

Supplementary Information



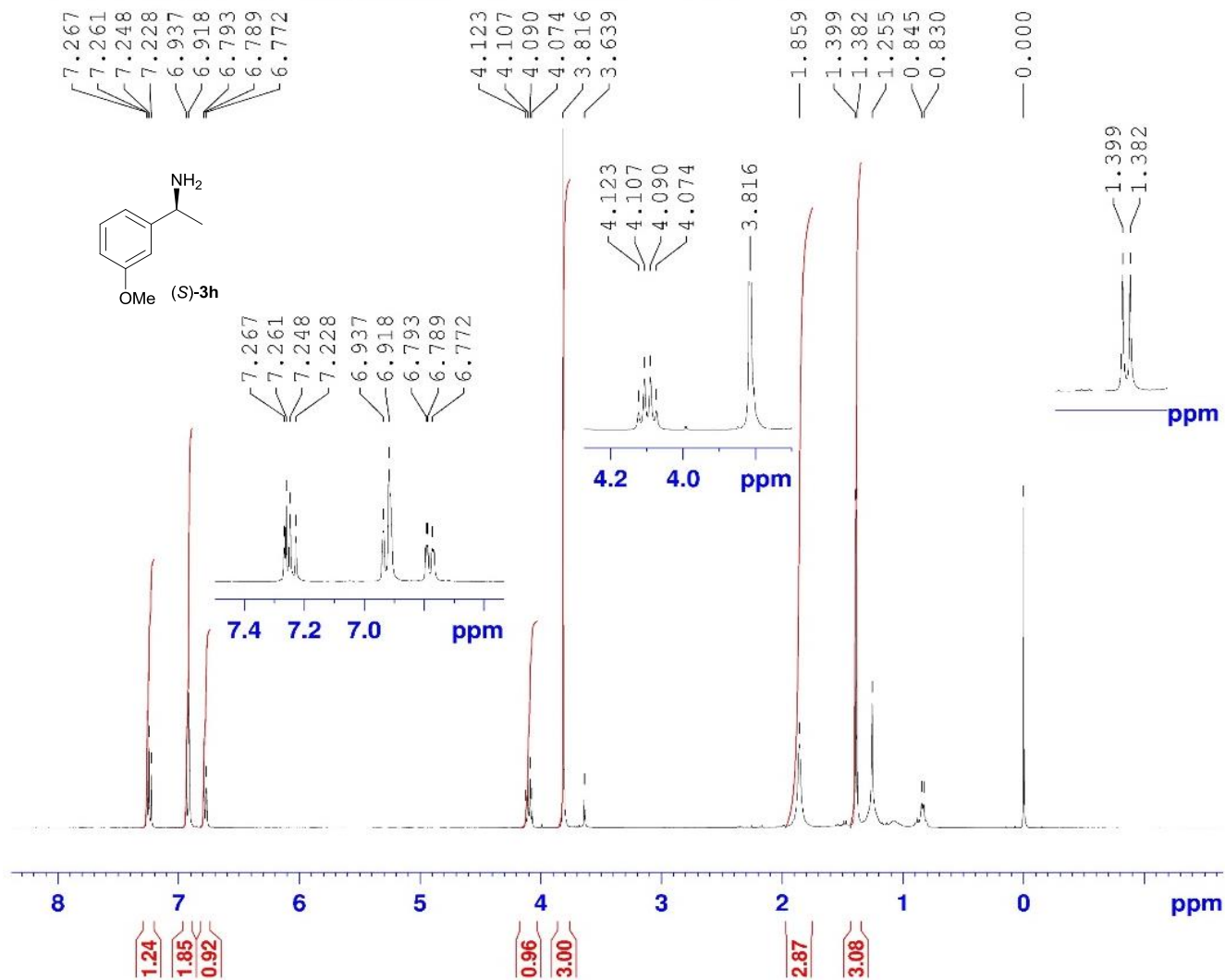
Deracemization of sec-Alcohols through Sequential Application of *C. albicans* and Ketoreductases

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1-(3-methoxyphenyl)ethanamine (3h) - CDCl₃ - Avance 400 MHz



