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A convenient chemoenzymatic synthesis of chiral 1-benzyl-5-(hydroxymethyl)-2-piperidone enabled by lipase AK desymmetrization of prochiral 1,3-diol and its diacetate

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Supporting Information

Contents

¹H and ¹³C NMR of the synthesized compounds:

Dimethyl 2-(3-(benzylamino)-3-oxopropyl)malonate 10	2
<i>N</i> -Benzyl-5-hydroxy-4-(hydroxymethyl)pentanamide 4	3
<i>N</i> -Benzyl-5-acetoxy-4-(acetoxymethyl)pentanamide 5	4
5-(benzylamino)-2-(hydroxymethyl)-5-oxopentyl acetate 3	5
(<i>R</i>)-1-benzyl-4-(hydroxymethyl)piperidin-2-one 1	6
HPLC diagrams of <i>racemic</i> -, (<i>R</i>)- and (<i>S</i>)- of monoacetate 3	7

Dimethyl 2-(3-(benzylamino)-3-oxopropyl)malonate **10**

diester N-benzyl amide substrate

diester N-benzyl amide

N-Benzyl-5-hydroxy-4-(hydroxymethyl)pentanamide **4**

N-Benzyl-5-acetoxy-4-(acetoxymethyl)pentanamide **5**

5-(benzylamino)-2-(hydroxymethyl)-5-oxopentyl acetate **3**

diolBn monoacetate

diolBn monoacetate ¹³C

(*R*)-1-benzyl-4-(hydroxymethyl)piperidin-2-one **1**

HPLC diagrams of *racemic*-, (*R*)- and (*S*)- of monoacetate **3**

racemic-**3**

(*R*)-**3**: $ee = 96.7\% - 3.3\% \approx 93\%$

(*S*)-**3** $ee = 96.4\% - 3.6\% \approx 93\%$