention time [min]
1d	A	1.0	30	<i>n</i> -hexane-IPA 99:1	15.3 (<i>R</i>); 19.0 (<i>S</i>)
2d	A	1.0	30	<i>n</i> -hexane-IPA 99:1	13.9 (<i>R</i>); 17.2 (<i>S</i>)
3d	B	1.0	30	<i>n</i> -hexane-IPA 95:5	19.5 (<i>S</i>); 30.1 (<i>R</i>)
4d	B	1.0	30	<i>n</i> -hexane-IPA 95:5	14.9 (<i>S</i>); 20.0 (<i>R</i>)
5d	B	1.0	30	<i>n</i> -hexane-IPA 95:5	11.2 (<i>S</i>); 16.8 (<i>R</i>)
6d	A	1.0	30	<i>n</i> -hexane-IPA 99:1	19.0 (<i>R</i>); 21.1 (<i>S</i>)

^a All the experiments were performed with isocratic eluent.

2. NMR Signals of the known compounds

(±)-Ethyl 2,3-dihydroxy-2-phenylpropanoate, (±)-**1d**: ¹H-RMN (300 MHz, CDCl₃): δ (ppm) 7.60 (d, 2H, *J* = 8.2 Hz), 7.39-7.30 (m, 3H), 4.37-4.25 (m, 3H), 4.13 (bs, 1H, OH), 3.75 (d, 1H, *J* = 11.2 Hz), 2.56 (bs, 1H, OH), 1.31 (t, 3H, *J* = 7.1 Hz). ¹³C-RMN (75.4 MHz, CDCl₃): δ (ppm) 173.6 (C=O), 138.1 (C_{Ar}), 128.3 (2CH_{Ar}), 128.2 (2CH_{Ar}), 125.3 (CH_{Ar}), 79.4 (C), 68.2 (CH₂), 62.8 (CH₂), 13.9 (CH₃).

(±)-Ethyl 2,3-dihydroxy-2-(4-methoxyphenyl)propanoate, (±)-**4d**: ¹H-RMN (300 MHz, CDCl₃): δ (ppm) 7.50 (d, 2H, *J* = 8.5 Hz), 6.89 (d, 2H, *J* = 8.5 Hz), 4.34-4.25 (m, 2H), 4.21 (d, 1H, *J* = 11.2 Hz), 4.10 (bs, 1H, OH), 3.80 (s, 3H), 3.72 (d, 1H, *J* = 11.2 Hz), 2.57 (bs, 1H, OH), 1.30 (t, 3H, *J* = 7.0 Hz). ¹³C-RMN (75.4 MHz, CDCl₃): δ (ppm) 173.8 (C=O), 159.4 (C_{Ar}), 130.2 (C_{Ar}), 126.4 (2CH_{Ar}), 113.7 (2CH_{Ar}), 79.1 (C), 68.2 (CH₂), 62.7 (CH₂), 55.2 (CH₃), 14.0 (CH₃).

(±)-Ethyl 2,3-dihydroxy-2-(thiophen-1-yl)propanoate, (±)-**5c**: ¹H-RMN (300 MHz, CDCl₃): δ (ppm) 7.25 (dd, 1H, *J* = 5.4, 1.7 Hz), 7.10 (dd, 1H, *J* = 3.4, 1.7 Hz), 6.98 (dd, 1H, *J* = 5.4, 3.4 Hz), 4.37-4.26 (m, 3H), 4.13 (d, 1H, *J* = 11.5 Hz), 3.80 (d, 1H, *J* = 11.5 Hz), 2.34 (bs, 1H, OH), 1.33 (t, 3H, *J* = 7.0 Hz). ¹³C-RMN (125 MHz, CDCl₃): δ (ppm) 172.7 (C=O), 142.2 (C_{Ar}), 127.1 (CH_{Ar}), 125.4 (CH_{Ar}), 124.4 (CH_{Ar}), 78.3 (C), 69.0 (CH₂), 63.2 (CH₂), 13.9 (CH₃).