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 PROCNO 1

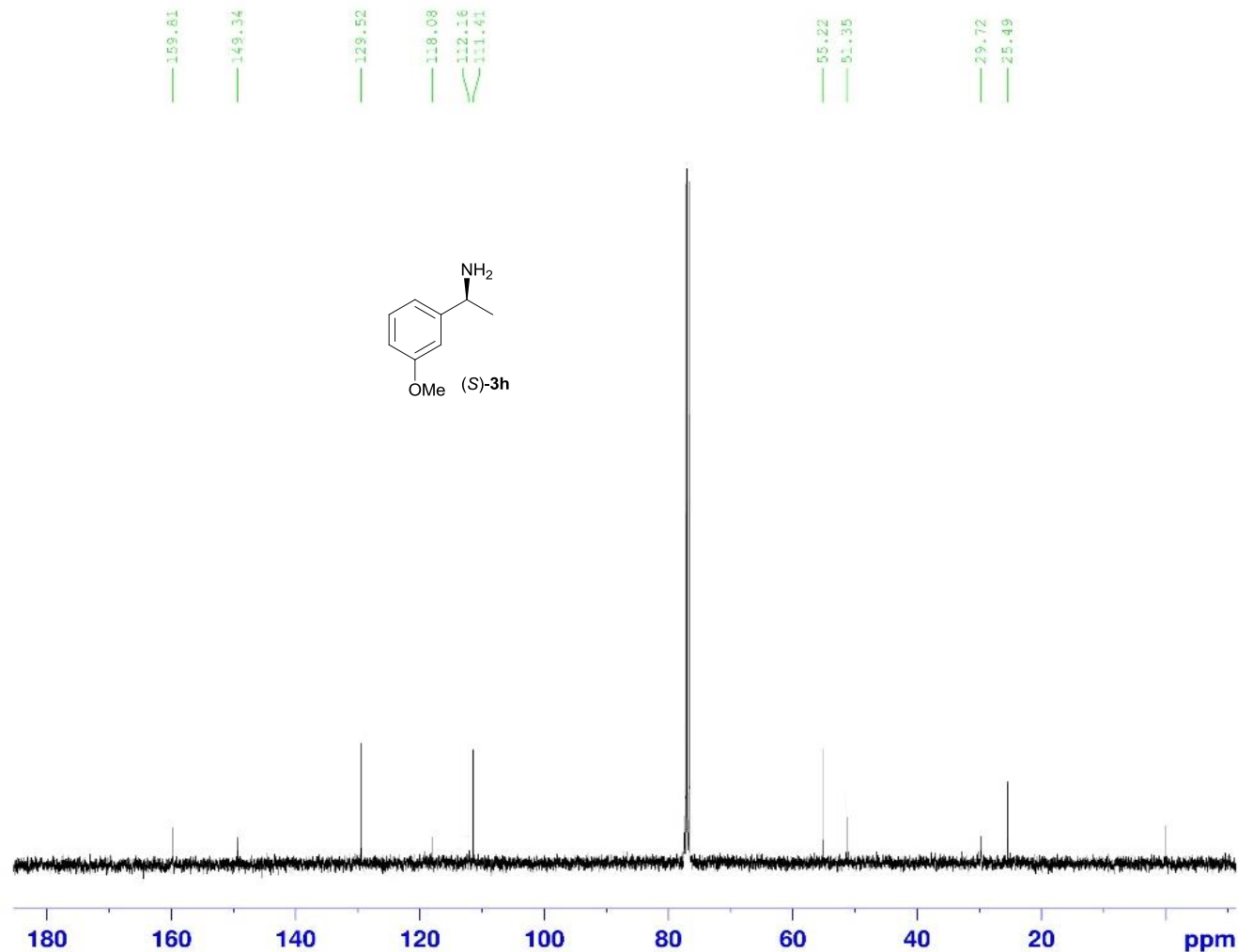
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 RG 161
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 DE 7.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

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 P1 8.50 usec
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F2 - Processing parameters
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 25.00

Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of (S)-3h (CAS number 82796-69-8).

1(3-methoxyphenyl)ethanamine (3h) - CDCl₃ - Avance 400 MHz - 13C



Current Data Parameters
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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FIDRES 0.733596 Hz
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D11 0.0300000 sec
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NUC2 1H
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PLW13 0.07691100 W

F2 - Processing parameters
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PC 1.40

Figure S2. ¹³C NMR (100 MHz, CDCl₃) spectrum of (S)-3h (CAS number 82796-69-8).

