Supporting Information

Kinetic resolution of secondary alcohols with *Burkholderia cepacia* lipase immobilized on biodegradable ternary blend polymer matrix; as a highly efficient and heterogeneous recyclable biocatalyst

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General Methods: All chemicals and solvents were purchased from M/S Sigma Aldrich, S. D. Fine Chemicals, and commercial suppliers. Burkholderia cepacia activity $\geq 30,000$ U/g, white colour powder purchased from Sigma Aldrich, India All solvents were distilled before use. The progress of the reaction was monitored by thin layer chromatography using Merck silica gel 60 F254 plates. Products were purified by column chromatography on silica gel (60–120 mesh). The ¹H and ¹³C NMR spectroscopic data were analysed with a Varian Inova 400 MHz spectrometer in either CDCl₃. Chemical shifts are reported in parts per million (δ) relative to tetramethylsilane as the internal standard. The coupling constants (J) are reported in Hz, and the splitting patterns of the proton signals are described as s (singlet), d (doublet), t (triplet), and m (multiplet). Mass is confirmed by GC-MS analysis by Shimadzu QP 2010 instrument (Rtx-17, 30 m × 25mmID, film thickness 0.25 µm df) column flow- 2 mL/min, 80 °C to 240 °C at 10°/min rise.. The IR spectra were recorded with an FTIR (Perkin-Elmer). Optical rotations were measured by using a Rudolph IV automatic Polarimeter. The enantiomeric excess values (ee) of the products were determined by HPLC analysis with an Agilent- HPLC on Daicel Chiralcel-OJ-H and Chiralcel OD-H chiral columns using propan-2-ol/hexane as the eluent.

General procedure for the kinetic resolution of secondary alcohols



In general procedure, a dry 10 ml glass stoppered tube was charged with 0.5 mmol (1 eq.) of secondary alcohol and 3 mL MTBE. After gentle stirring, 2 mmol (4 eq.) of vinyl acetate was added and to this 20 mg immobilized enzyme was added to initiate the reaction. The reaction mixture was placed at 40 °C in orbital shaker at 150 rpm speed given time span. Reaction progress was monitored by TLC, after completion of reaction the reaction mixture was filtered and biocatalyst was thoroughly washed 2-3 times with MTBE to remove any traces of reactant or product sticked to biocatalyst. The solvent was then evaporated under vacuum at very low pressure. The product residue obtained was then subjected for column chromatography (silica gel, mesh size 60–120) using pet ether: ethyl acetate (99:1) as eluent to afford pure products. The enantiomeric excess values (ee) of the product were determined by HPLC analysis with an Agilent- HPLC on Chiralcel OD-H chiral columns using propan-2-ol/hexane as the eluent.

(R)-1-Phenethyl acetate (2a); (Figure 2)



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OD-H column, *n*-hexane/ i-PrOH = 95/5, flow rate = 0.4 mL/min, 254nm; t_R = 15.6 min (one enantiomer); 99% ee. $[\alpha]_D^{22}$ 108.2 (Conc. 0.11 in CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.40-7.28 (m, 5H), 5.91 (q, *J*=8 Hz, 1H), 2.10(s, 3H), 1.55 (d, *J*= 8Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 170.31, 141.66, 128.46, 127.84, 126.07, 72.29, 22.17, 21, 32 ; Mass: GC-MS (EI, 70 eV): *m/z*: 164 [M]⁺, 164, 149, 122 (100), 104, 91,77,63,43.



Totals :

913.29526 47.72153



Racemic 1-phenylethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n hexane/IPA), flow rate: 0.4ml/ min, 254nm



Peak	RetTime Type	Width	Area	Height	Area
#	[min]	[min]	[mAU*s]	[mAU]	00
			-		
1	22.443 BB	0.3676	478.12885	19.96699	50.0622
2	26.566 BB	0.4377	476.94077	16.91815	49.9378
Total	.s :		955.06961	36.88515	

(*S*)-1-phenylethanol (1a); (Figure 2): The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.4ml/ min, 254nm.







(R)-1-(p-tolyl) ethyl acetate (2b); Figure 2



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, *n*-hexane/ i-PrOH = 99/1, flow rate = 0.5 mL/min, 254 nm; t_R = 16.2 min (major), t_R =30.8 min (minor), 99% ee; ¹H NMR (400 MHz, CDCl₃): 7.28-7.26 (d, *J*= 8Hz, 2H), 7.19-7.17 (d, *J*=8Hz, 2H), 5.88 (q, *J*= 8Hz, 1H), 2.36 (s, 3H), 2.08 (s, 3H), 1.55 (d, *J*=8Hz, 3H), Mass: GC-MS (EI, 70 eV): m/z: 178 [M]⁺, 178, 163,136,117(100), 103,91,77,65,43,41,40.









Racemic 1-(p-tolyl) ethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/ min, 220nm.

