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Supporting Information

Lipase Catalyzed Kinetic Resolution of *rac*-2-(3-Methoxy-4-methylphenyl) propan-1-ol and *rac*-2-(3-Hydroxy-4-methylphenyl)propyl propanoate for *S*-(+)-Xanthorrhizol

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Table 1. Conversions, enantiomeric excess and enantioselectivity of enzyme catalyzed hydrolysis reactions of *rac*-substrate V[a]

Enzyme	Time (h)	*c* (%)[c]	ee_s (%)[b]	ee_p (%)[b]	*E*[c]
Cal B	4	4	3	64	6
PLE	6	29	5	13	1
CRL	4	47	16	18	2
LAN	13	40	20	31	2
Acylase	13	64	23	13	2
LAK	5	49	17	18	2
PCL	4	75	25	8	1
LAH	3	69	29	13	2
AOL	19	53	99	87	80
PPL	19	67	99	50	14

[a]Reaction condition: 10 mg *rac*-substrate V, enzyme 30 mg, a mixture of acetone: phosphate buffer (pH 7.0) = 1:4 was shaken at 30 °C and 250 rpm. Here *c*: conversion, *E*: enantioselectivity, ee_s: enantiomeric excess of starting material, ee_p: enantiomeric excess of product. [b]Determined by HPLC using (R,R)-Whelk-01, 250 × 4.6 mm, 5 µm column, mobile phase: hexanes: ethanol: diethyl amine = 97:03:0.05 % v/v with flow rate 0.4 mL/min at RT. [c]Determined from the equation described in 2.7.

Table 2. Conversion, enantiomeric excess and enantioselectivity for enzyme catalyzed transesterification[a] and hydrolysis[b] reaction

Enzyme	Time (h)	Wt. (Substrate)	*c* (%)[e]	ee_s (%)	ee_p (%)	*E*[e]
AOL	34	10 g (II)[a]	58	98[c]	72[c]	27 ± 1
AOL	23	1 g (V)[b]	53	99[d]	88[d]	80 ± 3
Bi-phase reaction (hexanes : phosphate buffer pH 7.0 = 2:4)						
AOL	48	0.1 g (V)[b]	58	99[d]	72[d]	31 ± 3

[a]Reaction condition: *rac*-substrate II, vinyl propanoate (2.5 eq.), AOL Enzyme (3 mass equivalent), *tert*-BuOMe was shaken at 25 °C and 250 rpm. [b]Reaction condition: *rac*-substrate V, AOL Enzyme (3 mass eq.), a mixture of acetone: phosphate buffer (pH 7.0) = 1:4 was shaken at 30 °C and 250 rpm. Here *c*: conversion, *E*: enantioselectivity, ee_s: enantiomeric excess of starting material, ee_p: enantiomeric excess of product. [c]Determined by HPLC using Chiralpak AS-H, 250 × 4.6 mm, 5 µm column, mobile phase:hexanes:IPA = 95:05% v/v with flow rate 0.4 mL/min at RT. [d]Determined by HPLC using (*R*,*R*)-Whelk-01, 250 × 4.6 mm, 5 µm column, mobile Phase:hexanes:ethanol:diethyl amine = 97:03:0.05% v/v with flow rate 0.4 mL/min at rt. Values of *c*, ee_s and ee_p are the average of four determinations. [e]Determined from the equation described in 2.7 with average of *c* and ee_s.

Table 3. Solubility of the methyl protected and deprotected alcohol and propanoate ester

rac-compound	Solubility (g/L)[a]	Type
II	2.5	Slightly soluble
III	7.1	Slightly soluble
IV	0.052	Partially soluble
V	0.089	Partially soluble

[a]Solubility was measured with Nephelostar instrument from BMG Lab Tech. Values are the average of three determinations.