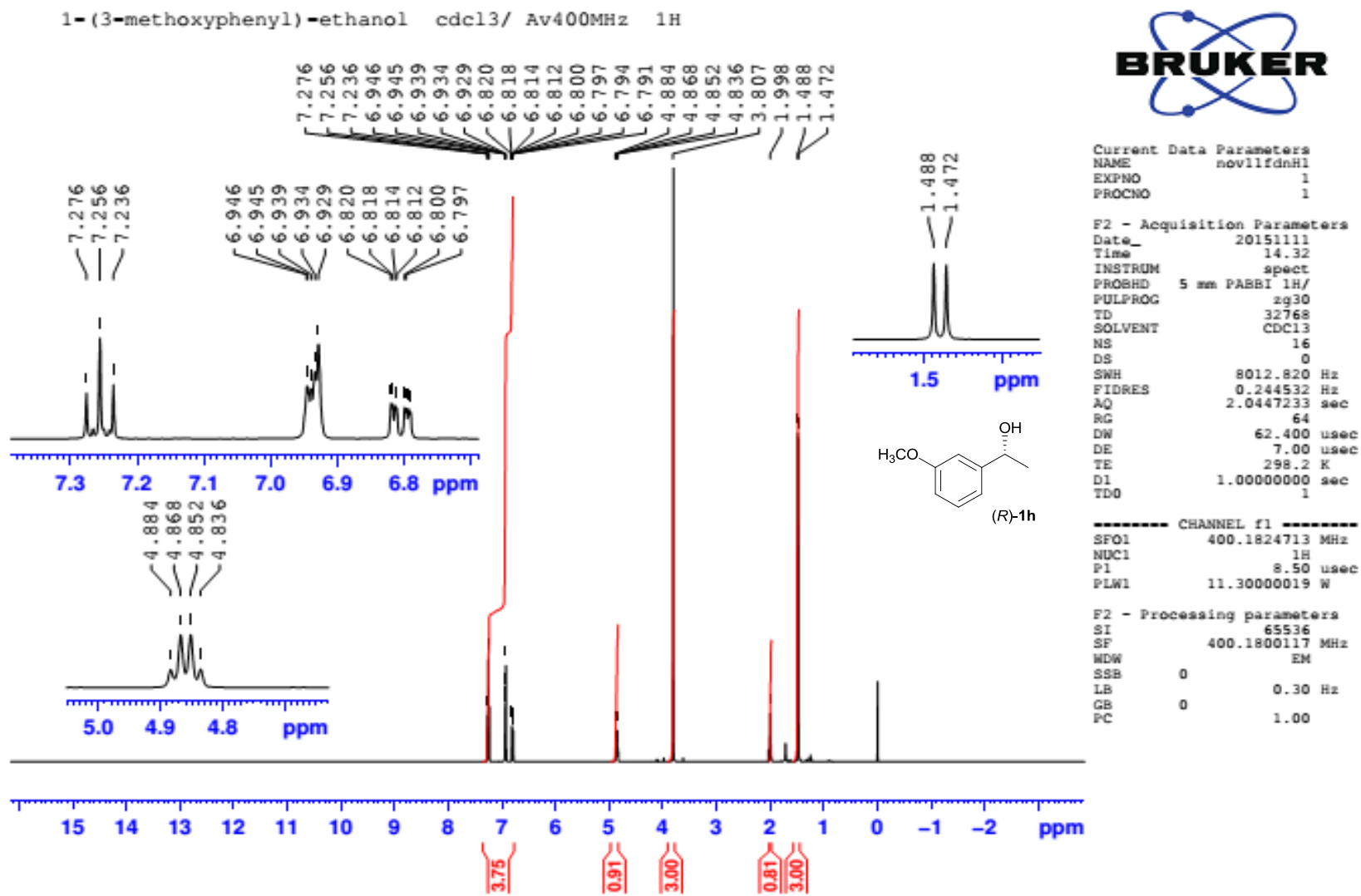


Figure S3. ¹H NMR (400 MHz, CDCl₃) spectrum of (R)-**1h** (CAS number 120523-12-8).