(S)-1-(p-tolyl) ethanol (1b); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (*n*-hexane/IPA), flow rate: 0.3 ml/ min, 220nm.





(*R*)-1-(4-methoxyphenyl) ethyl acetate (2c); (Figure 2):



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OD-H column, *n*-hexane/ i-PrOH = 95/5, flow rate = 0.3 mL/min, 254 nm; t_R = 18.4 min (major), t_R =19.3 min (minor). 97% ee; ¹H NMR (400 MHz, CDCl₃): δ 7.31-7.26 (m, 2H), 6.89-6.87 (m, 2H), 5.85(q, *J*=8Hz, 1H), 3.80 (s, 3H), 2.05 (s, 3H), 1.52 (d, *J*=8Hz, 3H); ¹³C NMR (100 MHz, CDCl₃):170.38, 159.24, 133.71, 127.56, 113.80, 71.98, 55.22, 21.90, 21.35; Mass: GC-MS (EI, 70 eV): *m/z*: 196 [M]⁺, 196, 179,152, 134 (100), 119, 105, 91,77,65,43,40.

Signal 1: VWD1 A, Wavelength=220 nm



Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type Width Height Area Area [mAU*s] [mAU] # [min] [min] 응 ----|-----|-----|-----| 1 18.478 BV 0.3248 3718.82056 175.78616 98.2910 19.350 VB 0.3121 64.66109 3.04898 1.7090 2 Totals : 3783.48164 178.83514





(*S*)-1-(4-methoxyphenyl) ethanol (1c); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/ min, 254nm.





(*R*)-1-(4-fluorophenyl) ethyl acetate (2d); (Figure 2):



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, *n*-hexane/ i-PrOH = 99/1, flow rate = 0.3 mL/min, 254nm; $t_R = 27.4$ min (major), $t_R = 32.0$ min (minor),

99% ee; ¹H NMR (400 MHz, CDCl₃): δ 7.34-7.26 (m, 2 H), 7.05-7.01(m, 2H), 5.85(q, *J*=8Hz, 1H), 2.06(s, 3H), 1.52 (d, *J*=8Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): 170.13, 163.52,161.08, 137.49, 137.45, 127.85, 115.43, 115.21, 71.62, 22.15, 21.28; Mass: GC-MS (EI, 70 eV): *m/z*: 182 [M]⁺, 167, 140,139, 122 (100), 103, 96,77,57,43, 41.







(*S*)-1-(4-fluorophenyl) ethanol (1d); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 98:2 (n-hexane/IPA), flow rate: 0.4ml/ min, 254nm.





(R)-1-(4-chlorophenyl) ethyl acetate (2e); Figure 2:



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, *n*-hexane/ i-

PrOH = 99/1, flow rate = 0.5 mL/min, 254 nm; t_R = 14.8 min (major). t_R =19.6 min (minor), 98 % ee; ¹H NMR (400 MHz, CDCl₃): δ 7.35-7.28 (m, 4H), 5.86(q, *J*= 8Hz, 1H), 2.09 (s, 3H), 1.54 (d, *J*= 8Hz, 3H); Mass: GC-MS (EI, 70 eV): *m/z*: 198 [M]⁺, 198, 183, 156, 140, 138, 121,103,91,77,63,43,41.



Retention Time	Area	Area %	Height	Height %
14.890	1302645	98.75	36133	98.78
19.662	16438	1.25	446	1.22
Totals				
	1319083	100.00	36579	100.00

Racemic 1-(4-chlorophenyl) ethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.4 ml/ min, 254nm



Signal 1: VWD1 A, Wavelength=254 nm

Peak	RetTime T	ype Width	Area	Height	Area
#	[min]	[min]	[mAU*s]	[mAU]	90
	-				I
1	20.491 B	B 0.3302	1121.06641	52.46633	49.4116
2	22.401 B	B 0.3709	1147.76526	47.62717	50.5884
Total	ls :		2268.83167	100.09350	

(*S*)-1-(4-chlorophenyl) ethanol (1e): Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.4 ml/ min, 254nm.





(R)-1-(4-bromophenyl) ethyl acetate (2f); Figure 2



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, *n*-hexane/ I PrOH = 99/1, flow rate = 0.5 mL/min, 254 nm; t_R = 16.0 min (major), 99% ee; ¹H NMR (400 MHz, CDCl₃): δ 7.51-7.48 (q, *J*=8Hz, 1H), 7.28-7.24(m, 2H), 5.84(q, *J*= 8 Hz, 1H), 1.53 (d, *J*=8Hz, 3H), ¹³C NMR (100 MHz, CDCl₃): δ 170.17, 140.71, 131.60, 1227.82, 121.72, 71.60, 22.80, 21.25; Mass: GC-MS (EI, 70 eV): *m/z*: 242 [M]⁺, 242, 227, 200, 182, 157, 121, 104, 91,77,63,43(100), 41.