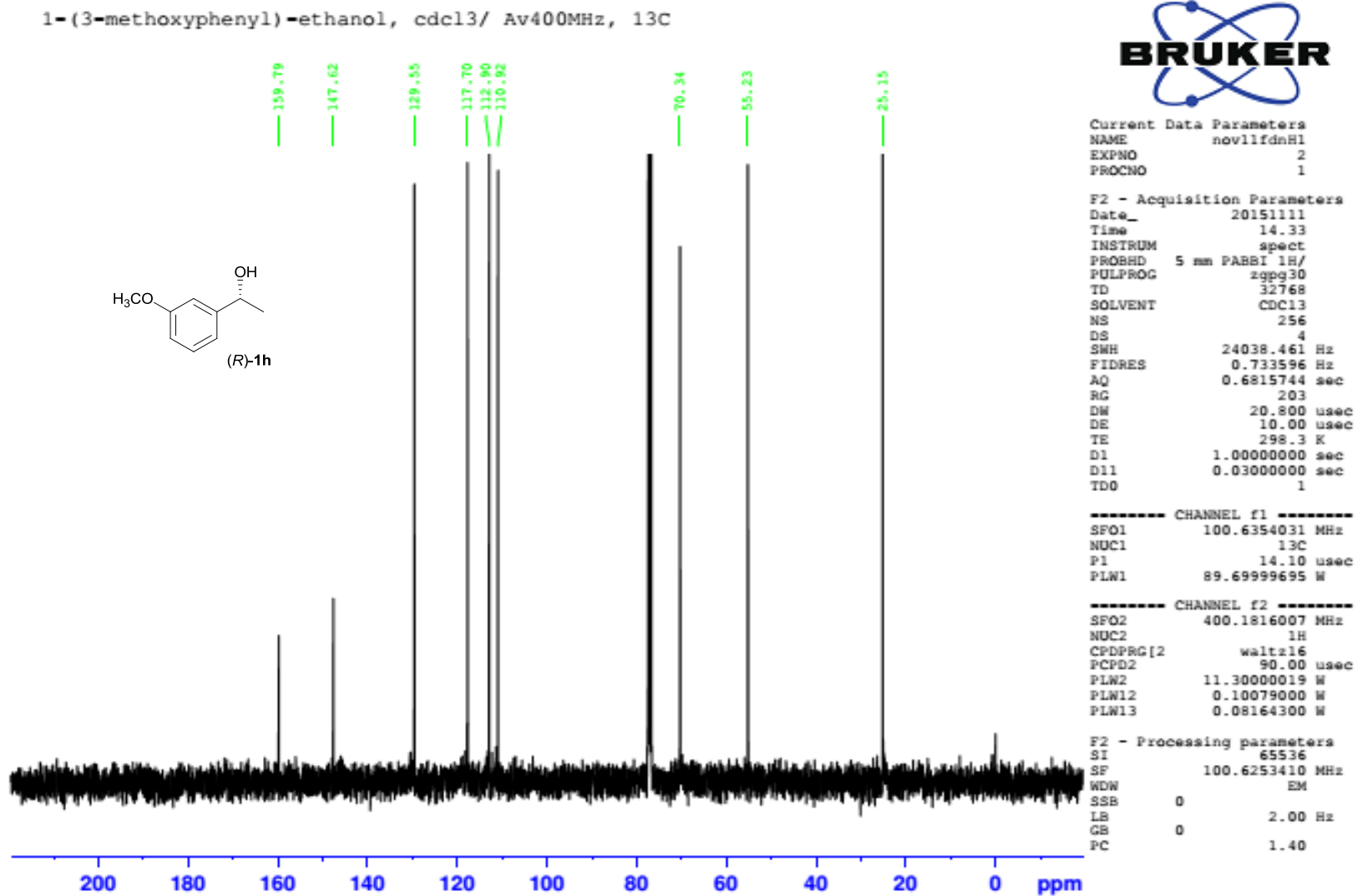


Figure S4. ^{13}C NMR (100 MHz, CDCl_3) spectrum of (R)-1h (CAS number 120523-12-8).

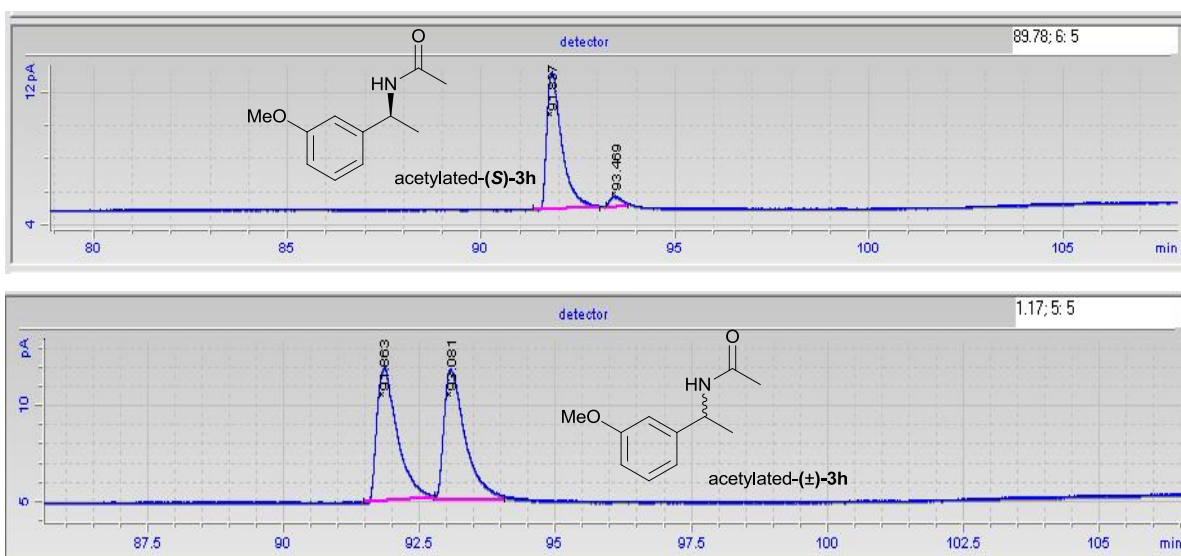


Figure S5. Chromatograms of acetylated (*S*)-3h and (±)-3h.

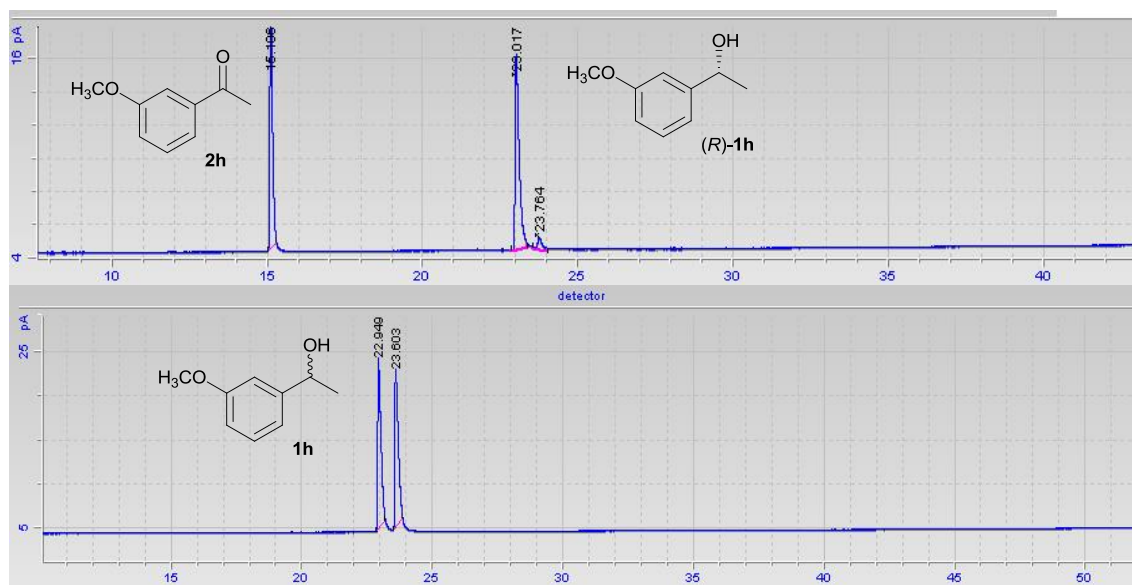


Figure S6. Chromatograms of (*R*)-1h and (±)-1h.