Racemic 1-(4-bromophenyl) ethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.4 ml/ min, 254nm



(*S*)-1-(4-bromophenyl) ethanol (1f); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.4 ml/ min, 254nm





(R)-1-(naphthalen-2-yl) ethyl acetate (2g); Figure 2



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OD-H column, *n*-hexane/ i-PrOH = 95/5, flow rate = 0.4 mL/min, 254 nm; t_R = 11.1 min (major), t_R =12.7 min (minor), 98% ee; ¹H NMR (400 MHz, CDCl₃): δ 7.85-7.80 (m, 4H), 7.50-7.48 (m, 3H), 6.05 (q, *J*= 8Hz, 1H), 2.11(s, 3H), 1.63 (d, *J*=8Hz, 3H); ¹³C NMR (100 MHz, CDCl₃):170.3,139,133.1, 133.0, 128.3, 128.0, 127.6, 126.2, 126.0, 125.0, 124.0, 77.2, 77.0, 76.7, 72.4, 22.1, 21.3; Mass: GC-MS (EI, 70 eV): m/z: 214 [M]⁺,

214,199,1172(100),158,154,129,115,101,89,76,63,43,





Racemic 1-(naphthalen-2-yl) ethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 98:2 (n-hexane/IPA), flow rate: 0.9 ml/ min, 254nm



Retention Time	Area	Area %	Height	Height %
39.433	2364116	50.06	53179	51.09
42.653	2358057	49.94	50912	48.91
Totals				
	4722173	100.00	104091	100.00

(S)-1-(naphthalen-2-yl) ethanol (1g); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 98:2(n-hexane/IPA), flow rate: 0.9ml/min, 254nm





(R)-1-(pyridin-4-yl) ethyl acetate (2h); Figure 2

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The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 80:20); The ee was determined by HPLC using a Daicel Chiralcel OD-H column, *n*-hexane/ i-PrOH = 99/1, flow rate = 0.7 mL/min, 254 nm; t_R = 38.7 min (major), t_R = 48.2 min(minor), 96% ee; Mass: GC-MS (EI, 70 eV): m/z: 165 [M]⁺, 165, 150, 123 (100), 106,94,78,65,43,40.



Totals	:

1.46004e4 194.94020



Racemic 1-(pyridin-4-yl) ethanol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.5 ml/ min, 254nm



Signal 1: VWD1 A, Wavelength=220 nm					
Peak RetTime Type	Width [min]	Area	Height	Area	
# [min]		[mAU*s]	[mAU]	%	
1 46.830 BB	0.9962	2392.83081	35.39092	50.0741	
2 53.065 BB		2385.74536	31.72638	49.9259	
Totals :		4778.57617	67.11730		

(S)-1-(pyridin-4-yl) ethanol (1h); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.5 ml/ min, 254nm



(R)-1, 2, 3, 4-tetrahydronaphthalen-1-yl acetate (2i); Figure 2



The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, n-hexane/ i-PrOH = 99/1, flow rate = 0.5 mL/min, 254 nm; $t_R = 12.7$ min (minor), $t_R = 16.4$ min (major), 89% ee; ¹H NMR (400 MHz, CDCl₃): δ 7.31-7.16 (m, 4H), 6.03(t, *J*=8 Hz, 1H), 2.92-2.80(m, 2H), 2.13 (s, 3H), 2.11-1.86 (m, 4H), 13C NMR (100 MHz, CDCl₃):170.78, 137.92, 134.55, 129.41, 129.06, 128.07, 126.06, 69.99, 29.07, 28.95, 21.47, 18.79; Mass: GC-MS (EI, 70 eV): *m/z*: 190 [M]⁺, 165, 148, 130 (100), 115,105, 91,77,65,43,40.





Racemic 1,2,3,4-tetrahydronaphthalen-1-ol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/ min, 254nm



(*S*)-1,2,3,4-tetrahydronaphthalen-1-ol (1i); Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/ min, 254nm.









The title compound was purified by silica gel chromatography (petroleum ether/ethyl acetate, 90:10); The ee was determined by HPLC using a Daicel Chiralcel OJ-H column, *n*-hexane/ i-PrOH = 99/1, flow rate = 0.5 mL/min, 254 nm; t_R = 13.3 min (minor), t_R =18.7 min (major), 91% ee; Mass: GC-MS (EI, 70 eV): m/z: 176 [M]⁺, 176, 154,133, 116 (100), 105, 91,77,65,43.





Racemic 2,3-dihydro-1H-inden-1-ol: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/ min, 254nm



(*S*)-2,3-dihydro-1H-inden-1-ol (1j);Figure 2: The ee was determined by HPLC using a Daicel Chiralcel OD-H column; 95:5 (n-hexane/IPA), flow rate: 0.3 ml/min, 254nm