Table S1. Deracemization of (\pm)-1-arylethanol by stereoinversion using immobilized *C. albicans* cells in calcium alginate beads and a commercial KRED

entry ^a	Substrate	R	Reduction catalyst	time / h	Alcohol	
					Conversion ^e / %	ee / %
1 ^b	1a	H	KRED-P1-A04	2	90	97 (R) ^f
2 ^b			KRED-P2-C11	2	92	96 (R) ^f
3 ^b			KRED-P2-H07	2	98	93 (R) ^f
4 ^b			KRED-P1-H10	2	98	92 (R) ^f
5 ^c	1b	4-Cl	ADH-PL	9	92	95 (R) ^f
6 ^d			ADH-PL	9	91	93 (R) ^f
7 ^b			KRED-P1-A04	19	> 99	84 (R) ^f
8 ^b			KRED-P2-C11	5	> 99	82 (R) ^f
9 ^b	KRED-P2-H07	5	> 99	83 (R) ^f		
10 ^b	KRED-P1-H10	5	> 99	83 (R) ^f		
11 ^c	1c	4-F	ADH-PL	12	> 99	84 (R) ^f
12 ^b			KRED-P1-A04	3	90	94 (R) ^f
13 ^b			KRED-P2-C11	3	92	95 (R) ^f
14 ^b			KRED-P2-H07	3	91	95 (R) ^f
15 ^b	KRED-P1-H10	3	91	92 (R) ^f		
16 ^c	1d	4-Br	ADH-PL	7	91	95 (R) ^f
17 ^b			KRED-P1-A04	19	> 99	89 (R) ^f
18 ^b			KRED-P2-C11	7	> 99	84 (R) ^f
19 ^b			KRED-P2-H07	7	> 99	83 (R) ^f
20 ^b	KRED-P1-H10	7	> 99	83 (R) ^f		
21 ^c	1e	4-CH ₃	ADH-PL	14	> 99	79 (R) ^f
22 ^b			KRED-P1-A04	19	80	93 (R) ^f
23 ^b			KRED-P2-C11	2	96	96 (R) ^f
24 ^b			KRED-P2-H07	2	97	95 (R) ^f
25 ^b	KRED-P1-H10	2	96	96 (R) ^f		
26 ^c	1f	4-OCH ₃	ADH-PL	9	95	94 (R) ^f
27 ^b			KRED-P1-A04	24	50	> 99 (R) ^f
28 ^b			KRED-P2-C11	24	55	75 (R) ^f
29 ^b			KRED-P2-H07	24	55	93 (R) ^f
30 ^b	KRED-P1-H10	24	55	92 (R) ^f		
31 ^c	1g	4-OH	ADH-PL	24	50	> 99 (R) ^f
32 ^b			KRED-P1-A04	40	49	83 (R) ^f
33 ^b			KRED-P2-C11	40	57	73 (R) ^f
34 ^b			KRED-P2-H07	40	50	86 (R) ^f
35 ^b	KRED-P1-H10	40	53	86 (R) ^f		
36 ^c	1h	3-OMe	ADH-PL	40	52	87 (R) ^f
37 ^b			KRED-P1-A04	19	95	93 (R) ^f
38 ^b			KRED-P2-C11	9	98	58 (R) ^f
39 ^b			KRED-P2-H07	3	99	93 (R) ^f
40 ^b	KRED-P1-H10	3	99	90 (R) ^f		

41 ^c			ADH-PL	10	96	91 (R) ^f
42 ^d			ADH-PL	7	95	90 (R) ^f
43 ^b	1i	3-OH	KRED-P1-A04	17	94	96 (R) ^g
44 ^b			KRED-P2-C11	40	96	62 (R) ^g
45 ^b			KRED-P2-H07	17	94	96 (R) ^g
46 ^b			KRED-P1-H10	21	93	92 (R) ^g
47 ^c			ADH-PL	40	92	96 (R) ^g

^a1st step: 0.5 mmol of **1a-i**, 0.150 mL of acetone, 11 g of immobilized *C. albicans*, 10 mL of H₂O; ²nd step: 1 mL of the reaction, 25 mg of dry Recycle Mix P, 0.100 mL of 2-propanol; ^b4 mg of KRED or ^c15 μL of ADH-PL; ^d10 mL of OKR (first step), 0.100 mL of ADH-PL, 1 mL of 2-propanol and 250 mg of dry Recycle Mix P; ^econversion monitored by GC-MS; ^fee determined by GC-FID; ^gee determined by HPLC.